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Optimising AI/ML: Beyond Gradients

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About Me

Dr Takfarinas Saber

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BSc, MSc and PhD Computer Science

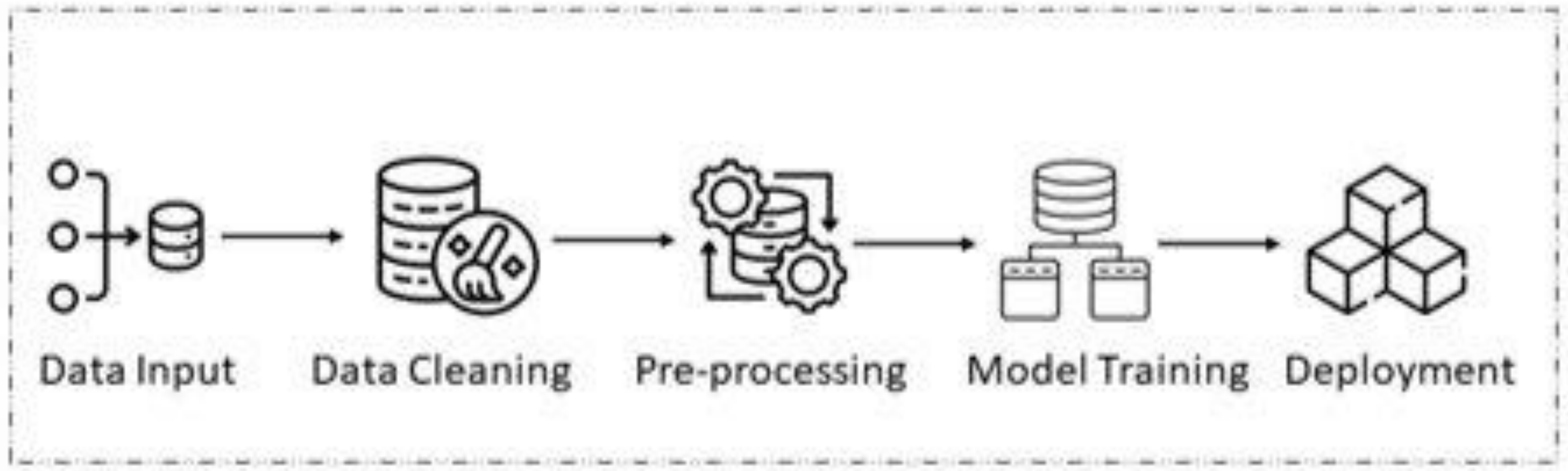
Research Areas:

- Resource Optimisation in Cloud
- Engineering, Testing and Optimisation of Software Applications

ML Pipeline

There are several ML Frameworks.

Why does your ML pipeline cost so much and run so slow?



The Optimization Maturity Ladder

- Level 0: Using default parameters (most software engineers using ML are here)
- Level 1: Manual tuning (most ML teams are)
- Level 2: Single-component optimization
- Level 3: Pipeline-level optimization
- Level 4: System-wide multi-objective optimization
- Level 4: Self-optimizing autonomous MLOps

At what level are your projects?

Phase 2 (★☆☆☆☆): Single component optimization

Hyperparameter tuning (Covered)
Resource allocation
Data sampling

Hyperparameter Optimization (HPO)

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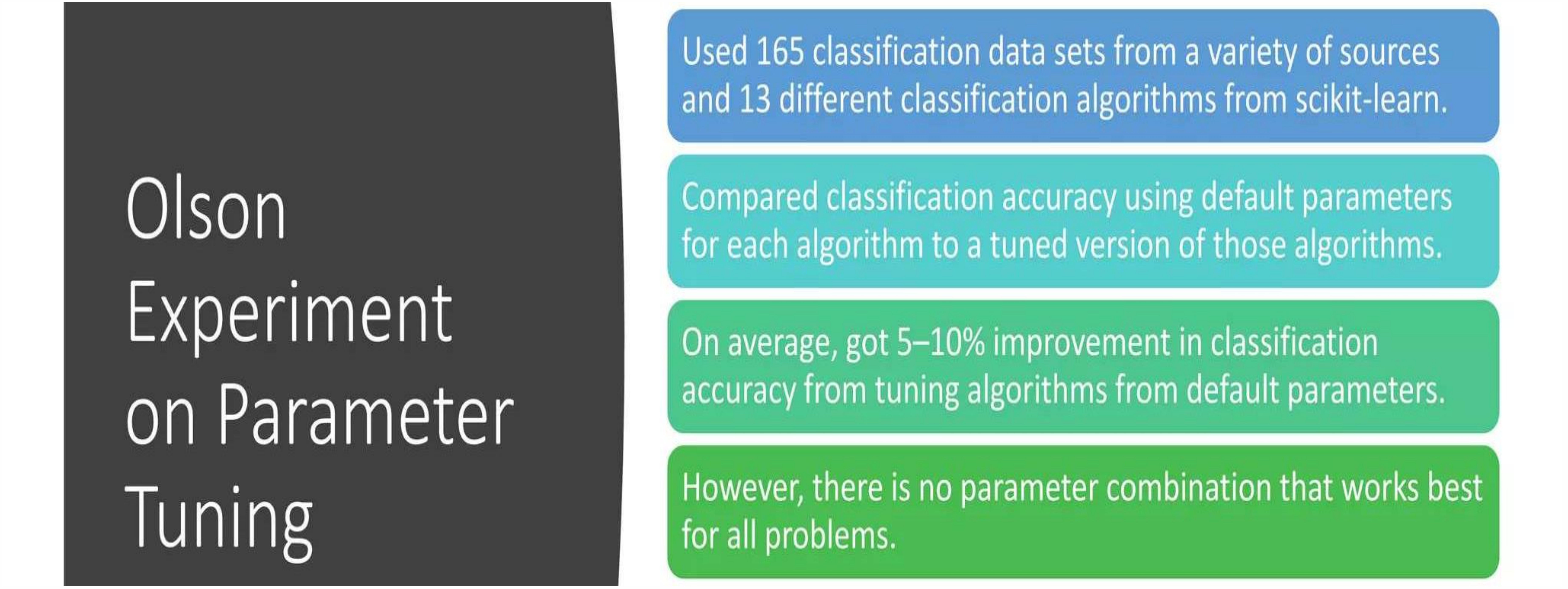


Tuning is mandatory to see improvement in ML algorithms

Olson, R.S., Cava, W.L., Mustahsan, Z., Varik, A. and Moore, J.H., 2018. Data-driven advice for applying machine learning to bioinformatics problems. In *Pacific symposium on biocomputing 2018: Proceedings of the pacific symposium* (pp. 192-203).

GridSearchCV

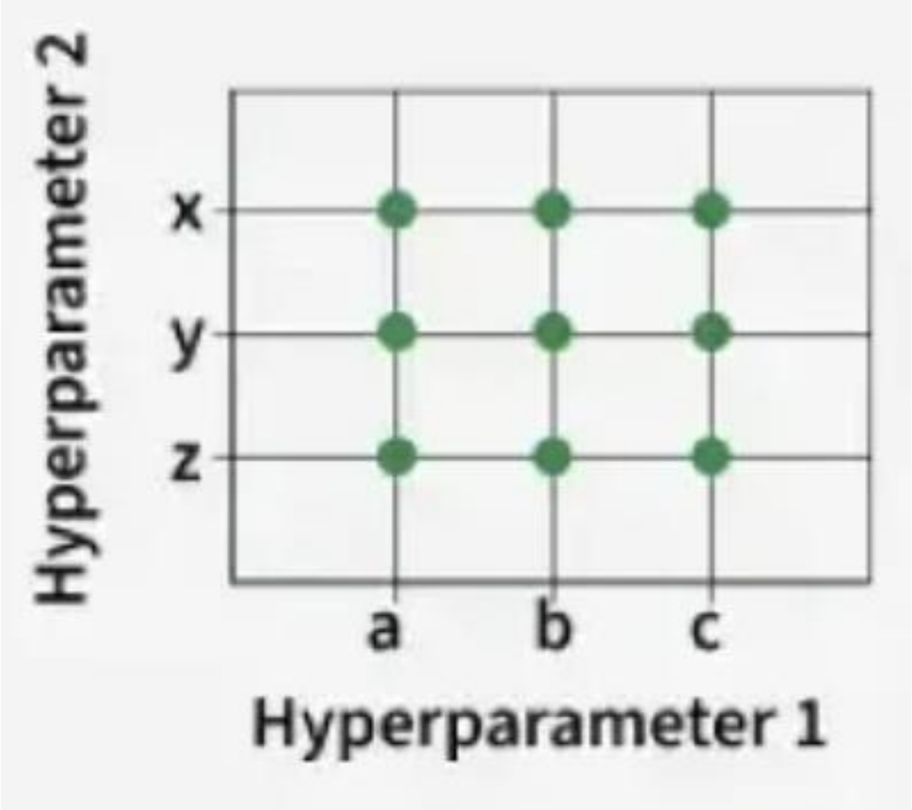
Brute-force technique for hyperparameter tuning.

It trains the model using all possible combinations of specified hyperparameter values.

It works using below steps:

- Create a grid of potential values for each hyperparameter.
- Train the model for every combination in the grid.
- Evaluate each model using cross-validation.
- Select the combination that gives the highest score.

It is slow and uses a lot of computer power which makes it hard to use with big datasets or many settings.



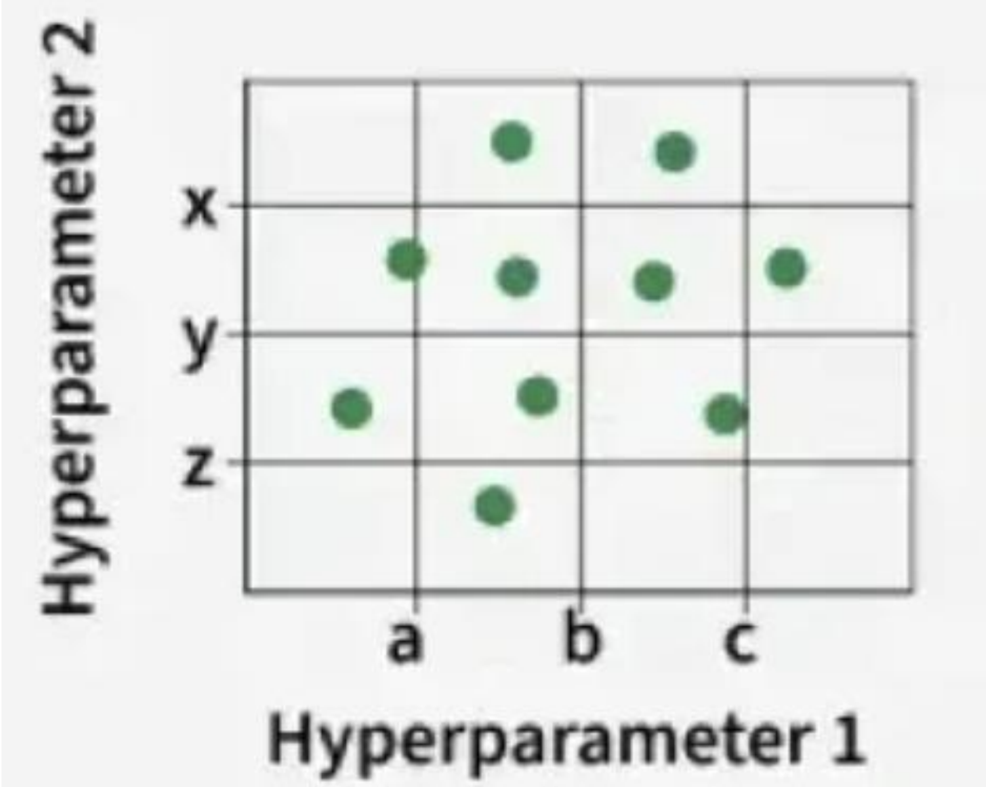
RandomizedSearchCV

Picks random combinations of hyperparameters from the given ranges.

In each iteration:

- It tries a new random combination of hyperparameter values.
- It records the model’s performance for each combination.

After several attempts it selects the best-performing set.

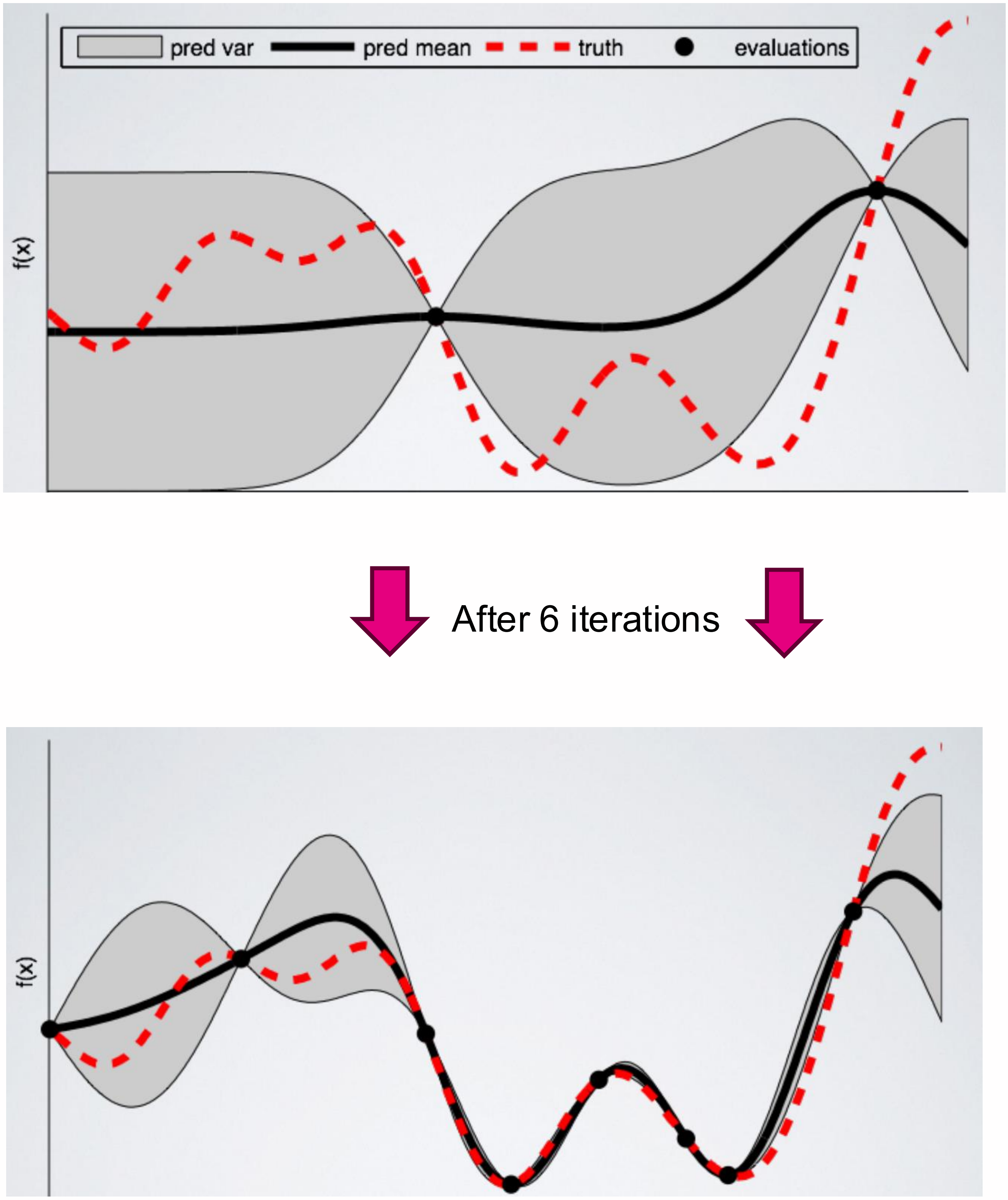


Bayesian Optimization

Grid Search and Random Search can be inefficient because they blindly try many hyperparameter combinations, even if some are clearly not useful.

Bayesian Optimization treats hyperparameter tuning like a mathematical optimization problem and learns from past results to decide what to try next:

1. Build **surrogate model** using initial evaluations of true objective function
2. Find the **hyperparameters** that perform best on the surrogate model
3. Apply these hyperparameters to the true objective function
4. Update the surrogate model incorporating the new results
5. Repeat steps 2–4 until max iterations or time is reached



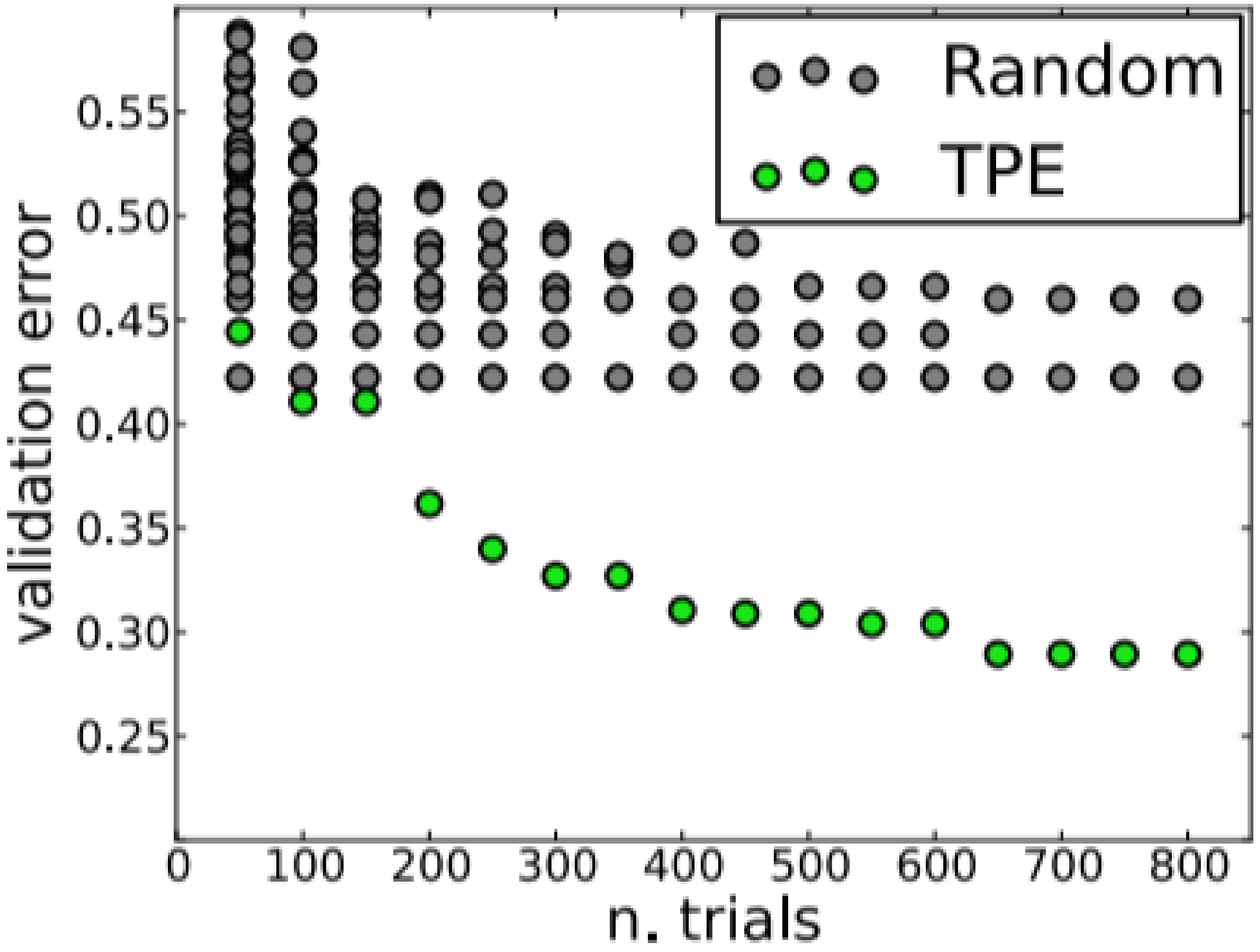
Bayesian Optimization vs Random Search

Common surrogate models used in Bayesian optimization include:

- Gaussian Processes
- Random Forest Regression
- Tree-structured Parzen Estimators (TPE)

Validation error for hyperparameter optimization of an image classification neural network [1] with:

- Random search in grey
- Bayesian Optimization (using the Tree Parzen Estimator or TPE) in green.



