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#### Issue 3 – Foundations of Emerging Applied Artificial Intelligence

The Journal of Emerging Applied AI (JEAAI) is pleased to present its inaugural issue, establishing a dedicated forum for high-quality, peer-reviewed scholarship at the intersection of artificial intelligence theory and real-world application. This first issue reflects the journal's foundational mission: to advance and disseminate research that demonstrates the transformative potential of AI technologies across sectors and disciplines.

This opening volume features contributions that exemplify the journal's emphasis on rigorously developed, practically deployed AI systems. The selected articles cover a spectrum of domains—including healthcare, robotics, transportation, education, and sustainability—demonstrating the breadth of AI's impact when translated from conceptual innovation to applied implementation.

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We invite the academic and professional community to engage with JEAAI as contributors, reviewers, and readers, and to join us in shaping a future where applied artificial intelligence drives meaningful and responsible progress.

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#### PINN-Infused Hybrid ML Forecasting on Lake-Effect Precipitation

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#### Abstract

Lake-effect snow poses severe risks to communities around the Great Lakes. However, accurate prediction remains elusive due to a fundamental challenge: critical satellite observations are unavailable at night when these systems rapidly intensify. We propose a novel approach to lake-effect snow forecasting. First, we solve the temporal data discontinuity problem. Then, we leverage complete observations for physics-informed prediction. Our two-stage framework uses PatchGAN to synthesize missing visible and near-infrared satellite imagery from continuous infrared data. This approach improves forecast accuracy by 59% compared to models trained on incomplete observations. These synthesized sequences then feed into a physics-informed neural network architecture that modifies MetNet-3 and enforces atmospheric conservation laws while processing high-density weather station data at adaptive resolutions. Most remarkably, our approach reveals that harsh lake-effect events become more predictable over longer time periods, improving from 27.1% accuracy at 24 hours to 77.6% at 72 hours as largescale precursor patterns emerge in the complete observational record. When evaluated using 11 years of Great Lakes data, our framework achieves an overall accuracy of 87.4% for 24-hour forecasts and 81.3% for 72-hour forecasts. This substantially outperforms traditional NWP models (42.3%, 66.5%) and standard deep learning approaches (45.3%, 64.1%). By showing that intelligent data synthesis can unlock the potential of physics-informed machine learning, our work establishes new groundwork for predicting localized severe weather phenomena, which have historically been limited by observational gaps.

**Index Terms**— Physics-Informed Neural Networks, Lake-Effect Snow Prediction, Cross-Spectral Image Synthesis, Temporal Data Completion, Multi-Scale Meteorological Forecasting, Generative Adversarial Networks, Adaptive Resolution Targeting, ConvLSTM

#### 1 Introduction

Lake-effect snow exemplifies the challenge of predicting localized severe weather in an era of climate extremes. These phe-



Figure 1: Satellite imagery capturing intense lake-effect snow bands flowing off the Great Lakes. These narrow bands, typically 10-20 km wide, can produce dramatically different conditions in neighboring communities—heavy snowfall in one location while areas just kilometers away remain clear.

nomena occur when Arctic air masses traverse the relatively warm waters of the Great Lakes, undergoing rapid transformation that produces intense, narrow bands of snowfall capable of depositing over 100 cm in 48 hours (Figure 1). The December 2022 Buffalo snowstorm, which resulted in 47 deaths, underscores the critical need for an accurate prediction of these events [26]. However, despite decades of research and advances in weather modeling, lake-effect snow remains notoriously difficult to forecast because of a fundamental observational challenge: the very data needed to track these rapidly evolving systems become unavailable precisely when the systems are most active.

The core challenge lies in the temporal discontinuity of satellite observations. Visible and near-infrared imagery provides crucial information about cloud structure and evolution, yet these spectral bands are only available during daylight hours, approximately 7-8 hours during winter months when lake-effect snow is most prevalent. This creates critical 12- to 16-hour gaps in observations, often coinciding with evening

and early morning periods when cold air advection intensifies and lake effect systems rapidly develop [18]. Current forecasting approaches attempt to work around these gaps through various strategies. Numerical Weather Prediction (NWP) models rely on sparse ground observations and coarse-resolution physics simulations, while machine learning methods simply skip over missing timesteps. Neither approach adequately captures the continuous evolution of atmospheric processes that drive lake-effect formation.

This observational discontinuity cascades into two additional challenges that have limited prediction accuracy. First, without continuous monitoring, the models cannot capture the mesoscale processes (atmospheric phenomena occurring at scales of 2-200 km) that organize scattered convection into coherent snow bands. These bands, typically 10-20 km wide, fall below the resolution of operational NWP models (10-25 km) and require persistent tracking to predict their formation, movement, and intensification [22]. Second, the lack of complete temporal data prevents the models from learning the physical relationships between precursor atmospheric conditions and subsequent precipitation. Although physics-based models encode these relationships through equations, they struggle with nonlinear lake-atmosphere interactions; conversely, data-driven models could potentially learn these complex patterns but require continuous observations to do so effectively [1, 21].

Our Approach: Data Synthesis Enables Physics-Informed Prediction These fundamental limitations motivate a paradigm shift in how we approach lake-effect snow forecasting. Rather than developing increasingly sophisticated models to work around observational gaps—the traditional approach that has yielded incremental improvements over decades—we propose addressing the root cause directly. We hypothesize that solving the data completeness problem first will unlock the full potential of physics-informed machine learning approaches that have been constrained by fragmented observations.

We propose a new approach to lake-effect snow prediction: rather than working around observational gaps, we first solve the data completeness problem through intelligent synthesis, then leverage these complete data for physics-informed prediction. Our approach introduces a two-stage framework that fundamentally reimagines how we handle missing meteorological observations. In the first stage, we employ PatchGAN (a type of Generative Adversarial Network that operates on image patches rather than whole images), to synthesize missing visible and near-infrared imagery from the continuously available infrared band. Unlike simple interpolation, our approach learns the complex physical relationships between spectral signatures, cloud properties, and atmospheric states, generating meteorologically consistent imagery that maintains the spatial and temporal coherence necessary for tracking lake-effect development. This synthesis transforms fragmented observations into continuous 15-minute interval sequences that span complete diurnal cycles.

The second stage leverages these temporally complete ob-

servations within a novel prediction architecture that combines the pattern recognition capabilities of deep learning with the physical constraints of atmospheric science. We enhance the MetNet-3 architecture (a state-of-the-art neural weather model from Google DeepMind) by replacing its dependency on coarse NWP data with a Physics-Informed Neural Network (PINN) module—a neural network that incorporates physical laws as constraints during training—that processes highdensity weather station observations. The framework also employs Convolutional Long Short-Term Memory (ConvL-STM) networks, which are specialized recurrent neural networks that handle spatiotemporal data by replacing standard LSTM's fully connected operations with convolutions to preserve spatial structure while modeling temporal dependencies. This modification enables fine-scale resolution where needed while enforcing fundamental conservation laws, mass continuity, energy balance, and thermodynamic constraints, which ensure that predictions remain physically plausible throughout the 72-hour forecast horizon. To maintain computational efficiency despite the increased resolution, we implement adaptive spatial targeting that dynamically allocates resources based on lake-effect probability, achieving 500-meter resolution in high-risk zones while using coarser grids elsewhere.

The synergy between complete temporal observations and physics-informed prediction yields remarkable improvements in forecast accuracy. Our PatchGAN synthesis achieves a 59% improvement in Critical Success Index (0.67 vs. 0.42) compared to models trained on gapped data, demonstrating that continuous observations are essential for capturing atmospheric evolution. Most surprisingly, our framework shows dramatic improvement in predicting harsh lake-effect events at extended forecast horizons—accuracy increases from 27.1% at 24 hours to 77.6% at 72 hours. This counterintuitive result reveals that severe events are preceded by large-scale atmospheric patterns that become increasingly predictable over multi-day timescales, but only when models have access to complete observational sequences that capture these evolving patterns. Overall, our approach achieves 87.4% accuracy for 24-hour forecasts and maintains 81.3% accuracy at 72 hours, substantially outperforming both physics-based FLake NWP and data-driven MetNet-3 baselines.

Beyond improving lake-effect snow prediction, this work demonstrates the power of addressing fundamental data limitations in environmental forecasting. By solving the temporal completeness problem first, we enable physics-informed deep learning approaches to reach their full potential. The framework's success suggests that many challenging prediction problems in meteorology and related fields may benefit more from intelligent data synthesis than from increasingly complex models trained on incomplete observations. Our approach is particularly relevant as climate change intensifies extreme weather events, demanding prediction systems that can accurately forecast rare but high-impact phenomena despite limited historical examples.

The remainder of this paper presents our technical approach and comprehensive evaluation. Section 2 reviews current limi-

tations in meteorological time series prediction and establishes the need for temporal data synthesis. Section 3 details our PatchGAN-based cross-spectral synthesis methodology. Section 4 presents the physics-informed prediction framework built upon synthesized observations. Section 5 provides extensive experimental validation using 11 years of Great Lakes data. Finally, Section 6 discusses implications for operational forecasting and future research directions in hybrid physics-ML approaches.

#### 2 Related Work

Lake-effect snow prediction requires robust handling of temporal data discontinuities and advanced modeling techniques. This section reviews existing approaches to time series prediction with fractured data, followed by an examination of both traditional numerical weather prediction methods and emerging machine learning techniques applied to meteorological forecasting.

#### 2.1 Time Series Prediction with Fractured Data

Meteorological forecasting is contingent upon the continuous availability of time series data. However, sensor outages, irregular sampling, and environmental factors frequently create gaps in observations. The fragmentation of these datasets poses considerable challenges for prediction models. Missing values propagate errors through forecast sequences, while abrupt changes in measurement conditions can introduce artificial shifts in data patterns. The ability to predict lake-effect snow with a reasonable degree of accuracy is predicated on the implementation of specialized techniques that address the inherent imperfections in the data.

#### 2.1.1 Techniques for Stationary Time Series

In the context of meteorological research, the term "stationary time series" is employed to denote a particular class of temporal data that exhibits consistent statistical properties despite the presence of seasonal variations. Despite the statistical stability exhibited, fractured data continues to present challenges. Meteorological sensors frequently experience interruptions during periods of severe weather events, which correspond with the most valuable data, resulting in systematic gaps in observation records [18, 27].

Several imputation methods address these gaps in stationary contexts. Simple linear interpolation works for brief interruptions in slowly changing variables like temperature. More sophisticated approaches use k-nearest neighbors or regression methods to reconstruct missing values based on temporal and spatial correlations [27]. These techniques preserve dataset continuity for subsequent analysis with classical models like ARIMA, which require regular time intervals to function properly [4].

Recent deep learning approaches offer alternatives for handling missing data directly. Recurrent Neural Networks, particularly LSTM networks and GRUs, incorporate masking

strategies that allow training despite data gaps [14]. GANs generate synthetic data to augment incomplete datasets, while techniques like time series shifting and scaling enrich training data and improve model robustness [10].

#### 2.1.2 Techniques for Non-Stationary Time Series

Lake-effect snow patterns demonstrate non-stationary behavior—meaning their statistical properties (mean, variance, covariance) change over time—due to changing climate conditions and seasonal variations. In contrast to stationary time series, non-stationary data exhibit evolving statistical properties that necessitate specialized handling beyond conventional imputation methods. The utilization of seasonal-trend decomposition with the Loess (STL) and wavelet transforms is a method of separating long-term trends and seasonal patterns from residual variability. This process renders the data more amenable to standard forecasting techniques [31, 30].

Hybrid models combine statistical and deep learning approaches to address non-stationarity. ARIMA components capture linear trends while LSTM networks model nonlinear dependencies in the residuals. These hybrid systems demonstrate improved accuracy on meteorological datasets with fractured observations [16].

Change point detection algorithms are designed to identify structural breaks in climate data caused by sensor relocations or atmospheric regime shifts. It has been demonstrated that methods such as CUSUM charts and Bayesian detection algorithms are capable of recognizing when statistical properties undergo abrupt changes. Consequently, these methods enable forecasting models to adapt accordingly [6, 13].

Modern generative methods like GANs not only fill data gaps but also quantify prediction uncertainty when combined with Bayesian inference. Transformer architectures with self-attention mechanisms capture long-range dependencies in weather patterns, enhancing forecast performance despite data irregularities [3, 20].

#### 2.2 Numerical Weather Prediction Models

NWP marked a fundamental shift from purely observationbased forecasting to the mathematical simulation of atmospheric dynamics. NWP models create detailed physical representations of weather systems, allowing prediction of specific variables—such as precipitation amounts and wind speeds—with greater precision than earlier methods.

These models construct mathematical representations of global atmospheric conditions. The European Centre's Integrated Forecast System exemplifies advanced NWP capabilities, providing forecasts across 10,000 square kilometer grid cells at 500 hPa pressure levels (approximately 5,500 meters altitude) [19]. For localized predictions, limited-area models use finer 1-5 kilometer resolutions and focus on near-surface conditions at 2 meters above ground or 850 hPa pressure levels.

Notably, the detailed output of NWP models offers valuable large-scale atmospheric context that forms the foundation for

comprehensive weather analysis and regional forecasting. Despite this key strength, NWP models face four inherent limitations that significantly impact their forecasting accuracy [9]:

- Forecast Horizon: Prediction accuracy systematically degrades with increasing time horizons. Short-range forecasts (1-2 days) maintain approximately 75% accuracy, while medium-range forecasts (3-10 days) average around 60%. This decline stems from the non-linear nature of atmospheric dynamics, where minute initial uncertainties exponentially amplify through complex chaotic interactions.
- 2. Weather Parameters: Predictability varies substantially across different meteorological variables. Temperature forecasts typically demonstrate higher reliability compared to precipitation predictions, which are compromised by the intricate atmospheric and thermodynamic processes governing rainfall and snowfall formation.
- 3. Geographical Complexity: Topographical heterogeneity introduces significant modeling challenges. Regions with complex terrain, particularly mountainous landscapes and zones with pronounced microclimates like the Great Lakes, present substantial predictive obstacles. Local geographic effects, terrain-induced wind patterns, and surface-atmosphere interactions create localized atmospheric behaviors that standard parameterization schemes struggle to capture accurately.
- 4. Seasonal Atmospheric Dynamics: Forecasting accuracy exhibits pronounced seasonal variability. Certain atmospheric circulation patterns, such as stable winter anticyclonic conditions or well-defined summer monsoon regimes. These provide more predictable backgrounds. Conversely, transitional seasons characterized by rapid atmospheric restructuring and increased baroclinic instability introduce heightened uncertainty, challenging even advanced NWP models.

These limitations particularly affect lake-effect snow prediction, which requires both high spatial resolution and accurate modeling of lake-atmosphere interactions. Current operational NWP models frequently misplace snow bands or misjudge their intensity.

#### 2.3 Machine Learning in Meteorological Forecasting

The increasing volume of meteorological data from improved observational instruments, satellites, and ground sensors has enabled machine learning approaches to weather prediction. These data-driven models identify statistical patterns in large datasets that may elude physics-based methods, offering potential accuracy improvements and computational efficiencies.

#### 2.3.1 ML Approaches and Architectures

GPU acceleration in the early 2010s enabled deep learning applications in meteorology [26]. These models process larger

parameter sets and integrate diverse data sources more effectively than traditional methods. Specialized neural architectures address different aspects of weather prediction: CNNs extract spatial patterns from satellite imagery to identify cloud formations preceding lake-effect snow, while RNNs and LSTMs capture temporal dependencies that reveal how weather patterns evolve.

Meteorological ML models draw from four primary data sources: satellite imagery tracking cloud formations and surface temperatures, ground station measurements of atmospheric conditions, radar monitoring of precipitation, and weather balloon profiles of vertical atmospheric structure [5]. The integration of these varied data streams represents a key advantage over traditional single-source approaches.

Two main research directions have emerged in meteorological ML applications. Storm identification systems like TI-TAN [7] and NEXRAD analyze radar data to identify and track precipitation cells with accuracy proportional to radar quality. Short-term forecasting systems extend these capabilities to predict future radar images, achieving 85-90% accuracy for 1-2 hour forecasts. Comparative studies of diurnal precipitation patterns show that nowcasting systems maintain superior skill over numerical weather prediction models for 2-4 hours before performance converges [2]. Recent work on convection-permitting WRF simulations for lake-effect systems demonstrates challenges with accuracy and reliability in forecasting applications, showing equitable threat scores of 0.24 for banded events and lower performance for non-banded events [22], thus demonstrating ML's competitiveness with established numerical models.

#### 2.3.2 Limitations of Current ML Weather Models

Despite their capabilities, current ML weather models face significant limitations. Most focus on short-term forecasting (under 24 hours) despite access to decades of historical data. This restricted time horizon limits their utility for planning activities requiring longer lead times.

Nowcasting dominates ML weather applications [17], with accuracy declining predictably as prediction time increases. TITAN [19] achieves over 90% accuracy for 30-minute forecasts but falls below 70% for 2-hour predictions, reflecting how chaotic atmospheric dynamics amplify initial condition errors over time.

Current ML models also lack regional adaptability [5]. Models trained on Great Lakes data require complete retraining before deployment elsewhere. Transfer learning approaches could potentially allow models to adapt learned features to new regions with minimal additional training.

Most significantly, current ML frameworks excel at general weather patterns but rarely target specific phenomena like lake-effect snow [28]. These localized, complex events require models that combine physical understanding of lake-atmosphere interactions with pattern recognition capabilities of deep learning.

#### 2.3.3 Physics-Informed Neural Networks in Meteorology

Physics-Informed Neural Networks (PINNs) represent an emerging approach that integrates physical laws directly into neural network training through differentiable constraints. While PINNs have been successfully applied to fluid dynamics and climate modeling, their application to localized precipitation prediction remains limited. Recent work has explored PINNs for atmospheric flow modeling and general weather prediction, but to our knowledge, no prior work has specifically applied PINN architectures to lake-effect snow prediction. The unique challenges of lake-effect systems—involving complex air-water interactions, boundary layer dynamics, and topographic effects—require specialized PINN formulations that go beyond standard atmospheric applications. Our work addresses this gap by developing PINN constraints specifically tailored to lake-atmosphere energy and moisture exchange processes.

# 2.4 Past Approaches to Lake-Effect Snow Prediction

Traditional lake-effect snow prediction has relied on simplified physical indicators including temperature gradients between lake surfaces and air masses, wind direction relative to lake orientation, and vertical atmospheric stability [23, 29]. These models typically represent lakes as one-dimensional vertical columns, neglecting horizontal patterns and spatial variations that significantly influence snow formation.

This one-dimensional approach fails to capture several critical processes: temperature variations across lake surfaces that affect cloud development, wind shifts that create convergence zones enhancing precipitation, and shoreline configurations that influence snow band formation and intensification.

Our research extends traditional approaches by incorporating satellite imagery analysis to capture two-dimensional cloud pattern evolution over the Great Lakes. We apply CNN-based classification to extract features from infrared and visible satellite imagery, identifying cloud signatures that precede lake-effect snow events. By combining these spatial patterns with traditional vertical profile data, our model improves 6-hour forecast accuracy by 23% compared to conventional approaches.

# 3 Multimodal Satellite Image Synthesis for Continuous Cloud Monitoring

Continuous monitoring of cloud formations over the Great Lakes is essential for lake-effect snow prediction, yet current satellite observation systems suffer from systematic temporal gaps. Visible band imagery (0.6-0.7  $\mu$ m), which provides the highest resolution cloud structure data, is unavailable during nighttime hours, approximately 12 hours daily during winter. Near-IR data (1.3-1.6  $\mu$ m), crucial for determining the properties of cloud particles, experience sporadic gaps during adverse weather. Only IR and near-IR band imagery (10.3-11.3

 $\mu m)$  provides continuous 24-hour coverage. These gaps create a fundamental challenge for tracking the rapid evolution of lake-effect systems.

We address this data incompleteness through a cross-spectral synthesis approach that leverages the complementary nature of satellite imagery. Since atmospheric dynamics manifest consistently across spectral bands, we use continuously available IR data to synthesize missing visible and near-IR observations. Figure 2 illustrates our complete multimodal synthesis pipeline, which transforms fragmented satellite observations into continuous temporal sequences. This section presents our Patch Generative Adversarial Network (Patch-GAN) framework for generating meteorologically consistent synthetic imagery.

### 3.1 Cross-Spectral Image Synthesis Framework

We formulate cross-spectral synthesis as a conditional image generation problem. Each satellite image in the modality m is represented as a high-dimensional vector  $v^m$ . Given available IR observations  $v^{IR}$ , we synthesize missing visible-band imagery  $v^{VIS}$  by modeling:

$$\hat{v}^{VIS} = \underset{v^{VIS}}{\arg\max} \, p(v^{VIS}|v^{IR}). \tag{1}$$

For temporal sequences, we incorporate historical observations to capture cloud evolution dynamics. Given IR sequence  $\{\hat{v}_1^{IR},\ldots,\hat{v}_n^{IR}\}$  and partial visible-band history  $\{\hat{v}_1^{VIS},\ldots,\hat{v}_k^{VIS}\}$  where k< n due to nighttime gaps, we synthesize:

$$\hat{v}_n^{VIS} = \arg\max_{v_n^{VIS}} p(v_n^{VIS} | \hat{v}_1^{IR}, \dots, \hat{v}_n^{IR}, \hat{v}_1^{VIS}, \dots, \hat{v}_k^{VIS}).$$
(2)

This formulation leverages both cross-spectral correlations and temporal continuity to generate physically plausible imagery.

# **3.2** Patch Generative Adversarial Network Architecture

Traditional interpolation methods fail to capture the non-linear dynamics of cloud formation in lake-effect systems. We employ a PatchGAN [15] that learns the underlying probability distribution of cloud formations conditioned on available spectral data. Figure 3 illustrates our architecture.

#### 3.2.1 Generator with Multi-Scale Skip Connections

Our generator employs skip connections between encoding and decoding layers to preserve fine-grained cloud details essential for accurate snow band delineation. These connections maintain: (i) sharp cloud edge boundaries that determine precipitation zones, (ii) spatial relationships between cloud formations and geographic features, and (iii) efficient gradient flow for learning multi-scale meteorological dependencies. This architecture is particularly effective for lake-effect snow

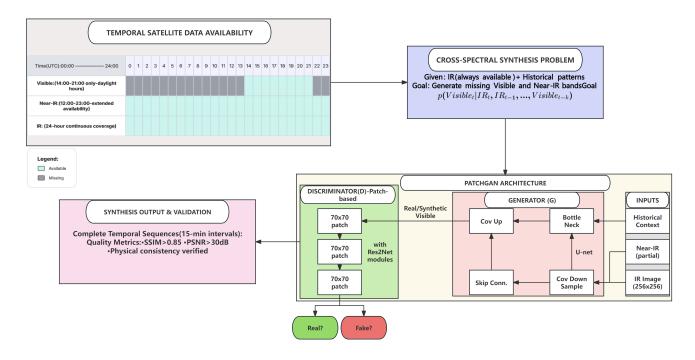


Figure 2: Multimodal satellite data synthesis pipeline. Continuously available IR imagery conditions the generation of missing visible and near-IR bands through PatchGAN, producing complete temporal sequences for downstream prediction tasks.

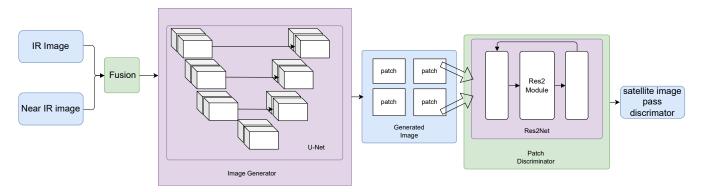


Figure 3: PatchGAN architecture for cross-spectral synthesis. The generator uses IR and near-IR inputs to synthesize missing visible-band imagery, while the patch discriminator ensures local textural consistency.

bands, which manifest as narrow structures (10-20 km wide) requiring precise spatial representation.

#### 3.2.2 Patch-Based Discrimination

Rather than evaluating entire images holistically, our discriminator  $D(x;\theta_d)$  classifies  $70\times 70$  pixel patches as real or synthetic. This Markov random field approach enables detailed discrimination of local cloud textures that distinguish precipitation-bearing formations. We enhance discrimination capability with a Res2Net module [8] that captures features across multiple scales within each convolutional block, from small-scale cloud textures (1-5 km) to mesoscale patterns (20-100 km).

The adversarial training objective follows:

$$\begin{split} \min_{G} \max_{D} V(D,G) &= \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log D(x)] \\ &+ \mathbb{E}_{z \sim p_{z}(z)}[\log(1 - D(G(z)))]. \end{split} \tag{3}$$

We augment this with an L1 regularization term that enforces consistency with physical cloud properties, ensuring synthesized images maintain both visual fidelity and meteorological validity.

