École chercheurs MEXICO, La Rochelle, Mars 2018

Model Based Optimization

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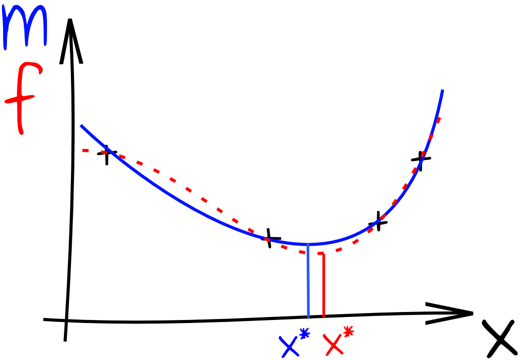
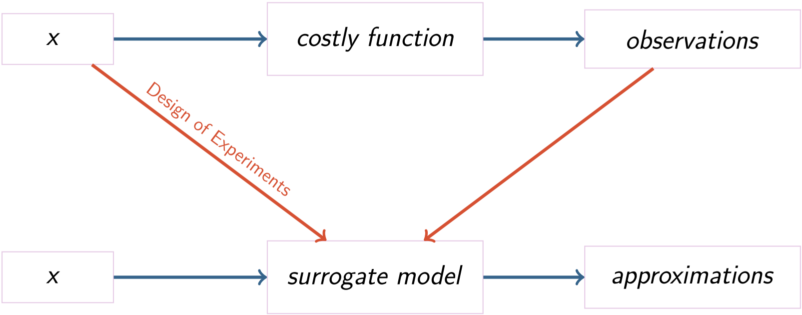
If the number of function evaluations is limited, we can run the optimization on the model instead of running it directly on the function



In the end, we hope that:

$$\text{argmin}(m) \approx \text{argmin}(f)$$
$$\min(m) \approx \min(f)$$

Overall framework



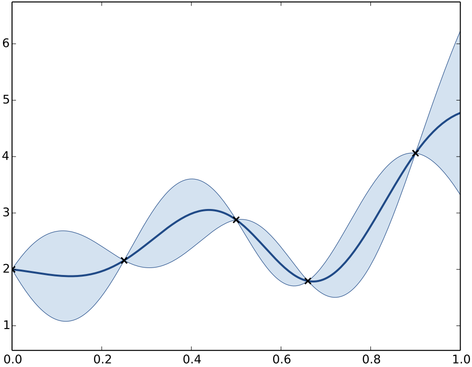
In practice, it is risky to take decisions based only on the model...

On the other hand, the model can be used to guide us in the search for the optimum.

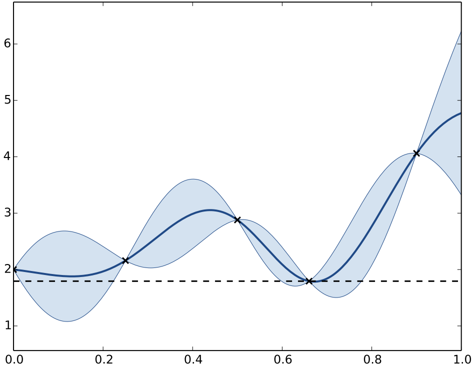
Global optimization methods are a trade-off between

- Exploitation of past good results
- Exploration of the space

How can GPR models be helpful?



In our example, the best observed value is 1.79

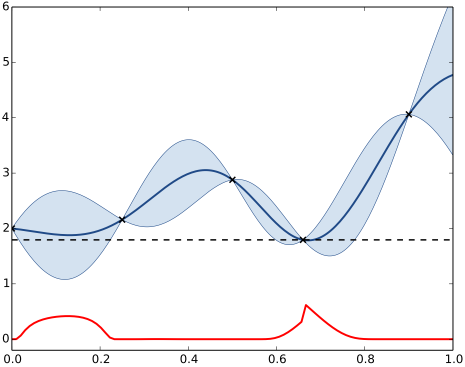


Various criteria can be studied

- probability of improvement
- Expected improvement

Probability of Improvement:

$$PI(x) = cdf\left(\frac{\min(F) - m(x)}{\sqrt{(c(x,x))}}\right)$$



The point with the highest PI is often very close to the best observed value. We can show that there is a x in the neighbourhood of x^* such that $PI(x) \geq 0.5$.

