Bayesian Optimization in High Dimensions via Random Embeddings

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Automated Parameter Tuning and Algorithm Configuration
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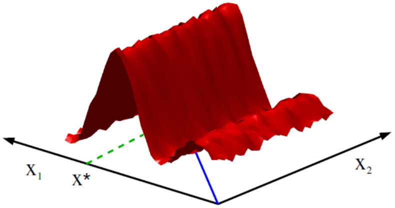
Low Effective Dimensionality



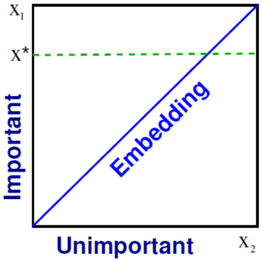


Table of Contents

Bayesian Optimization

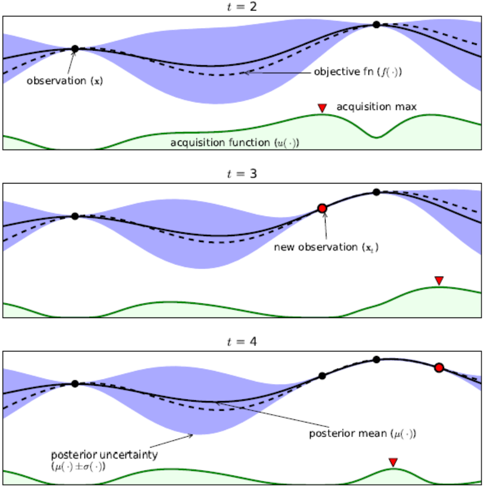


Table of Contents

Low Effective Dimensionality

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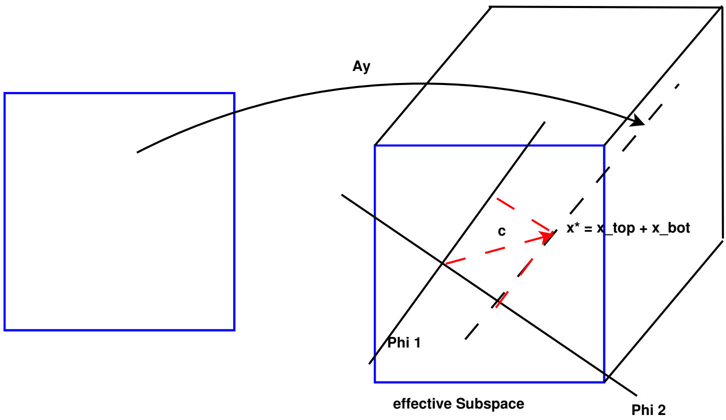
Definition

A function $f : \mathbb{R}^D \to \mathbb{R}$ has **effective dimensionality** d_e if:

- $\exists$ a linear subspace $\mathscr{T}$ of dimension d_e s.t. for all $x_\top \in \mathscr{T} \subset \mathbb{R}^D$ and $x_\perp \in \mathscr{T}^\perp \subset \mathbb{R}^D$ (orthogonal complement)
- $\Rightarrow f(x) = f(x_\top + x_\perp) = f(x_\top)$
- $\mathscr{T}$ is called the **effective subspace** of f and $\mathscr{T}^\perp$ the **constant subspace**

Theorem

If f has effective dimensionality d_e and a random Gaussian matrix $\mathbf{A} \in \mathbb{R}^{D \times d}$ with $d \geqslant d_e$:
$\Rightarrow$ with probability 1, for any $x \in \mathbb{R}^D$, $\exists$ a $y \in \mathbb{R}^d$ s.t. $f(x) = f(\mathbf{A}y)$.


Ay
c
x* = x_top + x_bot
Phi 1
effective Subspace
Phi 2

Proof Sketch.

Hence, $f(x) = f(x_\top + x_\perp) = f(x_\top)$

Proof Sketch.

