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Pattern Analysis & Machine Intelligence Praktikum: MLPR SS-24

Project Proposals

Project Timeline

Monday, 13th of May

- **Q&A Session**: Introduction to the project and initial assignment

24th, 27th, 31st of May

- **Informal Discussion**: Preliminary readings and initial thoughts on the project

17th, 24th of June

- **10-Minute Presentation**: Planned work and project scope

8th, 12th of July

- **Short Discussion**: Preliminary results

Summer Break (Dates TBA)

- **Presentation of Results**: Review and redefine the scope of the projects

Late September (Date TBA)

- Final Presentation, Code, and Report Submission

Project 1: Automatic and transparent inspection model

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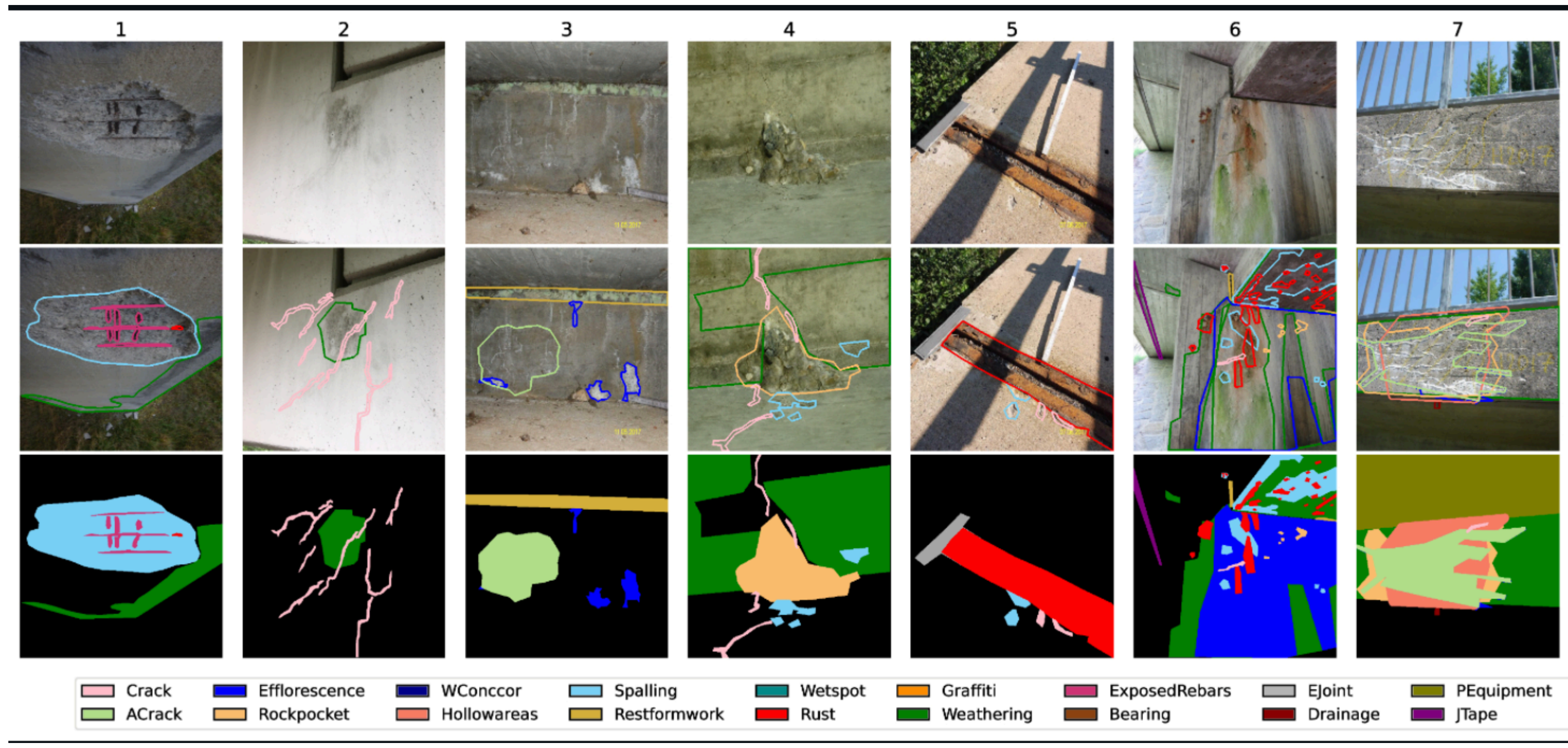
Objective: Develop an automatic and transparent inspection system using well understood Operators.

Description: This project aims to define and categorize various operators and explore different methodologies to design effective detectors for each class on the Dack10k dataset. The project will utilize Program Synthesis combined with Reinforcement Learning (RL) to identify optimal combinations of operators that address specific tasks effectively.

Approach: this project seeks to meta-learn the ideal decomposed design, including the number of parallel streams, operators, and layers for each task (i.e crack detection, rust localization etc.).



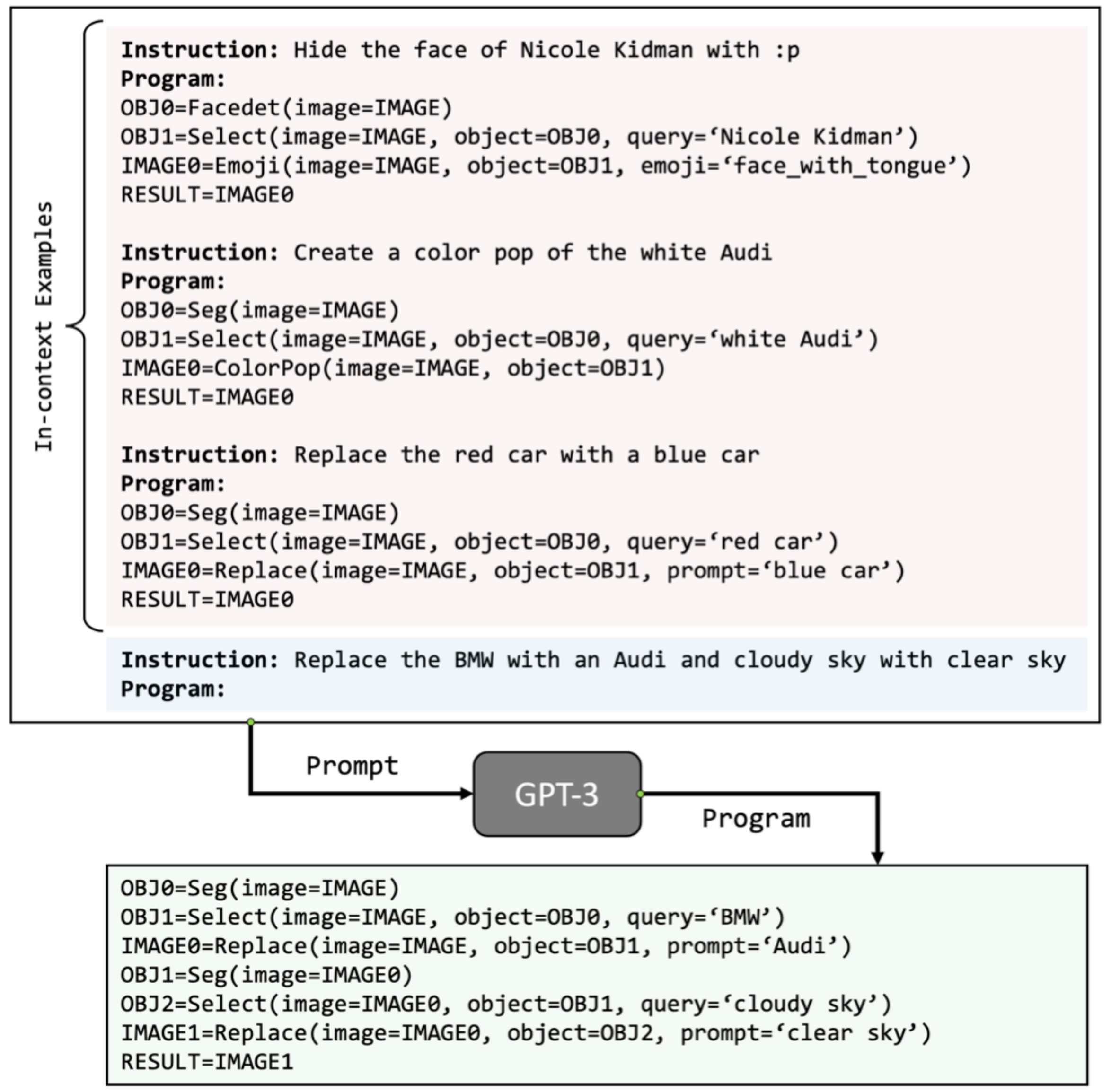


Figure 3. **Program generation in VISPROG.**

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Project 2: Multi-encoder networks with Meta-Learning and Brain Like representations

