Uncertainty Aware Semi-Supervised Learning on Graph Data

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Why is predicting uncertainty important?

Uncertainty vs. Misclassification

When our model only knows `car' and `road,'

1 *Incorrect prediction*

→ High Uncertainty

Misclassify "car" as "road"

2 *Out-of-distribution*

→ High Uncertainty

?

Misclassify "deer" (OOD object) as "car"

Is it important to know:

- ✓ **why we don’t know?**
- ✓ **how much we don’t know?**

So how can we predict the uncertainty based on its root cause?

Would it really help for our decision making?

Types of uncertainty

1 *Epistemic* uncertainty (a.k.a. model/parameter uncertainty)

- Measures what model doesn't know
- Due to **limited data and knowledge**

Aleatoric uncertainty (a.k.a. data uncertainty)

- Measures what you can't understand from the data
- Due to **randomness**

→ Probabilistic Uncertainty

2 ***Vacuity* uncertainty** (a.k.a. ignorance)

- Measures uncertainty due to **a lack of evidence**

***Dissonance* uncertainty**

- Measures uncertainty due to **conflicting evidence**

→ Evidential Uncertainty

Evidential Uncertainty

Task: 3 class image classification

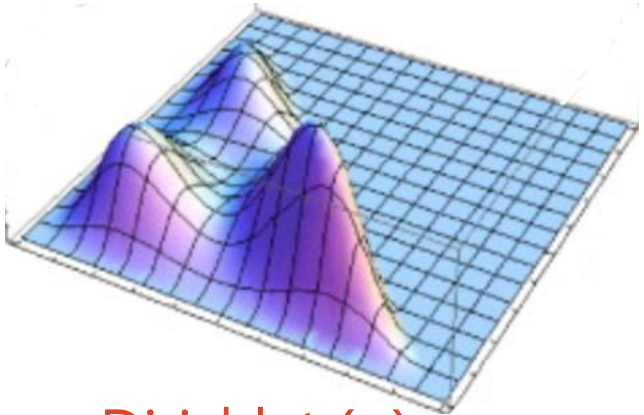
Training Data: Dog (e_1 =10 images) Cat (e_2 = 10 images) Pig (e_3 = 10 images)

$e = [e_1, \ldots, e_K]$ Evidence (Historical observations)

Subjective Opinion

$\omega = (\boldsymbol{b}, u, \boldsymbol{a})$

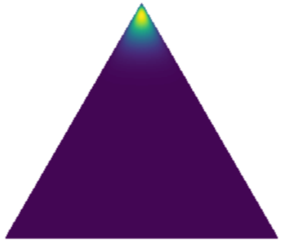
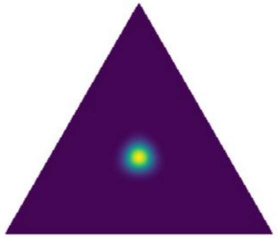
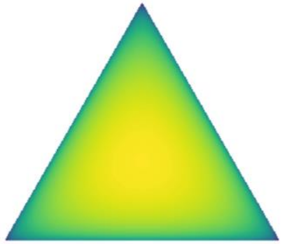
$\alpha = e + 1$



Dirichlet (α)

A subjective opinion modeled based on `Subjective Logic' which uses Dirichlet distribution to measure multiple dimensions of uncertainty in classification tasks

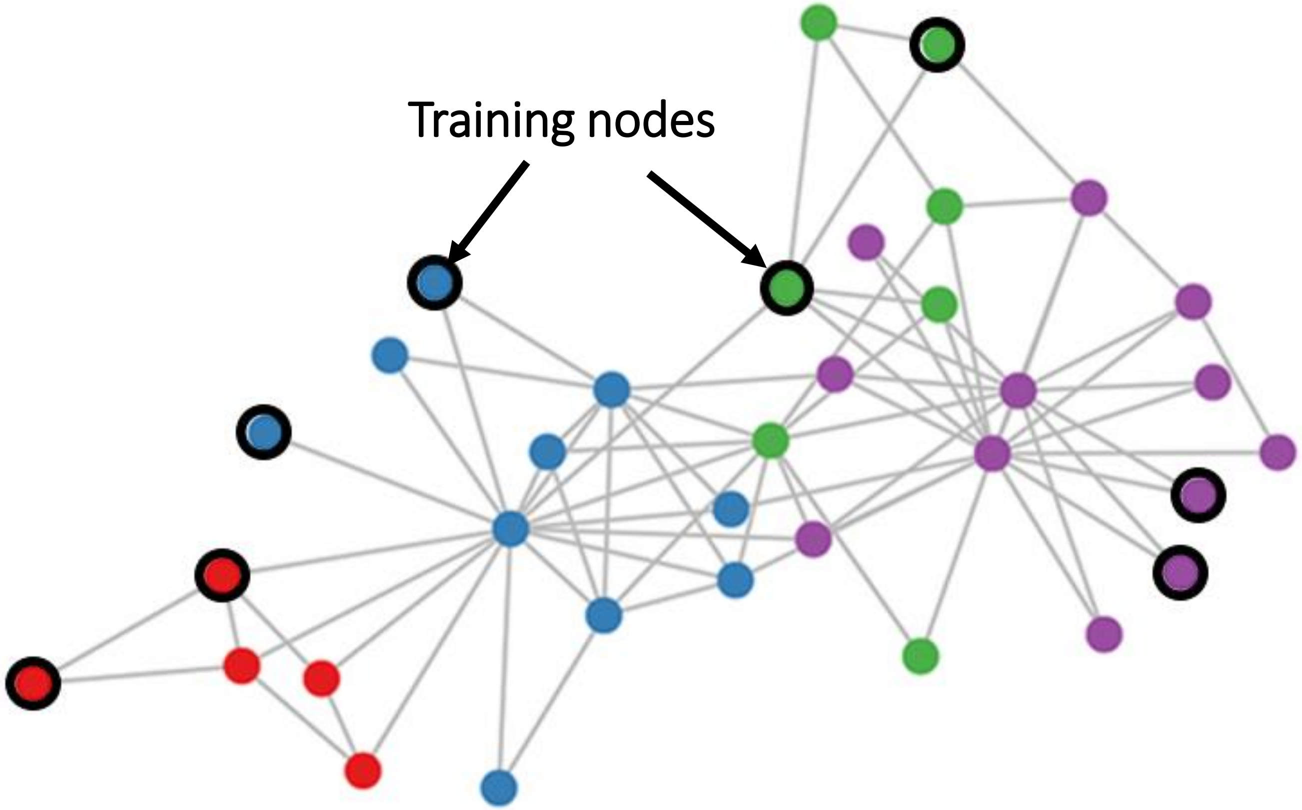
Why Evidential Uncertainty?

