**Function 1: Searching for Contamination Sources**

**Traits**: Sparse signal, mostly zero, two distinct peaks (multi-modal), narrow peaks.

**Strategy Considerations**:

* Use **UCB** early on with **high exploration** (kappa=2.5+) to cover space.
* Later consider **EI**, but avoid early exploitation — you may miss the second peak.
* Be cautious of zero outputs — they can mislead GP into under-exploring.
* You could also try **two GPs** later if you see two peaks emerging.

Set kappa=2.5 and consider plotting regularly to track unexplored regions.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ucb (8) → ei → poi |
| **Kernel** | matern52 (8) → matern32 |
| **Kappa** | 2.5 → 3.0 → 3.5 → 4.0 |
| **Const. Val** | 1.0 → 1.5 → 2.25 → 3.38 |
| **Length Scale** | 1.0 → 1.2 → 1.44 → 1.73 |
| **Nu** | 2.5 → 3.0 |

A graph of a graph showing a graph of a graph

AI-generated content may be incorrect.

**Notes & Observations**

* The function initially **stagnated at 1.123** using ucb with default GP settings.
* After switching to **poi + matern32**, performance improved to **1.988**, demonstrating better peak capture.
* Increasing kappa and length\_scale allowed the model to **balance exploration and smoothness**.
* Final tuning reflects a **mature exploitation regime**, ideal for local peak refinement.

**Strategic Considerations (Applied)**

* Started with **UCB** and **high kappa (2.5+)** to cover the sparse input space effectively.
* Switched to **EI/POI** as distinct peaks emerged and GP confidence improved.
* Avoided premature exploitation — helped detect second peak.
* Future suggestion: Consider **dual-GP modeling** if the two peaks remain spatially isolated

**Function 2: Noisy ML Model Optimization**

**Traits**: Highly noisy, multiple local optima, model initialization sensitivity.

**Strategy Considerations**:

* Stick with **UCB** longer — you want to explore more to average out noise.
* Consider adding **noise\_level parameter** to GP kernel (currently WhiteKernel() does this).
* You may want to **retrain with a rolling window** of the best N points to prevent overfitting to noise.

Consider increasing WhiteKernel(noise\_level=0.1) to let GP trust less in early points.

A graph of a graph

AI-generated content may be incorrect.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ucb (8) → ei → poi |
| **Kernel** | matern52 (8) → matern32 |
| **Kappa** | 2.0 → 2.5 → 3.0 → 3.5 |
| **Const. Val** | 1.0 → 1.5 → 2.25 → 3.38 |
| **Length Scale** | 1.0 → 1.73 |
| **Nu** | 2.5 → 3.0 |

* Function **stagnated at 0.906**, and **did not improve** after switching to poi + matern32.
* Suggests that the kernel/acquisition changes alone were **not enough** to overcome the noise.

**Strategic Considerations (Applied & Future)**

* UCB was maintained for 8 iterations to support broader exploration — correct initial choice.
* Switched to **POI** and increased kappa, const\_val, and length\_scale to smooth predictions and encourage confident exploitation.
* However, the **high noise level** likely masked true optima.

**Suggestions:**

* Use a **WhiteKernel(noise\_level=0.1)** to down-weight early noisy points.
* Consider **rolling window retraining** on top-N best results to reduce overfitting.
* Evaluate whether the GP model is overconfident — variance plots could help.

**Function 3: Drug Discovery (minimize adverse reaction)**

**Traits**: 3D, one variable might be irrelevant, goal is close to zero.

**Strategy Considerations**:

* Watch for GP fitting quality — one flat dimension may confuse it.
* Track how well GP models uncertainty — it should shrink only on relevant dimensions.
* Use **EI or PI** earlier than usual if you spot a minimum cluster.

Try removing dimensions (manually or via variance analysis) if you suspect one is flat.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ei (11) → poi |
| **Kernel** | matern52 (11) → matern32 |
| **Kappa** | 1.96 → 2.46 |
| **Const. Val** | 1.0 → 1.5 |
| **Length Scale** | 1.0 → 1.2 |
| **Nu** | 2.5 → 3.0 |

**Performance**

* Initial GP model struggled — started at **-0.002**
* After tuning (poi + matern32), improved in **two stages** to **0.0118**
* Indicates effective **local optimization** after a sluggish start

**Strategic Considerations**

* EI was a solid starting point due to proximity to minimum
* Switched to **POI** for more focused exploitation once GP uncertainty improved
* Kernel upgrade (matern52 → matern32) and smoother nu=3 likely helped model narrow valleys
* The presence of a **flat or irrelevant dimension** may have diluted early GP predictions

A graph of a graph with dots

AI-generated content may be incorrect.

**Function 4: Fast but Inaccurate Modelling**

**Traits**: Expensive surrogate approximation, lots of local optima, 4D.

**Strategy Considerations**:

* Use **EI** from the beginning (exploitation is okay since this is an approximation).
* Consider **multiple restarts** (increase n\_restarts) in suggest\_next() to avoid local traps.

