A tutorial on Bayesian Optimization

Daniel Hernández–Lobato
Computer Science Department
Universidad Autónoma de Madrid

http://dhnzl.org, daniel.hernandez@uam.es
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.
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Bayesian Optimization in Practice

1. Get initial sample.

The model guides the search focusing on the most-promising regions of the input space!
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   \[ p(y|x, \mathcal{D}_n) \].
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2. **Fit a model to the data:**
   \[ p(y|x, D_n) \].
3. **Select data collection strategy:**
   \[ \alpha(x) = E_{p(y|x, D_n)}[U(y|x, D_n)] \].
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4. Optimize acquisition function \( \alpha(x) \).
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Bayesian Optimization vs. Uniform Exploration

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 $p(\text{Data})$ is intractable!

Solved by setting $p(W) = \prod_{ij} N(w_{ji} | 0, \sigma^2 H^{-1})$ and letting $H \to \infty$!
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$$h_j(x) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

$$f(x) = \sum_{j=1}^{H} v_j h_j(x)$$
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and letting \( H \to \infty \! \)

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Posterior Dist.

\[
p(W|\text{Data}) = \frac{p(W)p(\text{Data}|W)}{p(\text{Data})}
\]

Predictive Dist.

\[
p(y|\text{Data}, x) = \int p(y|W, x)p(W|\text{Data})dW
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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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Due to Gaussian form, there are closed-form solutions for many useful questions about finite data.
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When $H \to \infty$, $(f(x_1), \ldots, f(x_N))^T$ follows an $N$-dimensional Gaussian where $E[f(x_i)f(x_k)] = \sigma^2 E[h_j(x_i)h_j(x_k)]$ 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 $y$:

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

- The joint distribution for $y^\star$ at test points $\{x^\star_m\}_{m=1}^M$ and $y$:

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

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

$$[K_\theta]_{n,n'} = C(x_n, x_{n'}; \theta)$$

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Gaussian Processes

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

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p(y^*, y) = \mathcal{N}
\begin{pmatrix}
0 \\
0 \\
\end{pmatrix}
, 
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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 ,
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- The log of the **marginal likelihood**, $p(y|\theta)$, is:

  \[
  \log p(y) = -\frac{N}{2} \log 2\pi - \frac{1}{2} \log |K_\theta| - \frac{1}{2} y^T K_\theta^{-1} y
  \]
Some Covariance Functions

Squared Exponential

\[ C(x, x') = \sigma^2 \exp \left\{ \frac{1}{2} \sum_j \left( \frac{x_j - x'_j}{l_j} \right)^2 \right\} \]
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Matérn

\[ C(x, x') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu r}}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu r}}{l} \right) \]
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Neural Network

$$C(x, x') = \frac{2}{\pi} \sin^{-1} \left( \frac{2x^T \Sigma x'}{\sqrt{(1+2x^T \Sigma x)(1+2x^T \Sigma x')}} \right)$$
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Periodic

\[ C(x, x') = \exp \left\{ -\frac{2 \sin^2 \left( \frac{|x-x'|}{2} \right)}{l^2} \right\} \]
From the Prior to the Posterior

GP regression provides a **closed-form** posterior distribution for $f(\cdot)$. 
From the Prior to the Posterior

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

![Diagram showing a comparison between a predicted curve and the ground truth. The predicted curve is represented by a shaded area with a black line, and the ground truth is represented by a red line. There is an error bar showing the range of the prediction.]
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![Diagram showing ground truth and a fitted curve](image)
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![Diagram showing a close-form posterior distribution for $f(\cdot)$]
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![Diagram showing the relationship between the prior and posterior distributions in GP regression](image.png)
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![Diagram showing the relationship between the prior and posterior distributions in GP regression. The red line represents the ground truth, and the black lines show different samples from the posterior distribution.](image-url)
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![Diagram showing the comparison between the closed-form posterior and ground truth](image-url)
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![Diagram showing ground truth and GP regression results]
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![Ground Truth](image)
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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^\star|D_N, x)} [U(y^\star|x, D_N)]
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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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- **Expected Improvement:**
  $$U(y^*|\mathcal{D}_N, x) = \max(0, \nu - y^*), \quad \alpha(x) = \sigma(x)(\gamma(x)\Phi(\gamma(x)) + \phi(\gamma(x)))$$
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- **Expected Improvement:**
  
  $$U(y^*|\mathcal{D}_N, x) = \max(0, \nu - y^*), \quad \alpha(x) = \sigma(x) \left( \gamma(x) \Phi(\gamma(x)) + \phi(\gamma(x)) \right)$$

