

# Bayesian and evolutionary optimization: searching from both sides

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# Bayesian and evolutionary optimization: searching from both sides

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### 11 July 2023 talk at the Hasso-Plattner Institut, Potsdam

R. Le Riche (CNRS LIMOS)

BO vs. EO searches

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### Context: global optimization

 $\min_{x\in\mathcal{S}}f(x)$ 

S: search space, continuous, discrete, mixed, others (graphs?). Default  $S \in \mathbb{R}^d$  (hyper-rectangle). d is the dimension.

Both evolutionary and Bayesian optimization algorithms (EO & BO) apply.

EO & BO have different scientific communities (computer science vs. applied math, but it is changing).

Goal of the talk : introduce BO through a comparison with EO and draw common perspectives.

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### Context: BO for costly optimization

 $\min_{x\in\mathcal{S}}f(x)$ 

*Costly*: one call to f takes more CPU than the rest of the optimization algorithm. Examples: nonlinear partial differential equations (finite elements), training of a neural network, real experiment ...

To save calls to f, build a model of it based on previous evaluations and rely on it whenever possible  $\longrightarrow$  metamodel / surrogate based optimization. Gaussian process as metamodel : Bayesian Optimization (BO).

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EO & BO both date from the 60s or 70s with the work of

- [Fogel et al., 1965], [Holland, 1973], [Rechenberg, 1973] and [Schwefel, 1977] for EO,
- and [Kushner, 1962], [Močkus, 1972] and [Saltenis, 1971] for BO.

Reference texts for BO : [Frazier, 2018], [Garnett, 2023].

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# Algorithms skeletons I

### BO

- make an initial design of experiments (DoE) X<sup>t</sup> and calculate F<sup>t</sup> = f(X<sup>t</sup>), t = length(F)
- build a Gaussian Proc. from  $(\mathbb{X}^t, \mathbb{F}^t) \to GP^t$
- $x^{t+1} = \arg \max_{x \in S} \operatorname{AcquisCrit}(x; GP^t)$
- $(X^{t+1}, F^{t+1}) =$  $(X^{t+1}, F^{t+1}) \cup (x^{t+1}, f(x^{t+1})),$ increment t

$${f i}$$
 stop  $(t>t^{\sf max},\ldots)$  or go to 2.

### EO

- make an initial DoE X and calculate  $\mathbb{F} = f(X)$ ,  $t = \text{length}(\mathbb{F})$
- Apply variation operators (selection, mutation, crossover) to get a new DoE:
   X' = Variation(X, F)

$$\begin{array}{ll} \textbf{3} \quad \text{calculate } \mathbb{F}' = f(\mathbb{X}'), \\ t = t + \text{length}(\mathbb{F}') \end{array}$$

• stop  $(t > t^{\max}, \ldots)$  or go to 2.

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# Algorithms skeletons II





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### Differences:

- Maximization of an acquisition criterion that depends on a Gaussian Process instead of the variation operators;
- EO is population oriented while all points are kept in BO. BO would be memory consumming for large *t* but not its typical range of use. The state of EO is implicitely stored in its population, efficient but loss prone.

### A SHORT INTRODUCTION TO BAYESIAN OPTIMIZATION

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### Gaussian Process Regression (kriging) – I



Y(x) is  $\mathcal{N}(\mu(x), k(x, x'))$   $Y(x)|Y(\mathbb{X})=\mathbb{F} \sim \mathcal{N}(m(x), c(x, x'))$  is also Gaussian, interpolating and depends on the kernel k(.,.) and  $\mu(.)$  through parameters  $\theta$ .

Example: 
$$k(x,x') = \sigma^2 \exp(-\sum_{i=1}^d rac{(x_i-x_i')^2}{2 heta_i^2})$$
 .

Note: kernels are defined over all kinds of spaces. Example of mixed continuous-discrete BO in [Cuesta-Ramirez et al., 2022].

