Scalable (and usable!) Bayesian Optimisation

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The University Of Sheffield.

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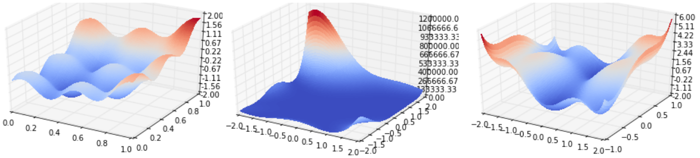
General goal of the talk

"Civilisation advances by extending the number of important operations which we can perform without thinking of them."
(Alfred North Whitehead)

- Scalable BO: models + parallelisation.
- Usable BO: new users + expert users.

Consider a *well behaved* function $f : \mathcal{X} \to \mathbb{R}$ where $\mathcal{X} \subseteq \mathbb{R}^D$ is (in principle) a bounded domain.

$$x_M = \arg\min_{x \in \mathcal{X}} f(x).$$

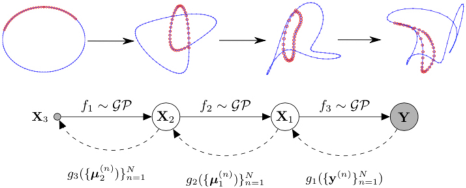


- f is explicitly unknown (computer model, process embodied in a physical process) and multimodal.
- Evaluations of f may be perturbed.
- Evaluations of f are (very) expensive.

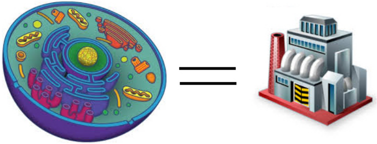
Expensive functions, who doesn't have one?

[Dai, Damianou, González and Lawrence, ICLR'2016]
[González et al. NIPS-ComBio 2014, 2015]

Model configuration: find learning rates, number of layers, etc



Design of experiments: Design synthetic genes that best enable cells to scale up the production of proteins of interest.



Probabilistic numerics approach?

http://www.probabilistic-numerics.org/, Michael Osborne, Philipp Hennig

Make a series of $x_1, \ldots, x_N$ evaluations of f to minimise *cumulative regret*

$$r_N = \sum_{n=1}^{N} f(x_n) - N f(x_M)$$

1. *Optimisation* as *decision*: Minimise the regret.
2. *Decision* as *inference*: need to model the *epistemic* uncertainty we have about f.

Probability theory to model uncertainty

Bayesian Optimisation

[Mockus, 1978]

Methodology to perform global optimisation of multimodal black-box functions.

1. Choose some *prior measure* over the space of possible objectives f.

2. Combine prior and the likelihood to get a *posterior measure* over the objective given some observations.

3. Use the posterior to decide where to take the next evaluation according to some *acquisition/loss function*.

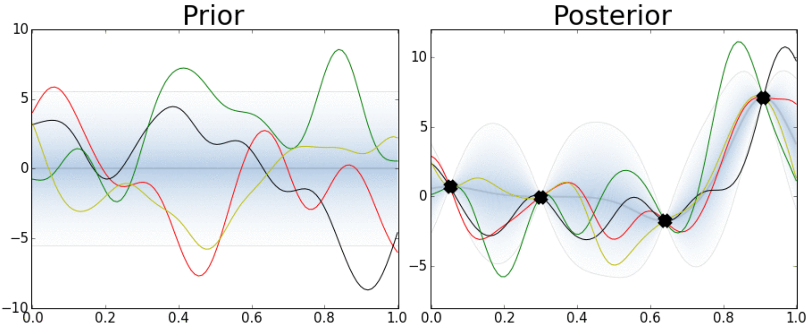
4. Augment the data.

Iterate between 2 and 4 until the evaluation budget is over.

Probability measure over functions

Gaussian processes [Rasmunsen and Williams, 2006]

Infinite-dimensional probability density, such that each linear finite-dimensional restriction is multivariate Gaussian.



- Fully determined by a covariance function $k(\mathbf{x}, \mathbf{x}'; \theta)$ operator.
- Marginals are Gaussians with known mean and variance.

