Sequential Design of Experiments with Gaussian Processes

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LIKE22 -Lifting Inference with Kernel Embeddings

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GP regression - recall from previous talk

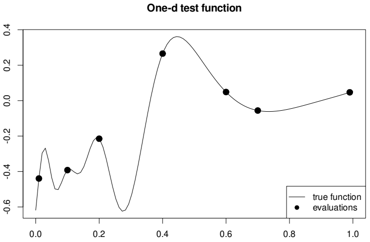
Data: $\mathcal{D} = (\mathbf{x}_i, y_i)_{i=1}^n$

$$y_i = f(\mathbf{x}_i) + \varepsilon_i$$

$$\varepsilon_i \sim N(0, \sigma_n^2)$$

$$\mathbf{x}_i \in D \subset \mathbb{R}^d$$

GP prior $Z \sim GP(m, k)$



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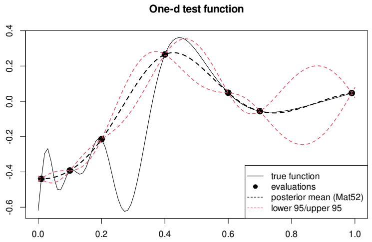


GP regression:

$$m_n(\mathbf{x}) = m(\mathbf{x}) + k(\mathbf{x}, X_n)(k(X_n, X_n) + \sigma_n^2 I_n)^{-1}\mathbf{y}_n$$

$$k_n(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}') - k(\mathbf{x}, X_n)(k(X_n, X_n) + \sigma_n^2 I_n)^{-1}k(X_n, \mathbf{x}')$$

A GP as a surrogate for f

We observe $y_i = f(\mathbf{x}_i) + \epsilon_i$, the function f can be

- expensive computer experiment
  (e.g., PDE solver, expensive MC simulation)
- truly unknown function
  (e.g., y are real measurements of a phenomenon)

We can build a Design of Experiments (DoE) to estimate f.

Examples of fixed (non-sequential) DoE:

- space-filling sequences (e.g., Sobol');
- deterministic designs (e.g., Latin hypercube sample);
- statistically optimal designs (A-optimality, D-optimality).

What do we mean by sequential design of experiments?

Initial dataset: n observations $(\mathbf{x}_i, y_i)_{i=1}^n$, where $y_i = f(\mathbf{x}_i) + \epsilon_i$, ϵ_i realization from i.i.d. noise.

Initial GP fit: proceed as in previous talk and obtain m_n, s_n.

Sequential DoE: strategies that sequentially add new points.

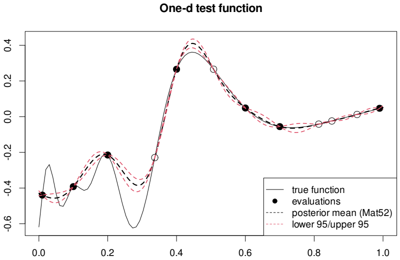
This talk

- what is the objective of adding new points?
  (learn f, finding global minimum of f, learn excursion set of f)
- strategies to achieve optimal DoE (e.g.: IMSE, EI, SUR)

What are the objectives of sequential DoE?

Today we will see

- improve the model and "learn" f,
  i.e. reduce posterior variance



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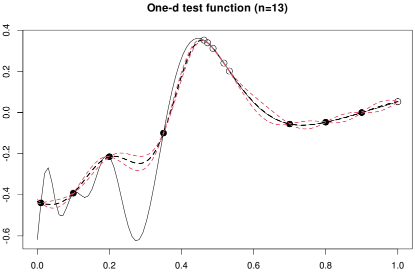
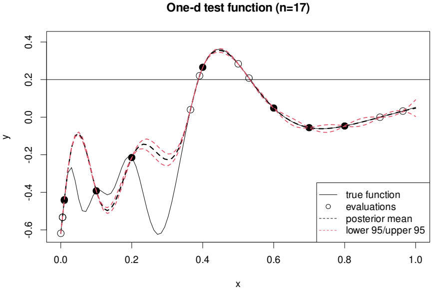
- improve the model and "learn" f
- Bayesian optimization:
  i.e. find $\mathbf{x}^* \in \arg\max_{\mathbf{x}\in D} f(\mathbf{x})$



What are the objectives of sequential DoE?

Today we will see

- improve the model and “learn” f
- Bayesian optimization
- learn level/excursion sets of f, i.e. estimate $\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \geq t\}$, fixed, known $t \in \mathbb{R}$.



Outline

Sequential DoE to improve the model
- MSE and IMSE criterion

Bayesian Optimization
- Upper Confidence Bound
- Expected Improvement
- Knowledge gradient
- Further topics

Target region estimation
- Targeted IMSE
- SUR for excursion set volume

Excursion set estimation
- Vorob'ev quantiles and Conservative estimates
- SUR strategies for conservative estimates

Sequential design of experiments

General procedure:

Start: train a surrogate model on an initial DoE;
Repeat until stopping criterion is met;

1. Use the surrogate model to define an **acquisition function**;
2. Optimize the acquisition function to find the next point(s);
3. Evaluate oracle to obtain new training data;
4. Update the surrogate model with new information;

What is the acquisition function? How to define it from a GP?

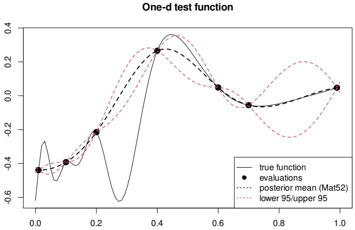
Outline

What does "improve the model" mean?

Regression data:

$\mathcal{D} = (\mathbf{x}_i, y_i)_{i=1}^n$

GP prior: $Z \sim GP(m, k)$



We compute the GP posterior $Z|\mathcal{D} \sim GP(m_n, k_n)$.

How can we improve this model? Reduce "error"

1. Mean Squared Error (MSE) criterion;
2. Integrated Mean Squared Error (IMSE) criterion.

GP regression as weighted interpolation

$Z \sim GP(m, k)$ with $m(\mathbf{x}) = 0$, $\mathbf{x} \in D$, k p.d. kernel.

Noiseless observations $Z_{\mathbf{x}_1}, \dots, Z_{\mathbf{x}_n}$ at $\mathbf{X}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$.

"Best" linear predictor for $Z_{\mathbf{x}}$?

We are looking for $\widehat{Z}_{\mathbf{x}} = \sum_{i=1}^{n} \lambda_i Z_{\mathbf{x}_i}$ which is

unbiased $\mathbb{E}[\widehat{Z}_{\mathbf{x}}] = \mathbb{E}[Z_{\mathbf{x}}]$

$\lambda \in \arg\min \mathrm{MSE}(\lambda) = \mathbb{E}[(\widehat{Z}_{\mathbf{x}} - Z_{\mathbf{x}})^2]$

We obtain $\lambda(\mathbf{x}) = k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x})$ and

$$\begin{aligned}\mathrm{MSE}(\lambda(\mathbf{x})) &= \lambda(\mathbf{x})^T k(\mathbf{X}_n, \mathbf{X}_n)\lambda(\mathbf{x}) - 2\lambda(\mathbf{x})^T k(\mathbf{X}_n, \mathbf{x}) + k(\mathbf{x}, \mathbf{x}) \\ &= k(\mathbf{x}, \mathbf{x}) - k(\mathbf{x}, \mathbf{X}_n) k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x})\end{aligned}$$

SK equations

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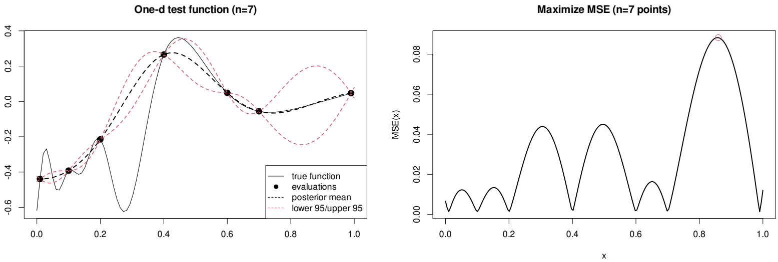
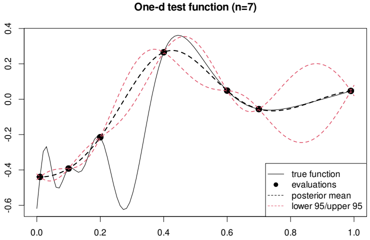
SK equations

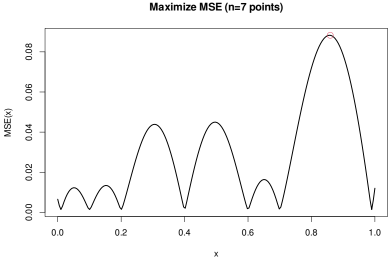
Improve the model by adding evaluations at maximum MSE points?



