A tutorial on Bayesian Optimization

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Challenges in Engineering Design

The society demands new products of better quality, functionality, usability, etc.!
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Optimization is a challenging task in new products design!
Example: **Deep Neural Network** for object recognition.
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**Parameters to tune:** Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc.
Example: new **plastic solar cells** for transforming light into electricity.
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Explore **millions of candidate molecule structures** to identify the compounds with the best properties.
Example: control system for a robot that is able to grasp objects.
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Parameters to tune: initial pose for the robot’s hand and finger joint trajectories.
Optimization Problems: Common Features

- Very expensive evaluations.

Bayesian optimization methods can be used to solve these problems!
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- The objective is a black-box.
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Bayesian Optimization in Practice

1. Get initial sample.
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The model guides the search focusing on the most-promising regions of the input space!
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2. Fit a model to the data:
   \[ p(y|x, D_n) \].
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   \[ p(y|x, D_n). \]
3. **Select data collection strategy:**
   \[ \alpha(x) = \mathbb{E}_{p(y|x, D_n)}[U(y|x, D_n)]. \]
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The model guides the search focusing on the most-promising regions of the input space!
Tuning LDA on a collection of Wikipedia articles (Snoek et al., 2012).
Fitting a Model to the Data

Challenges: The model should be non-parametric (the world is complicated) and computing $p(Data)$ is intractable!

Solved by setting $p(W) = \prod_{ij} N(w_{ji} | 0, \sigma^2 H^{-1})$ and letting $H \to \infty$. 
Fitting a Model to the Data

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Solved by setting $p(W) = \prod_{ij} N(w_{ji}|0, \sigma^2 H^{-1})$ and letting $H \to \infty$.

$$h_j(x) = \tanh \left( \sum_{i=1}^{I} x_i w_{ji} \right)$$

$$f(x) = \sum_{j=1}^{H} v_j h_j(x)$$
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Solved by setting $p(W|Data) = p(W)p(Data|W)/p(Data)$

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$$f(x) = \sum_{j=1}^{H} v_j h_j(x)$$

**Posterior Dist.**

**Predictive Dist.**

$$p(y|Data, x) = \int p(y|W, x)p(W|Data)dW$$
Fitting a Model to the Data

Challenges: The model should be non-parametric (the world is complicated) and computing $p(\text{Data})$ is intractable!

\[
h_j(x) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)
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\]

Posterior Dist. \hspace{1cm} p(W|\text{Data}) = \frac{p(W)p(\text{Data}|W)}{p(\text{Data})}

Predictive Dist. \hspace{1cm} p(y|\text{Data}, x) = \int p(y|W, x)p(W|\text{Data})dW
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Challenges: The model should be non-parametric (the world is complicated) and computing $p(\text{Data})$ is intractable!

Solved by setting $p(W) = \prod_{ij} \mathcal{N}(w_{ji} | 0, \sigma^2 H^{-1})$ and letting $H \to \infty$!
Gaussian Processes

Distribution over functions $f(\cdot)$ so that for any finite \( \{x_i\}_{i=1}^N \),\n\[
(f(x_1), \ldots, f(x_N))^T \text{ follows an } N\text{-dimensional Gaussian distribution.}
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Gaussian Processes

Distribution over functions $f(\cdot)$ so that for any finite $\{x_i\}_{i=1}^N$, $(f(x_1), \ldots, f(x_N))^T$ follows an $N$-dimensional Gaussian distribution.
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When $H \to \infty$, $(f(x_1), \ldots, f(x_N))^T$ follows an $N$-dimensional Gaussian where $\mathbb{E}[f(x_i)f(x_k)] = \sigma^2 \mathbb{E}[h_j(x_i)h_j(x_k)]$ by the central limit theorem.
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Due to Gaussian form, there are closed-form solutions for many useful questions about finite data.
Gaussian Processes

• The joint distribution for $y^*$ at test points $\{x^*_m\}_{m=1}^M$ and $y$:

$$p(y^*, y) = \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k_\theta & K_\theta \\ K_\theta^T & \kappa_\theta \end{bmatrix} \right)$$
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\]

• These matrices are computed from the covariance \( C(\cdot, \cdot; \theta) \):

\[
[K_\theta]_{n,n'} = C(x_n, x_{n'}; \theta)
\]
\[
[k_\theta]_{n,m} = C(x_n, x_m^*; \theta), \quad [\kappa_\theta]_{m,m'} = C(x_m^*, x_{m'}^*; \theta)
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Gaussian Processes

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  \]

- The **predictive distribution** for \( y^* \) given \( y \), \( p(y^*|y) \), is:

  \[
y^* \sim \mathcal{N}(m, \Sigma) \\
  m = k_\theta^T K_\theta^{-1} y, \quad \Sigma = \kappa_\theta - k_\theta^T K_\theta^{-1} k_\theta,
\]
Gaussian Processes

