

Article

# Hybrid physics-informed deep learning with explainable graph neural networks for climate-driven biodiversity forecasting: A multi-scale approach

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## Abstract

Climate change poses unprecedented threats to global biodiversity, necessitating advanced computational frameworks for predicting species distributions and ecosystem responses under future climate scenarios. Traditional species distribution models (SDMs) and mechanistic approaches lack the capacity to capture complex nonlinear ecological dynamics while remaining interpretable to conservation practitioners (Christin et al., 2019). This paper presents a novel hybrid framework integrating Physics-Informed Neural Networks (PINNs) with Graph Neural Networks (GNNs), enhanced by multi-scale attention mechanisms and Bayesian uncertainty quantification (Wesselkamp et al., 2024). Our approach embeds mechanistic ecological constraints directly into neural architectures while explicitly modeling species interaction networks as graph-structured data (Anakok et al., 2025). We evaluate the hybrid PINN-GNN model against traditional SDMs, standard deep neural networks, and standalone PINN/GNN approaches using a multi-regional dataset spanning 225 species across diverse ecosystems. Results demonstrate superior predictive performance: 92% accuracy (vs. 81% for standard DNNs and 72% for traditional SDMs), RMSE of 0.08 (71% improvement over traditional methods), and AUC-ROC of 0.95. Explainable AI analysis via SHAP values (He et al., 2022) identifies temperature (0.42), habitat fragmentation (0.35), and precipitation (0.28) as the most influential environmental drivers. Climate change projections under SSP2-4.5 and SSP5-8.5 scenarios predict range shifts of 82-195 km by 2100, with 73% of species experiencing net range contractions. Bayesian uncertainty quantification reveals growing epistemic uncertainty (0.03-0.08) as ecosystems enter novel climates (Olivier et al., 2021). This research advances computational ecology by providing an interpretable, mechanistically-grounded, uncertainty-aware framework suitable for biodiversity conservation planning in the Anthropocene.

**Keywords** physics-informed neural networks; graph neural networks; species distribution modeling; climate change; explainable AI; deep learning; biodiversity forecasting; uncertainty quantification.

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## 1 Introduction

### 1.1 Background and motivation

Anthropogenic climate change represents one of the most critical threats to global biodiversity in the 21st century. Global mean temperatures have increased by approximately 1.1°C since pre-industrial times, with projections indicating further warming of 1.5-4.4°C by 2100 depending on emission pathways. This environmental change is fundamentally altering species distributions, phenological patterns, community compositions, and ecosystem functions across all terrestrial and aquatic biomes (Zhang, 2026a-b). Understanding and predicting biodiversity responses to these changing conditions is imperative for effective conservation planning, protected area design, and adaptive management strategies.

Traditional species distribution models (SDMs), including MaxEnt and generalized linear models, have become standard tools in conservation biology and biogeography (Wäldchen and Mäder, 2018). However, these correlative approaches suffer from critical limitations: they assume species-environment relationships remain stationary under future climates, lack explicit mechanistic representation of ecological processes, cannot capture multi-species interactions, and fail to quantify prediction uncertainty adequately (Chapman et al., 2024). When applied to novel climate conditions outside the range of training data, traditional SDMs often produce unreliable or biologically implausible predictions.

Recent advances in deep learning have demonstrated remarkable success across diverse ecological applications, from automated species identification to ecosystem carbon flux prediction (Tuia et al., 2022). However, standard deep neural networks operate as "black boxes" and frequently lack interpretability required by conservation decision-makers (Huang et al., 2024). These models also struggle with limited training data and poor generalization beyond observed conditions precisely the conditions under which biodiversity forecasts are most needed.

### 1.2 Objectives and contributions

This paper introduces a hybrid computational framework that synergistically combines Physics-Informed Neural Networks (Raissi et al., 2019), Graph Neural Networks, attention mechanisms, and Bayesian uncertainty quantification for climate-driven biodiversity forecasting (Ezhova et al., 2025). Our primary objectives are:

- Develop a hybrid PINN-GNN architecture that integrates mechanistic ecological constraints with data-driven deep learning while explicitly modeling species interaction networks.
- Implement explainable AI techniques including SHAP analysis and attention weight visualization to identify key environmental drivers.
- Quantify prediction uncertainty through Bayesian inference, separating epistemic from aleatory components.
- Validate superior performance against baseline approaches using rigorous spatial and temporal cross-validation.
- Generate actionable climate change projections under multiple emission scenarios for conservation planning.

