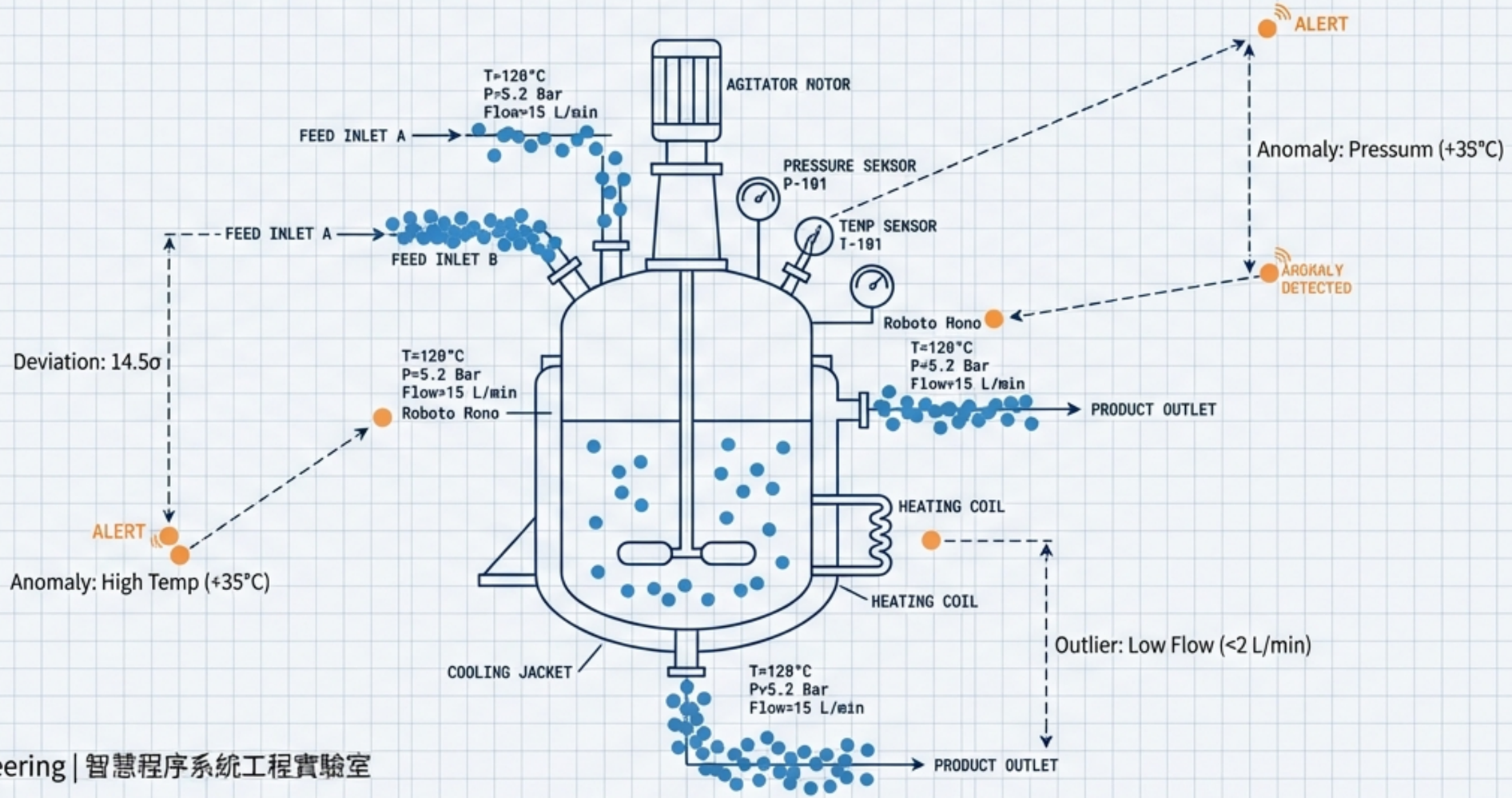
Unit 07 區域性離群因子 (LOF)