Objective: Enhance multi-encoder networks using meta-learning to mimic brain-like structures.
Description: Multi-encoder networks have traditionally had fixed architectures. This project proposes to use meta-learning to dynamically adjust and optimize the architecture of multi-encoder networks. By treating the architectural elements—such as the number of streams, the specific operators used, and the layer setup—as variables, the project will explore how a reinforcement learning agent can effectively learn and suggest the most efficient designs.
Approach: The project will experiment with different network configurations and compare the performance of these meta-learned models against traditional fixed designs, aiming to achieve closer performance to that of human brain-like processing capabilities in specific tasks.

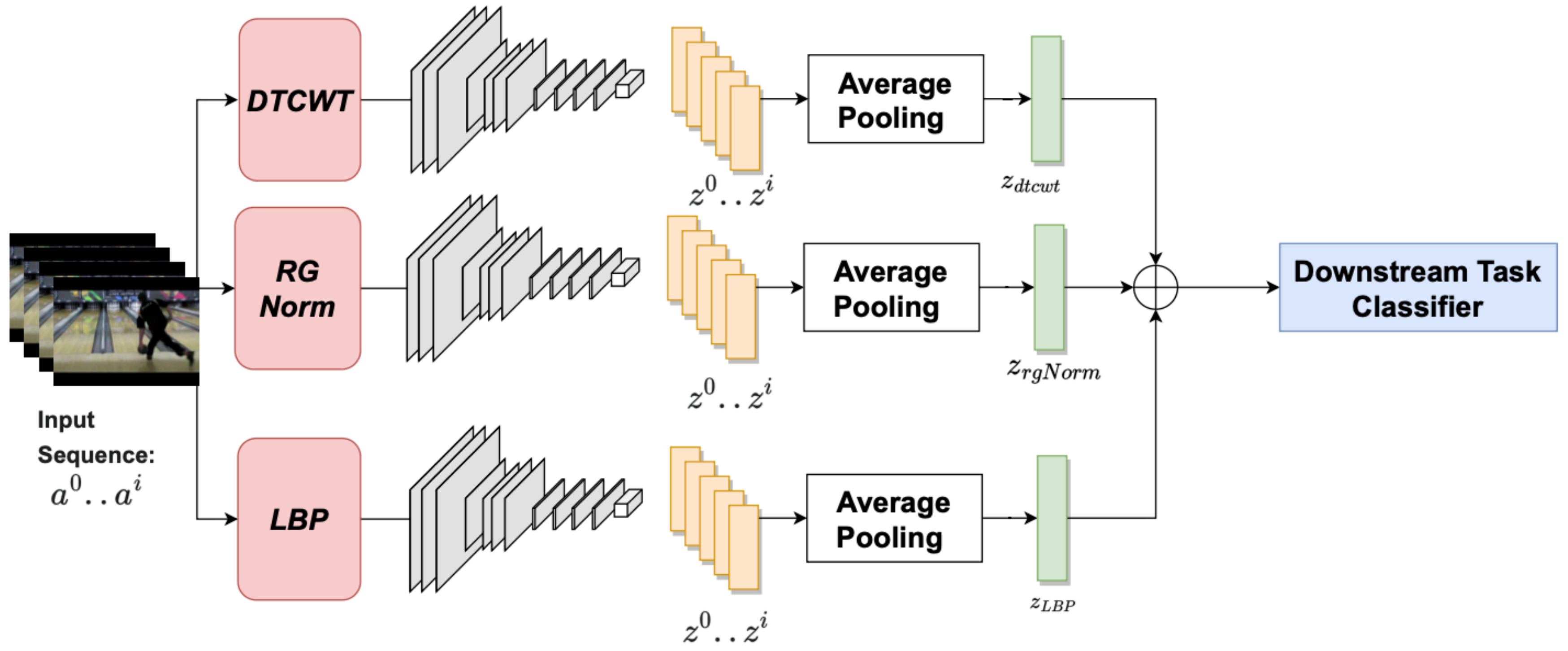


Figure 1. An illustration of the presented framework. Each encoder network is preceded by a transformation and is trained in a contrastive learning setting. Afterwards, the linear classifier is trained on a downstream classification task while the weights of the encoders are frozen.