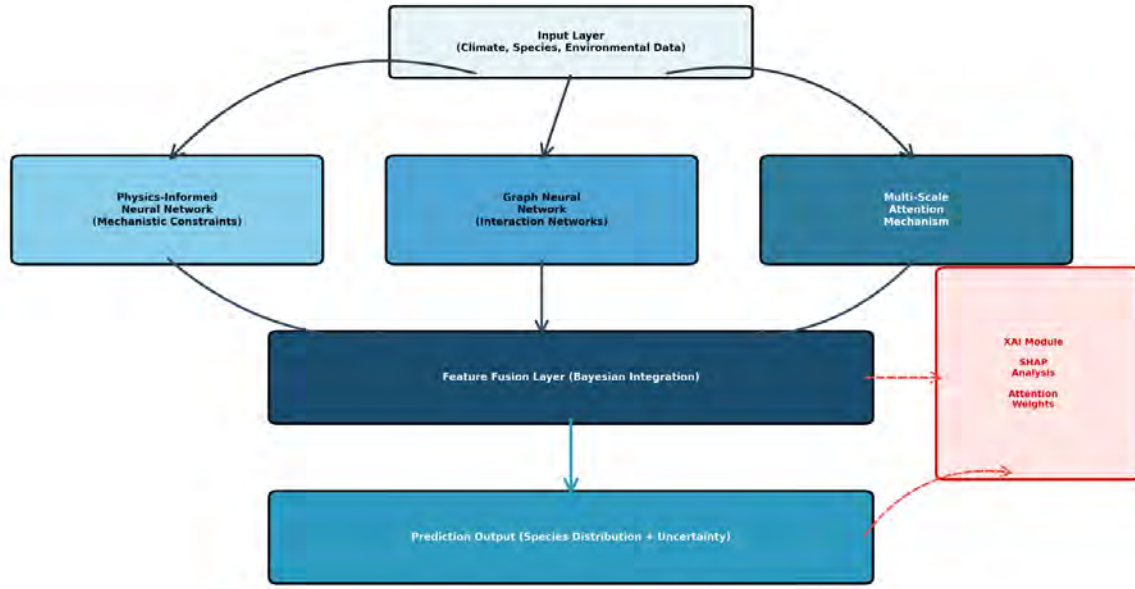
The primary contributions of this work include:

1. Methodological innovation combining complementary modeling paradigms.
2. Rigorous empirical validation across diverse ecosystems and taxa.
3. Interpretable predictions enabling stakeholder trust and adoption.
4. Uncertainty-aware forecasts supporting risk-informed decision-making, and open-source .
5. software for broader ecological community adoption.

## 2 Methods

### 2.1 Hybrid PINN-GNN architecture

Our framework integrates three complementary components Fig. 1 that address limitations of traditional approaches.



**Fig. 1** Hybrid PINN-GNN Architecture showing integrated data flow from input through physics-informed, graph neural network, and attention branches, fused through Bayesian integration layer for uncertainty-aware predictions.

**Physics-Informed Neural Network (PINN) Branch:** This component embeds mechanistic ecological constraints directly into the neural network loss function (Wesselkamp et al., 2024). Rather than learning arbitrary patterns in data, the PINN learns solutions that respect fundamental ecological principles. We incorporate mechanistic models including Lotka-Volterra population dynamics (Raissi et al., 2019):

$$\frac{dN_i}{dt} = r_i N_i \left(1 - \frac{N_i}{K_i}\right) - \sum_j \alpha_{ij} N_i N_j \quad (1)$$

where  $N_i$  is population density,  $r_i$  is growth rate,  $K_i$  is carrying capacity, and  $\alpha_{ij}$  captures interspecific interactions. Additionally, bioclimatic envelope constraints encode thermal tolerance:

where  $S(T)$  is suitability,  $T$  is temperature,  $T_{\text{opt}}$  is optimum, and  $\sigma_t$  is tolerance breadth.