	Confidence Prediction	Conflict Prediction	Out-of-Distribution
			
Dirichlet Distribution	α = [11, 1, 1]	α = [11, 11, 11]	α = [1, 1, 1]
Expected Probability	p = [0.83, 0.083, 0.083]	p = [1/3, 1/3, 1/3]	p = [1/3, 1/3, 1/3]
	Low Uncertainty	High Dissonance (conflicting evidence)	High Vacuity (lack of evidence)
Test image			

Different Evidential Uncertainty

Same probability

Problem Formulation



Given: graph $\mathcal{G} = (\mathbb{V}, \mathbb{E}, \mathbf{r}, \mathbf{y}_{\mathbb{L}})$

$\mathbb{V}$: Node

$\mathbb{E}$: Edge

$\mathbf{r}$: node-level feature

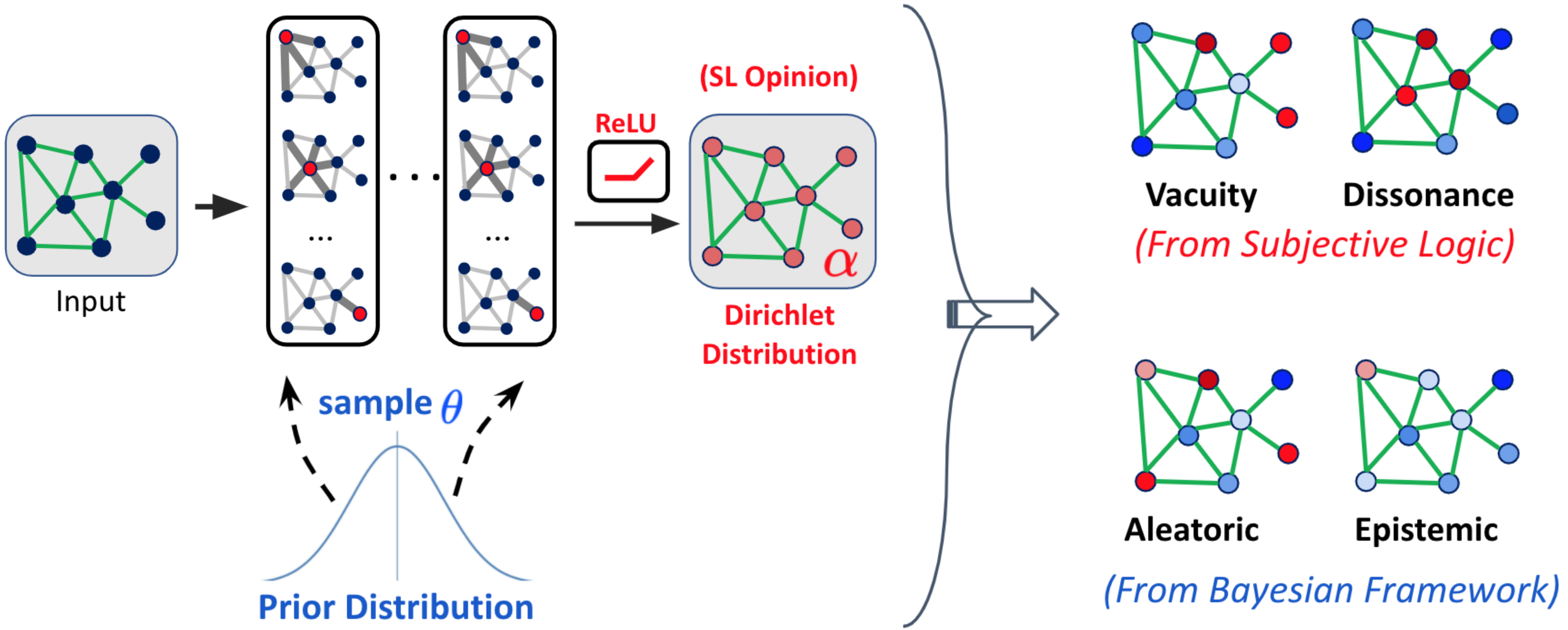
$\mathbf{y}_{\mathbb{L}}$: training labels (K classes)
a small set of training node (black circle)

Goal:

- class probabilities $\boldsymbol{p}$
- **multidimensional uncertainty $\boldsymbol{u}$**