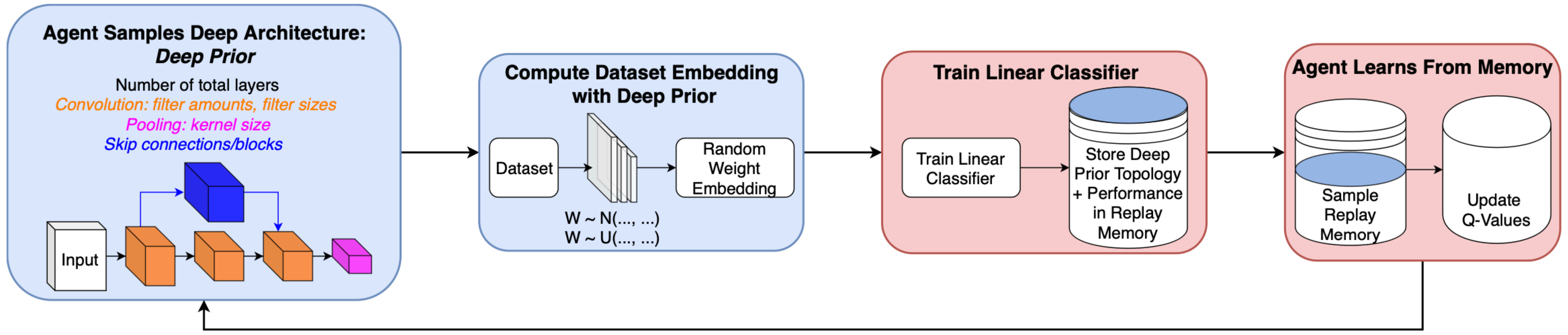


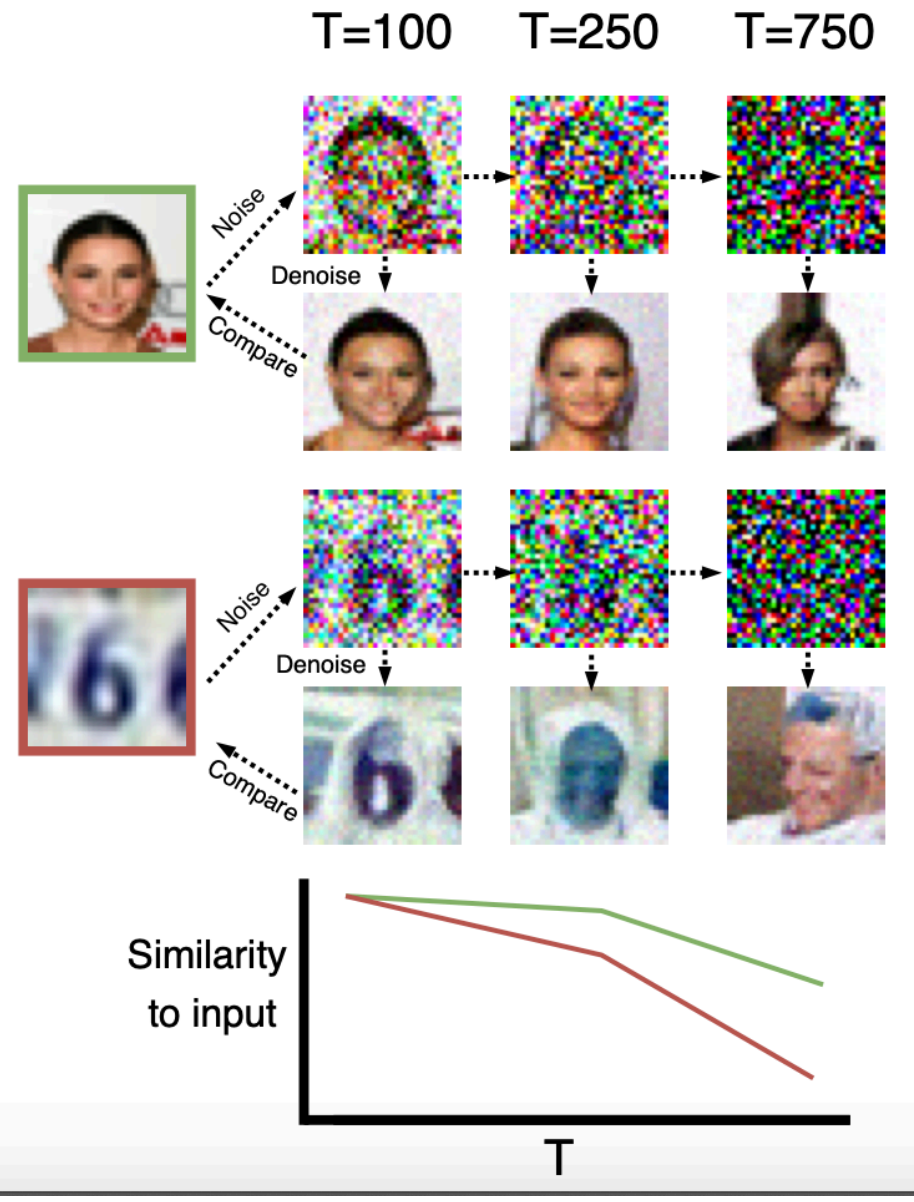
Figure 1. Illustration of the steps involved in Deep Prior Neural Architecture Search (DP-NAS). In DP-NAS, a reinforcement learning q-agent is trained to learn to assemble suitable architectures with random weights across a diverse range of options (illustrated in the first box). In contrast to conventional NAS, these architectures do not have their weights trained. Instead, a randomly projected dataset embedding is calculated (second box) and only a linear classifier is trained (third box). The essential premise is that suitable deep priors contain functional forms of selectivity with respect to low level data statistics, such that classes are easily linearly separable in the transformed space. The q-agent learns to find the latter for a given task (fourth box with outer loop). For convenience, parts of the algorithm that do not involve any parameter inference are colored in blue, with red parts illustrating the only trained components.

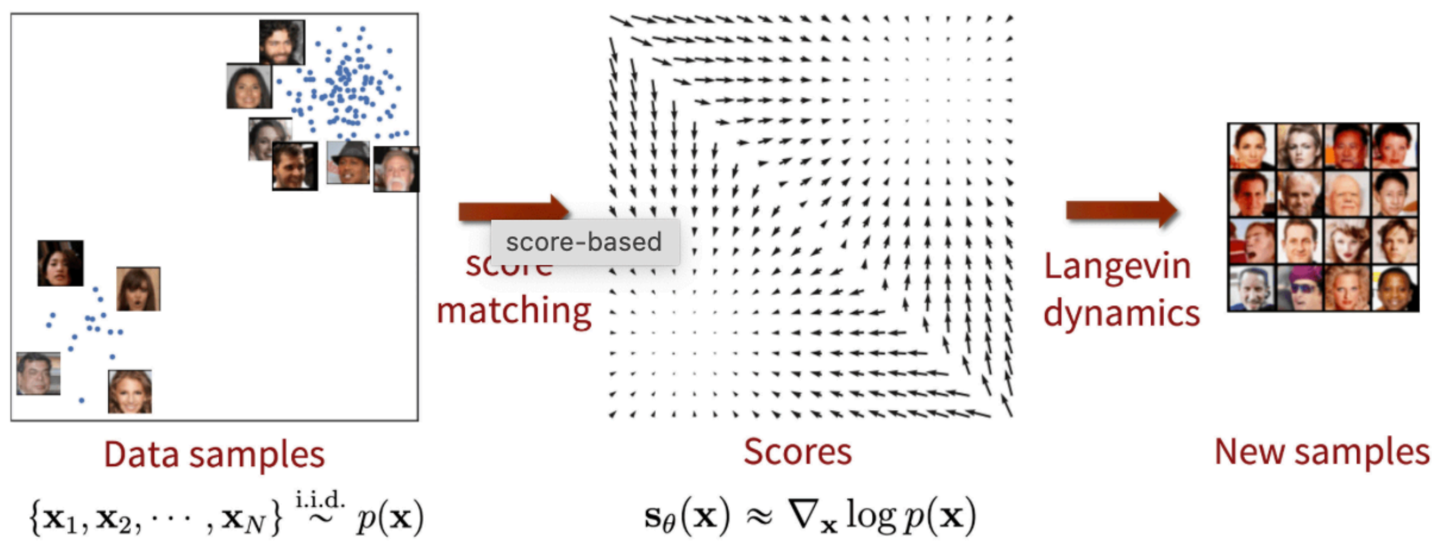
Project 3: Out of distribution detection with Diffusion Models

Objective: Improve out-of-distribution (OOD) detection in machine learning systems using diffusion models.

Description: Diffusion models are advanced generative models that have shown superior performance in high-resolution image reconstruction, outperforming GAN-based approaches. This project will focus on using these models for OOD detection, crucial for the safe deployment of AI systems. The project will explore both reconstruction-based and generative-based methods for OOD detection, leveraging the unique properties of diffusion models.

Approach: By investigating different datasets and types of OOD data (e.g., new classes, perturbed examples), the project will assess whether OOD detection quality correlates with the reconstruction or design quality of the models. This includes a detailed analysis of how the amount of noise and the size of the latent dimensions in diffusion models affect their performance in detecting OOD samples.





Score-based generative modeling with score matching + Langevin dynamics. Source: *Generative Modeling by Estimating Gradients of the Data Distribution*