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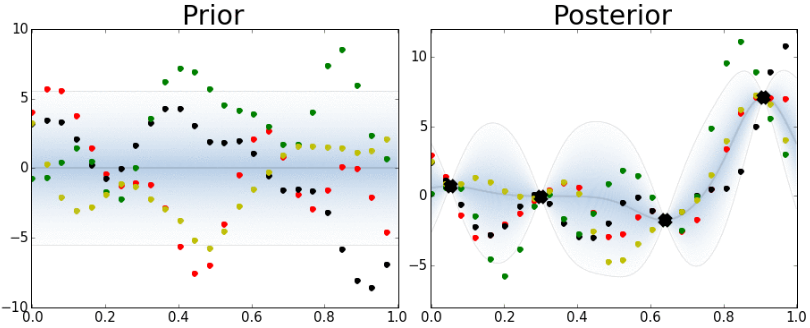

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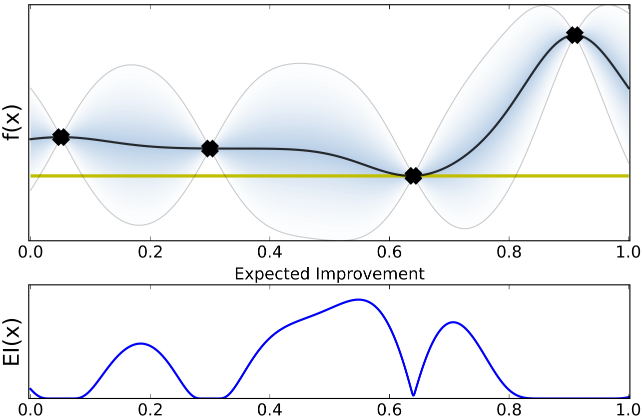
Expected Improvement

[Jones et al, 1998]

$$\alpha_{EI}(\mathbf{x};\theta,\mathcal{D}) \triangleq \mathbb{E}[\max(0, y_{best} - y)]$$



Exploration vs. exploitation to determine the next evaluation.