[1] Bergstra, J., Yamins, D. and Cox, D., 2013, February. Making a science of model search: Hyperparameter optimization in hundreds of dimensions for vision architectures. In *International conference on machine learning* (pp. 115-123). PMLR.

Advantages of Hyperparameter tuning

- **Improved Model Performance**:
  - Finding the optimal combination of hyperparameters can significantly boost model accuracy and robustness.
- **Reduced Overfitting and Underfitting**:
  - Tuning helps to prevent both overfitting and underfitting resulting in a well-balanced model.
- **Enhanced Model Generalizability**:
  - By selecting hyperparameters that optimize performance on validation data the model is more likely to generalize well to unseen data.
- **Optimized Resource Utilization**:
  - With careful tuning resources (e.g., computation time and memory) can be used more efficiently avoiding unnecessary work.
- **Improved Model Interpretability**:
  - Properly tuned hyperparameters can make the model simpler and easier to interpret.

Challenges in Hyperparameter Tuning

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- **Dealing with High-Dimensional Hyperparameter Spaces:**
  - The larger the hyperparameter space the more combinations need to be explored. This makes the search process computationally expensive and time-consuming especially for complex models with many hyperparameters.

- **Handling Expensive Function Evaluations:**
  - Evaluating a model's performance can be computationally expensive, particularly for models that require a lot of data or iterations.

- **Auxiliary problems:**
  - Resource Allocation for Single Training Job
  - Optimal subset from large dataset
  - Maximize model performance with minimum data

All maturity levels above inherit from these challenges and problems (at a larger scale)

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Phase 3 (★★★☆☆): Pipeline-level optimization

AutoML pipeline construction (Covered)
DAG scheduling
Distributed training

Optimizing ML Components Separately Often Fails

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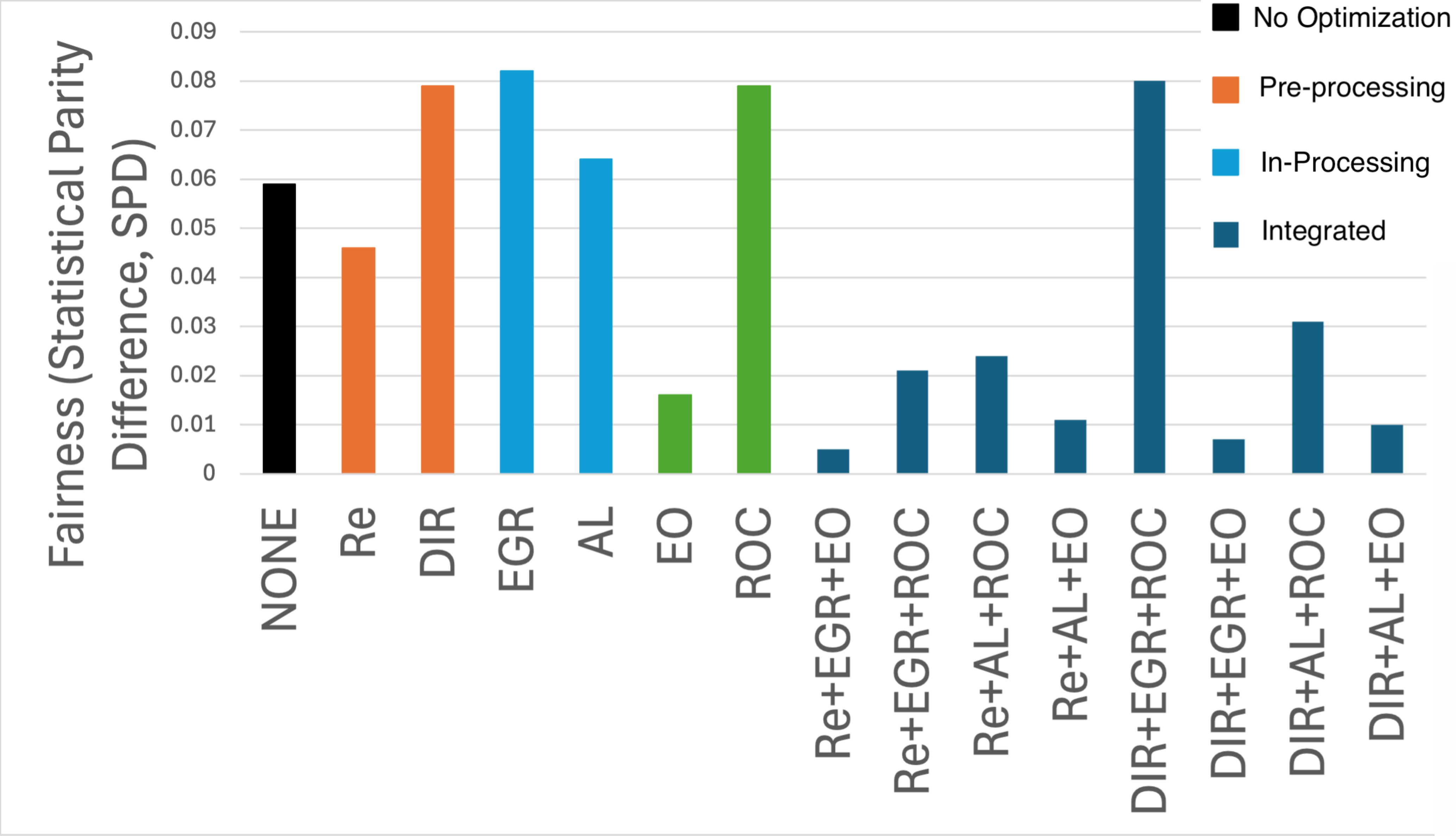
- Optimizing each component individually ignores interactions between stages.
- Locally optimal choices may lead to globally suboptimal pipelines.
    - E.g., Selecting the best data processing approaches for Fairness Optimisation [1].



The whole pipeline is more than the sum of its parts!

[1] Farayola, M.M., Tal, I., Saber, T., Connolly, R. and Bendechache, M., 2025. A fairness-focused approach to recidivism prediction: implications for accuracy, trust, and equity. *AI & SOCIETY*, pp.1-19.

AutoML Pipeline Construction

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Approach 1: Combined Algorithm Selection and Hyperparameter optimization (CASH)
Focuses on, searching a vast space to find the optimal "single model" and "its hyperparameters."

E.g., Generalizing the Bayesian Algorithm.

The search space is defined in two levels as fellows:

- Choices of classifier / regressor and preprocessing methods are top level categorical hyperparameters
- Hyperparameters of selected methods become active when they are chosen.

The combined space can then be searched with Bayesian Optimization methods.

- But need to be able to handle high-dimensional hierarchical spaces

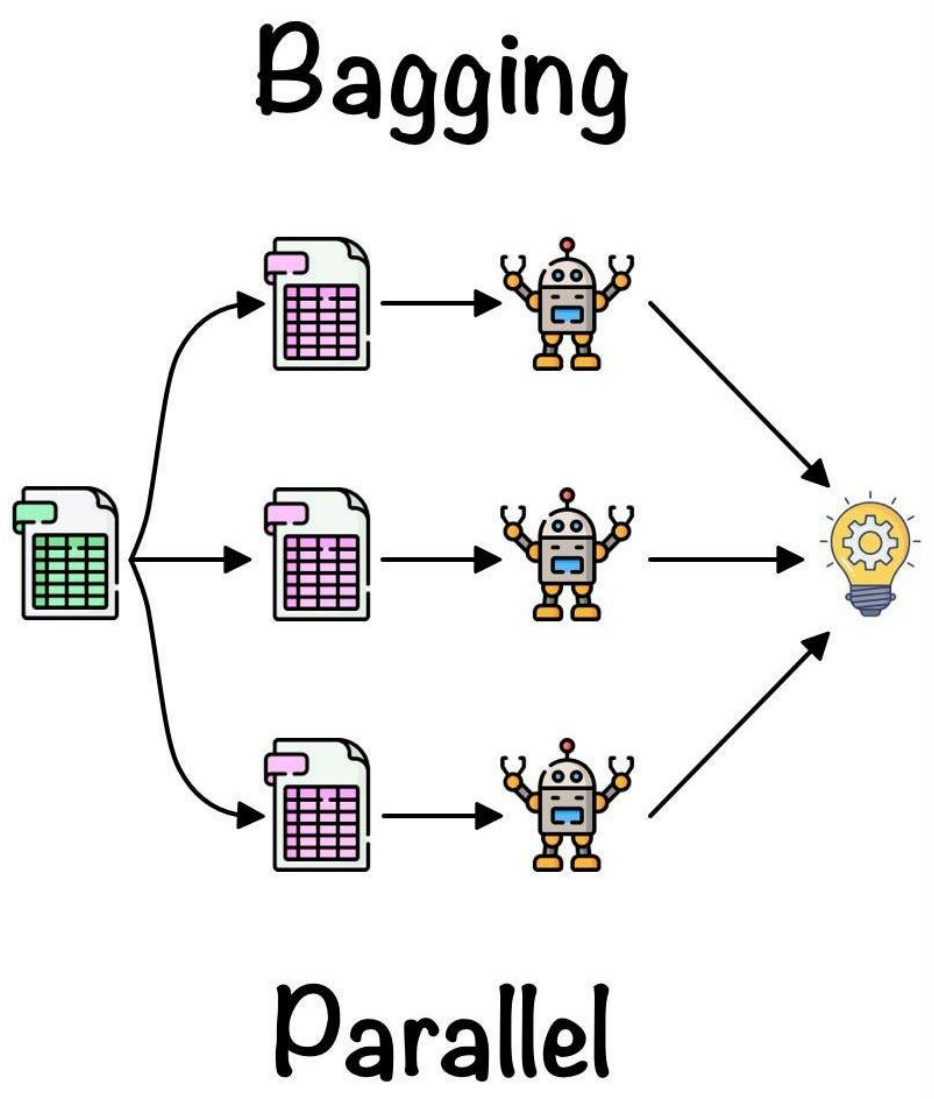
Auto-Sklearn

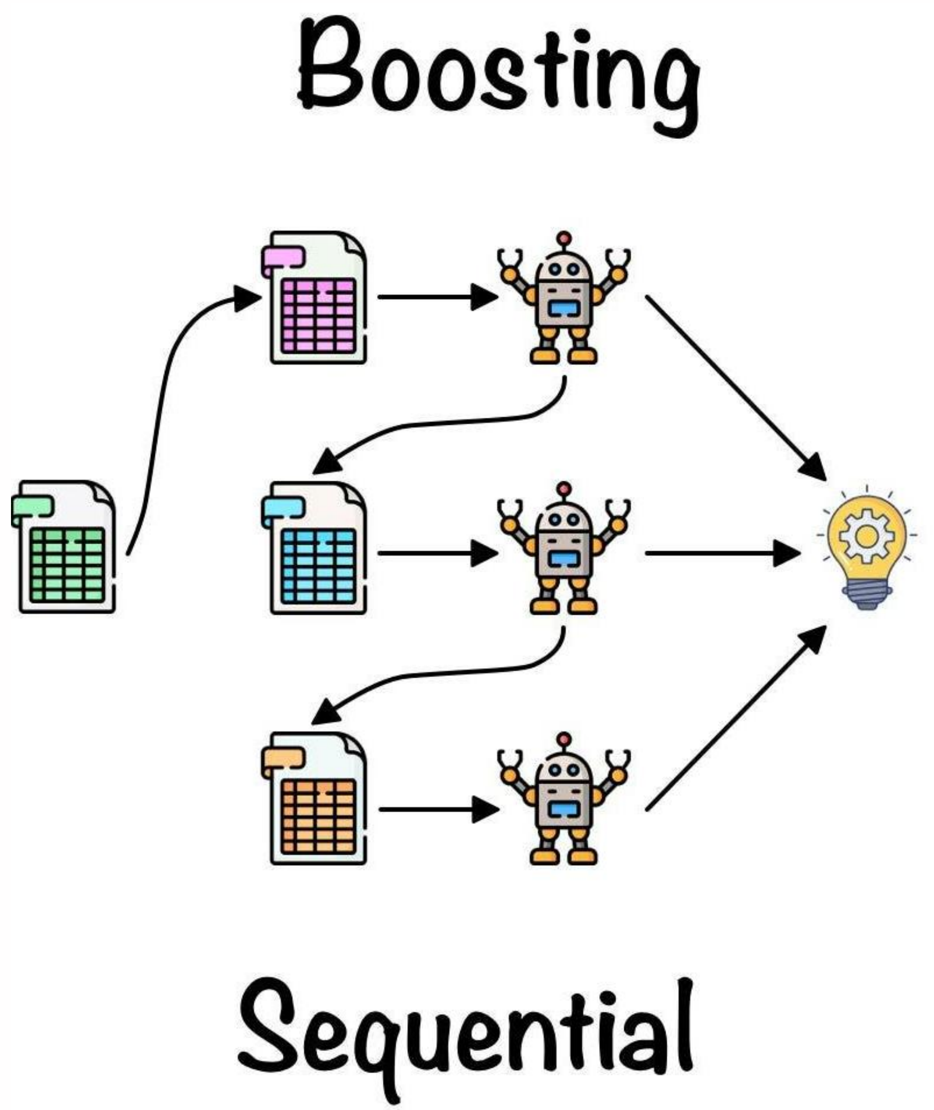
Issues various **common issues**, especially related to dependencies, system setup, and resource limits.

AutoML Pipeline Construction (Cont'd)

Approach 2: Ensembling
Achieves success by **ensembling** multiple models and stacking them in **multiple layers**.

The belief is that wisely combining many "good models" yields better results within a given time limit than searching for a "single perfect model."





AutoML Pipeline Construction (Cont'd)

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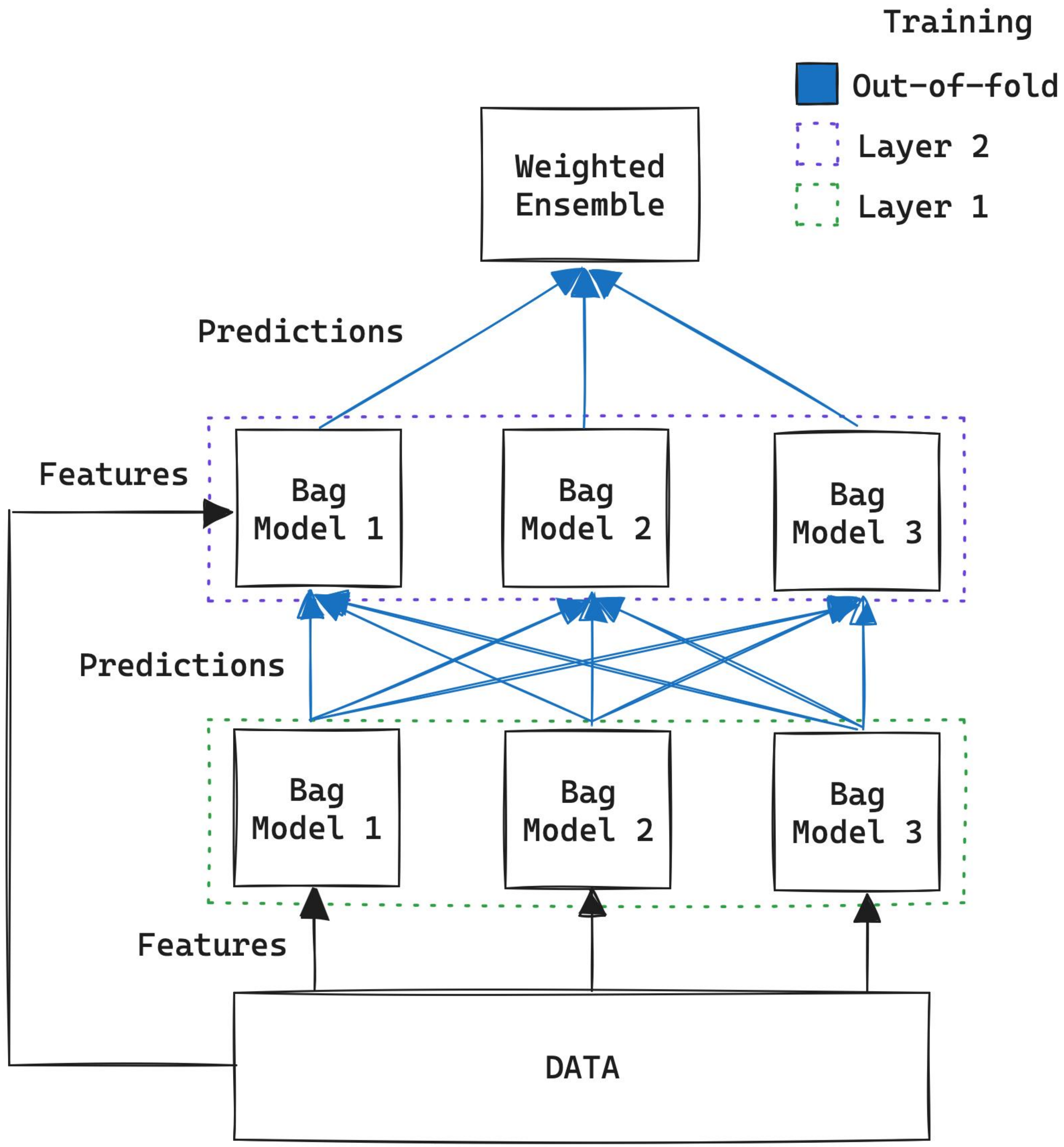
Approach 2: Ensembling

- Layer(s) of Models
- Weighted Ensemble
- Residual Connections

What Models To Use: pre-defined selection.

