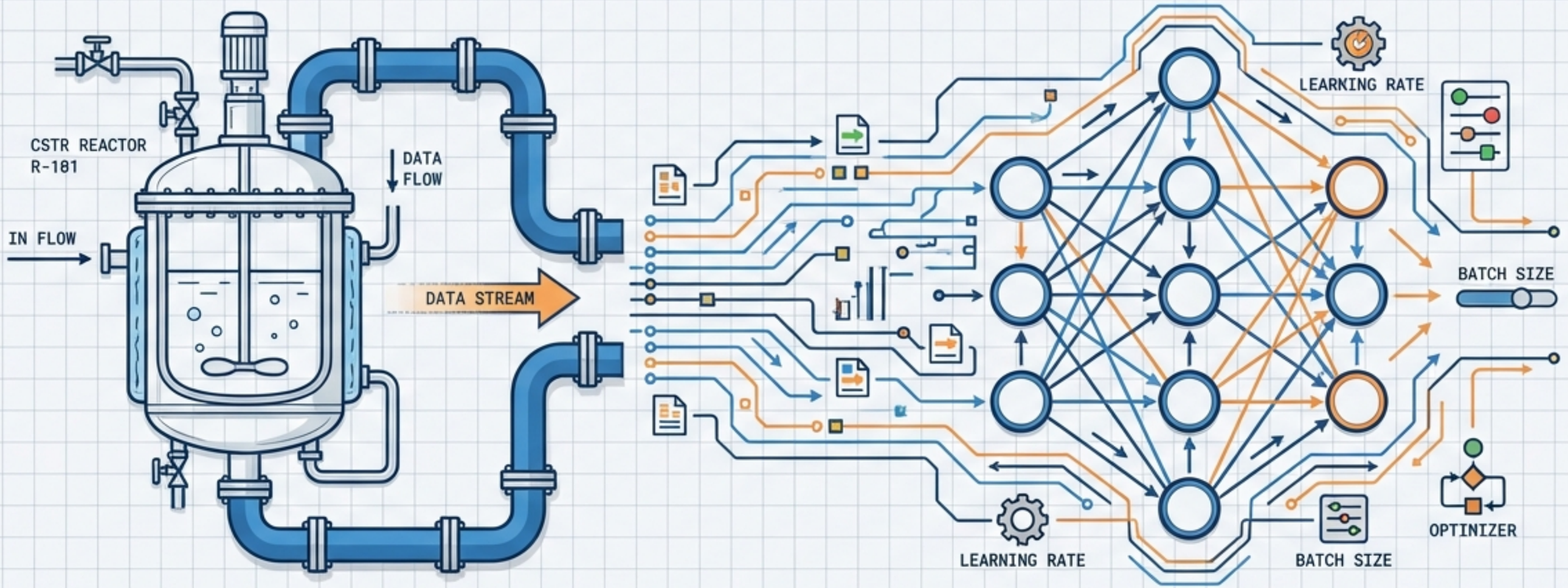
超參數調整 (Hyperparameter Tuning)

從經驗法則到貝氏最佳化：釋放模型的最大潛力



逢甲大學 化學工程學系 | 莊曜禎 助理教授

為什麼調參至關重要？ (Why Tuning Matters?)

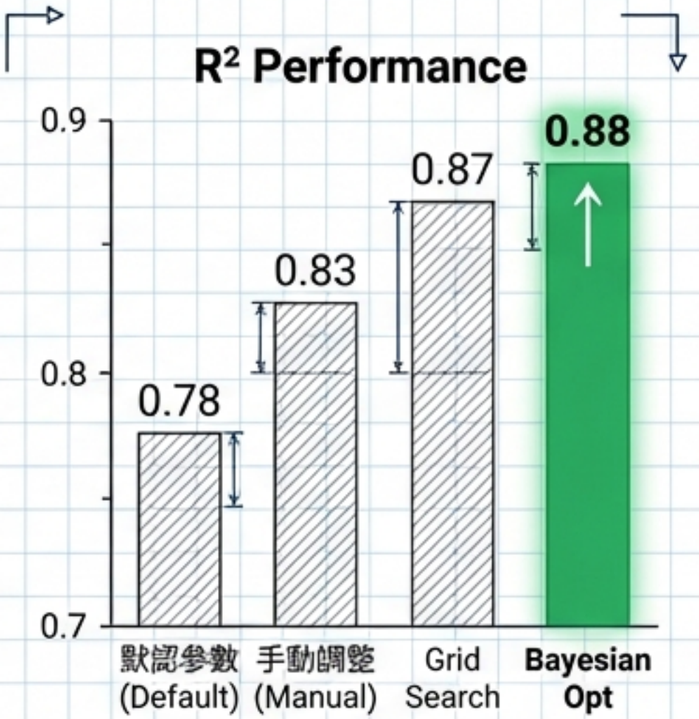
正確調參可提升 10-15% 性能，將模型從「堪用」提升至「高性能」。

Note

ChemE Challenges

- **小樣本** (Small Datasets): 實驗成本高，數據有限
- **多目標** (Multi-objective): 需兼顧產率、能耗與品質

配置	Test R^2	Time (s)
默認參數 (Default)	0.78	2.3s
手動調整 (Manual)	0.83	5.1s
Grid Search	0.87	45s
Bayesian Opt	**0.88**	**18s**

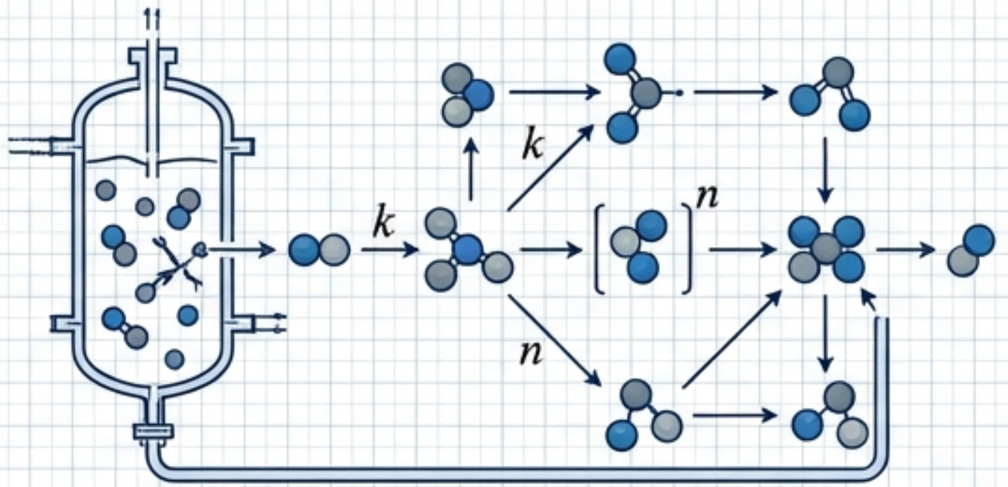


Industrial_Blueprint_v1		PROJECT: OPTIMIZATION-ML	
APPROVED	APPROVED	DRAWN BY: AI ENGINEER	DATE: 2024.06.15
	TECHNICAL SPECIFICATION	DWG NO: SLIDE_02_PROBLEM_STATEMENT	