Illustration of BO

Iteration 1

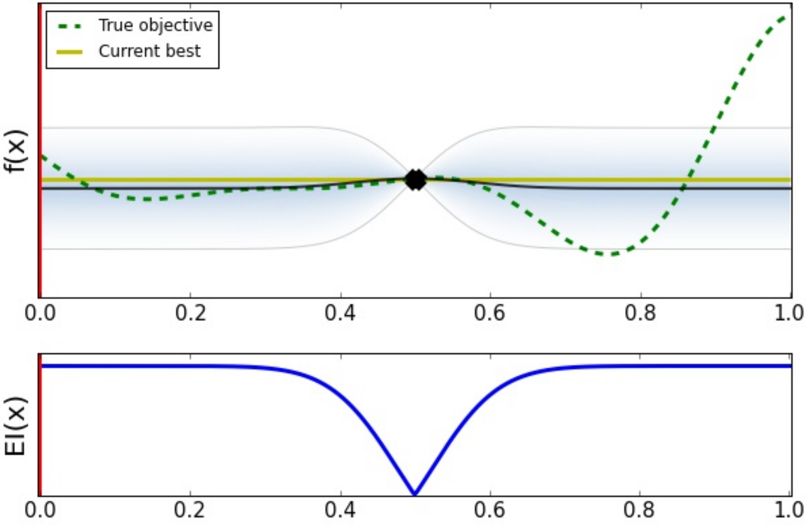


Illustration of BO

Iteration 2

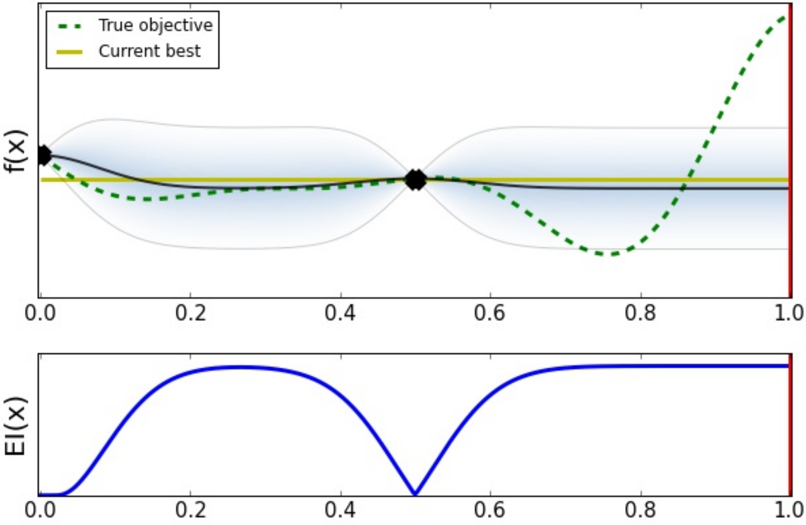


Illustration of BO

Iteration 3

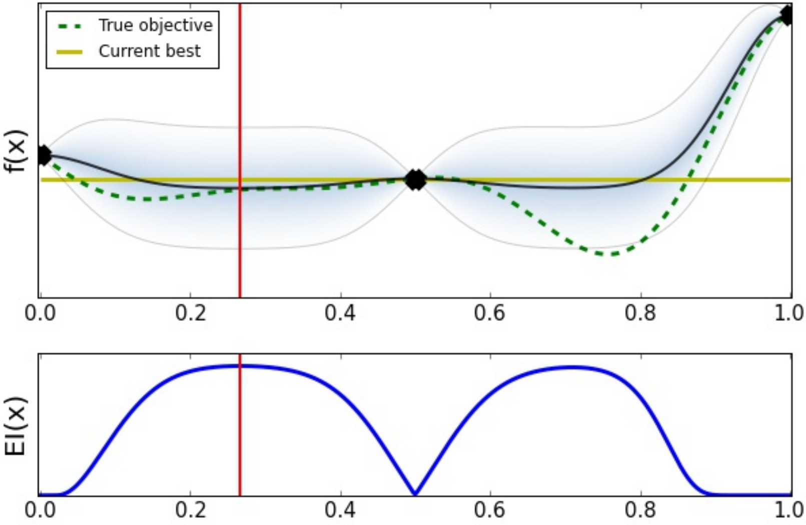


Illustration of BO

Iteration 4

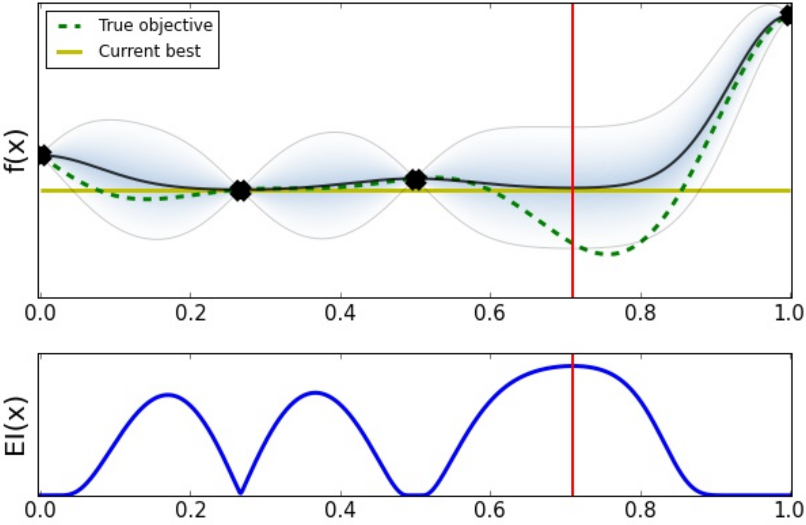