應對多密度化工數據的異常檢測方案



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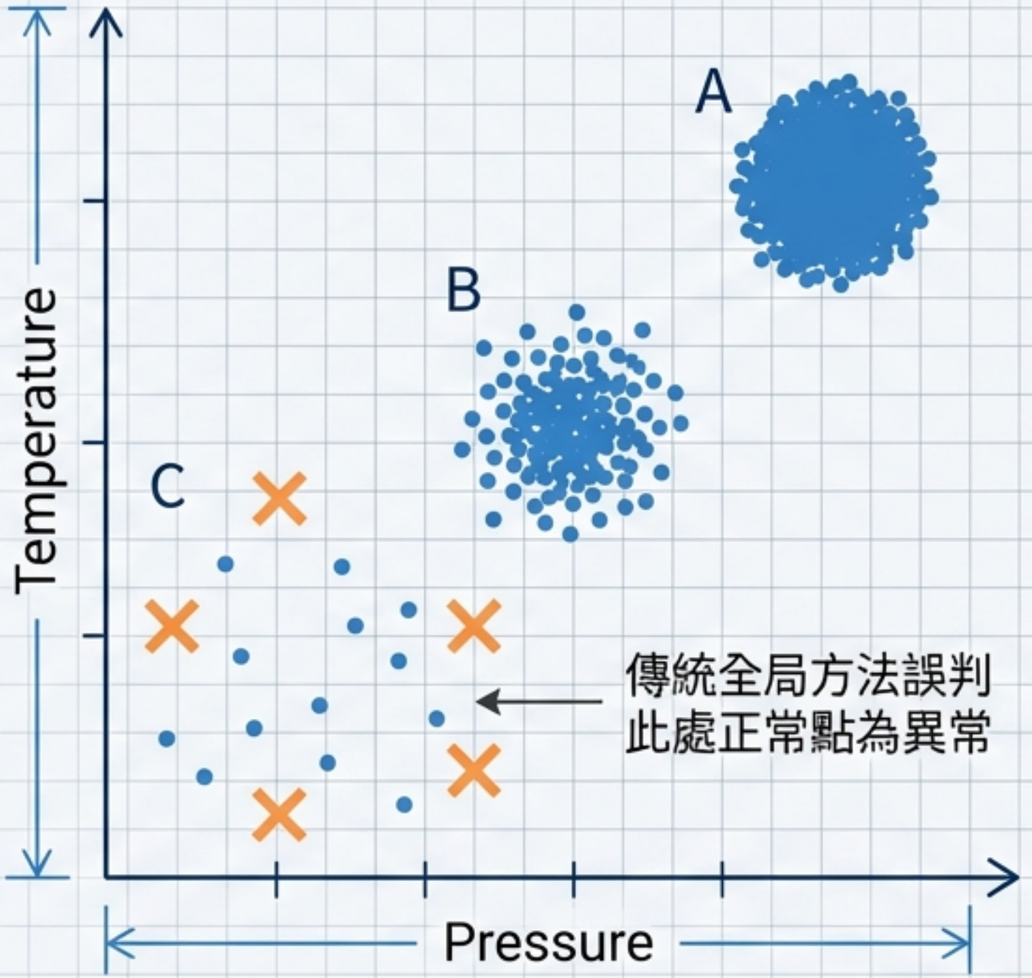
工業現場的挑戰：多模式製程數據 (Multi-Modal Processes)

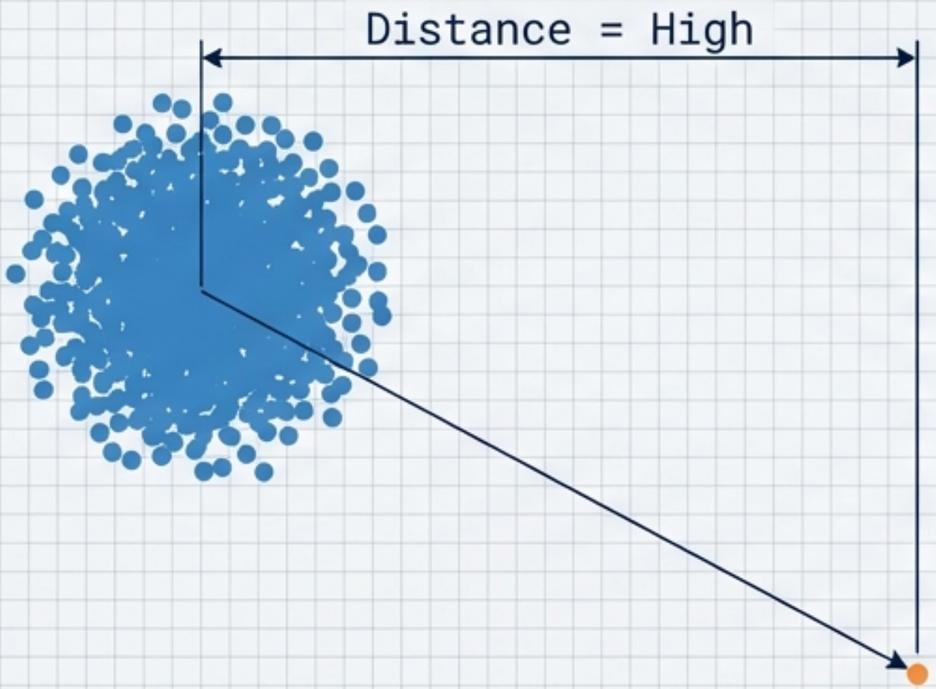
操作配方 (Operating Recipes)

- 1. Recipe A: 高溫高壓 (80-90°C)
  → [數據極度密集]
- 2. Recipe B: 中溫中壓 (60-70°C)
- 3. Recipe C: 低溫低壓 (40-50°C)
  → [數據相對稀疏]