Technical Specification

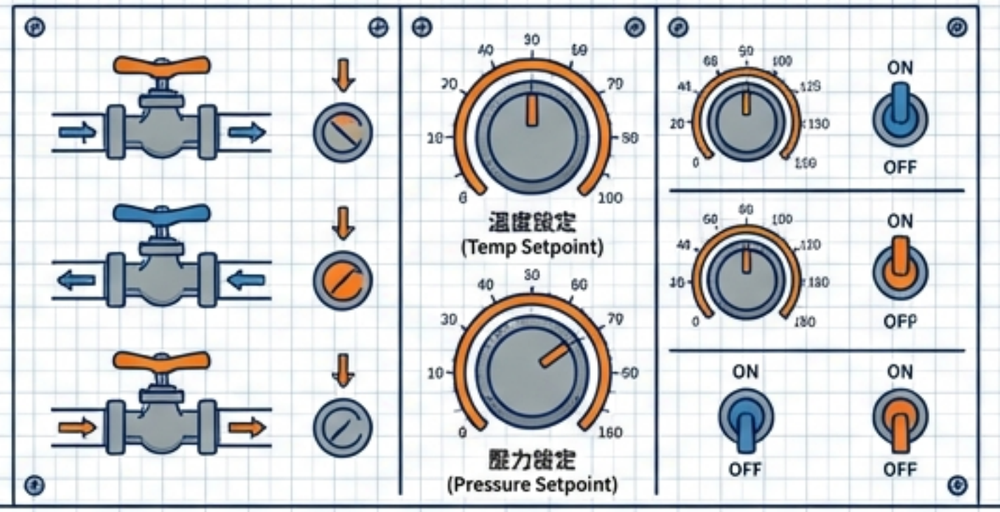
核心概念：參數 vs. 超參數

模型參數 (Model Parameters)



- 定義：模型從數據中自動學習的變量
- 類比：化學反應動力學機制 (k, n)
- 例子：Weights, Biases (w, b)

超參數 (Hyperparameters)



- 定義：訓練前人為設定的配置
- 類比：操作變數 (溫度、壓力設定點)
- 例子：Learning Rate, Tree Depth

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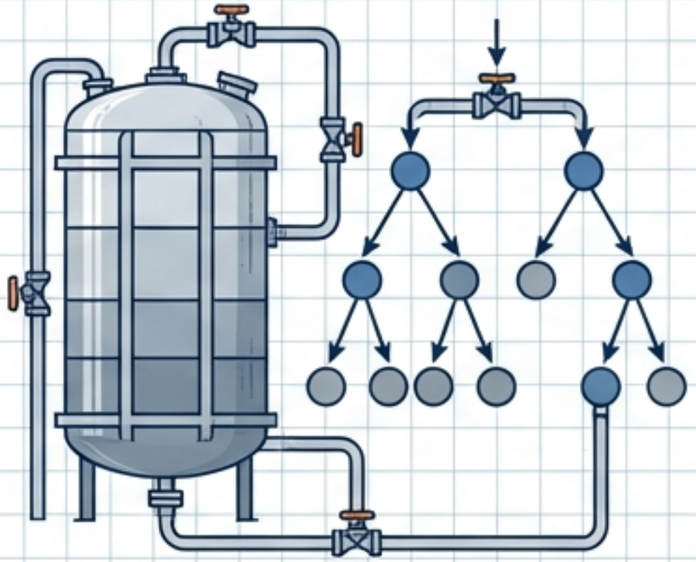
	Drawn by: AI ENGINEER	Title: OPTIMIZATION-ML
Technical Specification	Date: 2024.06.16	Drawing Number: SLIDE_03_PARAMS_VS_HYPERPARAMS
		Approved: -

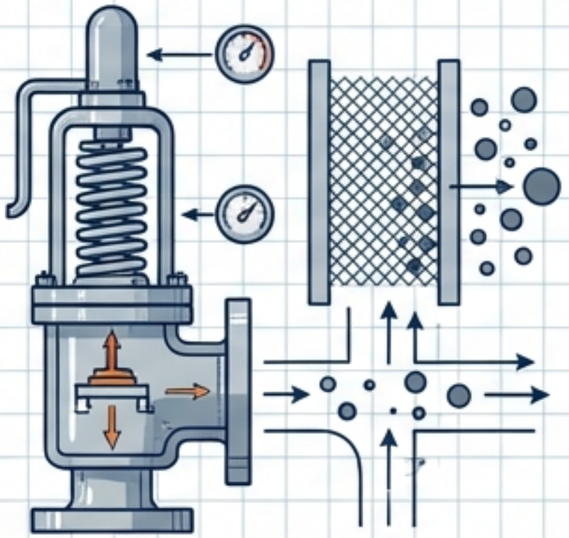
超參數解剖學：我們在調整什麼？

結構與容量 (Structure)



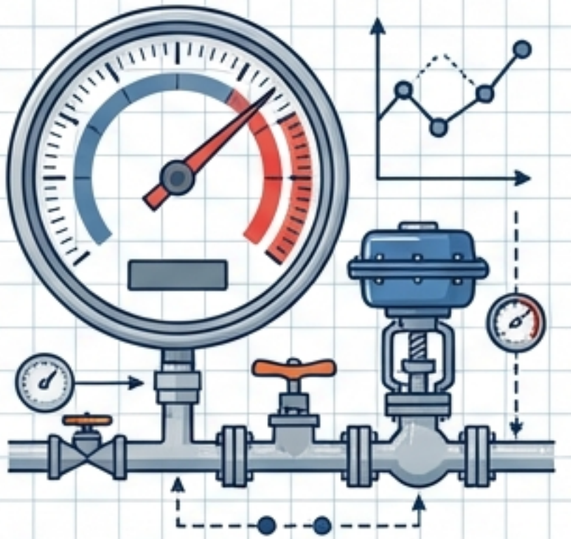
- 決定模型的複雜度
- 例子：Tree Depth, Layer Count, n_estimators