Mean Squared Error criterion

Criterion: select $\mathbf{x}_{n+1} \in \arg\max_{\mathbf{x} \in D} MSE_n(\mathbf{x})$





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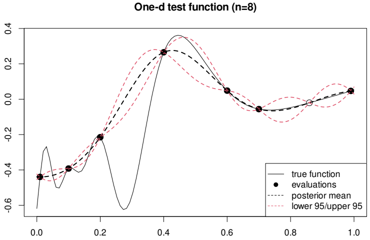

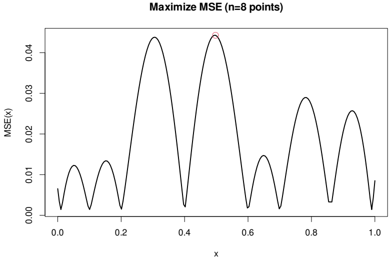

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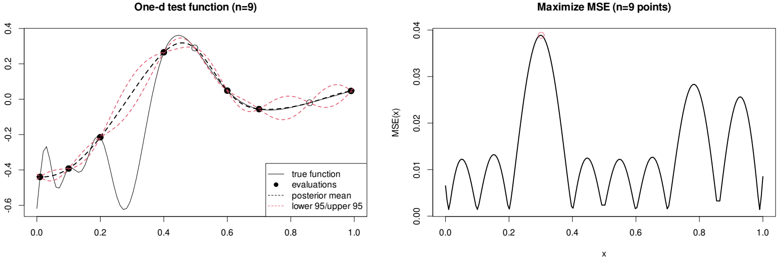

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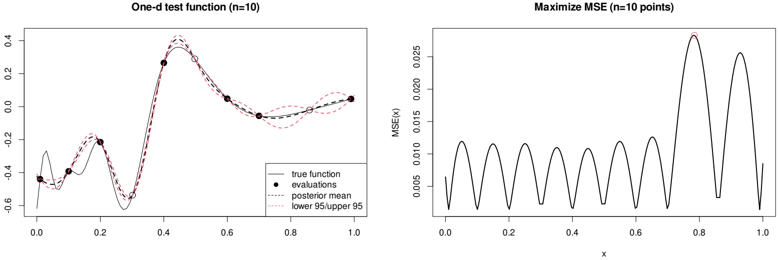

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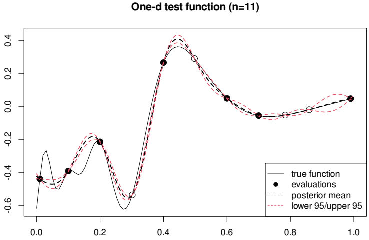

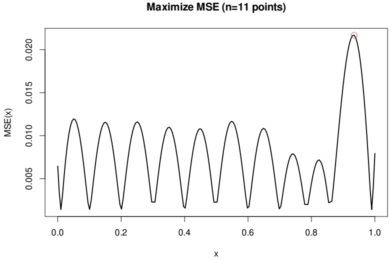

Integrated Mean Squared Error criterion

A global quantification of the uncertainty on the current model

$$H_n^{IMSE} = \int_D MSE_n(\mathbf{u}) d\mathbf{u},$$

(possible to generalize to a finite measure μ on D)

H_n^{IMSE} only considers the first n observations, can we "look-ahead"?

At step n we want $H_{n+1}^{IMSE} = \int_D MSE_{n+1}(\mathbf{u}; \mathbf{x}_{n+1}) d\mathbf{u}$,

where $MSE_{n+1}(\mathbf{u}; \mathbf{x})$ is the MSE for the model conditioned on $\{\mathbf{X}_n, \mathbf{x}\}$.

Can we compute $\mathbb{E}_n[H_{n+1}^{IMSE} \mid \mathbf{x}_{n+1} = \mathbf{x}]$?

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Integrated Mean Squared Error

In the GP case we can compute the criterion:

1. Compute $MSE_{n+1}(\mathbf{u})$ without the $n+1$ evaluation:

$$MSE_{n+1}(\mathbf{u};\mathbf{x}) = \lambda_{n+1}(\mathbf{u})^T k(\mathbf{X}_{n+1}(\mathbf{x}), \mathbf{X}_{n+1}(\mathbf{x}))^{-1} \lambda_{n+1}(\mathbf{u}) \\ - 2\lambda_{n+1}(\mathbf{u})^T k(\mathbf{X}_{n+1}(\mathbf{x}), \mathbf{u}) + k(\mathbf{u}, \mathbf{u}) = k_{n+1,\mathbf{x}}(\mathbf{u}, \mathbf{u})$$

where $\mathbf{X}_{n+1}(\mathbf{x}) = \{\mathbf{X}_n, \mathbf{x}\}$ is the augmented design.

2. the criterion then is

$$\mathbf{x}_{n+1} \in \arg\min_{\mathbf{x}\in D} \mathbb{E}_n[H_{n+1}^{IMSE}] = \arg\min_{\mathbf{x}\in D} \int_D k_{n+1,\mathbf{x}}(\mathbf{u}, \mathbf{u}) d\mathbf{u}$$

Sacks, J., Welch, W.J., Mitchell, T.J., Wynn, H.P. (1989). *Design and analysis of computer experiments.* Statistical Science 4(4), 409–435.

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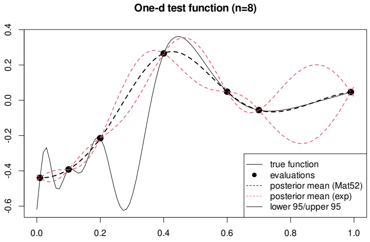

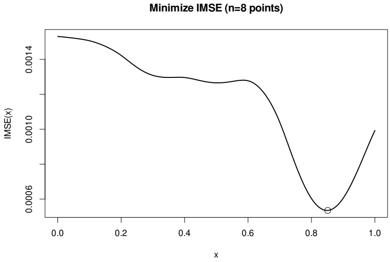

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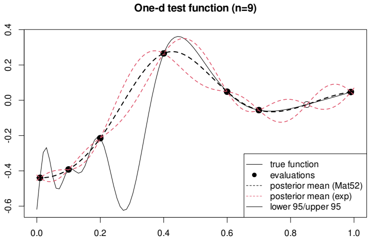

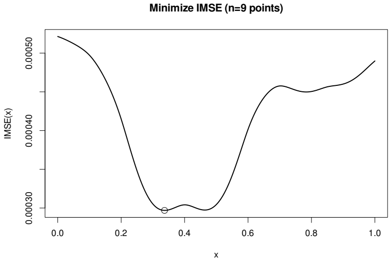

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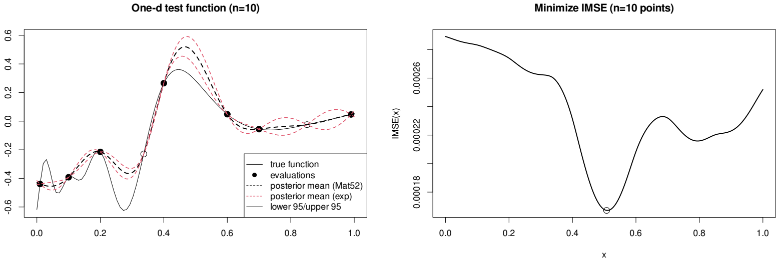