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### Gaussian Process Regression (kriging) – II



 $Y(x)|Y(X)=\mathbb{F} \sim \mathcal{N}(m(x), c(x, x'))$ , interpolating and depends on the kernel k(., .) and  $\mu(.)$  through parameters  $\theta$ .

$$m(x) = \mathbb{E}[Y(x)|Y(\mathbb{X})=\mathbb{F}] = \mu(x) + k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}(\mathbb{F}-\mu(x)\mathbb{1})$$
  
$$c(x,x') = \operatorname{Cov}[Y(x),Y(x')|Y(\mathbb{X})=\mathbb{F}] = k(x,x') - k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}k(\mathbb{X},x')$$

Learn the GP typically by max. (log) likelihood or leave-one-out crossvalidation,  $\theta^* = \arg \max_{\theta} LL(\theta; \mathbb{F})$ .

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### Gaussian Process Regression (kriging)

heta's as length scales,  $k(x, x') = \sigma^2 \prod_{i=1}^d \text{correlation}_i \left( \frac{|x_i - x'_i|}{\theta_i} \right)$ 



(Matérn kernel,  $\sigma = 1$ )

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### An example of acquisition criterion: the $\mathbb{E}I$

Measure of progress: the improvement,  $I(x) = \max \left(0, (\min(\mathbb{F}) - Y(x) \mid Y(\mathbb{X})=\mathbb{F})\right).$ 

Acquisition criterion:  $\mathbb{E}I$  [Saltenis, 1971, Schonlau, 1997], to maximize at each iteration.

The  $\mathbb{E}I$  is analytically known and does not involve calls to f,  $\mathbb{E}I(x) = \int_{-\infty}^{+\infty} I(x) \, dy(x) = \cdots = \sqrt{c(x,x)} \left[ w(x) \text{cdf}_{\mathcal{N}}(w(x)) + \text{pdf}_{\mathcal{N}}(w(x)) \right]$ with  $w(x) = \frac{\min(F) - m(x)}{\sqrt{(c(x,x))}}$ .

A parameter-less intensification (1st term) – exploration (2nd term) compromise.

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Let's see how it works... iteration 4



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$$x^{t+1} = { ext{arg max}}_{x \in \mathcal{S}} \, \mathbb{E} I(x)$$

Let's see how it works... iteration  $4{+}1$ 



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$$x^{t+1} = \arg \max_{x \in S} \mathbb{E}I(x)...$$
 iteration 4+2



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$$x^{t+1} = \operatorname{arg max}_{x \in S} \mathbb{E}I(x)...$$
 iteration 4+5



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### Expected Improvement: comments

There are other acquisition criteria:

- Upper Confidence Bound [Kushner, 1962, Srinivas et al., 2010], =  $m(x) - \alpha c(x, x)$ . Need to choose  $\alpha$ .
- Knowledge gradient [Močkus, 1972, Frazier and Powell, 2007], min<sub>x∈S</sub> m<sup>t</sup>(x) - E[min<sub>x∈S</sub> m<sup>t+1</sup>(x)]. No analytical expression.
- Criteria based on the reduction in entropy of the optimum [Villemonteix et al., 2009, Hernández-Lobato et al., 2014]. No analytical expression, complex.

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•  $\mathbb{E}I$  is a myopic criterion compared to the above criteria. It is still a good entry criterion thanks to its simplicity and ease of interpretation.

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Bayesian optimizers are competitive at low number of function evaluations but they loose this advantage with dimension.

- $\leftarrow$  Loss of GP accuracy?
- ← El sample too often at boundary?

Next slide: COCO tests [Hansen et al., 2016] from [Le Riche and Picheny, 2021]

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### Effect of dimension on Bayesian Optimization



### BO and trust regions

Principle: counteract the effect of increasing dimension (volume) by restricting the search to a smaller (controlled) trust region.



- TRIKE, Trust-Region Implementation in Kriging-based optimization with Expected Improvement, [Regis, 2016].
- TURBO, a TrUst-Region BO solver, [Eriksson et al., 2019].
- TREGO, a Trust-Region framework for EGO, [Diouane et al., 2023] : mix searches inside (local) and outside (global) the trust region.

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# TREGO algorithm



Parameters :  $\sigma_0$ ,  $\beta < 1$ Sufficient decrease condition for success of the local phase,  $f(x_{k+1}^{\text{local}}) \leq f(x_k^*) - 10^{-4}\sigma_k^2$ 

# **TREGO** properties

From [Diouane et al., 2023],

- TREGO iterates converge to a local minimum : by assuming f is bounded below, Lipschitz continuous near the point of convergence, and by considering a subsequence of the local iterates. No assumption on GP or x<sub>0</sub><sup>\*</sup>.
- Empirical COCO tests:
  - more local than global steps (4 to 1) is beneficial
  - TREGO is robust to the values of  $\sigma_{\rm 0}$  and  $\beta$
  - A local GP was thought an asset for non stationary functions. But it is a drawback on badly conditioned functions. Not kept.

