Enhancing DGEMO with Bayesian Optimization Properties: Towards DGEBO

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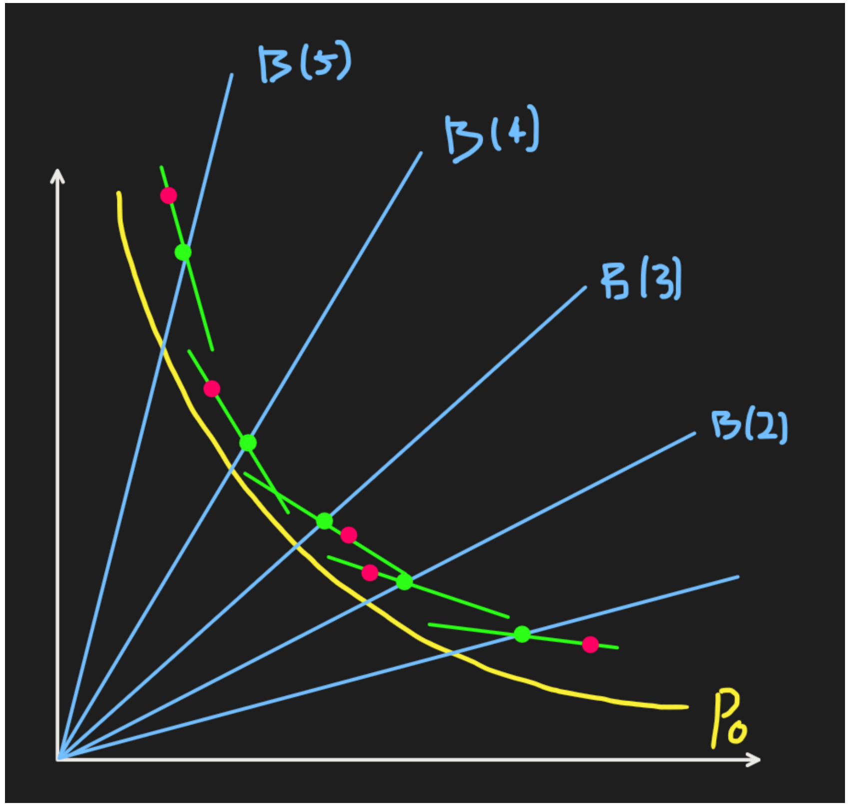

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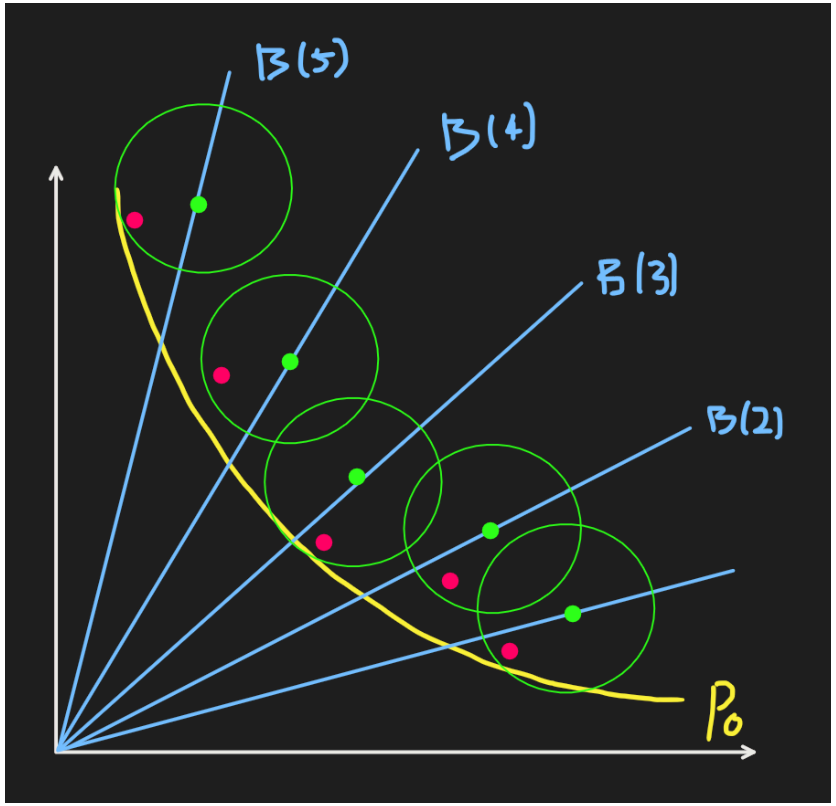