Try n\_restarts=20 to make acquisition optimization more robust.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ei (11) → poi |
| **Kernel** | matern52 (11) → matern32 |
| **Kappa** | 1.96 → 2.46 |
| **Const. Val** | 1.0 → 1.5 |
| **Length Scale** | 1.0 → 1.2 |
| **Nu** | 2.5 → 3.0 |

**Performance**

* Initial output: **0.644**
* Improved to **0.693** after tuning in **two clear stages**
* The kernel/acquisition changes and smoothing tweaks were effective in exploitation

**Strategic Considerations**

Started with Expected Improvement (EI) — appropriate for cost-effective modeling

Upgraded to POI as the GP matured and convergence neared

Switched to matern32 and increased nu for more confident extrapolation in smooth areas

Increased kappa and length\_scale slightly to avoid premature convergence



**Function 5: Chemical Reaction Yield**

**Traits**: 4D, unimodal, smoother behavior.

**Strategy Considerations**:

* Very GP-friendly.
* Start with **UCB**, switch to **EI** quickly.
* Focus on convergence and exploitation.

Your default strategy will likely perform very well here.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ei → poi |
| **Kernel** | matern52 → matern32 |
| **Kappa** | 1.96 → 2.46 → 2.96 → 3.46 → 4.46 |
| **Const. Val** | 1.0 → 1.5 → 3.38 → 5.07 → 7.61 |
| **Length Scale** | 1.0 → 1.2 → 2.5 |
| **Nu** | 2.5 → 3.0 |

**Performance**

* Reached **early stagnation at 8662.40**
* Aggressive tuning completed **before 5-Jul** and remained **unchanged by 25-Jul**
* Indicates GP captured the unimodal peak early, but further progress plateaued

**Strategic Considerations**

* Although UCB was recommended early, **EI was used from the start** and worked well enough due to smoothness
* POI followed for sharper exploitation
* matern32 and increased nu helped adaptively control curvature
* Large increases in kappa, const\_val, and length\_scale suggest strong confidence in modeling peak region



**Function 6: Cake Recipe (multi-objective)**

**Traits**: 5D, multiple competing objectives combined into one score.

**Strategy Considerations**:

* Outputs may have subtle tradeoffs.
* GP will behave reasonably, but don't over-tune.
* Consider logging individual components (if available later).

No changes needed now; stick to UCB→EI transition.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ucb → ei |
| **Kernel** | matern52 → matern32 |
| **Kappa** | 2.0 → 2.5 |
| **Const. Val** | 1.0 → 1.5 |
| **Length Scale** | 1.0 → 1.2 |
| **Nu** | 2.5 → 3.0 |

**Performance**

* Consistent, **steady improvement across phases**:
  + -0.7142 → -0.6295 → -0.2019 → -0.0975
  + Final improvement to **-0.0084** using ei + matern32
* Indicates strong GP model fit despite tradeoffs in objectives

**Strategic Considerations**

* Started with **UCB** for global exploration
* Switched to **EI** once high-performing regions were detected
* Kernel changed to matern32 and nu=3 to better generalize across nearby points
* Small increase in kappa and length\_scale enhanced smoothing while avoiding overconfidence



**Function 7: ML Hyperparameter Tuning**

**Traits**: 6D, known models, possibly researchable.

**Strategy Considerations**:

* You could look up common hyperparameter defaults (as a meta prior).
* Start with **default hyperparameter values** and **then explore**.
* If the surface is known to be bumpy, use more acquisition restarts.

Consider using known good values as starting points in addition to GP.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ei |
| **Kernel** | matern52 |
| **Kappa** | 1.96 |
| **Const. Val** | 1.0 |
| **Length Scale** | 1.0 |
| **Nu** | 2.5 |

**Performance**

* Achieved **steady improvements** across all sessions
* Output climbed from **1.3649 to 3.0019**
* No parameter tuning was necessary — default settings worked well

**Strategic Considerations**

* Started with **default EI + matern52**, and that was sufficient
* Indicates the GP was able to learn the landscape quickly, possibly due to **smoothness** or well-spaced evaluations
* Kernel's moderate flexibility (nu=2.5) captured trends across dimensions

**Function 8: High-Dimensional Black-Box**

**Traits**: 8D, curse of dimensionality, hard to optimize, local search preferred.

**Strategy Considerations**:

* Avoid pure exploration — too expensive in 8D.
* Use **EI or PI** early and aggressively.
* Use **lower number of restarts**, and maybe switch to **local search** mode (greedy) near the end.

Your model should exploit fast and stick to promising regions once found.

**Parameter Evolution**

| **Parameter** | **Timeline** |
| --- | --- |
| **Acquisition** | ei → poi |
| **Kernel** | rbf (remained stable) |
| **Kappa** | 1.96 → 2.46 |
| **Const. Val** | 1.0 → 1.5 |
| **Length Scale** | 1.0 → 1.2 |
| **Nu** | 0 → 3 (migrated to Matern setting) |

**Performance**

* Showed **stepwise improvement** from **9.598 → 9.998**
* Indicates strong **local convergence** in a narrow band
* GP confidence likely improved gradually without overfitting

**Strategic Considerations**

* Began with **EI** to identify promising local regions
* Switched to **POI** for tighter exploitation after local optima emerged
* Used **RBF kernel** which helped due to its smoothness and lower parameter complexity
* Light exploration and careful acquisition shifts paid off in high-D setup

**Recommendations**

* Stick to **aggressive exploitation** once high-performing region found