Illustration of BO

Iteration 5

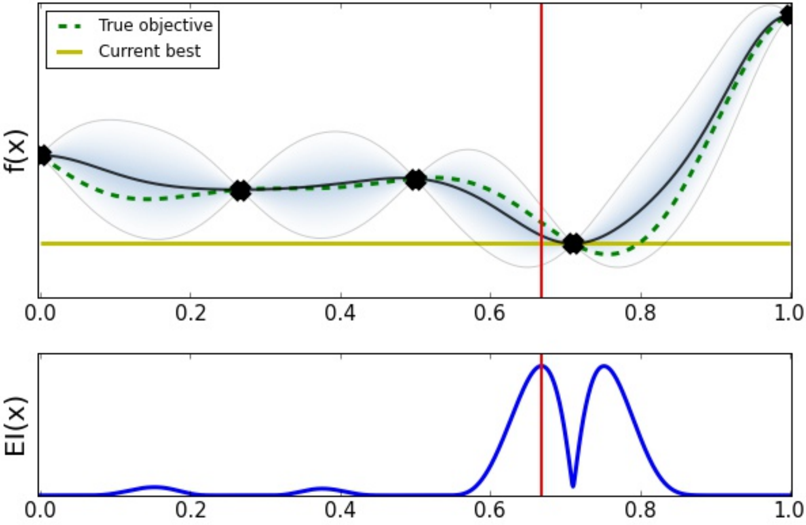


Illustration of BO

Iteration 6

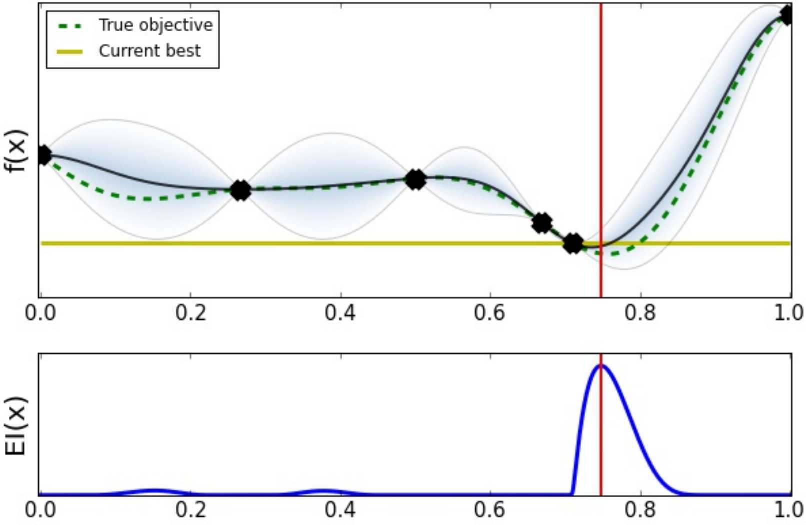


Illustration of BO

Iteration 8

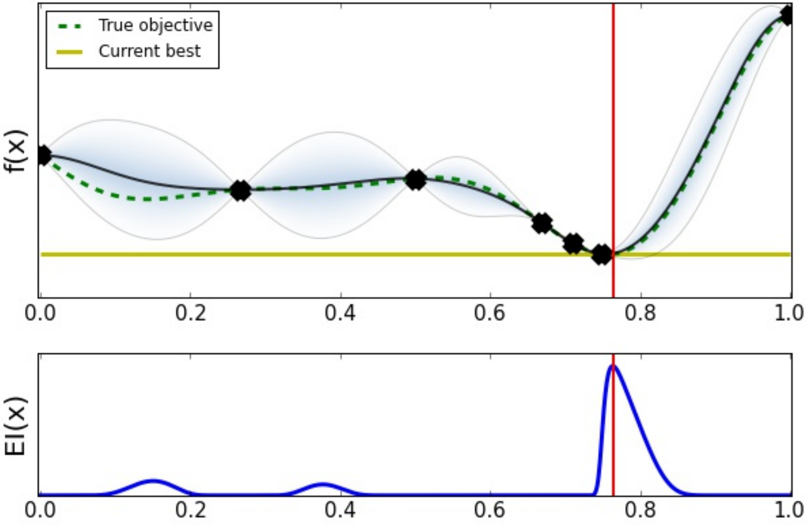
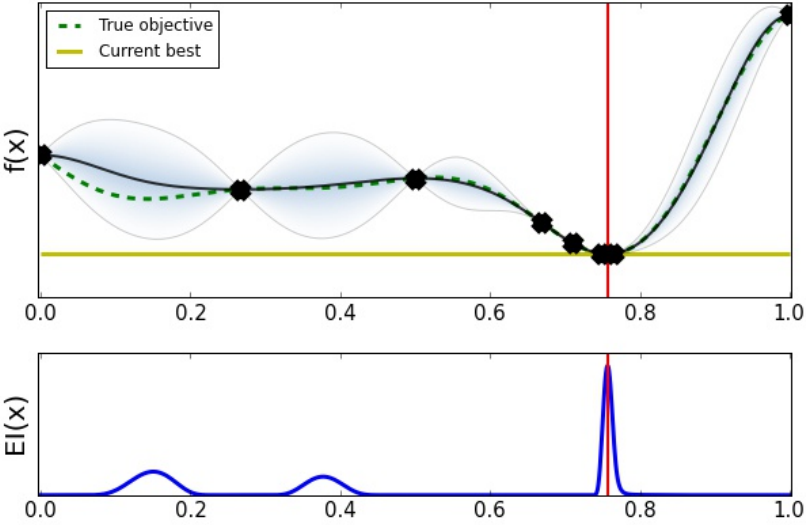