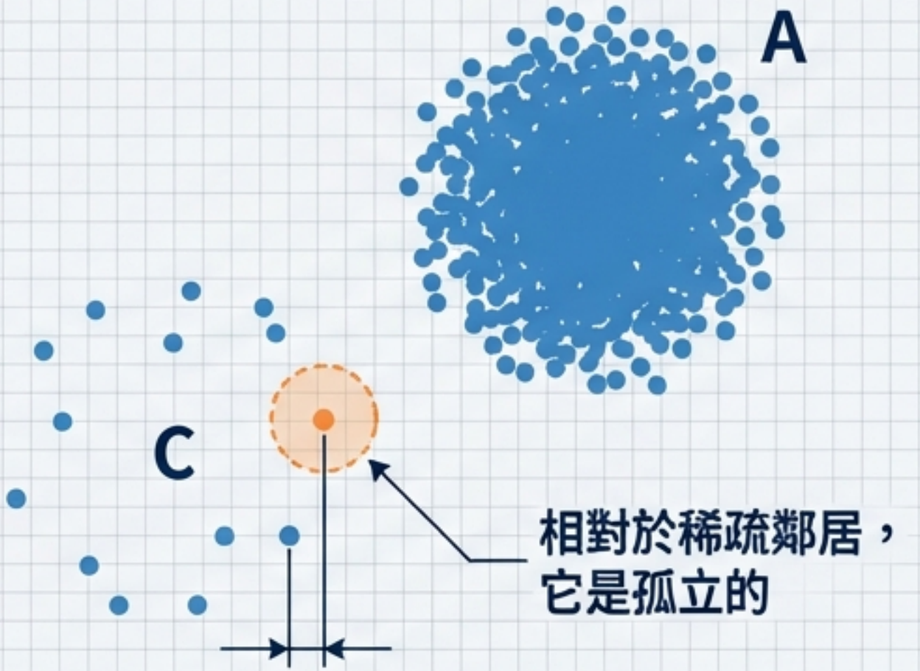


LOF 核心理念：異常是相對於鄰居而言

全局觀點 (Global View)

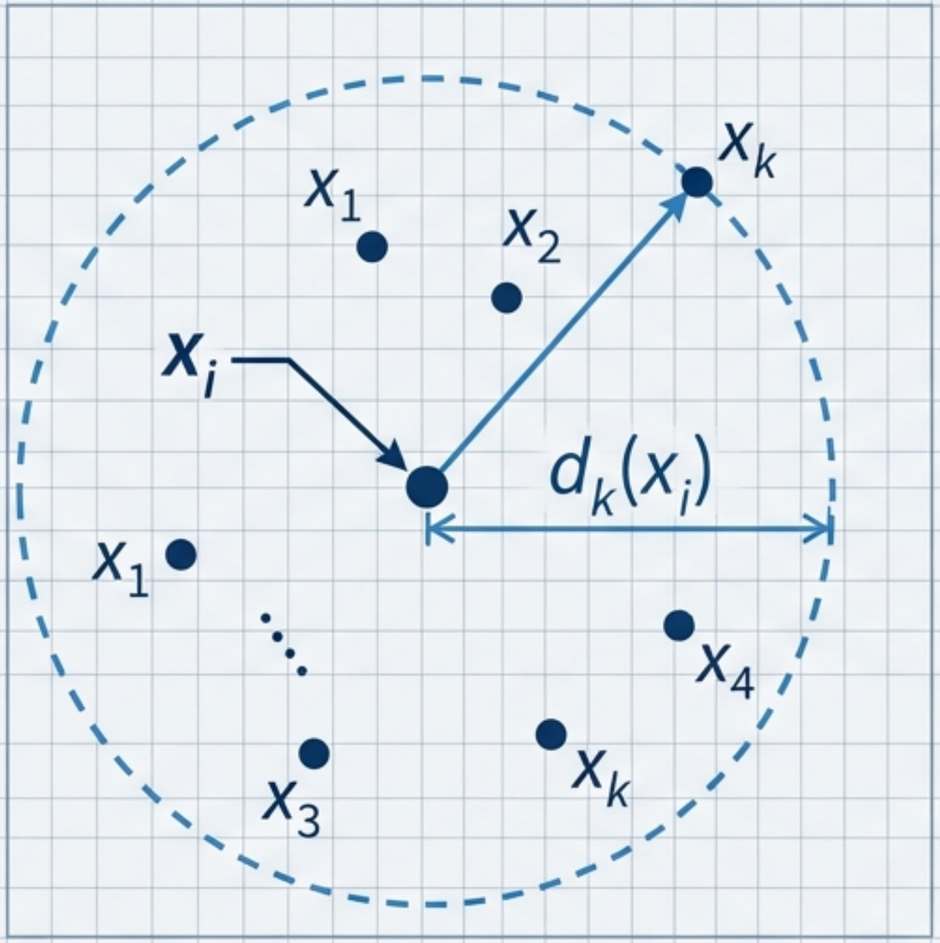


局部觀點 (Local View)



「異常點的局部密度明顯低於其鄰近點的局部密度。」

機制詳解 (1)：定義檢查範圍 (k-Distance)