Project 4: Self-supervision for Graph Neural Networks

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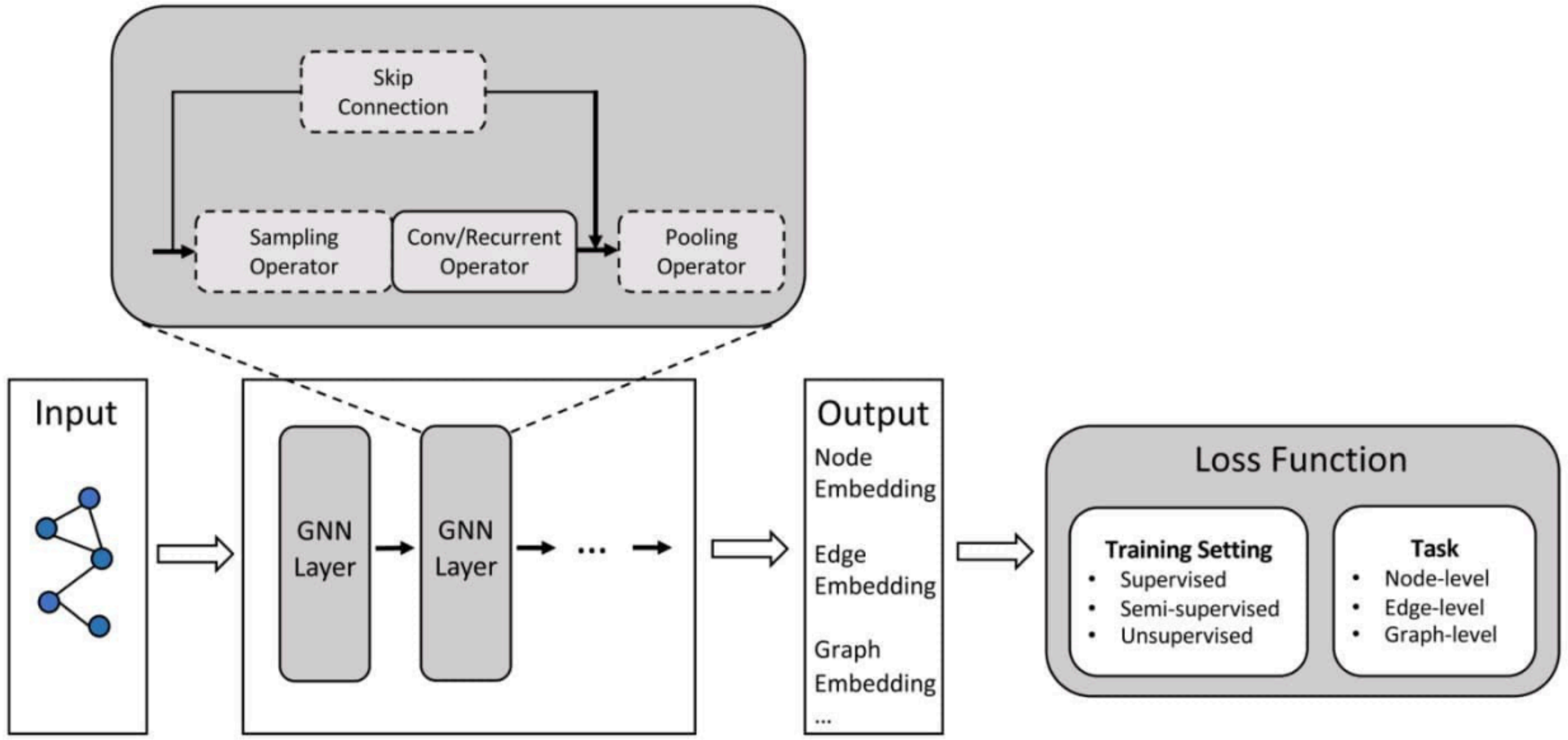
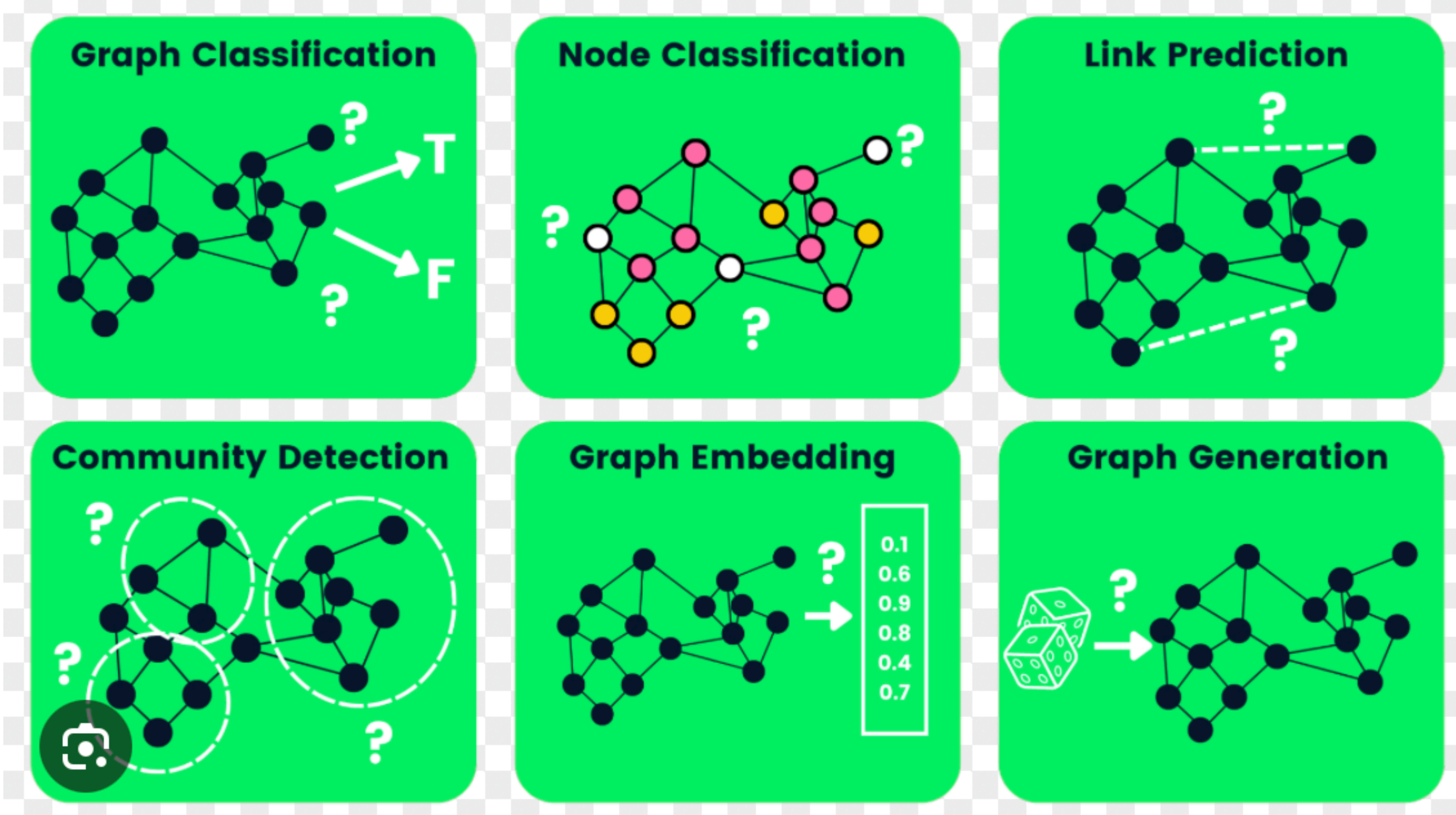
Objective: Enhance graph neural networks (GNNs) for predicting material properties in chemistry using self-supervised learning (SSL).

Description: GNNs are powerful tools for dealing with graph-structured data but often struggle with generalization, transferability, and robustness. This project aims to replicate existing results and extend the application of SSL methods to improve the learning capabilities of GNNs, particularly for chemistry-related problems where the stoichiometric formula can be treated as a dense weighted graph.

Approach: The project will explore SSL techniques tailored for graphs, evaluating their effectiveness in systematic learning and improvement of descriptors derived directly from data, thereby enhancing the predictive accuracy and applicability of GNNs in real-world chemical analysis.





