MAX-VALUE ENTROPY SEARCH FOR MULTI-OBJECTIVE BAYESIAN OPTIMIZATION

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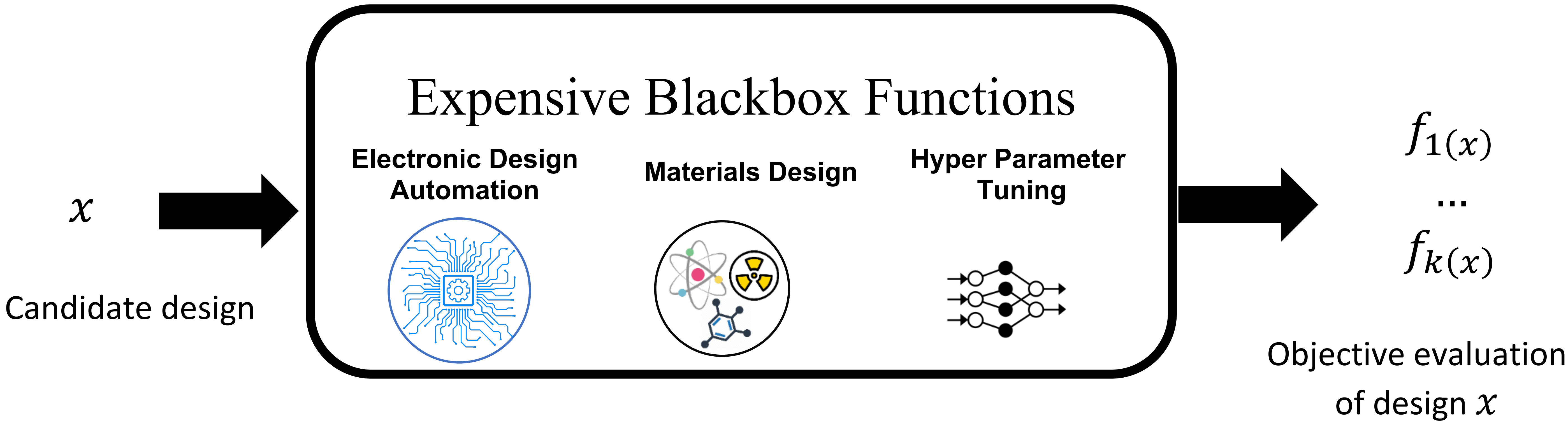
BLACKBOX OPTIMIZATION WITH MULTIPLE OBJECTIVES VIA EXPENSIVE EVALUATIONS

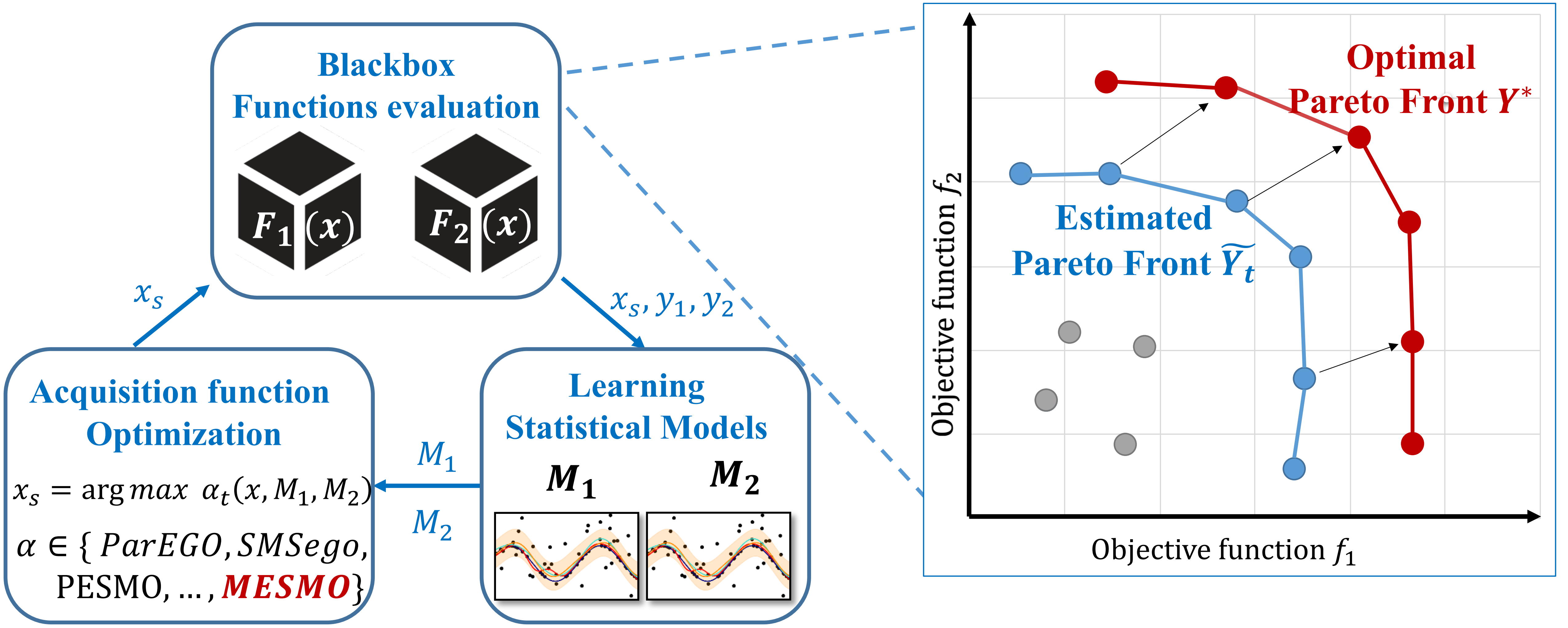


❑ Many scientific and engineering applications has following challenges

➢ Find the Pareto set of designs that trade-off multiple objectives
➢ Minimize the total resource cost for function evaluations for optimization