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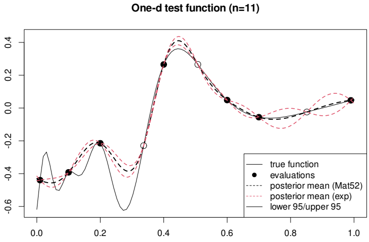

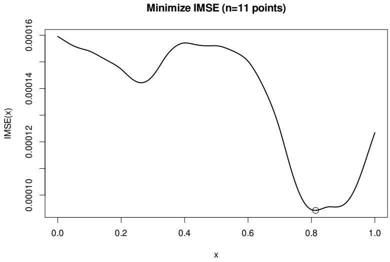

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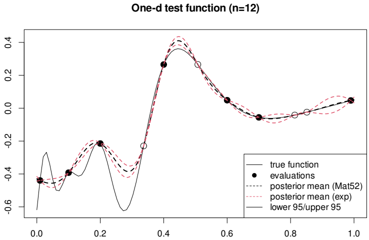

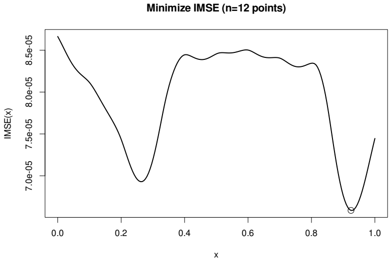

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Outline

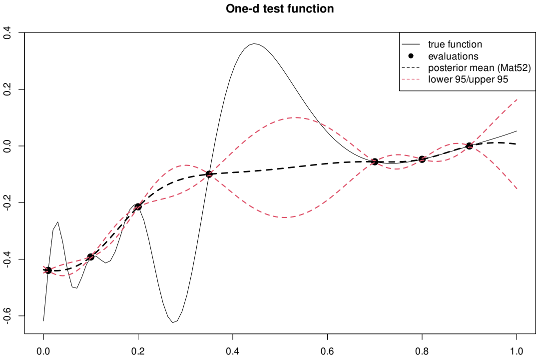
Bayesian optimization

Objective:

find global optimum

Tools:

GP predictions

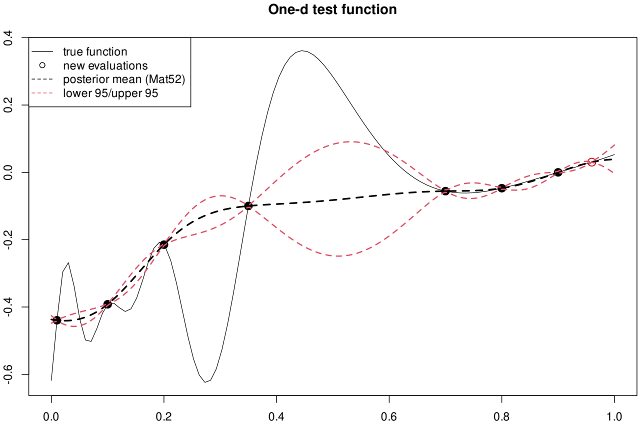


Questions:

1. where should we evaluate the function next?
2. what can we use to guide our exploration?

How to find the maximum?

First strategy: $\mathbf{x}_{n+1} \in \arg\max_{\mathbf{x} \in D} m_n(\mathbf{x})$ (maximizer of posterior mean)



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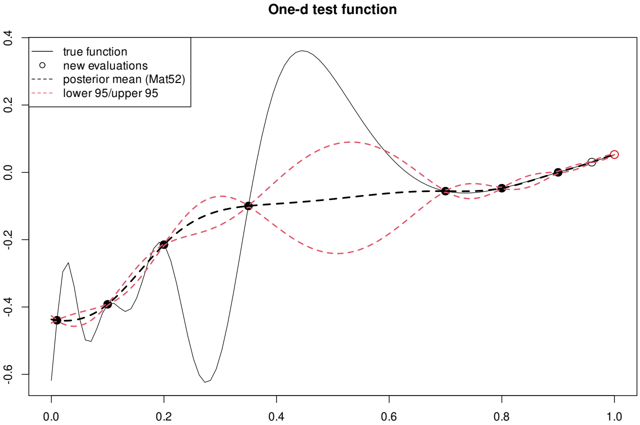

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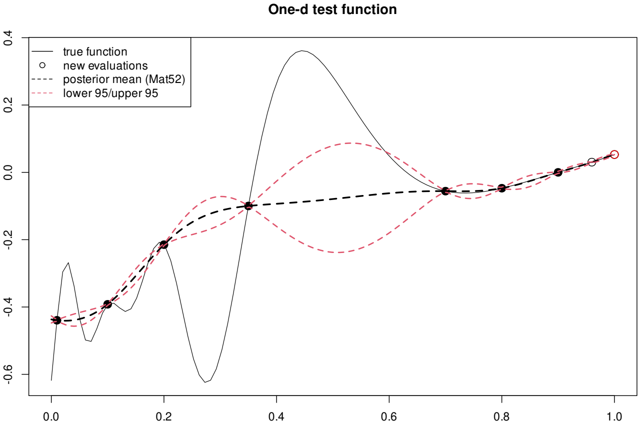

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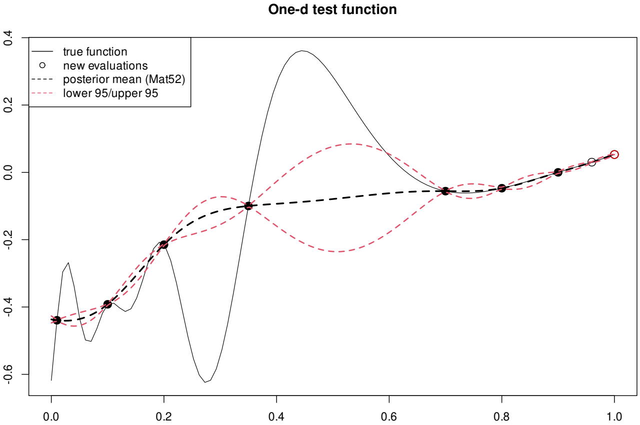

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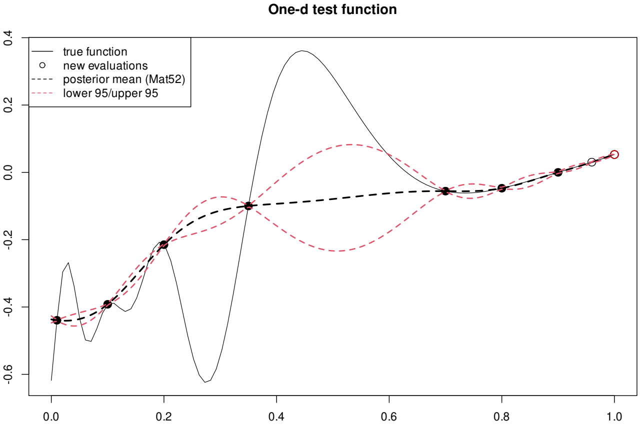
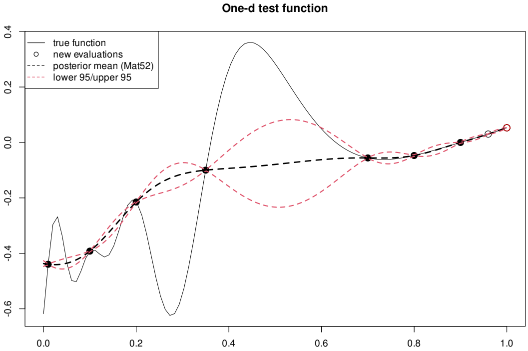