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# TREGO performance



Trust regions solve BO's oversampling of the boundaries in high-dim. while helping on unimodal functions (not the natural target for BO).

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### RELATIONS BETWEEN BAYESIAN AND EVOLUTIONARY OPTIMIZATION

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### The probabilistic representations of f

BO and EO represent f differently

BOEOGlobal model of the function<br/>(in  $\mathbb{R}$ )Model the distribution of good<br/>points (in  $\mathcal{S}$ ) $p(f \mid x) = \mathcal{N}(m(x), c(x, x))$  $p(x \mid f(x) \leq \text{threshold})$ <br/> $\approx \frac{1}{\operatorname{card}(\mathbb{X})} \sum_{x_i \in \mathbb{X}} \delta_{x_i}(x)$ 

Both views are tied by Bayes rule (see later).

### Fundamental degrees of freedom

#### BO

Choosing and learning the kernel = Choosing and learning the reprechoosing the feature space of the sentation and variation operators.  $\phi(x)$ 's: by Mercer's theorem, k(x, x') = | Quality metrics: ergodicity (com- $\sum_{i=1}^{D} \lambda_i \phi_i(x) \phi_i(x')$  (*N* possibly infinite). pletness), unbiasedness, locality Quality metrics: regression metrics (Q2, (genotype-phenotype local corre-LOO normality test).

Acquisition criterion: controls the exploration-intensification tradeoff. Quality metrics: optimization metrics (convergence, performance profiles,...).

#### EO

lation).

Both views will be linked later (perspectives).

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### EO for BO

BO has 2 internal optimizations that are not costly and multimodal: they benefit from EO (CMA-ES is a typical choice for maximizing the  $\mathbb{E}I$ ).



(from scikit-learn.org)

 $\max_{x} \mathbb{E}I(x; GP)$ 



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### BO for EO: adding a GP – I

Principle : EO algorithms need to order new x's for selection. Replace calls to f by calls to GPs.

Like surrogate-based EO, but with prediction uncertainties. Ranking from

- UCB [Büche et al., 2005],  $m(x) \alpha c(x, x)$ ,
- prob. of improvement [Ulmer et al., 2003],  $\mathrm{cdf}_{\mathcal{N}}\left((\min\mathbb{F}-m(x))/\sqrt{c(x,x)}
  ight)$ ,
- partial (Pareto) ranks of (function prediction,- function uncertainty) [Volz et al., 2017],  $(m(x), -\sqrt{c(x,x)})$ ,
- ... cf. [Bajer et al., 2019] for other criteria.

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# BO for EO: adding a GP – II

Algorithms are variants around the following sequence:

- X' = Variation(X)
- Rank points in X' using the GP and one of the ranking criteria (UCB, PI, EI, m, ...)
- Check the quality of the GP:
  - number of generations without GP update
  - OR compare ranking from true f and from GP on a small portion of X'
- GP update from a reduced number of points chosen in X' ∪ X where true f is calculated

a sequence which is decomposed, repeated, varied ... inside EO implementations.

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The aforementionned interfaces between BO and EO are external.

### **PERSPECTIVES**:

### A DEEPER LINK BETWEEN EO AND BO

through 2 examples.

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BO vs. EO searches

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### Crossover as a barycenter in feature space I

### Summary

- Feature learning (from data, through the kernels) can be seen as a search for an appropriate representation where linear reasoning works.
- Interprete crossover as a barycenter in feature space.

A kernel can always be seen as an inner product in feature space<sup>†</sup>,  $k(x, x') = \langle \phi(x), \phi(x') \rangle$ , where the feature is a map  $\phi : S \to \mathbb{R}^D$  and D can be infinite.