定義 Definition

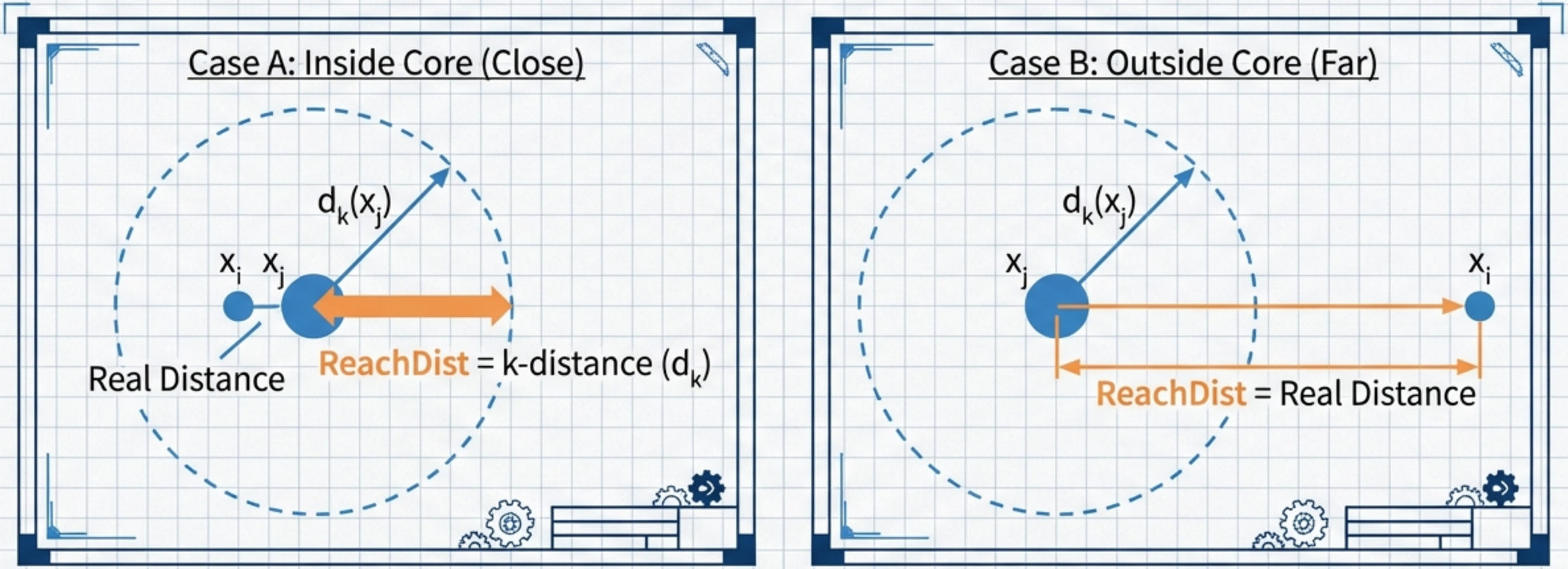
k-distance: 第 k 個最近鄰居的距離
k-neighborhood (N_k)：圓圈內的所有點

工程類比：為每個感測器讀值定義動態的檢查半徑

$$d_k(x_i) = \text{distance}(x_i, x_i^{(k)})$$

機制詳解 (2)：可達距離 (Reachability Distance)

目的：消除統計噪聲，確保密度估計的穩定性 (Stability).



$$\text{reach-dist}_k(x_i, x_j) = \max\{d_k(x_j), \text{distance}(x_i, x_j)\}$$

機制詳解 (3)：LRD 與 LOF 得分計算

Step 1: 局部可達密度 (LRD)

計算鄰居平均可達距離的倒數

$$\text{Density} \propto \frac{1}{\text{Distance}}$$

Step 2: 局部離群因子 (LOF)

比較：鄰居的平均 LRD / 我的 LRD

$$\text{Ratio} = \frac{\text{Neighbors' Density}}{\text{My Density}}$$

Step 3: 判讀結果 (Interpretation)

Ratio ≈ 1 ：正常 (Normal)
Ratio > 1.5：警告 (Warning)
Ratio > 2.0：**異常 (Anomaly)**

LOF Score

Python 實作：Scikit-Learn 工具箱

```python
from sklearn.neighbors import LocalOutlierFactor

# 初始化模型：針對多密度化工數據
lof = LocalOutlierFactor(
    n_neighbors=15,  # 關鍵參數 k（檢查範圍）
    contamination='auto',# 自動決定異常比例
    novelty=False        # False: 檢測歷史數據 (Outlier Detection)
)                        # True:  檢測新數據 (Novelty Detection)

# 訓練並取得結果 (-1 為異常，1 為正常)
y_pred = lof.fit_predict(X_train)
lof_scores = -lof.negative_outlier_factor_  # 轉為正數得分
```