Illustration of BO

Iteration 8



Why these ideas have been ignored for years?

- Lack of general software to apply these methods as a black optimisation boxes of for experimental design.
- Reduced scalability in dimensions, number of evaluations (parallelisation) and available models.

Usable BO: GPyOpt

http://sheffieldml.github.io/GPyOpt/

- Easy python interface (compatible with spearmint).
- Based on GPy: GPs, Sparse GPs, Warped GPs, Deep GPs, etc.
- MCMC integration of the acquisition functions.
- Parallel (synchronous batch) optimisation.
- Constrain optimisation.
- Armed bandits optimisation.
- Handles continous and discrete inputs.
- Several acquisition optimisers.
- More to come!

Open source code (BSD-3 license). You can contribute!

Scalable BO: Parallel/batch BO

Avoiding the bottleneck of evaluating f

- Cost of $f(\mathbf{x}_n)$ = cost of $\{f(\mathbf{x}_{n,1}), \ldots, f(\mathbf{x}_{n,nb})\}$.
- Many cores available, simultaneous lab experiments, etc.

Considerations when designing a batch

- Available pairs $\{(\mathbf{x}_j, y_i)\}_{i=1}^{n}$ are augmented with the evaluations of f on $\mathcal{B}_t^{n_b} = \{\mathbf{x}_{t,1}, \ldots, \mathbf{x}_{t,nb}\}$.
- Goal: design $\mathcal{B}_1^{n_b}, \ldots, \mathcal{B}_m^{n_b}$.

Notation:

- $\mathcal{I}_n$: data set $\mathcal{D}_n$ + $\mathcal{GP}$ structure ($\mathcal{I}_{t,k}$ in the batch context).
- $\alpha(\mathbf{x}; \mathcal{I}_n)$: generic acquisition function given $\mathcal{I}_n$.

Optimal greedy batch design

Design a batch optimally is intractable

Sequential policy: Maximise:

$$\alpha(\mathbf{x}; \mathcal{I}_{t,k-1})$$

Greedy batch policy, k-th element t-th batch: Maximize:

$$\int \alpha(\mathbf{x}; \mathcal{I}_{t,k-1}) \prod_{j=1}^{k-1} p(y_{t,j}|\mathbf{x}_{t,j}, \mathcal{I}_{t,j-1}) p(\mathbf{x}_{t,j}|\mathcal{I}_{t,j-1}) d\mathbf{x}_{t,j} dy_{t,j}$$

- $p(y_{t,j}|\mathbf{x}_{t,j}, \mathcal{I}_{t,j-1})$: predictive distribution of the $\mathcal{GP}$.
- $p(\mathbf{x}_j|\mathcal{I}_{t,j-1}) = \delta(\mathbf{x}_{t,j} - \arg\max_{\mathbf{x}\in\mathcal{X}} \alpha(\mathbf{x}; \mathcal{I}_{t,j-1}))$.

