From EHVI to Diffusion Models: Pareto Set Learning for Expensive Multi-Objective Bayesian Optimization

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Overview

1. Multi-Objective Bayesian Optimization (MOBO)
2. Hypervolume and Expected Hypervolume Improvement (EHVI)
3. EHVI-based Methods
4. Composite Diffusion Model for Pareto Set Learning (CDM-PSL)
5. Summary

Contents

Multi-Objective Optimization

We consider a black-box vector-valued objective:

$$\max_{x \in \Omega} f(x) = \left(f_1(x), f_2(x), \ldots, f_M(x)\right)^\top.$$

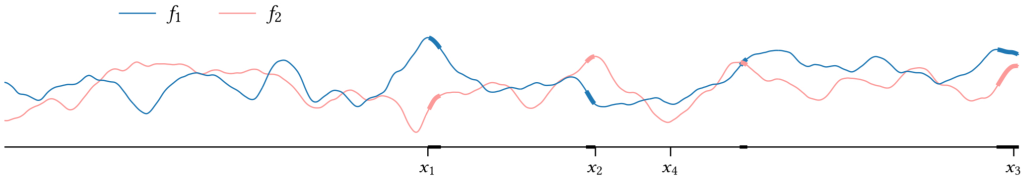


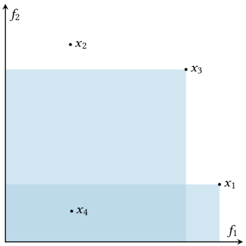
Figure: The first objective f_1 has its global maximum at x_1, which nearly coincides with the global minimum of the second objective f_2. Meanwhile, no rational agent would prefer x_4 to x_3 as the latter point achieves higher values for both objectives.

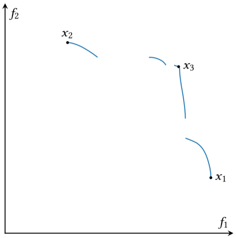
Pareto front

- We will say that a point x dominates y, denoted $y \prec x$, if

$$f_i(y) \leq f_i(x) \; \forall i, \qquad f_j(y) < f_j(x) \text{ for at least one } j.$$

- **Pareto optimal**: A point $x \in \mathcal{X}$ that is not dominated by any other point.
- **Pareto front**: The image of all Pareto optimal points.

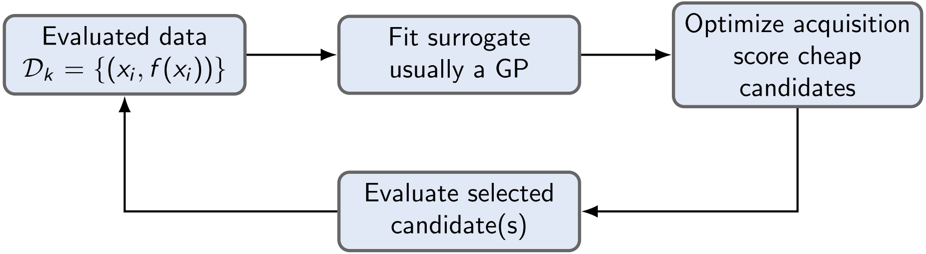




For minimization, we define $x \prec y$ if $f_i(x) \leq f_i(y) \; \forall i$, $f_j(x) < f_j(y)$ for at least one j.

Bayesian optimization loop

Bayesian optimization replaces repeated expensive evaluations with a cheaper probabilistic model.



For objective i, a GP surrogate gives a posterior mean and uncertainty:

$$f_i(x) \mid \mathcal{D}_k \sim \mathcal{N}\big(\mu_i(x), \sigma_i^2(x)\big).$$

The overall framework is called Multi-Objective Bayesian Optimization (MOBO).