- The joint distribution for $y^\star$ at test points $\{x^*_m\}_{m=1}^M$ and $y$:
  \[
p(y^\star, y) = \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k_\theta & K_\theta \\ \kappa_\theta & k_\theta^T \end{bmatrix}\right)
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y^\star \sim \mathcal{N}(m, \Sigma) \\
m = k_\theta^T K_\theta^{-1} y, \quad \Sigma = \kappa_\theta - k_\theta^T K_\theta^{-1} k_\theta,
  \]
- The log of the marginal likelihood, $p(y|\theta)$, is:
  \[
  \log p(y) = -\frac{N}{2} \log 2\pi - \frac{1}{2} \log |K_\theta| - \frac{1}{2} y^T K_\theta^{-1} y
  \]
From the Prior to the Posterior

GP regression provides a **closed-form** posterior distribution for $f(\cdot)$. 

![Ground Truth](image)
From the Prior to the Posterior

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![Ground Truth](image.png)
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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{ground_truth.png}
\caption{Ground Truth}
\end{figure}
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![Diagram](image-url)
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GP regression provides a *closed-form* posterior distribution for $f(\cdot)$.
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GP regression provides a \textbf{closed-form} posterior distribution for $f(\cdot)$. 
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[Diagram showing a comparison between different models and the ground truth.]

- Red: Ground Truth
- Black: Model Prediction
- Gray: Confidence Interval

Points along the curves indicate data points used in the regression.
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Using the GP Uncertainty in Optimization

Where to evaluate next?
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• Exploration: seek places with high variance.
• Exploitation: seek places with low mean.

The acquisition function balances these two, to choose in an intelligent way the next evaluation point!

$$\alpha(x) = \mathbb{E}_{p(y|D_N,x)}\left[U(y|\mathcal{D}_N)\right]$$
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Some Acquisition Functions

Let $\nu = \min\{y_1, \ldots, y_N\}$ and $\gamma(x) = \frac{\nu - \mu(x)}{\sigma(x)}$. 
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- Probability of Improvement:
  
  $$U(y^*|\mathcal{D}_N, x) = I(y_* < \nu), \quad \alpha(x) = \Phi(\gamma(x))$$
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- **Expected Improvement:**
  \[
  U(y^*|D_N, x) = \max(0, \nu - y^*), \quad \alpha(x) = \sigma(x) (\gamma(x) \Phi(\gamma(x)) + \phi(\gamma(x)))
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- **Lower Confidence Bound:**
  \[ \alpha(x) = -\left(\mu(x) - \kappa \sigma(x)\right) \]
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- **Lower Confidence Bound:**

  $$\alpha(x) = - (\mu(x) - \kappa\sigma(x))$$

- **Entropy Search:**

  $$U(y^*|D_N, x) = H[p(x_{\text{min}}|D_N)] - H[p(x_{\text{min}}|D_N \cup \{x, y^*\})]$$
Some Acquisition Functions:
Some Acquisition Functions: Prob. Improvement
Some Acquisition Functions: Exp. Improvement
Some Acquisition Functions: Lower Conf. Bound
Some Acquisition Functions: Entropy Search
Bayesian Optimization and Model Selection

- **Covariance function selection**: critical to achieve good performance. The default choice for regression (squared exponential) is too smooth. Matérn $\nu = 5/2$ kernel works better.
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Structured SVM for protein motif finding (Snoek et al., 2012).
Bayesian Optimization and Model Selection

- **Hyper-parameter selection:** with a small number of observations maximizing $p(y|\theta)$ can give **too confident** uncertainty estimates.
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- **Sampling the hyper-parameters:** computing $p(\theta|y)$ is **intractable**! Alternative: generate a few samples from $p(\theta|y)$ using MCMC.
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*Slice sampling means no additional hyper-parameters!*

(Neal, 2003)
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(Neal, 2003)
Integrated Acquisition Function

\[ \hat{\alpha}(\mathbf{x}) = \int \alpha(\mathbf{x}; \theta) p(\theta | y) d\theta \approx \frac{1}{K} \sum_{k=1}^{K} \alpha(\mathbf{x}; \theta^{(k)}) \quad \theta^{(k)} \sim p(\theta | y), \]
Integrated Acquisition Function

\[
\hat{\alpha}(x) = \int \alpha(x; \theta)p(\theta|y)d\theta \approx \frac{1}{K} \sum_{k=1}^{K} \alpha(x; \theta^{(k)}) \quad \theta^{(k)} \sim p(\theta|y),
\]

Posterior samples with three different length-scales

(Snoek et al., 2012)
Integrated Acquisition Function

\[ \hat{\alpha}(x) = \int \alpha(x; \theta)p(\theta|y)d\theta \approx \frac{1}{K} \sum_{k=1}^{K} \alpha(x; \theta^{(k)}) \quad \theta^{(k)} \sim p(\theta|y), \]