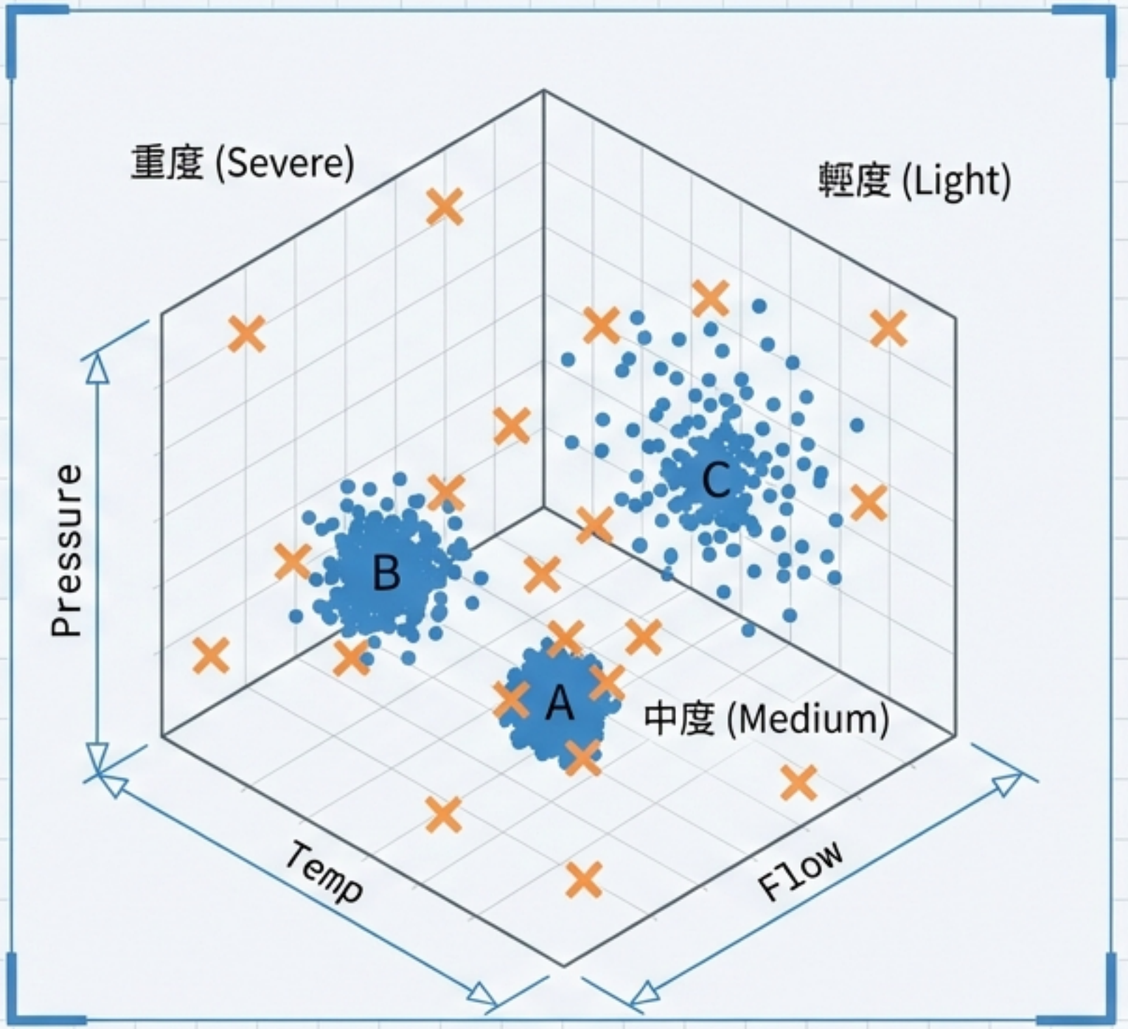
決定敏感度的核心參數

模式切換開關

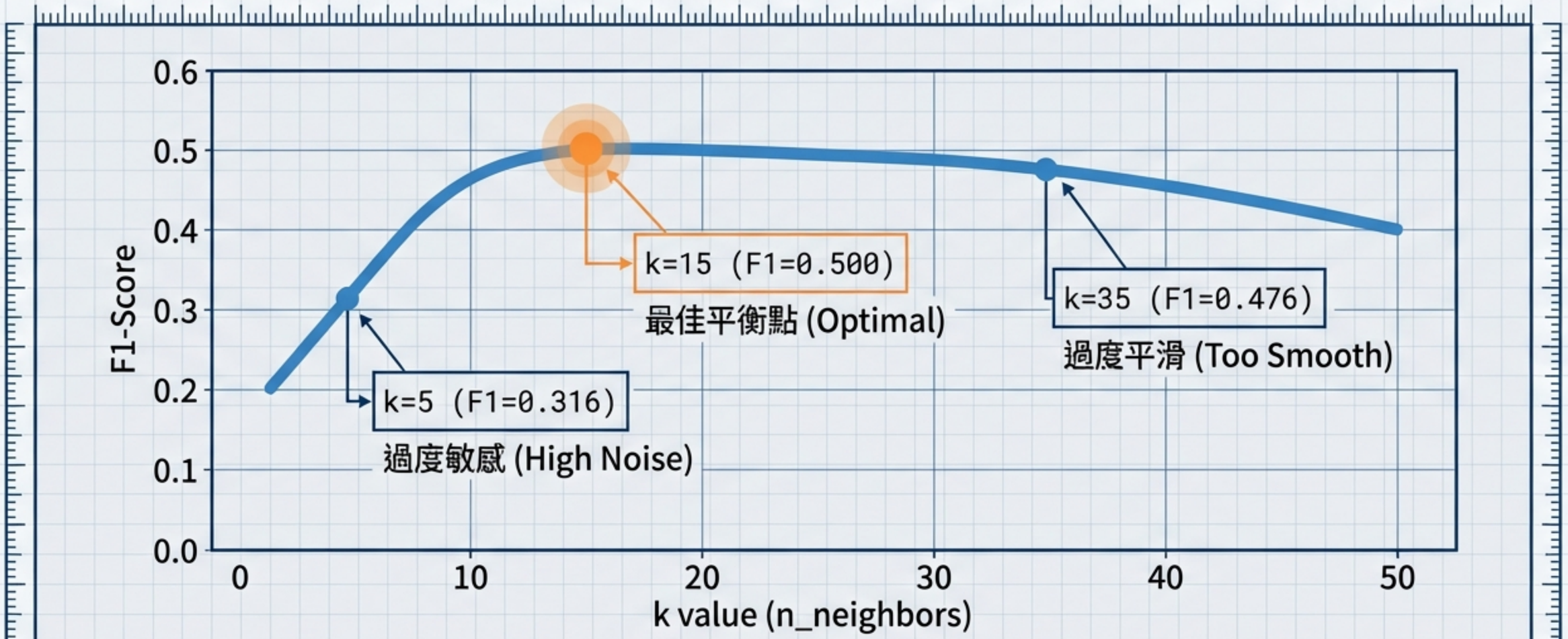
實驗設計：批次反應器模擬 (Batch Reactor Simulation)