Contents

Hypervolume

Let $P \subset \mathbb{R}^M$ be a non-dominated approximation set and let r be a reference point dominated by all relevant objective values [Zitzler and Thiele, 1999, Fleischer, 2002]. For minimization,

$$\mathrm{HV}(P; r) = \lambda_M \left(\bigcup_{y \in P} [y_1, r_1] \times \cdots \times [y_M, r_M] \right).$$

Given the non-dominated set P, the hypervolume improvement of a new objective value y is

$$\mathrm{HVI}(y \mid P, r) = \mathrm{HV}(P \cup \{y\}; r) - \mathrm{HV}(P; r).$$

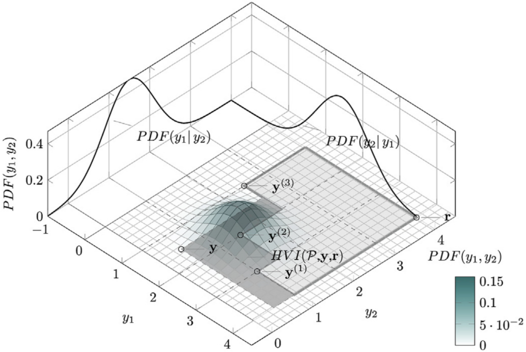
Expected Hypervolume Improvement (EHVI)

In MOBO, the value of a candidate x is uncertain under the surrogate posterior:

$$Y(x) \sim p\big(f(x) \mid \mathcal{D}_k\big).$$

EHVI averages hypervolume improvement under that posterior:

$$\mathrm{EHVI}(x) = \mathbb{E}_{Y(x)}\left[\mathrm{HVI}\big(Y(x) \mid P_k, r\big)\right].$$



Contents

Computation of EHVI

Efficient Computation of Expected Hypervolume Improvement Using Box Decomposition Algorithms. [Yang et al., 2019a]

1. **2-D case:** Partition the non-dominated space into $N_2 = n + 1$ vertical slices and sum closed-form EHVI contributions using Gaussian tail integrals and tail contributions.
2. **3-D case:** Use a sweep-line / AVL-tree box decomposition method, producing at most $N_3 = 2n + 1$ integration slices, with $2^{3-1} = 4$ closed-form terms per slice.
3. **Higher-dimensional case, $d > 3$:** Transform non-dominated-space partitioning into dominated-space partitioning using DKLV17 local lower bounds and LKF17 hyperbox decomposition, then compute EHVI.
4. **Computational costs:** For 2-D and 3-D, the cost is $O(n \log n)$ including sorting, or $\Theta(n)$ if P is already sorted; for $d > 3$, the cost is

$$O\left(2^{d-1} n^{\lfloor d/2 \rfloor}\right),$$

which is polynomial in n for fixed d but exponential in d.

Computation of qEHVI

Differentiable Expected Hypervolume Improvement for Parallel Multi-Objective Bayesian Optimization. [Daulton et al., 2020]

1. **qEHVI:** The batch version of EHVI; measures the expected hypervolume improvement from evaluating q candidate points jointly:

$$\alpha_{\mathrm{qEHVI}}(X_{\mathrm{cand}}) = \mathbb{E}\left[\mathrm{HVI}\left(f(X_{\mathrm{cand}})\right)\right].$$

2. **qEHVI cannot be calculated in closed form:** For $q > 1$, the joint HVI involves unions and intersections of improvement regions under the joint posterior, and no known analytical form exists for $q > 1$ or for correlated outcomes.

3. **Computation of qEHVI:** Use box decomposition and the inclusion–exclusion principle, then estimate the posterior expectation with Monte Carlo or quasi-Monte Carlo samples:

$$\hat{\alpha}^{N}_{\mathrm{qEHVI}}(X_{\mathrm{cand}}) = \frac{1}{N}\sum_{t=1}^{N}\sum_{k=1}^{K}\sum_{j=1}^{q}\sum_{X_j \in \mathcal{X}_j}(-1)^{j+1}\prod_{m=1}^{M}\left[z^{(m)}_{k,X_j,t} - l^{(m)}_{k}\right]_{+}.$$

   Then use auto-differentiation to compute exact gradients of this Monte Carlo estimator for gradient-based optimization.