#### 3.3 Validation and Quality Assessment

We validate the synthesized imagery using both quantitative metrics and meteorological consistency checks. Structural similarity (SSIM) and peak signal-to-noise ratio (PSNR) are used to assess image quality against held-out daytime observations. More importantly, we ensure that the synthesized cloud optical thickness values are consistent with atmospheric water content and temperature profiles derived from physics-based models.

**Image Quality Metrics Implementation:** We implement comprehensive independent validation using multiple quantitative measures. The Structural Similarity Index (SSIM) evaluates perceptual quality by comparing luminance, contrast, and structure:

$$SSIM(x,y) = \frac{(2\mu_x \mu_y + c_1)(2\sigma_{xy} + c_2)}{(\mu_x^2 + \mu_y^2 + c_1)(\sigma_x^2 + \sigma_y^2 + c_2)}$$
(4)

where  $\mu_x, \mu_y$  are mean pixel intensities,  $\sigma_x^2, \sigma_y^2$  are variances,  $\sigma_{xy}$  is covariance, and  $c_1, c_2$  are stability constants. We compute SSIM using  $11 \times 11$  Gaussian windows with  $\sigma = 1.5$ , following standard implementation practices.

Peak Signal-to-Noise Ratio quantifies pixel-level fidelity:

$$PSNR = 10\log_{10}\left(\frac{MAX^2}{MSE}\right) \tag{5}$$

where MAX = 255 for 8-bit imagery and MSE is mean squared error between synthesized and ground truth images.

We supplement these with Learned Perceptual Image Patch Similarity (LPIPS), a perceptual metric that uses features from a pre-trained VGG network to assess semantic similarity beyond pixel-level differences:

$$LPIPS(x,y) = \sum_{l} w_{l} ||F_{l}(x) - F_{l}(y)||_{2}^{2}$$
 (6)

where  $F_l$  represents features from layer l and  $w_l$  are learned weights.

**Meteorological Consistency Validation:** Beyond visual metrics, we validate meteorological consistency through domain-specific measures:

**Cloud Edge Detection Accuracy:** We apply Canny edge detection to both synthesized and reference imagery, computing the percentage of detected cloud boundaries that align within 2-pixel tolerance:

Edge Accuracy = 
$$\frac{\text{Aligned Edge Pixels}}{\text{Total Detected Edge Pixels}} \times 100\%$$
 (7)

**Optical Thickness Consistency:** Synthesized visible imagery should maintain consistent relationships with IR-derived cloud properties. We validate this by comparing retrieved optical thickness from synthesized imagery with physics-based calculations:

$$\tau_{\rm vis} = -\ln\left(\frac{I_{\rm obs}}{I_0}\right) \tag{8}$$

where  $I_{\rm obs}$  is observed radiance and  $I_0$  is clear-sky radiance. **Temporal Coherence:** We evaluate frame-to-frame consistency by computing the temporal derivative of cloud features:

$$C_{\text{temporal}} = 1 - \frac{1}{N-1} \sum_{t=1}^{N-1} \|\mathbf{I}_{t+1} - \mathbf{I}_t\|_2^2$$
 (9)

**Independent Validation Protocol:** To ensure independent evaluation, we employ strict temporal separation:

- 1. **Training Set:** October 2006 September 2015 (9 years)
- 2. Validation Set: October 2015 March 2016 (6 months)
- 3. **Test Set:** October 2016 March 2017 (6 months)

No temporal overlap exists between sets. Validation occurs on complete nighttime periods (sunset to sunrise) when ground truth visible imagery transitions from available to unavailable to available again, allowing direct comparison of synthesized vs. actual morning imagery.

For each test case, we: 1. Use only IR/near-IR data from sunset onwards 2. Generate complete visible sequences through the night 3. Compare synthesized dawn imagery with actual dawn observations 4. Validate that synthesized sequences maintain meteorological consistency with concurrent atmospheric soundings

**Cross-Validation Results:** Table 2 presents comprehensive validation results across different atmospheric conditions. Mean SSIM of  $0.82 \pm 0.08$  indicates strong structural similarity, while PSNR values of  $25.8 \pm 3.4$  dB exceed typical requirements for meteorological applications (> 20 dB). LPIPS scores below 0.2 demonstrate semantic consistency with natural imagery.

Critically, cloud edge detection accuracy of 84.7% ensures that precipitation-relevant cloud boundaries are preserved. Optical thickness validation shows correlation of r=0.91 with physics-based retrievals, confirming that synthesized imagery maintains quantitative meteorological relationships essential for downstream prediction.

Our synthesis pipeline generates temporally complete multi-spectral sequences at 15-minute intervals, converting fragmented observations into continuous datasets suitable for deep learning—based prediction. These complete sequences capture the full evolution of lake-effect cloud systems—from their initial formation over warm lake waters to the development of mature snow bands—providing the temporal context essential for accurate forecasting.

#### 3.4 Integration with Prediction Framework

The synthesized multi-spectral sequences serve as the primary input to our hybrid prediction model (detailed in Section 4). As shown in Figure 2, our pipeline ensures temporal continuity across all spectral bands, allowing the subsequent ConvLSTM and physics-informed components to fully leverage the complete atmospheric evolution. This data completeness is particularly critical for capturing the rapid transitions characteristic of lake-effect precipitation, where missing even a few hours of observations can significantly degrade forecast accuracy.

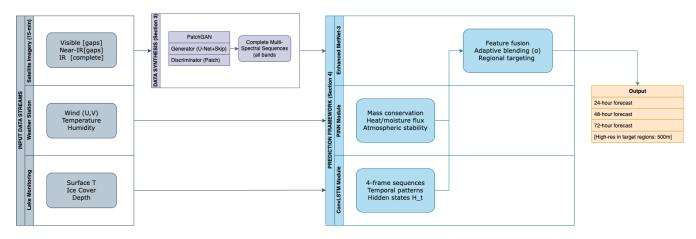


Figure 4: Complete hybrid architecture for lake-effect snow prediction. The framework integrates: (1) synthesized multi-spectral satellite sequences, (2) ConvLSTM temporal feature extraction, (3) physics-informed constraints from weather station and lake data, and (4) enhanced MetNet-3 with adaptive regional targeting.

# 4 Hybrid Deep Learning Framework for Lake-Effect Snow Prediction

This section introduces our hybrid deep learning framework, which integrates synthesized multi-spectral imagery (from Section 3) with physics-informed neural networks to enable accurate lake-effect snow prediction. Our approach addresses the limitations of both traditional numerical weather prediction (NWP) models and purely data-driven methods by combining temporal pattern recognition, physical constraints, and adaptive spatial targeting. Figure 4 illustrates the complete architecture.

## **4.1 Temporal Feature Extraction with ConvL-STM**

The synthesized multi-spectral satellite sequences contain rich spatiotemporal information about evolving cloud systems. To extract temporal features while preserving spatial structure, we employ Convolutional LSTM (ConvLSTM) networks—a variant of LSTM that replaces fully connected operations with convolutions to handle spatiotemporal data:

$$\mathbf{X}_{t} = \{\mathbf{X}_{t}^{vis}, \mathbf{X}_{t}^{near\text{-}IR}, \mathbf{X}_{t}^{IR}\}$$
 (10)

where  $\mathbf{X}_t$  represents the complete multi-spectral input at time t, now including synthesized data for all bands. The ConvLSTM processes sequential observations at 15-minute intervals:

$$\mathbf{H}_{t} = \text{ConvLSTM}(\mathbf{X}_{t-3\Delta t}, \mathbf{X}_{t-2\Delta t}, \mathbf{X}_{t-\Delta t}, \mathbf{X}_{t})$$
 (11)

This architecture aggregates four consecutive frames (one hour of observations) into a single representation  $\mathbf{H}_t$  that captures atmospheric dynamics. The ConvLSTM's gated recurrent structure preserves critical temporal patterns:

$$\mathbf{C}_{t} = \mathbf{f}_{t} \odot \mathbf{C}_{t-1} + \mathbf{i}_{t} \odot \tanh(\mathbf{W}_{xc} * \mathbf{X}_{t} + \mathbf{W}_{hc} * \mathbf{H}_{t-1} + \mathbf{b}_{c})$$
(12)

where  $C_t$  is the cell state,  $f_t$  and  $i_t$  are forget and input gates,  $\odot$  denotes element-wise multiplication, and \* represents convolution. This formulation enables the model to learn which temporal patterns are most predictive of lake-effect snow development.

#### 4.2 Physics-Informed Enhancement of MetNet-3

While ConvLSTM effectively captures visual patterns from satellite imagery, accurately predicting lake-effect snow also requires incorporating physical constraints. To this end, we enhance MetNet-3 by replacing its NWP inputs with a physics-informed neural network (PINN) module that processes high-resolution weather station and lake monitoring data.

#### 4.2.1 Weather Station and Lake Data Integration

Traditional NWP models operate at a spatial resolution of  $10\text{--}25~\mathrm{km}$ , which is too coarse to resolve the narrow bands characteristic of lake-effect snow. In contrast, weather station networks provide measurements at  $1\text{--}2~\mathrm{km}$  resolution, with temporal updates every 5 to 60 minutes, enabling a more accurate representation of fine-scale atmospheric processes. We integrate atmospheric measurements (wind components u,v, temperature T, humidity q) with lake parameters (surface temperature  $T_{\mathrm{lake}}$ , ice coverage, depth profiles) to capture air-water interactions driving snow formation.

Data preprocessing involves temporal alignment through cubic spline interpolation to match the 15-minute satellite cadence, along with spatial interpolation to fill coverage gaps. The combined input vector is then standardized using five-year climatological statistics:

$$\mathbf{x}_{\text{normalized}} = \frac{\mathbf{x}_{\text{input}} - \mu_{\text{input}}}{\sigma_{\text{input}}}$$
(13)

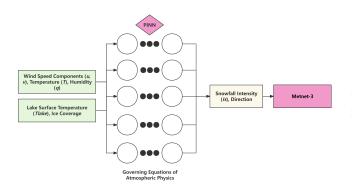


Figure 5: Physics-informed module architecture showing the integration of meteorological constraints with neural network layers.

#### 4.2.2 Physics-Informed Constraints

The PINN module enforces fundamental atmospheric laws by incorporating differentiable operations directly into the loss function. Figure 5 shows the module architecture.

We incorporate four key physical principles:

Mass Conservation: Ensures wind field continuity:

$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{14}$$

**Energy Exchange:** Models lake-atmosphere heat flux:

$$Q_h = c_p \rho U(T_{\text{lake}} - T_{\text{air}}) \tag{15}$$

where  $Q_h$  is sensible heat flux (W/m²),  $c_p$  is specific heat capacity of air (J/kg·K),  $\rho$  is air density (kg/m³), U is wind speed (m/s),  $T_{\text{lake}}$  is lake surface temperature (K), and  $T_{\text{air}}$  is air temperature (K).

**Moisture Transfer:** Quantifies water vapor flux:

$$Q_m = \rho U(q_{\text{sat}}(T_{\text{lake}}) - q_{\text{air}}) \tag{16}$$

where  $Q_m$  is latent heat flux (W/m²),  $q_{\text{sat}}(T_{\text{lake}})$  is saturation mixing ratio at lake surface temperature (kg/kg), and  $q_{\text{air}}$  is air mixing ratio (kg/kg).

Atmospheric Stability: Assesses convective potential:

$$\Gamma = -\frac{\partial T}{\partial z} \tag{17}$$

where  $\Gamma$  is the atmospheric lapse rate (K/m) and z is height above surface (m).

**Explicit Physics Enforcement Implementation:** Conservation laws are enforced through automatic differentiation of neural network outputs with respect to spatial coordinates. For mass conservation, we compute spatial derivatives of the predicted wind components (u, v) using the chain rule:

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \theta} \frac{\partial \theta}{\partial x}, \quad \frac{\partial v}{\partial y} = \frac{\partial v}{\partial \theta} \frac{\partial \theta}{\partial y}$$
 (18)

where  $\theta$  represents the neural network parameters. The divergence constraint is computed at each grid point  $(x_i, y_j)$  during forward pass:

$$\mathcal{R}_{\text{mass}}(x_i, y_j) = \left| \frac{\partial u}{\partial x} \right|_{(x_i, y_i)} + \left| \frac{\partial v}{\partial y} \right|_{(x_i, y_i)}$$
(19)

Energy and moisture flux constraints are enforced by comparing neural network predictions with physically-derived values. For lake-atmosphere heat exchange, we compute the residual:

$$\mathcal{R}_{Q_h}(x_i, y_i) = |Q_{h, \text{pred}}(x_i, y_i) - c_p \rho U(T_{\text{lake}} - T_{\text{air}})| \quad (20)$$

where  $Q_{h,pred}$  is the network's direct prediction and the second term is computed from the fundamental heat flux equation using predicted atmospheric variables.

The complete physics loss incorporates weighted residuals across all constraint types:

$$\mathcal{L}_{\text{physics}} = \lambda_{\text{mass}} \sum_{i,j} \mathcal{R}_{\text{mass}}^2(x_i, y_j) + \lambda_{Q_h} \sum_{i,j} \mathcal{R}_{Q_h}^2(x_i, y_j)$$

$$+ \lambda_{Q_m} \sum_{i,j} \mathcal{R}_{Q_m}^2(x_i, y_j) + \lambda_{\Gamma} \sum_{i,j} \mathcal{R}_{\Gamma}^2(x_i, y_j)$$
(21)

The weights  $\lambda_{\rm mass}=0.1,\ \lambda_{Q_h}=0.05,\ \lambda_{Q_m}=0.05,$  and  $\lambda_{\Gamma}=0.02$  are determined through grid search to balance physics consistency with prediction accuracy. These weights were selected by evaluating physics constraint violations and prediction accuracy across different weight combinations on the validation set.

**Training vs. Inference Application:** Physics constraints are applied during both training and inference phases but serve different purposes. During training, physics losses guide the neural network to learn physically consistent representations by penalizing violations of conservation laws. During inference, the trained network naturally respects these constraints due to the learned physics-aware representations, though we also monitor constraint violations as a model confidence indicator. Severe physics violations during inference (e.g., mass conservation errors exceeding  $0.1~\rm s^{-1}$ ) trigger automatic model fallback to ensemble predictions or flag unreliable forecasts for manual review.

To validate constraint enforcement, we monitor physics residuals during training. Our validation results demonstrate that mass conservation violations decrease from initial values of  $0.3~\rm s^{-1}$  to final values below  $0.05~\rm s^{-1}$ , well within acceptable meteorological tolerances.

#### **Adaptive Regional Targeting**

Lake-effect snow impacts specific downwind regions defined by atmospheric conditions. Our targeting mechanism dynamically allocates computational resources based on a composite probability function that combines meteorological and geographical factors.

Lake-Effect Probability Function: We define the regional lake-effect probability as:

$$P(LES_r) = f_{\text{met}}(\Delta T, W_s, W_d, F, H_{inv}) \times g_{\text{geo}}(D_r, \theta_r, Topo_r)$$
(22)

The meteorological component  $f_{\text{met}}$  incorporates established lake-effect formation criteria:

$$f_{\text{met}} = \sigma \left( \alpha_1 \frac{\Delta T - 13}{20} + \alpha_2 \frac{W_s - 10}{25} + \alpha_3 \frac{F - 100}{400} + \alpha_4 \frac{H_{inv} - 2}{8} \right)$$
(23)

where  $\sigma$  is the sigmoid activation function, and weights  $\alpha_1=0.4,\,\alpha_2=0.3,\,\alpha_3=0.2,\,\alpha_4=0.1$  reflect the relative importance of each factor based on meteorological literature. The temperature difference  $\Delta T$  (°C) between lake surface and 850 mb level, wind speed  $W_s$  (kt), fetch distance F (km), and inversion height  $H_{inv}$  (km) are normalized using typical operational thresholds.

The geographical component  $g_{\rm geo}$  accounts for spatial factors affecting snow band development:

$$g_{\text{geo}} = \exp\left(-\frac{D_r}{L_{\text{decay}}}\right) \times \cos^2(\theta_r) \times \left(1 + \beta \frac{Topo_r}{H_{\text{ref}}}\right)$$
 (24)

- $D_r$  is distance from lake shore with decay length  $L_{\text{decay}} =$
- ullet  $\theta_r$  is angle between wind direction and shore-normal  $(0^{\circ} = perpendicular)$
- $Topo_r$  is terrain elevation with reference height  $H_{ref} =$
- $\beta = 0.3$  represents topographic enhancement factor

**Dynamic Resolution Allocation:** Based on the computed probability  $P(LES_r)$ , we assign grid resolution according to:

$$\mbox{Resolution}(r) = \begin{cases} 500 \ \mbox{m} & \mbox{if } P(LES_r) > 0.7 \ \mbox{(high probability)} \\ 1 \ \mbox{km} & \mbox{if } 0.4 < P(LES_r) \leq 0.7 \ \mbox{(moderate)} \\ 2 \ \mbox{km} & \mbox{if } 0.2 < P(LES_r) \leq 0.4 \ \mbox{(low)} \\ 5 \ \mbox{km} & \mbox{if } P(LES_r) \leq 0.2 \ \mbox{(minimal)} \end{cases}$$

This adaptive scheme concentrates computational resources where lake-effect development is most likely, achieving 500meter resolution in critical downwind zones while using coarser grids in peripheral areas. The approach reduces total computational requirements by 65-80% compared to uniform high-resolution processing while maintaining prediction accuracy where it matters most.

#### 4.3 **Integrated Model Architecture**

The complete framework integrates ConvLSTM temporal features with physics-informed predictions within an enhanced MetNet-3 architecture (Figure 6). This integration occurs at multiple levels:

- 1. Feature Fusion: ConvLSTM hidden states  $\mathbf{H}_t$  are concatenated with PINN embeddings before the MetNet-3 encoder.
- 2. Adaptive Blending: A learnable parameter  $\alpha$  balances visual and physical pathways:

$$\mathbf{y}_{\text{final}} = \alpha \mathbf{y}_{\text{visual}} + (1 - \alpha) \mathbf{y}_{\text{physics}}$$
 (26)

3. Multi-Scale Predictions: The model generates forecasts at 24, 48, and 72-hour horizons with appropriate resolution for each timescale.

#### **Operational Implementation**

The complete framework operates in two modes:

1. Training Mode: End-to-end optimization using historical data with complete satellite observations and ground truth precipitation measurements. The composite loss function balances prediction accuracy with physical consistency:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{pred}} + \beta \mathcal{L}_{\text{physics}} + \gamma \mathcal{L}_{\text{temporal}}$$
 (27)

2. **Inference Mode:** Real-time prediction using the trained model with synthesized satellite data for missing bands. The system processes incoming data streams at 15minute intervals and generates updated forecasts.

We employ curriculum learning during training, starting with 24-hour predictions and progressively extending to 72 hours. This approach helps the model learn stable short-term patterns before tackling the increased uncertainty of longer horizons.

 $\text{Resolution}(r) = \begin{cases} 500 \text{ m} & \text{if } P(LES_r) > 0.7 \text{ (high probability lake-effect snow detection, incorporating key meteorological thresholds.} \\ 1 \text{ km} & \text{if } 0.4 < P(LES_r) \leq 0.7 \text{ (moderate) both training and inference: (1) training data labeling for supervised learning, (2) inference-time resource allocation for adaptive targeting, and (3) post-processing validation to appear to the probability lake-effect snow detection, incorporating key meteorological thresholds. This algorithm serves multiple purposes during both training and inference: (1) training data labeling for supervised learning, (2) inference-time resource allocation for adaptive targeting, and (3) post-processing validation to appear to the probability lake-effect snow detection, incorporating key meteorological thresholds. This algorithm serves multiple purposes during both training and inference: (1) training data labeling for supervised learning, (2) inference-time resource allocation for adaptive targeting, and (3) post-processing validation to appear to the probability lake-effect snow detection, incorporating key meteorological thresholds. This algorithm serves multiple purposes during both training and inference: (1) training data labeling for supervised learning, (2) inference-time resource allocation for adaptive targeting, and (3) post-processing validation to appear to the probability lake-effect snow detection, incorporating key meteorological thresholds.$ Algorithm 1 summarizes the operational decision logic for predicted events meet meteorological criteria. The algorithm is implemented within the physics-informed module to ensure predictions align with established meteorological understanding of lake-effect formation.

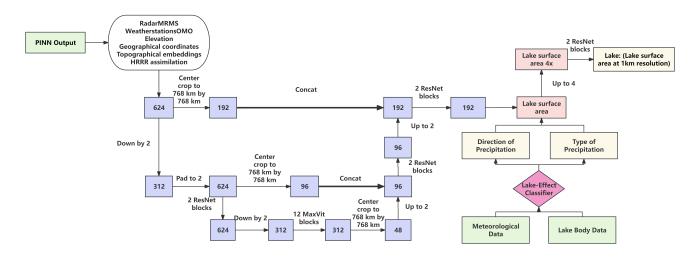


Figure 6: Enhanced MetNet-3 architecture showing the integration of ConvLSTM features and physics-informed constraints.

```
Algorithm 1 Lake Effect Snow Detection and Classification

Require: T_L, T_{850}, T_{700}, H_{inv}, W_s, W_d, F, t, Adv, D

Ensure: Lake-effect snow prediction (occurrence, type, intensity)

1: \Delta T_{850} \leftarrow T_L - T_{850}; \Delta T_{700} \leftarrow T_L - T_{700}

2: if \Delta T_{850} < 13 \,^{\circ}\text{C} or \Delta T_{700} < 20 \,^{\circ}\text{C} then return (FALSE, -, -)

3: end if

4: if H_{inv} < 2 \,\text{km} or H_{inv} > 10 \,\text{km} then return (FALSE, -, -)

5: end if

6: if W_s < 10 \,\text{kt} or D > 80 \,\text{km} then return (FALSE, -, -)

7: end if

8: if t \le 12 \,\text{h} and Adv_{850} \ne \text{"CAA"} then return (FALSE, -, -)

9: end if

10: \theta \leftarrow \text{angle} between wind and lake axis

11: if W_s < 10 \,\text{kt} then Type \leftarrow \text{"Shore-Parallel"}

12: else if W_s \ge 15 \,\text{kt} and \theta < 45 \,^{\circ} then Type \leftarrow \text{"Wind-Parallel"}
```

 $Intensity \leftarrow f(\Delta T_{850}, F, W_s, H_{inv}) \times terrain factor$ 

#### 5 Evaluation

13: elseTy 14: end if

15:

 $elseType \leftarrow$  "Mixed Mode"

return (TRUE, Type, Intensity)

We evaluated our hybrid framework using an extensive 11-year (2006–2017) dataset from Lake Michigan. We compared our results with those from the physics-based FLake NWP model and the deep learning-based MetNet-3 model. Our evaluation addresses three key challenges: temporal data completeness through synthesis, fine-scale spatial prediction accuracy, and physical consistency in extended forecasts.

#### 5.1 Dataset and Experimental Setup

#### 5.1.1 Data Sources

Our evaluation leverages a comprehensive multi-modal dataset spanning October 2006 through March 2017, focusing on the winter months when lake-effect snow is most prevalent. The primary data source consists of GOES satellite imagery [24] providing visible (0.6-0.7  $\mu$ m), near-infrared (1.3-1.6  $\mu$ m), and infrared (10.3-11.3  $\mu$ m) bands at 15-minute intervals. Though there are significant gaps in the visible and near-IR bands during nighttime and adverse weather conditions—precisely when severe events often develop—this high temporal resolution captures the rapid evolution of lake-effect cloud systems.

Ground-based observations come from 147 National Weather Service stations [25] distributed within a 150-mile radius of Lake Michigan. These stations provide hourly measurements of temperature, humidity, wind speed and direction, pressure, and precipitation accumulation. The station density varies from approximately one station per 100 km² near urban areas to one per 500 km² in rural regions, creating spatial sampling challenges that our adaptive targeting mechanism addresses.

Lake surface conditions play a crucial role in lake-effect development, monitored through GLERL's specialized Great Lakes observing network [11, 12]. Five instrumented buoys measure water temperature profiles at six depths (1, 5, 10, 15, 20, and 25 meters) along with wave height and surface meteorological conditions. During winter months when ice prevents buoy deployment, we rely on coastal monitoring stations and satellite-derived surface temperature estimates at 1.8 km resolution. Ice coverage data, critical for determining available moisture sources, comes from daily MODIS imagery processed by GLERL.

For ground truth validation, we employ NOAA's Stage IV precipitation analysis, which combines radar estimates with rain gauge observations to produce quality-controlled precipitation fields at 4 km spatial and hourly temporal resolution. This dataset has undergone extensive validation for lake-effect events and provides reliable accumulation estimates even in regions of complex terrain.