正則化 (Regularization)



- 防止過擬合 (Preventing Overfitting)
- 例子：Alpha, Dropout, min_samples_split

優化過程 (Optimization)



- 收斂速度與穩定性
- 例子：Learning Rate, Batch Size

⚠ 平衡關鍵：過大 → 過擬合 (Overfitting) | 過小 → 欠擬合 (Underfitting)

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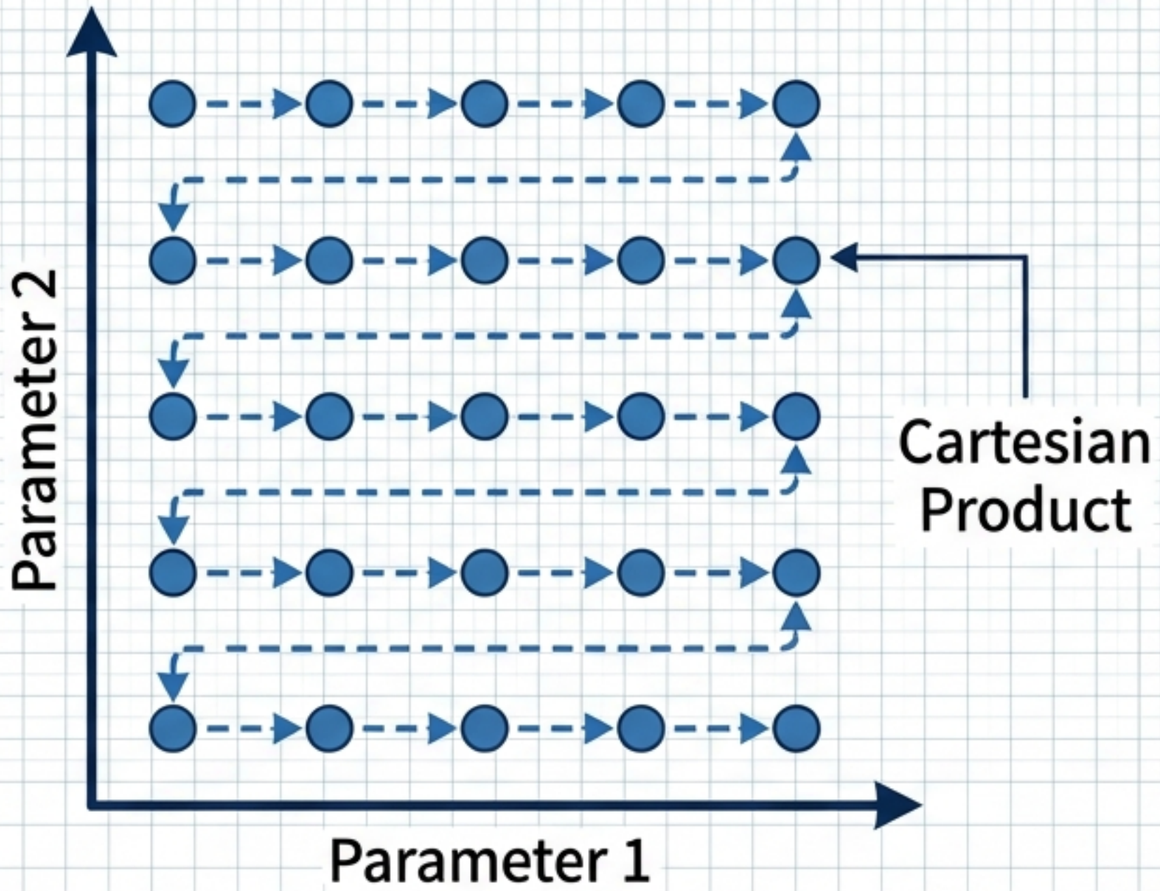
Technical Specification	Date: 2024.06.16	Drawing Number: SLIDE_04_HYPERPARAMETER_ANATOMY
		Approves: -

方法 1：Grid Search（網格搜索）

窮舉式搜索。定義候選值列表，生成所有可能的組合。



Pros & Cons

- **Pros:**
  - ✅ 完整性 (Completeness)
  - ✅ 可並行化 (Parallelizable)
- **Cons:**
  - ⚠️ 維度詛咒 (Curse of Dimensionality)

  10 parameters × 5 values = 5^{10} ≈ 9.7 million combinations

Combinatorial Explosion

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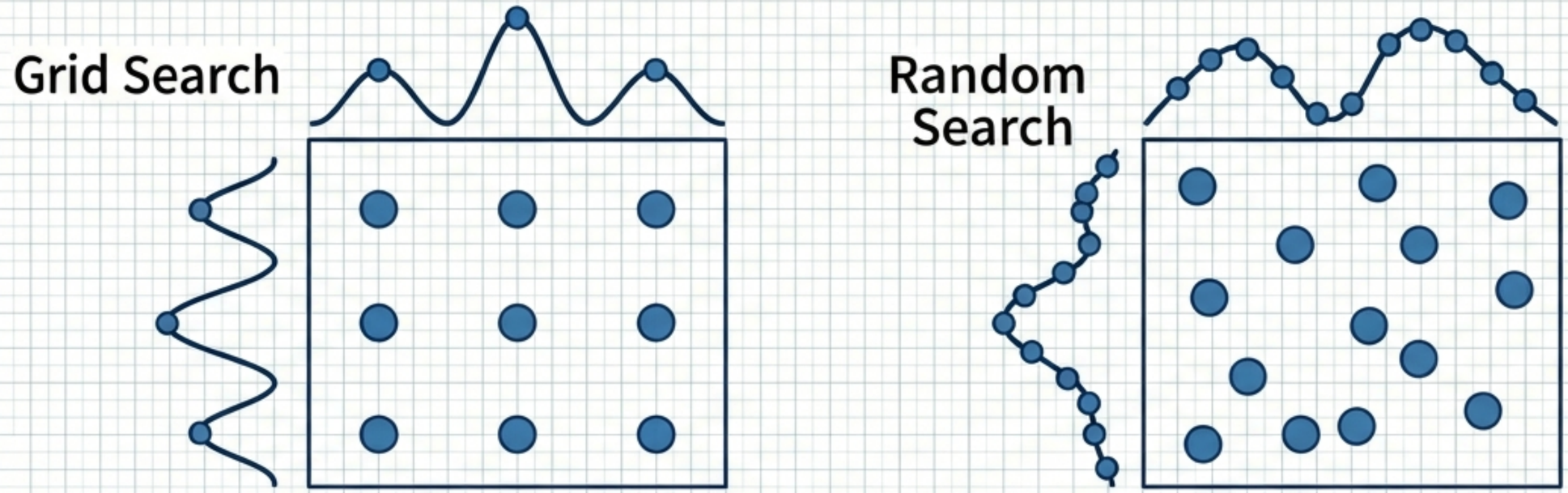
Technical Specification