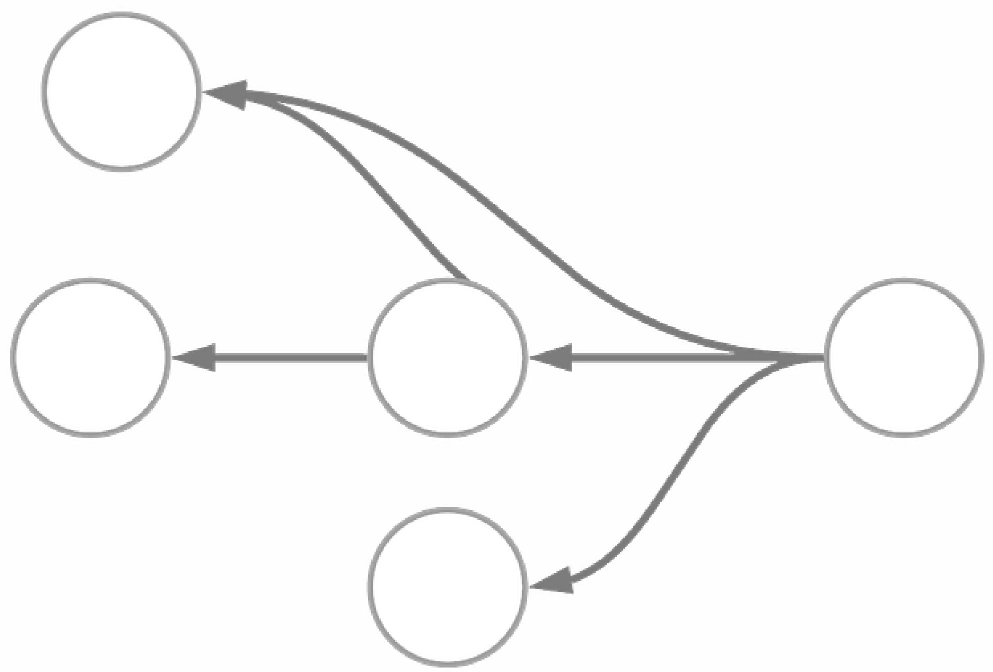
- Based on the comparison of 1,310 models on 200 distinct datasets with various configs/hyperparameters https://huggingface.co/spaces/TabArena/leaderboard



AutoML Pipeline Construction (Cont'd)

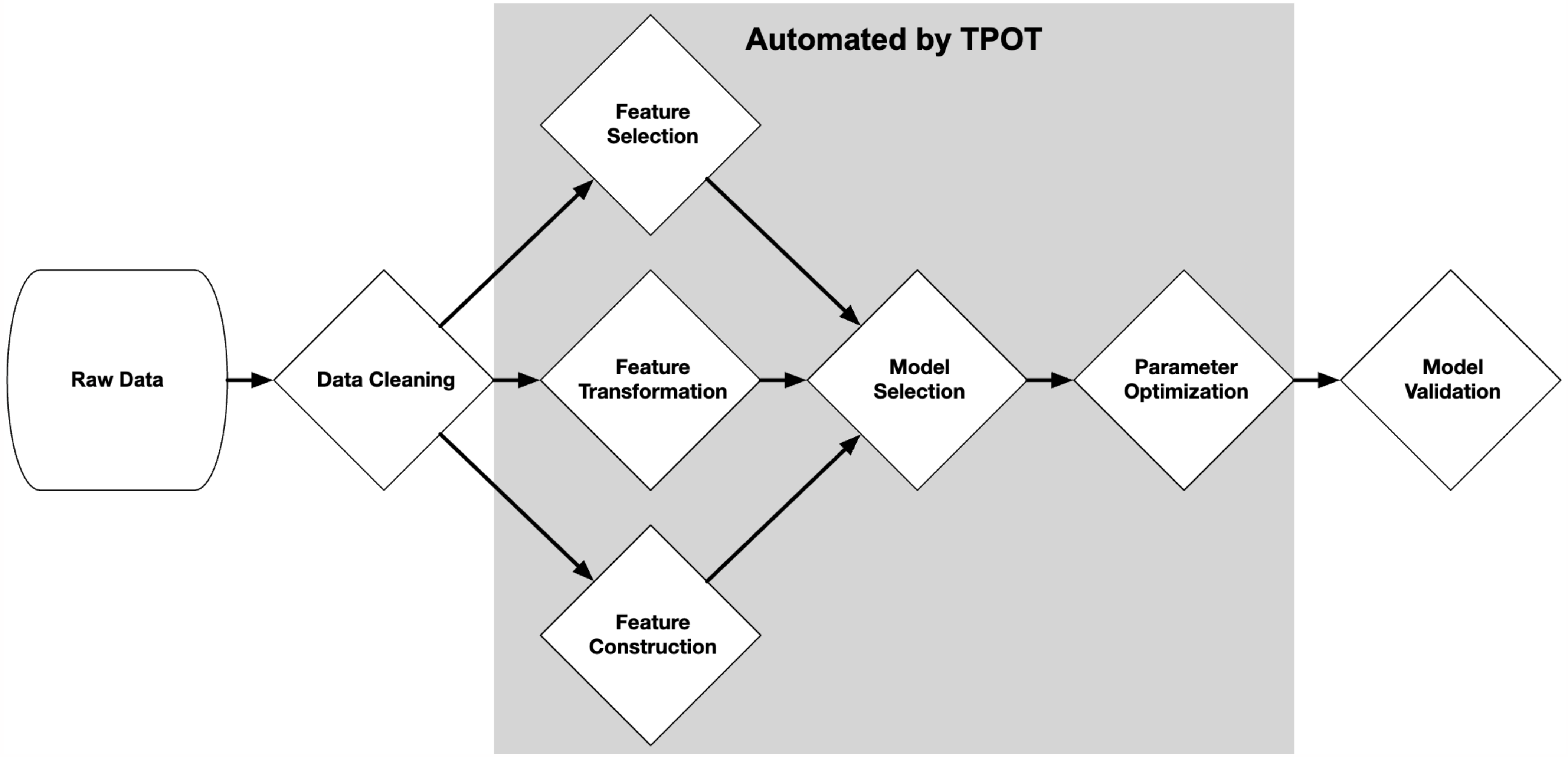
Approach 3: Directed Acyclic Graph (DAG)-Based Optimization

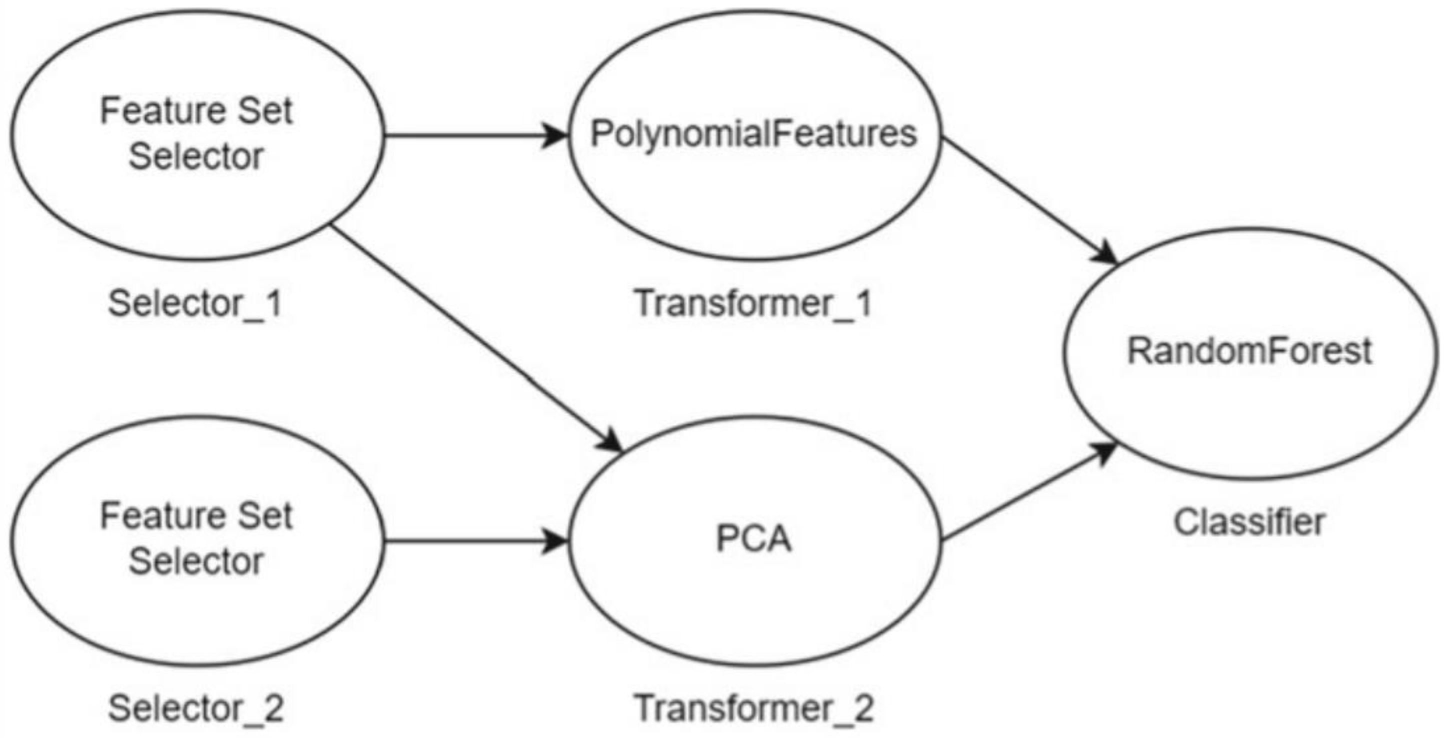
- Define the ML pipeline as a Directed Acyclic Graph (DAG) search space
- Search for the best DAG



AutoML Pipeline Construction (Cont'd)

Approach 3: Directed Acyclic Graph (DAG)-Based Optimization





Example of TPOT Pipeline

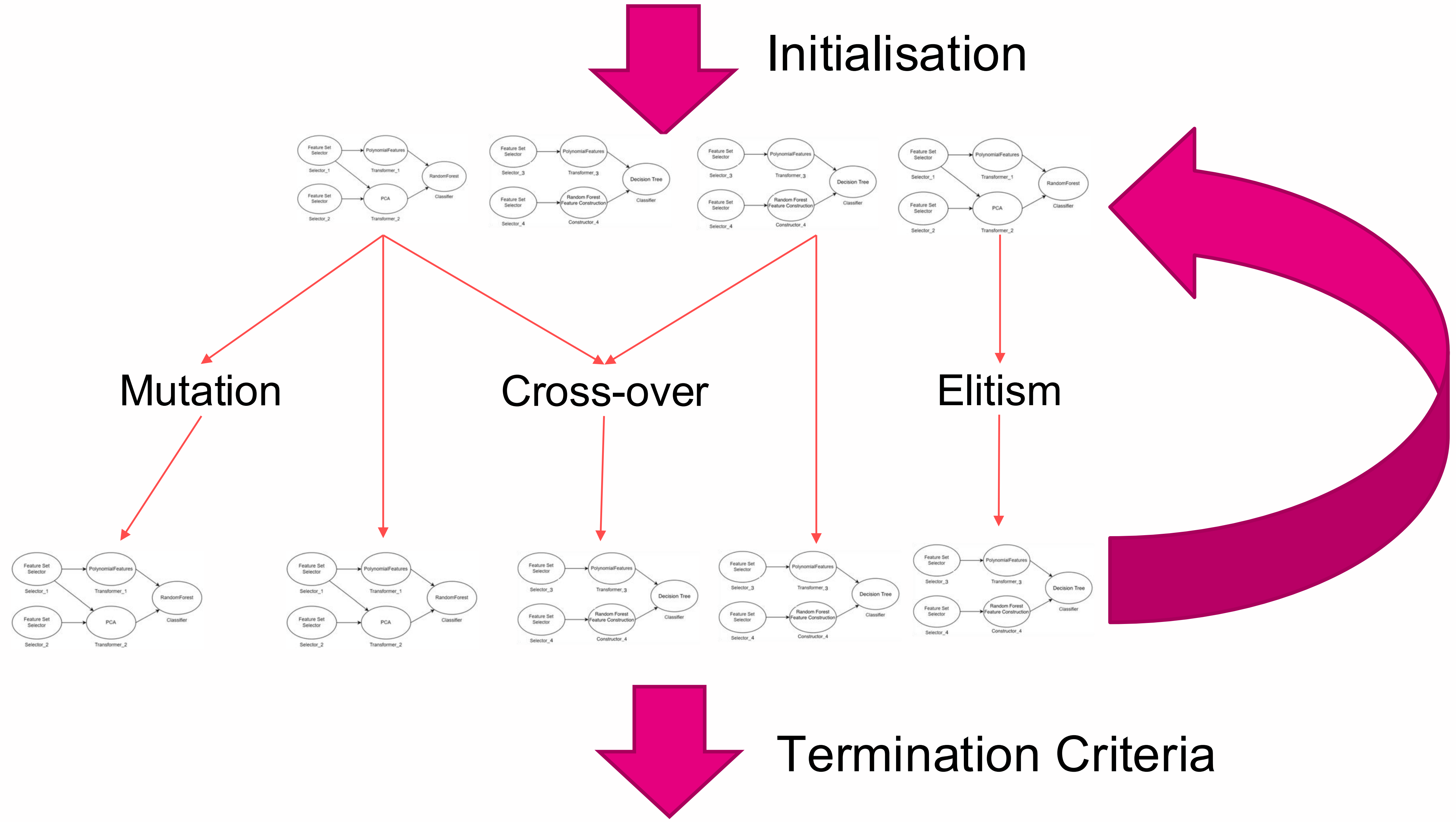
[1] Ribeiro, P., Saini, A., Moran, J., Matsumoto, N., Choi, H., Hernandez, M. and Moore, J.H., 2024. TPOT2: A New Graph-Based Implementation of the Tree-Based Pipeline Optimization Tool for Automated Machine Learning. In *Genetic programming theory and practice XX* (pp. 1-17). Singapore: Springer Nature Singapore.

AutoML Pipeline Construction (Cont'd)

Approach 3: Directed Acyclic Graph (DAG)-Based Optimization

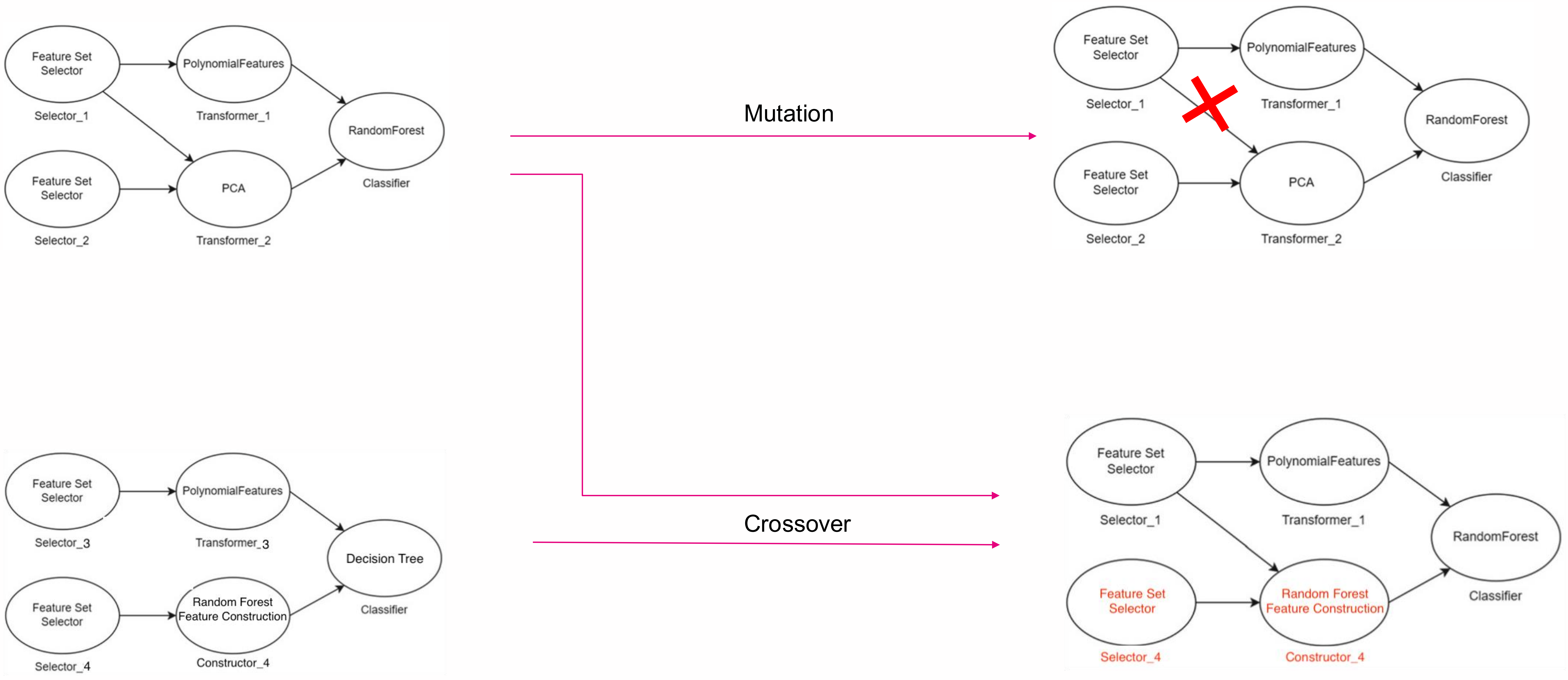
Using Genetic Programming

Returns the code of the pipeline



Keep **best** solutions for next generation

TPOT2 Evolutionary Operators



Comparison of AutoML frameworks

Library	Strengths	Weaknesses
AutoGluon	High performance, multi-data support, ensembling	Resource-heavy, MXNet backend
H2O AutoML	Robust, scalable, many model types	Steep learning curve, high memory use
TPOT	Customizable pipelines, exportable code	Slow, not ideal for large datasets
Auto-sklearn	Strong ML foundation, reproducible	Less deep learning support, tricky setup
MLJAR	User-friendly, explainable reports	Slightly lower performance, smaller community
PyCaret	Quick prototyping, low-code	Less control, may not reach top performance

Phase 4 (★★★★☆): System-wide multi-objective optimization

Balancing competing objectives across the entire MLOps lifecycle

MLOps

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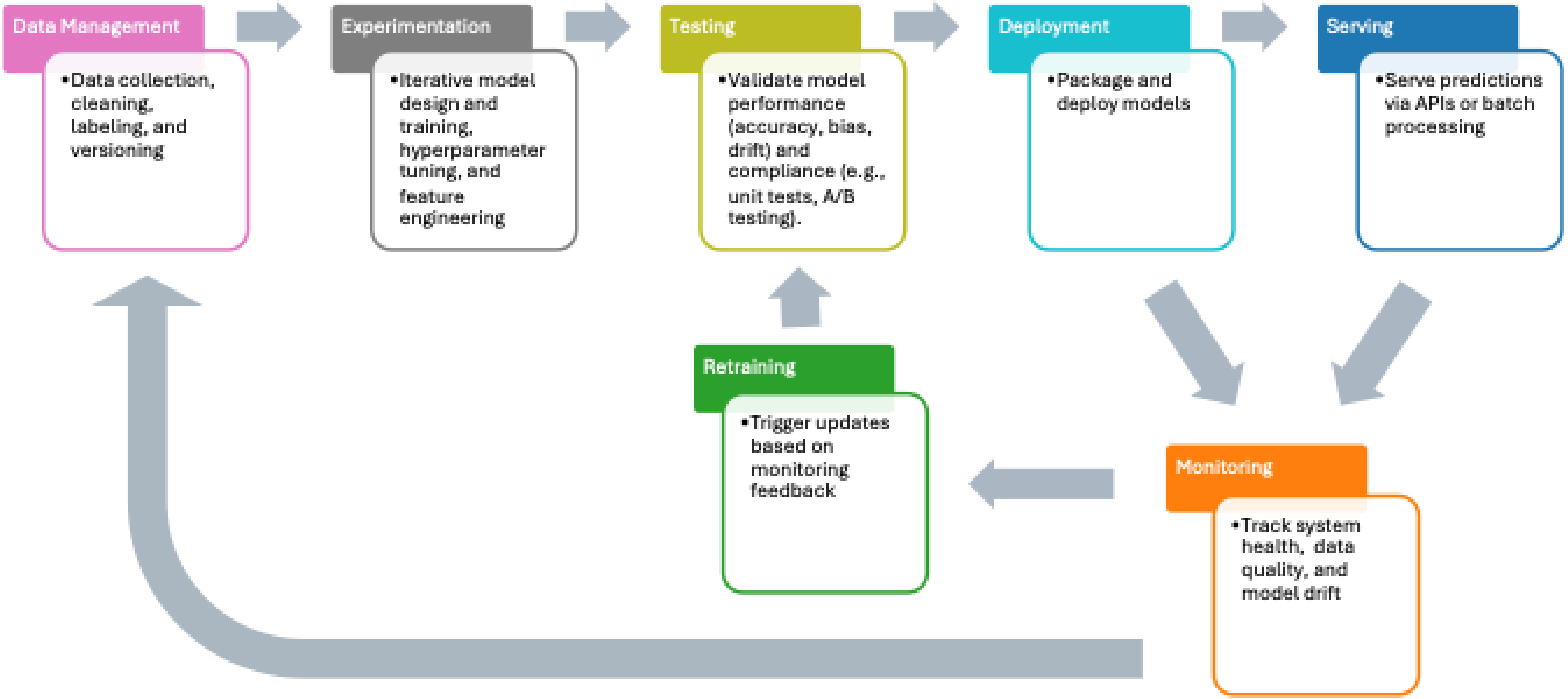


