

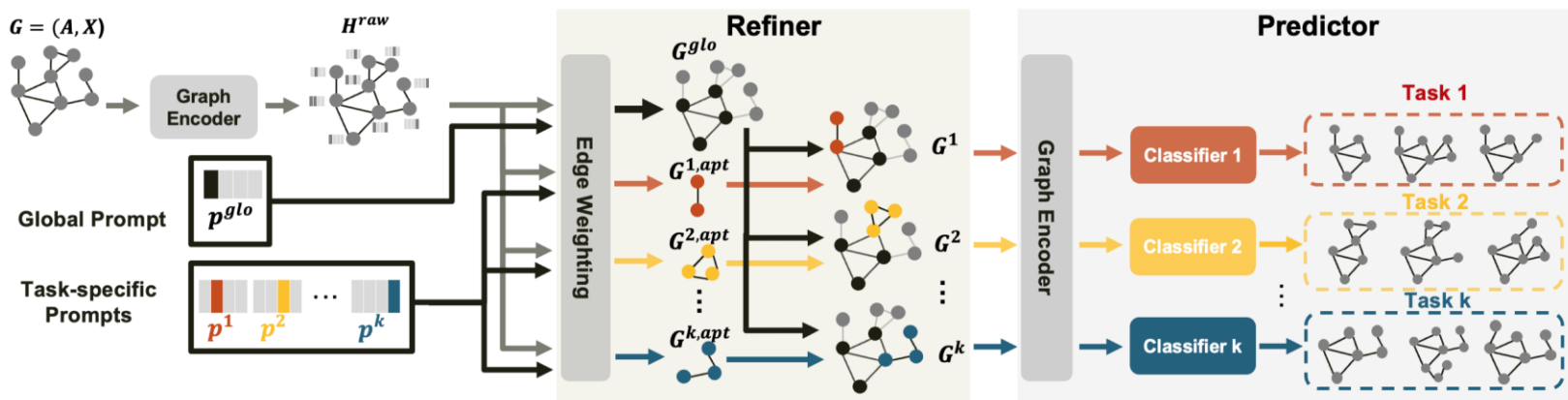
# Joint Task and Distribution Generalization via Graph Substructure Prompting

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# Problems & Ideas

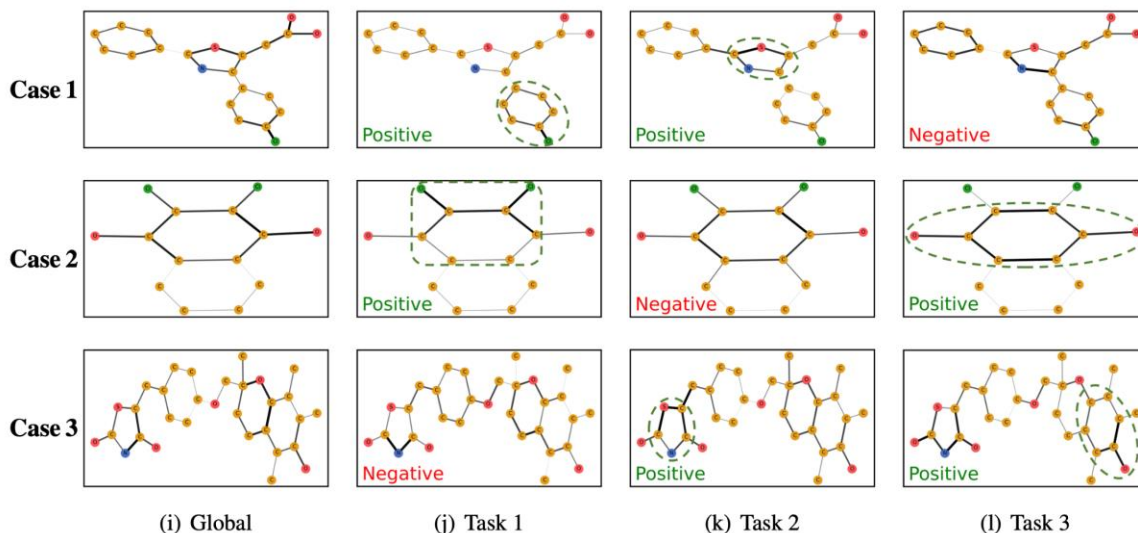
- The joint generalization challenge is common in graph-related tasks, such as molecular property graph prediction:
  - A single molecular sample often corresponds to different prediction tasks, which introduces **task generalization** challenges.
  - Test samples frequently exhibit significant distributional differences from training samples, which raises **distribution generalization** challenges.
- Ideas: We propose **Refiner** to assist GNNs in extracting task-specific critical subgraph information, thereby achieving joint task and distribution generalization. Additionally, we employ **subgraph prompting** to enable task adaptation.



Here the refiner highlights the key substructure for each task, and the predictor will classify based on the modified graph. To enable fast adaptation to new tasks, we introduce prompt vectors to control the behavior of the refiner: a global prompt shared across all tasks and task-specific prompts. During adaptation, we only learn a task-specific prompt vector and a classifier for each target task.

# Main Contributions

- Contributions:
  - We propose to address a novel and practical problem, i.e., joint task and distribution generalization.
  - We propose graph substructure prompting (GSP), which introduces a refiner to capture subgraph and employs prompts to adapt to new tasks.
  - Experiments show that GSP significantly outperforms recent state-of-the-art (SOTA) methods on both ID and OOD data.



Visualization of the substructures extracted by the refiner with global and task-specific prompts. Each row corresponds to a molecule from Tox21 dataset. Here thicker edges indicate larger learned weights. For Task 1, the discerned task-specific pattern is characterized by a hexagonal structure of carbon atoms (i.e., a benzene ring) connected with a chlorine atom (green node). For Task 2, the pivotal pattern encompasses a pentagonal structure incorporating sulfur and nitrogen atoms (pink and blue nodes). For Task 3, a typical pattern is a hexagonal benzene ring connected by an oxygen atom, known as Phenol. We outline the above key substructures by dashed circles as reference. We can observe that the edge weights learned by the refiner align with the pivotal patterns.