EHVI as HVI, qEHVI as a Sum of HVI Terms

Expected Hypervolume Improvement Is a Particular Hypervolume Improvement
[Deng et al., 2025]

1. **Key idea:** By **coordinate transformation**, the authors show that EHVI can be written as a particular HVI, and qEHVI can be written as a sum of HVI terms.
2. **EHVI:** The paper defines

$$\tilde{r}_j = \mathrm{EI}(0, \mu_j, \Sigma_{jj}), \qquad \tilde{f}_j^{(i)} = \tilde{r}_j - \mathrm{EI}(f_j^{(i)}, \mu_j, \Sigma_{jj}),$$

   and then computes EHVI by applying a standard hypervolume improvement algorithm to

$$\mathrm{EHVI}(A; \mu, \Sigma) = \mathrm{HVI}(\{\tilde{r}\}, \tilde{A}).$$

3. **How the paper computes qEHVI:** The paper expresses qEHVI as a finite inclusion–exclusion sum of transformed hypervolume improvement terms:

$$\mathrm{qEHVI}(A; \mu, \Sigma) = \sum_{\emptyset \neq I \subseteq \{1,\dots,q\}} (-1)^{|I|+1} \mathrm{HVI}(\{\hat{r}(I)\}, \hat{A}(I)),$$

   where $\hat{r}(I)$ and $\hat{A}(I)$ are constructed using qMinEI.

EHVI as HVI, qEHVI as a Sum of HVI Terms

Algorithm	KMAC (Yang et al. 2019a)		DBB (Daulton, Balandat, and Bakshy 2020)		This paper	
Dimension	$m = 2, 3$	$m \geq 4$	$m = 2, 3$	$m \geq 4$	$m = 2, 3$	$m \geq 4$
Compute EHVI	$\Theta(n \log n)$ time $O(n)$ space	$O(n^{\lfloor \frac{m}{2} \rfloor})$ time $O(n^{\lfloor \frac{m}{2} \rfloor})$ space	The same method as KMAC		$\Theta(n \log n)$ time $O(n)$ space	$\boldsymbol{\tilde{O}(n^{\frac{m}{3}})}$ **time** $\boldsymbol{O(n)}$ **space**
Compute qEHVI ($q > 1$)	N/A		Monte-Carlo method with the same complexities of DBB for EHVI		**Exact method** with the same complexities of our method for EHVI	

Contents

CDM-PSL

Expensive Multi-Objective Bayesian Optimization Based on Diffusion Models [Li et al., 2025].

Problem statement

Existing Pareto set learning methods can be unstable when only a limited number of expensive evaluations are available.

Proposed idea

CDM-PSL uses a **composite diffusion model** for Pareto set learning:

- unconditional diffusion generation for diversity
- conditional guided denoising for convergence
- entropy-based objective weighting to balance multiple objectives
- a GP surrogate and batch selection inside an MOBO loop

DDPM

To sample from $x_0 \sim p_{data}$, Denoising Diffusion Probabilistic Models (DDPMs) involve two distinct stochastic processes:

- The forward process (fixed encoder):

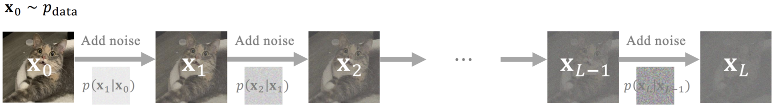


Figure: This process gradually corrupts data by injecting Gaussian noise over multiple steps.

- The reverse denoising process (learnable decoder):

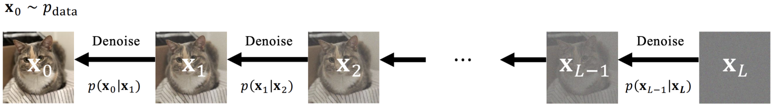


Figure: Starting from pure noise, this process iteratively denoises to generate realistic samples.