Multi-Objective Problem Formulation

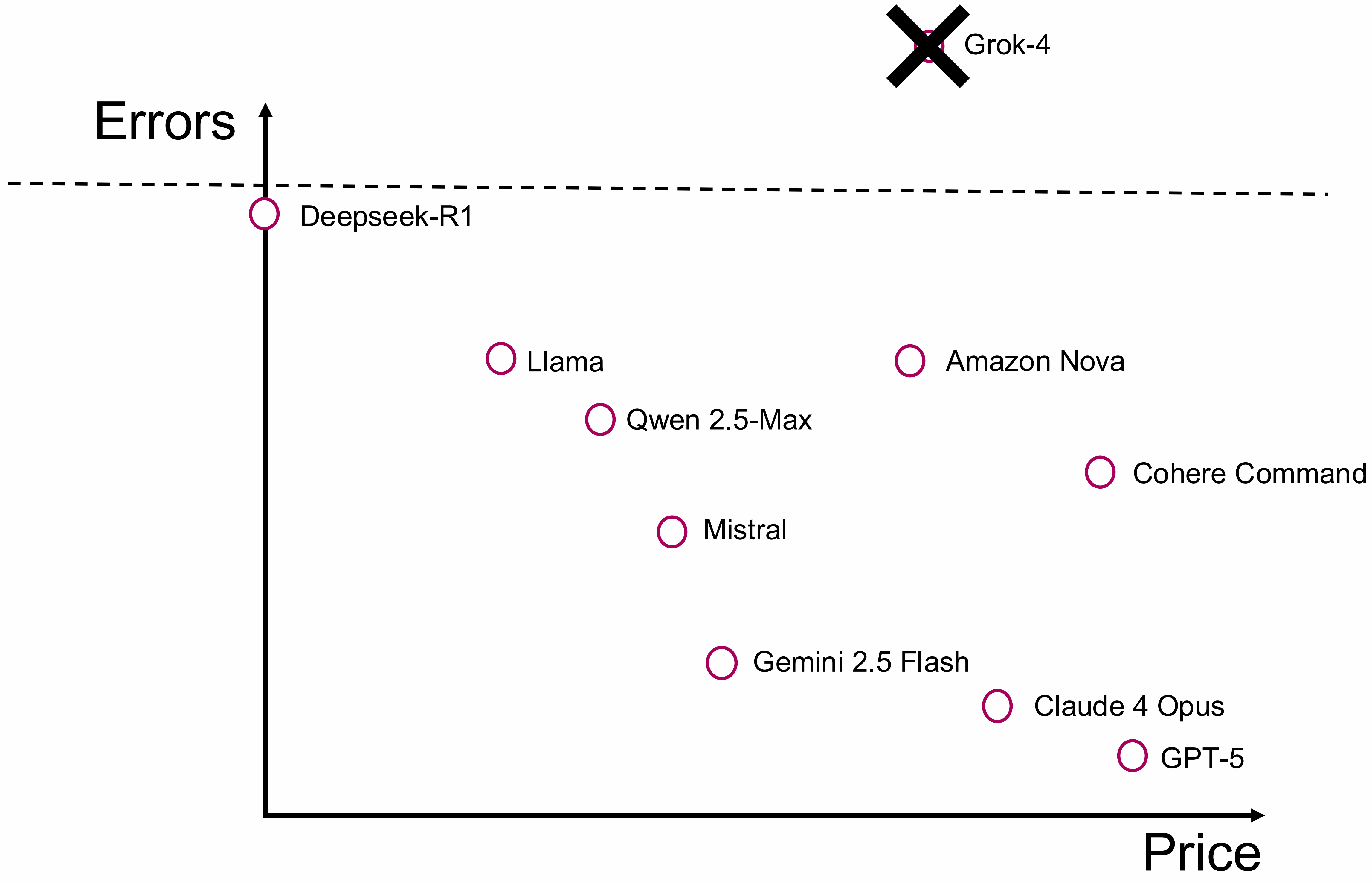
Competing Objectives:

- **Minimize**: Training cost, inference latency, model size, carbon footprint
- **Maximize**: Model accuracy, throughput, model freshness, system reliability

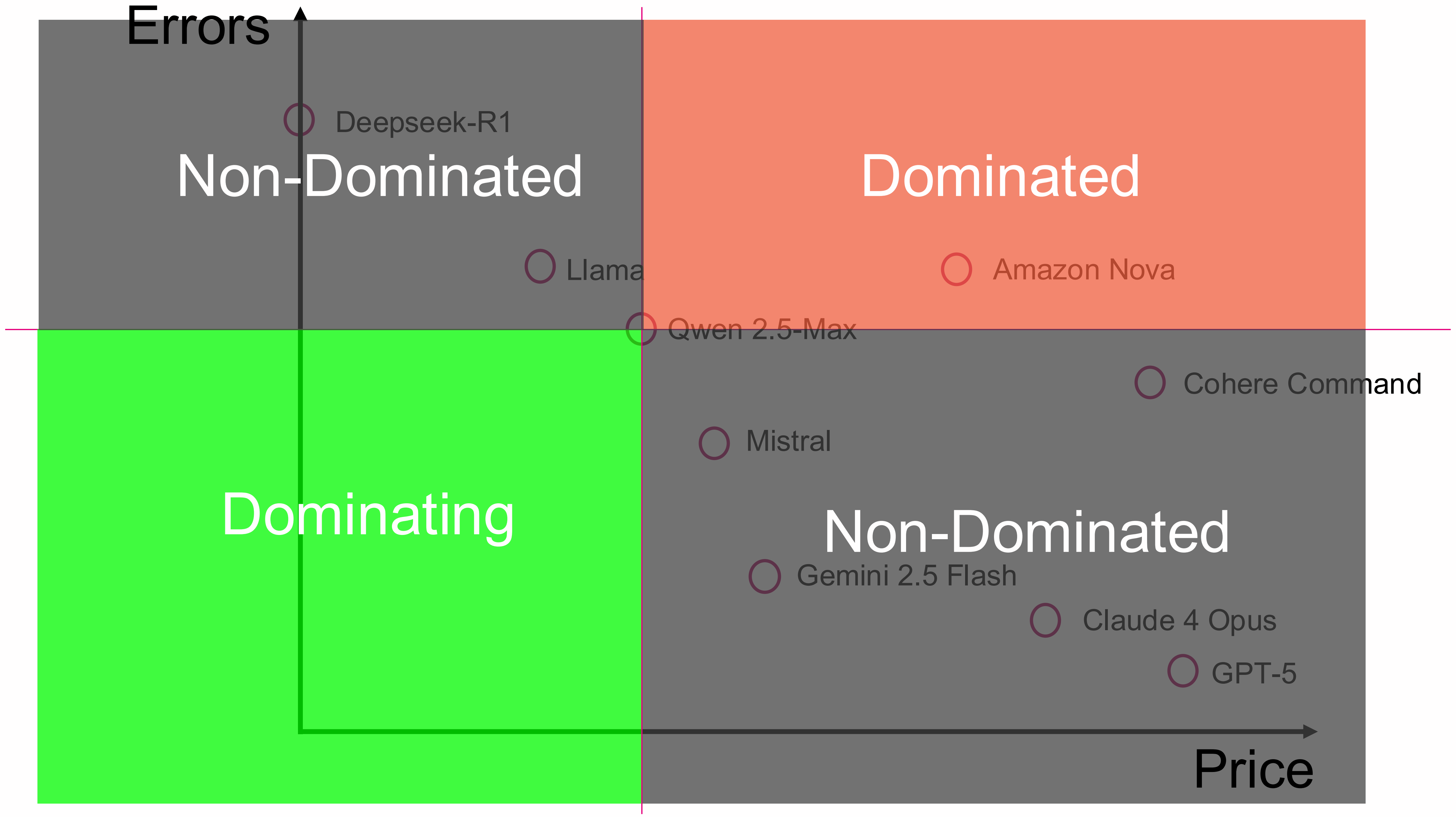
Challenge: No single optimal solution, only trade-offs

Two Objectives:

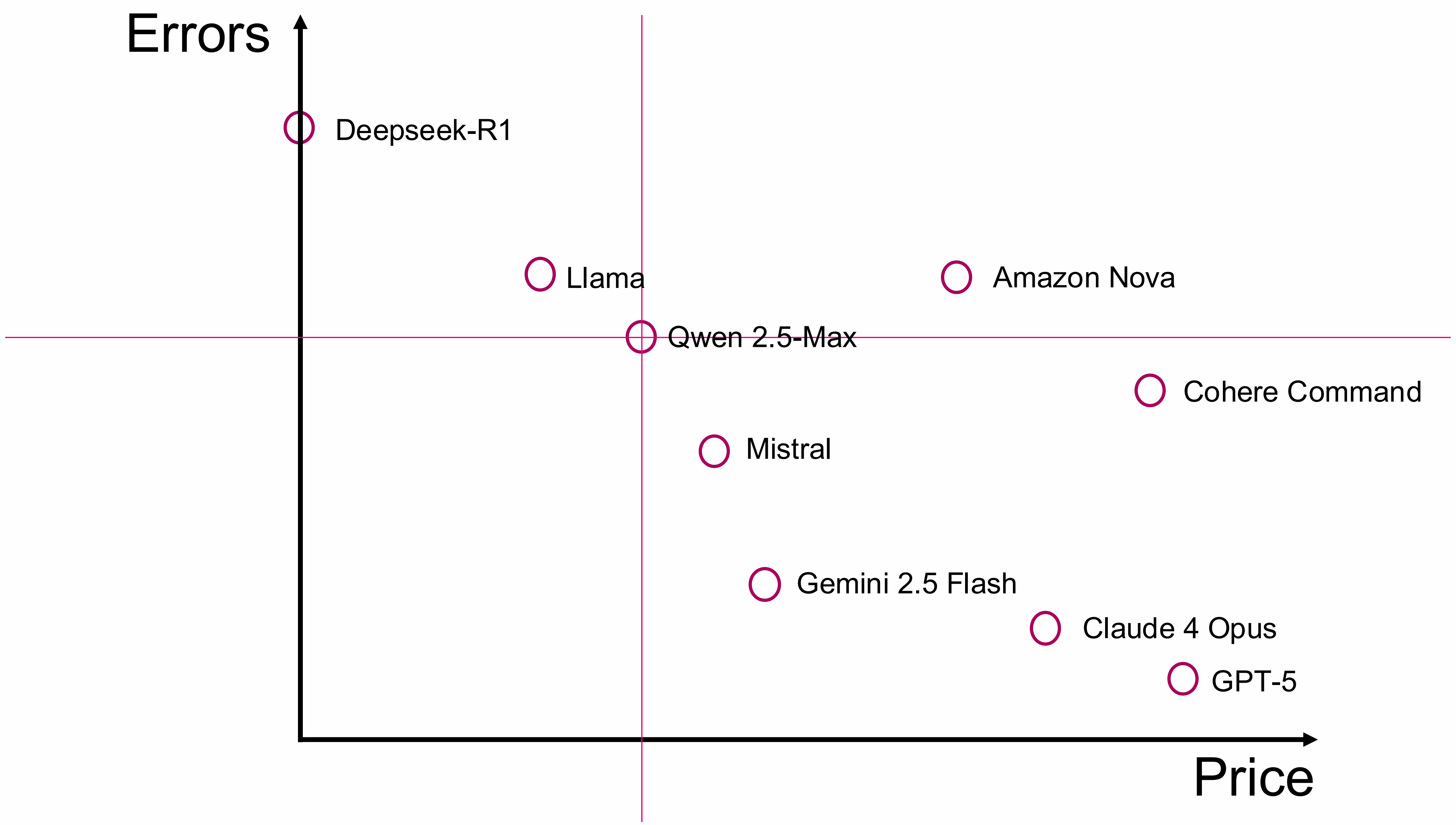
Cheap and Environmentally Friendly



Dominance


Errors
Deepseek-R1
Non-Dominated
Dominated
Llama
Amazon Nova
Qwen 2.5-Max
Cohere Command
Mistral
Dominating
Non-Dominated
Gemini 2.5 Flash
Claude 4 Opus
GPT-5
Price

Dominance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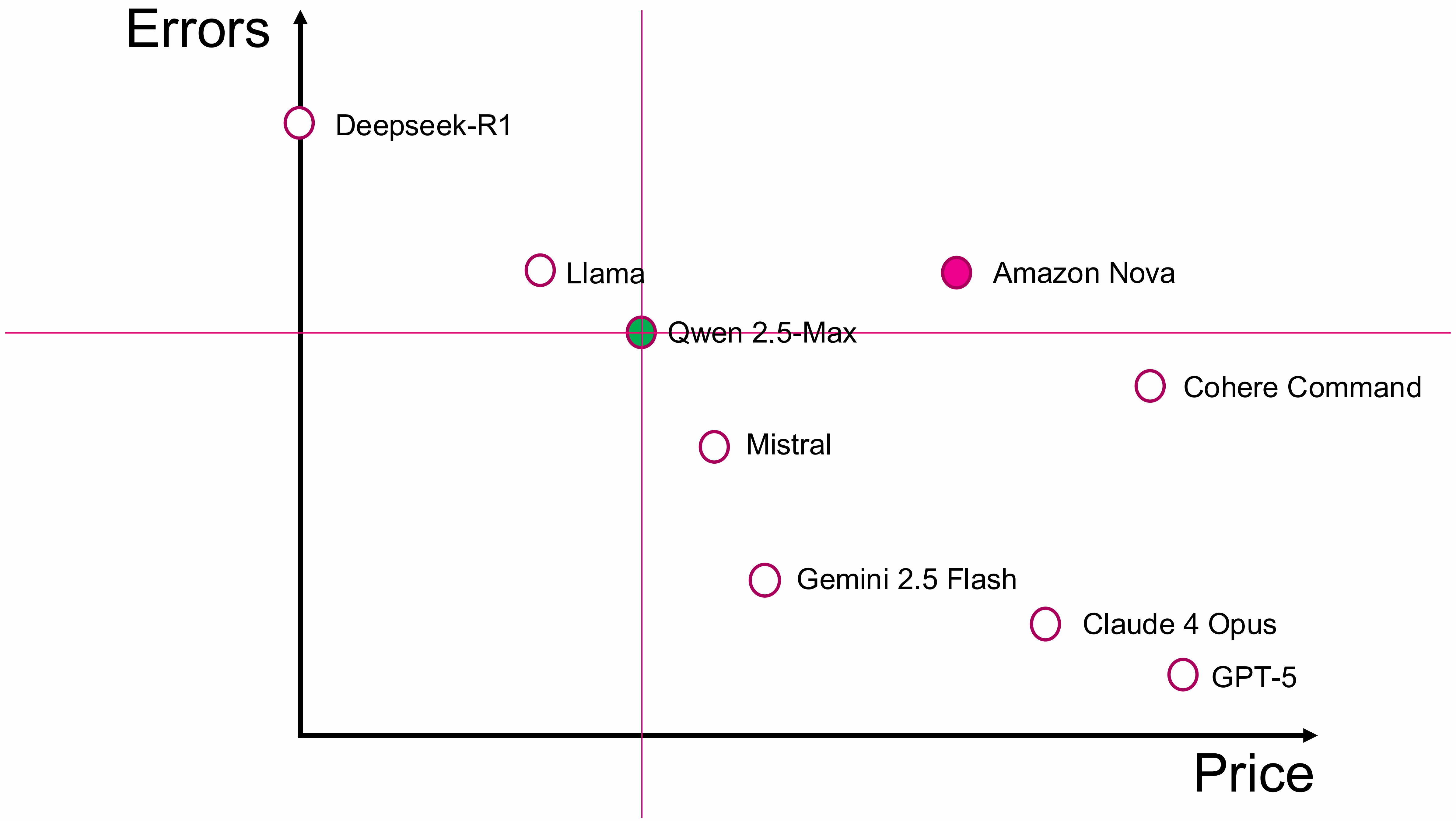