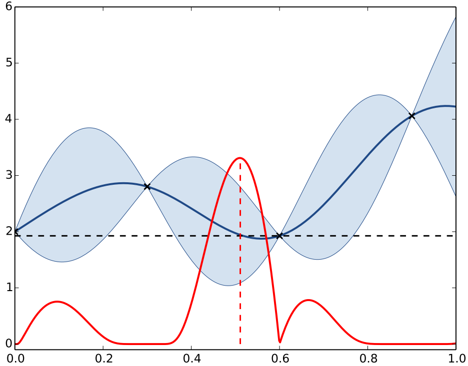
For such points, the improvement cannot be large...

Can we find another criterion?

Expected Improvement:

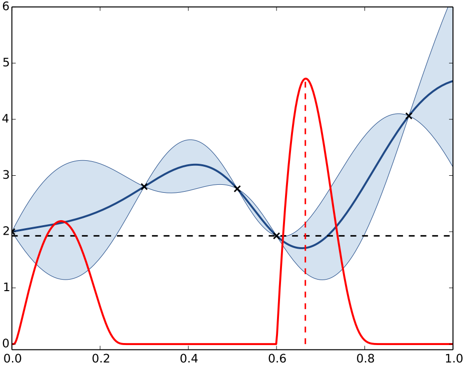
$$EI(x) = \int_{-\infty}^{\min(F)} \max\left(0, Y(x)\right)\ dy(x) = \cdots =$$

$$\sqrt{c(x,x)}(u(x)cdf(u(x)) + pdf(u(x))) \quad \text{with } u(x) = \frac{\min(F) - m(x)}{\sqrt{(c(x,x))}}$$



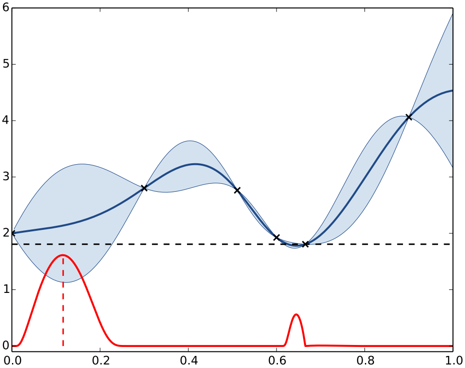
Expected Improvement

Let's see how it works... iteration 1



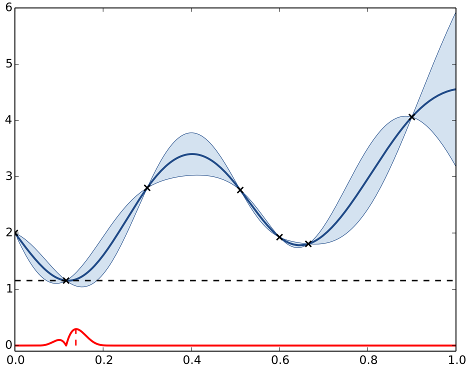
Expected Improvement

Let's see how it works... iteration 2



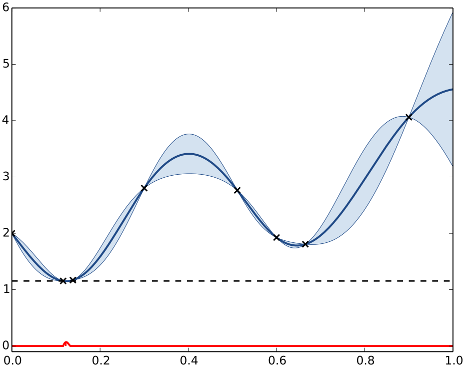
Expected Improvement

Let's see how it works... iteration 3



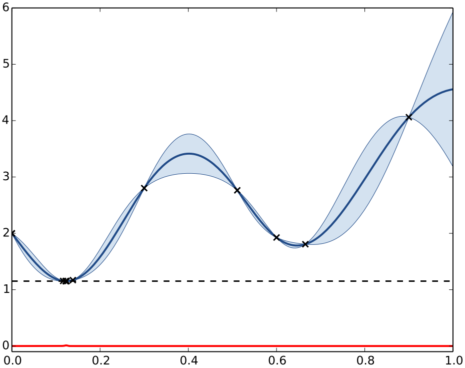
Expected Improvement

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



Expected Improvement

Let's see how it works... iteration 5



Expected Improvement

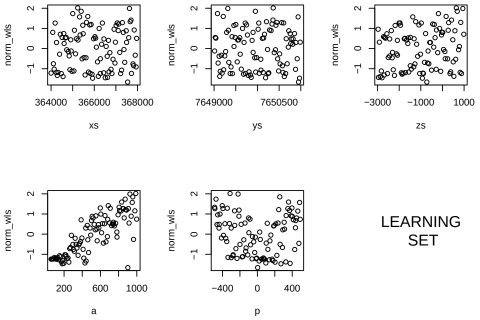
This algorithm is called **Efficient Global Optimization** (EGO, Jones et al., 1998):