方法 2：Random Search（隨機搜索）

從分佈中隨機抽樣，而非固定網格。



Bergstra & Bengio Insight: 在高維空間中，往往只有少數幾個超參數真正重要。

Random Search 在重要維度上能探索更多不同的值。

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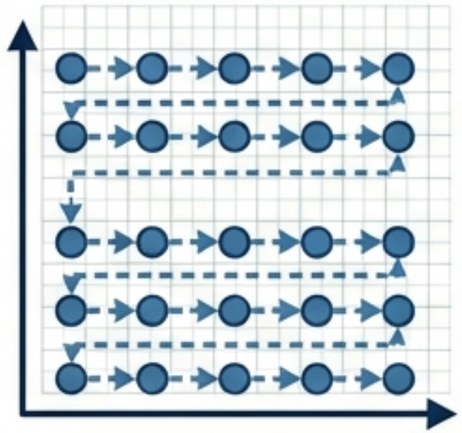
	Drawn by: AI ENGINEER	File: OPTIMIZATION-ML
Technical Specification	Date: 2024.06.16	Drawing Number: SLIDE_05_RANDOM SEARCH

Technical Specification

直觀對比：Grid vs. Random

Grid Search



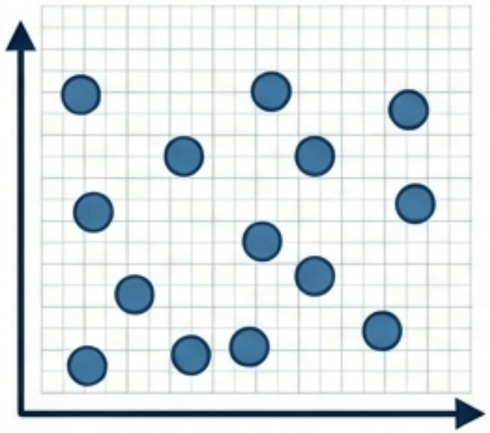
Trials: 256

Time: 45 Seconds

Result (R^2): 0.8534

WINNER

Random Search



Trials: 100

Time: 18 Seconds

Result (R^2): 0.8612

結論：Random Search 用更少的嘗試，覆蓋了更廣的有效空間。

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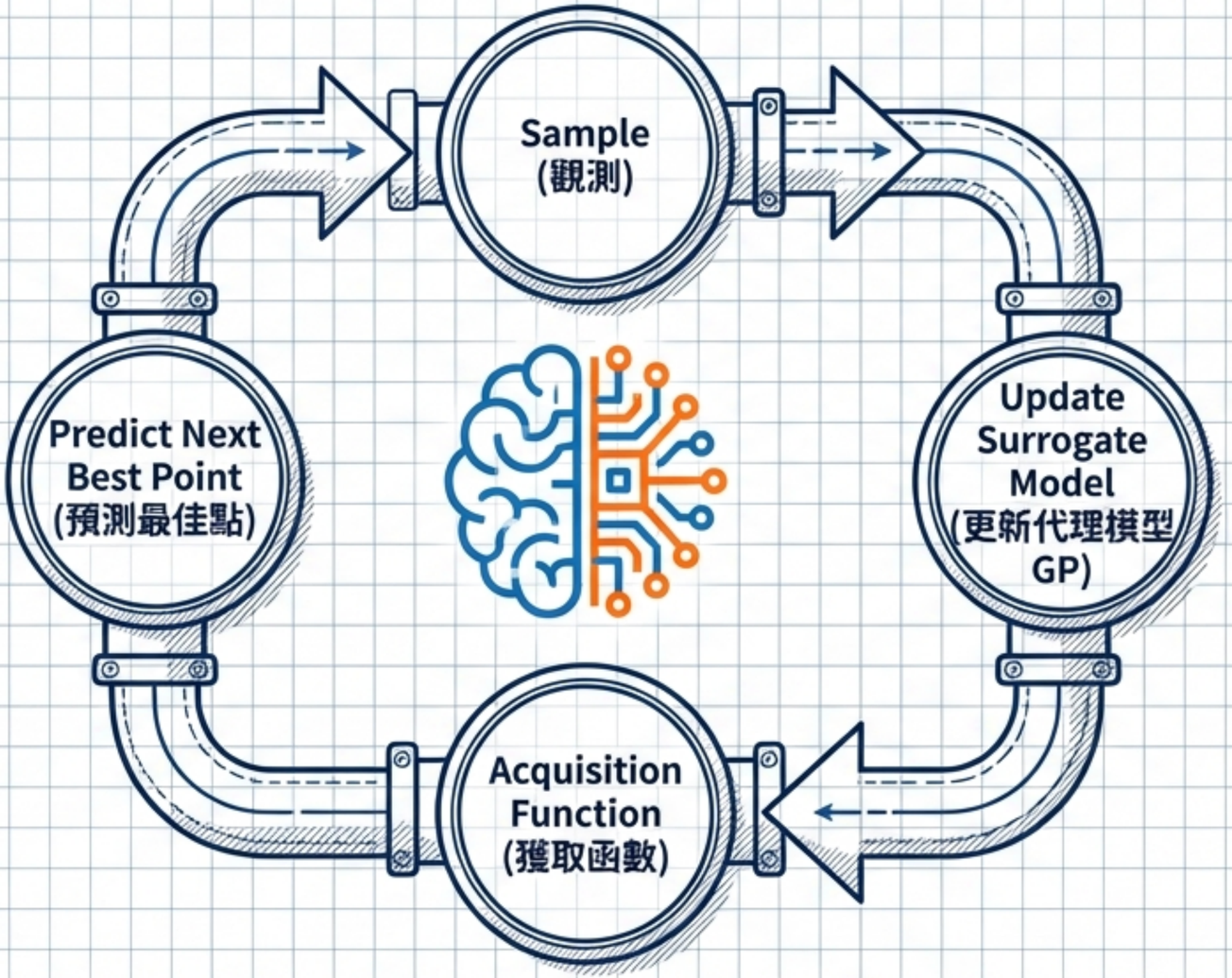
Technical Specification	Date: 2024.06.16	Drawing Number: SLIDE_06_GRID_VS_RANDOM

