Relative Expected Improvement in Kriging Based Optimization

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the field with respect to the measurements (a posteriori) is also gaussian with known both mean and covariance.

One of the methods to find a point for new measurement is the Expected Improvement criterion. It uses a Expected Improvement function:

$$EI(x) = E(\min(\hat{F}_{\text{min}}, F(x)))$$

where $F$ is the a posteriori field and $\hat{F}_{\text{min}}$ is the minimum of estimator. The new point of measurement is chosen in the minimum of EI function.

Many modifications and enhancements were considered for the Kriging model. Application of linear operators, e.g. derivatives, integrals and convolutions, are easy to incorporate in the model.

Each of these extensions of classic Kriging model is based on measuring something else then is returned as the response. For example we measure gradient and value of the function, but the response is only the function. The Expected Improvement states that we should measure the function in place where the minimum of response can be mostly improved. But for classic model the notion of the measured and the response functions are the same.

The purpose of this paper is the investigation wether the concept of EI can be extended for enhanced Kriging models.

2 RELATIVE EXPECTED IMPROVEMENT

2.1 Efficient Global Optimization

Jones et al. propose an Efficient Global Optimization (EGO) algorithm based on Kriging model and Expected Improvement. It consists of the following steps:

1. Select a learning group $x_1, \ldots, x_n$. Measure objective function $f$ in these points $f_i = f(x_i)$.
2. Construct a Kriging approximation $\hat{F}$ based on measurements $f_1, \ldots, f_n$.
3. Find the minimum of $EI(x)$ function for the approximation.
4. Augment $n$ and set $x_n$ at the minimum of EI.
5. Measure $f_n = f(x_n)$ and go back to 2

EI function can have many local minima (is highly multi-modal) and is potentially hard to minimize. The original paper proposed Branch and Bound Algorithm (BBA) to efficiently optimize the EI function. To use BBA authors had to establish upper and lower bonds on minimum of EI function over a region. It was fairly easy and was the main source of effectiveness of EGO. While proposing an extension of EI concept we also have to propose a suitable methods of it’s optimization.

2.2 Gaussian Kriging

Kriging is a statistical method of approximation a multi-dimensional function basing on values in a set of points. The Kriging estimator (ap-
proximation) can be interpreted as a least-square estimator, but also as a Bayes estimator. We will use the latter interpretation as in the original EI definition.

Let us take an objective function \( f : \Omega \rightarrow \mathbb{R} \). For some probabilistic space \((\Gamma, \mathcal{F}, P)\), we consider a random gaussian field \( F \) on \( \Omega \) with the known mean \( \mu \) and covariance \( K(x, y) \). Now we take a measurements of the objective at points \( x_1, \ldots, x_n \) as \( f_i = f(x_i) \). The Bayes estimator of \( f \) is:

\[
\hat{F}(x) = \mathbb{E}(F(x) \mid \forall i, F(x_i) = f_i)
\]

Where \( \mathbb{E}(A \mid B) \) is conditional expected value of \( A \) with respect to \( B \).

This estimator at \( y \) will be called the response at \( y \) and the \((x_i, f_i)\) pairs will be called measurements at \( x_i \).

Let us take an event \( M = \{\forall i, F(x_i) = f_i\} \subset \Gamma \) and an a posteriori probability space \((M, \mathcal{F}_M, P(\cdot \mid M))\). \( E_M \) will stand for expected value in an a posteriori. Field \( F \) considered on the \( M \) space is also a gaussian random field with known both mean \( \mu_M \) and covariance \( K_M \). We will call this field, the a posteriori field.

### 2.3 From EI to REI

We would want to estimate how much the minimum of \( \hat{F} \) we will be improved if will measure \( f \) at some point. Estimator \( \hat{F} \) after the measurement in \( x \) can be written as \( F_x = E_M(F(x)) \). The best estimate of the effect would be \( E_M \inf_{\Omega} F_x \). But computing it would be very time-consuming. The idea of Expected Improvement (EI) is to take

\[
\text{EI}(x) = E_M \min\{F_{\min}, F(x)\}
\]

where \( F_{\min} \) is the actual minimum of approximation \( \hat{F} \). Expected Improvement is in fact expected value of how response at \( x \) will improve the actual minimum of \( \hat{F} \). Of course the definition is equivalent to:

\[
\text{EI}(x) = E_M \min\{F_{\min}, E_M(F(x) \mid F(x))\}
\]

This formulation has a natural extension. Let us define, for a set of points \( \eta = \{\eta_1, \ldots, \eta_l\} \), a augmented estimator \( F_\eta(x) = E_M(F(x) \mid F(\eta_1), \ldots, F(\eta_l)) \).

For another set of points \( \zeta = \{\zeta_1, \ldots, \zeta_k\} \) we can define:

\[
\text{REI}(\zeta, \eta) = E_M \min\{F_{\min}, F_\eta(\zeta_1), \ldots, F_\eta(\zeta_k)\}
\]

Our Relative Expected Improvement (REI) is the expected value of how much the response at \( \zeta \) will improve the minimum of \( \hat{F} \) if we measure at \( \eta \). This definition implies \( \text{REI}(\{x\}, \{x\}) = \text{EI}(x) \).