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Project 5: Anomaly Detection with Diffusion Models for TS and Tabular Data

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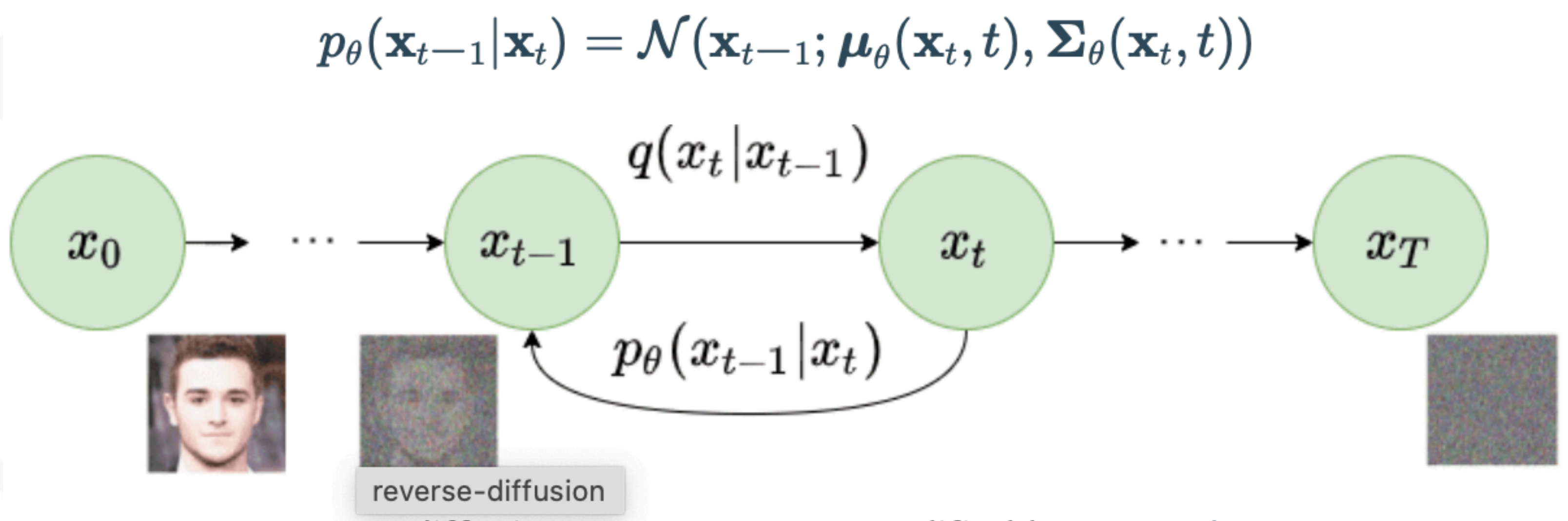
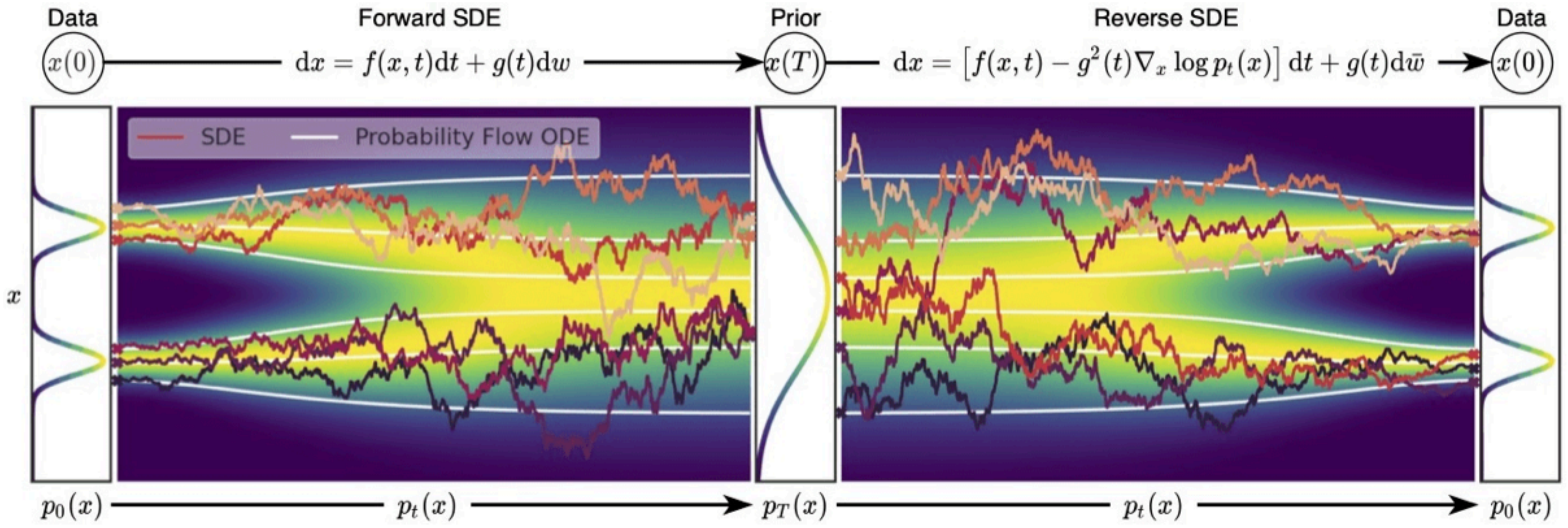
Objective: Apply diffusion models to anomaly detection in time series and tabular data.
Description: This project explores the application of diffusion models, typically used for image data, to time series and tabular data for detecting anomalies. By focusing on both reconstruction errors and layer-wise dynamics, the project aims to leverage advanced machine learning techniques, such as those used in Mahalanobis-Based Scores, to improve anomaly detection performance.
Approach: The research will involve adapting diffusion model architectures to handle the unique characteristics of time series and tabular data. It will also compare these methods with traditional anomaly detection techniques to evaluate improvements in detection accuracy and computational efficiency. The project will include extensive testing on various datasets to validate the models' effectiveness in real-world scenarios.



Reverse diffusion process. Image modified by Ho et al. 2020



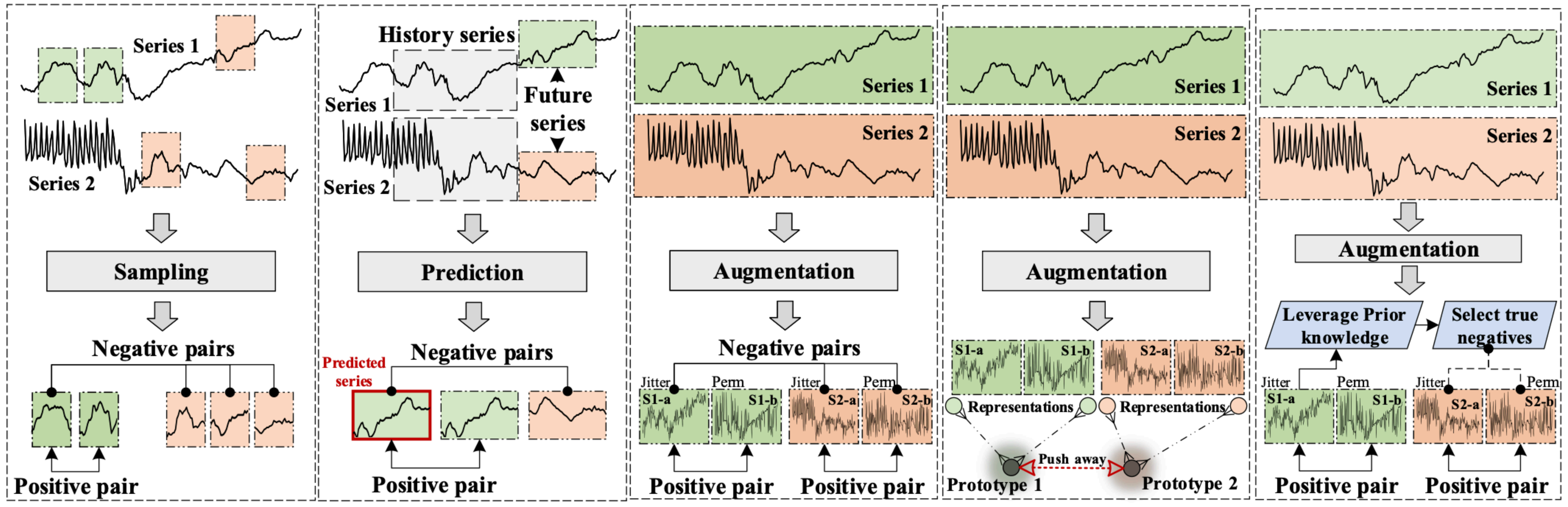
Overview of score-based generative modeling through SDEs. Source: Song et al. 2021

Project 6: Self-supervised Learning for Time Series

Objective: Enhance time series forecasting and anomaly detection using self-supervised learning methods.

Description: This project aims to explore and develop self-supervised learning (SSL) models specifically designed for time series data The focus will be on using soft contrastive learning approaches to improve the quality of forecasting and anomaly detection without relying on extensive labeled data.