方法 3：Bayesian Optimization (貝氏最佳化)

智能搜索：利用「過去的嘗試」指導「下一步的探索」。



Engineer Analogy：就像有經驗的工程師，根據上一次的實驗結果來調整反應器的旋鈕，而不是盲目猜測。

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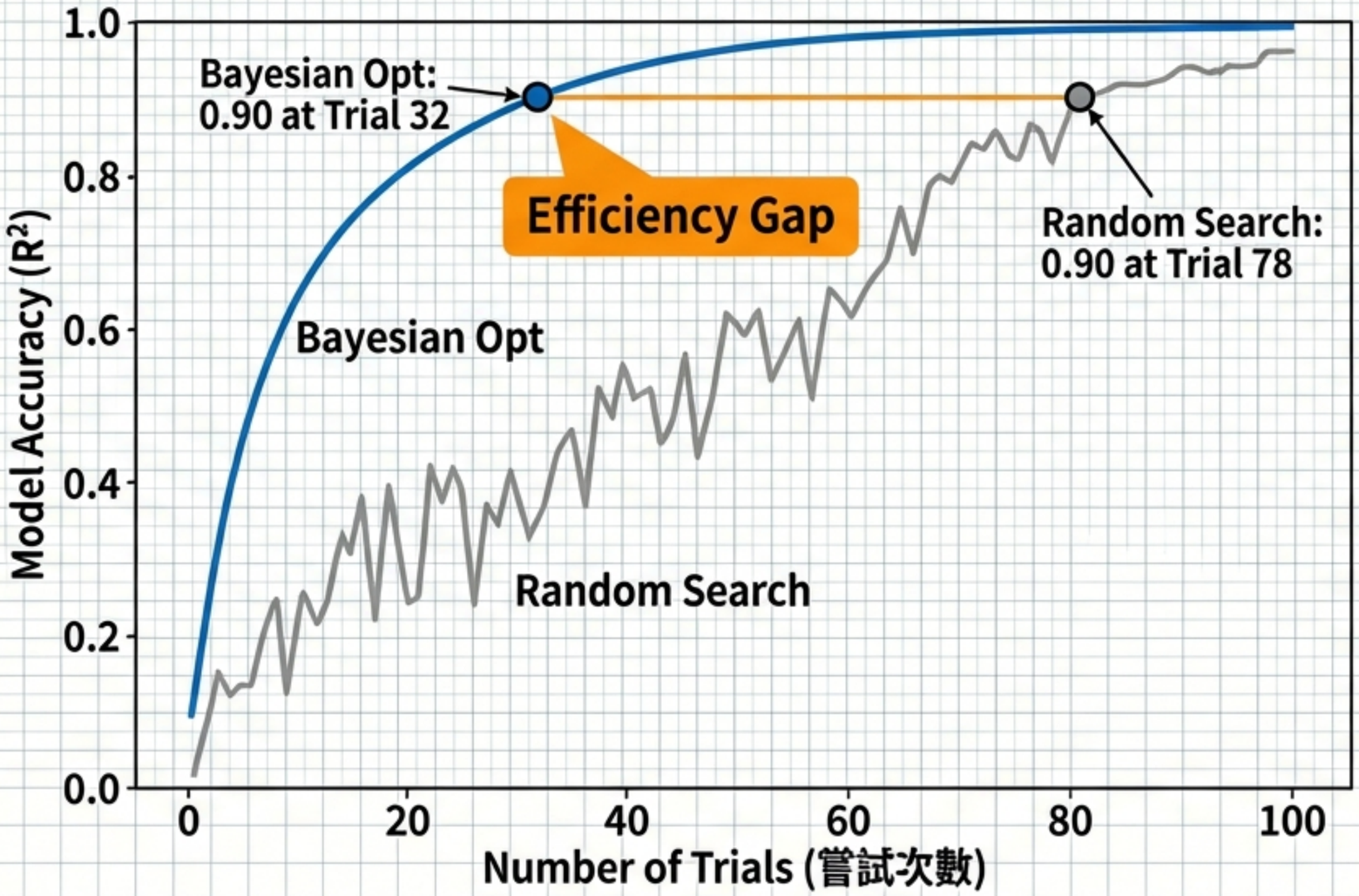
Project: Industrial_Blueprint_v1	
Date: 2024.06.16	
Title: SLIDE_07_BAYESIAN_OPTINIZATION	
Technical Specification	→ ←+→

Technical Specification

實戰表現：Optuna 框架



Scenario: Random Forest (6 params),
Target $R^2 > 0.90$

Random Search: 78 trials

Bayesian Opt: 32 trials
(High Sample Efficiency)