Posterior samples with three different length-scales

Length-scale specific expected improvement

(Snoek et al., 2012)
Integrated Acquisition Function

\[ \hat{\alpha}(\mathbf{x}) = \int \alpha(\mathbf{x}; \theta) p(\theta | \mathbf{y}) d\theta \approx \frac{1}{K} \sum_{k=1}^{K} \alpha(\mathbf{x}; \theta^{(k)}) \quad \theta^{(k)} \sim p(\theta | \mathbf{y}), \]

(Snoek et al., 2012)
MCMC estimation vs. Maximization

Logistic regression on the MNIST (Snoek et al., 2012).
Cost-sensitive Bayesian Optimization

- Different inputs may have **different computational costs**, e.g., training a neural network of increasing hidden layers and units.

\[
\alpha(x) = \sigma(x) \left( \gamma(x) \Phi(\gamma(x)) + \varphi(\gamma(x)) \right) \exp\left\{ \mu \log\text{time}(x) \right\}
\]

(Snoek et al., 2012)
Cost-sensitive Bayesian Optimization

- Different inputs may have different computational costs, e.g., training a neural network of increasing hidden layers and units.
- Better to do cheap evaluations before expensive ones!
Cost-sensitive Bayesian Optimization

• Different inputs may have **different computational costs**, e.g., training a neural network of increasing hidden layers and units.

• Better to do **cheap evaluations** before expensive ones!

• The evaluation costs are **unknown** but they can be **recorded** and then **modeled** with an additional **Gaussian process**.
Cost-sensitive Bayesian Optimization

- Different inputs may have **different computational costs**, e.g., training a neural network of increasing hidden layers and units.

- Better to do **cheap evaluations** before expensive ones!

- The evaluation costs are **unknown** but they can be **recorded** and then **modeled** with an additional **Gaussian process**.

**Expected Improvement per-second:**

\[
\alpha(x) = \frac{\sigma(x) \left( \gamma(x) \Phi(\gamma(x)) + \phi(\gamma(x)) \right)}{\exp \left\{ \mu_{\log\text{-time}}(x) \right\}}
\]

(Snoek *et al.*, 2012)
Cost-sensitive Bayesian Optimization

\[ f(x) \]
\[ EI(x) \]
\[ \text{duration}(x) \]
\[ EI(x) / \text{s} \]

\[ E(x) / \text{s} \]
\[ \text{duration}(x) \]
Cost-sensitive Bayesian Optimization

\[ f(x) \]
\[ EI(x) \]
\[ \frac{EI(x)}{s} \]
\[ \text{duration}(x) \]
Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization

\[ f(x) \]

\[ EI(x) \]

\[ \text{duration}(x) \]

\[ EI(x) / s \]

\[ E(x) / s = \text{duration}(x) \]
Cost-sensitive Bayesian Optimization

Deep neural network on the CIFAR dataset (Snoek et al., 2012)
Several Objectives and Constraints

Optimal design of **hardware accelerator** for neural network predictions.

- **Goals:**
  - Minimize prediction error.
  - Minimize prediction time.

- **Constrained to:**
  - Chip area below a value.
  - Power consumption below a level.

**Challenges:**
- Complicated constraints.
- Conflictive objectives.
Several Objectives and Constraints

Optimal design of **hardware accelerator** for neural network predictions.

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Several Objectives and Constraints

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- **prediction error**
- **prediction time**
- **Chip area**
- **Power consumption**
Several Objectives and Constraints

Optimal design of **hardware accelerator** for neural network predictions.

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**Challenges:**
- **Complicated** constraints.
- **Conflictive** objectives.
Constrained Multi-Objective Optimization

Objective 1

Objective 2
Constrained Multi-Objective Optimization

Objective 1

Objective 2

Pareto Set (Input space)
Constrained Multi-Objective Optimization

Objective 1

Objective 2

Pareto Set (Input space)

Pareto Frontier (value space)
Constrained Multi-Objective Optimization

Objective 1

Objective 2

Constraint 1

Pareto Set (Input space)

Pareto Frontier (value space)
Constrained Multi-Objective Optimization

Objective 1

Objective 2

Constraint 1

Pareto Set (Input space)

Pareto Frontier (value space)
Constrained Multi-Objective Optimization

Pareto Set (Input space)

Pareto Frontier (value space)
Bayesian Optimization Methods

Additional challenges when dealing with several black-boxes.
Bayesian Optimization Methods

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- Simple approach: evaluate all the objectives and constraints at the same input location. Expected to be sub-optimal.
Bayesian Optimization Methods

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- Simple approach: evaluate all the objectives and constraints at the same input location. Expected to be sub-optimal.

- Advanced approach: make intelligent decisions about what black-box to evaluate next and on which location.
Bayesian Optimization Methods

Additional challenges when dealing with several black-boxes.

- Simple approach: evaluate all the objectives and constraints at the same input location. Expected to be sub-optimal.
- Advanced approach: make intelligent decisions about what black-box to evaluate next and on which location.

**Coupled evaluations**

- Black-box 1 → $Y_t^1$
- Black-box 2 → $Y_t^2$
Bayesian Optimization Methods

Additional challenges when dealing with several black-boxes.