Looking for a better strategy

Consider the final GP fit with our previous strategy



We have predictive posterior **mean** m_n and **variance** s_n, *use both?*

Looking for a better strategy

If our next evaluation is

- point with **highest variance:** MSE criterion,
  pure exploration: we will improve the model everywhere

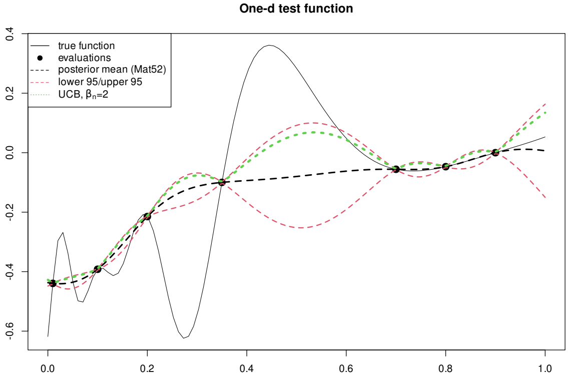
- point with **highest mean:** criterion above,
  pure exploitation: we believe that the current model is good enough

Idea: combine **exploitation** ($\max m_n$) and **exploration** ($\max s_n$)

How can we combine m_n and s_n?

Upper Confidence Bound: $\mathbf{x}_{n+1} \in \arg\max_{\mathbf{x} \in D} UCB_n(\mathbf{x})$,

$$UCB_n(\mathbf{x}) = m_n(\mathbf{x}) + \beta_n s_n(\mathbf{x})$$



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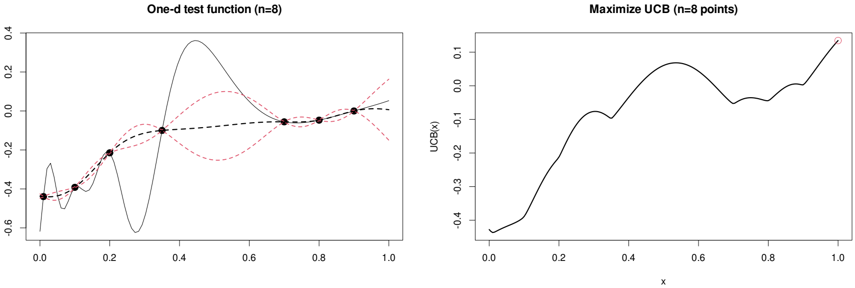

Here: $\beta_n = 2$, for all n.

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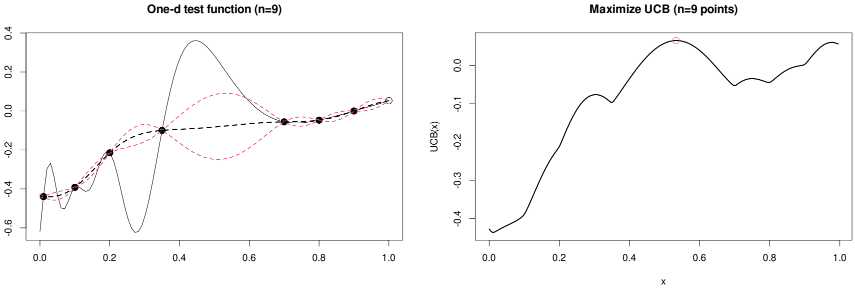

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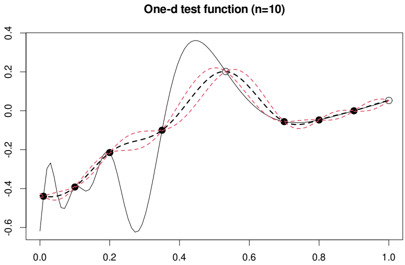

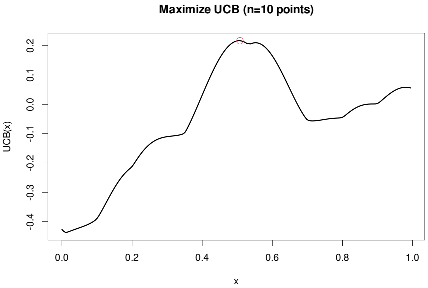

Here: $\beta_n = 2$, for all n.

Upper Confidence Bound

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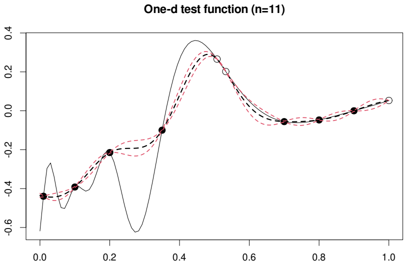

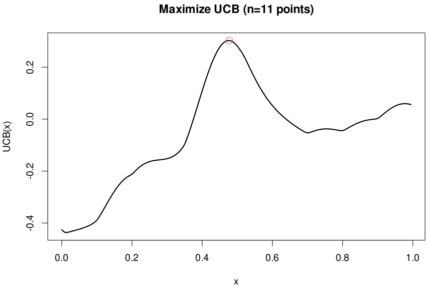

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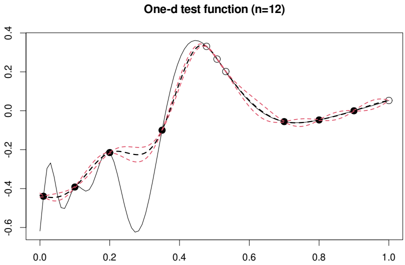

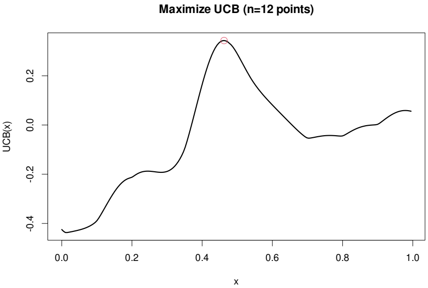

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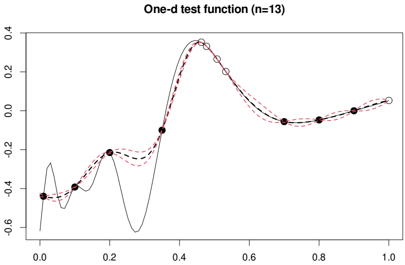
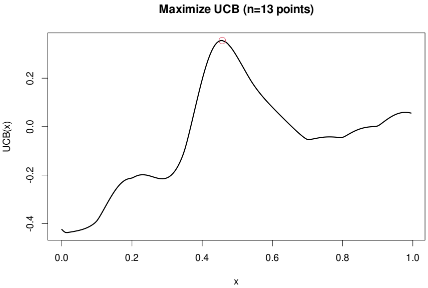




Here: $\beta_n = 2$, for all n.

Cumulative regret - a theoretical framework

- $\mathbf{x}^\star \in \arg\max_{\mathbf{x}\in D} f(\mathbf{x})$ (true maximizer of unknown function)
- **regret** at step n, $r_n = f(\mathbf{x}^\star) - f(\mathbf{x}_n)$;
  Note: $f(\mathbf{x}^\star)$ is unknown, so r_n is not computable.
- **cumulative regret:** $R_N = \sum_{n=1}^{N} r_n$

Regret and cumulative regret are tools used to

- build BO algorithms;
- analyze theoretical convergence of BO algorithms.

Upper Confidence Bound acquisition function

Properties

- Easy to implement: only requires m_n, s_n and β_n;
- Acquisition function easy to optimize;
- with variable β_n, provable convergence results
  (Simplest case: f assumed a GP sample on D,
  $\beta_n = 2\log(|D|n^2\pi^2/5\delta)$, γ_n maximum information gain
  then $R_N \leq \sqrt{C_1 N \beta_N \gamma_N}$ with high probability)

Srinivas N., Krause A., Kakade S., and Seeger M. (2010). *Gaussian process optimization in the bandit setting: no regret and experimental design.* ICML'10.