Vacuity, dissonance, epistemic, aleatoric

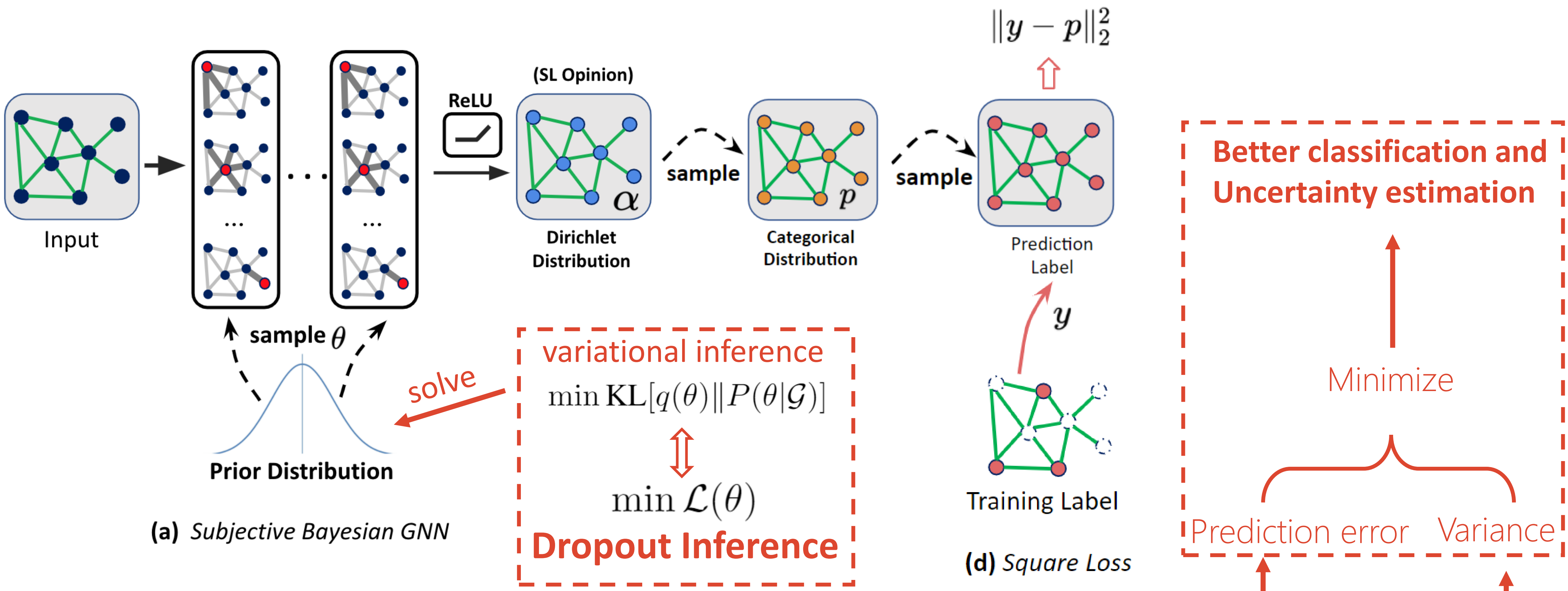
Uncertainty Aware Framework



Subjective Bayesian GNN

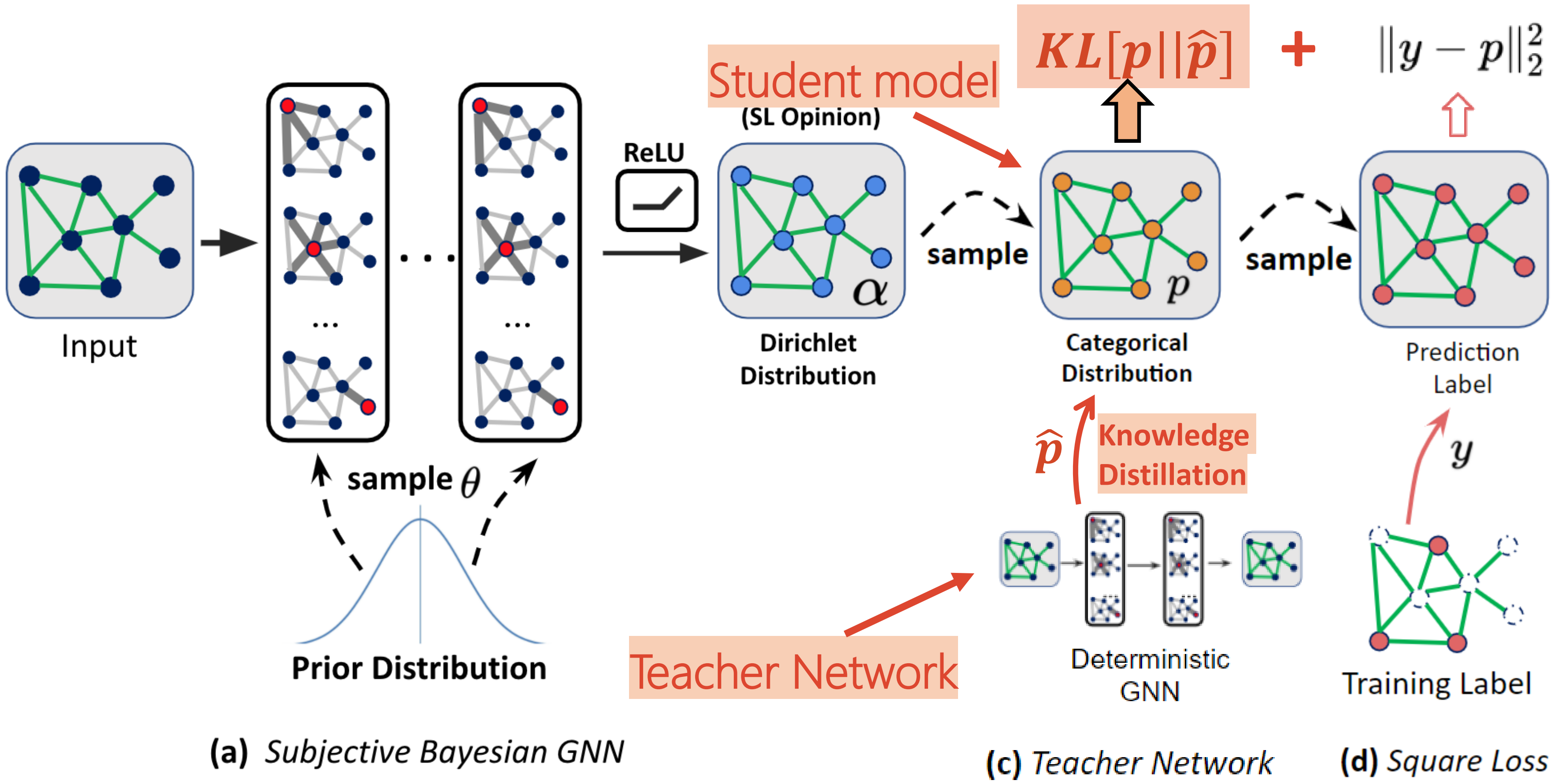
Multiple Uncertainties

Training Uncertainty Framework

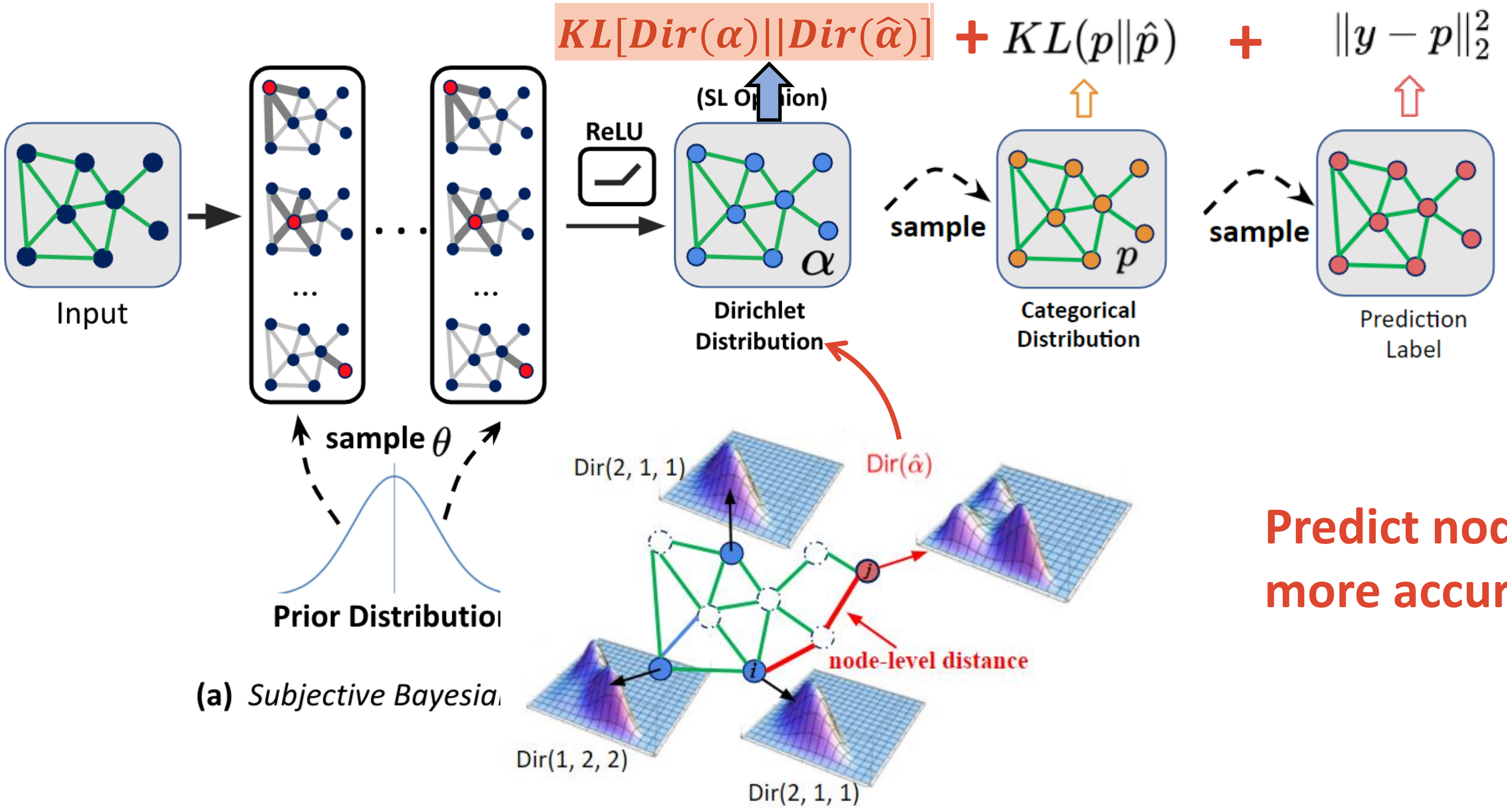


$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{i\in\mathbb{L}} \int \|\mathbf{y}_i - \mathbf{p}_i\|_2^2 \cdot P(\mathbf{p}_i|A,\mathbf{r};\boldsymbol{\theta})d\mathbf{p}_i = \sum_{i\in\mathbb{L}} \sum_{k=1}^{K} \left(y_{ik} - \mathbb{E}[p_{ik}]\right)^2 + \mathrm{Var}(p_{ik}),$$