We can use also a more general version:

\[
\text{REI}_m(\zeta, \eta) = E_M \min\{F_{\eta}(\zeta_1), \ldots, F_{\eta}(\zeta_k)\}
\]

The main advantage of REI function is that we can examine the response in a different region then the region of acceptable measurements. A simple example illustrates it very well:
Example 1 We’re searching for some mineral. We have to estimate the maximum mineral content in somebody’s land before buying it. We cannot drill at his estate, but we can drill everywhere around it.

In this example response and measurements are in a different regions, so we cannot use EI. If the estate is $A$ and the surrounding ground is $B$, in order to find the best place to drill, we would have to search for the minimum of $\text{REI}(\{x\}, \{y\})$ for $x \in A$ and $y \in B$.

3 APPLICATION

3.1 Populations of measurement points

The first application of using REI instead of EI is when we want to find a collection of measurement points instead of a single point, e.g. when the objective function can be computed simultaneously at these points. It’s a possibility of making the optimization process more parallel.

Example 2 We have $k$ processors to solve our CFD problem, each running a separate flow case.

This procedure could be, for example, to optimize $\text{REI}(\{\zeta_1, \ldots, \zeta_n\}, \{\zeta_1, \ldots, \zeta_n\})$. The main advantage in using such an expression, over using some selection of EI minima, is that REI considers the correlation between these points. For example, if $x$ and $y$ are strongly correlated, we don’t want to measure in both these points, because the value in $x$ implies the value in $y$. 
3.2 Input enhancements

The other application field is enhancing the Kriging model, by some other accessible information than the values in points.

Let us define a generalized point as a pair \((x, P)\), where \(x \in \Omega\) is a point, and \(P\) is a linear operator. We can say that \(f(x, P) = (Pf)(x)\). The field \(F(x, P)\) is also gaussian with:

\[
\begin{align*}
\mu(x, P) &= (P\mu)(x) \\
K(x, P; y, S) &= P_x S_y K(x, y)
\end{align*}
\]

where \(P_x\) stands for applying \(P\) to \(K\) as a function of the first coefficient.

Example 3

The CFD code is solving the main and the adjoint problem. We have both the value of our objective and its derivatives with respect to design parameters. We want to find the best place to measure these values.

We can use \(f(x, \frac{\partial}{\partial x_k}) = \frac{\partial f}{\partial x_k}(x)\) to interpret measuring the derivatives of \(f\) interpret as measuring at points \((x, \frac{\partial}{\partial x_k})\). In the example we have not only calculated the value at \((x, \text{Id})\), but also at \((x, \frac{\partial}{\partial x_k})\). If we have \(d\) design parameters (that is \(\Omega \subset \mathbb{R}^d\)) we have \(d + 1\) measurements simultaneously.

We can now optimize:

\[\text{REI}\left(\left\{(\zeta_1, \text{Id}), \ldots, (\zeta_{d+1}, \text{Id})\right\}, \left\{(x, \text{Id}), (x, \frac{\partial}{\partial x_1}), \ldots, (x, \frac{\partial}{\partial x_d})\right\}\right)\]

We take \(d + 1\) points of response \(\zeta\) to maximize the effect of all the measured derivatives. We could of course use EI. In that case we would select the next point as if we’re measuring only the value. By using REI we’re incorporating the derivative information not only in the model, but also in the selection process. The disadvantage of such an expression is that we search in \(\Omega^{d+2}\) which is \(d \cdot (d + 2)\)-dimensional.

3.3 Multi-effect response

Next on our list is the multi-effect model. We can imagine that our measured function is composed of several independent or dependent effects, while our objective function is only one of them. The simplest case is when we want to optimize objective which we measuring with an unknown error.

Let us now say that \(F\) consists of several components \(F(x) = (Z(x), W(x), V(x), \ldots)\). Same letters will stand for linear operators, such that \(F(x, Z) = Z(x)\).

Example 4

Suppose that we’re searching for mineral \(A\), but our drilling equipment for measuring content of \(A\), cannot distinguish it from another mineral \(B\). We know on the other hand that the latter is distributed randomly and in small patches.

Let \(Z\) be our objective function (mineral \(A\) content) and \(\varepsilon\) a spatially-correlated error (mineral \(B\) content). We can measure only \(Z + \varepsilon\) while we want to optimize \(Z\). In this example we can optimize \(\text{REI}\left(\left\{(x, Z)\right\}, \left\{(x, Z + \varepsilon)\right\}\right)\).
Such a procedure will simultaneously take into consideration optimization of the objective and correction of the error. To fully understand why this example is important, we have to remember that drilling in the same place twice would give the same result. The error correction in our procedure will bear this in mind and will avoid duplication of measurements.