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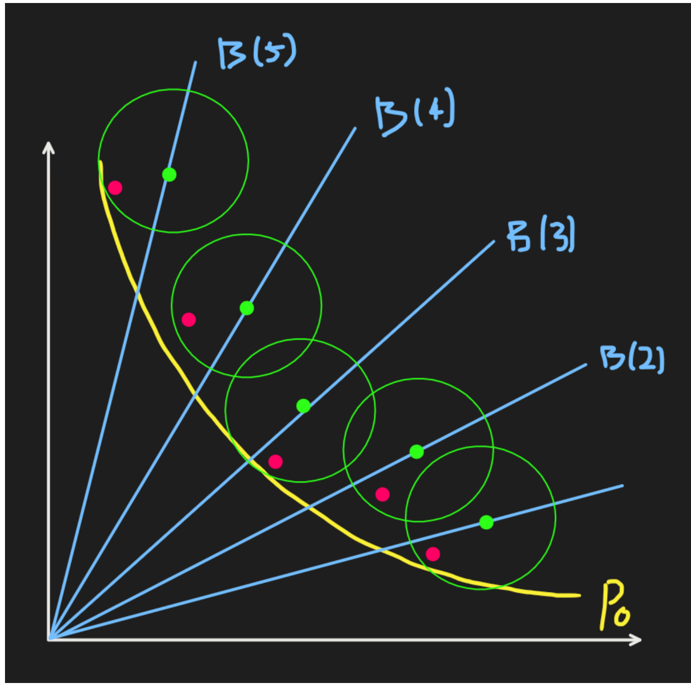
DGEBO Summary

- Utilize the posterior variance Σ from $F \sim N(\mu, \Sigma)$.
- Define the diversity region A_j as the dist. $A_j \sim N(x_j, C_j)$.
- Directly sample the batch X_B from A_j:

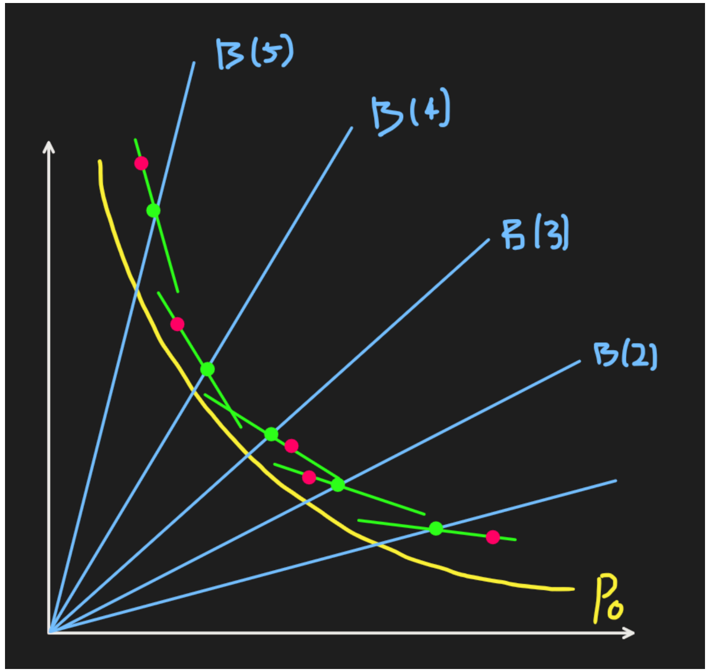
  i. For each performance buffer (diversity region):
    a. Sample candidates from $A_j \sim N(x_j, C_j)$.
    b. Evaluate the candidates using the utility function $U(x) = \mathrm{HVI}(P_f, x) - \lambda_{\mathrm{div}} \cdot (\mathrm{Diversity\ Discount})$
    c. Choose the one with the highest utility.
  ii. Add the batch to the dataset and update the posterior.



DGEMO Review

Methodology:

1. Partition the performance space into buffers $B(j)$ using Latin Hypercube Sampling (LHS).
2. For each $B(j)$, obtain K-best candidate points $\mathbf{x}_{jk}$ by repeating:
   i. Perform stochastic sampling in $B(j)$ to obtain $\mathbf{x}_j$.
   ii. Locally optimize $\mathbf{x}_j$ to get $\mathbf{x}_o$.
   iii. Maintain the K-best $\mathbf{x}_o$s.
3. Compute an affine subspace A_{jk} for each candidate $\mathbf{x}_{jk}$.
4. Use a Graph-cut algorithm to select A_j^* for each $B(j)$.
5. Sample X_B from each A_j^* using HVI optimization.