Training Uncertainty Framework



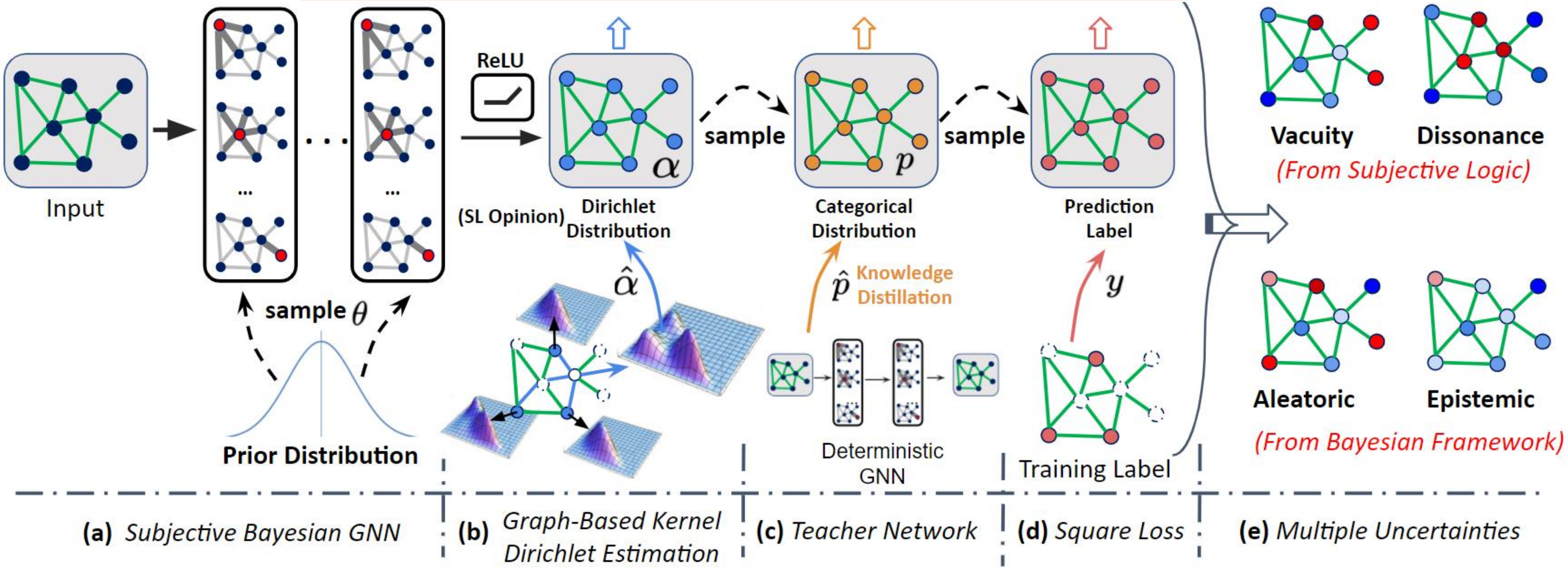
Training Uncertainty Framework



Predict node-level Dirichlet more accurately

Training Uncertainty Framework

$$Loss = KL[Dir(\alpha)||Dir(\hat{\alpha})] + KL[p||\hat{p}] + ||y-p||_2^2$$



Key Theoretical Results

- Relations between multiple uncertainties
- Impact of Graph-based Kernel Dirichlet distribution Estimation

Relationships Between Multiple Uncertainties

Consider a simplified scenario:

y: a multinomial random variable
y ~ Cal(p): follows a *K*-class categorical distribution
p ~ Dir(α): the class probabilities p follow a Dirichlet distribution

Probabilistic Uncertainty

$$\underbrace{\mathcal{I}[y, \mathbf{p}|\boldsymbol{\alpha}]}_{\text{Epistemic}} = \underbrace{\mathcal{H}\Big[\mathbb{E}_{\mathrm{Prob}(\mathbf{p}|\boldsymbol{\alpha})}[P(y|\mathbf{p})]\Big]}_{\text{Entropy}} - \underbrace{\mathbb{E}_{\mathrm{Prob}(\mathbf{p}|\boldsymbol{\alpha})}\Big[\mathcal{H}[P(y|\mathbf{p})]\Big]}_{\text{Aleatoric}}.$$

Relationships Between Multiple Uncertainties

Consider a simplified scenario:

y: a multinomial random variable
y ~ Cal(p): follows a *K*-class categorical distribution
p ~ Dir(α): the class probabilities p follow a Dirichlet distribution

Evidential Uncertainty

$$\mathrm{Dir}(\alpha) \Longleftrightarrow \omega = (\boldsymbol{b}, u, \boldsymbol{a})$$

$$vac(\omega) = K / \sum_{k=1}^{K} \alpha_k$$

Vacuity (lack of evidence)

$$diss(\omega) = \sum_{k=1}^{K} \left(\frac{b_k \sum_{j \neq k} b_j \mathrm{Bal}(b_j, b_k)}{\sum_{j \neq k} b_j} \right)$$

Dissonance (conflict evidence)

Relationships Between Multiple Uncertainties

General relations on all prediction scenarios.

vacuity + dissonance ≤ 1

- High vacuity → Low dissonance
- High dissonance → Low vacuity

Would not increase at same time!

Evidence	$e = [1,2]$	$e = [2,2]$	$e = [2,200]$	$e = [200,200]$
	lack of evidence	**lack of evidence**	confidence	**conflicting evidence**
Vacuity	**High**	**High**	Low	Low
dissonance	Low	Low	Low	**High**

Relationships Between Multiple Uncertainties

General relations on all prediction scenarios.

vacuity > epistemic

- vacuity is an upper bound of epistemic uncertainty
- On a sufficiently large amount of evidence available, vacuity and epistemic would close to zero.

Relationships Between Multiple Uncertainties

Special relations on the OOD

1 = vacuity = entropy > aleatoric > epistemic > dissonance = 0

Special relations on the Conflicting Prediction

entropy = 1, dissonance → 1, aleatoric → 1, vacuity → 0, epistemic → 0

entropy > aleatoric > dissonance > vacuity > epistemic

- entropy cannot distinguish different types of uncertainty due to different root causes.

Relationships Between Multiple Uncertainties

Special relations on the OOD

1 = vacuity = entropy > aleatoric > epistemic > dissonance = 0

Special relations on the Conflicting Prediction

entropy = 1, dissonance → 1, aleatoric → 1, vacuity → 0, epistemic → 0

entropy > aleatoric > dissonance > vacuity > epistemic

- a high aleatoric uncertainty value and a low epistemic uncertainty value are observed under both cases.