Hence, $f(x) = f(x_\top + x_\perp) = f(x_\top)$

- it suffices to show that $\exists y \in \mathbb{R}^d$ s.t $f(x_\top) = f(\mathbf{A}y)$.

Proof Sketch.

Hence, $f(x) = f(x_\top + x_\perp) = f(x_\top)$

- it suffices to show that $\exists y \in \mathbb{R}^d$ s.t $f(x_\top) = f(\mathbf{A}y)$.
- $\Phi \in \mathbb{R}^{D \times d_e}$ whose columns form an orthonormal basis for $\mathscr{T}$. For each $x_\top \in \mathscr{T}$ it exists a $c \in \mathbb{R}^{d_e}$ s.t. $x_\top = \Phi c$.

REMBO

Proof Sketch.

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- $rank(\Phi^\top A) = d_e$ and therefore we have $(\Phi^\top A)y = c$ for some y

REMBO

Proof Sketch.

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- $rank(\Phi^\top A) = d_e$ and therefore we have $(\Phi^\top A)y = c$ for some y
- orthogonal projection Ay onto $\mathscr{T}$ is given by $\Phi \Phi^T A y = \Phi c = x_\top$.

Proof Sketch.

Hence, $f(x) = f(x_\top + x_\perp) = f(x_\top)$

- it suffices to show that $\exists y \in \mathbb{R}^d$ s.t $f(x_\top) = f(\mathbf{A}y)$.
- $\Phi \in \mathbb{R}^{D \times d_e}$ whose columns form an orthonormal basis for $\mathscr{T}$. For each $x_\top \in \mathscr{T}$ it exists a $c \in \mathbb{R}^{d_e}$ s.t. $x_\top = \Phi c$.
- $rank(\Phi^\top A) = d_e$ and therefore we have $(\Phi^\top A)y = c$ for some y
- orthogonal projection Ay onto $\mathscr{T}$ is given by $\Phi\Phi^T Ay = \Phi c = x_\top$.
- $Ay = x_\top + x'$ with $x' \in \mathscr{T}^\perp$ and $f(Ay) = f(x_\top + x') = f(x_\top)$

$\square$

Table of Contents

Random Embeddings for Bayesian Optimization

The basic idea of REMBO:

- For any $x \in \mathbb{R}^D$ and a random matrix $A \in \mathbb{R}^{D \times d}$, there is a point $y \in \mathbb{R}^d$ such that $f(x) = f(Ay)$
- Thus, for any optimizer $x^\star \in \mathbb{R}^D$ it exists a $y^\star \in \mathbb{R}^d$ such that $f(x^\star) = f(\mathbf{A}y^\star)$
- Instead of optimizing in the high dimensional space, we optimize $g(\mathbf{y}) = f(\mathbf{Ay})$

for $t = 1, 2, ..$ **do**

Find $x_{t+1} \in \mathbb{R}^D$ by optimizing the acquisition function

$u : x_{t+1} = \arg\max_{x \in \mathscr{X}} u(\mathbf{x}|D_t)$

Augment the data $D_{t+1} = \{D_t, (x_{t+1}, f(\mathbf{x_{t+1}}))\}$

end

Algorithmus 1: Bayesian Optimization

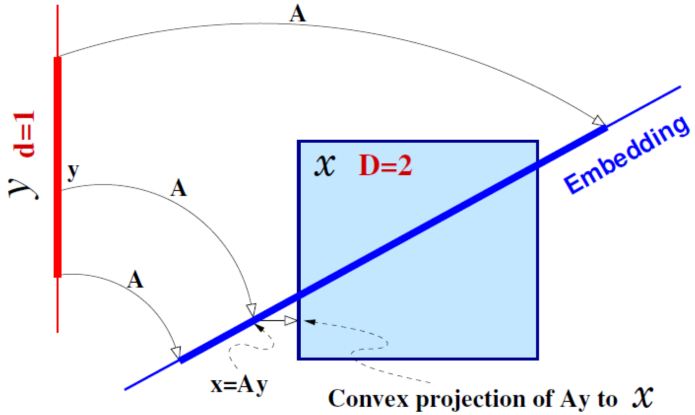
Random Embeddings for Bayesian Optimization