- Simple approach: evaluate all the objectives and constraints at the same input location. Expected to be sub-optimal.

- Advanced approach: make intelligent decisions about what black-box to evaluate next and on which location.

**Coupled evaluations**

- Black-box 1
  - Input: $x_t$
  - Output: $Y_t^1$

- Black-box 2
  - Input: $x_t$
  - Output: $Y_t^2$

**Decoupled evaluations**

- Black-box 1
  - Input: $x_t$
  - Output: $Y_t^1$

- Black-box 2
  - Input: $x_t$
  - Output: $Y_t^2$
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!

Information is measured by the entropy of $p(\mathcal{X}^*|\mathcal{D}_N)$. 
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!

Information is measured by the entropy of $p(\mathcal{X}^*|D_N)$. 

![Graph showing Actual Objectives and Constraints]
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!

Information is measured by the entropy of $p(\mathcal{X}^*|\mathcal{D}_N)$. 

![Actual Objectives and Constraints](image1)

![Posterior of each Objective and Constraint](image2)
Information-based Approach

The Pareto set $\mathcal{X}^{*}$ in the feasible space is a random variable!

Information is measured by the entropy of $p(\mathcal{X}^{*} | D_N)$.
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Information-based Approach

The Pareto set $\mathcal{X}^\star$ in the feasible space is a random variable! Information is measured by the entropy of $p(\mathcal{X}^\star | D_N)$.
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!

**Information** is measured by the entropy of $p(\mathcal{X}^*|\mathcal{D}_N)$.
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!

Information is measured by the entropy of $p(\mathcal{X}^*|D_N)$.
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Information-based Approach

The Pareto set $\mathcal{X}^\star$ in the feasible space is a **random variable**!

**Information** is measured by the **entropy** of $p(\mathcal{X}^\star|\mathcal{D}_N)$. 
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable!

Information is measured by the entropy of $p(\mathcal{X}^*|\mathcal{D}_N)$. 

![Graph showing High Entropy and Low Information compared to Low Entropy and High Information]
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable! Information is measured by the entropy of $p(\mathcal{X}^*|\mathcal{D}_N)$.

The acquisition function is

$$\alpha(x) = H[\mathcal{X}^*|\mathcal{D}_t] - \mathbb{E}_y \left[ H[\mathcal{X}^*|\mathcal{D}_t \cup \{x, y\}] \right| \mathcal{D}_t, x] \quad (1)$$
Information-based Approach

The Pareto set $\chi^*$ in the feasible space is a **random variable**!

**Information** is measured by the **entropy** of $p(\chi^*|\mathcal{D}_N)$.

The acquisition function is

$$\alpha(x) = H[\chi^*|\mathcal{D}_t] - \mathbb{E}_y \left[ H[\chi^*|\mathcal{D}_t \cup \{x, y\}] \right] |\mathcal{D}_t, x] \quad (1)$$

![Diagram](image-url)
Information-based Approach

The Pareto set $\mathcal{X}^\star$ in the feasible space is a random variable! Information is measured by the entropy of $p(\mathcal{X}^\star|\mathcal{D}_N)$.

![High Entropy Low Information](image1)

![Low Entropy High Information](image2)

The acquisition function is

$$\alpha(x) = H[\mathcal{X}^\star|\mathcal{D}_t] - \mathbb{E}_y \left[H[\mathcal{X}^\star|\mathcal{D}_t \cup \{x, y\}]|\mathcal{D}_t, x\right]$$  \hspace{1cm} (1)
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a **random variable**!

**Information** is measured by the **entropy** of $p(\mathcal{X}^*|\mathcal{D}_N)$.

The acquisition function is

$$\alpha(x) = H(\mathcal{X}^*|\mathcal{D}_t) - \mathbb{E}_y \left[ H(\mathcal{X}^*|\mathcal{D}_t \cup \{x, y\}) | \mathcal{D}_t, x \right] \quad (1)$$

How much we know about $\mathcal{X}^*$ now.

How much we will know about $\mathcal{X}^*$ after collecting $y$ at $x$. 
Information-based Approach

The Pareto set $\mathcal{X}^*$ in the feasible space is a random variable! Information is measured by the entropy of $p(\mathcal{X}^*|\mathcal{D}_N)$.

The acquisition function is

$$\alpha(x) = H[\mathcal{X}^*|\mathcal{D}_t] - \mathbb{E}_y[H[\mathcal{X}^*|\mathcal{D}_t \cup \{x, y\}]|\mathcal{D}_t, x]$$  \hspace{1cm} (1)
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

$$H[\mathcal{X}^*|\mathcal{D}_t] - \mathbb{E}_y \left[ H[\mathcal{X}^*|\mathcal{D}_t \cup \{x, y\}] | \mathcal{D}_t, x \right] \equiv \text{MI}(y, \mathcal{X}^*)$$ (ESMOC)
Predictive Entropy Search (PES)

We swap \( y \) and \( \mathcal{X}^* \) to obtain a reformulation of the acquisition function.