Relationships Between Multiple Uncertainties

Special relations on the OOD

1 = vacuity = entropy > aleatoric > epistemic > dissonance = 0

Special relations on the Conflicting Prediction

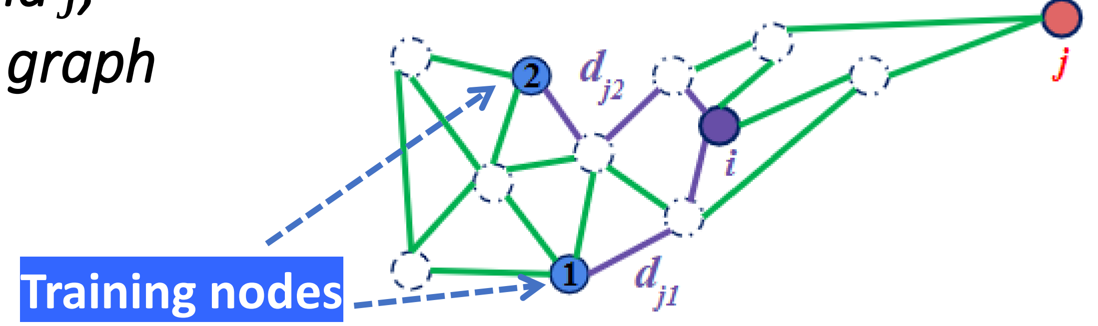
entropy = 1, dissonance → 1, aleatoric → 1, vacuity → 0, epistemic → 0

entropy > aleatoric > dissonance > vacuity > epistemic

- **vacuity and dissonance can clearly distinguish OOD from a conflicting prediction.**

Impact of Graph-based Kernel Dirichlet distribution Estimation

Given L training nodes and two testing nodes i and j,
Let $\boldsymbol{d}_i = [d_{i1}, \dots, d_{iL}]$, $\boldsymbol{d}_i = \left[d_{j1}, \dots, d_{jL}\right]$ *be the graph distance from training nodes.*

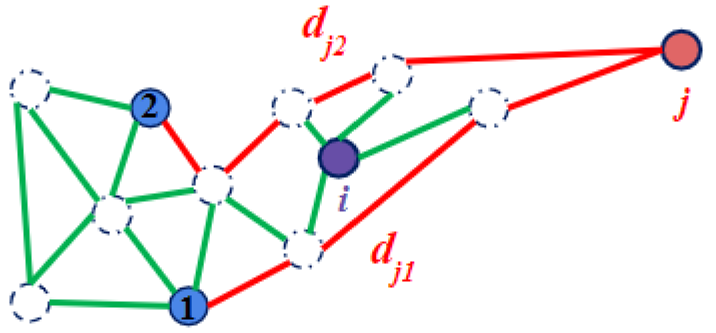


If for all $l \in \{1, \dots, L\}, d_{il} \le d_{jl}$*, we have*

$$d_{i1} < d_{j1}$$
$$d_{i2} < d_{j2}$$

$$\widehat{\boldsymbol{vacuity}}_i \le \widehat{\boldsymbol{vacuity}}_j$$

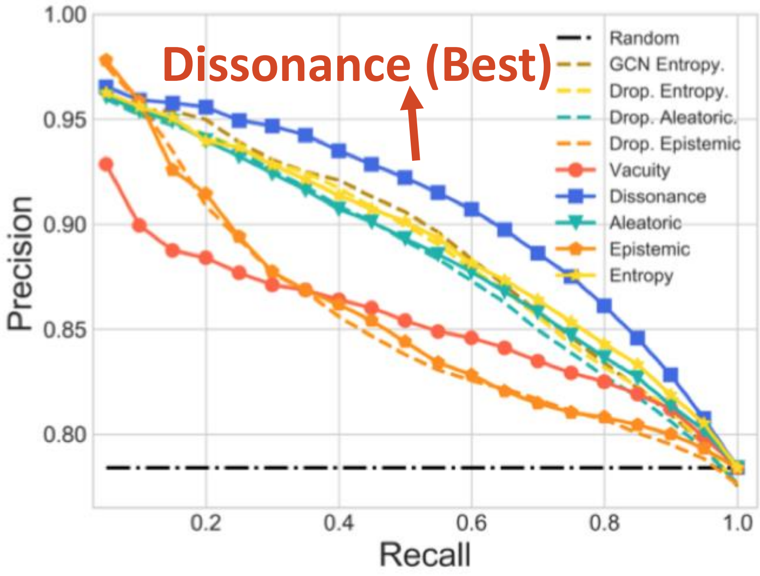
estimated based on GKDE.



High vacuity occurs when testing node is far away from training nodes.

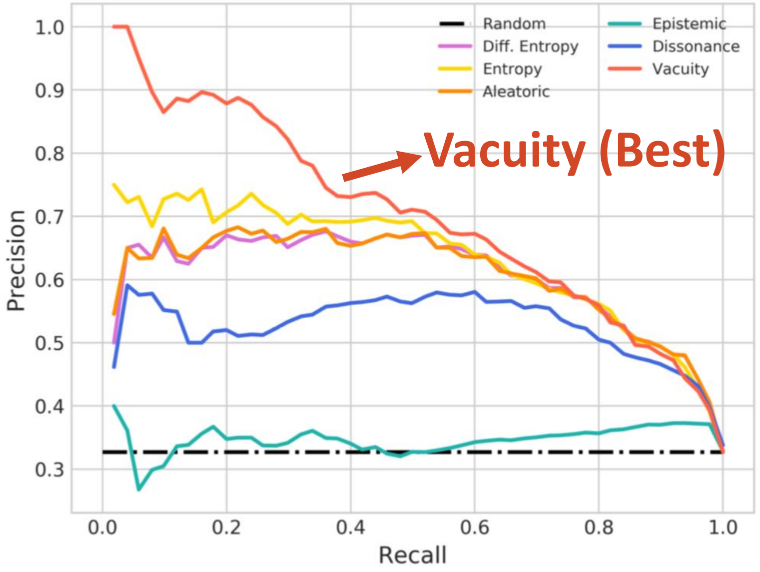
Key Experiment Result

Misclassification Detection



(c) PR curves on Pubmed

OOD Detection



(b) PR curves on Amazon Computers

Misclassification ← High Uncertainty → Out-of-distribution

Correct Prediction ← Low Uncertainty → In distribution

Why is Epistemic Uncertainty Less Effective than Vacuity?

