

Uncertainty Quantification on Graph Learning

**Chao CHEN, Chenghua GUO, Rui XU,
Cheng YANG, Xiangwen LIAO, Xi ZHANG,
Sihong XIE, Hui XIONG, Philip S. YU**

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Source of Uncertainty

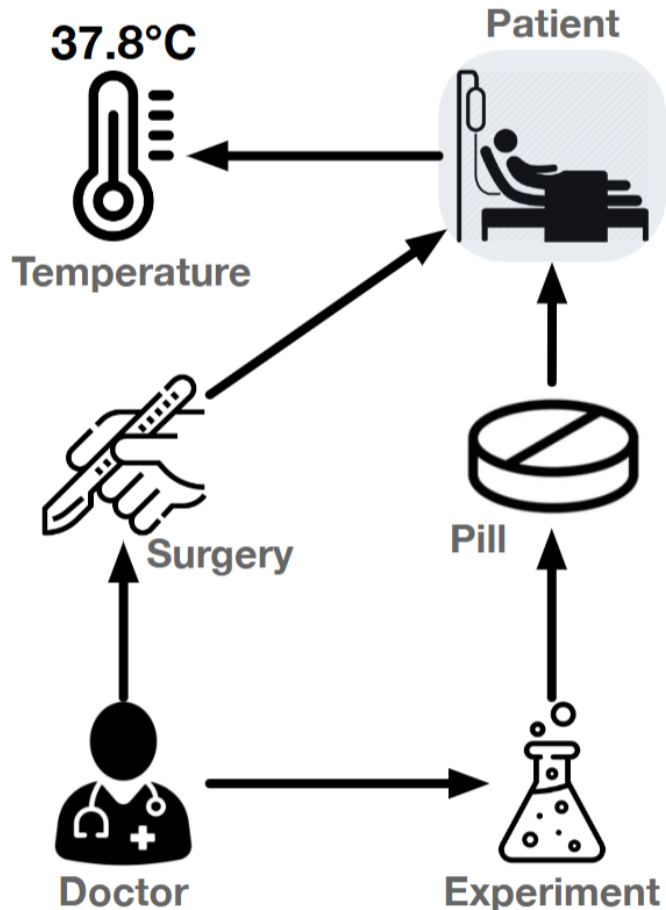


Figure 1: An example of graph-based prediction in a medical system, where the patient of interest (in gray) is connected to different treatment options.

- **Aleatoric uncertainty (AU)** captures the inherent randomness present in data, arising from noise in features or labels, and cannot be reduced by collecting additional data.

For example, body temperature measurements may vary due to unavoidable sensor noise.

- **Epistemic uncertainty (EU)** reflects a lack of knowledge caused by limited data coverage or model imperfections. In principle, it can be reduced by acquiring more information or improving the model.

For instance, access to a patient's medical records and history can enable more targeted treatment decisions.

Uncertainty Quantification

(a) OOD detection

$$P(\text{pill} \mid 37.8^\circ\text{C}) = 92\%$$

$$P(\text{pill} \mid 37.9^\circ\text{C}) = ?$$

Predicted probability

| | |
|------------------------|-----|
| Without OOD techniques | 20% |
| With OOD techniques | 90% |



Out-of-distribution (OOD) detection identify when a test graph or node deviates from the training distribution, effectively flagging high uncertainty.

(b) Conformalization

Desired coverage

$$P(\text{which pills}) \geq 90\%$$

Actual coverage

| | | |
|--------------------------|-----|---|
| Without Conformalization | 40% |  |
| With Conformalization | 95% |  |

Conformal prediction provides a distribution-free framework that constructs valid uncertainty sets with statistical guarantee of containing the ground truth.

(c) Calibration

Empirical accuracy

$$P(\text{lock}) = 25\%$$

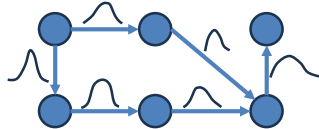
confidence ?

Predictive confidence

| | |
|---------------------|-----|
| Without Calibration | 10% |
| With Calibration | 25% |

Calibration techniques adjust a model's confidence scores to better align with empirical accuracy.

(d) Bayesian method



Distributional parameters to reflect randomness.

Predictive distribution

| | |
|------------------|--------------------------------|
| Without Bayesian | 10% |
| With Bayesian | $\mu = 25\%$ $\sigma = 5\%$ |

Bayesian probabilistic methods place probability distributions over model parameters or outputs and use Bayesian theorem to update beliefs.

Figure 2: Taxonomy of the methods to represent and handle uncertainty in graph models