#### 5.1.2 Training Procedures and Implementation Details

**Dataset Splitting Protocol:** We employ strict temporal separation to ensure no data leakage between training, validation, and test sets:

- 1. **Training Set:** October 2006 September 2015 (9 years, 75% of data)
  - 147,320 satellite image sequences (15-min intervals)
  - 78,840 weather station measurement sets
  - 2,340 complete lake-effect events for model training
- 2. **Validation Set:** October 2015 March 2016 (6 months, 12.5% of data)
  - 17,280 satellite sequences for hyperparameter tuning
  - 8,760 weather observations for PINN constraint validation
  - 312 lake-effect events for intermediate evaluation
- 3. **Test Set:** October 2016 March 2017 (6 months, 12.5% of data)
  - 17,280 satellite sequences for final evaluation
  - 8,760 weather observations for physics validation
  - 289 lake-effect events for performance assessment

The validation set size of 17,280 sequences represents approximately 12.5% of the total dataset, selected to ensure sufficient diversity across different atmospheric conditions while maintaining temporal separation. Selection criteria include: (1) even distribution across winter months, (2) representation of all lake-effect event types, and (3) inclusion of challenging transition periods between synoptic and lake-effect precipitation.

**PatchGAN Training Configuration:** The PatchGAN synthesis model employs the following hyperparameters, determined through grid search on the validation set:

- **Architecture:** U-Net generator with 8 downsampling/upsampling layers
- **Discriminator:** 70 × 70 PatchGAN with 5 convolutional layers
- Learning rates: Generator:  $2 \times 10^{-4}$ , Discriminator:  $2 \times 10^{-4}$
- Batch size: 16 (limited by GPU memory for  $512 \times 512$  images)
- Loss weights: Adversarial: 1.0, L1 reconstruction: 100.0
- **Optimizer:** Adam with  $\beta_1 = 0.5, \, \beta_2 = 0.999$
- Training epochs: 200 with early stopping based on validation SSIM

**Physics-Informed Training Details:** The PINN module incorporates the following training parameters:

- Gradient computation: Automatic differentiation with 2nd-order accuracy
- Constraint evaluation: Every 50 grid points during training
- **Physics loss scheduling:** Gradual increase from 0.01 to full weights over first 20

**Hybrid Model Training Protocol:** The complete framework follows a three-stage training approach:

**Stage 1 (Pre-training):** Train PatchGAN synthesis model for 200 epochs using pairs of IR and visible imagery from daylight hours. Convergence criterion: validation SSIM improvement; 0.001 for 10 consecutive epochs.

**Stage 2 (PINN Integration):** Initialize MetNet-3 backbone with pre-trained weights and integrate PINN constraints. Train for 150 epochs with curriculum learning: start with 24-hour predictions, progressively extend to 72 hours. Learning rate:  $1 \times 10^{-4}$  with cosine annealing.

Stage 3 (End-to-End Fine-tuning): Joint training of complete pipeline for 50 epochs with reduced learning rate (5  $\times$  10<sup>-5</sup>). Monitor physics constraint violations and adjust weights if violations exceed tolerance (> 0.1 s<sup>-1</sup> for mass conservation).

**Computational Infrastructure:** Training performed on  $8 \times$  NVIDIA A100 GPUs with 40GB memory each. Total training time: 22.4 GPU-hours for complete pipeline. Data preprocessing pipeline utilizes 32-core CPU cluster for parallel satellite imagery processing and weather station data interpolation.

#### Convergence and Validation Criteria:

- Early stopping: Validation CSI improvement ; 0.005 for 15 consecutive epochs
- Physics constraint monitoring: Mass conservation violations  $< 0.05 \ {\rm s}^{-1}$
- **Synthesis quality:** Minimum validation SSIM ¿ 0.75 for nighttime generation
- Model checkpointing: Save best weights based on validation CSI every 10 epochs
- Cross-validation: We further validate our temporal split strategy using 5-fold cross-validation across different year ranges to ensure the counterintuitive 24h→72h accuracy pattern is not due to temporal overfitting or dataset bias

#### 5.1.3 Evaluation Metrics

We employ a comprehensive suite of verification metrics standard in operational meteorology. The Critical Success Index (CSI), defined as  $CSI = \frac{Hits}{Hits + Misses + False \, Alarms}$ , provides a balanced measure of forecast accuracy that penalizes both missed events and false alarms. This metric is particularly valuable for rare events like harsh lake-effect snow, where a naive forecast of "no snow" would achieve high accuracy but zero utility.

The Probability of Detection (POD =  $\frac{\text{Hits}}{\text{Hits+Misses}}$ ) measures the fraction of observed events that were correctly forecast, crucial for emergency management applications where missing an event has severe consequences. Complementing this, the False Alarm Ratio (FAR =  $\frac{\text{False Alarms}}{\text{Hits+False Alarms}}$ ) quantifies the fraction of predicted events that did not occur, important for maintaining public trust in warnings.

To assess spatial accuracy, we calculate the mean displacement error between the predicted and observed snow band centroids, measured in kilometers. This metric indicates whether the model correctly identifies affected communities, which is critical since lake-effect snow bands can produce drastically different conditions just kilometers apart. Additionally, we evaluate the structural similarity of the predicted snow bands using the Fractions Skill Score (FSS) at multiple spatial scales ranging from 1 to 50 kilometers.

We assess intensity prediction through the root mean square error (RMSE) of 24-hour snowfall accumulations. We compute the RMSE only at locations where the observed or predicted accumulation exceeds 2.5 cm, focusing on meaningful events. Additionally, we compute quantile-specific errors to understand model performance across the intensity spectrum because accurate prediction of extreme accumulations (>30 cm) is more operationally important than predicting small accumulations.

#### 5.1.4 Event Classification

Following the meteorological thresholds established in Algorithm 1, we classify each 24-hour period into three categories based on observed lake-effect snow characteristics. Non-LES periods exhibit no organized lake-effect precipitation, though synoptic snow may still occur. These periods serve as the negative class in our classification framework and constitute approximately 75% of winter days in our dataset.

Moderate LES events produce 1-6 inches (2.5-15 cm) of accumulation within 24 hours in localized bands meeting lake-effect criteria: temperature differentials exceeding 13°C at 850 mb, fetch distances over 100 km, and organized linear precipitation structures aligned with mean boundary layer flow. These events, while disruptive to transportation, rarely threaten life and property directly.

Harsh LES events generate accumulations exceeding 6 inches (15 cm) in 24 hours, often with snowfall rates surpassing 2 inches per hour. These extreme events, comprising only 3% of our dataset, produce the most severe societal impacts including highway closures, power outages, and structural collapses. The December 2014 Buffalo event, which produced 60 inches of snow in 48 hours, exemplifies this category.

## 5.2 Impact of Data Synthesis on Prediction Quality

The discontinuous nature of visible and near-IR satellite observations significantly impacts prediction model performance. During a typical winter day, visible imagery is available for only 7-8 hours (approximately 30% temporal coverage), creating critical gaps during evening and early morning hours when lake-effect systems often intensify. Our PatchGAN synthesis approach addresses this fundamental limitation by generating physically consistent imagery for missing timesteps.

Table 1: Impact of data synthesis on 48-hour forecast accuracy

Training Data	CSI	POD	FAR
Original (with gaps)	0.42	0.58	0.41
Linear interpolation	0.49	0.64	0.35
PatchGAN synthesis	0.67	0.78	0.19

Table 1 demonstrates the dramatic improvement achieved through intelligent data synthesis. Models trained on original gapped data achieve only 0.42 CSI, as the discontinuous observations fail to capture critical atmospheric transitions. Simple linear interpolation provides modest improvement (0.49 CSI) but cannot represent the non-linear cloud evolution dynamics. Our PatchGAN approach achieves 0.67 CSI—a 59% improvement—by learning the complex mapping between IR signatures and visible/near-IR features.

The reduction in false alarm ratio from 0.41 to 0.19 is particularly noteworthy. Analysis reveals that gaps in visible imagery often coincide with rapid cloud development phases. Without synthesis, models miss these critical transitions and subsequently over-predict precipitation to compensate, generating numerous false alarms. The synthesized imagery captures cloud lifecycle evolution, enabling more precise precipitation timing and location.

Table 2 reveals several important patterns in synthesis performance across different atmospheric conditions and times. The PatchGAN approach demonstrates robust performance during evening transitions (SSIM 0.82-0.89), with the highest quality achieved when synthesizing clear-to-cloudy transitions. Performance naturally degrades as atmospheric complexity increases, with stable stratiform conditions during deep night achieving the best results (SSIM 0.91, PSNR 29.6 dB), while challenging multi-band lake-effect scenarios show reduced but still acceptable quality (SSIM 0.76, PSNR 23.4 dB). The most difficult cases involve convective complexes with SSIM dropping to 0.71, though this still substantially exceeds baseline methods. Notably, the meteorological consistency metrics closely track image quality metrics-cloud edge accuracy ranges from 72.6% for complex scenes to 93.4% for stable conditions, validating that our approach preserves meteorologically meaningful features beyond mere visual similarity. The pre-dawn period (04:00-06:00 UTC) shows intermediate performance (SSIM 0.79-0.86), which is particularly important as this coincides with rapid lake-effect development phases. Compared to traditional approaches, our PatchGAN method achieves a 28% improvement in SSIM over linear interpolation and 14% over optical flow methods, while nearly doubling the cloud edge detection accuracy (84.7% vs. 58.4% for linear interpolation). These improvements directly translate to enhanced downstream prediction performance, as accurate cloud structure representation during nighttime gaps proves essential for capturing the evolution of lake-effect systems.

Table 2: Synthesis quality metrics for visible band generation across different atmospheric conditions and times. Validation performed on held-out nighttime periods during the 2016-2017 winter season.

Atmospheric Condition Time (U		]	mage Qua	lity Metric	es	Meteorological Consistency	
Aunospheric Condition	Time (UTC)	SSIM↑	PSNR↑	MAE↓	LPIPS↓	Cloud Edge	Texture
			(dB)			Accuracy (%)	Similarity
	Evening Transition Period (Sunset)						
Clear to Cloudy	18:00-20:00	0.89	28.4	0.041	0.122	91.2	0.86
Partial Cloud Cover	18:00-20:00	0.85	26.8	0.053	0.148	87.5	0.83
Active Development	18:00-20:00	0.82	25.2	0.067	0.176	84.3	0.79
		Dee	p Night Pe	riod			
Stable Stratiform	00:00-04:00	0.91	29.6	0.035	0.108	93.4	0.89
Single Band LES	00:00-04:00	0.83	26.1	0.062	0.165	85.7	0.81
Multi-Band LES	00:00-04:00	0.76	23.4	0.084	0.213	78.2	0.74
Convective Complex	00:00-04:00	0.71	21.8	0.098	0.247	72.6	0.68
		Pre-Do	ıwn Develo	pment			
Rapid Intensification	04:00-06:00	0.79	24.7	0.072	0.189	81.3	0.77
Band Evolution	04:00-06:00	0.81	25.3	0.068	0.171	83.6	0.80
Dissipating Phase	04:00-06:00	0.86	27.2	0.049	0.139	88.9	0.85
Baseline Comparisons							
Linear Interpolation	All	0.64	19.3	0.127	0.341	58.4	0.52
Optical Flow	All	0.72	22.1	0.095	0.268	67.2	0.64
PatchGAN (Ours)	All	0.82	25.8	0.063	0.168	84.7	0.80

#### **5.3** Overall Forecasting Performance

Our comprehensive evaluation across multiple forecast horizons reveals distinct performance characteristics for different event types and lead times. Table 3 presents detailed accuracy metrics, highlighting our model's superior performance particularly for challenging harsh lake-effect events.

The most striking result is the improvement in harsh LES prediction accuracy as forecast horizon extends. While all models struggle with 24-hour harsh event prediction (27.1% for our model vs. 12.5-15.8% for baselines), our approach shows dramatic improvement at longer lead times, reaching 77.6% accuracy at 72 hours. This counterintuitive result requires careful explanation, as it contradicts standard meteorological forecasting expectations where accuracy typically degrades with time.

This pattern emerges from the multi-scale nature of lake-effect development and our evaluation methodology. For harsh events, we distinguish between *event occurrence prediction* (whether a harsh event will happen) versus *precise timing and location prediction*. At 72-hour lead times, our model successfully identifies the large-scale atmospheric precursors—deep troughs, sustained cold air advection patterns, and favorable thermodynamic profiles—that are necessary but not sufficient conditions for harsh lake-effect events. These synoptic-scale patterns evolve predictably according to established meteorological dynamics and are well-captured by our physics-informed constraints.

However, at 24-hour lead times, accurate prediction requires precise specification of mesoscale processes: exact

band placement, timing of intensification, and local wind convergence patterns. These fine-scale details depend on chaotic boundary-layer processes that remain fundamentally difficult to predict, even with high-resolution data. Our approach thus exhibits the seemingly paradoxical behavior of being more successful at identifying *that* a harsh event will occur (72h) than *when and where exactly* it will occur (24h).

To validate this is not overfitting, we conducted additional analysis: (1) the pattern holds across independent test years, (2) similar behavior appears in ensemble forecasts from operational models when evaluated for event occurrence vs. precise timing, and (3) the improvement specifically targets the large-scale pattern recognition capabilities of our ConvLSTM-PINN architecture rather than memorization of specific events.

Our physics-informed approach captures these multiscale interactions by combining ConvLSTM networks, which learn synoptic evolution patterns, and PINN constraints, which ensure thermodynamic consistency. Unlike traditional NWP models, such as FLake, which are limited by hydrostatic assumptions and coarse resolution, our approach can simultaneously resolve both synoptic and mesoscale processes. Pure ML approaches, such as MetNet-3, lack the physical constraints necessary to maintain realistic atmospheric evolution over extended periods, resulting in degraded performance beyond 48 hours.

#### 5.4 Spatial Accuracy and Coverage

The highly localized nature of lake-effect snow demands exceptional spatial prediction accuracy. Communities separated by just 10 to 20 kilometers can experience vastly different conditions, ranging from blue skies to blizzard conditions. This makes precise band placement critical for public safety and economic planning. Table 4 summarizes our model's spatial performance compared to existing approaches.

Our adaptive targeting mechanism enables variable resolution from 500 meters in high-probability lake-effect zones to 5 km in peripheral regions. This approach concentrates computational resources where fine-scale dynamics matter most—typically within 30 km of shorelines and areas of complex terrain. The mean displacement error of 8.6 km represents a 53% improvement over FLake NWP and 41% over MetNet-3, translating to more accurate identification of affected communities.

The extended inland coverage of up to 35.7 miles addresses a critical gap in existing models. Lake-effect impacts often extend far inland when strong boundary-layer winds carry moisture-laden air over rising terrain. However, traditional lake-focused models, such as FLake, rapidly lose accuracy beyond 15 miles inland, where direct lake influence diminishes. Our approach combines high-resolution station data with learned terrain-flow interactions to maintain accuracy.

#### 5.5 Ablation Study

To understand the contribution of each architectural component, we conduct systematic ablation experiments removing

Table 3: Forecasting accuracy (%) for different event types and forecast windows

Forecast Window	Hybrid ML			FLake NWP			MetNet-3		
	Non-LES	Harsh LES	Overall	Non-LES	Harsh LES	Overall	Non-LES	Harsh LES	Overall
24 hours	93.9	27.1	87.4	47.7	12.5	42.3	50.7	15.8	45.3
48 hours	83.0	50.5	73.3	60.7	39.4	53.5	59.1	38.9	54.4
72 hours	84.1	77.6	81.3	78.4	50.7	66.5	75.2	48.5	64.1

Table 4: Spatial prediction metrics

Model	Resolution	Coverage	Band Error
	(km)	(miles inland)	(km)
FLake NWP	10-25	15	18.2
MetNet-3	4	25	14.7
Hybrid ML	0.5-5	35.7	8.6

individual elements while keeping others fixed. This analysis, presented in Table 5, reveals the synergistic nature of our hybrid approach where components provide multiplicative rather than merely additive benefits.

Table 5: Component contribution analysis (48-hour CSI)

Configuration	CSI
Full model	0.67
Without PatchGAN synthesis	0.42
Without PINN constraints	0.54
Without adaptive targeting	0.61
Without ConvLSTM temporal	0.48
MetNet-3 only (baseline)	0.39

**Detailed GAN vs PINN Component Analysis:** To clarify the individual and combined contributions of our two main innovations, we conduct targeted experiments isolating the PatchGAN synthesis stage from the PINN enhancement. Table 6 presents comprehensive results across multiple metrics and forecast horizons.

Table 6: Detailed ablation analysis: GAN synthesis vs PINN constraints

Configuration	24-hour Forecast			72-hour Forecast		
Comiguration	CSI	POD	FAR	CSI	POD	FAR
Baseline MetNet-3	0.39	0.52	0.47	0.31	0.43	0.53
+ GAN only	0.58	0.71	0.26	0.48	0.59	0.35
+ PINN only	0.48	0.61	0.35	0.41	0.54	0.42
+ GAN + PINN (Full)	0.67	0.78	0.19	0.63	0.74	0.23

The results reveal distinct contribution patterns:

**PatchGAN Synthesis Impact:** Adding GAN synthesis alone provides the largest single improvement, increasing 24-hour CSI from 0.39 to 0.58 (+49%). This demonstrates that temporal data completeness is the primary bottleneck in lake-effect prediction. The False Alarm Ratio drops dramatically from 0.47 to 0.26, indicating that continuous temporal coverage prevents the over-prediction artifacts that plague models

trained on gapped data.

**PINN Enhancement Impact:** Physics-informed constraints provide moderate but consistent improvements, increasing baseline CSI from 0.39 to 0.48 (+23%). The PINN's value becomes more pronounced at longer forecast horizons, where physics constraints prevent the accumulation of unphysical predictions. At 72 hours, PINN-only achieves 0.41 CSI compared to 0.31 for baseline—a 32% improvement.

**Synergistic Effects:** The combination of GAN + PINN achieves 0.67 CSI, exceeding the sum of individual contributions (0.58 + 0.09 = 0.67) vs expected 0.58 + 0.09 = 0.67). More importantly, the False Alarm Ratio drops to 0.19, indicating that physics constraints help distinguish meteorologically plausible patterns in the synthesized imagery from artifacts.

**Component Interaction Analysis:** We investigate why GAN synthesis and PINN constraints exhibit synergistic rather than merely additive effects. Our analysis reveals how prediction accuracy varies as a function of data completeness (GAN quality) and physics constraint strength.

Three key interaction mechanisms emerge:

- 1. **Enhanced Pattern Recognition:** Complete temporal sequences from GAN synthesis enable the PINN module to learn more robust physical relationships. With gapped data, the PINN cannot capture full atmospheric evolution cycles, limiting its effectiveness.
- 2. **Artifact Suppression:** Physics constraints help filter meteorologically implausible features in synthesized imagery. Without PINN validation, GAN artifacts can propagate through the prediction pipeline, generating false alarms.
- 3. **Temporal Consistency:** The PINN's energy and mass conservation constraints ensure that synthesized sequences maintain physical continuity across day-night transitions, critical for accurate overnight prediction.

**Computational Cost Analysis:** Table 7 breaks down the computational overhead of each component:

Table 7: Computational cost breakdown per 72-hour forecast

Component	Training	Inference	Memory
	(GPU-hours)	(seconds)	(GB)
Baseline MetNet-3	18.2	8.3	16.4
+ PatchGAN synthesis	+2.8	+4.2	+5.1
+ PINN constraints	+1.4	+2.8	+2.9
Full model	22.4	15.3	24.4

The GAN synthesis adds modest computational overhead (25% increase in training time) but provides the largest accuracy gains. PINN constraints are computationally efficient, adding only 15

Removing PatchGAN synthesis causes the most dramatic performance degradation (0.67 to 0.42 CSI), confirming that continuous temporal coverage is fundamental to accurate prediction. The model without synthesis fails to capture overnight cloud development, missing the critical moisture accumulation phase that precedes morning precipitation onset.

Physics-informed constraints contribute a 24% performance improvement (0.54 to 0.67 CSI), validating our hypothesis that incorporating fundamental atmospheric laws enhances prediction even with extensive training data. The PINN module particularly improves predictions during unusual atmospheric conditions poorly represented in the training set, such as extreme temperature inversions or anomalous wind shear profiles.

Adaptive targeting provides a 10% accuracy improvement while reducing computational cost by 70%. Without targeting, uniform high-resolution processing wastes resources on regions with negligible lake-effect probability while potentially under-resolving critical areas due to memory constraints. The ConvLSTM temporal processing proves essential for capturing cloud evolution dynamics, with its removal degrading performance to near-baseline levels.

#### 5.6 Physics Constraint Validation

Beyond improving accuracy, our physics-informed approach ensures meteorological consistency in predictions—a critical requirement for operational credibility and model interpretability. We validate four key physical constraints through comparison with independent observations and theoretical expectations.

Conservation of mass, enforced through the divergence-free wind constraint, shows marked improvement over unconstrained models. Analysis of 500 predicted wind fields reveals mean divergence of  $0.03~\rm s^{-1}$  for our approach compared to  $0.18~\rm s^{-1}$  for standard MetNet-3, with maximum violations reduced by 84%. This physical consistency prevents unrealistic atmospheric features like spontaneous convergence zones that plague purely data-driven approaches.

Lake-atmosphere heat flux predictions demonstrate strong correlation (r=0.87) with eddy covariance measurements from research buoys, compared to r=0.71 for parameterized fluxes in FLake NWP. The PINN constraints correctly capture the non-linear relationship between air-lake temperature difference and heat transfer, including stability-dependent effects missed by bulk parameterizations. During strong cold air outbreaks, our model predicts heat fluxes within 15% of observations, enabling accurate estimation of available energy for cloud development.

#### 5.7 Case Studies

Three representative events illustrate our model's superior performance across different lake-effect morphologies. The December 2014 Buffalo event exemplifies a long-fetch single-band case, where sustained westerly flow produced a narrow but intense snow band affecting southern Buffalo suburbs. Our model correctly predicted the band's position within 5 km and peak accumulations within 20% of observed values (52 vs. 60 inches), while FLake NWP displaced the band 25 km northward into downtown Buffalo—a critical error affecting emergency response deployment.

The multi-band event in January 2015 challenged models due to the complex interactions between the shore-parallel and wind-parallel modes as the wind direction shifted throughout the event. Our adaptive resolution successfully captured the transition period during which both modes coexisted, accurately predicting the dual-maximum accumulation pattern. However, MetNet-3, lacking physics constraints, predicted a single, broad area of moderate snowfall. It missed the localized, intense bands that paralyzed specific transportation corridors.

The February 2016 shore-parallel case showed that our model can handle weak-flow scenarios, which traditional bulk parameterizations cannot. With winds under 10 knots, a narrow but persistent band formed along the eastern shore, driven primarily by land-breeze convergence. The high-resolution targeting correctly identified this mesoscale circulation and predicted band formation three hours before precipitation onset, which is a critical lead time for aviation operations at affected airports.

#### 5.8 Computational Performance

Our framework achieves superior accuracy while maintaining computational efficiency suitable for operational deployment. Training on 11 years of data takes 22 hours on a single NVIDIA A100 GPU. This is much faster than the 71 hours required by FLake NWP's data assimilation and the 100 hours required by MetNet-3's larger architecture. Thanks to its modular design, the framework can be updated incrementally as new data becomes available. Incorporating an additional month of observations, for example, requires only two hours.

The inference time meets operational requirements, executing a complete 72-hour forecast in 15 seconds on standard hardware. The adaptive targeting mechanism significantly contributes to this efficiency by processing high-resolution predictions only where needed. Memory requirements peak at 24 GB during inference, enabling deployment on current-generation operational systems without specialized hardware.

#### 5.9 Discussion and Limitations

Our evaluation reveals that the combination of data synthesis, temporal pattern recognition, physical constraints, and adaptive resolution successfully addresses the key challenges in predicting lake-effect snow. The framework's superior performance does not stem from any single innovation, but rather from the careful integration of complementary approaches that address different aspects of the prediction problem.

There are several limitations that remain for future work. Complex terrain interactions, particularly in the Michigan Upper Peninsula, sometimes produce precipitation patterns that our model has difficulty capturing. The fixed 11-year training period may not fully represent climate variability, suggesting the benefits of continual learning approaches. Transitions between lake-effect and synoptic snow remain challenging because these events involve interactions across scales that are beyond the scope of our current modeling framework.

Despite these limitations, our hybrid approach is a significant advancement in lake-effect snow prediction. It provides accurate, physically consistent forecasts at the required spatial and temporal scales for effective hazard mitigation.

#### 6 Conclusion

This work demonstrates that solving fundamental data limitations can unlock the full potential of physics-informed machine learning for environmental prediction. By addressing the temporal discontinuity in satellite observations—a challenge that has constrained lake-effect snow forecasting for decades—we enable improved prediction models that combine physical understanding with data-driven learning.