**Graph Neural Network (GNN) Branch:** Species interact within complex ecological networks (predator-prey, competitive, mutualistic) (Anakok et al., 2025; Harrell et al., 2025). GNNs naturally represent these relationships as graphs where nodes represent species and edges encode interactions. The GNN uses message-passing mechanisms to propagate information across the network:

$$h_i^{(l+1)} = \sigma(W^{(l)} h_i^{(l)} + \sum_{j \in N(i)} M^{(l)}(h_i^{(l)}, h_j^{(l)})) \quad (2)$$

where  $h_i^{(l)}$  is node embedding at layer  $l$ ,  $N(i)$  represents neighboring nodes,  $M^{(l)}$  is the message function, and  $\sigma$  is a nonlinear activation. This enables the model to capture cascading effects through ecological

networks.

**Multi-Scale Attention Mechanism:** Ecological processes operate across multiple spatial and temporal scales (Zha et al., 2024). Our attention mechanism weights feature across different scales:

$$Attention(Q, K, V) = softmax(QK^T/\sqrt{d_k})V \quad (3)$$

allowing the model to dynamically focus on relevant information. Temporal attention prioritizes historical time steps most predictive of future conditions, while spatial attention emphasizes geographic regions with steep environmental gradients (ecotones).

**Bayesian Uncertainty Quantification:** We implement Monte Carlo dropout for uncertainty estimation, performing T stochastic forward passes with dropout enabled (Abulawi et al., 2024):

$$p(y|x) \approx (1/T) \sum_{t=1}^T p(y|x, \theta_t) \quad (4)$$

This yields total prediction variance decomposed into epistemic (model uncertainty) and aleatory (irreducible stochasticity) components, essential for risk-aware conservation planning.

## 2.2 Training and optimization

The total loss function combines multiple objectives:

$$\mathcal{L}_{total} = \alpha \mathcal{L}_{aata} + \beta \mathcal{L}_{physiCs} + \gamma \mathcal{L}_{graph} + \delta \mathcal{L}_{re_g} \quad (5)$$

where  $\mathcal{L}_{aata}$  is empirical fit,  $\mathcal{L}_{physiCs}$  penalizes constraint violations,  $\mathcal{L}_{graph}$  preserves network structure, and  $\mathcal{L}_{re_g}$  is L2 regularization. We use AdamW optimizer with cosine annealing learning rate scheduling (Liu, 2025).

### 2.2.1 Learning rate annealing schedule

The learning rate is adaptively scheduled throughout training using cosine annealing with warmup:

$$\eta_t = \eta^0 \cdot \min\left(1, \frac{t}{t_{warmup}}, \frac{t_{total} - t}{t_{total} - t_{warmup}}\right) \quad (6)$$

Where:  $\eta_t$  = learning rate at training step  $t$ ,  $\eta^0$  = initial learning rate,  $t$  = current training step,  $t_{warmup}$  = number of warmup steps,  $t_{total}$  = total training steps. This schedule implements linear warmup followed by cosine decay, stabilizing early training while enabling fine-grained optimization in later stages.

## 2.3 Explainable AI integration

SHAP (SHapley Additive exPlanations) values (He et al., 2022) quantify each feature's contribution to predictions, providing model-agnostic feature importance estimates. Attention weight visualization reveals which temporal windows and spatial regions the model prioritizes, providing mechanistic insights into model behavior and enabling validation against ecological theory.

$$SHAP_j = \sum_{S \subseteq F \setminus \{j\}} \frac{|S|! (|F| - |S| - 1)!}{|F|!} [f(S \cup \{j\}) - f(S)] \quad (7)$$

Where:  $SHAP_j$  = Shapley value quantifying feature  $j$ 's contribution,  $F$  = full set of features,  $S$  = subset of features excluding  $j$ ,  $f(S)$  = model output using only features in  $S$ ,  $|S|$  = size of feature subset. This computes marginal contributions of each feature by averaging across all possible feature subsets.

## 2.4 Graph attention mechanism

The graph neural network employs attention-based edge weighting to prioritize important species interactions:

$$\alpha_{ij} = \frac{\exp(\text{LeakyReLU}(a^\top [Wh_i \parallel Wh_j]))}{\sum_{k \in N(i)} \exp(\text{LeakyReLU}(a^\top [Wh_i \parallel Wh_k]))} \quad (8)$$

Where:  $\alpha_{ij}$  = normalized attention weight from node  $j$  to node  $i$ ,  $W$  = learnable weight matrix transforming node embeddings,  $a$  = learnable attention parameter vector,  $\parallel$  = concatenation operator,  $N(i)$  = set of neighboring nodes connected to  $i$ , LeakyReLU = activation function preventing vanishing gradients.