Generate a random matrix A;
for $t = 1, 2, ..$ **do**
  Find $\mathbf{y_{t+1}} \in \mathbb{R}^d$ by optimizing the acquisition function $u : \mathbf{y_{t+1}} = \arg\max_{\mathbf{y} \in \mathscr{Y}} u(\mathbf{y}|D_t)$
  Augment the data $D_{t+1} = \{D_t, (\mathbf{y_{t+1}}, f(\mathbf{A}\mathbf{y_{t+1}})\}$
end

Algorithmus 2: REMBO

Table of Contents

Bounded Regions



Bounded Regions

How do we choose the bounded region $\mathscr{Y} \subset \mathbb{R}^d$ where REMBO performs the Bayesian Optimization?

- Is $\mathscr{Y}$ too small, it is more likely that it does not include the global optimizer
- Is $\mathscr{Y}$ too big, it is more time consuming

Bounded Regions

Theorem

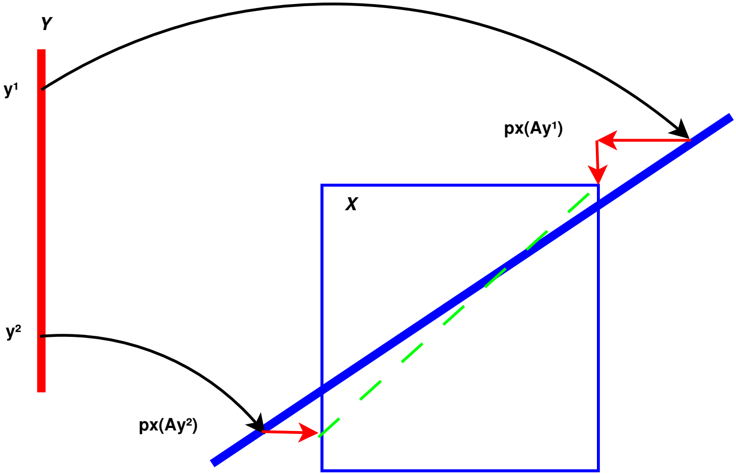
If $\mathbf{A}$ is a $D \times d$ random Gaussian matrix, there exists an optimizer $y^\star \in \mathbb{R}^d$ such that $f(\mathbf{A}y^\star) = f(x_\top^\star)$ and $\|y^\star\|_2 \leqslant \frac{\sqrt{d_e}}{\varepsilon}\|x_\top^\star\|_2$ with probability at least $1 - \varepsilon$.

Random Embeddings for Bayesian Optimization

- The Theorem says that with probability $1-\varepsilon$ the optimizer is in $\mathscr{Y}$ and that with probability $\delta \leqslant \varepsilon$ the optimizer lies outside of $\mathscr{Y}$
- To increase the success rate:
  - Run REMBO k times with different independently drawn random embeddings. This decreases δ to δ^k
  - Increase the dimensionality d. If $d > d_e$ there are $\binom{d}{d_e}$ different embeddings and it is more likely that the optimizer is included.

Table of Contents

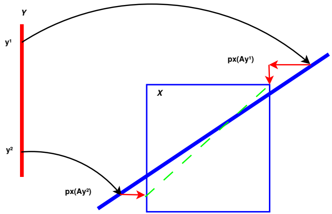
Kernels



Kernels

Low dimensional kernel:

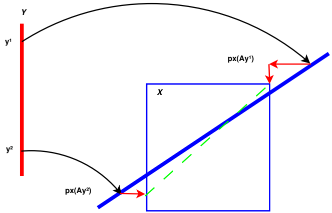
- $k_l^d(y^{(1)}, y^{(2)}) = \exp\left(-\frac{\|y^{(1)} - y^{(2)}\|^2}{2l^2}\right)$
- Squared exponential kernel in low dimensions
- It constructs a GP in the d-dimensional space
- Effective in continuous space