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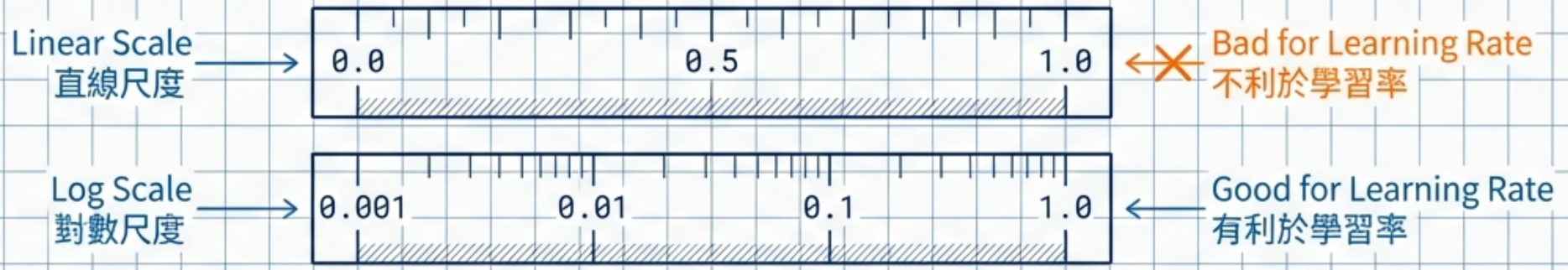
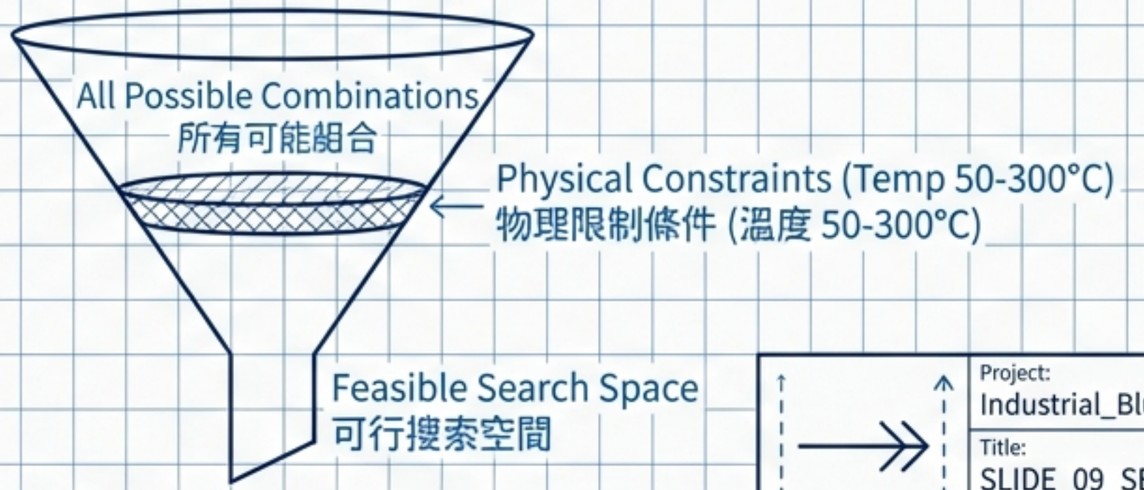
Technical Specification	Date: 2024.06.16	Drawing Number: SLIDE_08_OPTUNA_FRAMEWORK_PERFORMANCE

搜索空間設計：Garbage In, Garbage Out

Scale Matters (尺度選擇)



Domain Knowledge (領域知識)



利用化工限制條件縮減搜索空間。

	Project: Industrial_Blueprint_v1	Date: 2024.06.16
	Title: SLIDE_09_SEARCH_SPACE_DESIGN	
	Drawn by: AI ENGINEER	Approved Stamp

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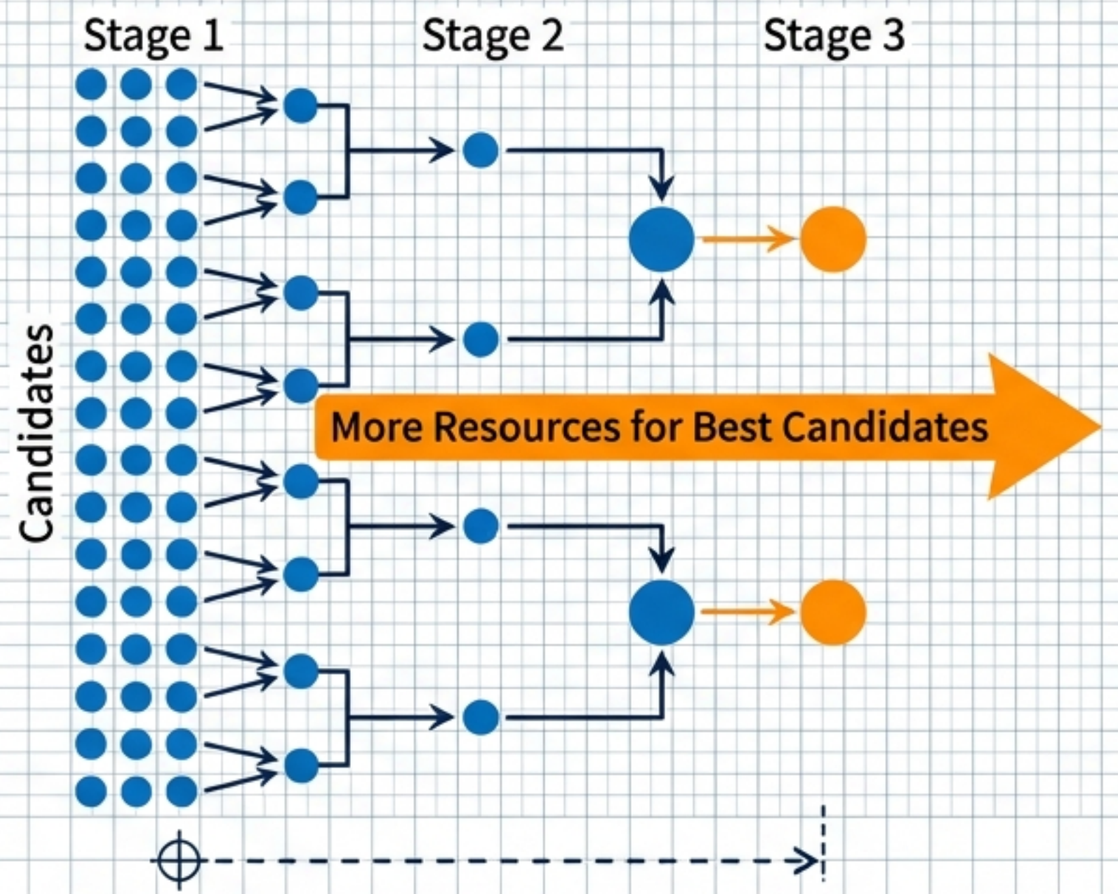
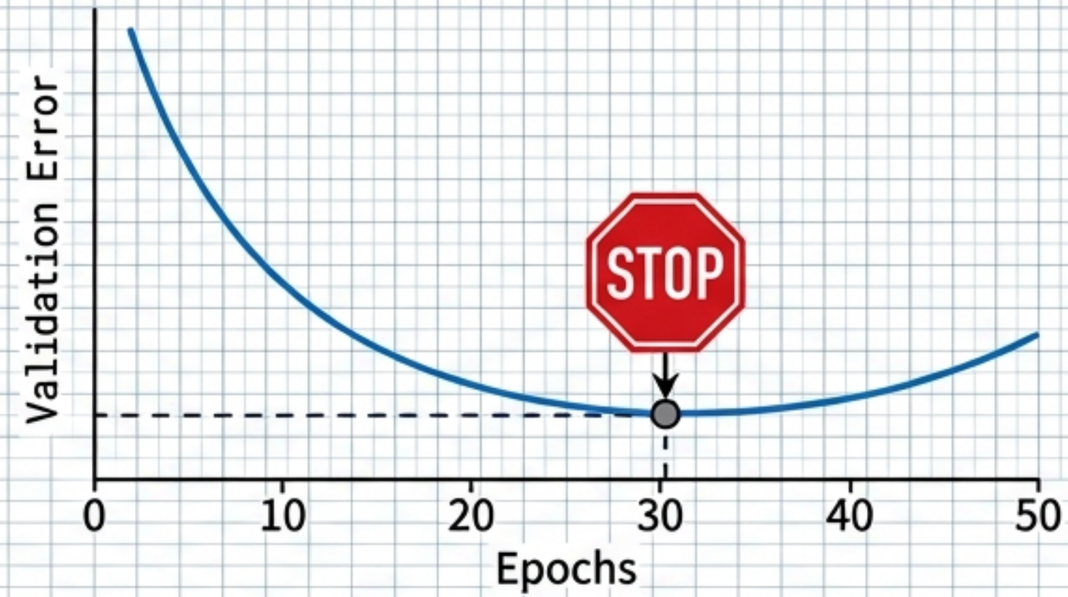
進階技巧：速度與效率