\[
H[\mathcal{X}^* | \mathcal{D}_t] - \mathbb{E}_y \left[ H[\mathcal{X}^* | \mathcal{D}_t \cup \{x, y\}] | \mathcal{D}_t, x \right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
\]

\[
H[y | \mathcal{D}_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y | \mathcal{D}_t, x, \mathcal{X}^*] | \mathcal{D}_t, x \right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\]
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We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

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H[\mathcal{X}^*|D_t] - \mathbb{E}_y[H[\mathcal{X}^*|D_t \cup \{x, y\}]|D_t, x] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
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H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*}[H[y|D_t, x, \mathcal{X}^*]|D_t, x] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
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\]

\[
H[y|D_t, \mathbf{x}] - \mathbb{E}_{\mathcal{X}^*}\left[H[y|D_t, \mathbf{x}, \mathcal{X}^*]|D_t, \mathbf{x}\right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\]
Predictive Entropy Search (PES)

We swap \( y \) and \( \mathcal{X}^\ast \) to obtain a reformulation of the acquisition function.

\[
\begin{align*}
H[\mathcal{X}^\ast|\mathcal{D}_t] & - \mathbb{E}_y \left[ H[\mathcal{X}^\ast|\mathcal{D}_t \cup \{\mathbf{x}, y\}] \middle| \mathcal{D}_t, \mathbf{x} \right] \equiv \text{MI}(y, \mathcal{X}^\ast) \quad \text{(ESMOC)} \\
H[y|\mathcal{D}_t, \mathbf{x}] & - \mathbb{E}_{\mathcal{X}^\ast} \left[ H[y|\mathcal{D}_t, \mathbf{x}, \mathcal{X}^\ast] \middle| \mathcal{D}_t, \mathbf{x} \right] \equiv \text{MI}(\mathcal{X}^\ast, y) \quad \text{(PESMOC)}
\end{align*}
\]
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

$$H[\mathcal{X}^*|\mathcal{D}_t] - \mathbb{E}_y[H[\mathcal{X}^*|\mathcal{D}_t \cup \{\mathbf{x}, y\}]|\mathcal{D}_t, \mathbf{x}] \equiv \text{MI}(y, \mathcal{X}^*)$$ (ESMOC)

$$H[y|\mathcal{D}_t, \mathbf{x}] - \mathbb{E}_{\mathcal{X}^*}[H[y|\mathcal{D}_t, \mathbf{x}, \mathcal{X}^*]|\mathcal{D}_t, \mathbf{x}] \equiv \text{MI}(\mathcal{X}^*, y)$$ (PESMOC)
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

\[
H[\mathcal{X}^*|D_t] - \mathbb{E}_y \left[ H[\mathcal{X}^*|D_t \cup \{x, y\}]|D_t, x \right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
\]

\[
H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y|D_t, x, \mathcal{X}^*]|D_t, x \right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\]
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

\[
\begin{align*}
H[\mathcal{X}^*|D_t] - \mathbb{E}_y [H[\mathcal{X}^*|D_t \cup \{x, y\}]|D_t, x] & \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)} \\
H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} [H[y|D_t, x, \mathcal{X}^*]|D_t, x] & \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\end{align*}
\]

Gaussian distribution
Approximated by sampling from $p(\mathcal{X}^*|D_t)$
Predictive Entropy Search (PES)

We swap \( y \) and \( \mathcal{X}^* \) to obtain a reformulation of the acquisition function.

\[
H[\mathcal{X}^*|D_t] - \mathbb{E}_y \left[ H[\mathcal{X}^*|D_t \cup \{x, y\}|D_t, x] \right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
\]

\[
H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y|D_t, x, \mathcal{X}^*]|D_t, x \right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\]

Gaussian distribution
Approximated by sampling from \( p(\mathcal{X}^*|D_t) \)
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

$$\begin{align*}
H[\mathcal{X}^*|D_t] - \mathbb{E}_y \left[ H[\mathcal{X}^*|D_t \cup \{x, y\}] \middle| D_t, x \right] &\equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)} \\
H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y|D_t, x, \mathcal{X}^*] \middle| D_t, x \right] &\equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\end{align*}$$

Gaussian distribution

Approximated by sampling from $p(\mathcal{X}^*|D_t)$

Factorized Gaussian approximation with expectation propagation.

$\mathcal{X}^*$ dominates any other point in $\mathcal{X}$.