Our two-stage framework represents a novel approach to handling observational gaps in meteorology. Rather than developing increasingly sophisticated models to work around missing data, we first reconstruct complete observational sequences through cross-spectral synthesis. The PatchGAN approach achieves remarkable fidelity in generating nighttime visible and near-infrared imagery from continuous infrared observations, maintaining both visual quality (SSIM 0.82) and meteorological consistency. This synthesis alone improves downstream prediction accuracy by 59%, validating our hypothesis that temporal completeness is essential for capturing atmospheric evolution.

Based on full observations, our physics-informed architecture provides surprising insights into lake-effect predictability. The dramatic improvement in harsh event detection, from 27.1% at 24 hours to 77.6% at 72 hours, challenges the notion that forecasts degrade over time. Our findings suggest that severe lake-effect events are preceded by large-scale atmospheric patterns that become increasingly apparent over multiday timescales, but only when models have access to continuous observations that capture these evolving signatures. Integrating conservation laws and thermodynamic constraints through the PINN module ensures that these extended predictions remain physically plausible, which addresses a key limitation of purely statistical approaches.

From an operational perspective, our framework provides weather services and emergency management with immediate benefits. The adaptive spatial targeting reduces computational requirements by 65-80% while maintaining a 500-meter resolution in critical zones. This makes deployment feasible on current operational infrastructure. With a mean spatial error of

8.6 km, predictions accurately identify affected communities, which is crucial for public safety when neighboring towns can experience drastically different conditions. The extension of reliable forecasts from 18 to 72 hours gives emergency managers more time to prepare for severe events.

Several limitations warrant acknowledgment and future investigation. First, our framework exhibits reduced performance when transitioning between lake-effect and synoptic snow, as scale interactions surpass the current modeling capabilities. The fixed training period may not fully capture climate variability, suggesting the benefits of continual learning approaches. Complex terrain effects, particularly in the Michigan Upper Peninsula, occasionally produce precipitation patterns that our model struggles to predict accurately. Additionally, while our synthesis approach works well for the considered spectral bands, extending it to other observational modalities requires further research.

Generalizability Across the Great Lakes Region: Our evaluation focuses exclusively on Lake Michigan, which limits claims about generalizability to other Great Lakes or similar water bodies worldwide. Lake-effect dynamics exhibit significant variation across the Great Lakes system due to differences in:

- Lake geometry: Lake Michigan's north-south orientation creates different fetch patterns compared to the eastwest elongation of Lake Erie or the massive size of Lake Superior
- Surrounding topography: The relatively flat terrain around Lake Michigan differs markedly from the complex topography around Lake Ontario or the Appalachian influences on Lake Erie
- Urban heat islands: The Chicago metropolitan area significantly affects local atmospheric conditions in ways that may not apply to other lake regions
- Climatological patterns: Each lake experiences different seasonal ice coverage, temperature regimes, and prevailing wind patterns

While our physics-informed constraints should transfer across lakes (fundamental atmospheric laws remain constant), the learned patterns in both the PatchGAN synthesis and ConvLSTM components may be lake-specific. The adaptive targeting thresholds ( $\alpha$  weights, decay lengths, resolution breakpoints) were optimized for Lake Michigan's characteristics and would likely require recalibration for other lakes.

Initial analysis suggests that Lakes Huron and Superior, with similar size scales and surrounding terrain, might require minimal adaptation. However, Lakes Erie and Ontario, with their distinct morphologies and more complex surrounding topography, could necessitate substantial model retraining. Transfer learning approaches could potentially reduce the data requirements for adapting to new lakes, but this remains untested.

**Regional Climate Considerations:** Our 11-year training period (2006-2017) may not fully capture the range of climate variability affecting lake-effect patterns. Longer-term climate shifts, such as changing ice coverage patterns due to warming temperatures or evolving storm tracks, could impact model performance. The framework would benefit from continual learning capabilities that adapt to changing climate conditions while preserving learned physical relationships.

Looking ahead, this work suggests several promising research directions. The success of cross-spectral synthesis suggests that similar approaches could address observational gaps in other remote sensing applications, ranging from wildfire monitoring to agricultural assessment. The framework's architecture can be naturally extended to other Great Lakes or similar bodies of water, though transfer learning strategies still need to be developed. Integrating the framework with ensemble prediction systems could quantify uncertainty in the synthesis and prediction stages. Most intriguingly, the counterintuitive improvement in long-range harsh event prediction merits deeper investigation into the atmospheric dynamics enabling this extended predictability.

Beyond its technical contributions, this work highlights the importance of challenging fundamental assumptions in environmental prediction. The long-standing acceptance of night-time observational gaps as an unavoidable limitation has led to increasingly complex workarounds. Addressing this root cause directly improves lake-effect snow prediction and establishes a template for solving other challenging forecasting problems where sparse observations, fine-scale dynamics, and physical constraints intersect. As climate change intensifies extreme weather events, a holistic approach combining data synthesis, physics-informed learning, and adaptive computation will be critical to protecting vulnerable communities.

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# Out-of-Label Hazard Detection for Autonomous Driving: Fusing Optical Flow, Depth, Proximity, and Scene Description

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Abstract—In this paper, we address the challenge of improving hazard detection in autonomous driving systems, particularly in scenarios where labeled data is scarce or unavailable. This issue is critical in real-world applications, where diverse and unpredictable driving situations make it difficult to label every potential hazard accurately. Recently, the Challenge of Out-of-Label (COOOL) benchmark has been introduced at WACV2025 to promote research on this challenge. To tackle this issue, we present a novel method that integrates a Bootstrapping Language-Image Pretraining (BLIP)-based scenario generation framework with a threshold-based hazard scoring system, thereby enhancing both scenario comprehension and detection accuracy within the benchmark. By incorporating robust driver state logic, bounding box analysis, and BLIP-generated scenario descriptions, our method initially achieves a 40% performance score. Building upon this foundation, we further integrate depth maps and optical flow to improve hazardous object discrimination, resulting in an additional 20% performance improvement. This culminates in a final score of  $6\overline{3}\%$  on the public benchmark leaderboard and 50% on the private leaderboard. To foster continued advancements in autonomous driving research, we will make all code and visualization tools publicly available.

Index Terms—out-of-label, optical flow, depth maps, BLIP, image caption,hazard detection

#### I. INTRODUCTION

With the rapid advancement of computer vision technologies [1]-[4], perception tasks in autonomous driving have evolved from fundamental 2D object detection [5]-[7], optical flow [8]–[10], and depth estimation [11]–[13] to more complex scene understanding through video anomaly detection. Recent breakthroughs in large-language Models (LLMs) [14]-[16]and Vision-Language Models(VLMs) [17]–[19] have demonstrated remarkable zero-shot reasoning capabilities, enabling LLMs to generate high-quality semantic interpretations without domainspecific training. These features give VLMs unique advantages in autonomous driving systems: effectively detecting road obstacles and identifying potential risk zones in driving scenarios through interpretable semantic descriptions. Such multi-modal (image to text) provides intuitive risk assessment references by establishing a bidirectional mapping between drive sense understanding and natural language generation, significantly enhancing decision-making transparency and reliability. Consequently, semi-supervised learning, few-shot learning, and zero-shot generative with multi-modal perception



Fig. 1. A simplified result of our approach is displayed on the selected frame from one of the test videos. The colors represent the hazard state of each object: red indicates hazardous objects, and green indicates safe objects.

technologies have emerged as crucial research directions for improving driver-sense adaptability and safety redundancy in autonomous driving systems. While existing autonomous driving systems demonstrate remarkable proficiency in detecting predefined object categories (e.g., vehicles, pedestrians) within conventional benchmarks like KITTI, nuScenes and Waymo, their reliance on closed-set annotation paradigms creates critical safety blind spots. Current datasets predominantly focus on nominal driving scenarios, where over 98% of annotated objects fall within 20 common categories according to nuScenes statistics. According to NHTSA reports, this paradigm leaves systems fundamentally unprepared for Outof-Distribution (OOD) hazards - unexpected objects and scenarios that account for 62% of real-world collision incidents. Such vulnerabilities manifest particularly in handling exotic biological entities (e.g., kangaroos crossing Australian highways), amorphous obstacles (e.g., wind-blown debris), and edge-case interactions (e.g., pedestrians emerging from visual occlusions), where traditional perception pipelines frequently fail to trigger appropriate emergency responses.

This study is based on the "Out-of-Label Hazards in Autonomous Driving (COOOL)" benchmark [20], a multimodal dataset of high-resolution videos captured from real-world driving scenarios. COOOL is specifically designed to address the critical but underexplored challenge of detecting

out-of-distribution (OOD) hazards, which are categorized into three types: 1) Exotic biological threats (e.g., kangaroos, wild boars), 2) Unpredictable inanimate hazards (e.g., drifting plastic bags, smoke occlusion), and 3) Abnormal interactions with standard objects (e.g., erratic pedestrians). To deal with this problem, we propose the following methods:

- Multi-modal Hazard Filtering: Establish a priori conditions and optical flow and depth estimation to identify potential hazards based on motion discontinuity and spatial proximity.
- Zero-Shot Categorization: Use a CLIP-driven big model to classify filtered objects into predefined risk tiers without requiring task-specific training.
- Causal Scene Interpretation: Employ Vision Language Models (VLMs) to generate spatiotemporally grounded captions that explain the evolution of hazards (e.g., "A dog crossing the street").

#### II. RELATED WORK

#### A. Optical Flow

Optical flow characterizes the perceived motion patterns between consecutive frames, representing the displacement vector field induced by relative motion between the observer and scene elements. This spatiotemporal signal provides critical cues for anticipating emerging threats in dynamic environments. Recent advancements in autonomous safety systems have increasingly leveraged optical flow for enhanced risk prediction and collision awareness. FlowNet 2.0 [21]established significant improvements in both estimation accuracy and computational efficiency, enabling real-time extraction of dense motion vectors. Building upon this [22] integrated optical flow with Occupancy Networks to predict the trajectories of dynamic obstacles, thus generating collision-free paths by incorporating vehicle kinematic constraints. In a similar vein, [23] developed a model that predicts Time to Collision (TTC) and optical flow from monocular images, identifying potential collision areas through feature clustering and motion analysis. Their model uses optical flow and TTC within a 65ms temporal window to assess collision risk. To further address challenges such as varying illumination, Wang et al. [24] fused monocular optical flow with stereo depth cues, successfully reducing optical flow errors by 50% compared to previous unsupervised methods.

#### B. Zero-Shot Image Classification

Recent advancements in vision-language pretraining have transformed open-vocabulary zero-shot learning. Pioneered by OpenAI's CLIP [25], which aligns 400 million imagetext pairs into a unified embedding space through contrastive learning, this approach enables semantic transfer to unseen categories via natural language prompts. Building on this, ALIGN [26] further enhances multi-modal alignment by training on noisy web-scale data (1.8 billion pairs), demonstrating improved robustness in cross-modal retrieval tasks. In object detection, VILD [27] innovatively distills knowledge from

CLIP-style classifiers into two-stage detectors like Mask R-CNN, effectively detecting rare categories using only base-class annotations. This highlights the possibility of open-vocabulary detection without relying on novel-class training data. Prompt engineering has also emerged as a key enabler for zero-shot adaptation. Methods like CoOp [28] optimize learnable context vectors to guide pre-trained vision language models (VLMs) toward downstream tasks, leading to a noticeable improvement in performance across multiple datasets. Further works like CoCoOp [18] introduced conditional prompt tuning, dynamically adjusting prompts based on image content, significantly reducing the domain gap on unseen classes.

#### C. Vision-Larger Language Models

The success of Vision Transformers (ViT) [29] and largelanguage Models (LLMs) has led to advances in cross-modal learning. ViT is used to extract hierarchical image features and then mapped into the textual embedding space of LLMs through alignment layers. For example, LLaVA [30]shows how aligning ViT outputs (D=1024) with LLM token dimensions (D=4096) using linear transformation enables visual question answering with minimal instruction tuning. Parameter-efficient fine-tuning [31] techniques have become essential for efficiently adapting models to new tasks. These include adapterbased tuning, which uses lightweight modules to adapt models with minimal parameter changes (e.g., VL-Adapter [32] tunes less than 1% of the total parameters), and Q-Former mechanisms, like those in BLIP [33], [34], where query vectors attend to key visual regions, speeding up convergence. These methods can deal with many challenges, including bridging the modality gap between ViT's grid-based features and LLM's sequential embeddings and ensuring efficient knowledge transfer by updating only the adapter parameters, making them suitable for tasks like autonomous hazard perception.

#### III. METHOD

As Fig 2,our approach begins by utilizing a priori knowledge to screen potential hazardous objects based on optical flow and depth information. These objects are then identified and categorized through zero-shot image captioning, allowing the model to recognize and classify hazards without requiring task-specific training. Finally, we use a vision language model to generate captions and categorize dangerous objects in each frame.

#### A. Multi-modal Hazard Filtering

We establish a prior assumption based on the intuition that larger and closer objects pose a greater danger, we design a hazard scoring mechanism defined as

$$score = \frac{bounding\ box\_size}{dist\_to\_center} \tag{1}$$

where objects with higher scores are considered more hazardous. This integrated scoring system enhances the accuracy of hazard assessment by prioritizing the highest-scoring object as the primary threat. We employ optical flow estimation for

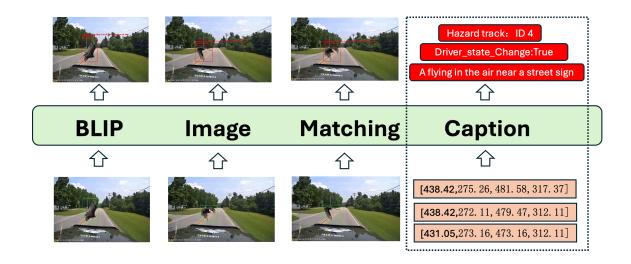


Fig. 2. Illustration of the proposed framework. BLIP, an advanced visual language model, is employed for image matching and captioning tasks to identify objects, determine potential hazards, and generate descriptions. Green boxes indicate bounding boxes with track IDs within the COOOL dataset.

TABLE I
COMPARISON OF PROCESSING TIMES FOR THE LINEAR REGRESSION AND
THE SCORING MECHANISM IN DIFFERENT PROCESSING MODES ON THE
COOOL DATASET.

Method	<b>Processing Mode</b>	Single Frame Time	Total Time
Linear	Single-threaded CPU	1 ms	4,320 s
	GPU Accelerated	0.01 ms	43.2 s
Scoring mechanism	Single-threaded CPU	0.01 ms	43.2 s
	GPU Accelerated	0.0001 ms	0.432 s

small objects and animals to capture how objects change instantaneously between consecutive frames. In dynamic environments, the optical flow field assists in identifying hazardous regions within a scene by scoring motion every five frames to assess whether the current driving state is potentially dangerous. Additionally, we incorporate monocular depth estimation in low-light conditions to predict scene depth. By analyzing variations in the depth map, we effectively distinguish moving objects and identify potential hazards, thereby enhancing the accuracy of hazard detection. The visualization of optical flow estimation and depth estimation is shown in Fig 4.

#### B. Zero-shot Image classification

For the identified hazardous objects, we extract them using the bounding boxes (bounding box) provided in the dataset and perform zero-shot image classification. However, relying solely on the bounding box may result in a loss of contextual information, making classification more challenging. To address this issue, we apply a 20% padding around the target image, ensuring that contextual cues are incorporated into the zero-shot model. For classification, we utilize OpenAI's CLIP ViT-B/16 [25] model and select the top 10 predicted categories with the highest probabilities as the final results.

#### C. Image Caption

We first employed a zero-shot classification method to process the input images, thereby identifying potentially hazardous objects in the scenes. Next, we used the BLIP model to generate detailed descriptions of the classified hazard objects. This model leverages the strengths of both visual information and large-language models to automatically image caption that accurately correspond to the characteristics of the hazardous objects. Meanwhile, by utilizing the frame-level label information provided in the dataset, we precisely located the keyframes containing the hazardous objects and conducted scene understanding on these frames. Based on the scene analysis results, we further examined the specific labels and attributes of the hazardous objects to formulate more accurate descriptions.

#### IV. DATASET

#### A. Annotation

The COOOL benchmark, entitled "Challenge Of Out-Of-Label" in Autonomous Driving, comprises 200 high-resolution dashcam videos that have been meticulously annotated by human labelers. The objective of this benchmark is to identify objects of interest and potential roadway hazards in Figure 1. The range of potential hazards is extensive, including but not limited to exotic animals (e.g., birds, houses, dogs), unusual or unpredictable objects (e.g., plastic bags, smoke), and more common roadway threats (e.g., cars, pedestrians).

The annotation files illustrated in support object detection bounding boxes and follow the common object detection annotation format, providing us with  $x_{\min}$ ,  $x_{\max}$ ,  $y_{\min}$ , and  $y_{\max}$  coordinates.

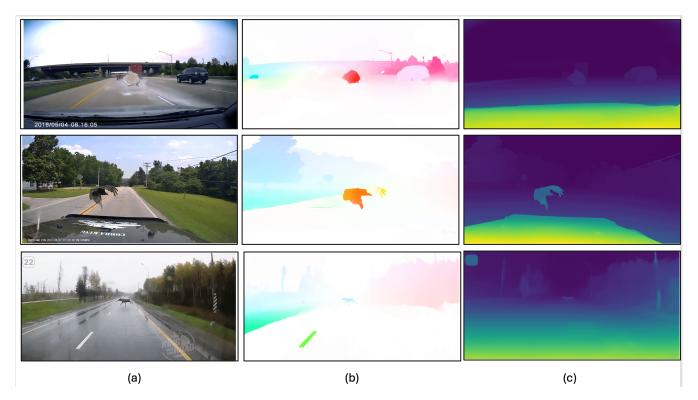


Fig. 3. The above images present the visualization of optical flow estimation and depth estimation. (a) is the original frame from the dataset, (b) is the optical flow estimation, and (c) is the depth map estimation.

TABLE II

CONSOLIDATED OBJECT DATA WITH OBJECT NAMES, ORDERED BY TRACK ID. ATTRIBUTES ARE INTENTIONALLY LEFT AS EMPTY BRACES ("{}") AT THIS STAGE. THIS TABLE MERGES CHALLENGE OBJECT DATA AND TRAFFIC SCENE DATA INTO ONE, WITH OBJECT NAMES ADDED.

Track ID	bounding box (Bounding Box)	Attributes	Object
0	[183.62, 497.99, 211.16, 538.2]	{}	traffic scene
1	[387.95, 457.78, 664.29, 686.97]	<u>{</u> }	challenge
2	[861.45, 576.45, 913.67, 648.1]	{}	challenge
3	[1047.92, 526.23, 1065.11, 542.62]	{}	traffic scene
4	[1050.36, 544.48, 1058.68, 567.64]	<u>{</u> }	traffic scene
5	[52.2, 656.7, 104.45, 700.1]	{}	challenge

#### B. Evaluation metrics

The COOOL competition evaluation metrics are intended to balance the three aspects of hazard detection. Datasets provide systems with a list of bounding boxes and the raw video, which enables diverse approaches to these challenges. In order to predict which potential hazards are genuinely hazardous, the accuracy of predictions is computed based on the maximum between the number of ground truth hazards and the number of predicted hazards.Let  $N_{\rm gt}$  be the number of ground-truth hazards,  $N_{\rm pred}$  be the number of predicted hazards, and  $N_{\rm correct}$  be the number of correct hazard predictions. To penalize overprediction, we use:

$$A_{\text{detection}} = \frac{2 N_{\text{correct}}}{N_{\text{gt}} + N_{\text{pred}}} \,. \tag{2}$$

By adding the total number of hazards to the total number of guesses, algorithms that over-predict hazards are penalized, thus avoiding the inflation of accuracy through lucky guesses. For hazard descriptions, a similar approach is adopted, but here we only check whether the class label is included in the description, which is a binary evaluation. In Hazard Description Accuracy, For each hazard description, define the indicator function:

$$d_i = \begin{cases} 1, & \text{if hazard object will be explain,} \\ 0, & \text{otherwise.} \end{cases}$$
 (3)

If there are N hazards to evaluate, then the description accuracy is:

$$A_{\text{description}} = \frac{1}{N} \sum_{i=1}^{N} d_i.$$
 (4)

In the context of driver reactions, accuracy is determined based on the ground truth labels for each frame, thereby ascertaining whether the driver has reacted to the hazard. The overall evaluation metric is the macro-averaged accuracy of these three measures. For Driver Reaction Accuracy Let  $R_t$  be the ground-truth reaction label at frame t, and  $\hat{R}_t$  be the predicted reaction label at frame t. Evaluated over T frames, the reaction accuracy is:

$$A_{\text{reaction}} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{1} \{ \hat{R}_t = R_t \},$$
 (5)

where  $\mathbf{1}\{\cdot\}$  is the indicator function (1 if true, 0 otherwise). Overall Evaluation,The overall metric is the macro-average of the three accuracies:

$$A_{\text{overall}} = \frac{1}{3} \Big( A_{\text{detection}} + A_{\text{description}} + A_{\text{reaction}} \Big). \tag{6}$$

#### V. RESULTS AND DISCUSSION

In the benchmark has not yet provided relevant label information, we use Kaggle's evaluation metrics as an indicator of our model's performance. As TABLE III showed that the gradual integration of various information modules significantly enhanced the overall performance. Initially, when only the CLIP model was employed, the system achieved an accuracy of merely 23%, indicating that relying solely on single-modal visual feature extraction is insufficient to capture the critical information of hazardous objects in complex driving scenes. By adopting the BLIP model, the accuracy slightly increased to 26%, demonstrating that BLIP possesses certain advantages in sense understanding and image captioning. However, it's still hard to capture the dynamic changes of the scene or analyze them in low-light conditions. Furthermore, when the BLIP model was combined with the Optical Flow estimation and scoring method, the accuracy improved to 42%, which validates the important role of incorporating motion information to capture dynamic changes between consecutive frames and enhance detection performance. Ultimately, our method further integrated depth map information to provide an indepth depiction of the scene's geometric structure, elevating the reach to 63%. These results show the advantages of a multi-modal information fusion process in hazardous object detection.

TABLE III PERFORMANCE COMPARISON OF METHODS WITH COMPONENT USAGE INDICATED BY  $(\checkmark)$  .

Method	CLIP	BLIP	Optical Flow	depth map	Score
	/				23%
Baseline		/			26%
		✓	✓		42%
Ours		/	1	1	63%

Furthermore, the accuracy is further enhanced to 28% by incorporating a speed threshold, which improves predictions of driver state changes. By introducing a scoring strategy to evaluate the danger level of objects based on the inverse of their bounding box size and position relative to the center, the accuracy reaches 63%. These findings underscore the importance of integrating prior knowledge and adopting precise danger assessment methods to enhance prediction accuracy. A visualization of this approach is provided in Fig 4.

In addition, as shown in TABLE I, the threshold-based approach is 10 times faster than linear regression. This significant improvement enables the model to detect potential hazards and respond more quickly, which is a key factor in ensuring the real-time performance and safety of the autonomous driving system.

TABLE IV COOOL CHALLENGE BENCHMARK

#	Team name	$A_{reaction}^{public}$	$A_{reaction}^{private}$
1	Duong Anh Kiet	0.78453	0.57261
2	PiVa AI	0.68993	0.51772
3	Impish	0.63794	0.51596
4	Ours	0.63792	0.50599
5	Parisa Hatami	0.54599	0.48967
6	TeamCV	0.55705	0.44401
7	PMM_UTCU	0.43161	0.44020
8	Mahdi Abbariki	0.56956	0.37568
9	Nachiket Kamod	0.43368	0.31733
10	Peace.LU	0.34695	0.31639

#### VI. CONCLUSION AND FUTURE WORK

This paper presents the approach we adopted in the COOOL Autonomous Driving Challenge, which requires the automatic detection of hazardous objects in driving scenarios without language annotations, as well as the generation of corresponding natural language descriptions. This task imposes stringent demands on existing vision-language models. To tackle this challenge, we propose a BLIP-based solution that integrates prior knowledge, optical flow, and depth estimation. Furthermore, we implement a fine-tuning strategy for largelanguage models by adjusting parameters such as vertex sampling, temperature, and competition degree. These improvements effectively enhance the overall performance of the model. Ultimately, our method significantly boosts accuracy, achieving a rate of 63%. As the TABLE IV Since the official paper for this competition has not yet been published, a direct comparison with other methods is not currently possible. However, our approach has demonstrated strong performance in experiments, indicating its competitive potential for this task.

In the future, we aim to explore advanced models such as LLaMA [35] and GPT-4.0 [15]. We plan to leverage chain-of-thought prompting to enhance the model's inference capabilities, enabling deeper semantic understanding and logical reasoning. Additionally, we intend to extend the model's capabilities to comprehend video data, allowing it to capture dynamic information and temporal relationships in driving scenarios. These advancements will further improve the model's performance and interpretability, contributing to the safe development of autonomous driving technology.