1. make an initial design of experiments X and calculate the associated F, $t = \texttt{length}(F)$
2. built a GP from (X, F) (max. log-likelihood on σ and θ_i's)
3. $X_{t+1} = \arg\max_x EI(x)$
4. calculate $F_{t+1} = f(X_{t+1})$, increment t
5. stop $(t > t^{\max})$ or go to 2.

+ EGO provides a good trade-off between exploitation and exploration without arbitrary parameters.
+ It requires few function observations (10 in the example) to get close to optimal regions.

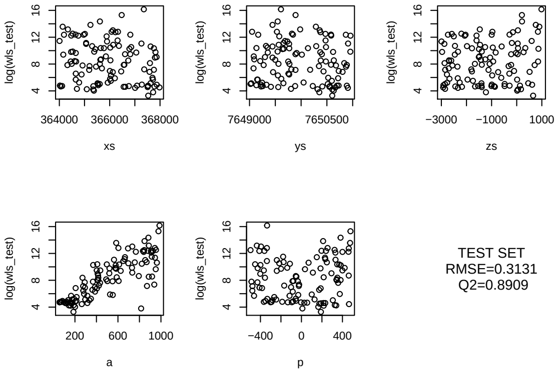
Example in 5d: surface displacements misfit minimization

$\Rightarrow$ demo with `mainInversionPunctualDisplSource.R`
!!! normalize the data: WLS has a few very large values, it is always > 0: make it more gaussian, $\texttt{wls}\_norm = \log(1 + \texttt{wls})$ and all x's and $\texttt{wls}\_norm$ between 0 and 1.



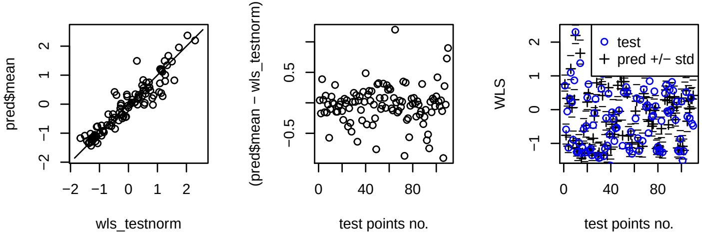
100 $\{xs, ys, zs, a, p\}$ points chosen through an optimized Latin Hypercube Sampling (R libraries `DiceDesign` or `lhs`).

(demo with `mainInversionPunctualDisplSource.R`, cont.)



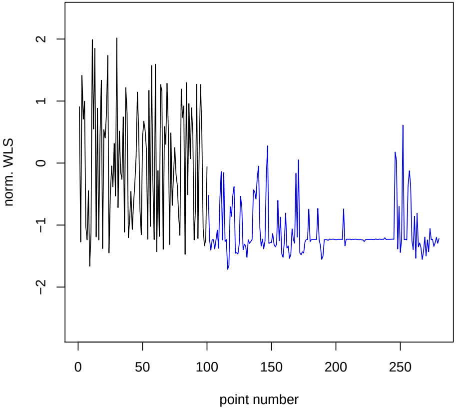
110 random $\{xs, ys, zs, a, p\}$ test points.

(demo with `mainInversionPunctualDisplSource.R`, cont.)



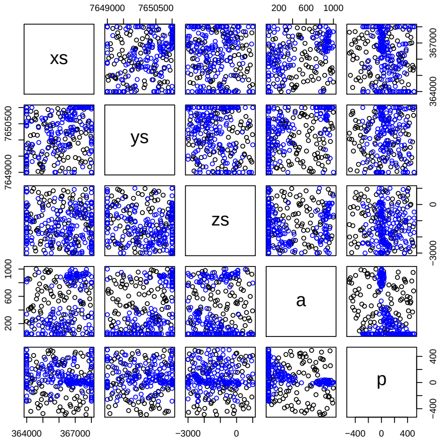
110 test points.