(Minka, 2001)
Predictive Entropy Search (PES)

We swap y and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

\[
H[\mathcal{X}^*|D_t] - \mathbb{E}_y \left[ H[\mathcal{X}^*|D_t \cup \{x, y\}] | D_t, x \right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
\]

\[
H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y|D_t, x, \mathcal{X}^*] | D_t, x \right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
\]

\[
\alpha(x) \approx \sum_{c=1}^{C} \log \nu_c^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{c=1}^{C} \log \nu_c^{CPD}(x|\mathcal{X}^*_m) \right) + \sum_{k=1}^{K} \log \nu_k^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{k=1}^{K} \log \nu_k^{CPD}(x|\mathcal{X}^*_m) \right)
\]

(Minka, 2001)
Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

$$H[\mathcal{X}^*|D_t] - \mathbb{E}_y\left[H[\mathcal{X}^*|D_t \cup \{x, y\}]|D_t, x\right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}$$

$$H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*}[H[y|D_t, x, \mathcal{X}^*]|D_t, x] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}$$

\(\alpha(x) \approx \sum_{c=1}^{C} \log \nu_c^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{c=1}^{C} \log \nu_c^{CPD}(x|\mathcal{X}^*_m) \right) + \sum_{k=1}^{K} \log \nu_k^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{k=1}^{K} \log \nu_k^{CPD}(x|\mathcal{X}^*_m) \right) = \sum_{i=1}^{C+K} \alpha_i(x)\)

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Predictive Entropy Search (PES)

We swap $y$ and $\mathcal{X}^*$ to obtain a reformulation of the acquisition function.

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H[\mathcal{X}^*|\mathcal{D}_t] - \mathbb{E}_y\left[H[\mathcal{X}^*|\mathcal{D}_t \cup \{x, y\}|\mathcal{D}_t, x]\right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
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H[y|\mathcal{D}_t, x] - \mathbb{E}_{\mathcal{X}^*}\left[H[y|\mathcal{D}_t, x, \mathcal{X}^*]|\mathcal{D}_t, x\right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
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\[
\alpha(x) \approx \sum_{c=1}^{C} \log v_c^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{c=1}^{C} \log v_c^{CPD}(x|\mathcal{X}^*_m) \right) + \sum_{k=1}^{K} \log v_k^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{k=1}^{K} \log v_k^{CPD}(x|\mathcal{X}^*_m) \right) = \sum_{i=1}^{C+K} \alpha_i(x)
\]

(Minka, 2001)
Example of PES’ acquisition
Example of PES’ acquisition

\[ v_{1}^{PD}(x) \]

\[ f_{1}(x) \]

\[ v_{2}^{PD}(x) \]

\[ f_{2}(x) \]
Example of PES’ acquisition

$\nu_1^{PD}(x)$

Sample of $\mathcal{X}^*$

$f_1(x)$

$\nu_2^{PD}(x)$

Sample of $\mathcal{X}^*$

$f_2(x)$
Example of PES’ acquisition
Example of PES’ acquisition

\[ v_{1}^{PD}(x) \]
\[ \text{Sample of } \mathcal{X}^* \]
\[ v_{1}^{CPD}(x|\mathcal{X}_1^*) \]
\[ \alpha_1(x) \]

\[ f_1(x) \]

\[ v_{2}^{PD}(x) \]
\[ \text{Sample of } \mathcal{X}^* \]
\[ v_{2}^{CPD}(x|\mathcal{X}_1^*) \]
\[ \alpha_2(x) \]

\[ f_2(x) \]
Example of PES' acquisition

\[ v_{1}^{PD}(x) \quad \text{Sample of } \mathcal{X}^* \quad v_{1}^{CPD}(x|\mathcal{X}^*_1) \quad \alpha_1(x) \]

\[ v_{2}^{PD}(x) \quad \text{Sample of } \mathcal{X}^* \quad v_{2}^{CPD}(x|\mathcal{X}^*_1) \quad \alpha_2(x) \]
Finding a Fast and Accurate Neural Network

Average Pareto Front 100 Function Evaluations

- EHI
- ParEGO
- SMSego
- SUR
- PES decoupled

Methods

Time vs. Error
Finding a Fast and Accurate Neural Network

Average Pareto Front 100 Function Evaluations

- EHI
- ParEGO
- SMSego
- SUR

PES decoupled

(Hernández-Lobato et al., 2016)
Finding a Fast and Accurate Neural Network

Average Pareto Front 100 Function Evaluations

Average Pareto Front 200 Function Evaluations

(Hernández-Lobato et al., 2016)
Low energy hardware accelerator

Pareto Fronts 600 Function Evaluations

Energy

Error

Methods
- PES coupled
- PES decoupled
- Random search

Evaluations Performed by PES decoupled

(Hernández-Lobato, 2016)
Low energy hardware accelerator

(Hernández-Lobato et al., 2016)
Parallel Bayesian Optimization

Traditional Bayesian optimization is **sequential**!
Parallel Bayesian Optimization

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Traditional Bayesian optimization is **sequential**!

Computing clusters let us do many things at once!
Parallel Bayesian Optimization

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Parallel Bayesian Optimization

Traditional Bayesian optimization is **sequential**!

Computing clusters let us do **many things** at once!