數據生成參數

- 配方數量: 3 (Dense, Medium, Sparse)
- 正常數據變異性: +30-40% (模擬真實噪聲)
- 異常設計 (Hierarchical Anomalies):
  - 輕度 (Light): 40%
  - 中度 (Medium): 40%
  - 重度 (Severe): 20%

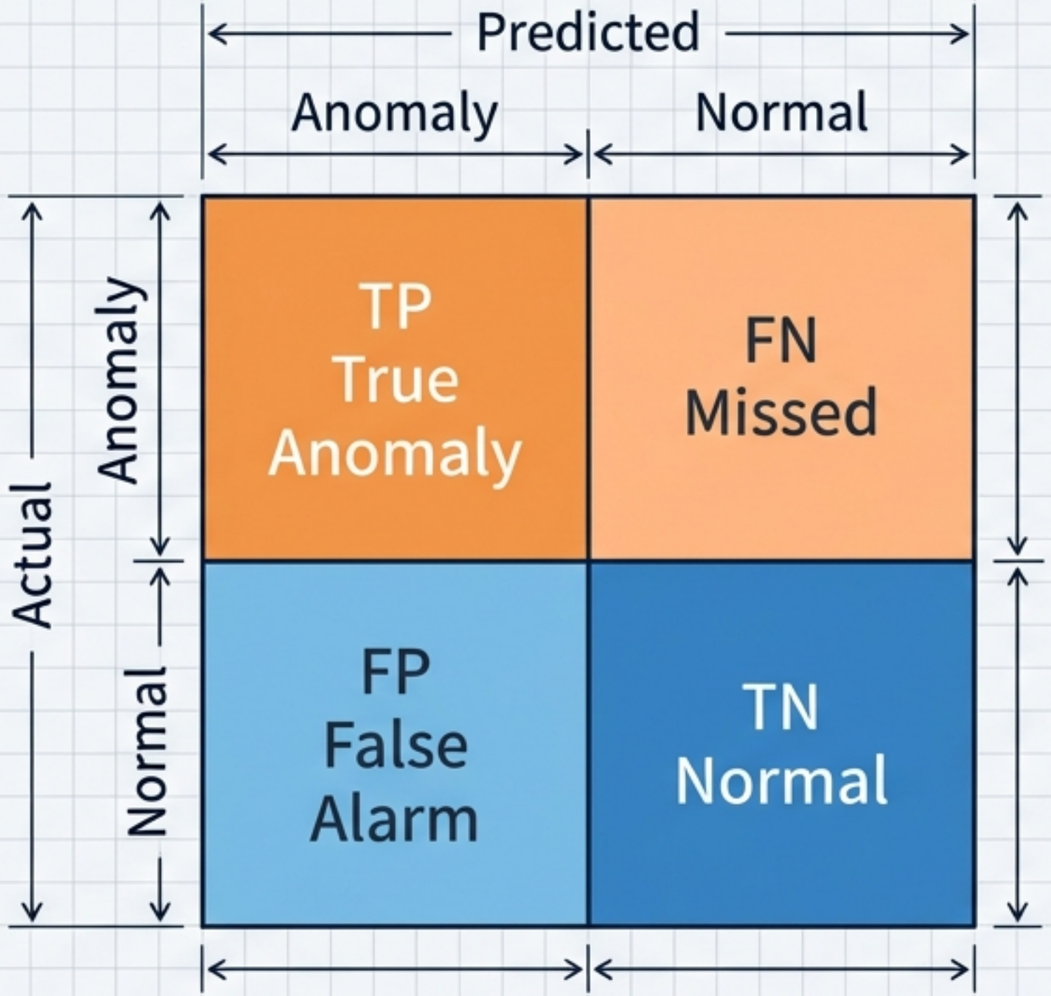


超參數分析：尋找最佳的 'k' (n_neighbors)



結論：對於中等規模數據 (n < 500)，k=10 ~ 20 通常是最佳範圍。

效能評估：真實數據的考驗



Model Metrics (k=15)

