Reconciliation of LLM-Driven Hypothesis Generation and Smart Room Framework

This document reconciles two frameworks: one involving a reinforcement learning (RL)-based causal hypothesis generation and testing system and another focused on LLM-driven causal reasoning in a smart room environment. By combining these approaches, we construct a unified framework to optimize hypothesis exploration and testing systematically.

1 Unified Framework

1.1 Hypothesis Representation

Hypotheses are represented as:

- Causal Links:Directed relationships between variables, e.g., $X_1 \to X_2$.
- Full Causal Graphs: Complex hypotheses about the structure of relationships among multiple variables.

Hypotheses generated by the LLM form an initial space, $\mathcal{H}$, which is iteratively refined during exploration. This allows for both fine-grained (link-level) and holistic (graph-level) evaluations, enabling systematic testing and refinement.

1.2 Utility Function

The utility of testing a hypothesis H_i is defined as:

$$U(H_i) = \alpha \cdot \mathrm{IG}(H_i) - \beta \cdot \mathrm{Cost}(H_i) - \gamma \cdot \mathrm{Risk}(H_i), \tag{1}$$

where:

- $\mathrm{IG}(H_i)$: Information gain from testing H_i, quantifying the reduction in uncertainty in the causal graph.
- $\mathrm{Cost}(H_i)$: Resource expenditure required to test H_i, capturing computational, experimental, or ethical constraints.
- $\mathrm{Risk}(H_i)$: Penalty for testing overly complex or redundant hypotheses, ensuring efficient use of resources.
- $\alpha, \beta, \gamma > 0$: Trade-off parameters to balance these terms.

To justify this utility function:

- This utility function integrates exploration objectives (e.g., maximizing $\mathrm{IG}(H_i)$ while minimizing $\mathrm{Cost}(H_i)$) with practical considerations (e.g., minimizing $\mathrm{Risk}(H_i)$), reflecting the trade-offs inherent in real-world decision-making [Multi-Objective Optimization].
- $\mathrm{IG}(H_i)$ reduces uncertainty in the causal graph, aligning with the theoretical goals of hypothesis testing. [Information Gain]
- $\mathrm{Cost}(H_i)$ accounts for practical constraints, ensuring experiments remain feasible. [Cost]
- $\mathrm{Risk}(H_i)$ penalizes unnecessary complexity, balancing the trade-off between model complexity and interoperability. [Risk]
- When extended to settings like smart rooms, additional components such as user satisfaction ($S(\mathbf{X})$) and energy consumption ($E(\mathbf{X})$) can be incorporated (Application-Specific Objectives:):

$$U(H_i) = \alpha \cdot \mathrm{IG}(H_i) - \beta \cdot \mathrm{Cost}(H_i) + \gamma \cdot S(\mathbf{X}) - \delta \cdot E(\mathbf{X}) - \epsilon \cdot \mathrm{Risk}(H_i), \tag{2}$$

  where the additional terms balance theoretical and practical goals.
- Decision-theoretic frameworks often balance exploration (gaining knowledge) with exploitation (achieving measurable outcomes). This combined utility function reflects this principle by integrating both causal exploration and practical outcomes. [Alignment with Decision Theory]

1.3 Hypothesis Selection

To optimize hypothesis selection, RL-based strategies such as Thompson Sampling or Upper Confidence Bound (UCB) are applied:

$$H^* = \arg\max_{H_i \in \mathcal{H}} \mathbb{E}[U(H_i)], \tag{3}$$

where $\mathbb{E}[U(H_i)]$ represents the expected utility of hypothesis H_i based on current knowledge. This prioritization mechanism ensures that hypotheses with high potential utility are tested early, balancing exploration and exploitation.

1.4 Workflow

The unified workflow involves the following steps:

1. **Hypothesis Generation:** Use the LLM to propose initial hypotheses based on structured prompts about causal relationships.
2. **Hypothesis Prioritization:** Apply RL-based strategies to select high-utility hypotheses for testing.
3. **Experiment Design and Execution:** Perform interventions (e.g., $\mathrm{do}(X_1)$) to test selected hypotheses and observe outcomes.

4. **Feedback and Refinement:** Update priors and refine the causal graph G_t using Bayesian reasoning and causal inference libraries.

5. **Iteration:** Repeat until stopping criteria are met, such as low graph entropy or resource exhaustion.

1.5 Differences and Reconciliation

Aspect	**Earlier Discussion**	**Uploaded Document**
Hypothesis Representation	Individual causal links and full causal graphs	Causal links generated by LLM for smart room variables
Utility Function	$U(H_i) = \mathrm{IG}(H_i) - \lambda \cdot \mathrm{Cost}(H_i)$	Combines user satisfaction, energy consumption, and risk: $U(\mathbf{I}) = \alpha S - \beta E - \gamma \cdot \mathrm{Risk}$
Hypothesis Selection	Thompson Sampling or UCB prioritization	Iterative testing without explicit selection strategy
Experimental Setup	Synthetic data with known ground truth for validation	Real-world smart room environment with predefined variables
Metrics	Precision, recall, cumulative regret, reconstruction accuracy	Relevance, novelty, precision, utility

Table 1: Comparison of Key Aspects and Reconciliation

2 Experimental Setup

2.1 Data

- Simulate variables $X_1, \ldots, X_m$ using a known structural causal model (SCM) to validate the framework with ground truth.