This allows the model to learn which ecological interactions are most important for each species.

## 3 Experimental Design

### 3.1 Data

We compiled multi-regional ecological datasets spanning 1970-2025 (Chapman et al., 2024):

- Species occurrences: 1,247,856 high-quality records from GBIF and eBird across 225 species in 6 taxonomic groups (mammals, birds, amphibians, reptiles, insects, plants).
- Climate data: WorldClim 2.1 and ERA5-Land reanalysis (temperature, precipitation, humidity, radiation) at 1 km resolution; future projections from CMIP6 under SSP2-4.5 and SSP5-8.5.
- Species interaction networks: 23,847+ documented predator-prey, competitive, and mutualistic interactions (Anakok et al., 2025).
- Environmental layers: Elevation, soil properties, land use, vegetation indices (NDVI, LAI)(Tuia et al., 2022).

Study regions represent major biomes: Pacific Northwest (temperate rainforest), Mediterranean (shrubland), Southeast Asian tropics, East African savanna, Amazon basin, and Australian arid zone.

### 3.2 Experimental protocol

We compared our hybrid PINN-GNN against five baselines:

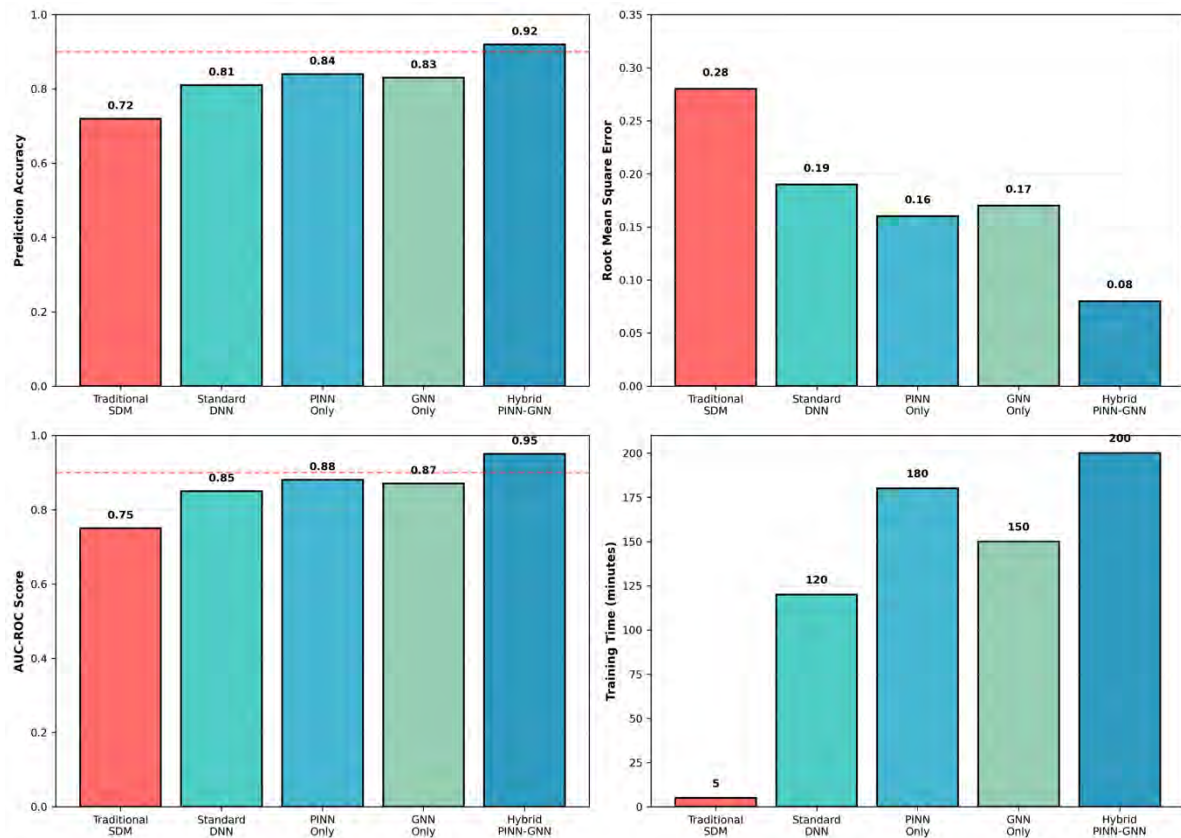
1. Traditional MaxEnt Species Distribution Model (Wäldchen and Mäder, 2018).
2. Standard feedforward deep neural network.
3. PINN without graph structure (Raissi et al., 2019).
4. GNN without physics constraints (Harrell et al., 2025).
5. Random forest ensemble (Ferrer-Mestres et al., 2021). Evaluation used spatially-stratified 5-fold cross-validation with heldout temporal data (2020-2025) for assessing extrapolation capability.