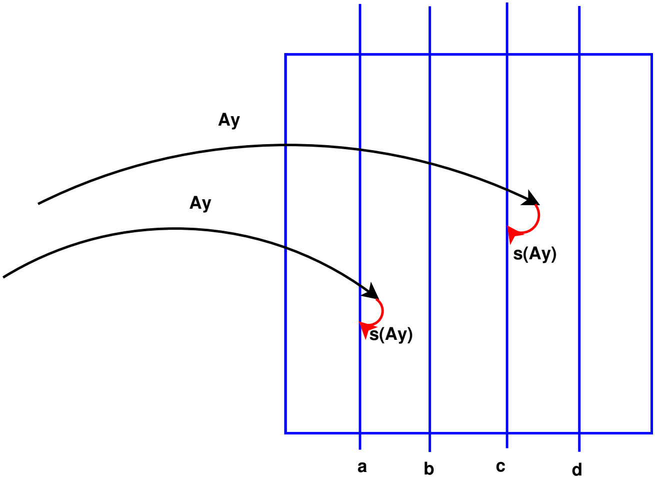
Kernels

High dimensional Kernel:

- $k_l^D(y^{(1)}, y^{(2)}) = \exp\left(-\frac{\|p_X(Ay^{(1)}) - p_X(Ay^{(2)})\|^2}{2l^2}\right)$ with $p_X : \mathbb{R}^D \to \mathbb{R}^D$ as the standard projection operator
- It constructs a GP in the D-dimensional space
- Search space is not $\mathscr{X}$ any more, it is now the smaller subspace $\{p_x(Ay) : y \in \mathscr{Y}\}$



Categorical Kernel:



Kernels

Categorical Kernel:

- $k_\lambda^D(y^{(1)}, y^{(1)}) = \exp\left(-\frac{\lambda}{2} g(s(Ay^{(1)}), s(Ay^{(2)}))^2\right)$
  with $g(x^{(1)}, x^{(2)}) = |\{i : x_i^{(1)} \neq x_i^{(2)}\}|$ as the Hamming distance and the function s that maps continuous vectors to discrete vectors
- Measures the distance between two low dimensional points as the distance between their high dimensional mappings

Table of Contents

Bayesian Optimization in a Billion Dimensions

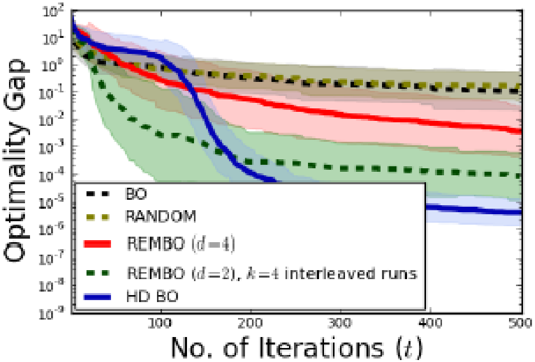
- Bayesian Optimization of the $d_e = 2$-dimensional Branin function embedded in a D-dimensional space with $D - d_e$ unimportant dimensions.
- The optimality gap as the performance measurement, i.e. the difference of the best function value and the optimal function value
- 500 function evaluations and $\frac{500}{k}$ for each run
- Tested with $D = 25$ and $D = 10^9$ and different internal dimensions d