DDPM: Two Markov Chains

Denoising Diffusion Probabilistic Models (DDPMs) use two stochastic processes:

Forward process: fixed encoder

Gradually corrupts real data by adding Gaussian noise:

$$x_0 \sim p_{\text{data}}, \qquad x_T \approx \mathcal{N}(0, I).$$

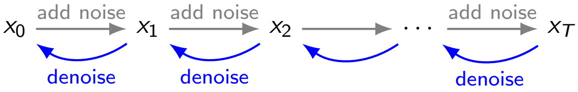
This process is fixed and non-trainable.

Reverse process: learned decoder

Starts from pure noise and denoises step-by-step:

$$x_T \sim p_{\text{prior}} = N(0, I), x_T \to x_{T-1} \to \cdots \to x_0.$$

The reverse transitions are learned by a neural network.



Forward Process: Fixed Gaussian Noise

One-step transition

For a pre-defined noise schedule $\{\beta_t\}_{t=1}^{T}$, define

$$\alpha_t := \sqrt{1 - \beta_t^2}.$$

Then

$$p(x_t \mid x_{t-1}) = \mathcal{N}\left(x_t;\, \alpha_t x_{t-1}, \beta_t^2 I\right).$$

Equivalently,

$$x_t = \alpha_t x_{t-1} + \beta_t \epsilon_t, \qquad \epsilon_t \sim N(0, I).$$

Forward Process: Fixed Gaussian Noise

Direct sampling at any noise level

Let
$$\bar{\alpha}_t := \prod_{k=1}^{t} \alpha_k.$$

Then the noisy sample at step t can be sampled directly from x_0:

$$p_t(x_t \mid x_0) = \mathcal{N}\left(x_t;\ \bar{\alpha}_t x_0, (1 - \bar{\alpha}_t^2) I\right),$$

or equivalently,
$$x_t = \bar{\alpha}_t x_0 + \sqrt{1 - \bar{\alpha}_t^2}\,\epsilon, \qquad \epsilon \sim N(0, I).$$

As t becomes large, x_t approaches pure Gaussian noise:

$$x_T \approx p_{\text{prior}} = N(0, I).$$

Reverse Process: Learned Denoising

Learned reverse transition

DDPM approximates the unknown reverse transition by a Gaussian model:

$$p_\phi(x_{t-1} \mid x_t) = \mathcal{N}\left(x_{t-1};\, \mu_\phi(x_t, t), \sigma_t^2 I\right),$$

where μ_ϕ is predicted by a neural network.

Conditioning trick

Instead of modeling the intractable marginal reverse kernel directly, DDPM uses the tractable conditional posterior:

$$p(x_{t-1} \mid x_t, x_0) = \mathcal{N}\left(x_{t-1};\, \mu(x_t, x_0, t), \sigma_t^2 I\right).$$

Thus training reduces to matching Gaussian means:

$$\mathcal{L}_{\mathrm{DDPM}}(\phi) = \sum_{t=2}^{L} \frac{1}{2\sigma_t^2} \mathbb{E}_{x_0} \mathbb{E}_{p(x_t \mid x_0)} \left[\|\mu_\phi(x_t, t) - \mu(x_t, x_0, t)\|_2^2 \right].$$

Reverse Process: Learned Denoising

Practical noise-prediction form

$$x_t = \bar{\alpha}_t x_0 + \sqrt{1 - \bar{\alpha}_t^2}\,\epsilon, \qquad \epsilon \sim \mathcal{N}(0, I),$$

DDPM commonly trains a network $\epsilon_\phi(x_t, t)$ to predict the added noise:

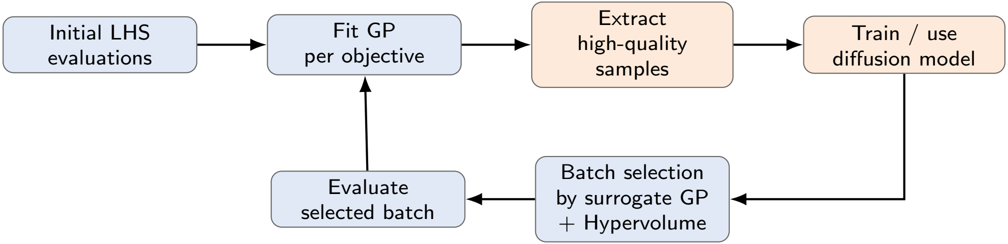
$$\mathcal{L}_{\text{simple}}(\phi) = \mathbb{E}_{t, x_0, \epsilon}\left[\|\epsilon_\phi(x_t, t) - \epsilon\|_2^2\right].$$

Sampling: Reverse Denoising After Training

The model recursively samples x_{t-1} using the learned reverse transition $p_\phi(x_{t-1} \mid x_t)$:

$$x_{t-1} \leftarrow \underbrace{\frac{1}{\alpha_t}\left(x_t - \frac{1 - \alpha_t^2}{\sqrt{1 - \bar{\alpha}_t^2}}\epsilon_\phi(x_t, t)\right)}_{\mu_\phi(x_t, t)} + \sigma_t \epsilon_t, \qquad epsilon_t \sim \mathcal{N}(0, I).$$

Algorithmic overview of CDM-PSL



Three main components

1. **Data extraction**: choose promising samples from evaluated data.
2. **Diffusion model training**: learn the distribution of good decision vectors.
3. **Composite generation**: combine guided conditional sampling with unconditional sampling.

Component 1: data extraction

The diffusion model is not trained on all evaluated points; it is trained on selected high-quality samples. The paper uses shift-based density estimation to score evaluated samples:

$$\mathrm{Fitness}(p) = \min_{q \in X^k \setminus \{p\}} \sqrt{\sum_{i=1}^{M} \left(\max\{0, f_i(q) - f_i(p)\}\right)^2}.$$

Intuition

- Keep samples that are promising for convergence and diversity.
- Use those samples as empirical evidence of the Pareto-set distribution.

Component 2: diffusion model training

Given selected samples X_k^*, the forward process gradually adds Gaussian noise:

$$X_{k,t}^* = \sqrt{1-\beta_t}\, X_{k,t-1}^* + \sqrt{\beta_t}\, \epsilon, \qquad \epsilon \sim \mathcal{N}(0, I).$$

The network learns to predict the added noise:

$$\mathcal{L}(\theta) = \frac{1}{H} \sum_{i=1}^{H} \left\| \epsilon - \epsilon_\theta(x_{k,i,t}^*, t) \right\|^2.$$

Component 3: conditional generation by guided denoising

To improve sample quality, CDM-PSL guides the reverse process using surrogate-gradient information:

$$X_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(X_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(X_t, t)\right) + \sigma_t^2 \hat{g} + \sigma_t z.$$

$$\hat{g} = \sum_{j=1}^{M} W_j \nabla a_j(x), \qquad a_j(x) : \text{GP-LCB surrogate for the } j\text{-th objective}$$

Denoising term

Moves noisy samples back toward the learned distribution of high-quality samples.

Guidance term $\hat{g}$

Uses GP surrogate gradients to bias the reverse trajectory toward improved objective values.

Component 3: entropy-based objective weighting

For each objective j, normalize objective values, form probabilities, and compute entropy:

$$\tilde{y}_{ij} = \frac{y_{ij} - \min(y_j)}{\max(y_j) - \min(y_j)}, \qquad P_{ij} = \frac{\tilde{y}_{ij}}{\sum_{k=1}^{N} \tilde{y}_{kj}},$$