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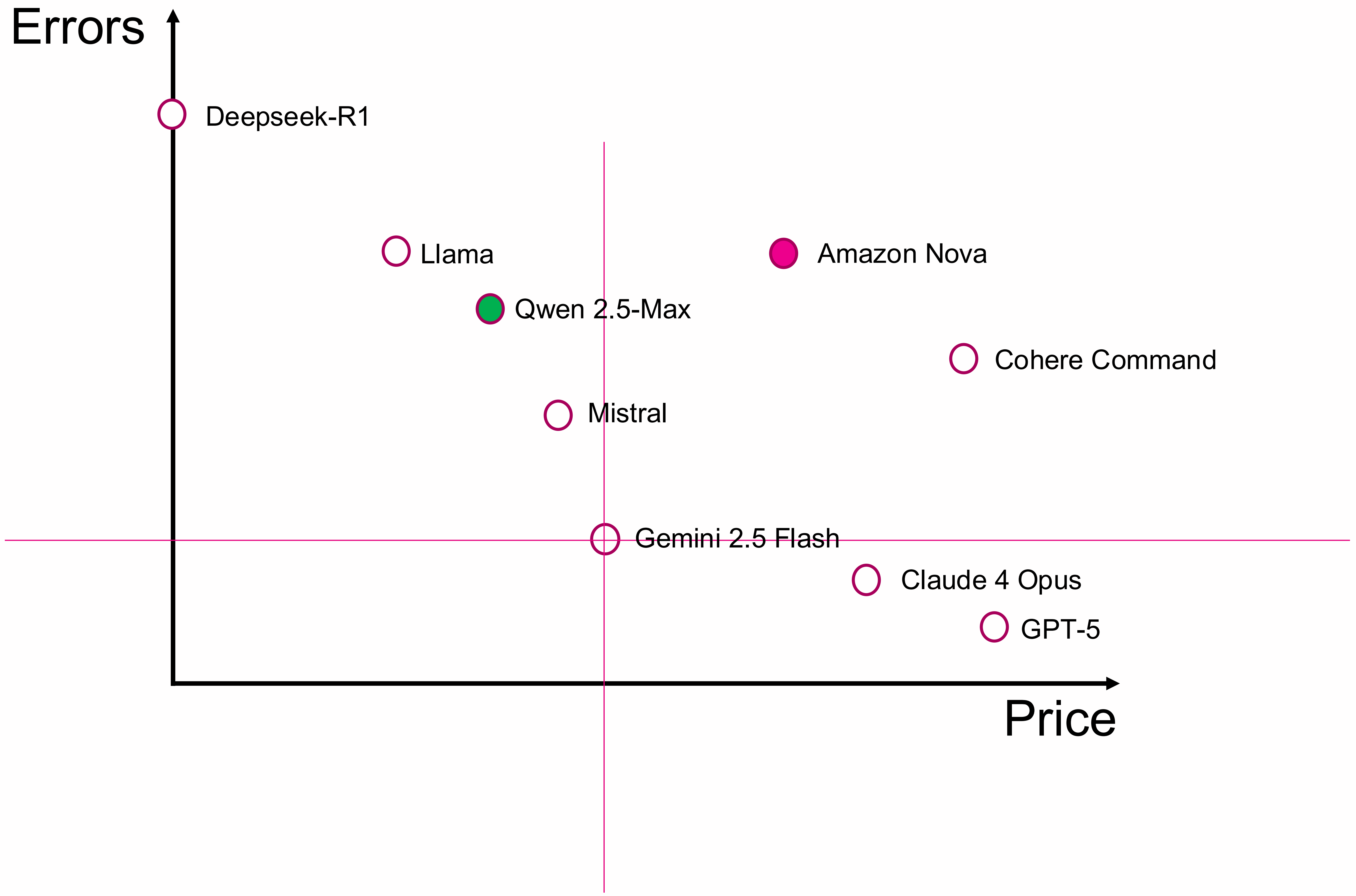
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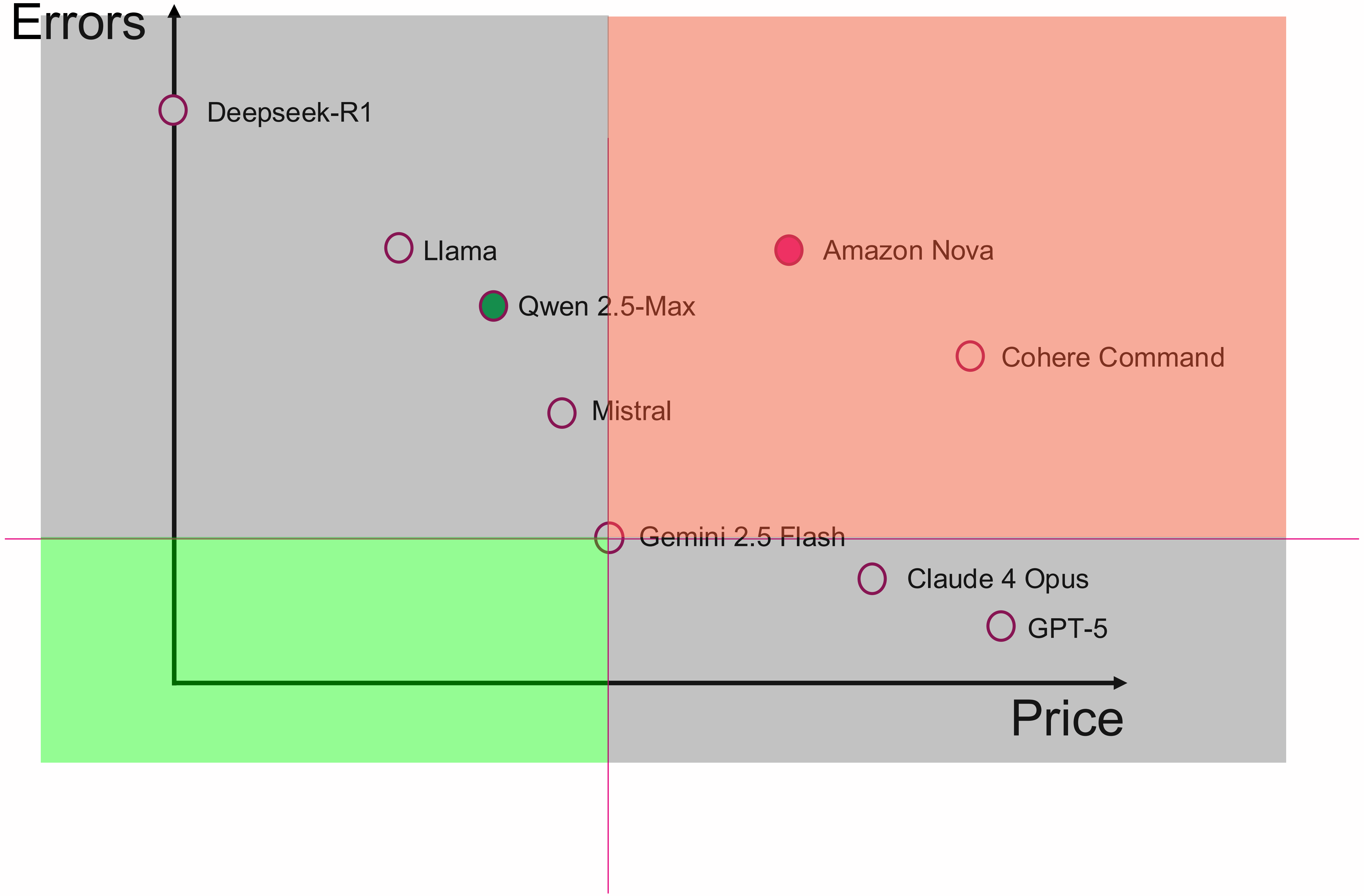

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Dominance

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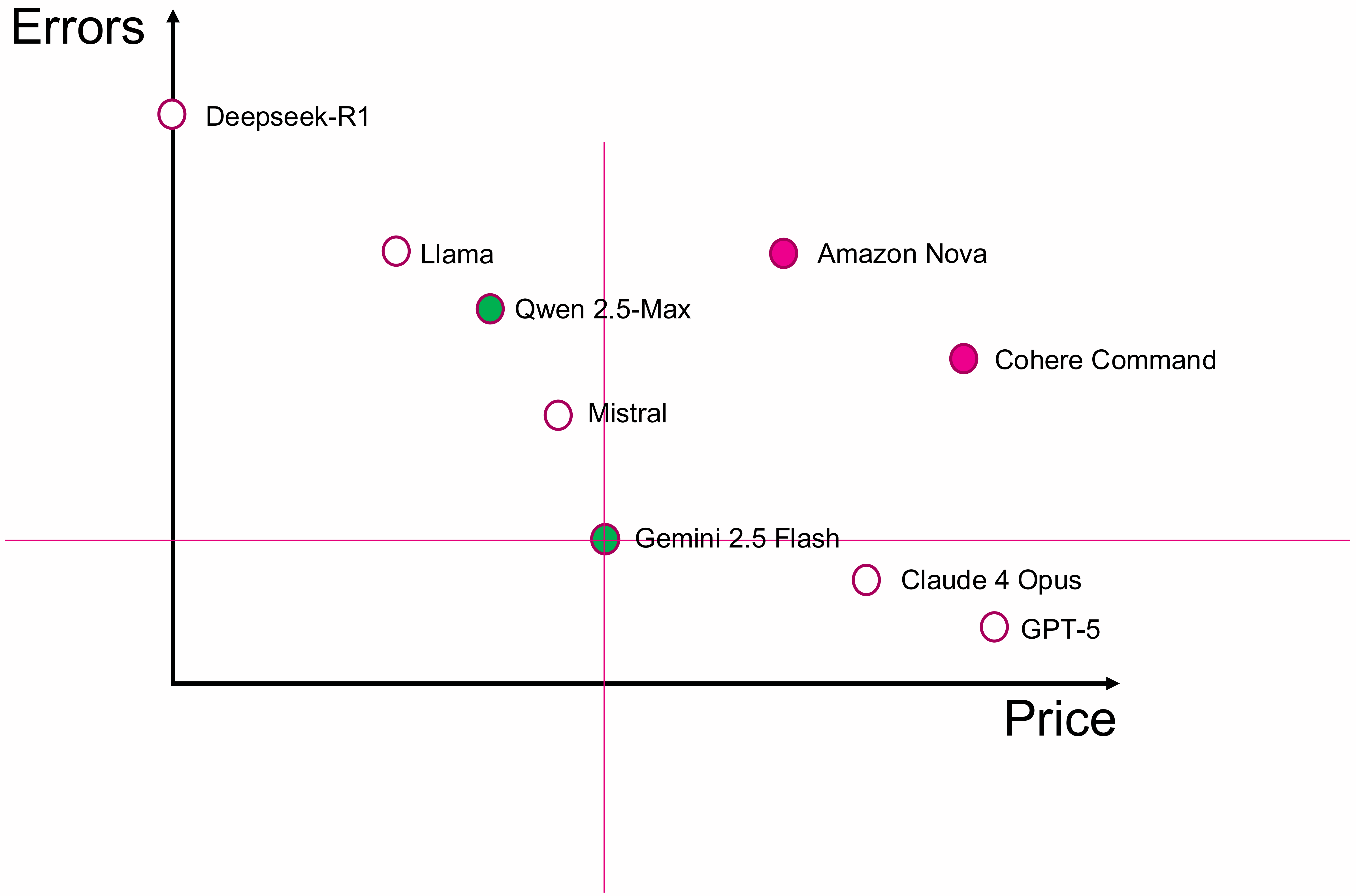
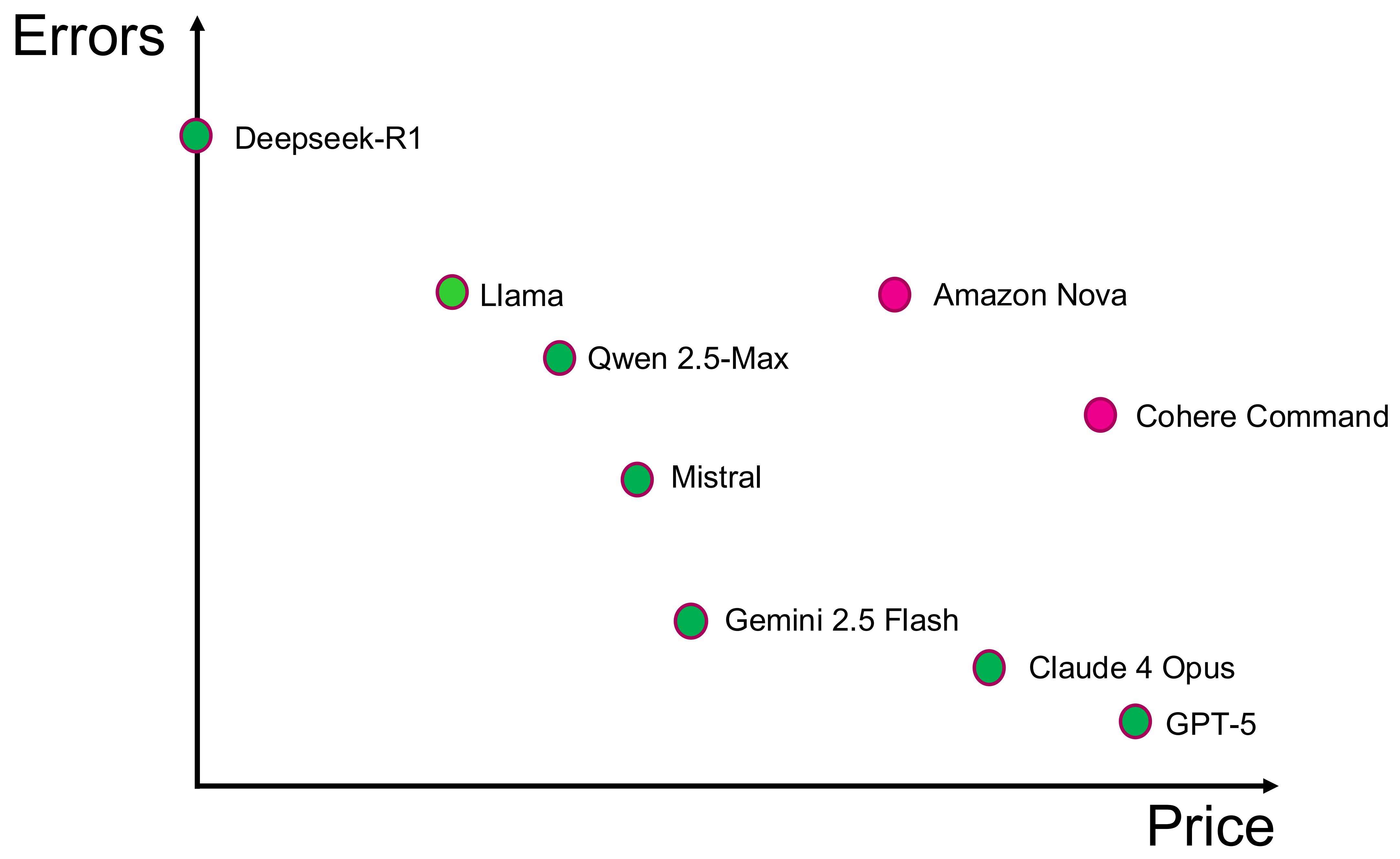
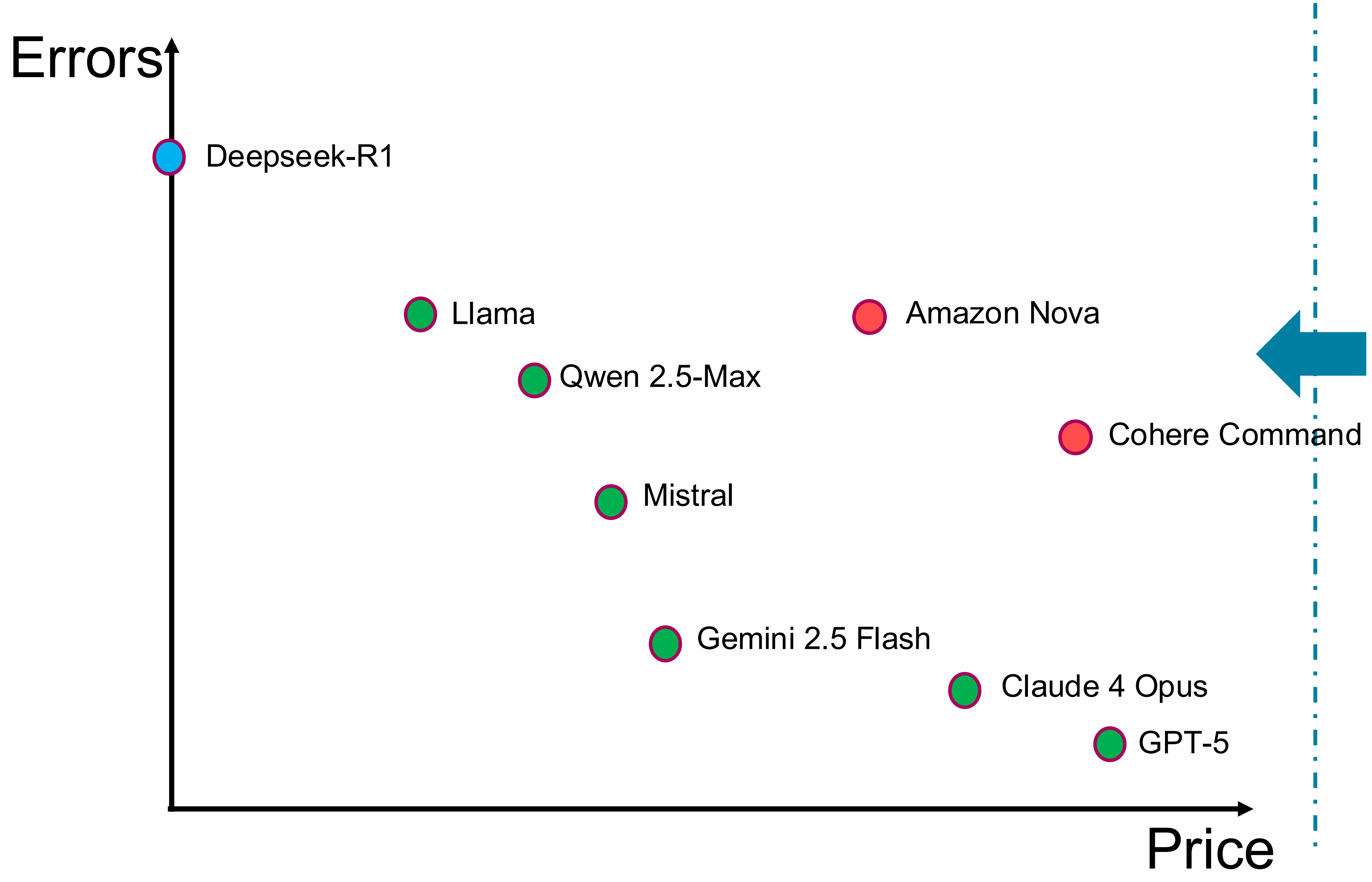


Non-Dominated Solutions (a.k.a., Pareto Front)



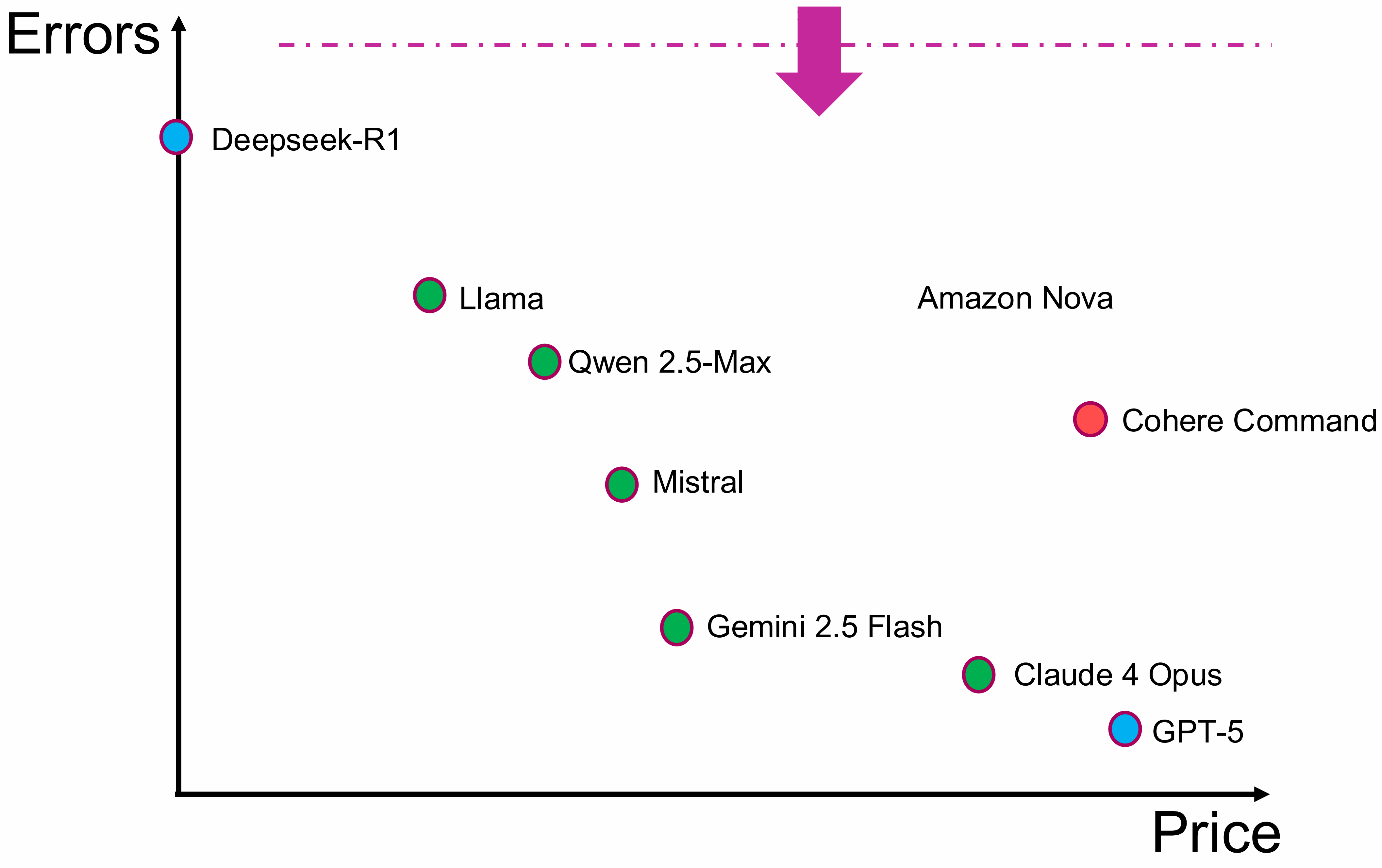
Pick One Objective

Minimize f = Price



Pick One Objective

Minimize f = Errors



Looking for a Trade-Off

Using a Weighted-Sum!