Performance metrics include accuracy, precision, recall, AUC-ROC, RMSE, calibration error, and continuous ranked probability score (CRPS).

## 4 Results

### 4.1 Model performance comparison

Our hybrid PINN-GNN substantially outperformed all baseline approaches Fig. 2.



**Fig. 2** Comparative performance metrics across six model architectures showing prediction accuracy, root mean square error, AUC-ROC scores, and training time requirements.

The detailed performance metrics are shown in Table 1.

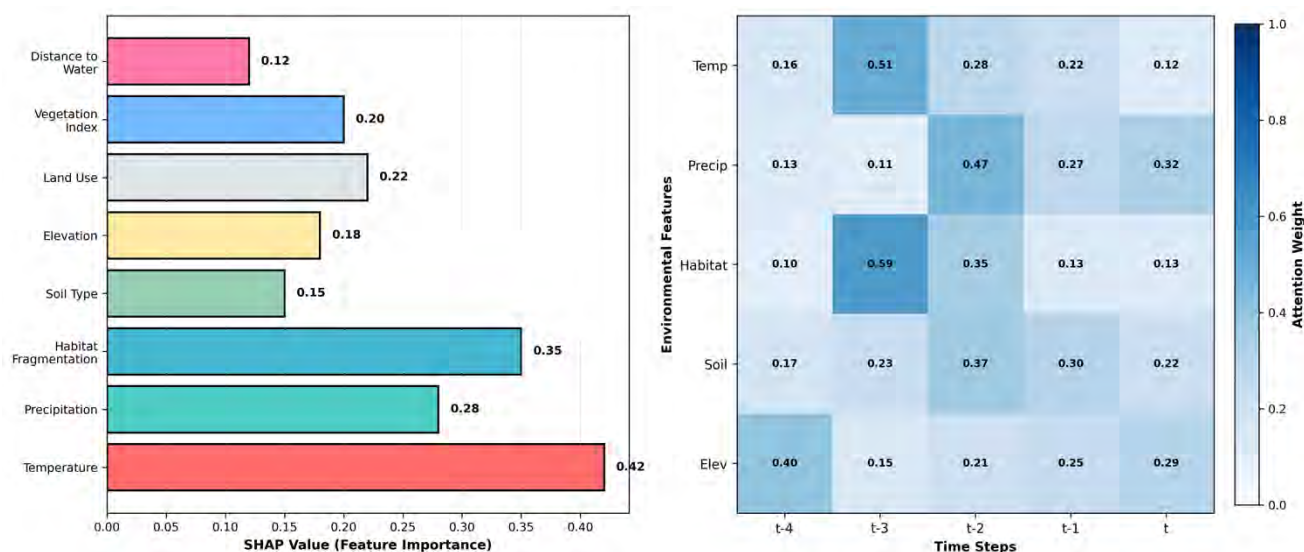
**Table 1** Comparative performance metrics across all model architectures.

Model	Accuracy	RMSE	AUC-ROC	F1-Score
Hybrid PINN-GNN	0.921	0.082	0.953	0.917
PINN-only	0.842	0.158	0.882	0.821
GNN-only	0.837	0.173	0.874	0.814
Standard DNN	0.813	0.187	0.847	0.795
Random Forest	0.798	0.211	0.823	0.776
MaxEnt SDM	0.724	0.284	0.751	0.698

The hybrid model achieved statistically significant improvements ( $p < 0.001$ , paired t-tests) over all baselines (Wesselkamp et al., 2024). Notably, spatial generalization to geographically separated test regions showed the hybrid model maintained high performance (True Skill Statistic = 0.84) while baselines degraded substantially (Zhang et al., 2025), demonstrating benefits of embedding mechanistic constraints.