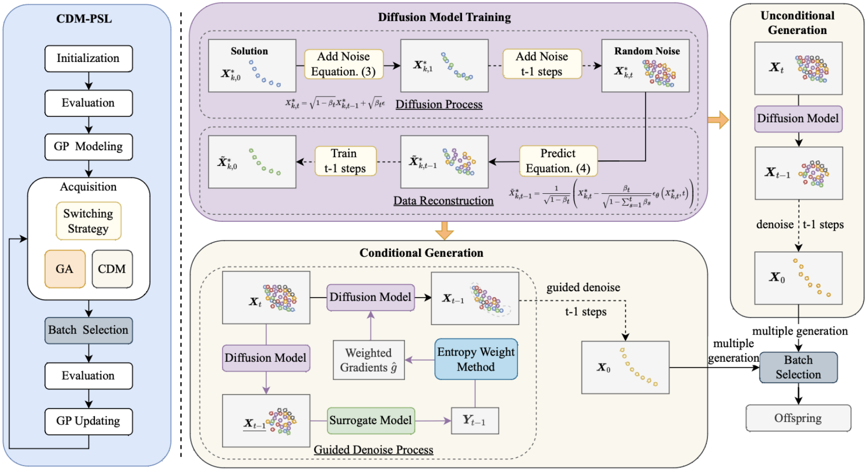
$$E_j = -\frac{1}{\ln N} \sum_{i=1}^{N} P_{ij} \ln(P_{ij} + \eta), \qquad W_j = \frac{1 - E_j}{\sum_{k=1}^{M} (1 - E_k)}.$$

Here, $i = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, M$, where N is the total number of samples and M is the number of objectives.

Intuition

E_j: minimized at 0 when $P_{1j} = 1, P_{ij} = 0 \forall i \neq 1$. W_j: maximized when $E_j = 0$. Therefore, this gives more weight to objectives with greater variation among individuals.

Diffusion model framework



Conditional Generation : Unconditional Generation $= 1 : 10$

Selection strategy after generation

Batch selection

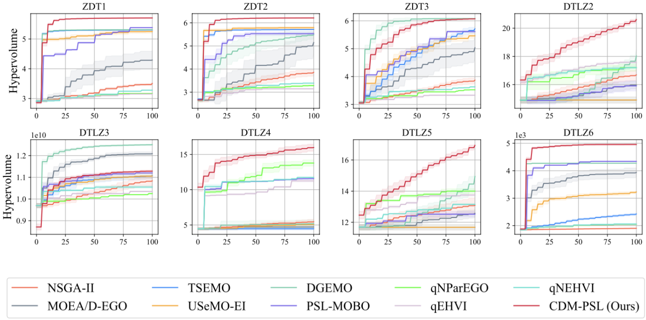
- Use the GP surrogate to estimate Hypervolume (HV).
- Select a small subset $X_k^B = \{x_b \mid b = 1, \ldots, B\}$ with high HV values.
- Evaluate only the selected batch with the expensive black-box function.

Operator switching

- Monitor hypervolume growth over an iteration window.
- If growth stagnates, switch the offspring generator to a genetic algorithm.
- This is intended to reduce local stagnation caused by a single operator.

Experimental Study

The paper evaluates CDM-PSL on synthetic benchmarks and real-world problems, comparing against classical and recent MOBO / EMO baselines.



Parameter settings

The DM is designed with two linear layers, each containing 128 hidden units, and is trained for 4000 epochs with a batch size of 1024. The hyperparameter step t is 25, and the noise level is defined in the range from 1e-5 to 0.5e-1.

Contents

Summary

Main problem

Multi-Objective Bayesian Optimization (MOBO) aims to optimize several expensive black-box objectives at the same time. Since objectives can conflict, the goal is not a single optimum but a set of Pareto-optimal solutions.

	EHVI as HVI [Deng et al., 2025]	**CDM-PSL** [Li et al., 2025]
Core idea	EHVI can be converted into a hypervolume-improvement HVI problem.	Uses a composite diffusion model to learn the distribution of Pareto-set samples.
Treatment of q batch optimization	qEHVI is expressed as a finite sum of particular HVI terms, giving an exact analytic expression for $q > 1$.	Supports batch optimization by generating many offspring candidates through CDM-PSL.
Candidate generation	Provides a more efficient exact acquisition-function computation that can be used inside an MOBO candidate-selection loop.	Generates candidates directly using the composite diffusion model: conditional and unconditional generation.

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