Epistemic uncertainty works well in CV applications (supervised learning for OOD detection).

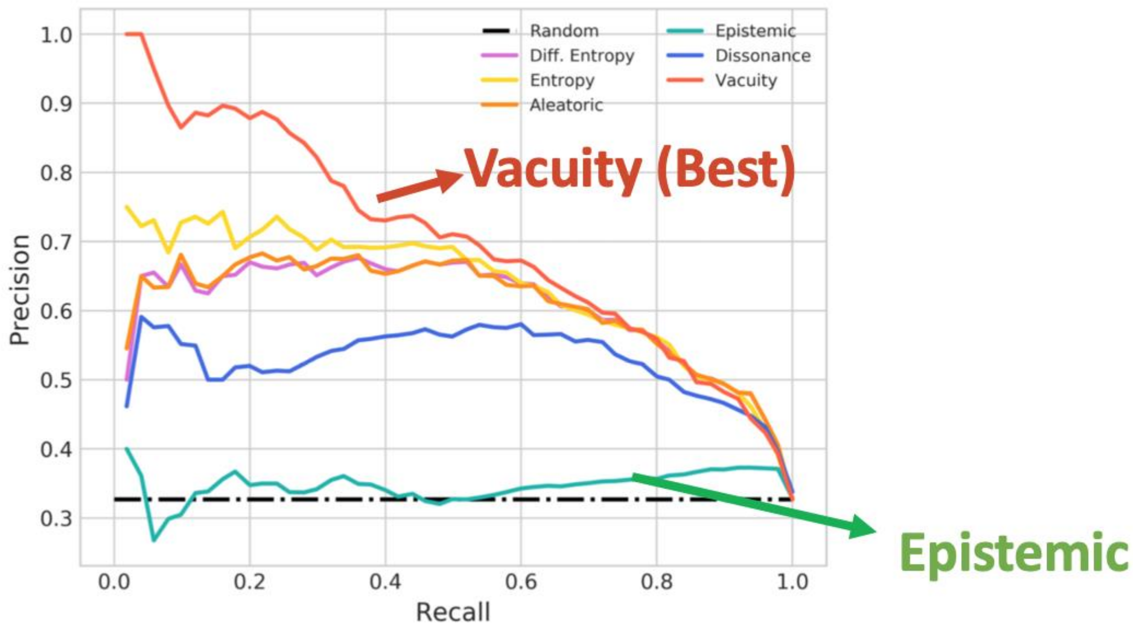
How epistemic uncertainty performances in SSL? **Not good.**

Semi-supervised ... ntains OOD)

	Epistemic	Pseudo Label
(MNIST)	**In-Distribut**	**0.041**
(FashionMNIST)	**Out-of-Dist**	0.020

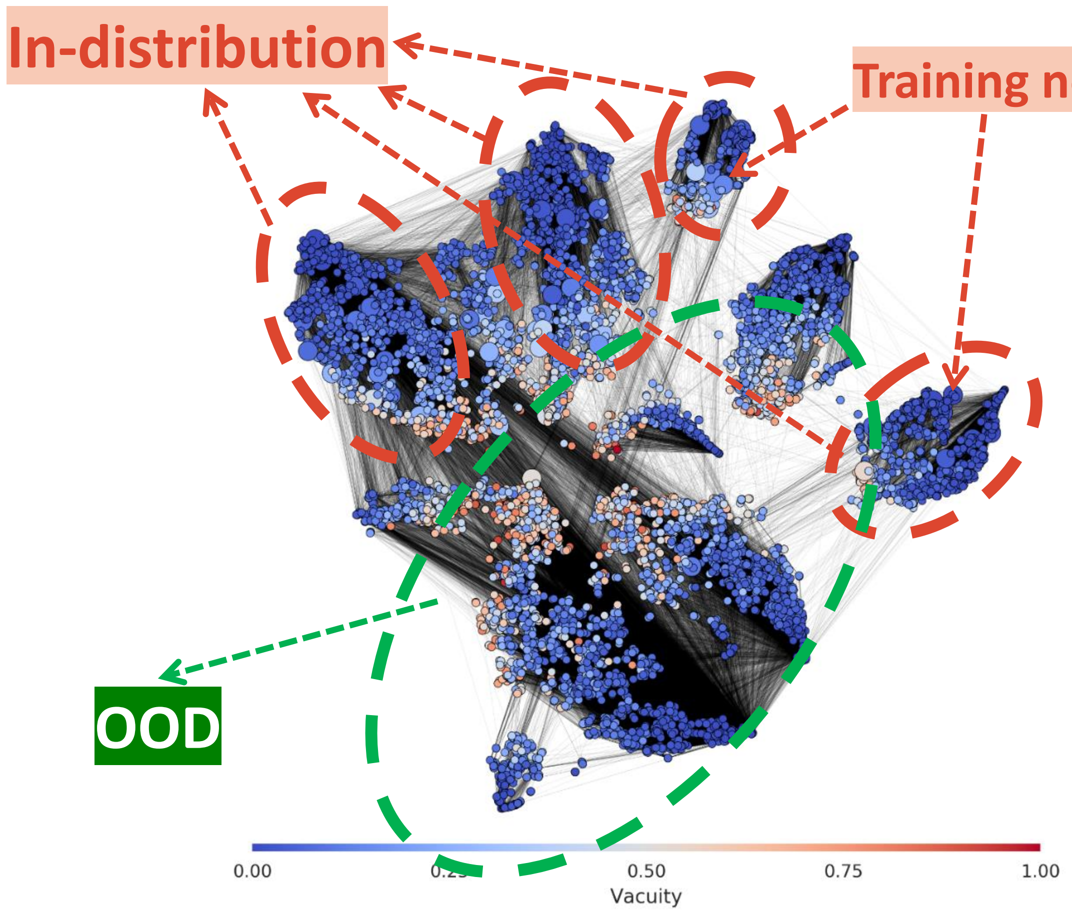
In semi-supervised le ... es are also fed to a model for training pr ... lence on its output.