Bayesian Optimization in a Billion Dimensions

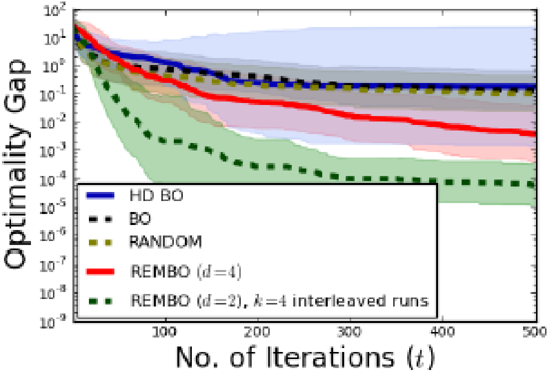
k	$d = 2$	$d = 4$	$d = 6$
10	0.0022 ± 0.0035	0.1553 ± 0.1601	0.4865 ± 0.4796
5	0.0004 ± 0.0011	0.0908 ± 0.1252	0.2586 ± 0.3702
4	0.0001 ± 0.0003	0.0654 ± 0.0877	0.3379 ± 0.3170
2	0.1514 ± 0.9154	0.0309 ± 0.0687	0.1643 ± 0.1877
1	0.7406 ± 1.8996	0.0143 ± 0.0406	0.1137 ± 0.1202

BO of the Branin function embedded in $D = 25$ dimensions

Bayesian Optimization in a Billion Dimensions



Bayesian Optimization in a Billion Dimensions



Bayesian Optimization in a Billion Dimensions

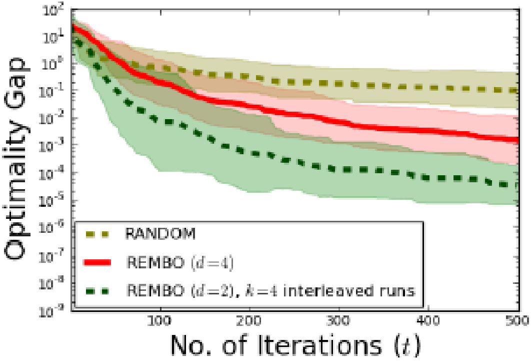


Table of Contents

Optimizing LPSOLVE

LPSOLVE

- Popular mixed integer linear programming solver

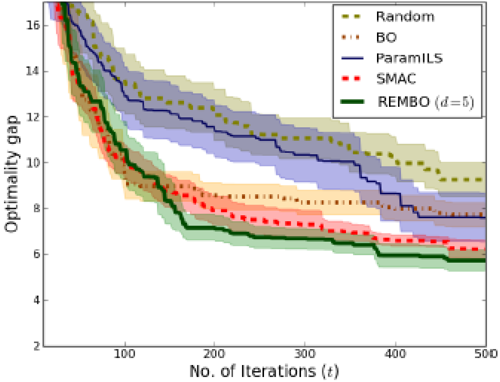
Problem instance

- Deterministic blackbox optimization problem
- The configuration problem includes 40 binary and 7 categorical parameters of LPSOLVE

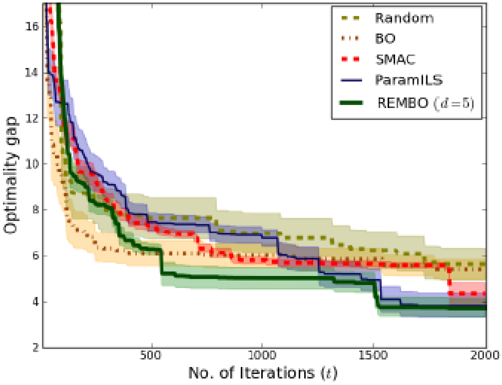
Experiment

- Comparison of BO, REMBO, ParamILS, SMAC and Random Search
- Due to the categorical parameters, the high-dimensional kernel is used for REMBO

Optimizing LPSOLVE



Optimizing LPSOLVE



Discussion

- REMBO performs Bayesian Optimization in a random embedded subspace in the high dimensional space of the objective function. The assumption is that the objective function has a low effective dimensionality.
- Normally no parameters are totally unimportant
- How do we choose the internal dimension d?
- It is not quite clear yet, how many practical problems fall into this class