DGEMO's Limitations

1. The posterior variance Σ_j is not used in the first-order approximation.
   - $\tilde{F} \triangleq [\mu_1, \cdots, \mu_d]$ where $f_j \sim N(\mu_j, \sigma_j)$ represents the posterior distribution.
2. Stochastic sampling is arbitrary and not aligned with the philosophy of BO.
   - $\mathbf{x}_s = \mathbf{x}^j + \frac{1}{2^{\delta_p}}\mathbf{d}_p$: random sampling
3. The objective function F is stochastic, but local opt. uses the L_2 norm.
   - $\mathbf{x}_o = \arg\min_{\mathbf{x}\in\mathcal{X}} \|F(\mathbf{x}) - \mathbf{z}(\mathbf{x}_s)\|^2$, where $F \sim N(\mu, \Sigma)$

Idea: DGEBO

Concepts I will retain from DGEMO:

1. Latin Hypercube Sampling (LHS)
2. The concept of performance buffers (diversity regions)
3. GP as a surrogate model, using the posterior $F \sim N(\mu, \Sigma)$
4. Diversity conditions such as continuity and neighboring buffers
5. HVI optimization within each diversity region

Concepts I want to revise:

1. Define the diversity region as a probability distribution $A_j \sim \mathcal{N}(\mathbf{x}_j, C_j)$ where:

- $[\mathbf{x}_1, \cdots, \mathbf{x}_B]$ are the LHS anchor point of each diversity region $B(1), \cdots, B(B)$.
- $C_j = C_j^{\text{local}} + \alpha \cdot C_j^{\text{diverse}}$, where:
  - $C_j^{\text{local}} = \lambda_1 \underbrace{J_\mu(x_j)J_\mu(x_j)^\top}_{\text{exploitation using mean}} + \lambda_2 \underbrace{J_\Sigma(x_j)J_\Sigma(x_j)^\top}_{\text{exploration using variance}}$
  - $C_j^{\text{diverse}} = \sum_{k \in \text{Neighbor}(j)} w_{jk}(v_{jk}v_{jk}^\top)$
    - $w_{jk} = \frac{1}{\|\mathbf{x}_j - \mathbf{x}_k\|^\beta} \in \mathbb{R}$: distance-based weighting
    - $v_{jk} = \frac{\mathbf{x}_j - \mathbf{x}_k}{\|\mathbf{x}_j - \mathbf{x}_k\|} \in \mathbb{R}^d$: direction from $\mathbf{x}_j$ to $\mathbf{x}_k$
  - α: a hyperparameter controlling the diversity level

2. A new Diversity Region-Based Batch Sampling Strategy

- For each diversity region (performance buffer) $B(j)$:
  - Directly sample K points $[\mathbf{x}_{j1}, \cdots, \mathbf{x}_{jK}]$ using $A_j \sim \mathcal{N}(\mathbf{x}_j, C_j)$
    - $X_K^j \triangleq [\mathbf{x}_{j1}, \cdots, \mathbf{x}_{jK}]$
  - Compute $U(\mathbf{x}_{jk}, \mathcal{D}) \triangleq \mathrm{HVI}(\mathbf{x}_{jk}, \mathcal{D}) - \lambda_{\mathrm{div}} \cdot (\mathrm{Diversity\ Discount})$
    - where $(\mathrm{Diversity\ Discount}) = \sum_{j' \neq j} \exp\left(-\frac{\|x_j - x_{j'}\|^2}{2\ell^2}\right)$
  - Select $\arg\max_{\mathbf{x}_{jk}} U(\mathbf{x}_{jk}, \mathcal{D})$
- Update $\mathcal{D} \leftarrow \mathcal{D} \cup \{\mathbf{x}_1^*, \cdots, \mathbf{x}_B^*\}$

DGEBO Procedure

1. From data $\mathcal{D}$, use GP as a surrogate model to get the posterior of $F \sim N(\mu, \Sigma)$.
2. Sample $[\mathbf{x}_1, \cdots, \mathbf{x}_B]$ using Latin Hypercube Sampling (LHS).
3. For each diversity region $B(j)$ for $j = 1, \cdots, B$
   i. Calculate $J_\mu(\mathbf{x}_j)$ and $J_\Sigma(\mathbf{x}_j)$ using autograd.
   ii. Sample K candidates using $A_j \sim N(\mathbf{x}_j, C_j)$ where $C_j = C_j^{\text{local}} + \alpha C_j^{\text{diverse}}$.
   iii. Calculate utilities of K candidates using $U(\mathbf{x}, \mathcal{D})$.
   iv. Let $\mathbf{x}_j^*$ be the candidate with the highest utility.
4. Update $\mathcal{D} \leftarrow \mathcal{D} \cup \{\mathbf{x}_1^*, \cdots, \mathbf{x}_B^*\}$

Visualized Comparison: DGEMO vs DGEBO

DGEMO	DGEBO