Another point of view: maximizing improvement

Denote by $t_n = \max_{i=1}^n f(\mathbf{x}_i)$, the current maximum of the evaluations.

At step n**:** we evaluate at $\mathbf{x}_{n+1}$, then

- if $f(\mathbf{x}_{n+1}) \geq t_n \Rightarrow f(\mathbf{x}_{n+1})$ is the new maximum;
- if $f(\mathbf{x}_{n+1}) \leq t_n \Rightarrow t_n$ is the maximum

The *improvement* brought by the new evaluation is
$\max(f(\mathbf{x}_{n+1}) - t_n, 0) := (f(\mathbf{x}_{n+1}) - t_n)_+$

Issue: at step n we don't know $f(\mathbf{x}_{n+1})$!

Expected improvement

Idea: use the GP assumption: $Z \sim GP(0, k)$ is a prior for f.

We obtain the random quantities $Z_{\mathbf{x}_{n+1}}$ and $T_n = \max_{i=1}^{n} Z_{\mathbf{x}_i}$ and

Expected improvement: $\mathbb{E}_n[(Z_{\mathbf{x}_{n+1}} - T_n)_+] = \mathbb{E}[(Z_{\mathbf{x}_{n+1}} - T_n)_+ | \mathcal{D}_n]$

T_n is known so we can define the acquisition function

$$EI_n(\mathbf{x}) = \mathbb{E}_n[(Z_{\mathbf{x}} - t_n)_+]$$

Močkus J. (1975) *On bayesian methods for seeking the extremum.* In: Marchuk G.I. (eds) Optimization Techniques IFIP Technical Conference Novosibirsk, July 1–7, 1974.

Jones, D. R., Schonlau, M., Welch, W. J. (1998). *Efficient global optimization of expensive black-box functions.* Journal of Global Optimization, 13(4), 455–492.

Expected improvement acquisition function

Expected improvement: $EI_n(\mathbf{x}) = \mathbb{E}_n[(Z_\mathbf{x} - t_n)_+]$.

There is analytical expression for the conditional expectation

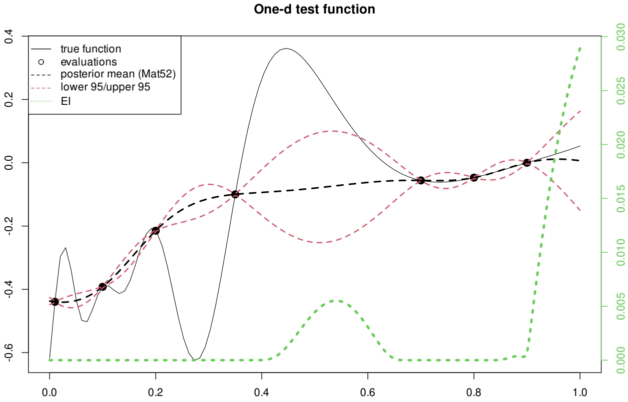
$$EI_n(\mathbf{x}) = \begin{cases} (u_n(\mathbf{x}))_+ & \text{if } s_n(\mathbf{x}) = 0 \\ (u_n(\mathbf{x}))_+ - |u_n(\mathbf{x})|\Phi\left(\frac{u_n(\mathbf{x})}{s_n(\mathbf{x})}\right) + s_n(\mathbf{x})\phi\left(\frac{u_n(\mathbf{x})}{s_n(\mathbf{x})}\right) & \text{else.} \end{cases}$$

Where $u_n(\mathbf{x}) = m_n(\mathbf{x}) - t_n$, $\Phi(\cdot)$ CDF of $N(0,1)$, $\phi(\cdot)$ PDF of $N(0,1)$.

Key take-away: EI one-step ahead can be computed with just m_n, s_n, t_n.

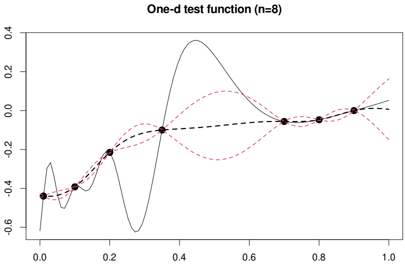
Expected improvement

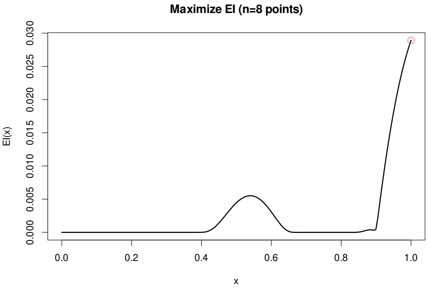
Consider our 1-d example, what is $EI(\mathbf{x})$?



Expected improvement

EI: $\mathbf{x}_{n+1} \in \arg\max_{\mathbf{x}\in D} EI_n(\mathbf{x}), \qquad EI_n(\mathbf{x}) = \mathbb{E}_n[(Z_{\mathbf{x}} - t_n)_+]$





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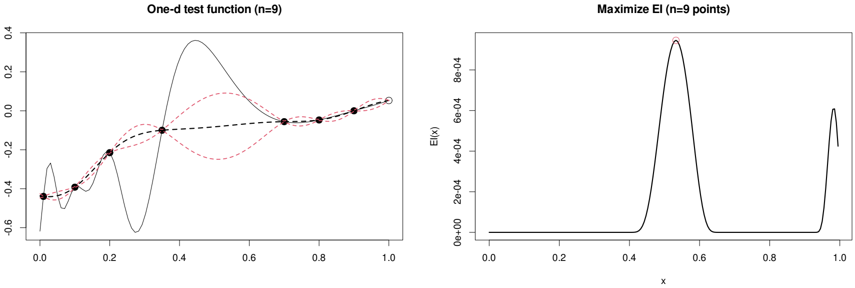

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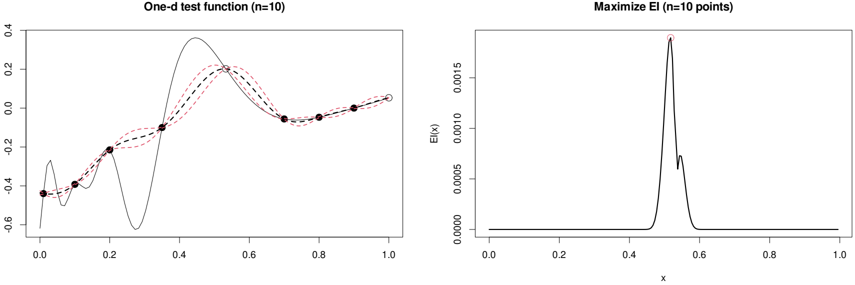

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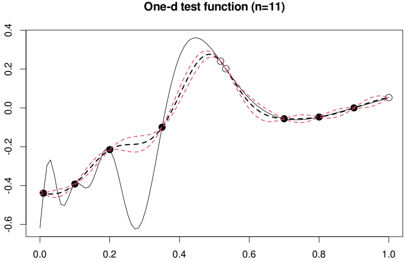

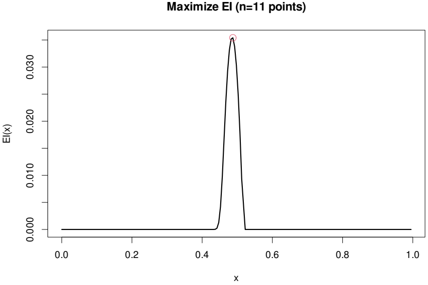

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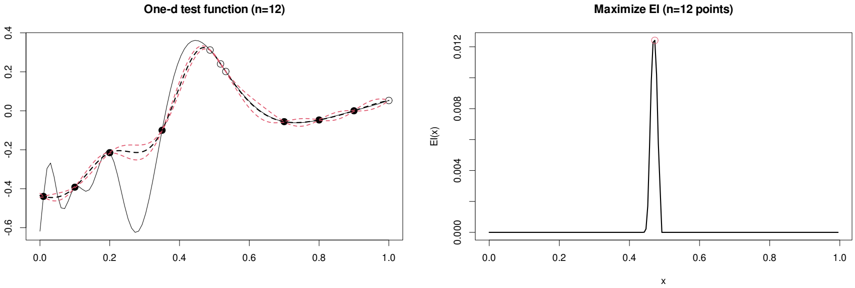