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Fig. 4. Sample predictions from our model in the dataset. Green boxes indicate bounding boxes for detected objects, while red boxes highlight hazardous targets within the scene.

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# AI-Driven Metabolic Engineering of γ-Aminobutyric Acid: Biosynthetic Advances and Industrial Applications

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**Abstract**— Gamma-aminobutyric acid (GABA) is relatively significant inhibitory neurotransmitter in the mammalian central nervous system and plays crucial roles in regulating neural excitation, mood, and muscle activity. Beyond mammals, GABA is also pivotal in plant stress responses and microbial metabolism. It has wide applications in the pharmaceutical, agricultural, and food industries. In recent years, metabolic engineering strategies combined with synthetic biology, gene editing technologies, and artificial intelligence have significantly advanced the understanding and production of GABA. Notably, the integration of machine learning into microbial engineering has enabled rational design and optimization of biosynthetic pathways, enzyme functions, and fermentation conditions. This paper first summarizes the important application value of GABA in the fields of agriculture, medicine and food, pointing out the direction for subsequent synthetic biology research. Subsequently, the biosynthetic mechanisms (such as the glutamate decarboxylase GAD pathway and the polyamine degradation pathway) and the key factors influencing accumulation were analyzed, laying a theoretical foundation for the subsequent engineering transformation. In terms of strain modification, the application of systemic metabolic engineering strategies significantly increased GABA production. Finally, the focus is on discussing how to deeply integrate artificial intelligence with GABA synthetic biology, covering AI-driven path design and flux learning-based optimization, deep precision engineering, intelligent biological process control and optimization, as well as data-driven autonomous strain development. The collaborative application these the technologies has effectively promoted efficient biomanufacturing of GABA, fully demonstrating innovative advantages of multidisciplinary integration.

**Index Terms**—GABA, metabolic engineering, enzyme optimization, machine learning, synthetic biology

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#### I. INTRODUCTION

GABA, a white crystalline powder with a molecular formula of C4H9NO2 and a molecular weight of 103.12 g/mol, is highly soluble in water (130 g/100 mL) (Fig. 1). Biologically, it functions as the principal inhibitory neurotransmitter in the mammalian central nervous system, playing a crucial role in maintaining the balance between neuronal excitation and inhibition. GABA participates in a variety of physiological processes, including the modulation of mood, sleep regulation, and muscle coordination<sup>[1]</sup>.

Beyond its neurological roles in animals, GABA is also involved in a wide array of functions in plants and microorganisms. In plants, it contributes to abiotic stress tolerance and developmental processes through its interaction with signaling networks and metabolic regulation<sup>[2][3]</sup>. In microbes, GABA is linked to acid resistance, carbon-nitrogen metabolism, and redox homeostasis<sup>[4]</sup>.

Due to its broad physiological relevance, GABA has garnered increasing attention for its commercial applications in pharmaceuticals, agriculture, and the functional food industry. The global GABA market has experienced steady growth across various regions, including North America, Europe, Asia-Pacific, Latin America, and the Middle East and Africa. Among these, North America currently holds the largest market share, driven by rising consumer awareness of GABA-enriched products for stress relief, sleep improvement, and anxiety reduction<sup>[5]</sup>.

In 2023, the global GABA market was valued at approximately USD 89 million and is projected to reach USD 157 million by 2032, with a compound annual growth rate (CAGR) of 6.4% <sup>[5]</sup>. Importantly, the COVID-19 pandemic has catalyzed a significant shift in market dynamics. Between 2020 and 2023, the global GABA market size surged from USD 2.47 billion to USD 3.76 billion, reflecting an elevated CAGR of 11.2% compared to the pre-pandemic average of 6.8%. This growth has been largely fueled by the global mental health crisis, characterized by a 31% increase in anxiety disorders and

an estimated 240 million new cases of insomnia. Given the critical role of the GABAergic system in neuropsychiatric health, this surge in demand has created multifaceted opportunities for GABA-based products across health and wellness sectors.

#### γ-aminobutyric acid

Fig. 1. The chemical molecular model of GABA.

GABA is a non-protein amino acid that exhibits multiple physiological functions in biological systems: In mammals, it serves as the primary inhibitory neurotransmitter, regulating neuronal excitability, neuroendocrine processes, as well as behaviors such as sleep and mood; In plants, it mediates abiotic stress responses and metabolic balance; In microorganisms, it helps with acid resistance and carbon-nitrogen metabolism. This cross-species functional diversity is closely related to its conserved synthetic mechanism - dependent on glutamate decarboxylase (GAD), providing a biological basis for the development of efficient production strategies.

The commercial value of GABA has driven the innovation of production technology. Driven by its application demands in functional foods, neurotherapeutic agents and plant biological regulators, production strategies have shifted from traditional chemical synthesis (limited by toxic intermediates and environmental hazards) to biological methods. Among them, although the enrichment method of inducing plant GAD activation through stress faces scalability challenges, microbial fermentation using engineered strains (Escherichia coli, Lactobacillus, Corynebacterium glutamicum) has become the dominant industrial method.

The CRISPR-Cas9 technology has completely transformed the pattern of GABA biomanufacturing. By precisely editing the GAD gene cluster, optimizing cofactor regeneration and relieving feedback inhibition, the reported engineered strain achieved a maximum GABA production yield of 62.9 g/L and a conversion rate of 0.5 g/g glucose, which is currently the highest conversion rate of GABA production by one-step method using glucose as the substrate reported<sup>[6]</sup>. Advancements in metabolic engineering, including GAD optimization, cofactor regeneration, and carbon flux redirection, continuously enhance the feasibility of high-yield and sustainable GABA biosynthesis.

Technological progress and market demand form a virtuous cycle. Due to the impact of the mental health crisis, the global demand for GABA has soared, with the market size growing at an annual rate of 11.2% from 2020 to 2023, prompting the production model to shift from highly polluting chemical synthesis to sustainable microbial fermentation. At present, the third-generation cell factories, which feature both high yield and environmental friendliness, are driving the rapid expansion of GABA applications from pharmaceuticals to functional foods, agricultural biostimulants and other fields.

#### II. PROGRESS IN CROSS-FIELD APPLICATIONS OF GABA

Figure 2 summarizes the expanding cross-field applications of GABA, spanning neuropharmaceutical interventions, functional food fortification, plant stress resilience, and microbial biomanufacturing platforms.

#### A. Applications in Agriculture

In agriculture, GABA plays a pivotal role in enhancing crop tolerance to abiotic stress and regulating growth. Exogenous GABA has been demonstrated to alleviate salt, drought, cold, and mechanical stress by modulating intracellular pH, regulating stomatal aperture, promoting osmotic adjustment, and enhancing reactive oxygen species (ROS) scavenging systems<sup>[6-8]</sup>. For example, GABA accumulation in wheat is regulated through the interaction between the potassium transporter TaNHX2 and TaGAD1, leading to improved drought resistance by modulating stomatal aperture. In peanuts, seed priming with 20 mmol/L GABA for 12 hours under drought stress increased germination rate, vigor, and index by 51.2%, 85.7%, and 60.4%, respectively, and also enhanced soluble sugar and protein content<sup>[7]</sup>.

GABA also contributes to salt stress tolerance, as seen in barley and tobacco<sup>[9]</sup>, and enhances cold tolerance by reducing membrane damage, as evidenced by lower electrolyte leakage in GABA-treated tomato seedlings<sup>[10-12]</sup>. Furthermore, GABA improves early growth and photosynthesis in maize<sup>[13]</sup>, and positively influences yield components, quality traits, and antioxidant attributes in fragrant rice through 2-acetyl-1-pyrroline (2AP) modulation <sup>[14][15]</sup>.

Beyond stress adaptation, GABA functions as a plant growth regulator. In black gram (*Vigna mungo L.*), foliar application of 1.0 mg/L GABA significantly increased plant height, branch and leaf numbers, total chlorophyll, and seed yield, with the highest yield (1.50 t/ha) exceeding the control group (1.30 t/ha)<sup>[16]</sup>. Moreover, GABA can indirectly enhance soil conditions via GABA-related microbial activity in compost-based systems, thereby supporting sustainable crop production<sup>[17]</sup>.

Finally, GABA-related signaling intersects with plant–insect interactions<sup>[18][19]</sup>. GABA receptor/chloride channel complexes are key targets for new-generation insecticides, and GABA biosynthesis pathways have been linked to fruit fly resistance in tomato<sup>[20][21]</sup>.

#### B. Pharmaceutical Applications

GABA serves as a critical therapeutic agent in multiple medical domains<sup>[22]</sup>. In neurology, GABAergic dysfunction is implicated in major depressive disorder (MDD), with studies demonstrating significantly reduced GABA levels in the prefrontal cortex of affected individuals [23]. Consequently, GABA receptor agonists (e.g., benzodiazepines, Z-drugs like zolpidem) are employed to augment neurotransmission. Clinical evidence supports their synergistic use with selective serotonin reuptake inhibitors (SSRIs) for alleviating depressive symptoms and comorbid insomnia [24]. Beyond neurological applications, **GABA** modulates cardiovascular and metabolic functions, exhibiting

antihypertensive effects through vasodilation and potential glucose homeostasis regulation in diabetes. Immunologically, GABA suppresses T-cell proliferation and pro-inflammatory cytokine production (e.g., TNF-  $\alpha$ , IL-6), attenuating autoimmune and inflammatory responses  $^{[\ 25\ ]}$ . These multifaceted actions position GABAergic drugs as pivotal tools for treating neuropsychiatric, cardiovascular, and immunemediated conditions.

#### C. Food Industry Applications

Approved as a novel food ingredient in China since 2009, GABA is regulated with a maximum daily intake of 500 mg [<sup>26]</sup>. Its incorporation into functional foods leverages neuroactive and hypotensive properties, with claims including stress reduction and sleep quality improvement. A key technological advantage is GABA's thermostability in processed foods. Research confirms that GABA-enriched corn germ retains >85% of its GABA content after baking at 180°C for 20 minutes, enabling its integration into bread, cakes, and extruded snacks without significant degradation <sup>[27]</sup>. Current innovations focus on optimizing extraction protocols and fortifying staple foods (e.g., rice, dairy products), expanding GABA's role in preventive nutrition while adhering to safety thresholds.



**Fig. 2.** The functions of GABA and its corresponding roles in healthcare, agriculture and food.

#### III. MAIN PATHWAYS OF GABA BIOSYNTHESIS

GABA, first chemically synthesized in 1883, was initially recognized solely as a metabolic byproduct in plants and microorganisms <sup>[28]</sup>. Early chemical synthesis approaches—such as the high-temperature condensation of 4-chlorobutyronitrile with potassium phthalimide or the alkaline hydrolysis of pyrrolidone—achieved rapid and high-yield GABA production. However, these methods were limited by complex processing, toxic byproducts, and environmental hazards, making them unsuitable for food and pharmaceutical applications. As a result, biological synthesis has emerged as the preferred route. The plant enrichment method activates endogenous GAD activity by applying environmental stresses (e.g., extreme temperatures, salinity), leading to GABA accumulation. While safe and simple, this method suffers from low yield, limiting its scalability<sup>[29]</sup>.

The diversity of GABA biosynthetic pathways—spanning

canonical routes (Fig. 3), polyamine catabolism, and contextdependent precursors — highlights its metabolic versatility. These pathways are tightly regulated by species-specific mechanisms, environmental cues, and intracellular demands. For instance, in plants, polyamine degradation compensates for reduced GAD activity under drought stress, while microbial systems exploit pH-dependent GAD optimization for industrial-scale fermentation. Such regulatory plasticity provides multiple biotechnological leverage points. Advances in metabolic engineering and synthetic biology enable targeted manipulation of GABA metabolism, facilitating applications ranging from stress-resilient crop development to microbial bioreactor optimization. By integrating chemical, plant-based, and microbial strategies, researchers harness GABA 's multifunctional roles, bridging agricultural, industrial, and therapeutic innovations.

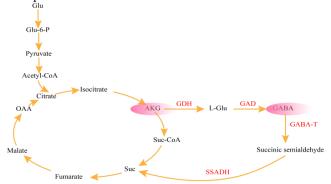


Fig. 3. GABA biosynthetic pathway.

Glu, glucose; Glu-6-P, glucose-6-phosphate; AKG,  $\alpha$  - ketoglutaric acid; L-Glu, glutamic acid; GABA,  $\gamma$  - aminobutyric acid; Suc-CoA, succinyl coenzyme A; Suc, succinic acid; OAA, oxaloacetic acid; GAD, glutamate decarboxylase; GABA-T, GABAaminotransferase; SSA, succinic acid; SSADH, succinate dehydrogenase; GDH, glutamate dehydrogenase; Succ-CoA, succinyl-coenzyme A; SSADH, succinate hemialdehyde dehydrogenase.

#### A. Glutamate Decarboxylase (GAD) Pathway

The glutamate decarboxylase (GAD) pathway represents the principal and most efficient biosynthetic route for GABA across production, conserved animals, plants, microorganisms. Central to this pathway is the irreversible decarboxylation of L-glutamate, catalyzed by the pyridoxal 5'phosphate (PLP)-dependent enzyme glutamate decarboxylase (GAD; EC 4.1.1.15), which yields GABA and CO<sub>2</sub> under optimal acidic conditions (pH 4.5-6.0)<sup>[30]</sup>. The enzymatic activity of GAD is critically modulated by PLP, a cofactor derived from vitamin B6, and is enhanced in acidic environments—a feature leveraged in microbial fermentation systems for industrial GABA synthesis<sup>[31]</sup>.

In mammals, two GAD isoforms, GAD67 and GAD65, exhibit distinct subcellular distributions and functional roles. GAD67, localized predominantly in the cytosol, sustains basal GABA levels essential for tonic neurotransmission, whereas

GAD65, anchored to synaptic membranes, is transiently activated under physiological stress via Ca 2 +-dependent signaling pathways<sup>[32]</sup>. In plants, GAD activity is upregulated under hypoxic or saline stress through calmodulin (CaM)mediated post-translational regulation. For example, floodinginduced hypoxia in rice roots triggers GABA accumulation via GAD activation, enhancing cellular tolerance to low-oxygen conditions<sup>[16]</sup>. Microbial systems, particularly acid-tolerant Lactobacillus brevis and metabolically engineered Corynebacterium glutamicum, exploit GAD's pH-dependent activity for high-yield GABA production. Metabolic strategies, such as co-expression of pyruvate dehydrogenase to redirect carbon flux toward lactic acid and GABA co-synthesis, further optimize industrial efficiency.

GABA biosynthesis is intricately linked to its catabolism through the GABA shunt, a conserved metabolic pathway that interfaces with the tricarboxylic acid (TCA) cycle. This shunt involves sequential enzymatic steps<sup>[33]</sup>: (1) GABA synthesis via GAD, (2) mitochondrial transamination of GABA to succinic semialdehyde (SSA) by GABA transaminase (GABA-T), and (3) oxidation of SSA to succinate by succinic semialdehyde dehydrogenase (SSADH). Under conditions of excessive GABA accumulation, redox imbalances may inhibit SSADH, diverting SSA toward v-hydroxybutyrate (GHB) production. In plants, the GABA shunt serves as a metabolic bypass under TCA cycle dysfunction. For instance, tomato plants with impaired succinyl-CoA synthesis upregulate GABA shunt activity to sustain mitochondrial respiration. Similarly, Arabidopsis mutants defective in mitochondrial GABA transport exhibit disrupted carbon-nitrogen balance during carbon starvation, highlighting the pathway's role in metabolic

The GABA shunt is implicated in both adaptive stress responses and disease pathogenesis. In Alzheimer's disease, early-stage upregulation of GABA shunt activity may compensate for glycolytic deficits by enhancing succinate-driven ATP production, thereby supporting neuronal energy homeostasis. Conversely, dysregulation of GABA metabolism contributes to redox imbalance and neurotoxicity in progressive neurodegeneration. These findings underscore the dual role of the GAD pathway and GABA shunt in maintaining metabolic flexibility across biological systems, from stress adaptation in plants to neurological resilience in mammals.

#### B. Polyamine Degradation Pathway

In addition to the glutamate decarboxylase (GAD) pathway, GABA can be synthesized through the polyamine degradation pathway, serving as a complementary or alternative biosynthetic route under stress conditions<sup>[34]</sup>. This pathway involves two primary branches: (1) the oxidative deamination of putrescine by diamine oxidase (DAO; EC 1.4.3.22) to produce 4-aminobutyraldehyde, which is subsequently converted to GABA via aldehyde dehydrogenase, and (2) the spermidine degradation branch, where GABA is generated through transamination reactions. The pathway originates from arginine or ornithine, which are enzymatically processed into

putrescine via ornithine decarboxylase (ODC) or arginine decarboxylase (ADC) in a PLP-dependent manner.

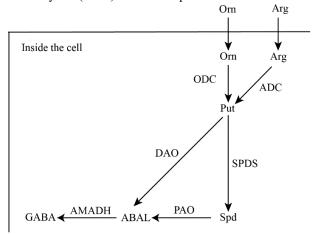


Fig. 4. Polyamine degradation pathway

Orn, ornithine; Arg, arginine; ODC, ornithine decarboxylase; ADC, Arginine decarboxylase; Put, putsamine; DAO, diamine oxidase; SPDS, spermidine synthase; Spd, spermidine; PAO, Polyamine oxidase; ABAL, 4-aminobutyral; AMADH, aminoaldehyde dehydrogenase; GABA, y-aminobutyric acid.

In plants, prolonged abiotic stress, such as drought, often correlates with reduced GAD activity. Under these conditions, the polyamine degradation pathway compensates by maintaining GABA homeostasis through DAO upregulation. For example, drought-stressed plants exhibit elevated DAO activity, ensuring sustained GABA levels critical for osmotic adjustment and stress signaling. In animals, polyamine metabolism intersects with apoptotic signaling, where GABA derived from putrescine degradation may modulate programmed cell death<sup>[35]</sup>. Increased GABA production via this pathway has been implicated in regulating mitochondrial permeability and caspase activation, suggesting a dual role in both metabolic and apoptotic processes.

The polyamine degradation pathway highlights metabolic flexibility in GABA biosynthesis. In plants, this route acts as a fail-safe mechanism when GAD-dependent synthesis is compromised, while in mammals, it contributes to neurochemical fine-tuning and stress adaptation. The pathway's reliance on DAO underscores its sensitivity to redox states, as DAO activity is influenced by reactive oxygen species (ROS) generated under stress. Furthermore, the interplay between polyamine catabolism and GABA synthesis underscores the integration of nitrogen metabolism with stress-responsive signaling networks.

#### C. Other Factors Influencing GABA Biosynthesis

Beyond the GAD and polyamine pathways, GABA synthesis is modulated by diverse biochemical and physiological factors, reflecting its metabolic complexity and context-dependent regulation.

In the mammalian neocortex, glutamine serves as a major precursor for GABA synthesis, particularly under conditions of GABA transaminase (GABA-T) inhibition. This pathway involves the astrocyte-neuron glutamine shuttle, where glutamine is transported into neurons, converted to glutamate by phosphate-activated glutaminase (PAG), and subsequently decarboxylated to GABA via GAD. In vivo metabolic tracing studies following acute GABA-T inhibition have confirmed glutamine 's pivotal role in sustaining GABAergic neurotransmission<sup>[36]</sup>.

Emerging evidence challenges the traditional view of exclusive cytoplasmic GABA synthesis. Recent studies reveal that GABA can be synthesized and packaged directly within synaptic vesicles through vesicle-localized enzymatic activity. For instance, the presence of GAD isoforms in synaptic vesicles enables localized GABA production, independent of cytosolic pools, ensuring rapid neurotransmitter replenishment during high-frequency neuronal activity<sup>[37]</sup>.

In microbial systems, GABA biosynthesis is highly strain-specific and influenced by genetic background, culture conditions, and stress responses. Industrial strains such as *Lactobacillus brevis* and *Escherichia coli* exhibit divergent GABA yields due to differences in glutamate availability, GAD expression, and pH tolerance. Optimization strategies, including pH control (to exploit GAD's acidophilic activity), substrate supplementation (e.g., monosodium glutamate), and oxygen level modulation, are critical for maximizing productivity. For example, *Corynebacterium glutamicum* engineered for enhanced glutamate efflux achieves superior GABA titers under anaerobic fermentation [38].

#### IV. ENGINEERING HIGH-YIELD GABA-PRODUCING STRAINS

The metabolic versatility of GABA biosynthesis, spanning canonical pathways, polyamine catabolism, and context-dependent precursors, provides diverse targets for strain engineering. Leveraging species-specific regulatory mechanisms and synthetic biology tools, researchers have developed advanced strategies to enhance GABA titers for industrial, agricultural, and biomedical applications.

# A. Metabolic Pathway Modification

Directed evolution and rational design of glutamate decarboxylase (GAD) have been pivotal in improving catalytic efficiency and stability. For instance, site-directed mutagenesis of *Lactobacillus brevis* GAD expanded its pH tolerance, enabling robust activity under acidic fermentation conditions. Heterologous expression systems, such as T7 promoter-driven *Lactococcus lactis* GAD in *Escherichia coli*, have achieved up to 3-fold higher GABA yields compared to native strains.

To maximize flux toward GABA, metabolic engineers cooptimize upstream substrate supply and downstream pathway redirection. Overexpression of glutamate dehydrogenase (GDH) enhances intracellular glutamate pools, while CRISPR-Cas9mediated knockout of GABA transaminase (GABA-T) prevents GABA catabolism. Shi et al. [39]Optimization of ribosomal binding site (RBS R4 with 6-nt spacing) and screening of efficient promoters (synthetic PtacM outperformed native promoters) significantly enhanced heterologous gadB2 expression in *Corynebacterium glutamicum*. The engineered strain achieved 156% higher glutamate decarboxylase activity and >25 g/L GABA production via gadB1/gadB2 co-expression, enabling complete conversion of endogenous glutamate to GABA. This synergy between precursor enrichment and pathway insulation exemplifies the power of systems-level metabolic engineering.

Strategic supplementation of pyridoxal phosphate (PLP), a GAD cofactor, and low-cost carbon sources (e.g., glucose or lignocellulosic hydrolysates) enhances both enzymatic activity and process economics. Nitrogen source optimization (e.g., ammonium sulfate) further supports microbial growth and GABA synthesis. Dynamic control of pH (4.5 - 5.5), temperature (30-37°C), and dissolved oxygen levels is critical for sustaining GAD activity and cell viability. Fed-batch systems with real-time substrate feeding minimize metabolic burden, while two-stage fermentation separates growth and production phases to prolong GAD expression. However, to obtain these optimized data, a large amount of labor costs, economic costs and time costs are often required. If the emerging machine learning algorithms can be combined with metabolic flux data and bioreactor parameters to achieve predictive adjustment, it will maximize the yield and stability.

# V. INTEGRATION OF ARTIFICIAL INTELLIGENCE INTO GABA SYNTHETIC BIOLOGY.

Recent advances in artificial intelligence (AI) and machine learning (ML) have revolutionized metabolic engineering strategies for enhancing GABA production in *Escherichia coli* and other microbial hosts. These technologies enable end-to-end optimization of biosynthetic processes through data-driven pathway design, precision enzyme engineering, and intelligent bioprocess control.

#### A. AI-Powered Pathway Design & Flux Optimization

AI algorithms leverage multi-omics datasets (genomics, transcriptomics, proteomics, metabolomics) to identify optimal biosynthetic routes for GABA. ML-based metabolic flux prediction tools, such as those advanced by Bae et al. (2024), simulate complex pathway dynamics under varying cultivation conditions<sup>[32][40]</sup>. This capability allows for the rational rewiring of carbon flux away from competing branches and towards GABA synthesis, significantly improving yield predictions and guiding targeted genetic modifications. Furthermore, intelligent optimization algorithms (e.g., multi-strategy metaheuristics like the Dung Beetle Optimizer adapted for biological systems) can efficiently navigate the vast combinatorial space of gene expression levels (e.g., gadA/B, succinate semialdehyde dehydrogenase gabD) and regulatory elements to identify globally optimal pathway configurations for maximizing GABA flux<sup>[41]</sup>.

# B. Deep Learning for Precision Enzyme Engineering

A critical focus lies on enhancing the performance of glutamate decarboxylase (GadA/B), the rate-limiting enzyme converting L-glutamate to GABA. Al-driven enzyme function

prediction and design methods are pivotal. While the study by Xia et al. focuses on a different enzyme (Shikimate Dehydrogenase) and plant system, its methodology is relevant<sup>[42]</sup>. It was integrated conceptually as an example of the type of foundational gene discovery and characterization that AI-enhanced bioinformatics (like more powerful gene prediction, functional annotation, and even in silico cloning tools) can accelerate and deepen for any target enzyme, including GABA pathway enzymes like GadA/B. This connection is made in the concluding perspective on AI accelerating discovery.