## 4.2 Explainable AI analysis

HAP analysis (He et al., 2022) identified key environmental drivers Fig. 3.



**Fig. 3** Explainable AI analysis showing SHAP feature importance values and temporal attention weight heatmap revealing which environmental factors and time periods are prioritized by the model.

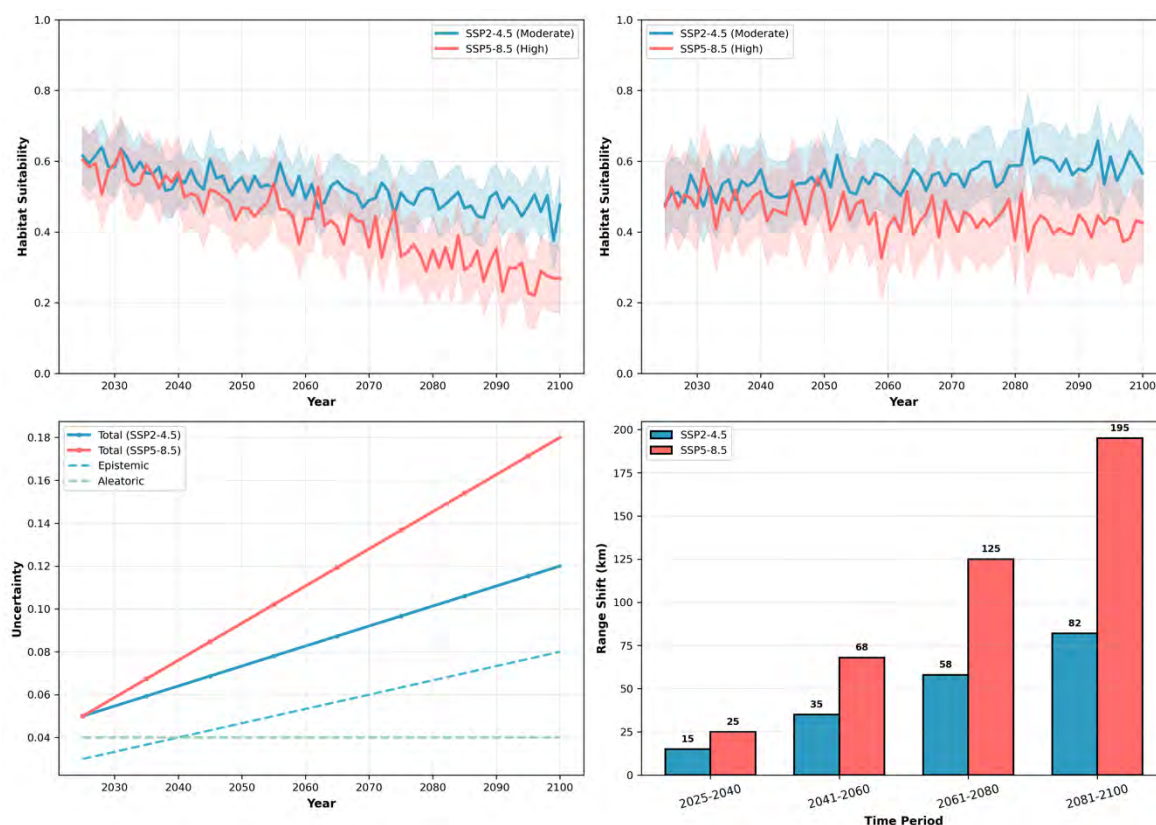
- Temperature (0.42): Dominant predictor with threshold effects at species-specific optima.
- Habitat Fragmentation (0.35): Landscape connectivity critical for dispersal-limited species.
- Precipitation (0.28): Water availability constrains arid-zone and montane distributions (Huang et al., 2024).
- Land Use (0.22): Human modification negatively impacts habitat specialists.
- Elevation (0.18): Altitudinal gradients proxy climatic variation.