(demo with `mainInversionPunctualDisplSource.R`, cont.)
EGO parameters: anisotropic Matèrn 5/2 kernel, GP updated (log-likelihood maximized) every 5 added points, BFGS with bounded variables (from `optim()` function) restarted from random initial points for maximizing log-likelihood and EI.



Preferential sampling of good regions of S, but global therefore sometimes increasing WLS. Lower bound on θ_i's increased from 0.08 to 0.1 at $t = 250$ (x_i's and θ_i's normed between 0 and 1).

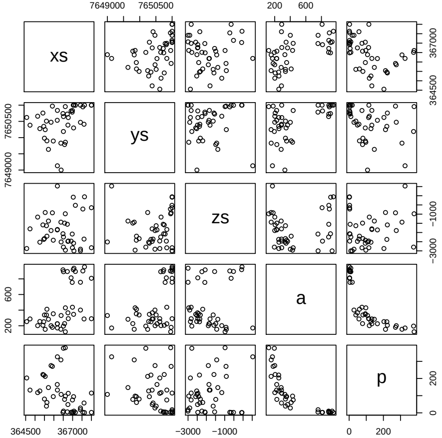
(demo with `mainInversionPunctualDisplSource.R`, cont.)



Black: LHS initial points.
Blue: EGO points.

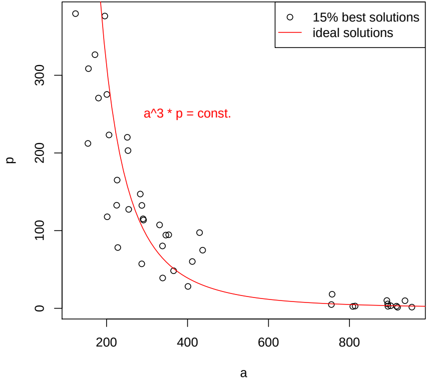
Note the patterns in new points. Accumulation at lower bound of a and mid interval of p before $t = 250$.

(demo with `mainInversionPunctualDisplSource.R`, cont.)



15% best sampled points. Note the "function" for the (a, p) pair, i.e., $a^\star(p^\star)$.

(demo with `mainInversionPunctualDisplSource.R`, cont.)



Mogi model only dependency in a and p is through $a^3 \times p$: it is not identifiable.

EGO tells it by preferential sampling in the valley

$$a^3 \times p = \text{const.} = a^{\star 3} \times p^\star$$

Other EGO output: a statistical model of WLS.
The last length scales are an indication of the sensitivity of WLS to each variable: a, p and zs are very sensitive (θ_i's small, in $[0.08, 0.1]$), xs a little sensitive (θ in $[0.1, 2.5]$) and ys insensitive ($\theta \approx 3$).

Difficulties and challenges with EGO

- Standard GPs are limited to $n \approx 1000$ points (covariance matrix inversion).
- EGO clusters points in good regions, the covariance matrix may become ill-conditionned if length scales θ_i are too large w.r.t. X.
- Although the method perfectly applies to large dimensional spaces ($d > 100$), larger d may require larger n, back 2 lines above.
- EGO does not converge in the traditional sense: it creates dense samples in the volume of S. The efficiency comes from the order in which points are sampled.

$\Rightarrow$ these are the topics of current research. Let's mention a few extensions next.

EGO continuations

- Parallelized EGO: estimate the *EI* of groups of points, cf. Ginsbourger et al.
- Finite budget: *EI* of a single x is only optimal at the last iteration. Theory of dynamic *EI*, cf. Ginsbourger et al.
- EGO and bad covariance matrix conditioning: replace points that are close-by by one point and the associated derivatives (cf. M. Osborn, L. Laurent), regularizations (cf. Le Riche et al.)
- SUR strategies: (Step-wise Uncertainty Reduction), reduce the entropy of the optimum (cf. Vasquez et al.), or the average probability of incursions below $min(F)$ (cf. Picheny).

Related problems addressed with GPs

- EGO with constraints: $\min_x f(x)$ s.t. $g(x) \leq 0$, multiply the *EI* by the probability of constraints satisfaction.
- GP for target attainment: find the set of x s.t. $f(x) = T$, change the *EI* into $c(x,x) \times \text{pdf}\left((T - m(x))/sqrt(c(x,x))\right)$, cf. Picheny et al.
- GP for probability estimation: find $\mathbb{P}(f(x,U) \leq T)$ where U is a random vector.
- GP for multi-objective optimization: $\min_x\{f_1(x), \ldots f_m(x)\}$, cf. Binois et al.