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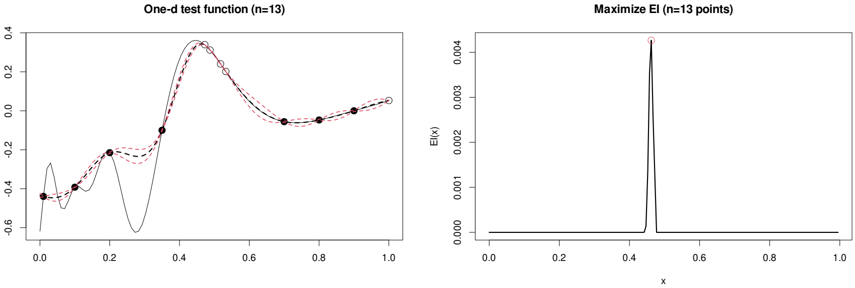


Expected improvement - Properties

The acquisition function EI_n

- non-negative, vanishes at evaluations;
- generally not convex/concave and highly multi-modal;
- regularity driven by k_n;
- under technical condition on k and f, EI fills the space;
- convergence for EI recently proven in Bect et al. (2019).

Bect J., Bachoc F., Ginsbourger D. (2019) *A supermartingale approach to Gaussian process based sequential design of experiments.* Bernoulli 25 (4A) 2883 - 2919.

Expected improvement - Limits and extensions

Only one step ahead? $EI_n(\mathbf{x})$ provides the **next** evaluation $\mathbf{x}_{n+1}$.

Can we have a **batch** of q evaluations at each step?

Parallel (multi-point) EI: analytical formulae for multi-point EI (See Ginsbourger et al. (2010), Chevalier, Ginsbourger (2013), Marmin et al. (2015))

Noisy evaluations: up until now observations $y_i = f(\mathbf{x}_i) \Rightarrow$ no noise.

What if $y_i = f(\mathbf{x}_i) + \epsilon_i$?

EI and noisy observations

Data: $y_i = f(\mathbf{x}_i) + \epsilon_i$ with $\epsilon_i \sim N(0, \sigma_n^2)$, $\sigma_n^2 > 0$.

Recall:

$$EI_n(\mathbf{x}) = \mathbb{E}_n[(\overbrace{Z_{\mathbf{x}}}^{\text{not reachable}} - \overbrace{\max_{i=1}^{n} Z_{\mathbf{x}_i}}^{\text{not known}})_+]$$

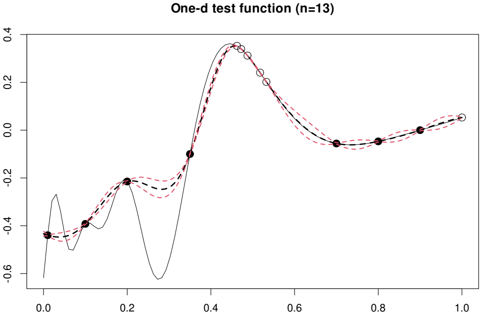
Possible fixes:

- **plug-in:** EI with highest expected value of the observed points.
- **Expected Quantile Improvement:** measure improvement on quantiles. "Best" point at highest quantile. See Picheny et al. (2013).

Acquisition function that handles well noise is **knowledge gradient**.

Knowledge gradient - a different point of view

EI: “best point” $=$ highest **evaluated** point;



Another option: return a non evaluated point

Example: $\hat{\mathbf{x}} = \arg\max_{\mathbf{x}\in D} m_n(\mathbf{x})$

Knowledge gradient - a different "improvement":

"Best" point determined as $\hat{\mathbf{x}} = \arg\max_{\mathbf{x} \in D} m_n(\mathbf{x})$

at step n "best value" $m_n^\star = m_n(\hat{\mathbf{x}})$

at step $n+1$ $m_{n+1}^\star = \max_{\mathbf{x} \in D} m_{n+1}(\mathbf{x})$

(random and unknown until $\mathbf{x}_{n+1}$ given)

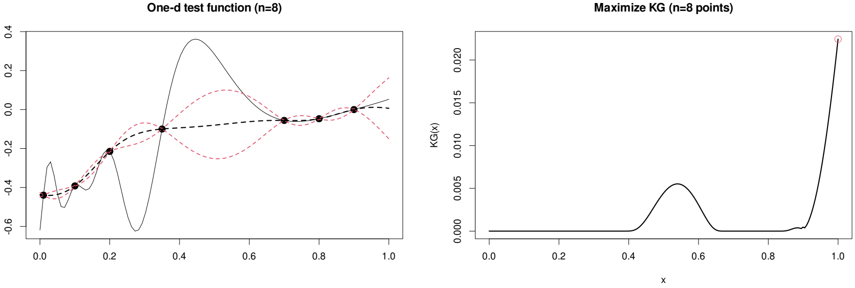
We would like $\mathbf{x}_{n+1}$ that maximizes $m_{n+1}^\star - m_n^\star$

Knowledge gradient: $KG(\mathbf{x}) = \mathbb{E}_n[m_{n+1}^\star - m_n^\star | \mathbf{x}_{n+1} = \mathbf{x}]$

Frazier P., Powell W., Dayanik S., (2009) *The Knowledge-Gradient Policy for Correlated Normal Beliefs.* INFORMS Journal on Computing 21(4):599-613.

Knowledge gradient

KG: $\mathbf{x}_{n+1} \in \arg\max_{\mathbf{x}\in D} KG_n(\mathbf{x}), \qquad KG_n(\mathbf{x}) = \mathbb{E}_n[m^\star_{n+1} - m^\star_n | \mathbf{x}_{n+1} = \mathbf{x}]$



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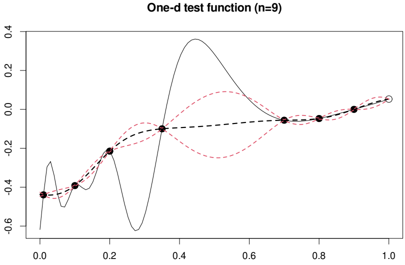

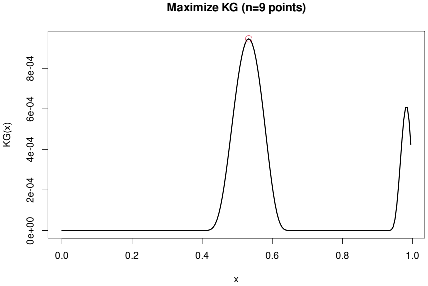

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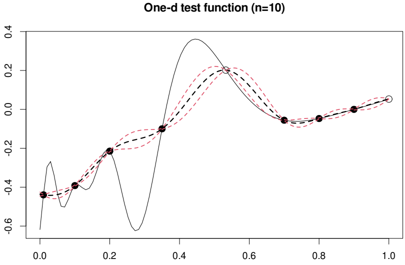

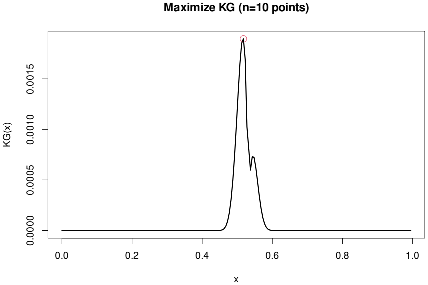

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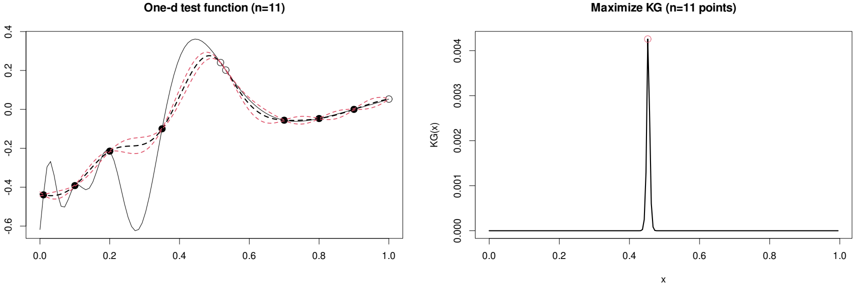