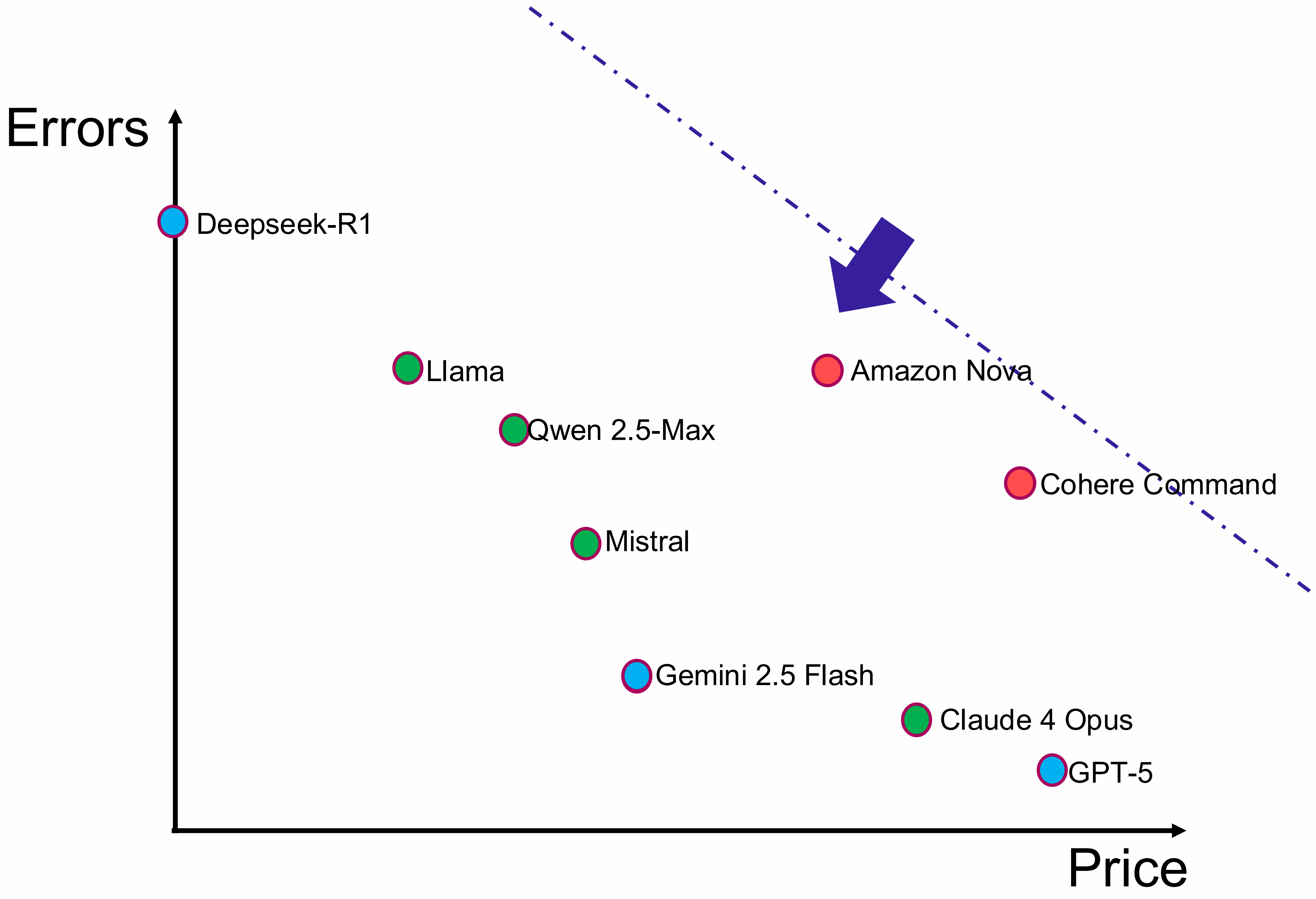
Minimize:

$$\sum_{i=0}^{\#Objectives} W_i \,.\, Objective_i$$

But, what weights to select?

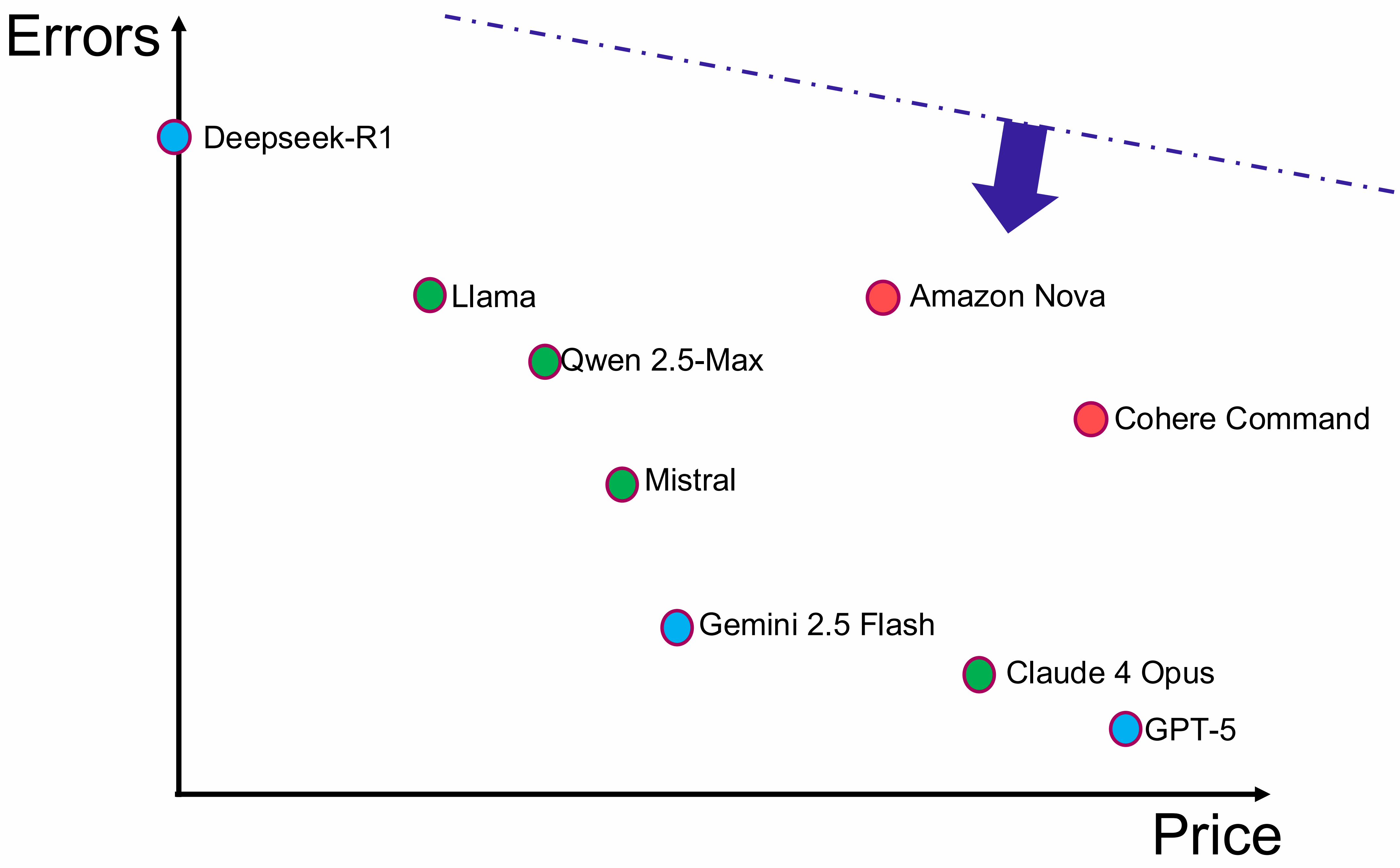
Visual Optimization of Weighted-Sum

Minimize f = **50%** Errors + **50%** Price



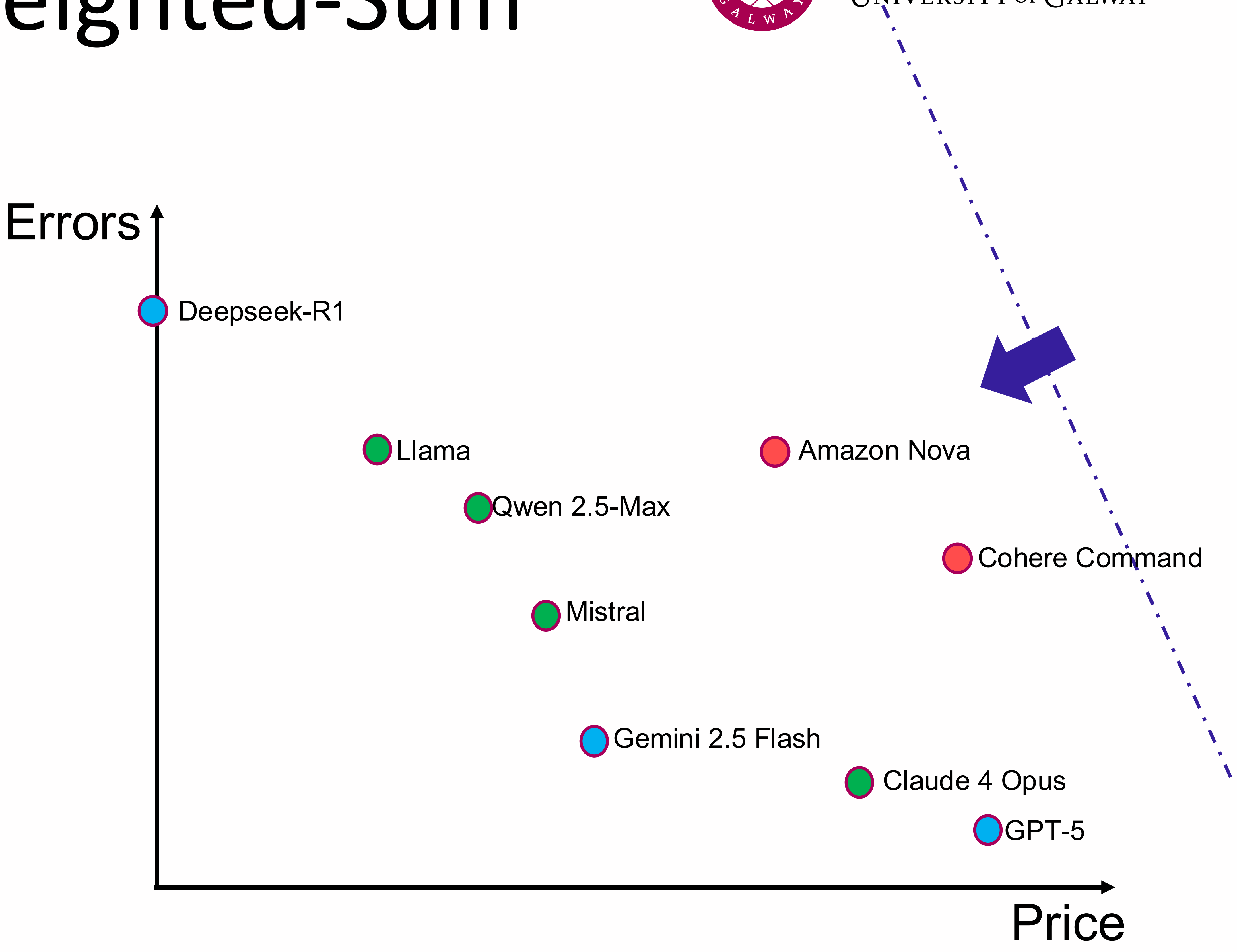
Visual Optimization of Weighted-Sum

Minimize f = **25%** Errors + **75%** Price



Visual Optimization of Weighted-Sum

Minimize f = **75%** Errors + **25%** Price



Visual Optimization of Weighted-Sum

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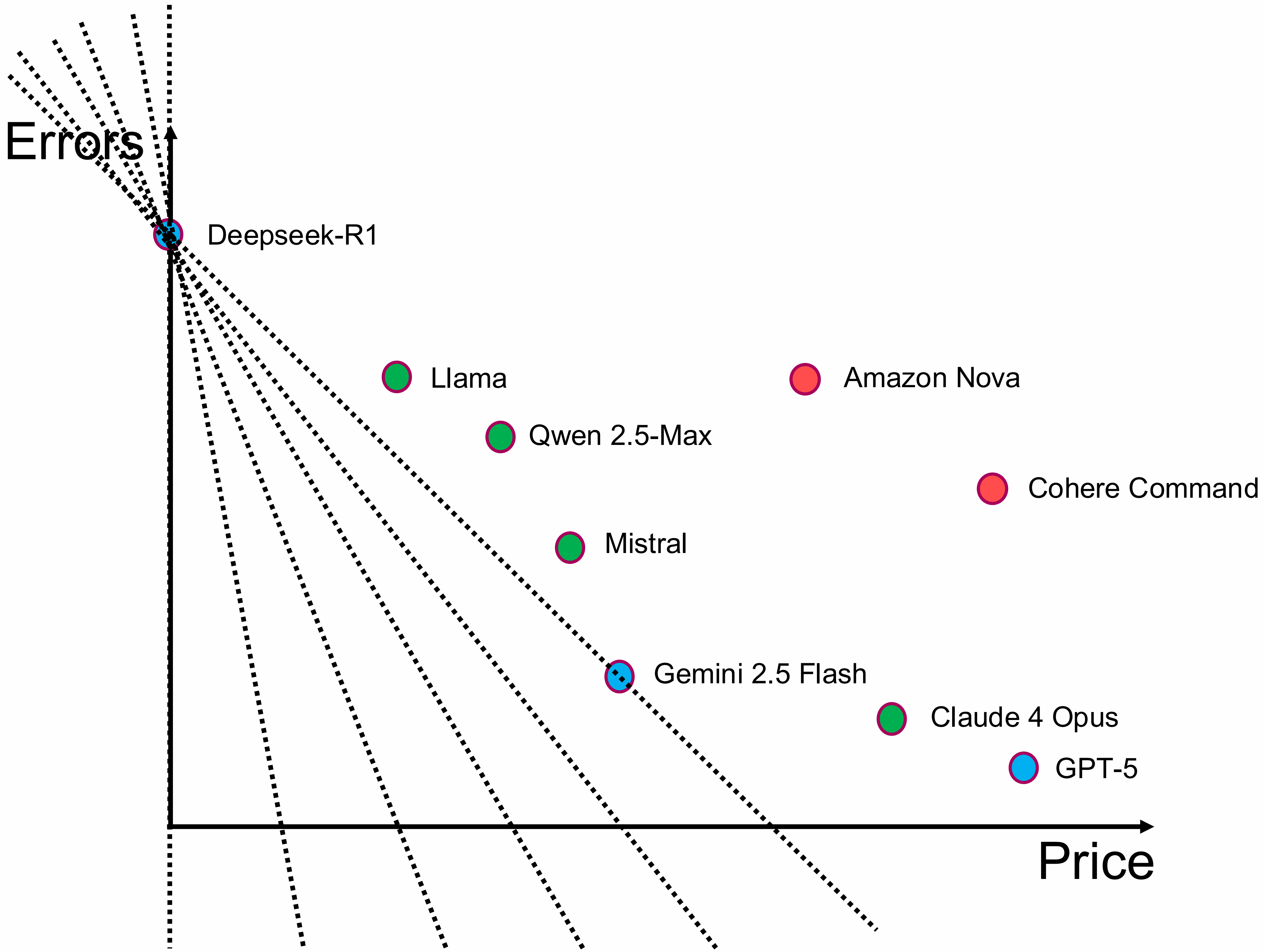
Minimize f = **0%** Errors + **100%** Price

Minimize f = **25%** Errors + **75%** Price

Minimize f = **50%** Errors + **50%** Price

. . .

Minimize f = **100%** Errors + **0%** Price



Visual Optimization of Weighted-Sum

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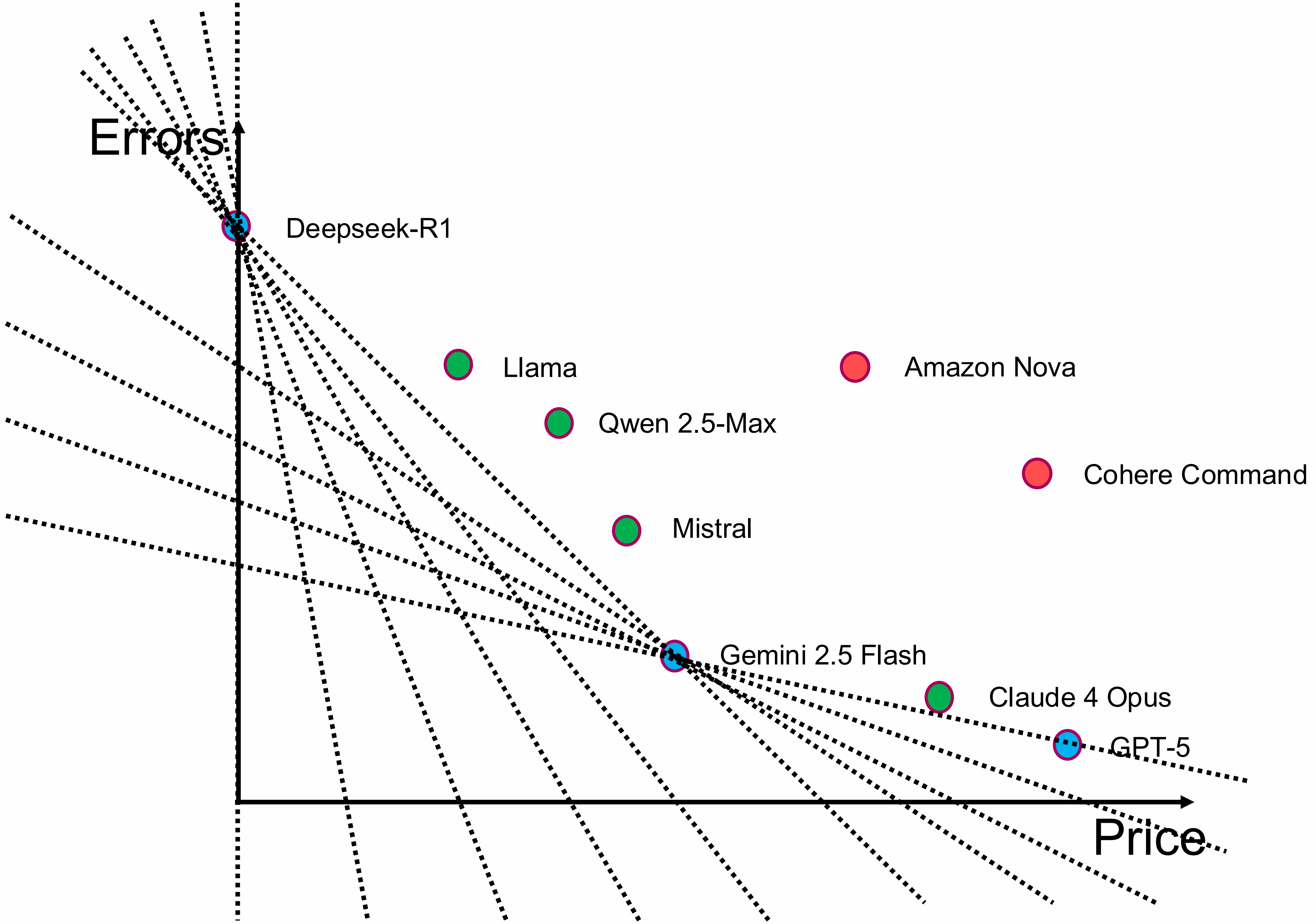
Minimize f = **0%** Errors + **100%** Price

Minimize f = **25%** Errors + **75%** Price

Minimize f = **50%** Errors + **50%** Price

. . .