Robust optimization

Can EGO be adapted when observations are noisy?

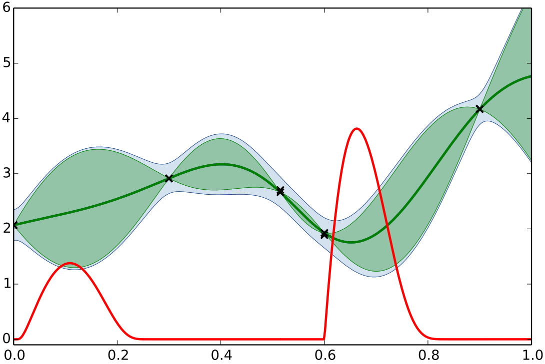
First of all, using the current best observation as a minimum does not make much sense...

Some solutions are

- S1 Build a new model that interpolates $m(X)$ at X where $m(X)$ accounts for the noise (non interpolating GP, e.g. with a white noise part in the kernel).
- S2 Include observation noise and replace $\min(F)$ by $\min(m(X))$ in the EI expression
- S3 Similar to 2 but consider an Expected Mean Improvement (V. Picheny).

Solution 1

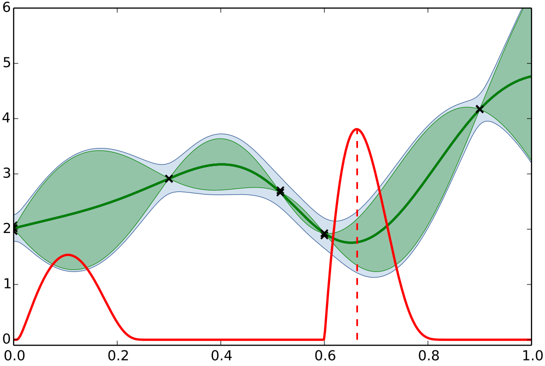
iteration 0



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

iteration 1



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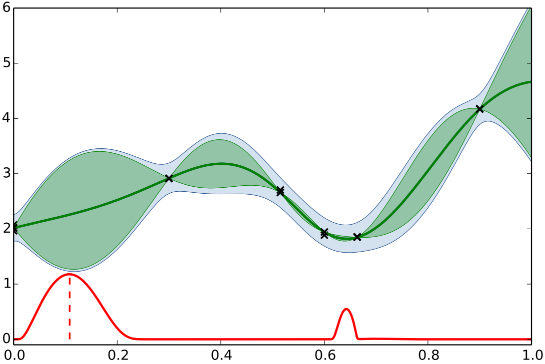
Solution 1

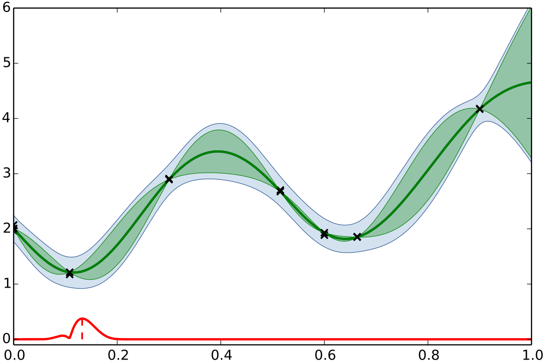
iteration 2



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

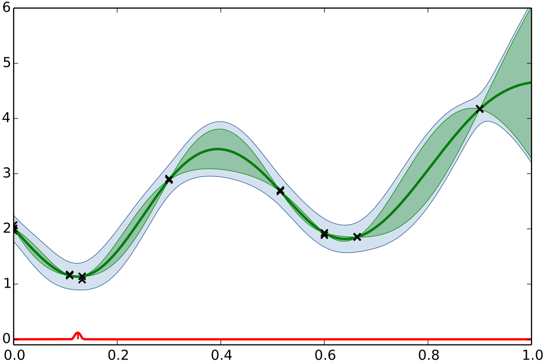
iteration 3



(noisy observations and their denoised versions are both shown as black crosses)

Solution 1

iteration 4



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