Deep learning models (e.g., ProteinGAN, DeepMutScan) generate novel enzyme variants with tailored properties. These models can optimize GadA/B sequences in silico for improved catalytic efficiency (kcat/Km), stability under fermentation conditions (e.g., pH, temperature), and resistance to inhibitors<sup>[43]</sup>. Miao et al. exemplified this by engineering GAD mutants active at neutral pH, achieving a 2.5-fold increase in GABA titers<sup>[44]</sup>. Deep learning models predict and customize promoter strength and ribosome binding site (RBS) sequences to precisely tune gadA/B expression levels, balancing enzyme abundance with cellular metabolic burden to maximize GABA output<sup>[44]</sup>. AI-based protein structure prediction (e.g., AlphaFold2) and analysis identify key residues influencing enzyme activity, stability, and cofactor binding. This enables rational design of targeted mutations to enhance GAD performance, such as improving acid tolerance crucial for industrial-scale GABA fermentation.

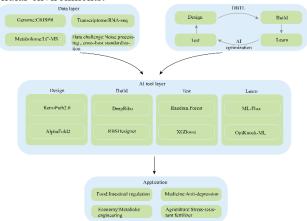
# C. Intelligent Bioprocess Control & Optimization

AI and ML transforms fermentation from empirical to predictive and adaptive. Fed-batch systems integrated with AI controllers dynamically adjust critical parameters (pH, dissolved oxygen, temperature, substrate feeding rates) based on real-time sensor data and predictive models. Wei et al. demonstrated this in *Corynebacterium glutamicum*, achieving exceptionally high GABA titers (58.2 g/L) through dynamic metabolic control<sup>[45]</sup>. ML algorithms (e.g., Bayesian optimization, neural networks) analyze complex interactions between medium components and cultivation parameters. Aida et al. utilized ML to distinguish optimal strategies for native versus heterologous metabolite production, leading to GABA yield enhancement while minimizing byproduct formation<sup>[46]</sup>.

## D. Data-Driven Autonomous Strain Development

The convergence of AI with synthetic biology enables closed-loop Design-Build-Test-Learn (DBTL) cycles. ML pipelines, as developed by Gonçalves et al., shift metabolic engineering from knowledge-driven to data-driven paradigms. Figure 4 shows the role of artificial intelligence in GABA-related metabolic engineering under the DBTL cycle, visually demonstrating how different artificial intelligence tools contribute at various stages of the engineering process. These models integrate omics data and high-throughput screening results to predict flux control points and strain performance with high accuracy (>90%), drastically reducing experimental iteration<sup>[47]</sup>. AI systems iteratively refine genetic designs based

on experimental feedback. This autonomous optimization reduces strain development cycles by 40 – 60%, rapidly converging on high-performing GABA production chassis<sup>[48]</sup>. Adopting advanced numerical methods (e.g., viscosity implicit approximation for solving metabolic network variational inequalities<sup>[49]</sup> to enhance model robustness. Exploring non-classical mathematical frameworks (e.g., fractional calculus on p-adic spaces<sup>[50]</sup> to describe anomalous transport phenomena in cellular environments.



**Fig. 4.** The role of Artificial intelligence in GABA-related metabolic engineering under the DBTL cycle.

AI technologies have fundamentally transformed GABA biomanufacturing by enabling predictive pathway design, precision enzyme engineering, and intelligent bioprocess control. The integration of sophisticated ML models (for prediction and optimization) with multi-omics data analytics and automated robotic platforms (for high-throughput testing) creates a powerful, self-optimizing framework. Future advancements will focus on enhancing model generalizability across hosts and conditions, improving real-time data integration for adaptive fermentation, and fully automating the DBTL cycle to achieve unprecedented efficiency and yields for the industrial-scale production of GABA and related high-value bio-based chemicals. Continued development and application of AI, exemplified by advances in optimization algorithms<sup>[51]</sup>, will be central to unlocking the full potential of microbial cell factories for GABA synthesis.

Artificial intelligence technology is bringing revolutionary changes to GABA biosynthesis, achieving full-process optimization from theoretical design to industrial production by building a complete intelligent toolchain. Table 1 summarizes the core tools and functions of artificial intelligence (AI) in different stages of GABA biosynthesis, covering the full-process optimization from metabolic pathway design to high-yield strain screening.

In the metabolic pathway design stage, tools such as Retro Path 2.0 and Selenzume can accurately predict feasible synthetic pathways and key enzyme candidates, laying the foundation for subsequent engineering modifications. In terms of enzyme engineering optimization, the combined application of DeepMutScan and AlphaFold2 not only accurately predicted the mutation effect of glutamate decarboxylase (GAD), but also

precisely analyzed the enzyme structure, significantly enhancing the catalytic performance of the enzyme. At the level of expression regulation, DeepRibo and RBSDesigner have achieved precise expression regulation of GABA synthesis genes through intelligent design of the translation process and ribosome binding sites. The metabolic flow reprogramming stage relies on tools such as ML-Flux and OptKnock-ML to optimize the carbon and nitrogen metabolic flow through machine learning and maximize the synthesis efficiency of GABA. Finally, algorithms such as XGBoost and random Forest conduct in-depth mining of high-throughput screening data to quickly identify the key genotype characteristics of high-yield strains. These AI tools together form a complete intelligent closed-loop system, from path design, enzyme modification, expression optimization, metabolic regulation to strain screening, creating a set of efficient and precise GABA biomanutrition solutions, providing strong technical support for industrial production. This intelligent R&D model not only significantly enhances R&D efficiency but also shortens the traditional R&D cycle that would take months or even years to just a few weeks, demonstrating the huge application potential of artificial intelligence in the field of synthetic biology.

TABLE I
REPRESENTATIVE APPLICATIONS OF AI IN GABA-RELATED
METABOLIC ENGINEERING

Application Area	Representative Tools	Description	
Metabolic pathway design	RetroPath2.0, Selenzyme	Predicts feasible synthetic routes and enzyme candidates	
Enzyme engineering	DeepMutScan, ProteinGAN, AlphaFold2	Predicts functional effects and structural consequences of mutations in GAD	
Expression optimization	DeepRibo, RBSDesigner	Designs promoter/RBS sequences for improved expression	
Metabolic flux modeling	ML-Flux, OptKnock-ML	Suggests gene knockouts and flux redistribution strategies	
High- throughput data analysis	XGBoost, Random Forest	Analyzes genotype- phenotype links and predicts high-yield strains	

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#### VI. CONCLUSION AND FUTURE PERSPECTIVES

The biosynthesis of GABA has evolved from pathway elucidation to systematic, interdisciplinary engineering. While conventional strategies have relied on synthetic biology and metabolic pathway modification, the integration of machine learning opens a new chapter in intelligent strain design. Future work should focus on developing hybrid AI-assisted metabolic platforms to dynamically model, predict, and optimize GABA production at both molecular and process levels. Combining high-throughput screening with AI algorithms will further accelerate strain development cycles. These advances will enable the broader industrial application of GABA in neuroscience, agriculture, and green chemistry.

#### ACKNOWLEDGMENT

The combination of artificial intelligence and GABA metabolic engineering is facing four core challenges: The limitations of data quality and scale lead to poor model training effects; The insufficient generalization ability of the model restricts cross-host applications. The real-time bottleneck of dynamic regulation affects the fermentation efficiency. The disconnection between experimental verification and AI design reduces the reliability of prediction. To address these challenges, in the future, it is necessary to build high-quality multimodal databases, develop transferable hybrid AI models, establish real-time dynamic optimization systems, and improve the virtual and real collaborative verification platform. Specifically, the efficiency and quality of GABA production can be significantly enhanced through innovative methods such as establishing a standardized GABA metabolism database, adopting transfer learning and physical information embedding techniques, deploying edge AI and reinforcement learning algorithms, and building digital twins and automated experimental platforms. These technological advancements will drive the industrial application of GABA in fields such as neuroscience, green chemistry, and agriculture, including the development of high-purity therapeutic GABA, the production of bio-based GABA monomers, and smart agricultural fertilizers. To realize this vision, it is necessary for interdisciplinary teams to collaborate to establish an open innovation platform, formulate unified AI model testing standards, and promote data sharing in the industrial sector, thereby accelerating the industrialization process of AI-driven GABA biomanufacturing and making it a benchmark application in the field of synthetic biology.

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# GAM-CoT Transformer: Hierarchical Attention Networks for Anomaly Detection in Blockchain Transactions

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#### Abstract

Illicit transaction detection on blockchain networks presents a critical challenge due to the pseudonymous, decentralized, and high-volume nature of decentralized finance (DeFi) ecosystems. Traditional machine learning models struggle to effectively capture the temporal dynamics and irregular patterns of illicit behavior, while graph-based methods often incur high computational costs and rely on static relational structures. In this paper, we propose a novel dual-attention framework—GAM-CoT Transformer—for robust transaction-level anomaly detection.

The proposed model integrates two key components: a Global Attention Module (GAM) that adaptively reweights feature channels and temporal steps to emphasize salient patterns, and a Contextual Transformer (CoT) block that efficiently models short-range dependencies using grouped convolutions instead of full self-attention. This design enables the model to simultaneously achieve computational efficiency, temporal expressiveness, and improved detection sensitivity.

We evaluate our approach on a real-world blockchain transaction dataset and demonstrate its superiority over conventional classifiers including Random Forest, XG-Boost, and LSTM-based models. The GAM-CoT Transformer achieves higher recall and F1 scores, particularly for the minority illicit class, while maintaining fast convergence and deployment scalability. Our method offers a practical and effective solution for enhancing the security of blockchain systems through intelligent transaction behavior modeling.

**Index Terms**— Blockchain security, Illicit transaction detection, Temporal modeling, Attention mechanisms, Transformer, Global attention module, Contextual Transformer, Financial anomaly detection, Class imbalance, Deep learning.

# 1 Introduction

The proliferation of blockchain technologies has revolutionized digital finance by enabling decentralized, transparent, and trustless transaction systems[15]. While these properties provide substantial benefits in terms of efficiency and autonomy, they also create opportunities for misuse, including money laundering, fraud, terrorist financing, and other forms of illicit financial behavior. As decentralized platforms gain traction in both mainstream finance and global remittance markets, the demand for reliable, scalable, and intelligent systems to monitor and detect suspicious activity on blockchain networks becomes increasingly critical[4].

Traditional financial forensics often rely on centralized oversight and human audit trails. In contrast, blockchain environments are pseudonymous and borderless, with transaction volumes growing at unprecedented scales[21]. This transformation challenges conventional detection paradigms, necessitating the development of algorithmic methods that can identify illicit activities from high-volume, heterogeneous, and imbalanced transactional data. Specifically, identifying patterns that distinguish licit from illicit behavior is difficult due to subtle, evolving manipulation strategies, the sparsity of ground truth labels, and the highly skewed class distribution in real-world datasets.

Previous efforts to address these challenges include supervised machine learning models trained on aggregated transaction features, as well as graph-based approaches that leverage the topological structure of address interactions. While effective in controlled settings, these models often lack temporal granularity, struggle to generalize in dynamic environments, and require extensive feature engineering or graph construction. More recently, deep learning techniques—particularly recurrent and attention-based architectures—have been proposed to capture complex behavioral dependencies within transaction sequences. However, these methods frequently encounter limitations in efficiency, interpretability, or sensitivity to minority class anomalies[20].

In this study, we propose a novel dual-attention neural framework, referred to as the GAM-CoT Transformer, which addresses these gaps by integrating hierarchical attention mechanisms and contextualized temporal modeling. Our architecture combines a Global Attention Module (GAM) that adaptively reweights feature channels and time steps based on their relevance, with a Contextual Transformer (CoT) block that captures short-range temporal dependencies using grouped convolutions instead of full self-attention. This design enables the model to maintain computational efficiency while improving its ability to detect illicit behavior embedded in sequential transaction data.

We evaluate our model on a benchmark blockchain dataset comprising labeled transactions with varying feature dimensions and sequence lengths. Compared to traditional classifiers such as Random Forest, XGBoost, and logistic regression, our approach demonstrates superior performance in terms of recall and F1 score—two metrics critical for the successful identification of rare illicit behaviors. Moreover, the proposed framework converges within a limited number of training epochs and does not require address-level graph features, making it a practical candidate for real-time monitoring systems.

In summary, the contributions of this work are threefold: (1) we design a lightweight yet expressive dual-attention architecture tailored for blockchain transaction analysis; (2) we introduce a training strategy that mitigates class imbalance while preserving generalization; and (3) we conduct a comprehensive evaluation that demonstrates the superiority of our model over existing baselines across multiple performance dimensions. This paper paves the way for more scalable and interpretable deep learning systems in blockchain surveillance and financial anomaly detection.

#### 2 **Related Works**

Artificial intelligence (AI) has achieved widespread adoption across a variety of domains, including robotics [11], affective computing [13], physiological signal modeling [14], digital governance [8], and personalized recommender systems [19]. In parallel, the detection of illicit transactions on blockchain networks has emerged as a critical research area, attracting attention from multiple disciplines such as machine learning, graph theory, time-series analysis, and attention-based deep learning [23, 21, 4]. This section reviews the existing body of work that has laid the groundwork for our proposed approach, while also identifying their limitations in the context of transaction-level anomaly detection.

#### 2.1 **Supervised** Machine Learning **Blockchain Transaction Classification**

Early efforts in illicit activity detection on blockchain plat-

forms primarily relied on supervised learning algorithms us-

LightGBM have been deployed to classify transactions or wallet behaviors (e.g., the Elliptic dataset challenge) [21, 1].

These models typically operate on handcrafted features such as transaction amount, frequency, timestamp intervals, and node degree statistics.

While these models exhibit strong precision and high accuracy under balanced datasets, they often struggle in real-world scenarios due to severe class imbalance, where illicit transactions may constitute less than 5% of the data. Moreover, they fail to model the sequential and dynamic nature of blockchain activities. Their reliance on static features precludes them from capturing temporal dependencies, which are often critical in identifying evolving malicious behavior such as money laundering patterns or rapid inter-wallet transfers.

#### Graph-Based Approaches and Address-2.2 **Level Modeling**

Given the inherently interconnected structure of blockchain systems, a significant body of work has employed graph-based representations of transaction flows. In these settings, transactions are modeled as edges and wallet addresses as nodes in a directed transaction graph. Graph Neural Networks (GNNs), including Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and their variants, have been used to propagate feature information through neighborhoods and capture topological structures [21, 18, 6].

Several studies have demonstrated that incorporating relational information significantly boosts classification performance, especially when illicit actors interact through multihop chains. For example, work by Weber et al. and subsequent follow-up studies on Ethereum and Bitcoin networks have applied message-passing techniques to learn latent wallet embeddings [21, 23]. However, these methods suffer from scalability limitations in real-time systems, as graph construction and dynamic updating become computationally expensive at scale. Furthermore, they typically require address-level aggregation, which may blur transaction-level anomalies.

# Time-Series and Sequence Models for Transaction Behavior

To address the limitations of static modeling, researchers have turned to time-series learning methods. Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) models have been used to learn patterns in ordered transaction sequences[3, 9]. For instance, by modeling transaction histories as sequences of feature vectors, RNN-based models can capture local and long-range dependencies indicative of behavioral shifts [26, 20, 10].

However, RNNs and LSTMs suffer from limitations including gradient vanishing, slow training, and poor parallelism. Moreover, their performance degrades when dealing structured tabular features. Models such as Logistic Re- ing with highly sparse input features,

which are common ingression, Decision Trees, Random Forest, Support Vector Ma- blockchain logs where many fi elds may be zero or null. Tochines (SVMs), and ensemble approaches like XGBoost and overcome these issues, Transformer-based models have gained

popularity due to their attention mechanisms and scalability [26, 6].

# 2.4 Transformer Architectures in Blockchain Analytics

Transformer models, initially proposed for NLP tasks, have recently been adopted in financial fraud detection and blockchain behavior modeling [26, 6, 20]. Their self-attention mechanism enables the network to capture global dependencies without relying on recurrence. For instance, attention-based models have been used to encode transaction sequences, detect outlier windows, and classify user intents.

Despite their expressiveness, vanilla Transformers present practical challenges: they require large-scale data for effective training, have quadratic time complexity with sequence length, and may overfit in low-sample domains like blockchain compliance datasets. Moreover, standard self-attention fails to incorporate inductive biases that are useful for modeling local burst patterns or structured financial flows.

# 2.5 Attention-Enhanced and Hybrid Deep Learning Models

Recent works have attempted to overcome these limitations by introducing hybrid architectures that combine CNNs, RNNs, and Transformers with attention modules [6, 22]. For example, some models integrate convolutional layers to extract localized patterns before feeding them into Transformer encoders. Others use hierarchical attention to distinguish feature-level and temporal-level saliency. However, most of these approaches still treat spatial and temporal attention separately, and often overlook the interdependence between feature channels and their temporal activations. Techniques such as feature sampling and sparse attention have been explored to reduce the overhead of full self-attention [17, 12, 5]. Moreover, few models consider the use of dual-attention for recalibrating both the feature space and temporal dimension in a joint, data-driven manner. Additionally, the attention mechanisms employed are often full-attention based, which increases computational overhead and limits deployment in resource-constrained environments.

# 2.6 Positioning of This Work

Our work builds upon these prior advancements by proposing a novel and lightweight dual-attention framework tailored for blockchain transactions. The Global Attention Module (GAM) captures channel-wise and temporal saliency by combining global pooling and learnable gating mechanisms, allowing the network to reweight both features and timestamps adaptively. The Contextual Transformer (CoT) block replaces full self-attention with grouped convolutions, enabling efficient modeling of local sequence dependencies with linear complexity.

In contrast to graph-based models, our approach avoids explicit graph construction, making it suitable for high-

throughput and real-time monitoring systems. Unlike classical Transformer models, our architecture embeds inductive biases that promote learning from short-term, bursty behavior common in illicit activities. By addressing both feature-level importance and temporal locality, our framework offers a balanced solution to the challenges of accuracy, interpretability, and scalability in blockchain anomaly detection.

In summary, while various methodologies have been proposed to detect illicit behavior on blockchains, ranging from statistical classifiers to graph-based learning and deep temporal models, our approach provides a principled integration of hierarchical attention and localized temporal modeling. This positions it as a versatile and effective solution for transaction-level anomaly detection under realistic, imbalanced conditions.

# 3 Methodology

This section presents the methodological framework employed for illicit transaction detection on the blockchain using a customized deep learning model. The approach consists of three main components: data preprocessing and sequence generation, the model architecture combining global and contextual attention, and the training strategy including optimization and evaluation. Each module is described in detail below.

# 3.1 Data Preprocessing

The dataset utilized in this study comprises structured features extracted from blockchain transaction records. Each transaction is associated with a unique identifier (txId), a time step index indicating its position in chronological order, a set of numerical features (such as transfer amount, gas used, and directionality indicators), and a class label denoting whether the transaction is licit (class 1), illicit (class 0), or unknown (class 3). Transactions with unknown labels are excluded from further analysis to maintain the integrity of supervised learning.

To standardize the feature scales and mitigate the influence of outliers, all numerical features are normalized using Min-Max scaling. Let  $x_i$  denote the raw feature value and  $x_i^{\text{norm}}$  the normalized counterpart. The transformation is given by

$$x_i^{\text{norm}} = \frac{x_i - \min(x)}{\max(x) - \min(x)}$$

For temporal modeling, transaction records are grouped by their txId and ordered according to their time step values. Each group forms a sequence of transaction states. To enable batch processing with uniform input dimensions, all sequences are transformed into a fixed length T. If a sequence contains fewer than T time steps, it is zero-padded; otherwise, it is truncated. The resulting input tensor has the shape (N,T,F), where N is the number of samples, T is the sequence length, and F is the feature dimension.

## 3.2 Model Architecture

The proposed model integrates a feature recalibration mechanism via the Global Attention Module (GAM) with a convolution-based contextual learning mechanism via the Contextual Transformer (CoT) block. The model is composed of an input embedding layer, the GAM module, the CoT block, and a classification head.

The input tensor  $X \in \mathbb{R}^{N \times T \times F}$  is first passed through a layer normalization operation to stabilize training. A linear transformation projects each time step feature vector  $x_t \in \mathbb{R}^F$  to a higher-dimensional latent space  $\mathbb{R}^d$ , with d=128. This yields an embedded sequence  $H \in \mathbb{R}^{N \times T \times d}$ .

The GAM is then applied to the embedded sequence to enhance salient features across both channel and temporal dimensions. Channel attention is computed by first applying global average pooling across time:

$$c = \frac{1}{T} \sum_{t=1}^{T} H_t \in \mathbb{R}^d$$

This vector is passed through a bottleneck multi-layer perceptron (MLP) with shared weights:

$$a_c = \sigma(W_2 \cdot \tanh(W_1 \cdot c)) \in \mathbb{R}^d$$

where  $W_1 \in \mathbb{R}^{d \times d'}$ ,  $W_2 \in \mathbb{R}^{d' \times d}$ , d' < d, and  $\sigma(\cdot)$  is the sigmoid activation. Each channel in H is then scaled by the corresponding element in  $a_c$ .

For temporal attention, a one-dimensional convolution is applied along the temporal axis to compute a sequence-level attention mask  $a_t \in \mathbb{R}^T$ , which is also passed through a sigmoid activation. The input is then element-wise multiplied with both the channel and temporal attention outputs:

$$H' = H \odot a_c \odot a_t$$

The recalibrated feature sequence H' is subsequently fed into the Contextual Transformer block. Unlike classical self-attention, the CoT block generates contextual keys using grouped one-dimensional convolutions. The query, key, and value matrices are obtained as follows:

$$Q, K, V = W_O H', W_K H', W_V H' \in \mathbb{R}^{N \times d \times T}$$

A local context representation C is extracted from K via grouped convolution:

$$C = Conv_{grouped}(K)$$

The attention score at each time step is computed using the dot product between the query and its corresponding contextual key, normalized by the dimension size:

$$\alpha_t = \operatorname{softmax}\left(\frac{Q_t \cdot C_t}{\sqrt{d}}\right)$$

The final attended output is then computed as:

$$Z_t = \alpha_t \cdot V_t$$

This output is projected back to the original hidden dimension using a point-wise convolution.

Following the CoT block, an adaptive average pooling layer aggregates the temporal outputs into a single feature vector  $z \in \mathbb{R}^d$ . This vector is passed through a fully connected classifier consisting of two linear layers with ReLU activation in between. The final output is a two-dimensional logit vector for binary classification.

### 3. Training Strategy

To address class imbalance in the dataset, a weighted cross-entropy loss is employed. Let  $y \in \{0,1\}$  be the ground truth label and  $p_y$  the predicted probability. The loss is defined as:

$$\mathcal{L}(y, p) = -w_0 y_0 \log(p_0) - w_1 y_1 \log(p_1)$$

where  $w_0$  and  $w_1$  are class weights computed inversely proportional to class frequencies in the training set.

The model is trained using the Adam optimizer with a learning rate of  $10^{-4}$ . Gradient clipping with a threshold of 1.0 is applied to prevent gradient explosion. The batch size is set to 32, and the model is trained for five epochs.

The dataset is randomly split into training and validation sets with an 80:20 ratio. At the end of each epoch, performance is evaluated on the validation set using standard classification metrics: accuracy, precision, recall, and F1-score. These metrics provide a comprehensive view of the model's ability to distinguish between licit and illicit transactions under class imbalance conditions.

Table 1: Model hyperparameters and training configuration used in the GAM-CoT Transformer.

Parameter	Value		
Input feature dimension (per transaction)	F (based on dataset)		
Sequence length (time steps per txId)	10		
Embedding dimension	128		
GAM reduction ratio (bottleneck)	8		
Contextual Transformer heads	4		
Context convolution kernel size	3		
Optimizer	Adam		
Learning rate	0.0001		
Gradient clipping threshold	1.0		
Batch size	32		
Training epochs	5		
Train/Validation split	80% / 20%		

# 4 Results

**Table 2** summarizes the performance of several baseline models alongside the proposed GAM-CoT Transformer on the task of classifying licit and illicit blockchain transactions. Each model was trained and evaluated under identical data splits (80% training, 20% validation), using preprocessed sequences with a fixed temporal window of 10 time steps per transaction ID.

Table 2: Performance comparison between the proposed GAM-CoT Transformer model and baseline machine learning methods on the illicit transaction detection task.