Minimize f = **100%** Errors + **0%** Price



Visual Optimization of Weighted-Sum

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Minimize f = **0%** Errors + **100%** Price

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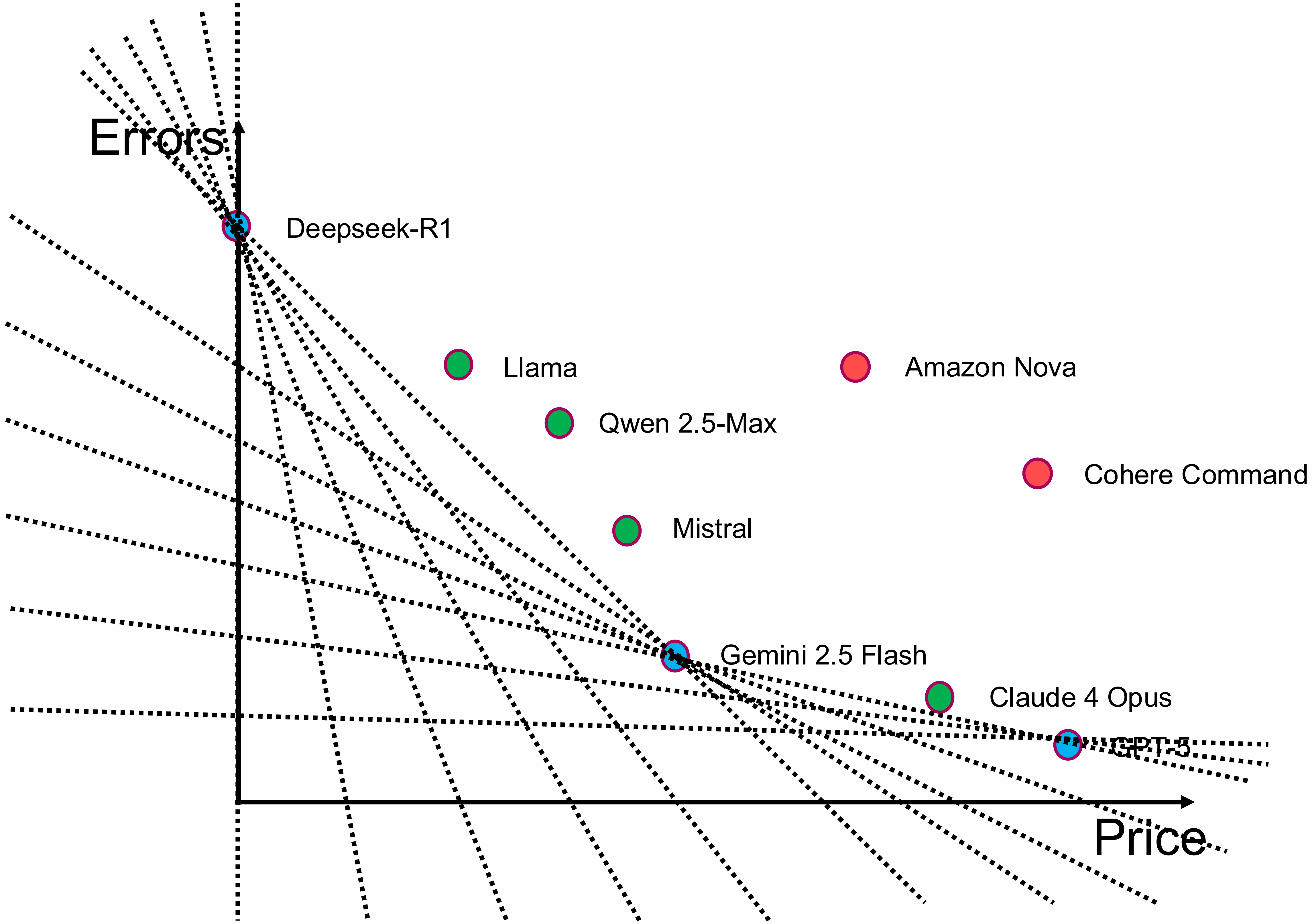
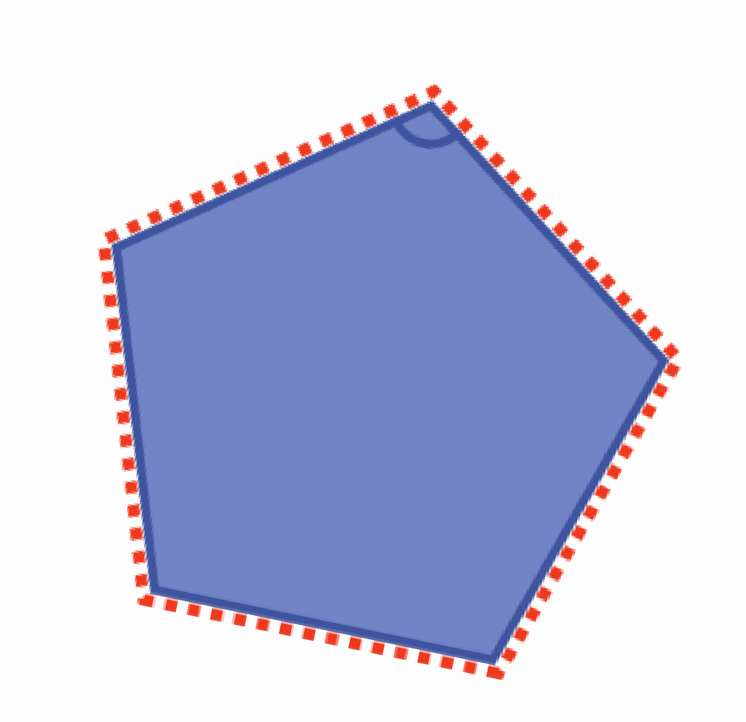
...

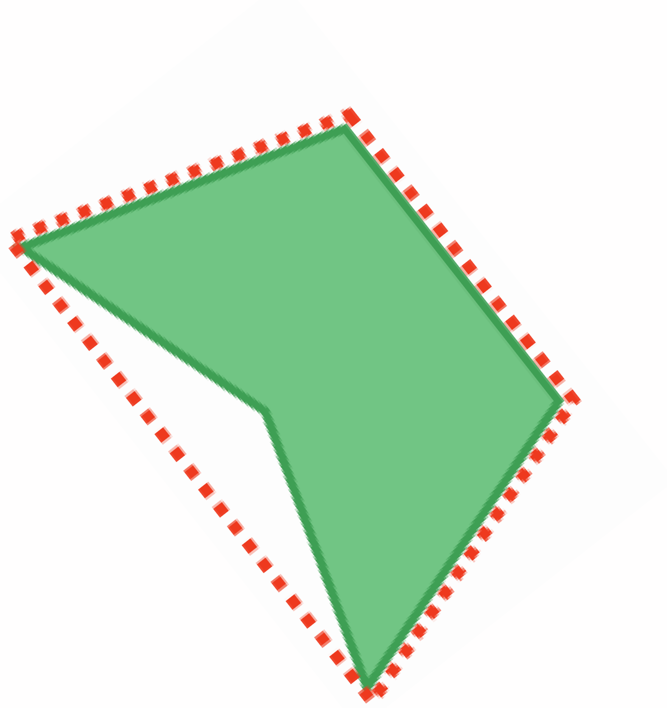
Minimize f = **100%** Errors + **0%** Price



Convex *vs.* Concave



Convex

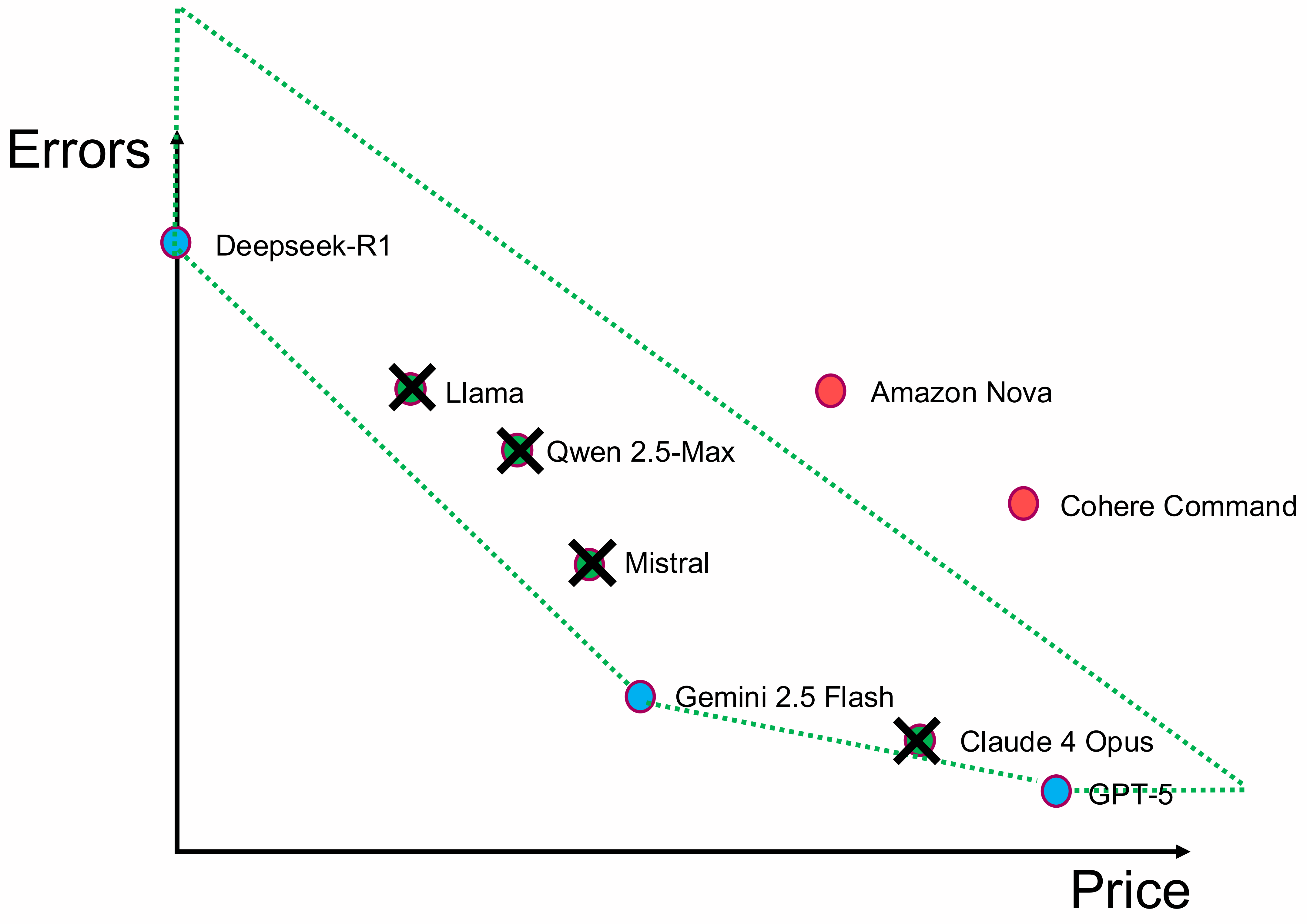


Concave

Rule:

- Weighted-Sum will only allow you to find non-dominated (best) solutions that are in the Convex Hull

Visual Optimization of Weighted-Sum



What If I still want All Non-Dominated Solutions?

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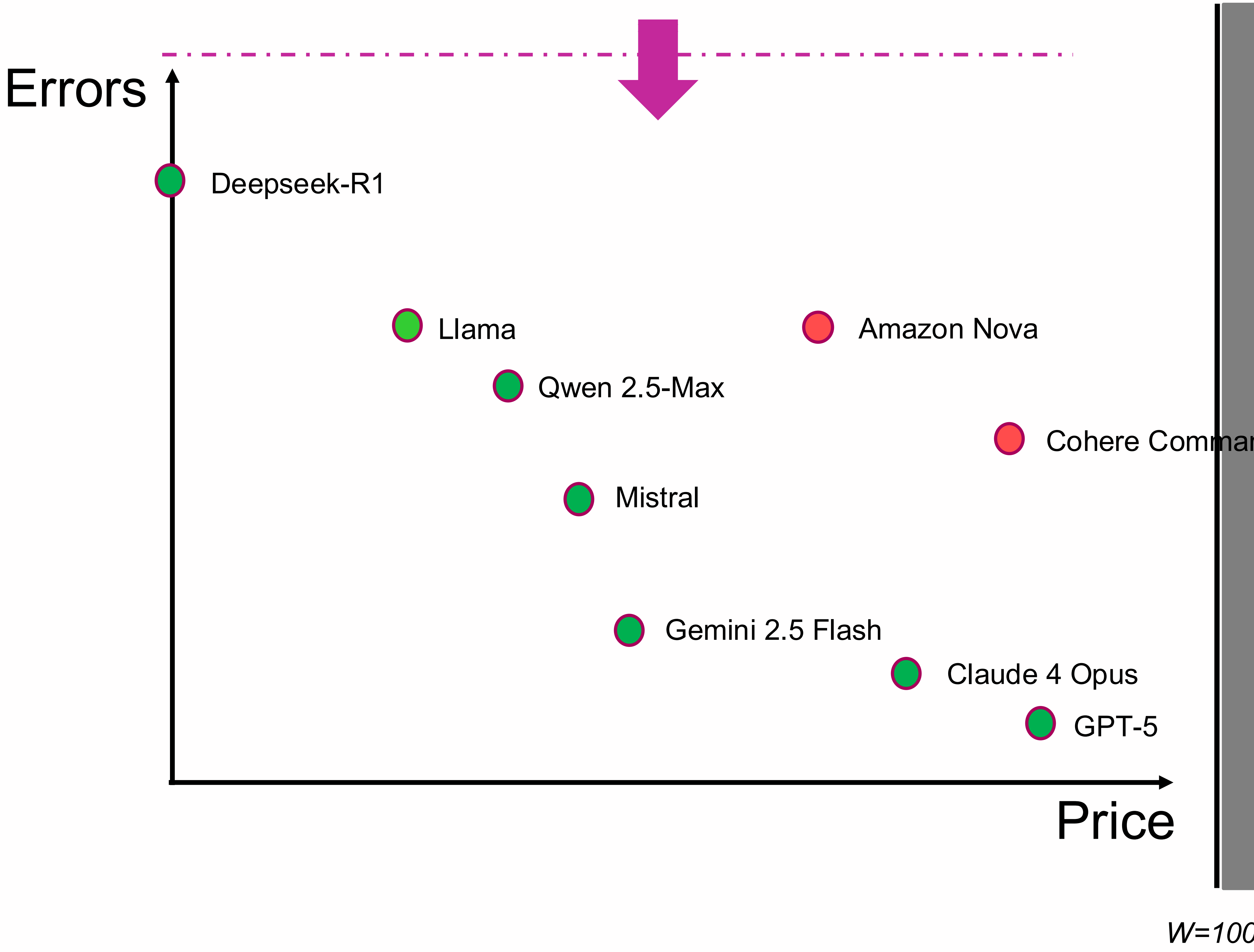
What if I Still Only Want All Non-dominated Solutions?

Better use **ε**-Constraints

Repeat with <u>various</u> values for W

Minimize: Errors
Subject to:
Price < W



Multi-Objective Optimization with TPOT

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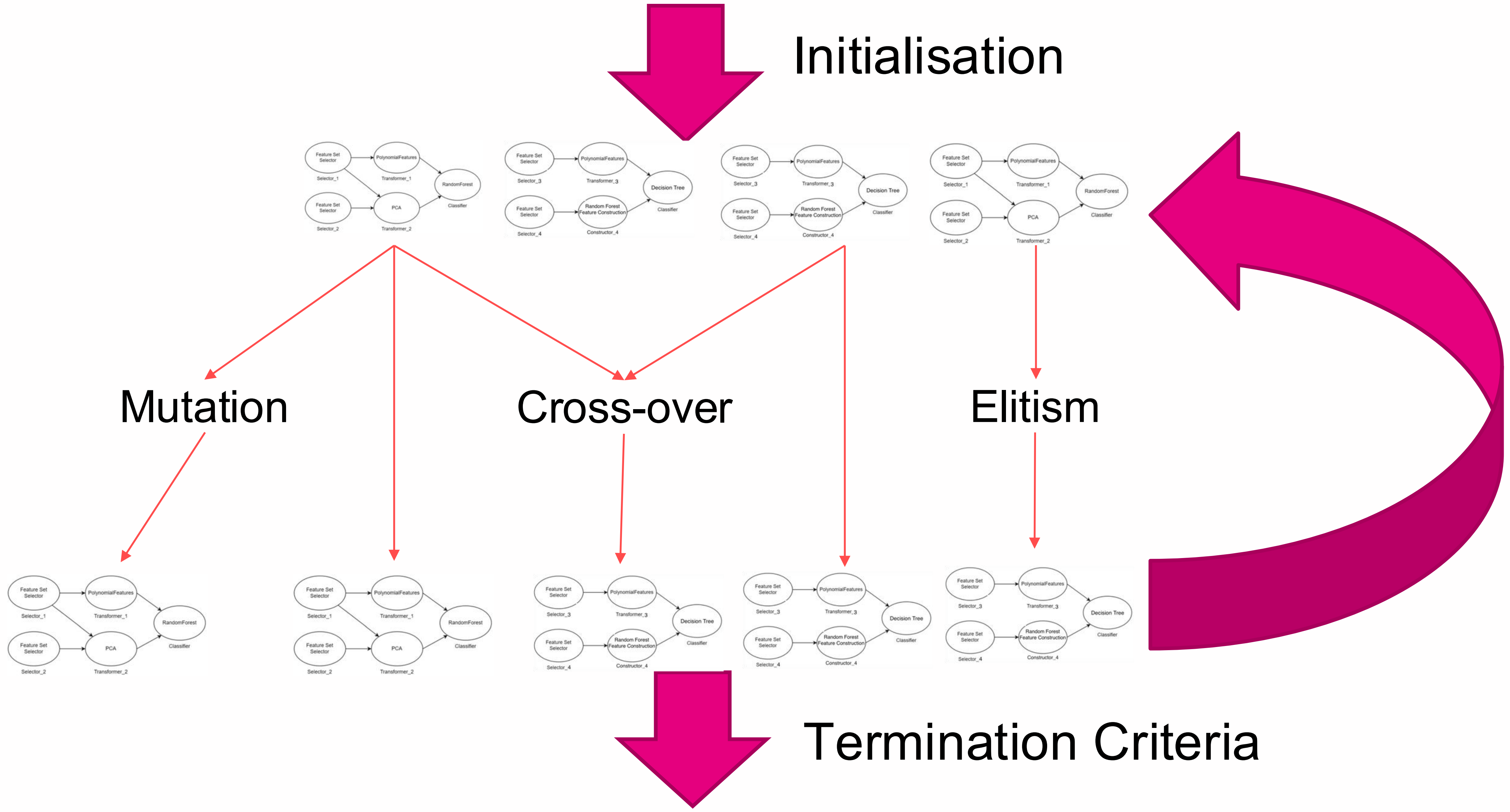

non-dominated and most spread

Keep ~~best~~ solutions for next generation

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Phase 5 (★★★★★): Advanced topics