Available approaches

[Azimi et al., 2010; Desautels et al., 2012; Chevalier et al., 2013; Contal et al. 2013]

Bottleneck

Available methods require to iteratively update $p(y_{t,j}|\mathbf{x}_j, \mathcal{I}_{t,j-1})$ to model the iteration between the elements in the batch: $\mathcal{O}(n^3)$

How to design batches reducing this cost? Local penalisation

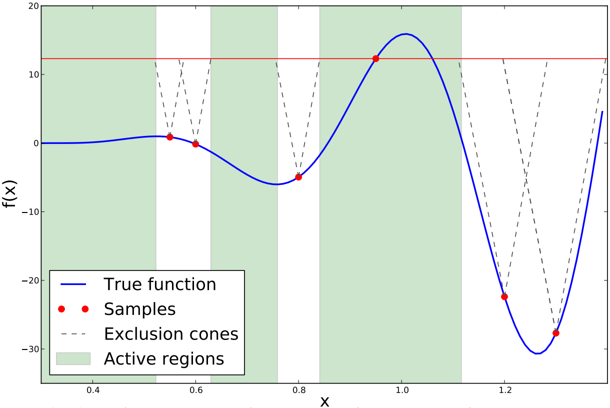
Lipschitz continuity

$$|f(\mathbf{x}_1) - f(\mathbf{x}_2)| \leq L\|\mathbf{x}_1 - \mathbf{x}_2\|_p.$$

Interpretation of the Lipschitz continuity of f

$M = \max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$ and $B_{r_{x_j}}(\mathbf{x}_j) = \{\mathbf{x} \in \mathcal{X} : \|\mathbf{x} - \mathbf{x}_j\| \leq r_{x_j}\}$ where

$$r_{x_j} = \frac{M - f(\mathbf{x}_j)}{L}$$



$x_M \notin B_{r_{x_j}}(\mathbf{x}_j)$ otherwise, the Lipschitz condition is violated.

Probabilistic version of $B_{r_x}(\mathbf{x})$

We can do this because $f(\mathbf{x}) \sim \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$

- r_{x_j} is Gaussian with $\mu(r_{x_j}) = \frac{M-\mu(\mathbf{x}_j)}{L}$ and $\sigma^2(r_{x_j}) = \frac{\sigma^2(\mathbf{x}_j)}{L^2}$.

Local penalisers: $\varphi(\mathbf{x}; \mathbf{x}_j) = p(\mathbf{x} \notin B_{r_{\mathbf{x}_j}}(\mathbf{x}_j))$

$$\begin{aligned}\varphi(\mathbf{x}; \mathbf{x}_j) &= p(r_{\mathbf{x}_j} < \|\mathbf{x} - \mathbf{x}_j\|) \\ &= 0.5\mathrm{erfc}(-z)\end{aligned}$$

where $z = \frac{1}{\sqrt{2\sigma_n^2(\mathbf{x}_j)}}(L\|\mathbf{x}_j - \mathbf{x}\| - M + \mu_n(\mathbf{x}_j))$.

- Reflects the size of the ‘Lipschitz’ exclusion areas.
- Approaches to 1 when $\mathbf{x}$ is far form $\mathbf{x}_j$ and decreases otherwise.

Idea to collect the batches

Without using explicitly the model.

Optimal batch: maximisation-marginalisation

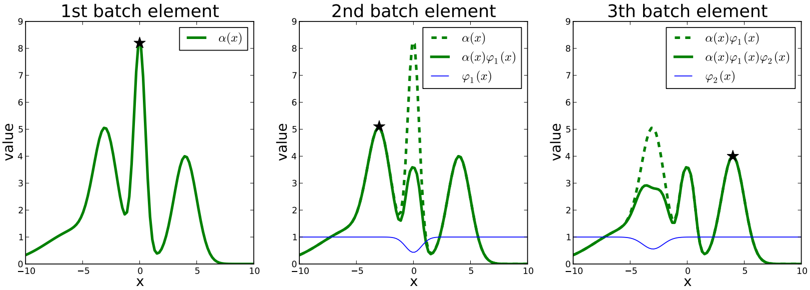
$$\int \alpha(\mathbf{x}; \mathcal{I}_{t,k-1}) \prod_{j=1}^{k-1} p(y_{t,j}|\mathbf{x}_{t,j}, \mathcal{I}_{t,j-1}) p(\mathbf{x}_{t,j}|\mathcal{I}_{t,j-1}) d\mathbf{x}_{t,j} dy_{t,j}$$

Proposal: maximisation-penalisation.