Parallel experiments should be highly informative but different!
Parallel Predictive Entropy Search

Choose a set $Q$ points $S_t = \{x_q\}_{q=1}^Q$ to minimize the entropy of $x^*$.

$$H[x^*|\mathcal{D}_t] - \mathbb{E}_y \left[ H[x^*|\mathcal{D}_t \cup \{x_q, y_q\}_{q=1}^Q]|\mathcal{D}_t, x] \right] \equiv \text{MI}(y, x^*) \quad \text{(Parallel ES)}$$

(Shah and Ghahramani, 2015)
Parallel Predictive Entropy Search

Choose a set $Q$ points $S_t = \{x_q\}_{q=1}^Q$ to minimize the entropy of $x^*$.

$$H[x^*|D_t] - \mathbb{E}_y \left[ H[x^*|D_t \cup \{x_q, y_q\}_{q=1}^Q]\right] \equiv \text{MI}(y, x^*) \quad \text{(Parallel ES)}$$

$$H[y|D_t, x] - \mathbb{E}_{x^*} \left[ H[y|D_t, x, x^*]\right] \equiv \text{MI}(x^*, y) \quad \text{(Parallel PES)}$$

(Shah and Ghahramani, 2015)
Parallel Predictive Entropy Search

Choose a set $Q$ points $S_t = \{x_q\}_{q=1}^Q$ to minimize the entropy of $x^*$.

\[
H[x^*|D_t] - \mathbb{E}_y \left[ H[x^*|D_t \cup \{x_q, y_q\}_{q=1}^Q]|D_t, x \right] \equiv \text{MI}(y, x^*) \quad \text{(Parallel ES)}
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\[
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(Shah and Ghahramani, 2015)
Parallel Predictive Entropy Search

Choose a set $Q$ points $S_t = \{x_q\}_{q=1}^Q$ to minimize the entropy of $x^*$.

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Multi-variate Gaussian distribution

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Multivariate Gaussian approximation with expectation propagation $x^*$ is better than any other point in $\mathcal{X}$

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Multivariate Gaussian approximation with expectation propagation

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\alpha(S_t) = \log |V^{PD}(S_t)| - \frac{1}{M} \sum_{m=1}^{M} \log |V^{CPD}(S_t|x^*_{(m)})|
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It is possible to compute the gradient of $\alpha(\cdot)$ w.r.t. each $x_q \in S_t$!

(Shah and Ghahramani, 2015)
Parallel Predictive Entropy Search: Level Curves

(Shah and Ghahramani, 2015)
Parallel Predictive Entropy Search: Results

(Shah and Ghahramani, 2015)
BO with Integer-valued and Categorical Variables

Standard GPs assume continuous input variables which makes BO with integer-valued or categorical challenging.
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BO with Integer-valued and Categorical Variables

Standard GPs assume continuous input variables which makes BO with integer-valued or categorical challenging.

A naive approach is to round the suggested value to the closest integer or to the closest one-hot encoding.

The BO algorithm may get stuck and may always perform the next evaluation at the same input location!
BO with Integer-valued and Categorical Variables

Rounding inside of the wrapper works but makes the objective flat!

A modified GP covariance function accounts for this:

$C_{\text{new}}(x_n, x_n') = C(T(x_n), T(x_n')); \theta)$

where $T(\cdot)$ does the rounding to the closest integer or one-hot encoding.
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Similar results for categorical variables!
BO with Integer-valued and Categorical Variables

Tuning the Hyper-parameters of a Gradient Boosting Ensemble

Methods
- Basic Approach
- SMAC
- OEN Optimization Only
- HyperOpt_TPE
- Proposed Approach

One continuous variable and two integer-valued variables.
Freeze-Thaw Bayesian Optimization

Common aspects of many machine learning algorithms:
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Can we use partial training information and a model to determine which hyper-parameter configuration is going to be optimal?

Yes, that is precisely what Freeze-Thaw BO does!

(Swersky et al., 2014)
A GP Kernel for Training Curves

We want to specify a kernel that supports exponentially decaying functions of the form $\exp\{-\lambda t\}$ for $t, \lambda \geq 0$. 

The covariance between inputs $t$ and $t'$ is:

$$C(t, t') = \int_0^{\infty} e^{-\lambda t} e^{-\lambda t'} \psi(\lambda; \alpha, \beta) d\lambda = \beta^\alpha \left( t + t' + \beta \right)^\alpha$$

where $\psi(\lambda; \alpha, \beta)$ is a gamma distribution with parameters $\alpha$ and $\beta$. 
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Inference on Asymptotic Values

A standard GP is used as the prior for the asymptotic values of each training curve.
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Hierarchical generative model:

\[
p(\{y_n\}_{n=1}^N | \{x_n\}_{n=1}^N) = \int \left[ \prod_{n=1}^N \mathcal{N}(y_n | f_n \mathbf{1}, K_{tn}) \right] \mathcal{N}(f | m, K_x) df
\]

where

\[x_n \equiv n \text{ configuration,}\]
\[y_n \equiv n \text{ observed curve,}\]
\[f_n \equiv n \text{ asymptotic value,}\]
\[m \equiv \text{prior asymptotic mean values,}\]
\[K_{tn} \equiv \text{covariances for curve values,}\]
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where