<sup>†</sup>For example it can be the eigendecomposition of Mercer's theorem seen earlier,  $k(x, x') = \sum_{i=1}^{\infty} \sqrt{\lambda_i} \phi_i(x) \sqrt{\lambda_i} \phi_i(x')$  with the usual L2 scalar product, or the canonical decomposition in the RKHS,  $k(x, x') = \langle k(x, .), k(x', .) \rangle_{\mathcal{H}}$ .

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### Definition (Crossover as barycenter of features)

Let  $x_C \in S$  be the result of the crossover of  $x_A \in S$  with  $x_B \in S$ . The features of  $x_C$  are the  $\alpha$ -barycenter of the features of  $x_A$  and  $x_B$ ,  $0 \le \alpha \le 1$ :

$$\mathbf{x}_{\mathcal{C}}\coloneqq rgmin_{\mathbf{x}\in\mathcal{S}} lpha \|\phi(\mathbf{x})-\phi(\mathbf{x}_{\mathcal{A}})\|^2 + (1-lpha)\|\phi(\mathbf{x})-\phi(\mathbf{x}_{\mathcal{B}})\|^2$$

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### Crossover as a barycenter in feature space III

Calculation:  $\begin{aligned} \|\phi(x) - \phi(x_A)\|^2 &= \langle \phi(x) - \phi(x_A), \phi(x) - \phi(x_A) \rangle \\ &= \langle \phi(x), \phi(x) \rangle + \langle \phi(x_A), \phi(x_A) \rangle - 2 \langle \phi(x), \phi(x_A) \rangle \\ &= k(x, x) + k(x_A, x_A) - 2k(x, x_A) \\ \text{and idem with } \|\phi(x) - \phi(x_B)\|^2. \end{aligned}$ Assume stationarity,  $k(x, x) = k(x_A, x_A) = k(x_B, x_B) = \sigma^2$ , then

$$x_{C} = \arg\min_{x \in S} 2\sigma^{2} - 2\alpha k(x, x_{A}) - 2(1 - \alpha)k(x, x_{B})$$

or equivalently

$$x_C = \arg \max_{x \in S} \alpha k(x, x_A) + (1 - \alpha)k(x, x_B)$$

i.e., maximize weighted similarities with  $x_A$  and  $x_B$  as seen by the (learned) kernels.

For a crossover, choose  $\alpha \sim \mathcal{U}[0, 1]$ .

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### A Bayesian variation operator I

Link the probabilistic representations of BO and EO (cf. earlier slide) to define a variation (crossover and mutation) operator.

- T, a threshold (e.g.,  $T = \min \mathbb{F}$ ) •  $F(x) \coloneqq Y(x) \mid f(\mathbb{X}) = \mathbb{F} \sim \mathcal{N}(m(x), c(x, x))$ , the GP • F(x) < T, a logical random variable. It can be written  $F(X) < T \mid X = x, X$  random variable in S • Bayes:  $p(F(X) < T \mid X = x) \cdot p(X = x) =$ p(X = x | F(X) < T). p(F(X) < T)• GP :  $p(F(X) < T | X = x) = cdf_{\mathcal{N}} \left( (T - m(x)) / \sqrt{c(x,x)} \right)$
- p(X = x) = U[S]. Other more intensifying choices possible, at the risk of premature convergence.

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### A Bayesian variation operator II

p(X = x | F(X) < T) is the model for the variation operator of EO. It is sampled through

$$p(X = x | F(X) < T) \propto \operatorname{cdf}_{\mathcal{N}} \left( (T - m(x)) / \sqrt{c(x,x)} \right) p(X = x)$$

by a Metropolis-Hastings (or any appropriate MCMC) scheme.

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### References I



Bajer, L., Pitra, Z., Repickỳ, J., and Holeňa, M. (2019). Gaussian process surrogate models for the CMA evolution strategy. *Evolutionary computation*, 27(4):665–697.



Büche, D., Schraudolph, N. N., and Koumoutsakos, P. (2005).
Accelerating evolutionary algorithms with Gaussian process fitness function models. *IEEE Transactions on Systems, Man, and Cybernetics, Part C (Applications and Reviews)*, 35(2):183–194.



Cuesta-Ramirez, J., Le Riche, R., Roustant, O., Perrin, G., Durantin, C., and Gliere, A. (2022).

A comparison of mixed-variables Bayesian optimization approaches. Advanced MOdeling and Simulation in engineering sciences, 9(1).