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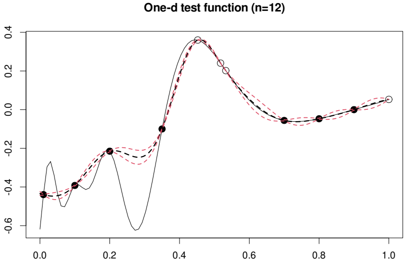

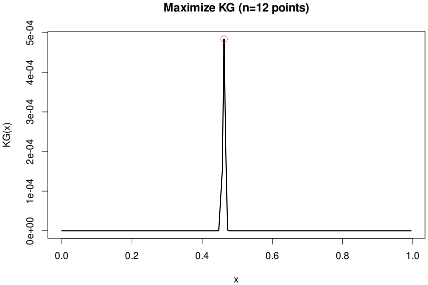

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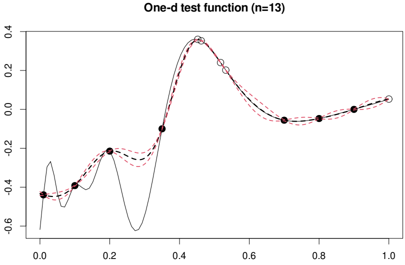
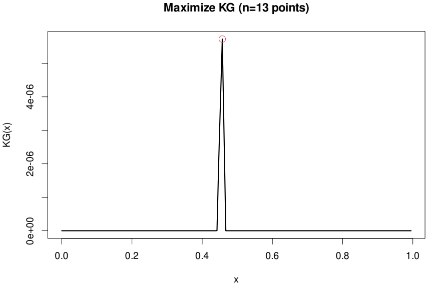
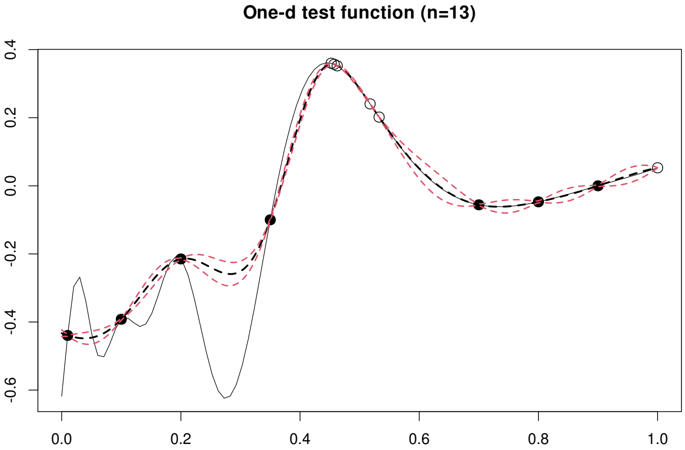




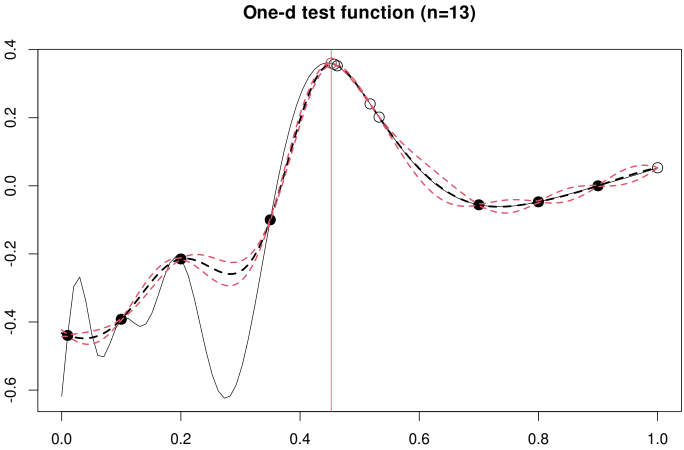
Knowledge gradient - final iteration

Where is our maximum?



Knowledge gradient - final iteration

Where is our maximum? **Recall:** best point is $\arg\max_{\mathbf{x}\in D} m_n(\mathbf{x})$



Knowledge gradient - further details

Computation: $KG_n(\mathbf{x})$ can be computed

- via simulation (Frazier et al. 2009)
- multi-start stochastic gradient ascent (more efficient, see Wu and Frazier (2016))
- parallelizable (see Wu and Frazier (2016))

Noisy evaluations

- *KG* does not use directly function evaluations
- on noisy functions showed good performances

Wu, J. and Frazier, P. (2016). *The parallel knowledge gradient method for batch Bayesian optimization.* In Advances in Neural Information Processing Systems.

Quick and partial summary on BO

	Pros	Cons
UCB	+ fast to implement	- no one-step optimality
	+ convergence guarantees	
EI	+ one-step optimal	- not adapted to noisy data
	+ convergence guarantees	
KG	+ one-step optimal	- no convergence guarantee
	+ handle noisy data	

Further topics not covered here

Other notable strategies: Thomson sampling, Entropy sampling, Predictive entropy sampling, ...

Constrained optimization

Multi-fidelity optimization

Non-myopic strategies

High-dimensional BO

Gray-box (using derivative information on f)

A very nice tutorial

Frazier P. (2018). *A Tutorial on Bayesian Optimization.* arXiv:1807.02811 [stat.ML]

Partial list of software

Python: BOtorch (pytorch), GPflowOpt (tensorflow), Cornell-MOE, GPyOpt(end of life),Spearmint (no longer actively maintained)

R: DiceOptim, laGP

Matlab: DACE (no longer actively maintained)

References (1)

Srinivas N., Krause A., Kakade S., and Seeger M. (2010). *Gaussian process optimization in the bandit setting: no regret and experimental design.* ICML'10.

Močkus J. (1975) *On bayesian methods for seeking the extremum.* In: Marchuk G.I. (eds) Optimization Techniques IFIP Technical Conference Novosibirsk, July 1–7, 1974.

Jones, D. R., Schonlau, M., Welch, W. J. (1998). *Efficient global optimization of expensive black-box functions.* Journal of Global Optimization, 13(4), 455–492.

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Bect J., Bachoc F., Ginsbourger D. (2019) *A supermartingale approach to Gaussian process based sequential design of experiments.* Bernoulli 25 (4A) 2883 - 2919.

References (2)

Marmin S., Chevalier C., Ginsbourger D. (2015) *Differentiating the Multipoint Expected Improvement for Optimal Batch Design.* In: Machine Learning, Optimization, and Big Data. MOD 2015.

Picheny V., Ginsbourger D., Richet Y., Caplin G. (2013) *Quantile-Based Optimization of Noisy Computer Experiments With Tunable Precision.* Technometrics, 55:1, 2-13

Frazier P., Powell W., Dayanik S., (2009) *The Knowledge-Gradient Policy for Correlated Normal Beliefs.* INFORMS Journal on Computing 21(4):599-613.

Wu, J. and Frazier, P. (2016). *The parallel knowledge gradient method for batch Bayesian optimization.* In Advances in Neural Information Processing Systems.

Outline

The framework

Consider now $\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \in T\} = f^{-1}(T)$
where $D \subset \mathbb{R}^d$ is compact, $f : D \longrightarrow \mathbb{R}$ is continuous, $T \subset \mathbb{R}$.

Particular case: $T = (-\infty, t]$ for a fixed $t \in \mathbb{R}$.
$\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \leq t\}$ is the excursion set of f below t.

