Uncertainty Quantification on Graph Learning

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

Frontiers of Computer Science, DOI: 10.1007/s11704-026-51464-7

Source of Uncertainty

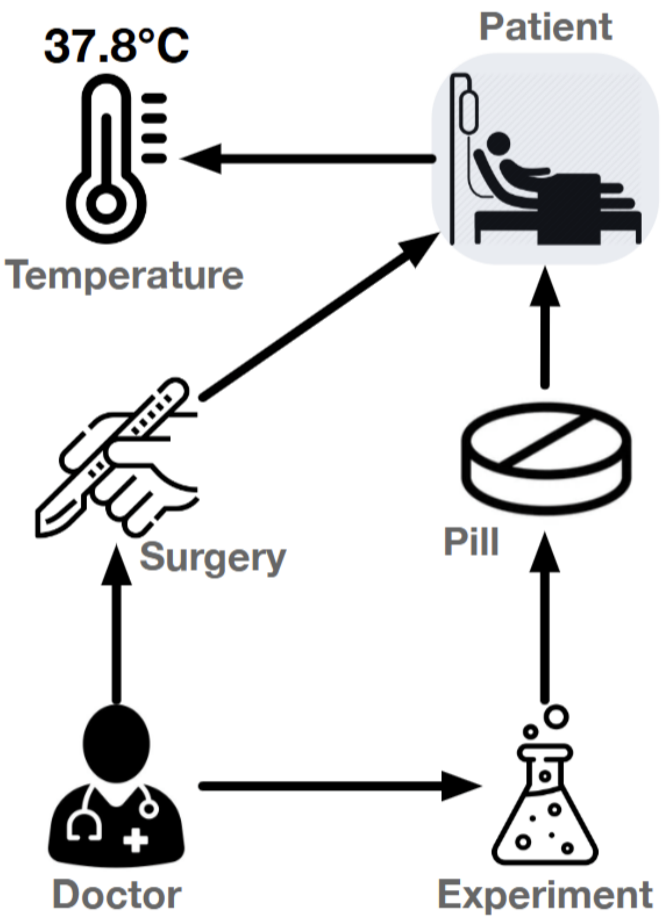


Figure 1: An example of graph-based prediction in a medical system, wherethe patient of interest (in gray) is connected to different treatment options.

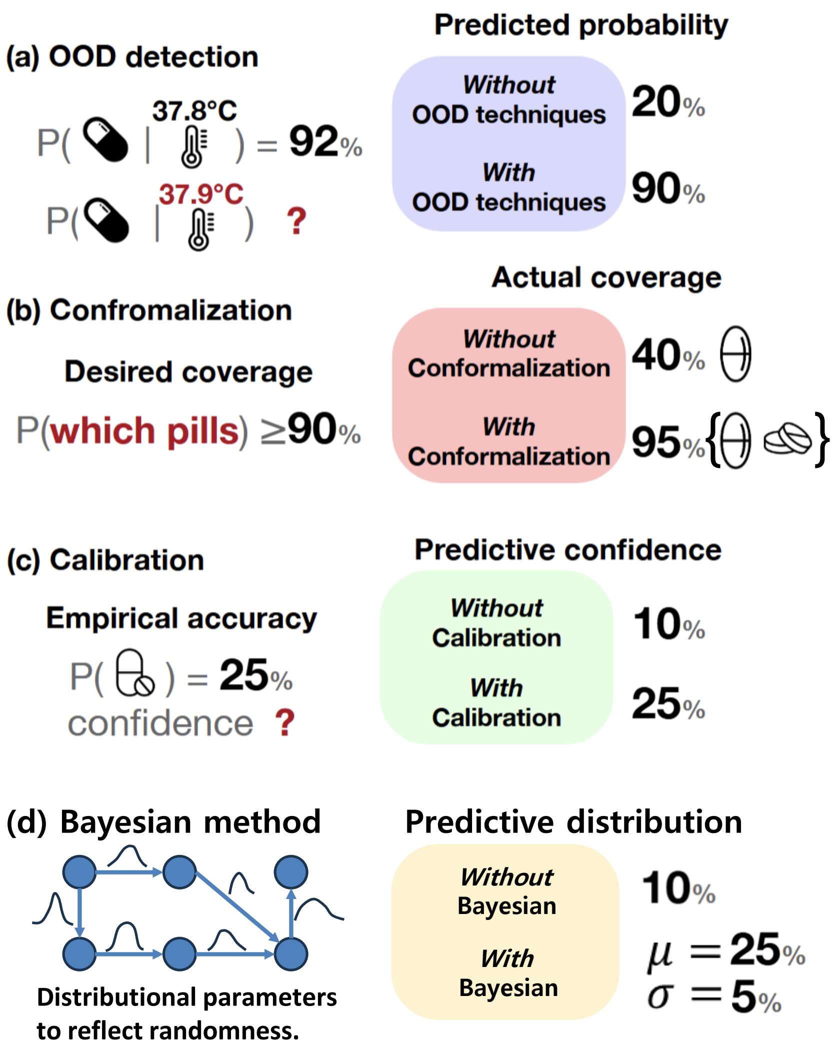
- **Aleatoric uncertainty (AU)** captures the inherent randomness present in data, arising from noise in features or labels, and cannot be reduced by collecting additional data.

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



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

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

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

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