

Phase 6.2 — Heteroscedastic GP Surrogate

Feature map

Let \mathcal{P} denote the space of PACKAGE configurations. A package $p \in \mathcal{P}$ is encoded as a fixed-length feature vector

$$\mathbf{x} = \varphi(p) \in \mathbb{R}^d$$

where φ concatenates one-hot encodings of the model slot, a binary skill-presence vector, and one-hot encodings of the named system-prompt and template-value variants (the Phase 3.1 slot-space schema).

Observations

After N completed trials we have a dataset $\mathcal{D}_N = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$ where each $\mathbf{y}_i \in \mathbb{R}^5$ records the five Pareto-axis values

$$\mathbf{y}_i = (\bar{\tau}_i, \bar{c}_i, s_i, \bar{q}_i, r_i) \quad (\text{tokens, dollars, scaling slope, quality, subjective})$$

Trials without a subjective score contribute only the first four components; the subjective head is trained on the subset of fully-scored trials.

Heteroscedastic single-task GP (per output head)

For each output $j \in \{1, \dots, 5\}$ we place an independent GP prior:

$$f^{(j)}(\mathbf{x}) \sim \mathcal{GP}\left(0, k^{(j)}(\mathbf{x}, \mathbf{x}')\right)$$

with a squared-exponential (RBF-ARD) kernel

$$k^{(j)}(\mathbf{x}, \mathbf{x}') = \sigma_{f,j}^2 \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{x}')^\top \mathbf{\Lambda}_j^{-1}(\mathbf{x} - \mathbf{x}')\right)$$

where $\mathbf{\Lambda}_j = \text{diag}(\ell_{j,1}^2, \dots, \ell_{j,d}^2)$ are per-dimension length-scales (automatic relevance determination).

Input-dependent noise. Rather than assuming a fixed noise level, we model the log noise variance with a second GP:

$$g^{(j)}(\mathbf{x}) \sim \mathcal{GP}\left(0, k_\varepsilon^{(j)}(\mathbf{x}, \mathbf{x}')\right) \quad \sigma^{2,(j)}(\mathbf{x}) = \exp\left(g^{(j)}(\mathbf{x})\right)$$

The observation model is then

$$\mathbf{y}_i^{(j)} = f^{(j)}(\mathbf{x}_i) + \varepsilon_i^{(j)}, \quad \varepsilon_i^{(j)} \sim \mathcal{N}\left(0, \sigma^{2,(j)}(\mathbf{x}_i)\right)$$

Posterior

Let $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]^\top$, $\mathbf{y}^{(j)} = [y_1^{(j)}, \dots, y_N^{(j)}]^\top$, and $\Sigma^{(j)} = \text{diag}(\sigma^{2,(j)}(\mathbf{x}_1), \dots, \sigma^{2,(j)}(\mathbf{x}_N))$.

The posterior over $f^{(j)}$ at a new point \mathbf{x}_* is Gaussian:

$$\mu_N^{(j)}(\mathbf{x}_*) = \mathbf{k}_*^{(j)\top} [\mathbf{K}^{(j)} + \Sigma^{(j)}]^{-1} \mathbf{y}^{(j)} \quad (1)$$

$$\sigma_N^{2,(j)}(\mathbf{x}_*) = k^{(j)}(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^{(j)\top} [\mathbf{K}^{(j)} + \Sigma^{(j)}]^{-1} \mathbf{k}_*^{(j)} \quad (2)$$

where $\mathbf{K}_{ij}^{(j)} = k^{(j)}(\mathbf{x}_i, \mathbf{x}_j)$ and $\mathbf{k}_*^{(j)} = [k^{(j)}(\mathbf{x}_*, \mathbf{x}_i)]_{i=1}^N$.

Hyperparameters $\theta_j = \{\sigma_{f,j}^2, \Lambda_j, \theta_{\epsilon,j}\}$ are optimised by maximising the log marginal likelihood.

Bootstrap discipline

Define the trial count threshold $N_0 \approx 10$. The proposer operates in two regimes:

$$\text{next proposal} = \begin{cases} \text{RandomFromSlotSpace} & N < N_0 \\ \arg \max_{\mathbf{x} \in \mathcal{X}} \alpha_{\text{EHVI}}(\mathbf{x}; \mathcal{D}_N) & N \geq N_0 \end{cases}$$

where \mathcal{X} is the discrete set of un-evaluated packages and α_{EHVI} is the expected hypervolume improvement over the current 5D Pareto frontier (Phase 6.3).

Note

A few design notes embedded in the math:

- **ARD kernel:** length-scales $\ell_{j,k}$ let the model learn which slots actually matter per axis — useful since model is likely far more predictive of dollars than `system_prompt`.
- **Independent heads:** simpler than a multi-task GP and sufficient here; cross-axis correlations (e.g. tokens \leftrightarrow dollars) can be captured later if needed.
- **Heteroscedastic noise:** the subjective head in particular will have high variance at low trial counts and should narrow as more scores arrive — homoscedastic noise would mask that.
- **Bootstrap at $N_0 \approx 10$:** the GP is unreliable below this; pure random exploration avoids over-exploiting a badly-conditioned posterior.