Approach: The project will test various SSL methods to determine their impact on the accuracy and reliability of time series forecasting models , such as TimesNet and NLinear models and anomaly detection. It will also assess the capability of these models to generalize across different types of time series data and conditions, aiming to improve model robustness and applicability in practical settings.

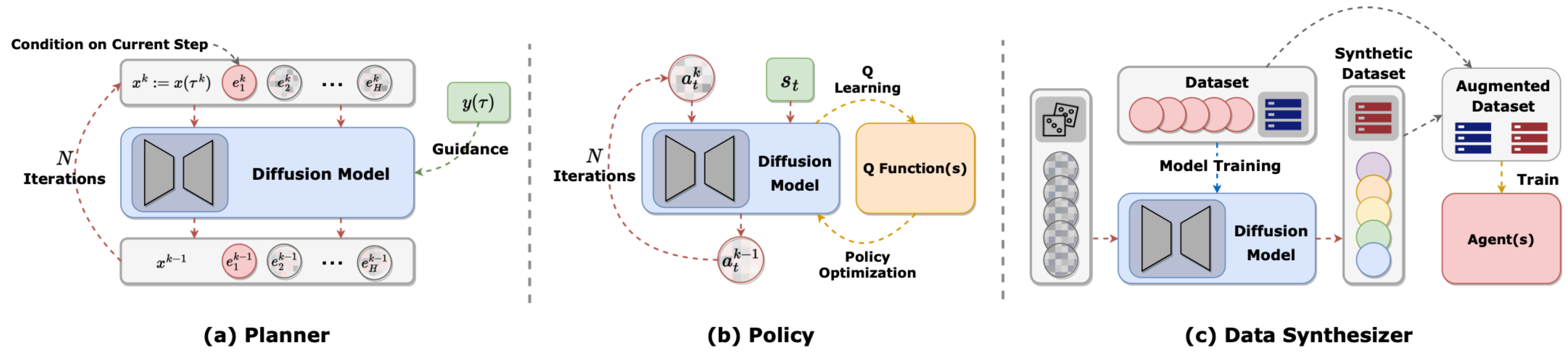


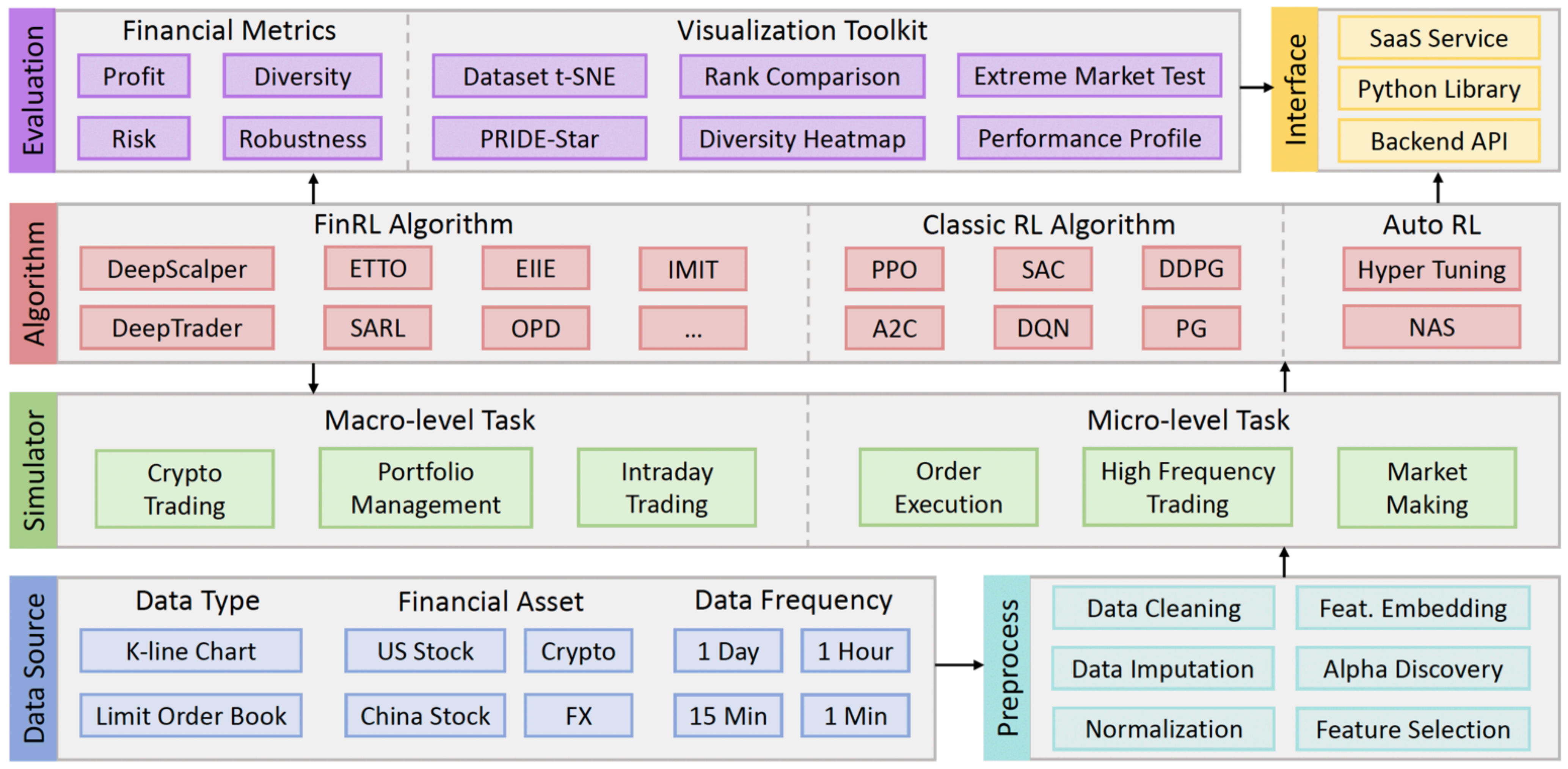
(a) Sampling contrast (b) Prediction contrast (c) Augmentation contrast (d) Prototype contrast (e) Expert knowledge contrast

Fig. 3: Five categories of contrastive-based SSL for time series data.

Project 7: Generative NeuralSDE Models for RL

Objective: Optimize options trading strategies using reinforcement learning (RL).
Description: This project explores the application of modern RL algorithms on TradeMaster—a holistic quantitative trading platform designed for RL experiments. The project will investigate various enhancements like curriculum learning, generative models and adjustments for non-stationarity in financial markets.
Approach: The project will involve developing and testing different RL algorithms to identify the most effective strategies for options trading. It will consider various market conditions and trading scenarios to refine these strategies, aiming to increase profitability and minimize risk. The research will also compare the developed methods against traditional trading algorithms to benchmark performance improvements.