Use the $\varphi(\boldsymbol{x}; \boldsymbol{x}_j)$ to penalise the acquisition and predict the expected change in $\alpha(\boldsymbol{x}; \mathcal{I}_{t,k-1})$.

Local penalisation strategy

[González, Dai, Hennig, Lawrence, 2016]

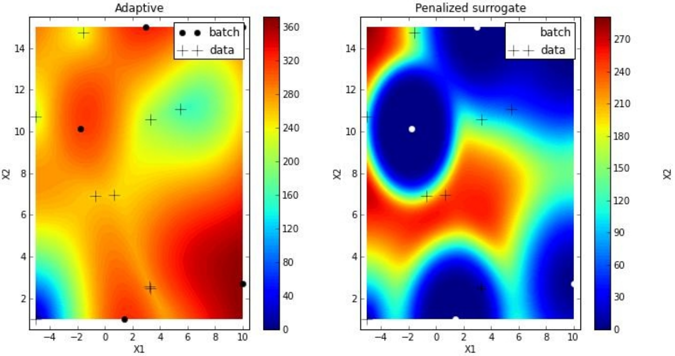


The maximization-penalisation strategy selects $\mathbf{x}_{t,k}$ as

$$\mathbf{x}_{t,k} = \arg\max_{x \in \mathcal{X}} \left\{ g(\alpha(\mathbf{x}; \mathcal{I}_{t,0})) \prod_{j=1}^{k-1} \varphi(\mathbf{x}; \mathbf{x}_{t,j}) \right\},$$

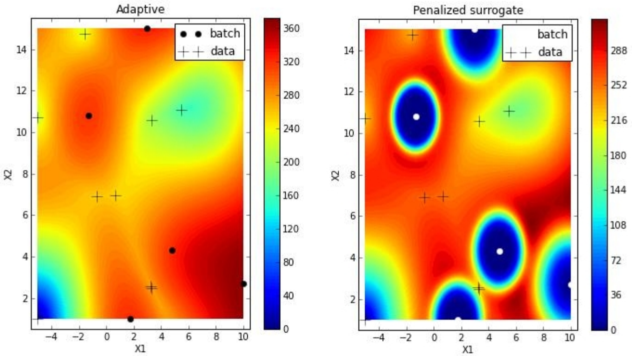
g is a transformation of $\alpha(\mathbf{x}; \mathcal{I}_{t,0})$ to make it always positive.

Example for $L = 50$



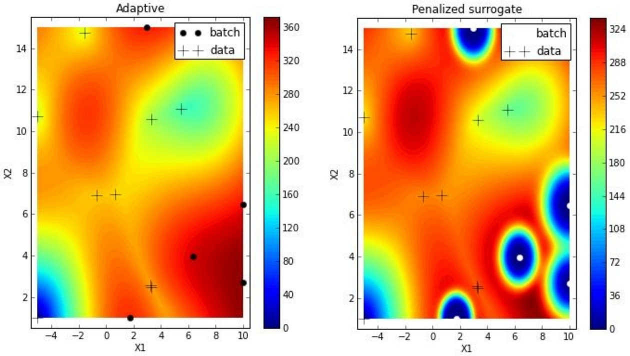
L controls the exploration-exploitation balance within the batch.

Example for $L = 100$



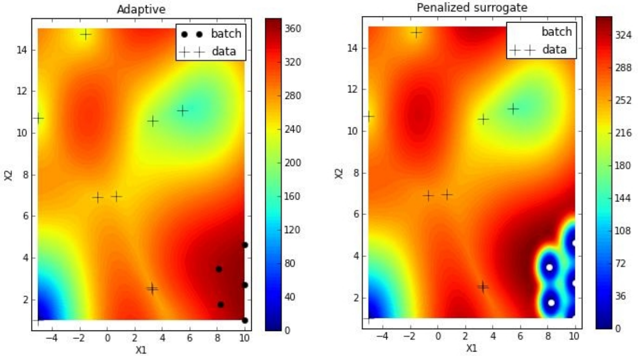
L controls the exploration-exploitation balance within the batch.