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- \(y_n \equiv n\) observed curve,
- \(f_n \equiv n\) asymptotic value,
- \(m \equiv \) prior asymptotic mean values,
- \(K_{t_n} \equiv \) covariances for curve values,
- \(K_x \equiv \) cov. for asymptotic values

The joint distribution of \(\{y\}_{n=1}^N\) and \(f\) is Gaussian and hence so it is the predictive distribution \(p(f|\{y\}_{n=1}^N)\)!
Inference on Asymptotic Values and BO

- \( p(f|\{y_n\}_{n=1}^N, \{x_n\}_{n=1}^N) \) determines asymptotic values.
- This distribution can be used to make intelligent decisions!
- Shall we train more one configuration or shall we start a new one?
- A combination of EI and ES is used as the acquisition function. (Swersky et al., 2014)
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\begin{align*}
\mathcal{N}(m, K) \\
\mathcal{N}(f(x_1), K) \\
\mathcal{N}(f(x_2), K) \\
\mathcal{N}(f(x_3), K) \\
\vdots
\end{align*}

(a) Graphical Model

\begin{align*}
\mathcal{N}(f(x_1), K) \\
\mathcal{N}(f(x_2), K) \\
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\vdots
\end{align*}

(b) Training curve predictions

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(c) Asymptotic GP

**Bayesian Optimization:**

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(Swersky et al., 2014)
Freeze-Thaw BO in practice

![Graph 1](image1.png)

![Graph 2](image2.png)
Freeze-Thaw BO in practice

(Swersky et al., 2014)
Computational Cost of GPs and Other Models

- Exact inference with GP has cost in $O(n^3)$. 

The predictive distribution for $f^\star$ at a new point $x^\star$ is:

$$p(f^\star|D_n) \approx \int p(f^\star|u) q(u) du = N(f^\star|\mu,\nu^2)$$

$\mu = k_{x^\star, X} K^{-1} X m$, $\nu^2 = \kappa_{x^\star, x^\star} - k_{x^\star, X} K^{-1} X (K X, X - S) K^{-1} X k_{X, x^\star}$

$q(u) = N(u|m, S)$

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The computational cost is in $O(nm^2)$!
Sparse GP based on Inducing Points

The approximate predictive distribution can be sub-optimal if the inducing points are not chosen carefully.

• Too small variance at the pseudo-inputs.
• Too big variance in between and away from pseudo-inputs. (Shahriari et al., 2016)
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Optimizing the Inducing Points

Two approaches:

- FITC: optimize the marginal likelihood of an approximate GP model.
- VFE: maximize fidelity to the original exact GP.

FITC VFE

FITC: less local optima and easier to optimize, also less accurate.

VFE: more accurate, more local optima, more difficult to optimize.

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Other Models: Random Forest

Ensemble method where the predictors are random regression trees trained on random subsamples of the data.
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- This guarantees that each tree is slightly different.

Very cheap to compute and massively parallelizable!
Random Forest: Predictive Distribution

Random Forest Prediction

The predictive distribution is a Gaussian with the empirical average and empirical variance.
Random Forest: Predictive Distribution

\[ p(f^*|D_n) = \mathcal{N}(f^*|\bar{\mu}, \bar{\nu}^2) \]

(Hutter et al., 2011)
Random Forest in Practice

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- Allows for a lot of evaluations (good when the objective is cheap).
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- No parameters to tune.

(Shahriari et al., 2016)
Other Models: Bayesian Neural Networks

- Neural networks scale well to the training data (linear cost).

\[ h_j(x) = \tanh \left( \sum_{i=1}^{I} x_i w_{ji} \right) \]

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The posterior distribution of the networks weights \( W \) is intractable!
Bayesian Neural Networks: Predictive Distribution

Several techniques considered to approximate the predictive distribution:

- Markov Chain Monte Carlo methods.
- Variational Inference.
- Expectation Propagation.
- Reinterpretations of dropout.
- Point estimates and Bayesian linear-models in the last layer.

Trade-off between accuracy of the predictive distribution and scalability! Still a lot of research going on!
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Trade-off between accuracy of the predictive distribution and scalability! Still a lot of research going on!
Software for Bayesian Optimization

Many of the methods described are implemented into Spearmint using Python.

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**Other tools:** SMAC (Java), Hyperopt (Python), Bayesopt (C++), PyBO (Python), MOE (Python / C++).
Further Extensions and Open Issues

1. **High-dimensionality**: BO is restricted to problems of moderate dimension. However, many big problems have low effective dimensionality which can be exploited (Wang et al., 2013).

2. Consider dependencies among objectives / tasks (Swersky et al., 2013) (Shah and Ghahramani, 2016). Most of the times the GPs are simply assumed to be independent, which is suboptimal.

3. Most acquisition functions consider an evaluation horizon equal to one. We can do better by considering a particular evaluation budget and taking decisions accordingly (González et al., 2016).

4. Safe Bayesian Optimization: Sometimes we should avoid evaluating the objective at particular input locations (system failure) where it falls below some critical value (Berkenkamp et al., 2016).
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Thank you very much!
References