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Project 8: Disentanglement and Path Dynamics of Normalising Flows and Diffusion Models

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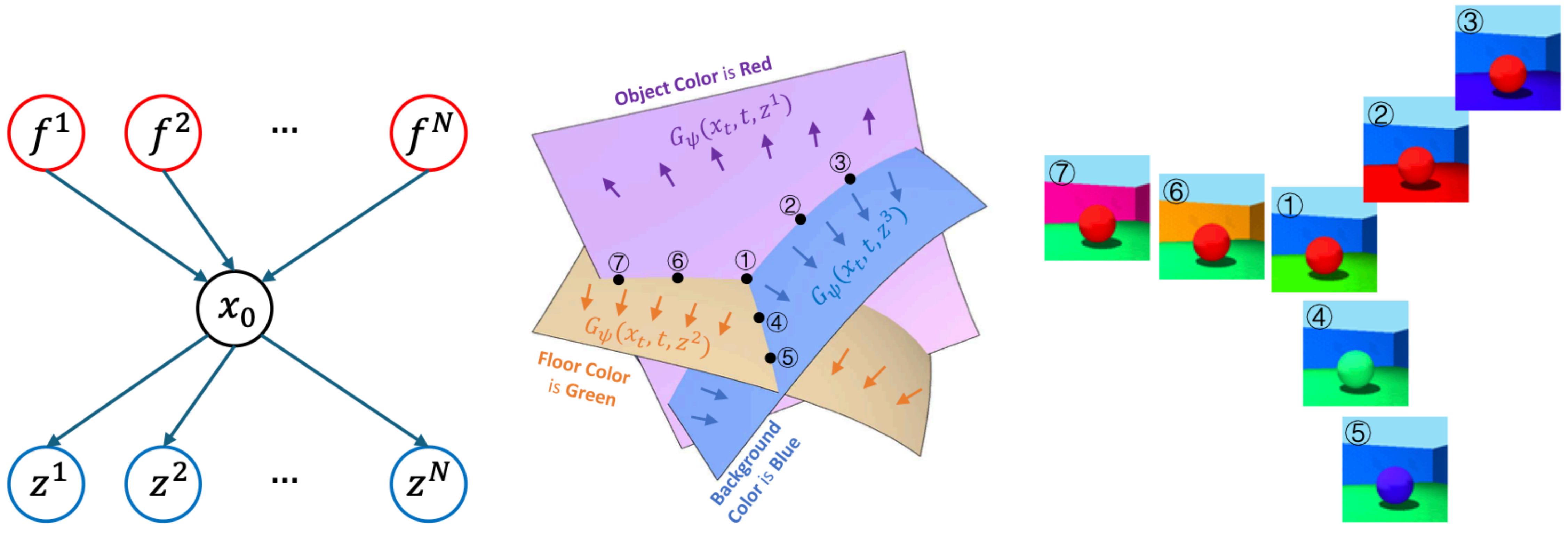
Objective: Analyze and improve the robustness of score-based generative models through input disentanglement and path dynamics study.

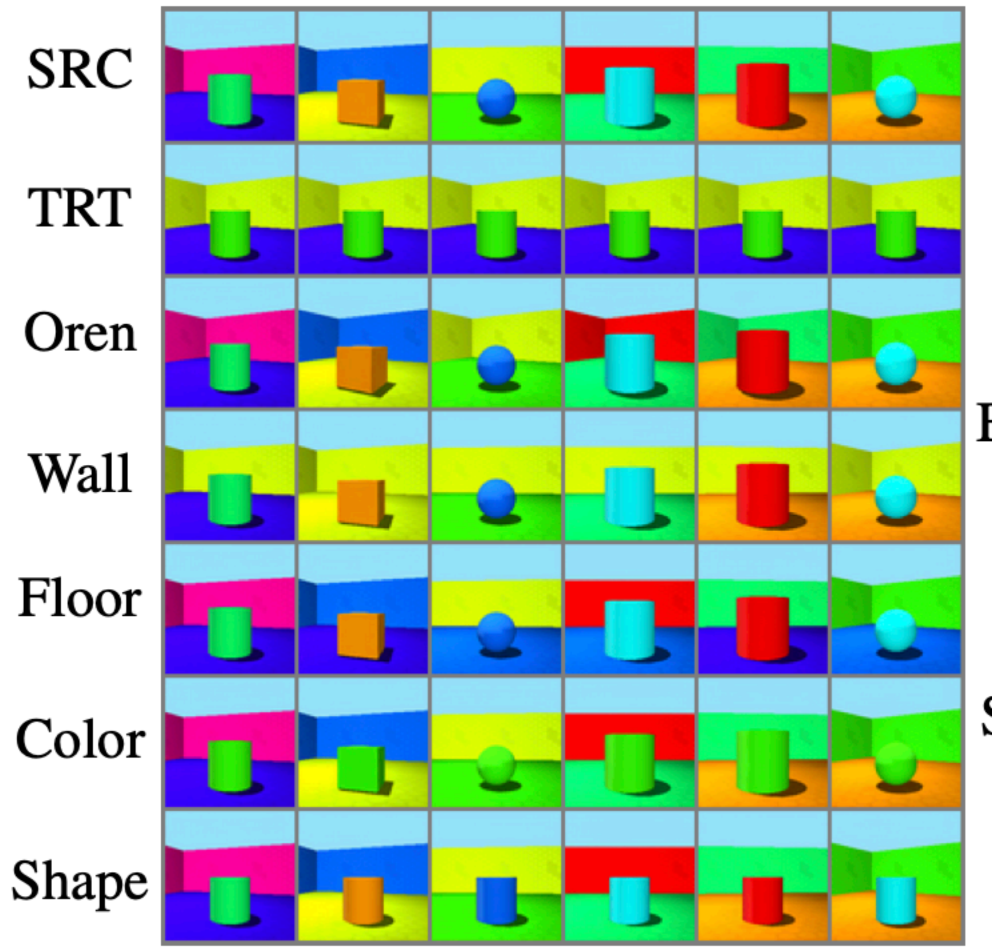
Description: This project focuses on comparing the trajectory paths of score-based generative models, such as normalizing flows and diffusion models, when subjected to varying inputs. It aims to quantify and analyze how slight changes in inputs affect the generative paths and subsequently, the model's output. The goal is to disentangle these inputs into clearer, distinct paths to enhance model robustness and understanding.

Approach: The research will involve detailed simulations and analytical studies to trace and compare paths within generative models. Techniques for disentangling these paths will be developed and tested, aiming to identify best practices that improve robustness and predictability of model behavior under varied input conditions.



(a) PGM of disentanglement (b) Image Space (c) Sampled Images

Figure 1: Illustration of disentanglement of DPMs. (a) is the diagram of Probabilistic Graphical Models (PGM). (b) is the diagram of image space. (c) is the demonstration of sampled images in (b). Surface indicates the conditional data distribution of a single factor $p(x|f^c)$. Different colors correspond to various factors. Here, we show three factors: object color, background color, and floor color. Arrows are gradient fields $\nabla_{x_t} \log p(f^c|x_t)$ modeled by using a decoder $G^c_\phi(x_t, t, z^c)$. The black points are the sampled images shown in (b).



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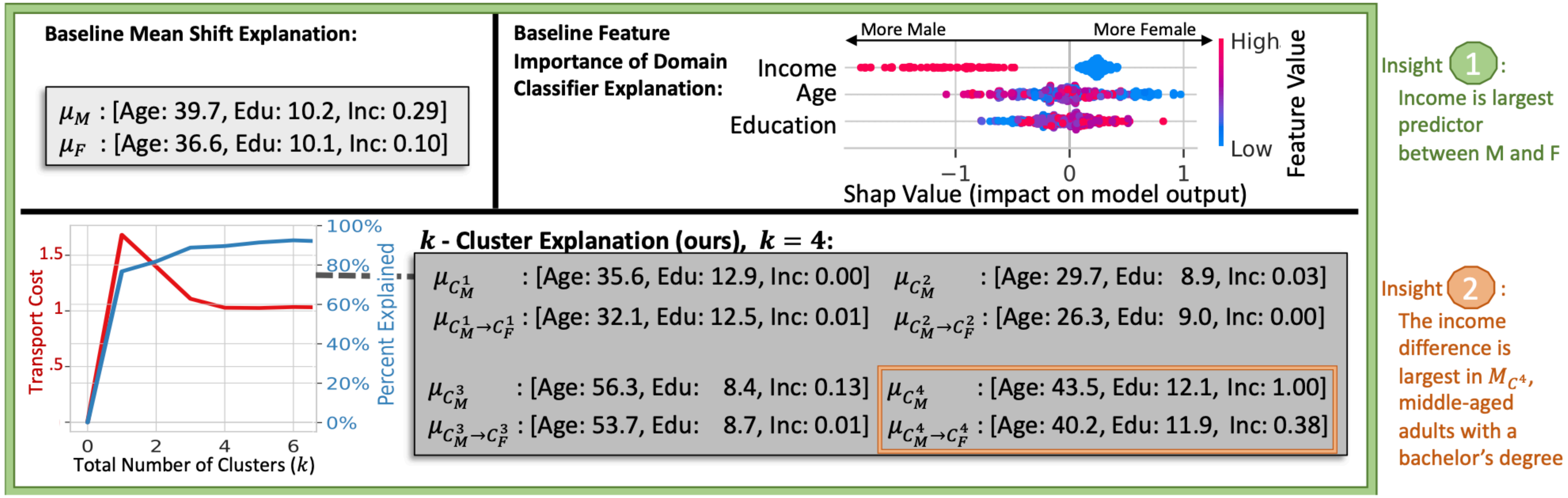
Project 9: Explanation Shift

Objective: Develop methods for detecting and explaining shifts in data distributions in tabular datasets.