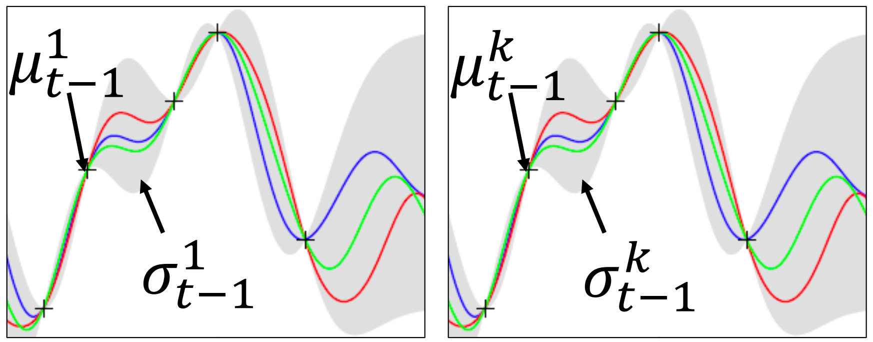
MULTI-OBJECTIVE BAYESIAN OPTIMIZATION

- Bayesian optimization (BO) is a framework to **optimize expensive black-box functions** using the following elements:
  - **Statistical models** as a prior for the functions: Gaussian processes (GPs) can provide prediction $\mu(x)$ and uncertainty via variance $\sigma(x)$
  - **Acquisition function** to score the utility of evaluating input x
  - **Optimization procedure** to select the best input x for evaluation



MESMO: OUTPUT SPACE ENTROPY SEARCH ALGORITHM

Posteriors estimation



Sample a set of optimal pareto fronts Y^*

Define the acquisition function $\alpha_t(x) = I(\{x, y\}: Y^* \mid D_t)$

Evaluate the functions $f_1, \dots, f_k$ at $x_t = \arg max\, \alpha_t(x)$

OUTPUT SPACE ENTROPY SEARCH VS. INPUT SPACE ENTROPY SEARCH

- **Output space entropy-based acquisition function**

$$\begin{aligned}
\alpha(\mathbf{x}) &= I(\{\mathbf{x}, \mathbf{y}\}, \mathcal{Y}^* \mid D) \\
&= H(\mathcal{Y}^* \mid D) - \mathbb{E}_y[H(\mathcal{Y}^* \mid D \cup \{\mathbf{x}, \mathbf{y}\})] \\
&= H(\mathbf{y} \mid D, \mathbf{x}) - \mathbb{E}_{\mathcal{Y}^*}[H(\mathbf{y} \mid D, \mathbf{x}, \mathcal{Y}^*)]
\end{aligned}$$

Information gain about the optimal Pareto front

Equivalent to expected reduction in entropy over the pareto front

Symmetric property of information gain

Entropy of factorizable gaussian distribution

Closed form using properties of truncated gaussian distribution

$$\boxed{\alpha(\mathbf{x}) \simeq \frac{1}{S} \sum_{s=1}^{S} \sum_{j=1}^{K} \left[\frac{\gamma_s^j(\mathbf{x}) \phi(\gamma_s^j(\mathbf{x}))}{2\Phi(\gamma_s^j(\mathbf{x}))} - \ln \Phi(\gamma_s^j(\mathbf{x})) \right]}$$

Closed-form

OUTPUT SPACE ENTROPY SEARCH VS. INPUT SPACE ENTROPY SEARCH

- **Output space entropy-based acquisition function**

$$\alpha(\mathbf{x}) = I(\{\mathbf{x},\mathbf{y}\}, \boxed{\mathcal{Y}^*} \mid D)$$

Output dimension *k* < < *d*

$$= H(\mathcal{Y}^* \mid D) - \mathbb{E}_y[H(\mathcal{Y}^* \mid D \cup \{\mathbf{x},\mathbf{y}\})]$$

$$= H(\mathbf{y} \mid D, \mathbf{x}) - \boxed{\mathbb{E}_{\mathcal{Y}^*}[H(\mathbf{y} \mid D, \mathbf{x}, \mathcal{Y}^*)]}$$

Sum of truncated Gaussians

$$\boxed{\alpha(\mathbf{x}) \simeq \frac{1}{S}\sum_{s=1}^{S}\sum_{j=1}^{K}\left[\frac{\gamma_s^j(\mathbf{x})\phi(\gamma_s^j(\mathbf{x}))}{2\Phi(\gamma_s^j(\mathbf{x}))} - \ln \Phi(\gamma_s^j(\mathbf{x}))\right]}$$

Closed-form

- **Input space entropy-based acquisition function**

$$\alpha(\mathbf{x}) = I(\{\mathbf{x},\mathbf{y}\}, \boxed{\mathcal{X}^*} \mid D)$$

Input dimension *d*

$$= H(\mathcal{X}^* \mid D) - \mathbb{E}_y[H(\mathcal{X}^* \mid D \cup \{\mathbf{x},\mathbf{y}\})]$$

$$= H(\mathbf{y} \mid D, \mathbf{x}) - \boxed{\mathbb{E}_{\mathcal{X}^*}[H(\mathbf{y} \mid D, \mathbf{x}, \mathcal{X}^*)]}$$

Requires approximation

Thank You