Halving Search (優勝劣汰)



Early Stopping (早停)



若驗證分數不再改善，立即停止訓練。

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	Title: SLIDE_10_ADVANCED_TECHNIQUES	
	Drawn by: AI ENGINEER	Approved Stamp

化工案例 1：蒸餾塔軟測量

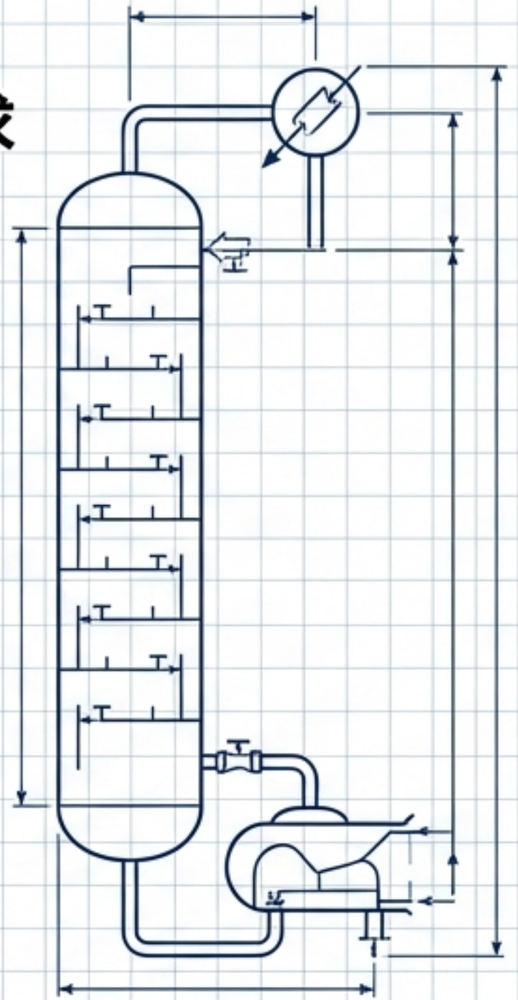
目標：預測塔頂溫度 (Top Temperature) | 挑戰：即時控制需求

Inputs

- Flow
- Reflux
- Reboiler Duty

Model: XGBoost + Bayesian Opt

Output: Top Temp (T_{top})



Results Dashboard

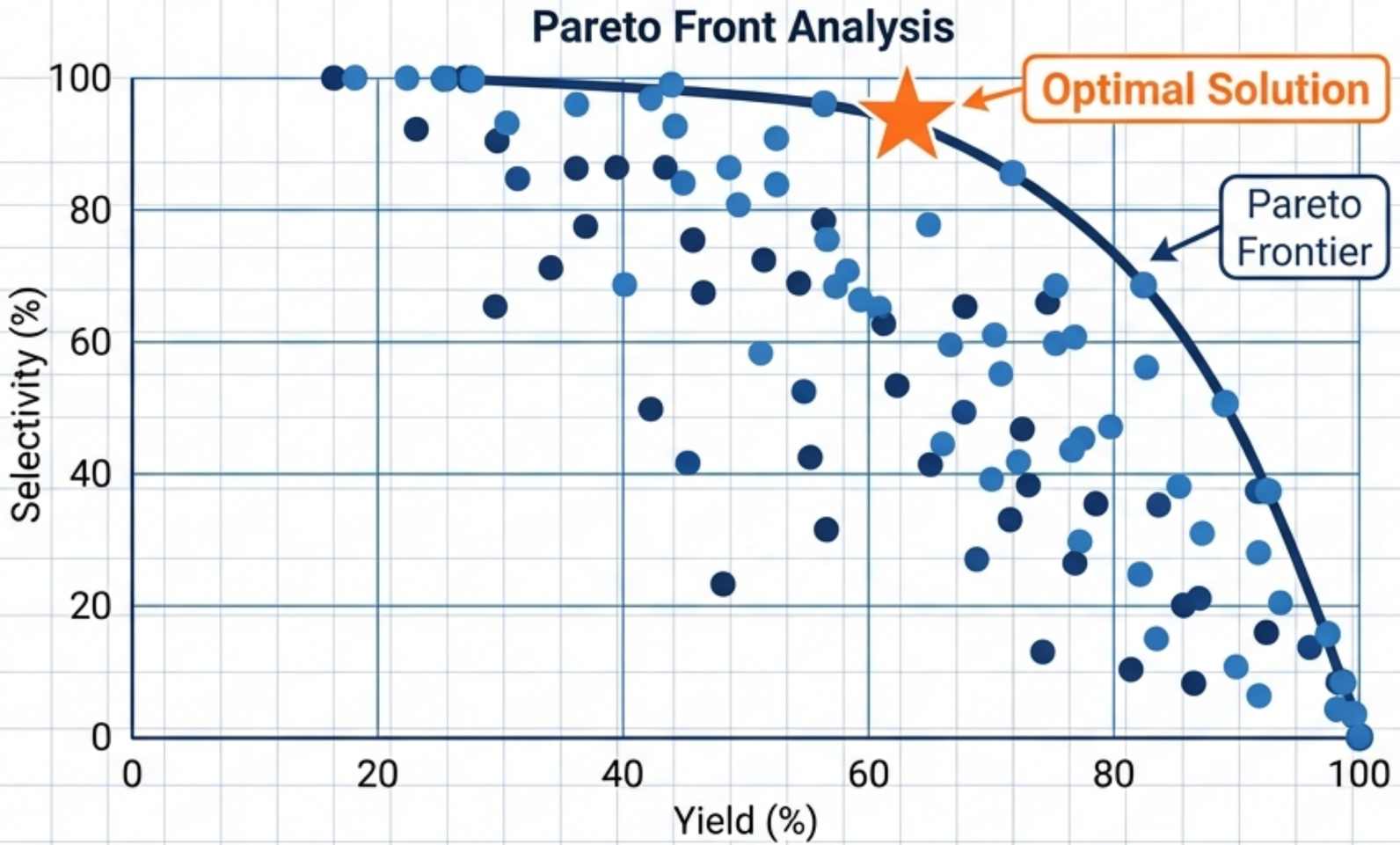
- **Accuracy:** MAE < 0.87°C
- **Speed:** Inference < 0.23ms