Example for $L = 150$



L controls the exploration-exploitation balance within the batch.

Example for $L = 250$

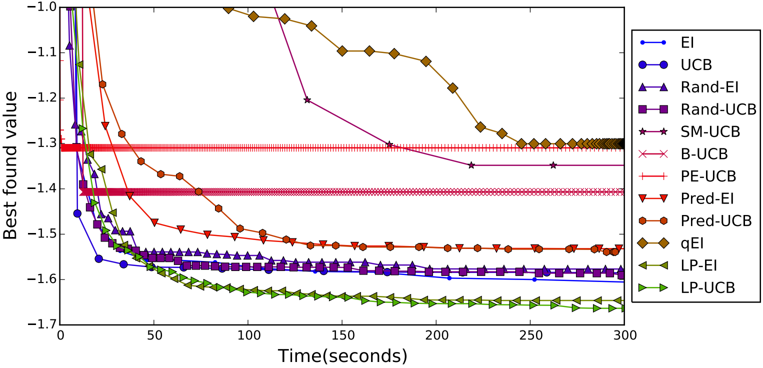


L controls the exploration-exploitation balance within the batch.

We choose $\hat{L} = \max_{\mathcal{X}} \|\mu_{\nabla}(\mathbf{x}^*)\|$.

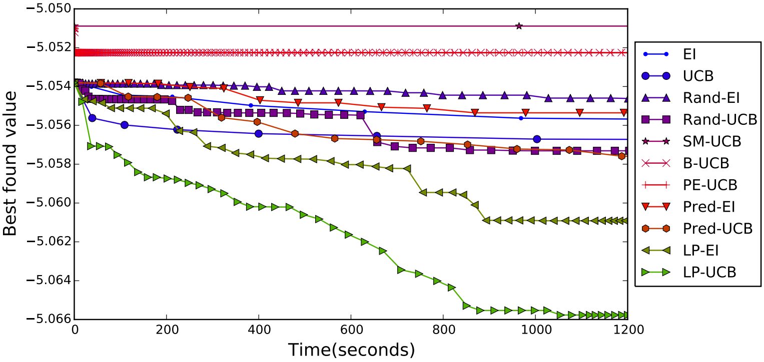
2D experiment with 'large domain'

Comparison in terms of the wall clock time



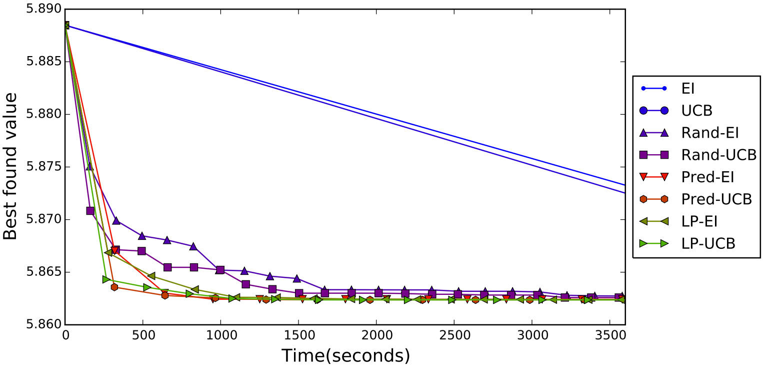
Optimisation of a fitted model for gene design

70 dimensions (gene features), emulator of the protein production by cells.



Support Vector Regression

- Minimisation of the RMSE on a test set over 3 parameters.
- 'Physiochemical' properties of protein tertiary structure?
- 45730 instances and 9 continuous attributes.



Wrapping up

- BO is fantastic tool for global parameter optimisation in ML and experimental design.
- To parallelise BO requires modelling the interaction between the elements in the batches to design. This can be done without updating the model explicitly after each batch element is collected.
- Software available! Use GPyOpt!