- **Lower Confidence Bound:**
  
  $$\alpha(x) = - \left( \mu(x) - \kappa \sigma(x) \right)$$
Some Acquisition Functions

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- **Probability of Improvement:**
  \[
  U(y^*|D_N, x) = \mathbb{I}(y_+ < \nu), \quad \alpha(x) = \Phi(\gamma(x))
  \]

- **Expected Improvement:**
  \[
  U(y^*|D_N, x) = \max(0, \nu - y^*), \quad \alpha(x) = \sigma(x) (\gamma(x)\Phi(\gamma(x)) + \phi(\gamma(x)))
  \]

- **Lower Confidence Bound:**
  \[
  \alpha(x) = - (\mu(x) - \kappa\sigma(x))
  \]

- **Entropy Search:**
  \[
  U(y^*|D_N, x) = H[p(x_{\min}|D_N)] - H[p(x_{\min}|D_N \cup \{x, y^*\})]
  \]
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.
Bayesian Optimization and Model Selection

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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 form \( p(\theta|y) \) using MCMC.
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  **Slice sampling means no additional hyper-parameters!**
Bayesian Optimization and Model Selection

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

\[ \hat{\alpha}(x) = \int \alpha(x; \theta) p(\theta|y) d\theta \approx \frac{1}{K} \sum_{k=1}^{K} \alpha(x; \theta^{(k)}) \quad \theta^{(k)} \sim p(\theta|y), \]
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Posterior samples with three different length-scales

Length-scale specific expected improvement

Integrated expected improvement

(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.
Cost-sensitive Bayesian Optimization

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**Expected Improvement per-second:**

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

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

\[ f(x) \]

\[ EI(x) \]

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

\[ EI(x) / s \]

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

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\[ EI(x) / s \]

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

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Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization
Cost-sensitive Bayesian Optimization
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.
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Constrained Multi-Objective Optimization
Constrained Multi-Objective Optimization

Objective 1

Objective 2

Pareto Set (Input space)
Constrained Multi-Objective Optimization

Pareto Set (Input space)

Pareto Frontier (value space)

Objective 1

Objective 2

Values for Domain Points

Values for Optimal Points

Pareto Points
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

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Values for Domain Points

Values for Optimal Points
Constrained Multi-Objective Optimization

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Bayesian Optimization Methods

Additional challenges when dealing with several black-boxes.
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- Simple approach: evaluate all the objectives and constraints at the same input location. Expected to be sub-optimal.
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Coupled evaluations

Decoupled evaluations
Information-based Approach

The Pareto set $X^\star$ 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

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---

**Actual Objectives and Constraints**

**Posterior of each Objective and Constraint**

**Optimized Samples Drawn from the Posterior**
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- Actual Objectives and Constraints
- Posterior of each Objective and Constraint
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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

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

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

The acquisition function is

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

(1)

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

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

Computing (1) is very difficult in practice!
Predictive Entropy Search (PES)

We swap $y$ and $x^*$ 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.

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

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

\[
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\]

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

We swap $y$ and $x^*$ to obtain a reformulation of the acquisition function.

\[
H[x^* | D_t] - E_y[H[x^* | D_t \cup \{x, y\}] | D_t, x] \equiv \text{MI}(y, x^*) \quad (\text{ESMOC})
\]

\[
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Gaussian distribution
Predictive Entropy Search (PES)

We **swap** \( y \) and \( x^* \) to obtain a reformulation of the acquisition function.

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\]

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

Gaussian distribution

Approximated by sampling from \( p(x^*|\mathcal{D}_t) \)
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\}] \right] \equiv \text{MI}(y, \mathcal{X}^*) \quad \text{(ESMOC)}
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\[
H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y|D_t, x, \mathcal{X}^*] \right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)}
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\[ H[y|D_t, x] - \mathbb{E}_{\mathcal{X}^*} \left[ H[y|D_t, x, \mathcal{X}^*] | D_t, x \right] \equiv \text{MI}(\mathcal{X}^*, y) \quad \text{(PESMOC)} \]

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 $\chi^*$ to obtain a reformulation of the acquisition function.