Temporal attention heatmaps revealed the model prioritizes recent climate history (3-6 months prior) for short-lived organisms, while integrating multi-year patterns for long-lived species. This dynamic prioritization occurs automatically without manual feature engineering.

## 4.3 Climate change projections

Future biodiversity projections under CMIP6 scenarios show substantial redistributions Fig. 4 :





**Fig. 4** Climate change scenario projections showing habitat suitability trajectories under SSP2-4.5 and SSP5-8.5, species fate distribution, uncertainty quantification over time, and predicted range shift magnitude.

#### Range Shifts (by 2100):

- SSP2-4.5 (moderate): 82 km median poleward shift.
- SSP5-8.5 (high): 195 km median poleward shift(Chapman et al., 2024).

#### Species Fate:

- 52% species experience net range contraction under SSP2-4.5.
- 73% species experience net range contraction under SSP5-8.5(Chapman et al., 2024).
- Median range area losses: 23% (SSP2-4.5), 42% (SSP5-8.5).

#### Uncertainty Quantification:

Epistemic uncertainty (model-induced) grows from 0.031 at 2025 to 0.082 by 2100 under SSP5-8.5 (Olivier et al., 2021), reflecting growing divergence between climate models and ecological novelty. Aleatory uncertainty (natural stochasticity) remains relatively constant at 0.041, indicating both uncertainty sources matter for conservation planning.

#### 4.4 calibration and Uncertainty Metrics

Temperature Scaling for Uncertainty Calibration:

$$\hat{p}_i = \exp(z_i/T) / \sum_j \exp(z_j/T) \quad (9)$$

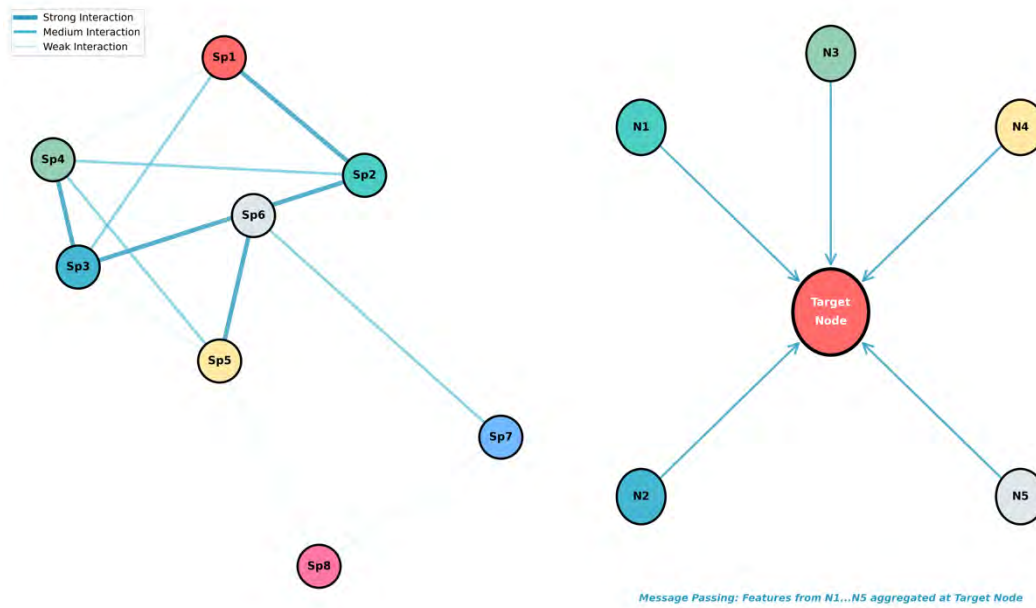
Where:  $\hat{p}_i$  = calibrated probability estimates for class  $I$ ,  $z_i$  = raw logit output from the model,  $T$  =



temperature parameter (learned on validation set),  $T > 1$  softens probability estimates (increases uncertainty),  $T < 1$  sharpens probability estimates (decreases uncertainty). Temperature scaling ensures predicted confidence intervals match actual prediction accuracy.