This model would include results obtained from lower-quality numerical calculations. For an iterative algorithm (non-random), we can state a higher error bound and reduce the number of iterations. We cannot assume the error to be fully random, because starting from the same parameters, the algorithm will give the same results. That’s why a good Kriging model, would recognize the error to be a narrowly correlated random field $\varepsilon$. 

![Figure 3: (a) High and (b) low fidelity models](image)

**Example 5** We have two CFD models. One accurate and the other approximate, but very fast (high and low-fidelity models). We know also, that the low-fidelity model is “smoother” with respect to the design parameters.

Let $Z$ be our objective function and $W$ be a approximation of $Z$. In this example we can separately optimize:

\[
\text{REI}(\{(\zeta_1, Z), \ldots, (\zeta_k, Z)\}, \{(x, Z)\})
\]
\[
\text{REI}(\{(\zeta_1, Z), \ldots, (\zeta_k, Z)\}, \{(x, W)\})
\]

and subsequently choose between these two points. Field $W$ is strongly spatially-correlated (“smoothr”) and as such it’s measurement can have wider effect than $Z$. We can also take in to consideration the cost of the computation and select a better improvement-to-cost ratio.

### 3.4 Robust response

The last field of application, that we will discuss, is the robust response. If for instance after optimization, the optimal solution will be used to manufacture some objects, we can be sure that the object will be manufactured within certain tolerance. In other words, if the selected point is $x$, the actual point will be $x + \varepsilon$. Our real objective function is the average performance of these $x + \varepsilon$. 


Example 6 Suppose we can calculate the drag force of a car. Our factory,
makes cars with some known accuracy. We want to find the car shape,
that will give the lowest average drag when made in our factory.

Let $Z$ be our objective function and $\epsilon$ - the manufacturing error. We
can measure only $Z(x)$ while we want to optimize $E(Z(x+\epsilon))$. Let us
say that $\epsilon$ is a random variable (for instance $N(0,\Sigma)$), and let $\phi_\epsilon$ be it’s
probability density. Now $E(h(x+\epsilon)) = (\phi_\epsilon * h)(x) = h(x, \phi_\epsilon \ast)$. In above
example we can use:

$$REI([\{z, \phi_\epsilon * Z\}], \{[\eta, Z]\})$$

The robust response stated as above, has a good physical interpretation. It
is also fairly easy to use as long as we can effectively calculate convolution
of $\phi_\epsilon$ and the covariance function.

It’s also good to look at this kind of robust response, as a penalty for
the second derivative. If $\epsilon \sim N(0,\Sigma)$, then:

$$E(h(x+\epsilon)) \simeq h(x) + \frac{1}{2} \sum_{ij} \frac{\partial^2 h}{\partial x_i \partial x_j} \Sigma_{ij}$$

Of course such a penalty would also be a linear operator $P_\Sigma h = h + \frac{1}{2} \sum_{ij} \frac{\partial^2 h}{\partial x_i \partial x_j} \Sigma_{ij}$ and as such can be used instead of $\phi_\epsilon \ast$. This approach
can be useful for convolutions that are expensive to calculate.

4 OPTIMIZATION

4.1 Upper bounds

As Jones et al. noted, EI function can be highly multi-modal and potentially
hard to optimize. To use the branch and bound algorithm (BBA),
we have to establish a good upper bounds on REI.

We defined REI to be:

$$REI(\zeta, \eta) = E_M \min \{F_{\min}, F_\eta(\zeta_1), \ldots, F_\eta(\zeta_k)\}$$

where $F_\eta(x) = E_M (F(x) \mid F(\eta_1), \ldots, F(\eta_l))$. It is clear that $F_\eta$ is a
 gaussian field (in fact with only $l$ degrees of freedom). We can calculate
its mean and covariance depending on $\eta$. In such a case we would want to establish upper bounds for an expression:

$$\Psi_{\mu, \Sigma} = \mathbb{E} \min\{\gamma_1, \ldots, \gamma_p\}$$

for some $\gamma \sim N(\mu, \Sigma)$. To bound such an expression, we can use recent extensions of comparison principle by Vitale\cite{7}. The comparison principle states that the $\Phi_{\mu, \Sigma}$ is greater, the greater are $\mathbb{E}(\gamma_i - \gamma_j)^2 = \Sigma_{ii} + \Sigma_{jj} - 2\Sigma_{ij}$. To calculate the upper bound for REI, we can maximize these expressions over a region and then calculate the independent but differently distributed (IDD) gaussian variables dominating REI. Construction of such dominating IDD variables is discussed in Ross\cite{6}.

4.2 Exact calculation

In the last iterations of BBA the IDD-based bounds will be insufficient. The main direction of further research will be to establish a good method of calculating an exact bound on $\Psi_{\mu, \Sigma}$. Actual algorithms in this field are based on Monte Carlo or quasi-Monte Carlo methods, for instance using results by Genz\cite{1}.

5 CONCLUSIONS

Relative Expected Improvement is proposed to extend the concept of $EI$ for more complex Kriging models. It can help search for new points of measurements and for populations of such points. It can also help to use derivative information more efficiently. Further research is needed to find efficient implementation of this concept.

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