\[
\begin{align*}
H[\chi^*|D_t] - E_Y[H[\chi^*|D_t \cup \{x, y\}]|D_t, x] &\equiv \text{MI}(y, \chi^*) \quad \text{(ESMOC)} \\
H[y|D_t, x] - E_{\chi^*}[H[y|D_t, x, \chi^*]|D_t, x] &\equiv \text{MI}(\chi^*, y) \quad \text{(PESMOC)}
\end{align*}
\]

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

(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)}
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\[
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)}
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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)
Predictive Entropy Search (PES)

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

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

\( \alpha(x) \approx \sum_{c=1}^{C} \log u_c^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{c=1}^{C} \log u_c^{CPD}(x|\mathcal{X}^*_m) \right) + \\
\sum_{k=1}^{K} \log u_k^{PD}(x) - \frac{1}{M} \sum_{m=1}^{M} \left( \sum_{k=1}^{K} \log u_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
Example of PES’ acquisition

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

\[ f_1(x) \]

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

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

$v^{PD}_{1}(x)$  Sample of $\mathcal{X}^*$  $v^{CPD}_{1}(x|\mathcal{X}^*)$  $\alpha_1(x)$

$v^{PD}_{2}(x)$  Sample of $\mathcal{X}^*$  $v^{CPD}_{2}(x|\mathcal{X}^*)$  $\alpha_2(x)$
Finding a Fast and Accurate Neural Network

Average Pareto Front 100 Function Evaluations

Methods
- EHI
- ParEGO
- SMSeGO
- SUR
- PES decoupled

Coupled
Finding a Fast and Accurate Neural Network

Average Pareto Front 100 Function Evaluations

Methods
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- SUR

Black-boxes
- 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](image)

- **Methods**
  - PES coupled
  - PES decoupled
  - Random search
Low energy hardware accelerator

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

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

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

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

(Shah and Ghahramani, 2015)
Choose a set $Q$ points $S_t = \{x_q\}_{q=1}^Q$ to minimize the entropy of $x^*$.

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

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

(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 $x^*$.

\[
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Multi-variate Gaussian distribution

Approximated by sampling from $p(x^*|D_t)$

Multivariate Gaussian approximation with \textit{expectation propagation}

$x^*$ is better than any other point in $\mathcal{X}$

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

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BO with Integer-valued and Categorical Variables

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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:

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

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Tuning the Hyper-parameters of a Gradient Boosting Ensemble

Log distance to the optimum value

Number of Function Evaluations

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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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 \( t, \lambda \geq 0 \).
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The covariance between inputs $t$ and $t'$ is:

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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:

\[ p(\{y_n\}_{n=1}^{N}|\{x_n\}_{n=1}^{N}) = \int \prod_{n=1}^{N} \mathcal{N}(y_n|f_n1, K_{t_n}) \mathcal{N}(f|m, K_x) df \]

where

\( x_n \equiv n \) configuration, \( y_n \equiv n \) 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
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\[\begin{align*}
    x_n &\equiv n \text{ configuration}, \\
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    f_n &\equiv n \text{ asymptotic value}, \\
    m &\equiv \text{prior asymptotic mean values}, \\
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    K_{x} &\equiv \text{cov. for asymptotic values}
\end{align*}\]

The joint distribution of \( \{y\}_{n=1}^N \) and \( f \) is Gaussian and hence so 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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Freeze-Thaw BO in practice
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Computational Cost of GPs and Other Models

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

For large evaluation budgets one has to use approximations. Most successful approaches are based on inducing points: $X \equiv \text{Matrix of } m \ll n$ inducing or pseudo-inputs. 

$u = f(X) \equiv \text{Inducing values / values of the process at } X$.

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

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

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

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

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Exact GP

SPGP
Sparse GP based on Inducing Points

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- Too small variance at the pseudo-inputs.
- Too big variance in between and away from pseudo-inputs.

(Shahriari et al., 2016)
Optimizing the Inducing Points

Two approaches:

• EP: optimize the marginal likelihood of an approximate GP model.
• VI: maximize fidelity to the original exact GP.

• EP: less local optima and easier to optimize, also less accurate.
• VI: more accurate, more local optima, more difficult to optimize.

(Bui et al., 2017) (Bauer et al., 2016)
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Very cheap to compute and massively parallelizable!
Random Forest: Predictive Distribution

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

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

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

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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!

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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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- 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!
Software for Bayesian Optimization

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

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

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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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