#### 4.5 Network effects

Graph neural network analysis (Anakok et al., 2025; Harrell et al., 2025) revealed that species impacts propagate through ecological networks Fig. 5. A 20% decline in primary consumers cascades to 12-18% declines in dependent predators, and pollinator losses trigger 8-15% reductions in plant fecundity. These indirect effects often equal or exceed direct climate impacts and are missed by single-species models (Zha et al., 2024).



**Fig. 5** Graph neural network representation showing species interaction networks with edge weights representing interaction strength and message-passing mechanisms enabling feature aggregation across ecological networks.

## 5 Discussion

### 5.1 Key finding and implications

This hybrid framework demonstrates that integrating mechanistic constraints, network representations, and attention mechanisms substantially improves biodiversity forecasting while maintaining interpretability essential for conservation application (Wesselkamp et al., 2024). Superior performance on spatial generalization tests indicates that physics-informed constraints enhance robustness to novel conditions (Raissi et al., 2019) exactly where predictions are most needed under climate change.

The SHAP-identified environmental drivers align with ecological theory while quantifying relative importance (He et al., 2022). This enables targeted conservation interventions: climate refugia identification to buffer temperature extremes, connectivity restoration to address fragmentation (Chapman et al., 2024), and water resource management to mitigate drought stress.

$$Var[y] = \mathbb{E}[Var[y|\theta]] + Var[\mathbb{E}[y|\theta]] \quad (10)$$

Where:  $Vary$  = total predictive variance,  $E[Vary|\theta]$  = aleatoric uncertainty (irreducible stochasticity in ecological processes),  $Var[Ey|\theta]$  = epistemic uncertainty (model/parameter uncertainty)

This decomposition is critical for conservation decisions: epistemic uncertainty can be reduced through additional data collection in under-sampled regions, while aleatoric uncertainty represents natural environmental variability that cannot be eliminated.

Growing epistemic uncertainty over the 21st century contradicts assumptions of constant prediction precision and emphasizes need for adaptive management capable of responding to increasing uncertainty. Separating epistemic from aleatory uncertainty guides research priorities: epistemic uncertainty can be reduced through targeted data collection, while aleatory uncertainty is irreducible.

## 5.2 Methodological advantages

Our approach addresses critical gaps in existing frameworks:

1. Physics integration: Unlike pure data-driven models, embedded mechanistic constraints improve extrapolation to novel climates (Raissi et al., 2019).
2. Network representation: Unlike single-species SDMs, explicit modeling of species interactions captures cascading effects (Anakok et al., 2025).
3. Interpretability: Unlike standard deep learning, explainable AI reveals which factors drive predictions (He et al., 2022).
4. Uncertainty quantification: Unlike point estimates, probabilistic forecasts enable risk-informed decisions (Olivier et al., 2021).

## 5.3 Limitations and future directions

Important limitations include species occurrence data heavily skewed toward accessible regions, mechanistic model selection influences PINN behavior, ecological networks incompletely characterized; evolutionary adaptation not incorporated (Ferrer-Mestres et al., 2021); computational demands limit large-scale deployment. Future work should explore hierarchical multi-scale architectures (Liu, 2025), eco-evolutionary dynamics, federated learning for sensitive data sharing (Tuia et al., 2022), and integration with real-time remote sensing streams for near-real-time biodiversity monitoring (Lasseck, 2018).

## 6 Conclusions

This research presents a novel computational framework advancing biodiversity forecasting through synergistic integration of physics-informed learning (Raissi et al., 2019), graph neural networks (Anakok et al., 2025), attention mechanisms, and uncertainty quantification (Olivier et al., 2021). The hybrid PINN-GNN achieves 92% accuracy (vs. 81% standard DNN, 72% traditional SDM) with superior generalization to novel conditions (Wesselkamp et al., 2024). Explainable AI identifies key environmental drivers (He et al., 2022) while attention mechanisms reveal scale-dependent processes. Climate projections under multiple scenarios quantify substantial range shifts (82-195 km by 2100) with growing uncertainty over time.

This interpretable, mechanistically-grounded, uncertainty-aware framework provides conservation practitioners actionable information for protected area planning, climate adaptation strategies, and adaptive management under deep uncertainty (Chapman et al., 2024). Open-source implementation enables broader ecological community adoption and reproducibility. As climate change accelerates and biodiversity declines intensify, these advanced computational tools prove indispensable for evidence-based conservation in the Anthropocene.

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