OOD Detection



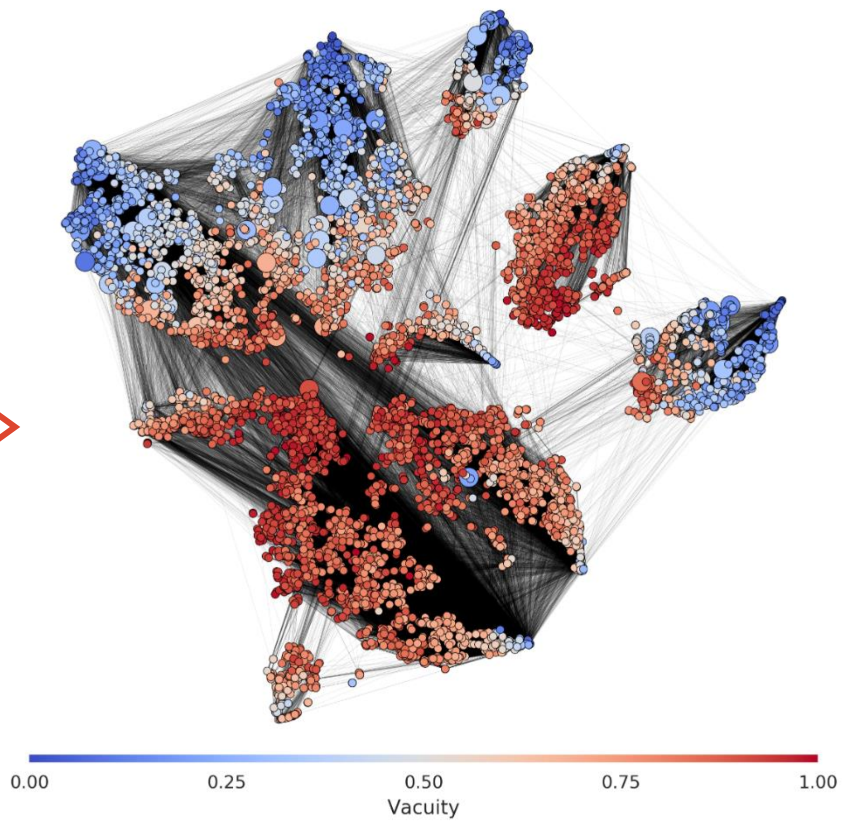
(b) PR curves on Amazon Computers

Key Merits of GKDE



OOD Detection
AUROC: 64%

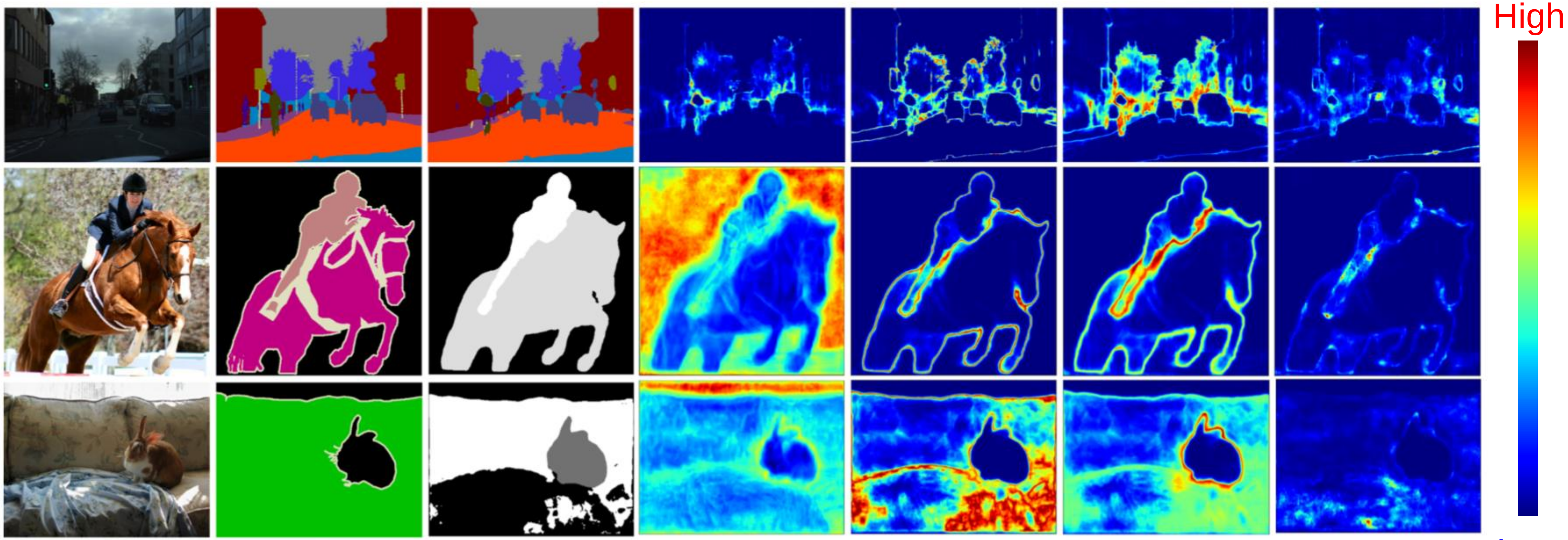
add GKDE



OOD Detection
AUROC: 93%

Extension to other Deep Learning Model (CNN)

Provide pixel-level predictive uncertainties by replacing GNN with CNN



(a) Input Image (b) Ground Truth (c) Semantic Segmentation (d) Vacuity Uncertainty (e) Dissonance Uncertainty (f) Aleatoric Uncertainty (g) Epistemic Uncertainty

Summary

- Proposed a multi-source uncertainty framework of GNNs.
- Provided a theoretical analysis about the relationships between different types of uncertainties.
- Demonstrate the use of vacuity for OOD detection and dissonance for misclassification detection.

Thank you!

Any Question & Comments?

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