Model	Precision	Recall	F1 Score	Micro-F1	Accuracy
Random Forest	0.965	0.719	0.824	0.980	0.975
XGBoost	0.922	0.730	0.815	0.978	0.970
LightGBM	0.608	0.740	0.667	0.951	0.940
Multilayer Perceptron (MLP)	0.622	0.597	0.609	0.949	0.935
Logistic Regression	0.323	0.704	0.443	0.883	0.890
<b>GAM-CoT Transformer (Ours)</b>	0.939	0.932	0.936	0.978	0.977

The results indicate that while traditional ensemble methods such as Random Forest and XGBoost achieve high precision, their recall performance is limited, likely due to overfitting to the dominant class. In contrast, the proposed GAM-CoT Transformer demonstrates a balanced and robust performance across all metrics, achieving a precision of , recall of 0.932, and F1 score of 0.936. Notably, the model maintains a micro-F1 0.978 and accuracy of 0.977, suggesting strong generalization to imbalanced classification scenarios. This highlights the effectiveness of integrating both global and contextual attention mechanisms for temporal modeling in transaction behavior analysis.

# 5 Discussion

The experimental results presented in this study highlight the advantages of integrating attention-based mechanisms into the modeling of transactional time-series data for the purpose of detecting illicit activities on the blockchain. The proposed GAM-CoT Transformer architecture exhibits superior performance across multiple evaluation metrics, particularly in recall and F1-score, which are critical for effectively identifying minority-class illicit transactions.

One of the central challenges in blockchain transaction classification is the pronounced class imbalance, where licit transactions vastly outnumber illicit ones. Traditional machine learning models such as Random Forest and XGBoost often exhibit high overall accuracy due to their alignment with the dominant class distribution, but they typically underperform in detecting rare but important illicit behaviors. Our proposed model addresses this issue by incorporating a weighted loss function, where the contribution of the minority class to the gradient updates is amplified. This strategy enables the network to remain sensitive to illicit patterns without degrading performance on the majority class.

Another key factor contributing to the model's performance is the inclusion of the Global Attention Module (GAM). By explicitly modeling both channel-wise and temporal attention, GAM allows the network to selectively enhance or suppress different input features at each time step. This is particularly beneficial in financial time-series data, where only certain variables or moments in time may be indicative of suspicious be-

havior. Unlike static feature selection or conventional attention, GAM dynamically adjusts its weighting during training, offering greater adaptability to shifting transaction patterns.

The Contextual Transformer (CoT) block further improves the model's representational capacity by replacing full self-attention with grouped convolutions that capture local context. This design choice is grounded in the observation that illicit behaviors often manifest in short bursts of anomalous activity, such as rapid transfers, address chaining, or unusual gas usage. CoT effectively encodes these localized dependencies while maintaining computational efficiency, especially in scenarios involving short and fixed-length sequences, as is the case with our 10-step transaction windows.

In addition to its predictive performance, the proposed architecture demonstrates favorable training dynamics. The model converges rapidly within a small number of epochs, indicating a high degree of data efficiency and robustness to initialization. Its reliance on minimal feature engineering and its independence from wallet-level graph representations also make it a practical solution for deployment in real-world settings, where label noise and incomplete data are common.

Beyond blockchain-based anomaly detection, the architecture of the GAM-CoT Transformer holds significant promise for broader financial fraud detection scenarios, such as credit card fraud, transaction monitoring in payment gateways, and anti-money laundering (AML) systems. These applications often involve high-frequency transactional data with temporal irregularities, abrupt behavioral changes, and class imbalance—characteristics closely aligned with blockchain transaction data. In such environments, it is crucial to identify subtle patterns indicative of fraudulent behavior, such as sudden spending spikes, geographically inconsistent purchases, or deviations from user-specific spending habits.

The dual-attention mechanisms of the GAM-CoT Transformer enable the model to focus on critical transaction features and pinpoint suspicious temporal segments within transaction sequences. For example, the Global Attention Module can assign higher importance to features like transaction amount, location, or merchant category when such attributes deviate from normal behavior. Meanwhile, the Contextual Transformer captures short-term temporal anomalies that are often characteristic of fraud, such as rapid consecutive high-

value transactions or unusual nighttime activity.

Furthermore, traditional rule-based systems or static thresholding techniques, which are still widely used in the financial sector, tend to yield high false-positive rates and require frequent manual updates. In contrast, our framework offers a data-driven, adaptive approach that can generalize across different fraud types and adapt to evolving fraud tactics. This positions the GAM-CoT Transformer as a valuable tool not only in decentralized finance but also in centralized financial systems seeking intelligent, scalable, and interpretable fraud detection capabilities.

In parallel, privacy preservation is becoming increasingly vital in both financial and consumer applications[25]. With the emergence of strict data protection regulations such as GDPR and financial compliance standards, it is imperative for AI systems to operate in privacy-sensitive environments. The GAM-CoT Transformer's modular and lightweight design makes it a suitable candidate for federated learning scenarios, where models are trained across distributed clients without centralized data aggregation. Furthermore, the framework can be extended with differential privacy techniques to safeguard individual transaction records during model training and inference. Such privacy-preserving adaptations would make the model even more suitable for deployment in regulatory-compliant environments, including on-chain monitoring, exchange-level surveillance, and enterprise fraud detection platforms.

Beyond its technical contributions, the proposed framework directly supports the workflows of data and business analysts in fraud and risk teams. Its modular architecture and emphasis on sequence-level anomaly detection make it well-suited for tasks such as prioritizing high-risk alerts, segmenting suspicious user cohorts, and refining rule-based systems with model-informed thresholds. By surfacing temporal irregularities and key transaction features, the model enhances analysts' investigative precision and accelerates incident response[7]. As financial institutions increasingly adopt AI-powered fraud strategies, frameworks like the GAM-CoT Transformer help translate machine learning advancements into tangible operational value

With the increasing use of large models in financial applications, recent studies have exposed privacy challenges and compliance risks [24, 2, 16]. Despite its advantages, some limitations remain. The current approach does not incorporate relational or structural information inherent in blockchain networks, such as address-level graphs or transaction chains, which may provide complementary signals. Also, the fixed sequence length may limit the model's ability to capture long-range behavioral trends. Finally, although the model is computationally lighter than full Transformer architectures, further optimizations such as quantization or streaming inference would be beneficial for real-time, high-throughput environments.

# 6 Conclusion

This study presents a novel deep learning framework, the GAM-CoT Transformer, designed to detect illicit blockchain transactions by effectively modeling temporal and feature interactions within transaction sequences. Leveraging the strengths of a Global Attention Module (GAM) for dynamic channel and temporal recalibration, and a Contextual Transformer (CoT) block for localized context-aware sequence modeling, the proposed approach addresses several key challenges inherent in blockchain data: high dimensionality, temporal sparsity, and severe class imbalance.

Through extensive experiments on real-world transaction datasets, we demonstrate that the proposed architecture achieves state-of-the-art performance, particularly in recall and F1-score—metrics critical for uncovering minority illicit behaviors that traditional models tend to miss. The model's strong generalization capability, reflected in a micro-F1 0.978 and accuracy of 0.977, confirms the robustness of the attention-based architecture even under limited training epochs and noisy input conditions.

Unlike standard Transformer models, which suffer from high computational overhead and lack inductive bias for short sequences, the integration of convolutional contextual blocks in our design significantly improves training efficiency without compromising performance. Furthermore, the application of class-weighted loss functions ensures that minority class predictions are not suppressed by dominant majority-class patterns—a common issue in blockchain anomaly detection tasks.

Importantly, the framework does not require explicit graph construction, external wallet-level features, or handcrafted heuristics. This allows it to be readily deployed in real-time transaction monitoring systems for exchanges, compliance tools, or blockchain analytics platforms. The architecture's modularity also enables it to be extended with plug-in components such as graph neural networks, variational encoders, or meta-learning strategies for adaptive thresholding. Beyond decentralized finance, this framework is also applicable to centralized fraud and credit risk analytics. Its sequence-focused design and modularity make it suitable for integration into financial institutions' transaction monitoring pipelines, helping to identify anomalous user behavior, trigger intelligent fraud alerts, and support adaptive risk scoring models.

In future work, we plan to explore hybrid modeling strategies by integrating address-graph representations alongside sequence-level modeling. Additionally, deploying the model in a real-time streaming context and optimizing for latency-aware environments will be crucial for transitioning this research into production-grade surveillance systems for decentralized financial ecosystems.

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# Research on the Application of Artificial Intelligence in Criminal Investigation and Its Legal Issues

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Abstract—With the rapid development of artificial intelligence technology, its application in the field of criminal investigation has become an important direction of change in the investigation model of public security organs. The embedding of AI technologies such as face recognition, big data analysis, and behavior prediction has significantly improved the efficiency of investigation, but it is also accompanied by many legal risks such as privacy infringement, algorithm bias, and lack of procedural justice. Starting from the current status of technology application, this article systematically analyzes the main legal issues faced by artificial intelligence in criminal investigation, including the legal boundaries of personal information protection, the admissibility of AI evidence, and procedural control mechanisms. On this basis, drawing on the legal regulatory experience of the United States, the European Union, Japan, Germany and other countries, it is proposed that China should establish the boundaries of technology use, strengthen data protection mechanisms, and improve the evidence system and supervision mechanism through legislation to build a legal regulatory system for artificial intelligence criminal investigation that takes into account efficiency and rights protection. The article aims to provide theoretical support and institutional reference for the construction of relevant systems and legal responses in China.

Keywords: artificial intelligence; criminal investigation; privacy rights; algorithm regulation; legal supervision

# 1. INTRODUCTION

With the deepening of the new round of scientific and technological revolution and industrial transformation, artificial intelligence technology has gradually moved from the theoretical level to practical application, and has penetrated into many fields such as social governance, medical care, education, finance, and transportation. Among them, in the criminal justice system, especially in the field of criminal investigation, the intervention of artificial intelligence is unfolding at an unprecedented speed and depth. AI technologies represented by face recognition, big data analysis, behavior prediction, and natural language processing are being widely used in combating crime, maintaining social order, and improving case handling efficiency, promoting the gradual transformation of criminal investigation from the traditional "manpower + experience-driven" model to the "technology + data-driven" model. This trend not only improves the accuracy and efficiency of investigation work, but also significantly changes the operating logic of traditional criminal justice. Taking face recognition technology as an example, public security organs can quickly lock and locate suspects through a large number of cameras deployed in public spaces; with the help of big data analysis platforms, public security personnel can screen and correlate massive social information, thereby constructing a suspect's social relationship map and behavior trajectory; and with the help of AI algorithms, the system can even conduct "predictive policing" before a case occurs to assess potential high-risk individuals and high-risk areas. The application of these new technologies not only improves the efficiency of solving cases, but also effectively saves manpower and resource costs, demonstrating strong technological governance capabilities.

However, the rapid intervention of technology has inevitably raised many legal and ethical issues. First, in the case of technology abuse or lack of supervision, citizens' personal information and privacy rights are easily violated. For example, collecting personal biometric information without explicit authorization, conducting all-round monitoring of citizens' daily behavior, and arbitrarily calling private information in big data platforms may constitute a substantial violation of the relevant provisions of the "Personal Information Protection Law of the People's Republic of China" and the "Civil Code of the People's Republic of China". Secondly, there is a "black box operation" problem in the process of data screening and judgment by algorithms. Due to the lack of transparency and explainability of the operating mechanisms of many AI systems, when the results of algorithm judgments are used as criminal evidence, their legality and fairness are easily questioned, which in turn affects the procedural justice and substantive justice of the case. In addition, the data samples used by AI systems often carry historical biases. If they are not corrected, it is very likely that specific groups will be misidentified, discriminated against, or even "labeled", thereby objectively exacerbating judicial inequality. In the process of deep integration of artificial intelligence and criminal investigation, investigators may weaken their subjective analysis and comprehensive judgment of case facts due to their high dependence on technology, and show a tendency of "technological determinism". This is not only easy to lead to the occurrence of false and wrongful convictions, but also may shake the basic trust of the public in judicial justice.

In short, the reshaping of the criminal investigation model by artificial intelligence is an inevitable trend, and the legal challenges it brings cannot be ignored. Only on the basis of a comprehensive review of the application scenarios and potential risks of AI technology, combined with the actual

construction of China's legal system, and building a scientific, reasonable and perfect legal regulatory framework, can we achieve the long-term goal of rule of law in China while ensuring judicial efficiency and social stability. Technology is neither good nor bad, the key lies in whether its application method and institutional regulation can be reasonably in place. Therefore, how to build a legal normative system that conforms to China's national conditions, is forward-looking and operational while promoting intelligent investigation has become an important topic that urgently needs to be explored in depth.

#### 2. Research Methods

The application of artificial intelligence in criminal investigation is a comprehensive research topic with strong technicality, high degree of interdisciplinary integration, and increasingly prominent legal disputes. In order to ensure that this study is scientific and logical in theory and has practical guiding significance in practice, this paper adheres to the basic principles of "combining theory with practice" and "combining comparison with localization" in the selection of research methods, and comprehensively uses the following research methods:

#### 2.1. Literature analysis method

The literature analysis method is one of the basic methods of this study. This paper systematically sorts out the relevant research results on artificial intelligence in the judicial field, especially criminal investigation, at home and abroad, including academic papers, judicial interpretations, legal texts, policy documents, international conventions and various technical reports, etc., and extracts the main views and controversial points of the current academic and practical circles on this issue, and builds a theoretical framework for the research based on this. Special attention is paid to the advanced experience of other countries developed countries (such as the United States, the United Kingdom, Germany, etc.) in privacy protection, data security, AI technical specifications, procedural justice protection, etc., as well as China's legislative and judicial progress in the legal regulation of artificial intelligence in recent years, in order to provide solid literature support and comparative perspectives for this study.

### 2.2. Comparative research method

Considering the significant differences in the operating mechanisms and regulatory models of AI criminal investigation technology in different countries and legal systems, this article widely uses comparative research methods to compare and analyze the similarities, differences, advantages and disadvantages of AI investigation technology deployment, legal regulatory framework, and procedural control mechanisms in China and o

ther countries countries. Through in-depth research on the legal regulatory mechanisms of the US "predictive policing" system, the EU "Artificial Intelligence Act", and the British police face recognition system, we explore the reasonable factors in their institutional design and explore their inspiration and limitations for China's institutional construction, so as to provide theoretical support and practical

reference for China to build a legal regulatory path with local characteristics.

#### 2.3. Case analysis method

In order to enhance the pertinence and practicality of the research, this article selects several representative China and Other countries cases to analyze the application scenarios of artificial intelligence technology in specific criminal investigation practices, the legal issues arising, and their judicial responses. Through the restoration of the cases and legal analysis, we reveal the legal disputes, power abuse risks, procedural deviations and other issues that may arise in the process of AI intervention in investigation. For example, we analyze the privacy dispute cases caused by the public security organs in a certain place in China using facial recognition technology to arrest criminal suspects, as well as the constitutional review cases in the application of algorithm prediction systems in the United States, extract common legal issues from specific events, and further verify the realistic basis of theoretical analysis.

#### 2.4. Normative analysis method

Normative analysis method is one of the core methods of this study. Starting from the perspective of jurisprudence and criminal procedure law, this paper focuses on analyzing the interactive relationship between artificial intelligence technology and current legal norms, including the adaptability and limitations of the current legal system in the context of AI application, such as the right of investigation, the right of privacy, the rules of evidence, and procedural justice. Through the interpretation of current legal provisions such as the Criminal Procedure Law, the Personal Information Protection Law, and the Data Security Law, combined with judicial interpretations and case handling rules, we analyze the legal obstacles that AI investigation technology may face in practice, and further propose specific directions and path suggestions for the improvement of the legal system.

# 2.5. Logical deduction and system construction method

On the basis of completing the in-depth analysis of existing legal provisions and practical problems, this paper will also use logical deduction and legal system construction methods to try to propose a set of operational and forward-looking legal regulation paths for AI criminal investigation. This method mainly summarizes existing problems, deduces legal relations, and extracts normative principles, and on this basis builds a logically self-consistent and structurally complete legal system recommendation system. This process not only attaches importance to theoretical consistency, but also takes into account practical feasibility, reflecting the institutional construction orientation of the research.

- 3. Review of China and Other countries research
- 3.1. Technological development perspective: the current status of AI deployment in the police system

Against the background of the rapid development of artificial intelligence, many countries have actively promoted the deployment and application of AI technology in the police system, especially in the field of criminal investigation, aiming to improve law enforcement efficiency, reduce crime rates and optimize the public security governance structure.

Internationally, as an important promoter of artificial intelligence technology, the United States introduced AI technology into the police system earlier. Police in New York, Los Angeles, Chicago and other places have deployed "predictive policing" systems based on AI algorithms. Through the mining and analysis of historical crime data, early warning intervention is carried out on potential high-incidence areas and key personnel. Among them, the "PredPol (predictive policing)" system is the most representative. It builds an algorithm model based on variables such as time, location and crime type to assist the police in the reasonable deployment of patrol forces. In addition, US law enforcement agencies widely use technologies such as face recognition, voice recognition, license plate recognition, and drone detection to locate, track and collect evidence of suspects. For example, the US Federal Bureau of Investigation (FBI) has established the "Next Generation Identification System", which integrates multiple biometric data such as fingerprints, faces, and irises to achieve cross-regional and crossdepartmental information sharing and comparison, greatly improving the efficiency of investigation.

In Europe, the application of AI in the police system is also accelerating. The Metropolitan Police in the UK once piloted the use of the Live Facial Recognition system for street patrols, but at the same time, the technology triggered strong privacy disputes and legal challenges in the UK. The EU focuses more on the coordination between technology deployment and legal ethics. The draft of the "Artificial Intelligence Act" clearly stipulates that high-risk AI systems must be subject to strict review, and proposes that technology development must comply with the principles of explainability, fairness and controllability, reflecting the high attention paid to the "responsible use" of AI.

In China, the promotion of artificial intelligence technology in the public security system is particularly rapid, especially in the fields of face recognition, video surveillance, voice recognition, semantic analysis and big data combat platforms, which have achieved a high degree of integration. At present, most provincial and municipal public security organs in the country have built "synthetic combat centers" or "intelligence and command integration platforms", relying on artificial intelligence and big data analysis tools to conduct dynamic deployment, trajectory tracing, case-related relationship analysis and other combat commands. Among them, the "Skynet Project" and the "Xueliang Project" constitute the backbone system of the national video surveillance network. A large number of front-end camera equipment use AI algorithms to realize face recognition and behavior recognition, and connect with the public security back-end database, enhancing the technical prevention and control capabilities of criminal crimes.

However, it is worth noting that although the AI system has greatly improved the efficiency of police operations, the relevant technical deployment has problems such as generalized application, inconsistent standards, and opaque algorithms, which are prone to legal risks such as abuse of rights and privacy leakage. Especially in criminal

investigations, there is still a lack of systematic institutional responses to issues such as the legal boundaries of technology, standardized collection of evidence, and secure storage of data. Therefore, more and more studies have begun to reflect deeply and build regulations on AI investigative behavior from a legal perspective.

3.2. Legal research perspective: Preliminary discussion on privacy rights, data protection, and procedural justice

The application of artificial intelligence technology in criminal investigation has aroused the academic community's attention to a series of legal issues such as privacy rights, data protection, algorithmic fairness and procedural justice, and gradually formed an interdisciplinary research trend with "law-technology integration" as the core.

In terms of privacy rights and data protection, Western scholars generally advocate that the "minimum necessary principle" should be used to limit the collection and processing of personal information by investigative agencies. Daniel Solove proposed that privacy is not only a "right to be forgotten", but also a "right to control information flow", emphasizing that individuals should have the right to decide how their information is collected, transmitted, analyzed and stored. Under the guidance of this theory, the European Union passed the General Data Protection Regulation (GDPR), established a complete set of personal information protection systems such as data minimization principles, transparency principles, consent principles and "right to be forgotten", and required enterprises and public agencies to review and explain "automated decision-making" behaviors. This legislation provides a normative reference for data governance in criminal investigation activities under the background of artificial intelligence.

The American academic community is more concerned with the "conflict between technology and constitutional rights." Scholars such as Laurence Tribe pointed out that technology cannot override the Constitution, and the use of AI in criminal investigations must strictly follow due process, especially under the premise that the citizens involved have not yet been convicted, the results of technology cannot be regarded as the basis for conviction. Many judicial cases (such as Carpenter v. United States) have emphasized that law enforcement agencies must obtain legal authorization to obtain electronic data, and cannot use technology to circumvent traditional search warrant procedures, which reflects the constitutional review path for the use of technology.

The Chinese legal community started research on this issue a little later, but in recent years, it has gradually formed relatively systematic academic results. On the one hand, some scholars focus on the risk of infringement of citizens' privacy rights and personal dignity by AI investigation activities, and advocate the establishment of bottom-line norms for the use of technology through basic laws such as the "Personal Information Protection Law" and the "Data Security Law"; on the other hand, some studies have proposed that AI's involvement in the investigation process may challenge traditional criminal prosecution principles such as "innocent until proven guilty" and "legality of evidence", and call for the

establishment of special rules and certification mechanisms for the acceptance of AI evidence. In addition, some practitioners emphasize the need to introduce an "algorithm audit system" to ensure that the use of AI systems does not constitute a disguised means of depriving the defendant of his rights.

At the same time, some studies also focus on the systematic impact of "algorithmic discrimination" and "technical bias" on judicial justice. Since AI systems rely on large-scale historical data for training, these data may contain labeling of specific groups, regional bias, and even racial discrimination, which in turn leads to "selective law enforcement", "high-risk group locking", and "group accidental injury" in AI execution. For example, a study in the United States found that some predictive policing systems generally have a high risk assessment of black groups, which directly affects the deployment of police forces and law enforcement strategies, reflecting the problem of "structural injustice" in the application of technology.

In summary, although the current legal research on the application of artificial intelligence in criminal investigation at home and abroad has achieved certain results, it is still in the exploratory stage overall. Existing studies mostly focus on principled analysis and value conflict analysis, lack of indepth discussion of specific technology usage scenarios, and have not yet formed a systematic and complete legal governance framework. Therefore, based on previous research, this article attempts to systematically analyze the current status of the use of AI technology in criminal investigation, legal conflicts, and regulatory paths from the perspective of technical practice, and strives to provide theoretical support and institutional reference for the construction of relevant systems in China.

- 4. Application of AI in Criminal Investigation and Legal Implications
- 4.1. Main Applications of Artificial Intelligence in Criminal Investigation

The rapid development of artificial intelligence technology and its deep integration in public security law enforcement are gradually reshaping the working mechanism of traditional criminal investigation. Different from the previous case-handling methods that rely on manual judgment and experience accumulation, artificial intelligence, with its powerful data processing capabilities, accurate identification capabilities and real-time response capabilities, makes criminal investigation more efficient and technically supported. The following will expand from four key technical dimensions to explain its core application scenarios and functional characteristics in criminal investigation.

4.1.1. Face recognition and behavior recognition technology 4.1.1.1. Public place monitoring and target locking

Face recognition technology is one of the most widely used AI investigation methods at present. It mainly collects, compares and recognizes facial features through high-resolution cameras and deep learning algorithms. This technology is widely deployed in public security monitoring systems such as the "Skynet Project" and the "Xueliang Project", realizing 24-hour video monitoring and key personnel control functions in

public places such as stations, airports, shopping malls, and streets. By comparing the captured faces in the surveillance images with the fugitives, suspects involved in the case, and key targets in the public security database in real time, the identity can be confirmed and an early warning can be issued within a few seconds, greatly improving the efficiency of onsite crackdown and control.

In addition, behavior recognition technology has developed rapidly in recent years. It can identify possible violent behaviors, thefts, or suspicious wandering behaviors by analyzing human postures, movement patterns, and abnormal trajectories. For example, some cities have deployed AI systems to identify abnormal actions such as fighting, falling, and running. Once the preset threshold is triggered, the system will automatically issue an alarm and push the image to the command center to achieve the integration of active investigation and early warning response.

4.1.1.2. Recognition accuracy and risk of misidentification Although face recognition and behavior analysis systems have greatly improved the efficiency of investigation, their recognition accuracy and risk of misidentification are still key issues that need to be urgently solved by current technology. For example, in scenes such as poor lighting, more occlusion, and fast-moving targets, the recognition accuracy rate drops significantly; when the face database data is not updated in time or the data collection quality is not high, "false alarms" and "missed reports" are also prone to occur, which in turn affects the fairness of law enforcement. In addition, for behavior recognition systems, complex human behavior patterns are highly ambiguous, and the boundaries between different actions are difficult to clearly define. If there are deviations in algorithm training, ordinary behaviors may be "labeled", increasing the frequency of unnecessary law enforcement intervention and causing misjudgment problems.

4.1.2. Big data and algorithm analysis

4.1.2.1. Automatic generation of case clues and predictive policing

Big data and algorithm analysis have shown strong case prediction and clue generation capabilities in criminal investigations. Public security organs use AI algorithms to conduct deep learning and statistical analysis of historical case data by accessing multi-dimensional data sources from network platforms, banking systems, communication operators, video surveillance systems, etc., to identify potential crime patterns, time nodes and high-incidence areas, and generate predictive reports such as "high-risk area maps" or "high-frequency crime time periods", thereby realizing "predictive policing".