Description: This project addresses the challenge of understanding shifts in data distributions within a well-defined simulator model for tabular data. It seeks to establish methodologies not only for detecting these shifts but also for providing explanations for why these shifts occur, thereby contributing to better model interpretability and reliability.

Approach: Initially, the project will focus on creating a robust detection system for shifts in dataset distributions. Following detection, the project will explore various strategies to explain the shifts effectively. This involves developing a comprehensive framework that facilitates these explorations, providing insights into the underlying causes of distribution changes.



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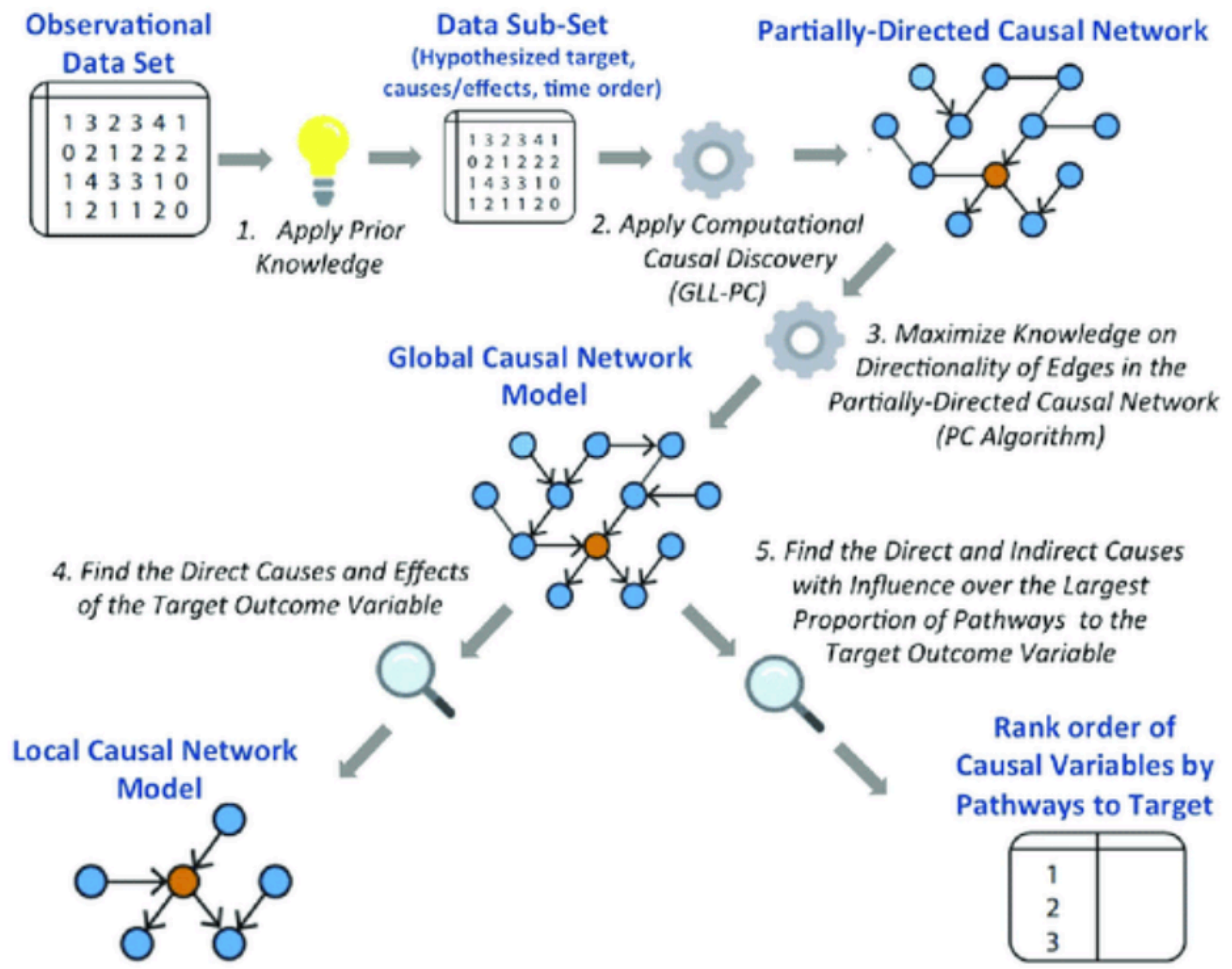
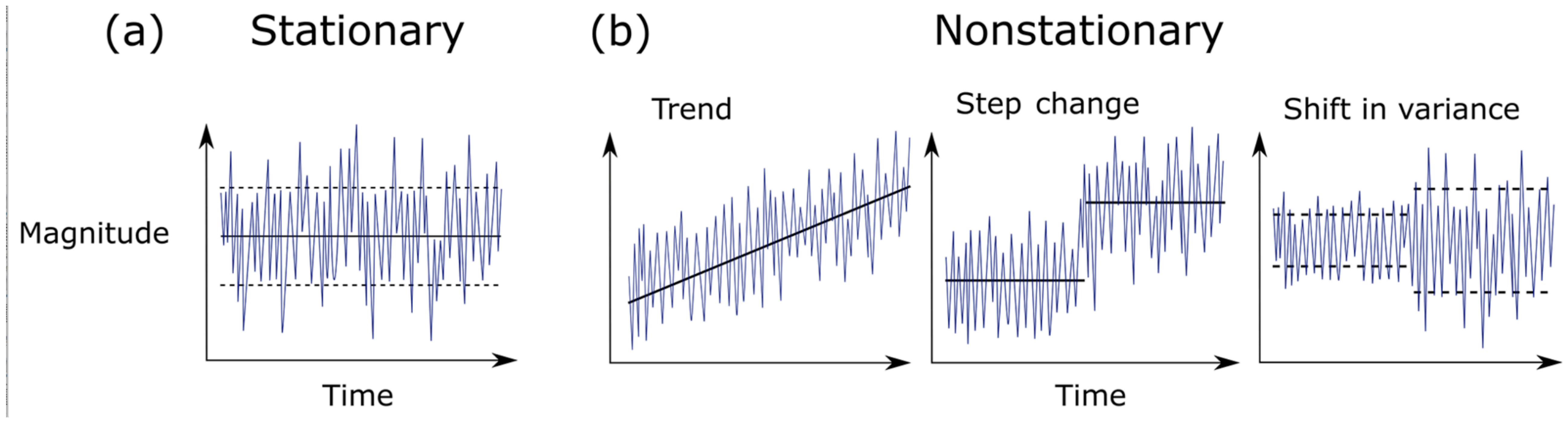
Project 10: Causal Discovery in Logistics

Objective: Design and implement a versatile toolbox for exploring correlations, causality, and non-stationarity in various datasets, with a focus on logistics (other publicly available data can be used).
Description: This project proposes the creation of a comprehensive toolbox that integrates classical machine learning techniques with advanced methods in causal discovery. The toolbox will be used to investigate different correlations, causal relationships, and instances of non-stationarity across diverse datasets. The aim is to provide a deep analysis tailored to the logistics sector, among others.
Approach: The project will involve the development and implementation of various analytical methods within the toolbox. It will be applied to a range of datasets, including those specific to the logistics industry, to uncover meaningful patterns and causal links. The results will be used to enhance data-driven decision-making processes in the logistics field and beyond.





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