Precision: 0.500
50% Reliability

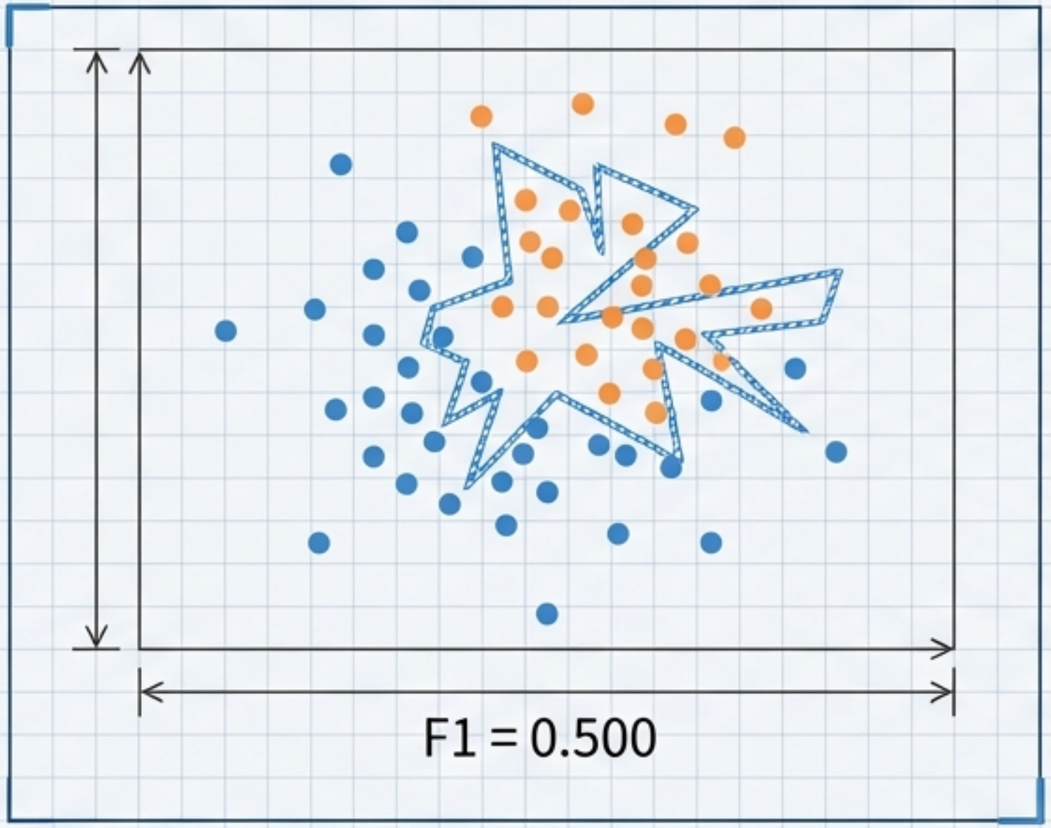
Recall: 0.500
Caught 50% anomalies

AUC: 0.835
Good Separability

Why not AUC 1.0?
真實工業數據存在模糊邊界與輕微異常。
這是合理的現實結果 (Realistic Outcome).

進階應用：新穎性檢測 (Novelty Detection)

Outlier Detection (Mixed Data)



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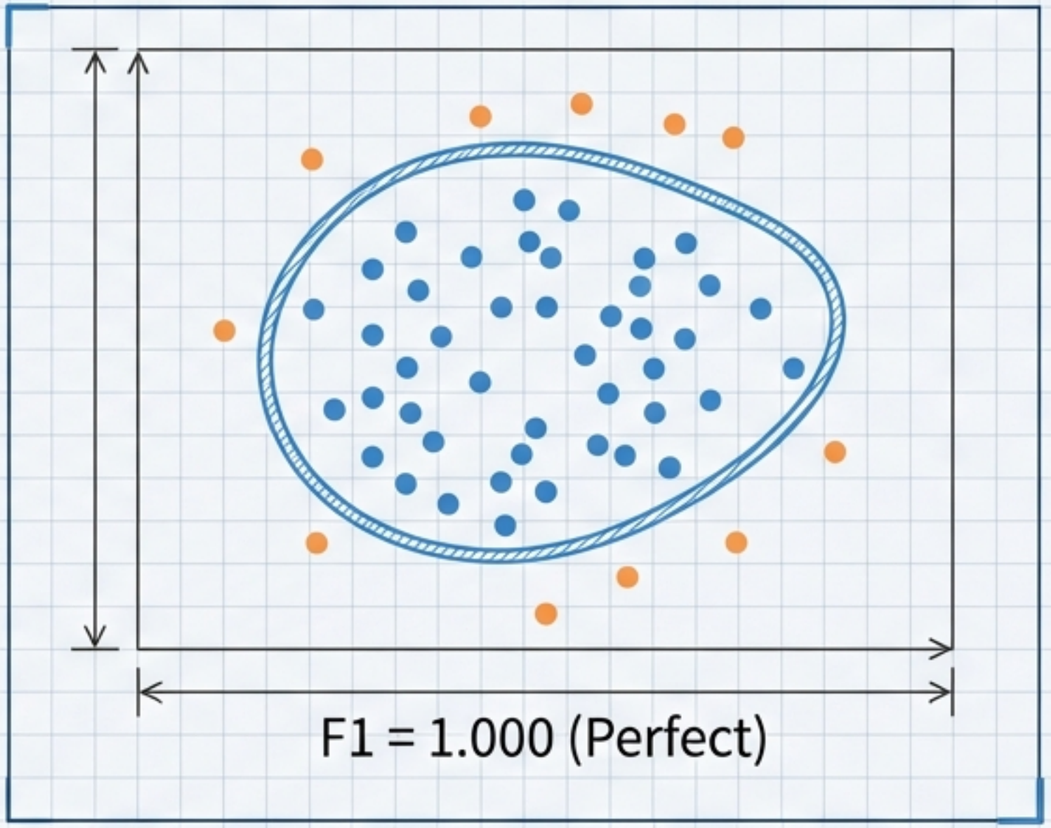
Novelty Detection (Clean History)