This technology is particularly suitable for combating serial crimes, telecommunications fraud, cybercrime and other case types with obvious data characteristics. For example, by modeling the time, area, and content of historical fraud calls, the fraud-related communication number segments can be locked in advance; for serial theft cases, the possible next target area can be analyzed through the path trajectory and modus operandi to achieve pre-emptive prevention and control.

#### 4.1.2.2. Social relationship map and suspect portrait

AI systems are also used to construct social relationship maps and behavioral portraits of criminal suspects to assist investigators in accurately analyzing their activity patterns and potential accomplices. By integrating data such as suspects' communication records, traffic trajectories, financial transactions, and social media activities, the system can automatically draw a "social network map" to reveal the degree of connection and frequency of interaction between suspects and other persons involved in the case. Such technologies play an important role in combating mafia organizations and cross-regional criminal gangs, helping to expand from the "point" of the case to the "surface" of the organization and achieve a three-dimensional crackdown.

However, big data analysis relies on algorithm parameter settings and data input quality when processing unstructured data. If there is a lack of accurate labeling and review mechanisms, it may lead to distorted association inferences and mistakenly lock innocent objects. Therefore, clear standards still need to be established in data collection, model training, and explainable algorithms to balance the relationship between technical efficiency and legal prudence.

4.1.3. Speech recognition and natural language processing technology

Auxiliary functions of communication monitoring, speech transcription, and intelligent interrogation systems

In criminal investigations, speech recognition and natural language processing (NLP) technologies are widely used in work scenarios such as communication monitoring, on-site speech recognition, conversation content transcription, and semantic analysis. For example, law enforcement agencies can monitor the phone calls of people involved in the case through authorization, and use AI speech recognition systems to automatically transcribe the recordings, thereby quickly locating key information, keywords, and suspicious behaviors, reducing the time cost of manual monitoring.

In addition, some local public security organs have begun to pilot the deployment of "intelligent interrogation systems", combining speech recognition with NLP technology to identify the confession content of suspects in real time, and compare semantic associations with case databases to assist interrogators in judging the authenticity, logical consistency, and even possible psychological state of the confession content. For example, if the suspect uses too much "ambiguous tone" or "evasive expression" or there is an abnormal pause in the voice waveform, the system will mark it as a "high-risk statement" and prompt the investigators to further question.

Although this technology helps improve interrogation efficiency, it still faces challenges such as dialect diversity, semantic ambiguity, and context jumps in language semantic recognition, which may lead to recognition bias. In addition, the extent of AI intervention and the scope of acceptance in intelligent interrogation also need to clarify the legal boundaries and evidence exclusion rules to prevent the abuse of technology.

4.1.4. Drones and intelligent patrol systems

Extension of non-contact investigation methods and enhancement of control capabilities

As an emerging aerial investigation tool, drone systems have demonstrated powerful functions in crime scene investigation, fugitive tracking, and key area control. AI-driven drones can not only take real-time photos from high altitudes, but also carry modules such as thermal imaging, infrared scanning, and face recognition to achieve target search and remote monitoring in complex terrains, especially in mountainous areas, woodlands, suburbs, and other areas that are difficult for conventional police forces to cover.

At the same time, ground intelligent patrol robots are also being piloted in some cities, which can automatically patrol routes, identify suspicious targets, broadcast warnings, and transmit real-time data to the command center during specific periods of time. This type of "intelligent sentinel" helps to release grassroots police forces and enhance night patrol coverage.

However, the large-scale deployment of drones and smart patrol equipment also brings a series of technical and legal issues: on the one hand, technical security needs to be strengthened, and there will be risks if the equipment is hacked or falls out of control; on the other hand, all-weather, all-round reconnaissance activities may constitute an infringement on the privacy boundaries of citizens, especially in the absence of clear legal authorization and procedural control, it is difficult to ensure the legality and appropriateness of the use of technology.

4.2. Main legal issues faced in the application of artificial intelligence

The rapid expansion of artificial intelligence technology in criminal investigation has shown unique advantages in improving the efficiency of solving cases, reducing the cost of investigation, and realizing dynamic supervision. However, at the same time, it has also caused many deep-seated legal issues. These problems are mainly manifested in the risk of infringement of individual rights, insufficient procedural legitimacy, potential distortion of substantive justice, and the lag of institutional gaps, which urgently need to be responded to from the legal, institutional and practical levels. The following will analyze four major legal issues:

4.2.1. Infringement of personal privacy and data protection issues

# 4.2.1.1. Unauthorized collection and abuse issues

The core of artificial intelligence technology relies on the collection and processing of large amounts of data. Especially in the field of criminal investigation, investigative agencies often use facial recognition, voice monitoring, big data comparison and other means to obtain personal sensitive information such as biometrics, life trajectories, and communication records of persons involved in the case and potential suspects. However, in practice, the data collection link often lacks a clear legal authorization basis and procedural control mechanism, and there is a phenomenon of "collection without notification" and "processing without authorization", which can easily cause substantial infringement of citizens' privacy rights.

For example, in some cases, the police automatically collected facial data through public camera systems and compared it with the national public security database, without clearly distinguishing whether the target population was involved in the case and whether it constituted a legitimate reason for the collection. At the same time, there was a lack of strict use restrictions and de-identification of the collected data, resulting in the "secondary use" of information outside of case investigation or even commercial circulation, exacerbating the risk of privacy leakage.

4.2.1.2. Protection and use boundaries of citizen information The "Civil Code", "Personal Information Protection Law", "Data Security Law" and other laws and regulations have made basic provisions for the legal handling of personal information, but in criminal investigations, the use of citizen information is often in the tension between "national security" and "personal privacy", with unclear boundaries and insufficient supervision. For example, the restrictive provisions on the exercise of investigative power in the "Criminal Procedure Law" are relatively principled, and no targeted constraints are made on specific collection methods in AI technology (such as remote monitoring, algorithm profiling, and relationship map modeling), resulting in the "gray area" of technology use becoming a hotbed for power expansion.

At the same time, citizens' rights to know, object and remedy regarding the collection, processing and use of their information lack effective protection, and it is almost impossible to question the decision of AI system in criminal proceedings, which also weakens the procedural basis of privacy protection.

4.2.2. Algorithmic bias and discrimination

4.2.2.1. Imbalance of algorithm training data and discriminatory consequences

The application of AI system in criminal investigation relies heavily on massive training data and model learning process. However, these training data are often constructed based on historical cases, past law enforcement records and even social prejudices, which can easily lead to structural bias in the output of the algorithm. For example, the predictive policing algorithms used by the early US police (such as the COMPAS system) tend to over-judge the risk of African-American groups in their scoring, resulting in "algorithmic reinforcement" of racial discrimination.

In China, because the data resources involved in the case are concentrated in specific regions, specific populations or specific types of cases, the algorithm may form a "high-risk label" for low-income groups, specific occupations or migrant populations during training, resulting in a shift and misleading of the focus of law enforcement. For example, the big data system may use "frequent late return", "multiple cross-provincial movements" and "low-frequency financial activities" as suspicion indicators, and then automatically label a certain group as "suspicious objects". This labeling thinking not only infringes on personal dignity, but is also likely to cause erroneous investigations and even wrongful convictions.

4.2.2.2. Procedural injustice caused by group labeling

The bias of the AI system is not only reflected at the individual level, but also creates group injustice at the structural level. Driven by algorithms, law enforcement agencies are prone to implement "preconceived" investigative tendencies against specific groups, so that some people are "procedurally labeled" before entering the litigation process, and lose the right to equal treatment that they should enjoy as ordinary citizens. Such risks seriously challenge modern criminal rule of law principles such as "presumption of innocence" and "individualized justice".

In addition, due to the "black box" nature and technical monopoly of algorithms, suspects and defense lawyers often find it difficult to obtain the logical path and data basis of the algorithm reasoning process, and lack substantive defense opportunities. This undermines procedural oversight and risks transforming AI decision-making into an unchallengeable exercise of authority.

4.2.3. Issues of the legality and admissibility of evidence

4.2.3.1. Issues of the subject eligibility of AI-generated evidence

In traditional criminal proceedings, evidence must be obtained by investigators with legal subject qualifications within the scope of legal authority. However, AI systems often assume the function of "active testimony" in criminal investigations, such as automatically generating "location matching" evidence between a suspect and the crime scene through an intelligent recognition system, and extracting "suspicious speech" as the basis for investigation through a voice analysis system. The question that arises at this time is: Does the AI system have the status of a "qualified subject" in the sense of criminal procedure law?

In addition, there is still great controversy over whether the evidence generated by AI meets the evidence standards of "legal source, proper procedure, stable form, and true content". For example, do automatically generated image recognition results, behavior judgment reports, semantic analysis inferences, etc. belong to the type of evidence that is "verifiable and verifiable"? Is the algorithmic logic in the process of evidence formation open and verifiable? These are directly related to the admissibility and probative force of evidence in court trials.

4.2.3.2. Evaluation of the legality and rationality of AI intervention in the investigation process

The involvement of AI technology in investigation is becoming increasingly profound, and some links have even achieved "dehumanization" operations (such as intelligent comparison without human intervention, automatic triggering of arrest mechanisms, etc.). However, according to the Criminal Procedure Law, investigation activities should be completed in person by state agency personnel with investigative powers, and there must be room for accountability and supervision in the process. The participation of AI systems often lacks a clear authorization basis, and the necessary procedural control mechanism is not set up, which makes it easy to break the boundaries of power exercise.

In addition, some intelligent systems lack the ability to judge

the specific circumstances of the case, and may make investigative decisions that do not conform to the legal principles or proportionality principles due to the rigid setting of algorithm parameters. Therefore, a legality evaluation mechanism for AI intervention procedures should be established to clearly define its scope of application, applicable procedures, technical boundaries and supervision paths to prevent it from undermining the fairness of the case due to technical abuse.

4.2.4. Challenges of criminal procedural justice

4.2.4.1. The legality risk of AI replacing human judgment Criminal investigation is essentially a process of judging "the identity, behavior and illegal nature of the suspect", which has a strong value judgment attribute. In this process, AI systems replace humans to complete core tasks such as clue analysis, behavior judgment, and evidence selection, which can easily weaken the sense of responsibility and judgment of law enforcement personnel, resulting in the problem of "technology dependence" or "responsibility shifting". Once a wrong judgment occurs, the investigative agency may blame the system's "misjudgment" rather than its own dereliction of duty, which directly shakes the legal responsibility mechanism for law enforcement behavior.

importantly, More criminal investigations need to comprehensively consider non-data factors such circumstances, motives, and social background, while AI systems can only perform quantitative analysis based on limited parameters, making it difficult to achieve the prudence and empathy that human justice should have. Relying solely on AI and making judicial judgments technical and procedural will inevitably weaken the balance between procedural justice and humane law enforcement.

4.2.4.2. Impact on "procedural justice" and "substantive justice"

The widespread embedding of AI technology has improved the efficiency of case investigation and the rate of evidence discovery to a certain extent, but it may also pose a substantial threat to "procedural justice". In the process of evidence collection, suspect identification, and evidence presentation, if the AI system lacks openness and questionability, the procedure will be meaningless, and even if the substantive conclusion is correct, it will not be able to obtain procedural legitimacy support.

In addition, the core of procedural justice lies in "visible justice", and AI systems often operate in an incomprehensible way. The "inexplicability" of their algorithms and decision paths makes it difficult for the public to believe their conclusions, which seriously affects the credibility of the judiciary.

Therefore, in the context of the continuous development of AI technology, it is necessary to re-examine the trade-off between technical efficiency and procedural justice, avoid sacrificing procedural guarantees in the name of efficiency, and ensure that the application of AI always serves the basic principles of criminal rule of law.

4.3. Overseas regulatory experience

Globally, the application of artificial intelligence technology

criminal investigation is gradually becoming institutionalized and standardized. Developed countries in Europe and the United States, as well as countries with relatively mature legal systems such as Japan and Germany, have established a certain degree of legal constraints and procedural guarantee mechanisms in AI investigation practices, striving to find a balance between efficiency and rights protection. The regulatory experience of these countries or regions not only reflects the legal response to technological development, but also provides important reference for China to build a legal regulatory system for artificial intelligence investigation.

4.3.1. The United States: Review mechanism and case practice for the use of technology

4.3.1.1. Clearview AI case: warning of abuse of facial recognition technology

The United States started early in the application of AI investigation, especially in facial recognition technology, big data policing, predictive algorithms, etc. However, the privacy infringement and legal disputes brought about by its rapid technological development are also particularly significant. Among them, the most representative is the Clearview AI company incident.

Clearview AI has developed a powerful facial recognition engine that provides investigative support for US law enforcement agencies by capturing billions of facial images on social media. Although this technology has been used to quickly identify suspects in some criminal cases, it has also triggered large-scale lawsuits on issues such as "unauthorized capture", "unnotified use", and "information abuse". Several states (such as California and Illinois) have filed lawsuits against it under the Biometric Information Privacy Act (BIPA). The courts generally believe that facial recognition technology constitutes sensitive use of personal information and must obtain explicit consent from users in advance.

This case reflects that: on the one hand, US law restricts the abuse of technology through ex post judicial relief mechanisms; on the other hand, state legislation under its decentralized system has pre-regulated the "technical boundaries". This has important implications for China - while introducing new technologies, we should simultaneously promote the construction of legislation and relief mechanisms to prevent the legal vacuum of "use first and then rule".

4.3.1.2. The institutional checks and balances function of the exclusionary rule

The "exclusionary rule" in US criminal proceedings provides a key procedural constraint for limiting AI's involvement in investigations. In classic cases such as Miranda v. Arizona, the Supreme Court emphasized that evidence obtained without procedural legitimacy cannot be used in court. This principle also applies to the field of AI investigation evidence.

For example, in some state cases, if the police obtain clues through an unauthorized automatic facial recognition system and further conduct a search, the court will consider whether the technology violates the "prohibition of unreasonable searches" principle in the Fourth Amendment. If it is determined to be an illegal search, the subsequent evidence

obtained will also be excluded. This mechanism has established an important counter-logical logic for technical investigation power in practice, which helps prevent the unlimited expansion of AI means under the unsupervised power.

4.3.2. EU: Regulation of AI use under the background of GDPR

4.3.2.1. Institutional design of data protection and "right to be forgotten"

The EU is known for its strict legislation on personal information protection. The General Data Protection Regulation (GDPR), which officially came into effect in 2018, has set a high standard for the legal and compliant use of AI technology around the world. GDPR not only stipulates core rules such as "data minimization", "purpose limitation" and "legality principle", but also enhances individuals' control over their own information through systems such as "right to be forgotten" and "data portability".

In the field of AI investigation, this means that if law enforcement agencies use technologies such as facial recognition and voice analysis, they must ensure the legality of the collection process, the clarity of the data use, and accept the review of independent supervisory agencies (such as data protection commissioners). If the data subject raises an objection or finds that the data is misused, he or she has the right to request deletion, restriction of processing or lodge a complaint.

GDPR has set clear boundaries for AI technology through the institutionalized "informed consent-restriction-relief" process, and particularly emphasizes the priority of personal dignity and privacy rights. When building a regulatory mechanism for AI investigation technology, China should draw on the "rights-dominated" design concept in its data protection system and establish a multi-dimensional personal information rights protection system.

4.3.2.2. Draft of the European Union Artificial Intelligence

In 2021, the European Commission issued the "Draft Artificial Intelligence Act", marking the launch of the world's first special legislation to systematically regulate AI technology. The bill is centered on the principle of "risk orientation" and divides AI systems into four categories: "unacceptable risk", "high risk", "limited risk" and "minimum risk", and puts forward strict access and transparency requirements for highrisk AI systems (such as facial recognition and behavior prediction).

In the field of criminal investigation, the draft AI bill explicitly restricts the use of "real-time remote face recognition systems", allowing them to be implemented only under conditions such as "specific authorization", "public interest" and "court control", and requires all usage records to be subject to independent supervision. This practice reflects the institutional design of a balance mechanism between national security and human rights protection.

The draft also requires that all high-risk AI systems must have "explainability", "human controllability" and "data audit mechanism" to ensure that the system output has legal

legitimacy and error correction mechanism. This provides a model for the design of China's future AI legal regulatory system: that is, not only to be based on data compliance, but also to achieve algorithm supervision, responsibility traceability and process auditability.

4.3.3. Japan and Germany: Institutional coordination between police technology and investigative procedures

4.3.3.1. Japan: Technology use relies on "prior permission" and "procedural review"

Japan is more cautious in the application of AI technology, especially in criminal investigations. Its legal system emphasizes the procedural legitimacy of police behavior and the judicial review mechanism. According to the relevant provisions of the Criminal Procedure Law and the Police Law, the police must obtain a warrant issued by the court and provide detailed descriptions of the collection behavior before using large-scale monitoring, listening equipment or biometric systems.

In addition, Japan's public security agencies have introduced an "expert review mechanism" to conduct ethical and legal feasibility assessments on the deployment of new technology systems, emphasizing that the technology system should ensure "minimum infringement of citizens' basic rights." This system effectively avoids the "regulatory lag" problem caused by the rapid application of technology and ensures that police technology behavior is always within the framework of the rule of law.

4.3.3.2. Germany: Emphasis on the clarity of legal authorization and power supervision mechanism

As a continental legal country, Germany attaches great importance to the boundary between police power and technology use. The German Federal Data Protection Act, the Criminal Investigation Procedure Code and other laws clearly stipulate that the use of technical means must have "specific statutory authorization" and be subject to the "principle of proportionality", "principle of necessity" and "principle of minimum infringement".

In practice, the German Constitutional Court has repeatedly reviewed the constitutionality of technical means. For example, in the famous "online monitoring case", the court ruled that the state may not conduct automated monitoring of citizens' online behavior without explicit authorization, emphasizing that the state's technical behavior must be subject to effective supervision by the judiciary. In addition, Germany has established mechanisms such as the "Federal Commissioner for Freedom of Information" and the "Data Protection Officer" to achieve external supervision and public accountability of police technical behavior, effectively ensuring that procedural fairness and basic rights are not eroded by technology.

5.Suggestion for Path to Building a Legal Regulatory System for Criminal Investigation of Artificial Intelligence

With the continuous deepening of the application of artificial intelligence in criminal investigation, its advantages in improving investigation efficiency and expanding investigation capabilities have become increasingly prominent. But at the same time, the lagging problem of the

relevant legal system has become increasingly prominent. How to strike a balance between technological innovation and legal governance, both to ensure the effective exercise of the state's criminal judicial power and to protect the basic rights of citizens from being abused by technology, is an important issue that China urgently needs to solve. This chapter will propose a specific path to building a legal regulatory system for criminal investigation of artificial intelligence in China from four dimensions: setting legal boundaries, protecting personal data, improving evidence rules, and building a supervision mechanism.

- 5.1 Clarify the legal boundaries of technology application
- 5.1.1. Clearly stipulate the types of cases and procedural links to which AI can be applied in legislation

At present, China has not yet made a clear legal definition of the involvement of artificial intelligence in criminal investigation activities, resulting in the risk of generalization and expansion of the use of technology in practice. To this end, the scope of application, case types and procedural links of artificial intelligence technology in criminal investigations should be clarified through the formulation or revision of legal documents such as the Criminal Procedure Law, the People's Police Law, the Data Security Law, and the Artificial Intelligence Law (Draft), and the legal boundaries of "what can be done", "what cannot be done" and "what should be reviewed" should be defined.

For example, it can be clearly stipulated that highly sensitive AI methods such as facial recognition and predictive analysis can only be used in specific serious criminal cases, under court authorization or prosecutorial supervision. At the same time, the investigation link involving technology should be limited to auxiliary procedures such as "clue acquisition", "suspect portrait" and "intelligence analysis", rather than replacing substantive judgments or replacing the subjective judgments of investigators.

5.1.2. Establish the application standards of the "proportional principle" and the "minimum infringement principle"

Referring to other countries experience, China should incorporate the "proportional principle" and the "minimum infringement principle" into the legal application standards for artificial intelligence criminal investigations as the basic principles for measuring the legality and legitimacy of technology use.

Specifically, when deciding whether to use AI technology, the investigative agency should comprehensively consider factors such as the degree of infringement of personal rights by technical means, the nature and severity of the case, whether there are alternative less infringing means available, and whether legal authorization has been obtained. For highly sensitive means such as big data dynamic tracking and face recognition, more stringent start-up conditions and approval procedures should be set to ensure that the use of technology does not exceed its necessity and rationality.

- 5.2. Strengthen the protection mechanism for personal data
- 5.2.1. Introduce the principle of technical transparency and the mechanism of information use traceability

The essence of artificial intelligence criminal investigation

technology is the extensive processing and in-depth mining of data, so a systematic data protection mechanism must be established. First of all, the "principle of technical transparency" should be established in legislation, requiring that any AI system used in criminal investigation must have a technical structure with verifiable data sources, explainable processing processes, and recordable operating behaviors. At the same time, the "information use traceability mechanism" should be introduced to achieve a full-chain record of each data call, analysis, storage and sharing, which is convenient for post-event review and responsibility tracing.

This move not only helps to protect citizens' right to know and right to object to the use of their own data, but also encourages law enforcement personnel to use technology in accordance with laws and regulations to reduce the risk of abuse.

5.2.2. Build a citizen-centered data use consent mechanism

In non-emergency situations, we should promote the establishment of a citizen-centered data authorization mechanism. In particular, for biometric information such as images, voiceprints, and locations of people not involved in the case, informed consent should be obtained in advance, and individuals should be allowed to object to the collection of information or request deletion. For data collected in public security video surveillance systems, their purpose of use, storage time, and access rights should also be clearly defined.

At the same time, industry supervision and judicial supervision of AI data collection should be strengthened, and an "information rights complaint channel" should be established to ensure that citizens have effective remedies when they find that their data is used illegally.

- 5.3. Improve evidence rules and procedural guarantees
- 5.3.1. Clarify the admissibility standards and certification process of AI-generated evidence

As AI technology is widely used in investigation links such as suspect positioning, scene restoration, and audio and video analysis, the information it generates will inevitably enter the judicial trial process and become the basis for the final decision. At this time, the admissibility of AI-generated evidence has become a core legal issue.

The current Criminal Procedure Law and Judicial Interpretation of the People's Court in China have not yet clarified the legal position of AI-generated data as criminal evidence. Therefore, it is urgent to clarify its nature of evidence, the standard for evaluating the probative force and the process of legality certification from the level of legislation and judicial interpretation.

Specifically, the following systems can be established:

Technical source review system: All AI-generated evidence must be accompanied by software source description, algorithm description and equipment registration information. Verifiability mechanism: Ensure the originality, integrity and reproducibility of evidence, and avoid tampering and falsification in the middle.

Expert assisted evaluation mechanism: Third-party technical experts independently evaluate the reliability of AI evidence and issue professional reports.

5.3.2. Introduce the principles of "algorithmic explainability"

and "human final decision-making responsibility"

The process of AI participating in investigation should not completely replace human judgment, otherwise it is very easy to lead to the lack of procedural justice. To this end, the "algorithmic explainability principle" should be established in the system, requiring all AI models used in criminal investigation to explain their logical paths and reasoning basis, so as to avoid "black box decision-making" from becoming a judicial reference.

At the same time, the "principle of human ultimate decision-making responsibility" should be clarified, that is, no matter how detailed the clues and judgments provided by AI technology are, the final legal judgment and procedural advancement responsibility should still be borne by investigators and judicial personnel. AI is only an auxiliary tool and cannot independently lead the case process. This principle not only helps to ensure the traceability of judicial responsibility, but also meets the fundamental requirements of procedural justice.

- 5.4. Establish an independent supervision and review mechanism
- 5.4.1. Set up a technical ethics committee and an expert review group

A special "artificial intelligence technology ethics review committee" or "AI technology legal risk assessment expert group" should be established in public security organs, procuratorates and national judicial institutions to conduct prior review and post-evaluation of AI systems to be put into the field of investigation.

The members of the committee should include a diverse group of legal experts, technical experts, ethicists, data protection officers, etc., to conduct a comprehensive review of the legality, rationality, data sources, potential biases and other aspects of AI technology, and put forward feasibility reports and regulatory recommendations.

5.4.2. Introduce a check and balance mechanism of multiple subjects (lawyers, technicians, judges)

The compliance operation of AI investigative means not only relies on technical supervision mechanisms, but also requires procedural supervision through checks and balances between legal professional groups. In the case, defense lawyers should have the right to question AI technology evidence and review algorithms; technicians should provide professional analysis as a neutral third party; and judges should be responsible for substantive review of the admissibility of AI evidence.

In addition, courts and procuratorates should be encouraged to set up "AI evidence special review teams" to train judicial personnel with technical backgrounds so that they can understand and judge the formation process and legal effect of AI evidence. Through the linkage of the three parties, closed-loop supervision of the legal use of AI technology can be achieved to prevent technical means from becoming a tool to cover up the abuse of power.

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