Diouane, Y., Picheny, V., Le Riche, R., and Di Scotto, A. (2023). TREGO: a trust-region framework for efficient global optimization. *Journal of Global Optimization*, 86(1):1–23.

Eriksson, D., Pearce, M., Gardner, J., Turner, R. D., and Poloczek, M. (2019). Scalable global optimization via local Bayesian optimization.

In Wallach, H., Larochelle, H., Beygelzimer, A., d'Alché-Buc, F., Fox, E., and Garnett, R., editors, *Advances in Neural Information Processing Systems 32*, pages 5496–5507. Curran Associates, Inc.

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### References II

#### Fogel, L., Owens, A., and Walsh, M. (1965).

Artificial intelligence through a simulation of evolution, in biophysics and cybernetics systems.

In Proceedings of the Second Cybernetics Sciences Symposium, ed. by M. Maxfield, A. Callahan, and LJ Fogel, Spartan Books, Washington.

#### Frazier, P. and Powell, W. (2007).

The knowledge gradient policy for offline learning with independent normal rewards. In 2007 IEEE International Symposium on Approximate Dynamic Programming and Reinforcement Learning, pages 143–150. IEEE.



-

#### Frazier, P. I. (2018).

A tutorial on Bayesian optimization. arXiv preprint arXiv:1807.02811.



Garnett, R. (2023). Bayesian optimization. Cambridge University Press.



Hansen, N., Auger, A., Mersmann, O., Tusar, T., and Brockhoff, D. (2016). COCO: A platform for comparing continuous optimizers in a black-box setting. *arXiv preprint arXiv:1603.08785*.

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# References III



Hernández-Lobato, J. M., Hoffman, M. W., and Ghahramani, Z. (2014). Predictive entropy search for efficient global optimization of black-box functions. Advances in neural information processing systems, 27:918–926.



Holland, J. H. (1973).

Genetic algorithms and the optimal allocation of trials. SIAM journal on computing, 2(2):88–105.



Kushner, H. J. (1962).

A versatile stochastic model of a function of unknown and time varying form. Journal of Mathematical Analysis and Applications, 5(1):150–167.



Le Riche, R. and Picheny, V. (2021). Revisiting Bayesian optimization in the light of the COCO benchmark. Structural and Multidisciplinary Optimization, 64(5):3063–3087.

Močkus, J. (1972). On Bayesian methods of search for extremum. Automatics and Computers, 3:53-62.

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(4) (日本)

# **References IV**



#### Rechenberg, I. (1973).

Evolutionsstrategie: Optimierung technischer Systeme nach Prinzipien der biologischen Evolution.

Frommann-Holzboog-Verlag, Stuttgart.



#### Regis, R. G. (2016).

Trust regions in kriging-based optimization with expected improvement. 48:1037–1059.



#### Saltenis, V. R. (1971).

#### One method of multiextremum optimization.

Avtomatika i Vychislitel'naya Tekhnika (Automatic Control and Computer Sciences), 5(3):33–38.



#### Schonlau, M. (1997).

*Computer experiments and global optimization.* PhD thesis, University of Waterloo.

#### 

#### Schwefel, H.-P. (1977).

Numerische Optimierung von Computer Modellen mittels der Evolutionsstrategie. Birkhaeuser, Basel/Stuttgart. volume 26 of ISR.

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### References V

	-6

Srinivas, N., Krause, A., Kakade, S. M., and Seeger, M. (2010).

Gaussian process optimization in the bandit setting: No regret and experimental design. In ICML.



Ulmer, H., Streichert, F., and Zell, A. (2003).

Evolution strategies assisted by Gaussian processes with improved preselection criterion. In *The 2003 Congress on Evolutionary Computation, 2003. CEC'03.*, volume 1, pages 692–699. IEEE.

Villemonteix, J., Vazquez, E., and Walter, E. (2009). An informational approach to the global optimization of expensive-to-evaluate functions. *Journal of Global Optimization*, 44(4):509.



Volz, V., Rudolph, G., and Naujoks, B. (2017). Investigating uncertainty propagation in surrogate-assisted evolutionary algorithms. In *Proceedings of the Genetic and Evolutionary Computation Conference*, pages 881–888.

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