Roboto Mono

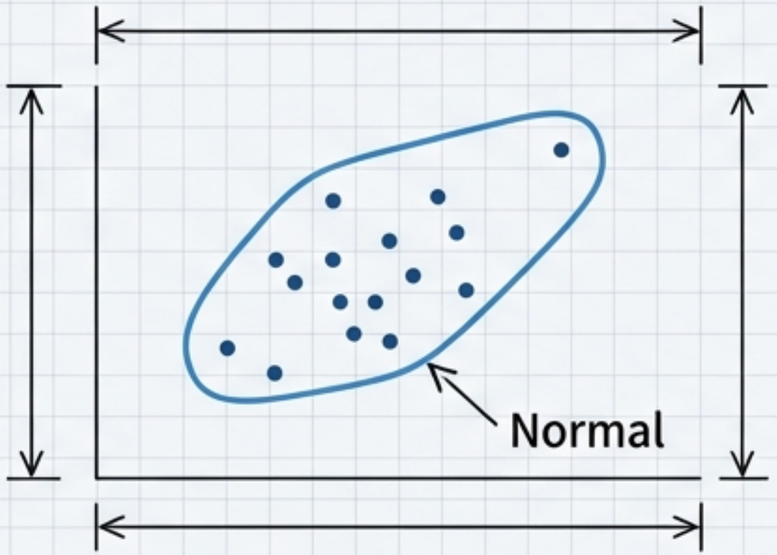
Training on Golden Batch only

應用場景：當擁有純淨的歷史數據時，切換 `novelty=True` 可實現最佳即時監控。

演算法對決：LOF vs. Isolation Forest

LOF (Local Outlier Factor)

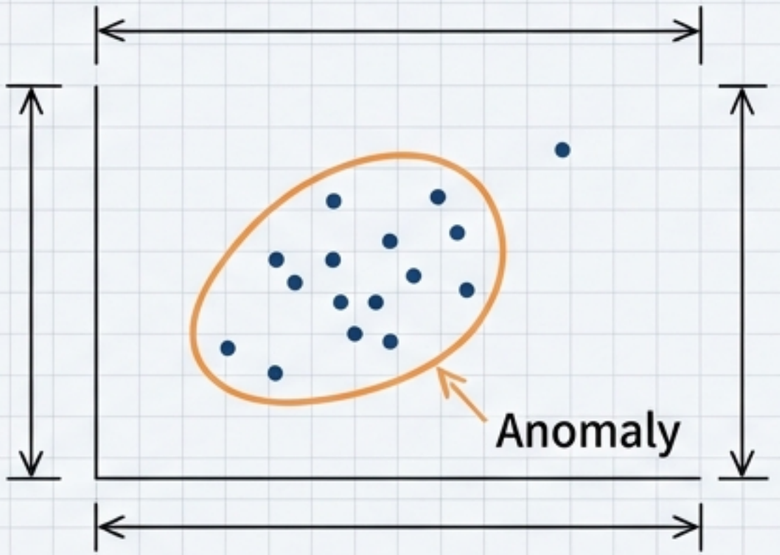
F1 Score: 0.500 ✅



適應局部密度：正確識別稀疏配方為正常。

Isolation Forest

F1 Score: 0.400 ⚠️



全局隔離：誤判稀疏配方為異常 (False Alarm)。

Isolation Forest 難以處理多密度 (Multi-Density) 數據集。

策略總結：LOF 的優勢與代價

優勢 Advantages

- ✓ 處理多密度數據 (Multi-Density Handling)
- ✓ 無需假設分佈 (No Gaussian Assumption)
- ✓ 提供量化異常分數 (Quantifiable Score)

劣勢 Disadvantages

- ⚠ 計算成本較高 $O(n^2)$ (Computationally Expensive)
- ⚠ 對參數 k 敏感 (Sensitive to Hyperparameters)
- ⚠ 高維度表現下降 (Curse of Dimensionality)

最佳適用：複雜、中等規模的製造業數據集 (Complex, Medium-sized Manufacturing Data)。

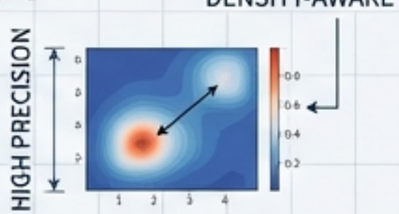
實務部署指南 (Deployment Guide)

↳ Code is read much more often than it is written. — 請保持代碼與模型的可維護性。

結論與下一步

核心價值

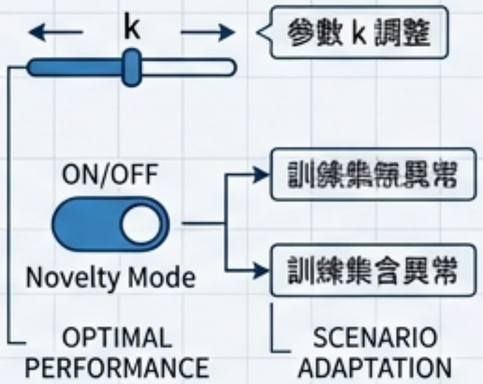
LOF 是應對「非均勻密度」工業數據的最佳檢查員。



關鍵洞察

從「全局距離」轉向「局部密度」視角，大幅降低誤報。

實作建議



注意參數 k 的調整，並針對不同場景選擇 Novelty 模式。

下一步 (Next Step):
開啟 Unit07_LOF.ipynb
開始實作練習