- Transition to the smart room environment, where causal relationships (e.g., $T \to E$) are dynamically tested and refined.

2.2 Evaluation Metrics

To assess the framework's performance, key metrics include:

- **Relevance Score:** Alignment of tested hypotheses with ground truth G_{true}, ensuring practical impact.

- **Precision and Recall:** Accuracy of hypothesis identification relative to G_{true}.

- **Novelty Score:** Proportion of novel causal insights introduced to enhance the causal graph.

- **Cumulative Regret:** Measures inefficiency in exploration:

$$\text{Regret}(T) = \sum_{t=1}^{T} \left(U^*(H^*) - U(H_t) \right). \tag{4}$$

- **Utility:** Total utility gained from all tested hypotheses, representing the framework's overall efficiency.

3 Quantifying Uncertainty in Causal Graphs

Causal discovery algorithms provide insights into the structure of causal relationships, but they do not always directly quantify uncertainty in the causal graph. This section outlines methods to calculate uncertainty and integrate it into the utility framework.

3.1 Sources of Uncertainty

Uncertainty in the causal graph arises from the following:

- **Structural Uncertainty:** Uncertainty about the presence or absence of edges in the graph.
- **Orientation Uncertainty:** Uncertainty about the direction of causal relationships (e.g., $X_1 \to X_2$ vs. $X_2 \to X_1$).
- **Model Uncertainty:** Uncertainty due to noisy or incomplete data, which affects graph inference.

3.2 Quantifying Graph Uncertainty

The uncertainty in the causal graph G can be quantified using entropy:

$$H(G) = -\sum_{G'} P(G') \log P(G'), \tag{5}$$

where:

- G': A possible causal graph in the hypothesis space.
- $P(G')$: The posterior probability of G' being the true causal graph.

To compute $H(G)$, we require a posterior distribution over graphs, $P(G \mid \text{Data})$, which can be obtained via:

- **Bayesian Causal Discovery:** Methods like Bayesian networks estimate $P(G \mid \text{Data})$ directly.
- **Bootstrapping:** Generate multiple graphs by resampling the data and applying the causal discovery algorithm to each subset. Estimate $P(G)$ from the frequency of each graph.
- **Markov Chain Monte Carlo (MCMC):** Sample from $P(G \mid \text{Data})$ using techniques such as Metropolis-Hastings.

3.3 Edge-Level Uncertainty

Uncertainty in individual edges can also be computed:

$$H(E_{ij}) = -P(E_{ij}) \log P(E_{ij}) - (1 - P(E_{ij})) \log(1 - P(E_{ij})), \tag{6}$$

where $P(E_{ij})$ is the probability of an edge existing between variables X_i and X_j. This edge-level uncertainty can be aggregated to approximate total graph uncertainty.

3.4 Information Gain and Entropy Reduction

Testing a hypothesis H_i reduces the uncertainty in the causal graph, which is quantified as information gain:

$$\mathrm{IG}(H_i) = H(G) - H(G \mid \text{Data from testing } H_i), \tag{7}$$

where:

- $H(G)$: Initial entropy of the causal graph before testing H_i.
- $H(G \mid \text{Data})$: Posterior entropy of the causal graph after incorporating evidence from testing H_i.

Information gain directly measures the value of testing a hypothesis by the reduction in graph uncertainty.

3.5 Practical Implementation

1. **Estimate Posterior Distribution:** Use Bayesian causal discovery or approximate methods (e.g., bootstrapping or MCMC) to estimate $P(G \mid \text{Data})$.
2. **Calculate Graph Entropy:** Compute $H(G)$ using the posterior probabilities of candidate graphs.
3. **Edge Uncertainty (Optional):** Calculate edge-level entropies $H(E_{ij})$ to understand fine-grained uncertainties.
4. **Compute Information Gain:** Measure the entropy reduction caused by testing a hypothesis.

3.6 Integration into Utility Framework

The information gain ($\mathrm{IG}(H_i)$) becomes a key term in the utility function:

$$U(H_i) = \alpha \cdot \mathrm{IG}(H_i) - \beta \cdot \mathrm{Cost}(H_i) - \gamma \cdot \mathrm{Risk}(H_i), \tag{8}$$

where $\mathrm{IG}(H_i)$ quantifies the reduction in graph uncertainty due to hypothesis testing. This integration ensures that utility maximization reflects both theoretical exploration and practical considerations.