Self-optimizing systems (Covered)
Federated MLOps

Self-Optimizing MLOps Systems

Vision: **MLOps Holy Grail**
- Learns from optimization history
- System monitors itself to detect and propose optimization opportunities

Technologies:
- Meta-learning: Learning to optimize
- Neural Architecture Search for optimizers
- Automated problem formulation
- Optimization as a Service

Early Results:
- Google's AutoML Zero:
  - Automatically evolve entire ML pipelines (algorithms + architectures + optimization strategies) form scratch.
  - Minimise Human-designed bias

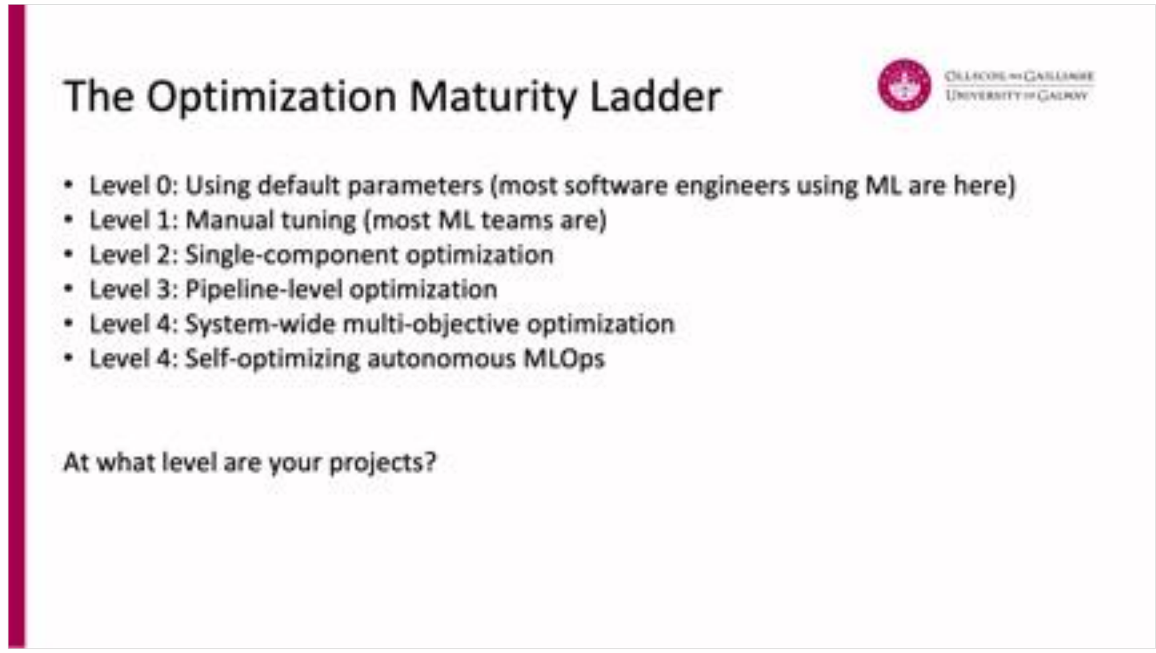
Final Takeaways

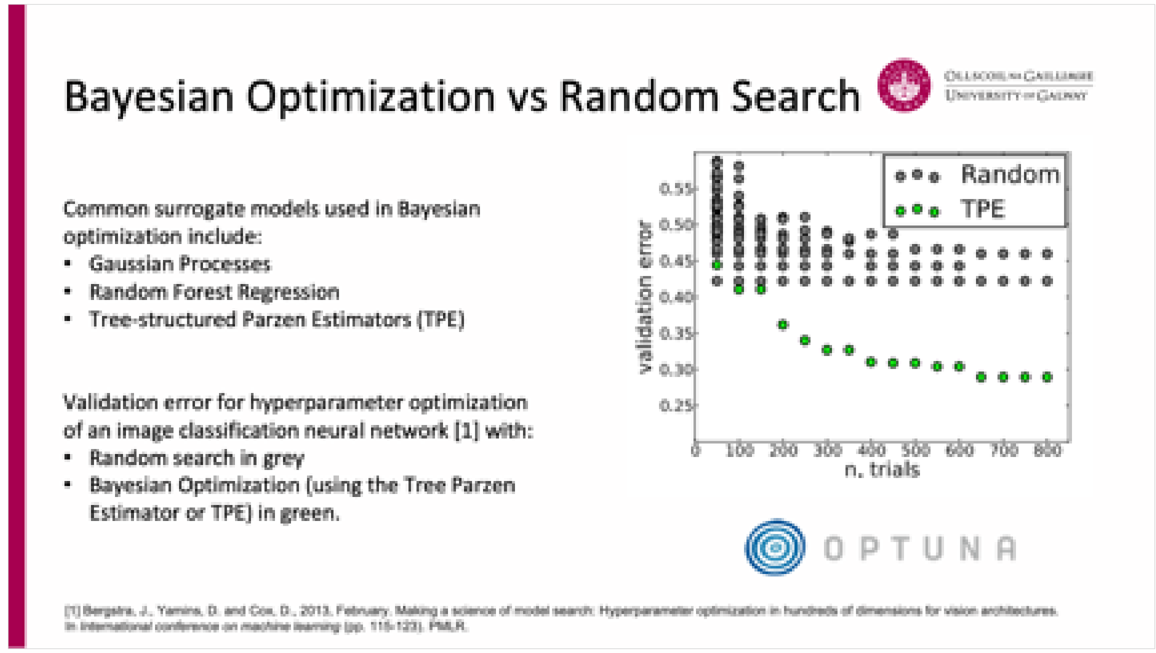
Key Messages:

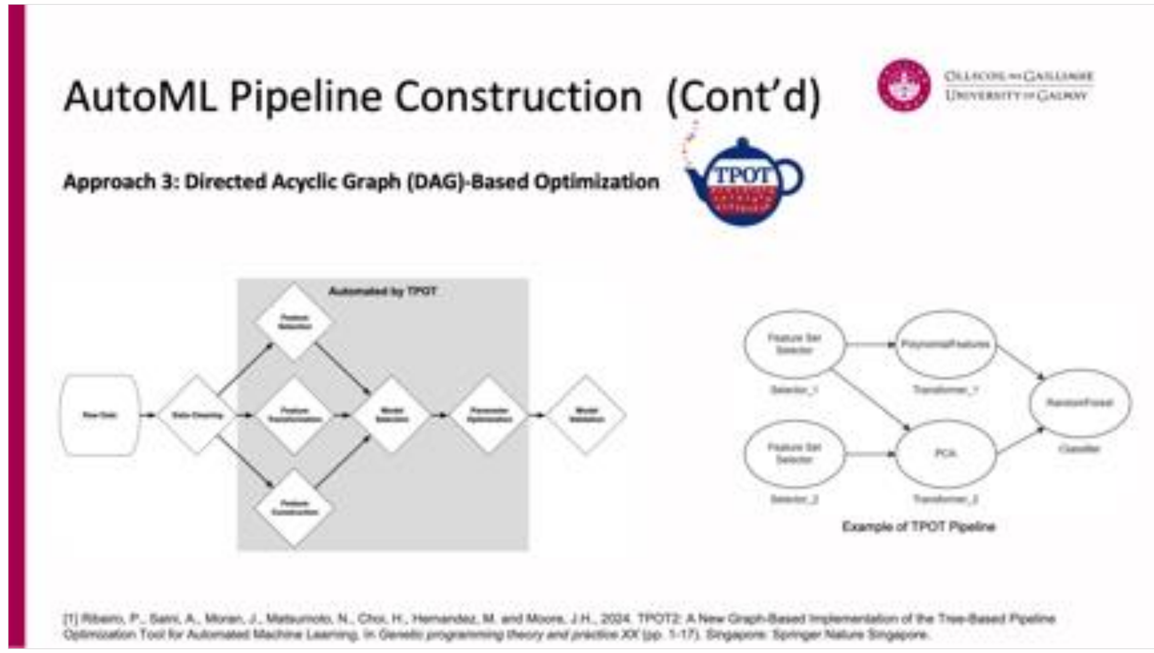
- Optimization is accessible and pays off
  - Open-source tools are production-ready
  - 30-60% improvements are common
- Main advantage is not saving time, but doing things that were not possible before due to the lack of time
  - E.g., Collaboration between Data Scientist and Business Experts, Multi-Criteria Decision Analysis, etc.
- Continuous journey: Optimization is never "done"

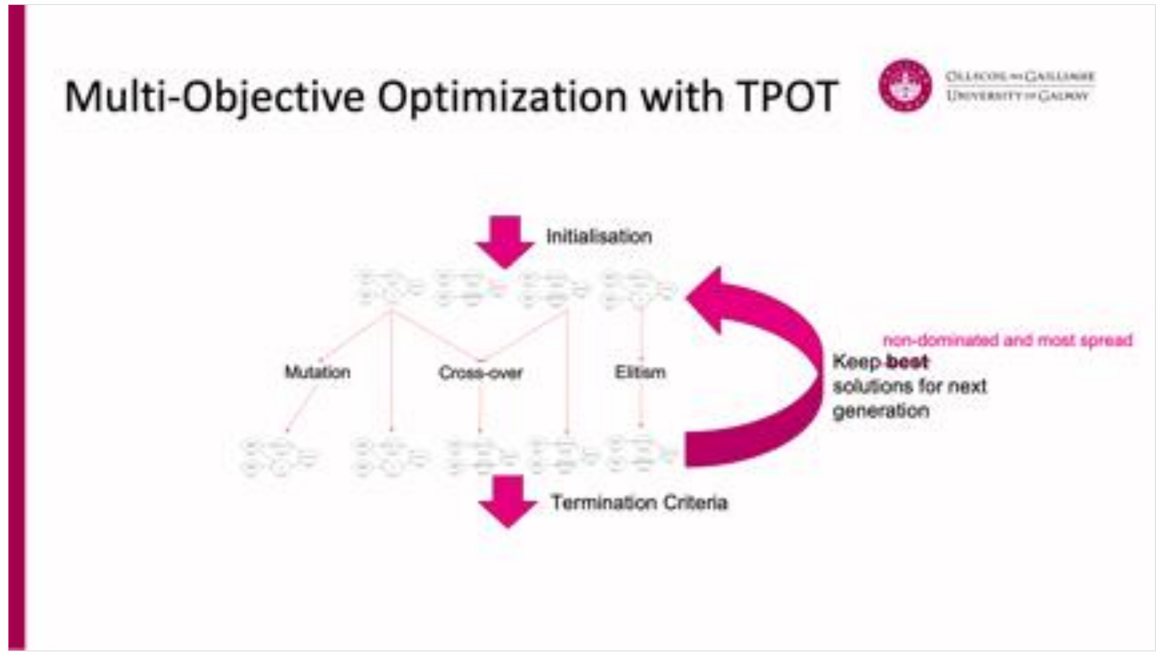
Closing Statement: "The future of MLOps isn't just automated. It is optimized."
The question isn't whether to optimize, but how fast you can move up the maturity ladder.

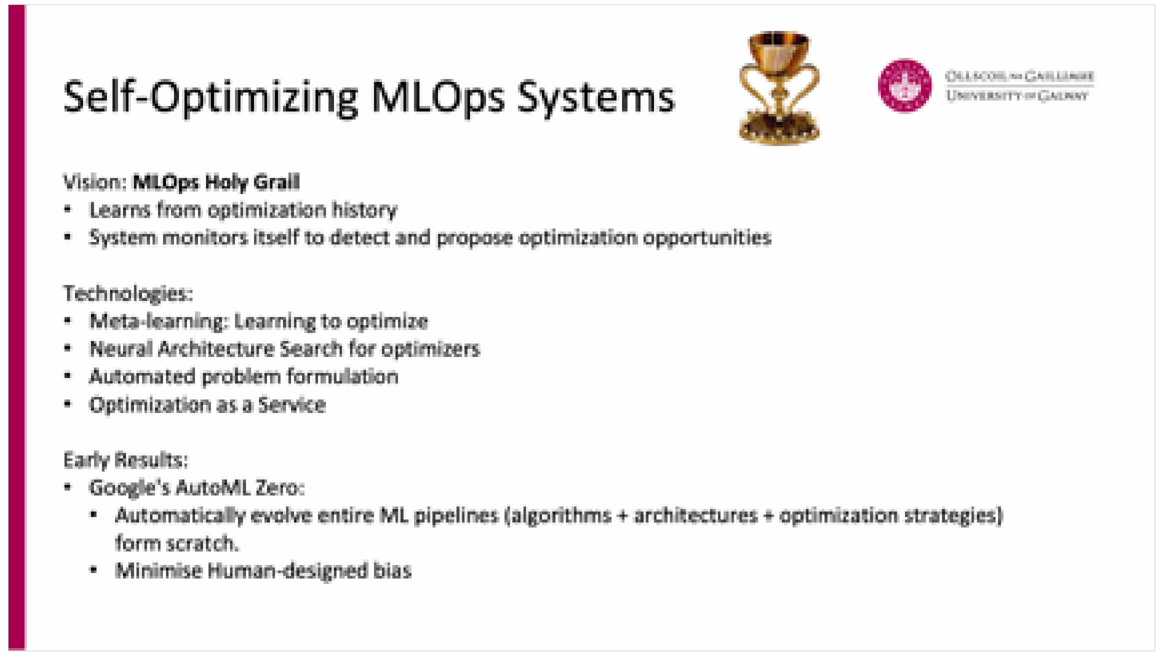
Q&A

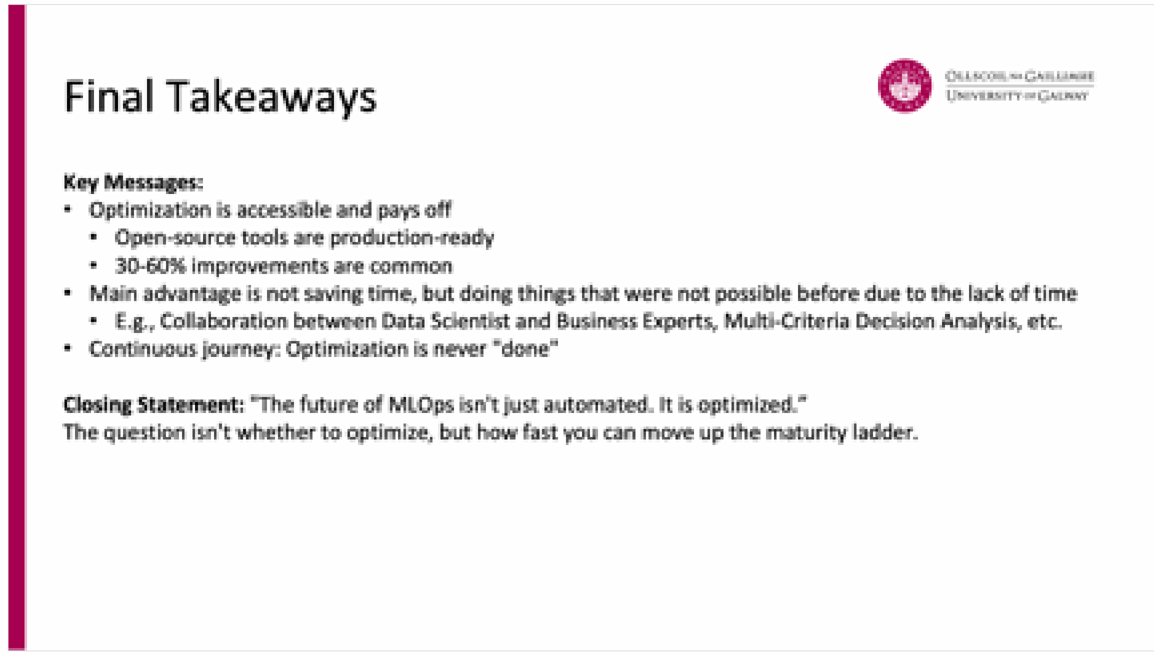

The Optimization Maturity Ladder
Level 0: Using default parameters (most software engineers using ML are here)
Level 1: Manual tuning (most ML teams are)
Level 2: Single-component optimization
Level 3: Pipeline-level optimization
Level 4: System-wide multi-objective optimization
Level 4: Self-optimizing autonomous MLOps
At what level are your projects?


Bayesian Optimization vs Random Search
Common surrogate models used in Bayesian optimization include:
Gaussian Processes
Random Forest Regression
Tree-structured Parzen Estimators (TPE)
Validation error for hyperparameter optimization of an image classification neural network [1] with:
Random search in grey
Bayesian Optimization (using the Tree Parzen Estimator or TPE) in green.
Random
TPE
validation error
n. trials
OPTUNA
[1] Bergstra, J., Yamins, D. and Cox, D., 2013, February. Making a science of model search: Hyperparameter optimization in hundreds of dimensions for vision architectures. In International conference on machine learning (pp. 115-123). PMLR.


AutoML Pipeline Construction (Cont'd)
Approach 3: Directed Acyclic Graph (DAG)-Based Optimization
TPOT
Automated by TPOT
Example of TPOT Pipeline
[1] Ribeiro, P., Saini, A., Moran, J., Matsumoto, N., Choi, H., Hernandez, M. and Moore, J.H., 2024. TPOT2: A New Graph-Based Implementation of the Tree-Based Pipeline Optimization Tool for Automated Machine Learning. In Genetic programming theory and practice XX (pp. 1-17). Singapore: Springer Nature Singapore.


Multi-Objective Optimization with TPOT
Initialisation
Mutation
Cross-over
Elitism
non-dominated and most spread
Keep best solutions for next generation
Termination Criteria


Self-Optimizing MLOps Systems
Vision: MLOps Holy Grail
Learns from optimization history
System monitors itself to detect and propose optimization opportunities
Technologies:
Meta-learning: Learning to optimize
Neural Architecture Search for optimizers
Automated problem formulation
Optimization as a Service
Early Results:
Google's AutoML Zero:
Automatically evolve entire ML pipelines (algorithms + architectures + optimization strategies) form scratch.
Minimise Human-designed bias


Final Takeaways
Key Messages:
Optimization is accessible and pays off
Open-source tools are production-ready
30-60% improvements are common
Main advantage is not saving time, but doing things that were not possible before due to the lack of time
E.g., Collaboration between Data Scientist and Business Experts, Multi-Criteria Decision Analysis, etc.
Continuous journey: Optimization is never "done"
Closing Statement: "The future of MLOps isn't just automated. It is optimized."
The question isn't whether to optimize, but how fast you can move up the maturity ladder.