Optimization Focus: Accuracy vs. Real-time Speed

Project: Industrial_Blueprint_v1	Date: 2024.06.16
Title: SLIDE_12_CHEME_CASE_STUDY_1	
Drawn by: AI ENGINEER	Approved Stamp

化工案例 2：催化劑高通量篩選

目標：最大化產率 (Yield) 與選擇性 (Selectivity)



關鍵參數與成果

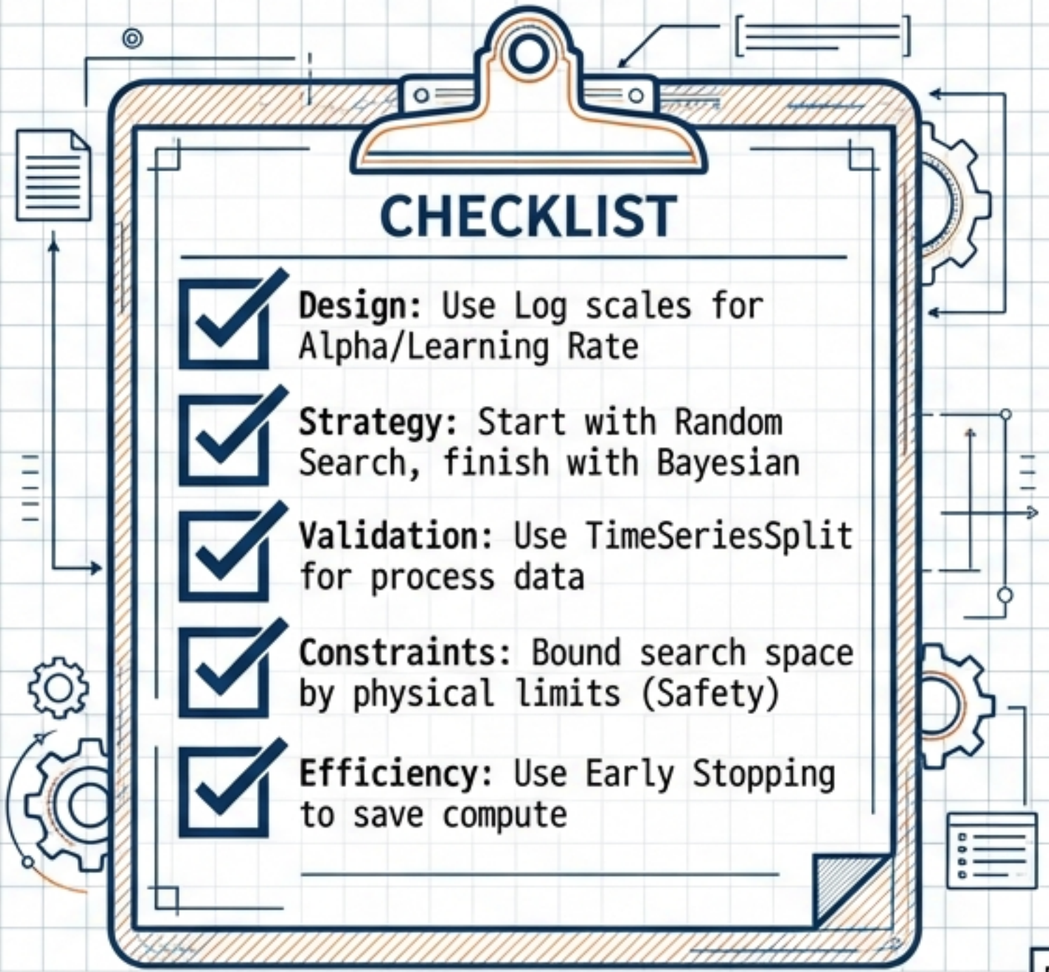
- Constraint: Expensive Experiments (>10k NTD/run)
- Method: Multi-objective Bayesian Opt
- Outcome: Found solution in 25 runs (40% cost saving)

Technical Specification

Approved Stamp

Project: Industrial_Blueprint_v1	Date: 2024.06.16
Title: SLIDE_14_CHEME_CASE_STUDY_2	
Drawn by: AI ENGINEER	

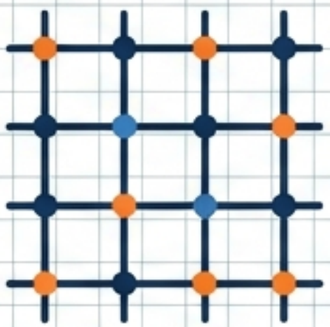
最佳實踐清單 (Best Practices Checklist)



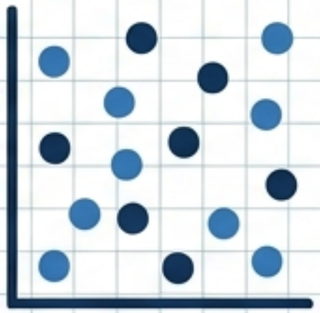
"Correct tuning moves AI from Lab Prototype to Industrial Grade."

Project: Industrial_Blueprint_v1	Date: 2024.06.16
Title: SLIDE_16_BEST_PRACTICES_CHECKLIST	
Drawn by: AI ENGINEER	Approved Stamp

總結：您的調參工具箱



Grid Search
(Small Space)



Random Search
(Baseline)

Bayesian Opt
(Precision)

超參數調整是連接「模型理論」與「工業落地」的橋樑。

Next Step: Unit 15 - Complete Chemical Engineering Case Study Integration

Project: Industrial_Blueprint_v1	Date: 2024.06.16
Title: SLIDE_17_CONCLUSION	
Drawn by: AI ENGINEER	Approved Stamp