Objectives

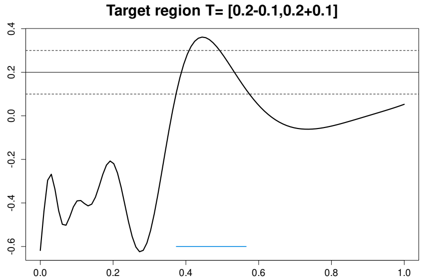
Starting from evaluations of f at $\mathbf{X}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset D$

- Obtain a good regression model for values of f in $[t - \epsilon, t + \epsilon]$
- Estimate the volume of $\Gamma^\star$, $\alpha_\mu = \mu(\Gamma^\star)$ and reduce its uncertainty.
- Estimate $\Gamma^\star$ and quantify uncertainty on it

Example

Consider the function f and

$$\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \in T\} = f^{-1}(T)$$



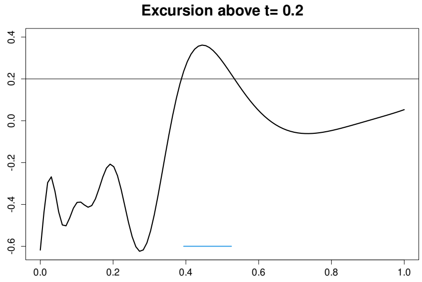
- target region: $T = [t - \epsilon, t + \epsilon]$, $t = 0.2$, $\epsilon = 0.1$;
- excursion region

  $T = [t, +\infty)$, $t = 0.2$.

Example

Consider the function f and

$$\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \in T\} = f^{-1}(T)$$



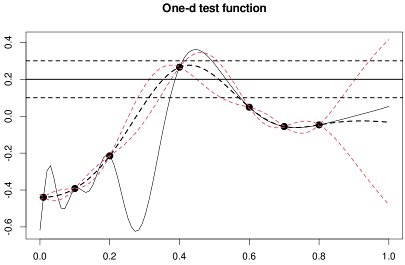
- target region: $T = [t - \epsilon, t + \epsilon]$, $t = 0.2$, $\epsilon = 0.1$;
- excursion region

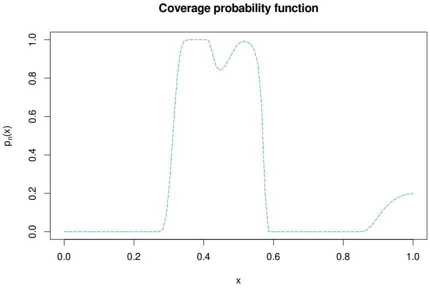
  $T = [t, +\infty)$, $t = 0.2$.

The coverage probability function - target region case

GP model $(Z_{\mathbf{x}})_{\mathbf{x}\in D} \sim GP(m, k)$ and n evaluations $\mathbf{y}_n$ at points $\mathbf{X}_n$.
The **(posterior) coverage probability function** is

$$p_{n,t,\epsilon}(\mathbf{x}) = P(\mathbf{x} \in \Gamma | Z_{\mathbf{X}_n} = \mathbf{y}_n) = \Phi\left(\frac{t+\epsilon-m_n(\mathbf{x})}{\sqrt{k_n(\mathbf{x},\mathbf{x})}}\right) - \Phi\left(\frac{t-\epsilon-m_n(\mathbf{x})}{\sqrt{k_n(\mathbf{x},\mathbf{x})}}\right)$$

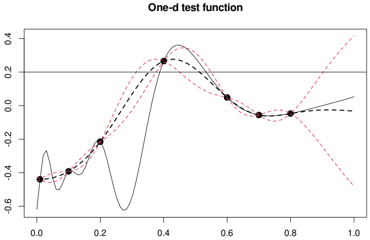


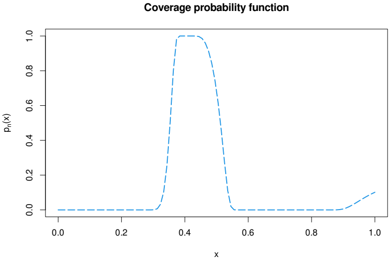


The coverage probability function - excursion case

GP model $(Z_{\mathbf{x}})_{\mathbf{x}\in D} \sim GP(m,k)$ and n evaluations $\mathbf{y}_n$ at points $\mathbf{X}_n$.
The **(posterior) coverage probability function** is

$$p_n(\mathbf{x}) = P(\mathbf{x} \in \Gamma | Z_{\mathbf{X}_n} = \mathbf{y}_n) = \Phi\left(\frac{m_n(\mathbf{x}) - t}{\sqrt{k_n(\mathbf{x},\mathbf{x})}}\right)$$





Stepwise Uncertainty Reduction (SUR) framework

Start: initial design $\mathbf{X}_n$, $\mathbf{y}_n = f(\mathbf{X}_n)$, prior model $(Z_\mathbf{x})_{\mathbf{x} \in D} \sim GP(m, k)$.

1. First model for f from posterior mean of $Z_\mathbf{x}$ given $Z_{\mathbf{X}_n} = \mathbf{y}_n$
2. define uncertainty measure H_n
3. next evaluation $\mathbf{x}_{n+1}$ as the minimizer of expected future uncertainty ($\mathbf{x}_{n+1} \in \arg\min_\mathbf{x} \mathbb{E}_n[H_{n+1} \mid \mathbf{x}_{n+1} = \mathbf{x}]$)
4. update the model
5. repeat steps 2-4 until convergence or until computational budget is exhausted.

Target region exploration - targeted IMSE

Define the targeted IMSE with target t and tolerance ϵ as

$$H_n^{tIMSE} = \mathbb{E}_n[\int_D MSE_n(\mathbf{u})\mathbf{1}_{[t-\epsilon,t+\epsilon]}(Z_{\mathbf{u}})\mu(d\mathbf{u})]$$
$$= \int_D k_n(\mathbf{u},\mathbf{u})p_{n,t,\epsilon}(\mathbf{u})\mu(d\mathbf{u})$$

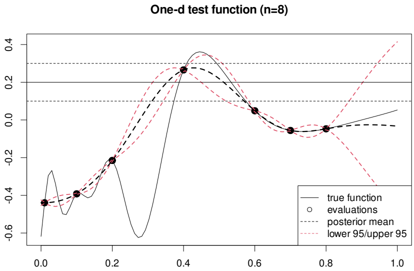
The corresponding criterion is

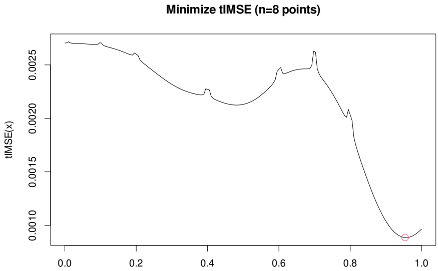
$$J_n^{tIMSE}(\mathbf{x}) = \mathbb{E}_n[\int_D k_{n+1,\mathbf{x}_{n+1}}(\mathbf{u},\mathbf{u})p_{n,t,\epsilon}(\mathbf{u})\mu(d\mathbf{u}) \mid \mathbf{x}_{n+1} = \mathbf{x}]$$

Picheny V., Ginsbourger D., Roustant O., Haftka R.T., Kim N. (2010). *Adaptive Designs of Experiments for Accurate Approximation of a Target Region.* ASME. J. Mech. Des. 132(7):071008-071008-9.

targeted IMSE - Example

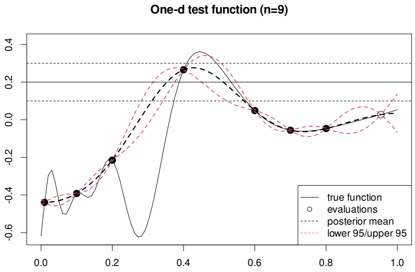
Initial design $n = 7$, add 10 points.

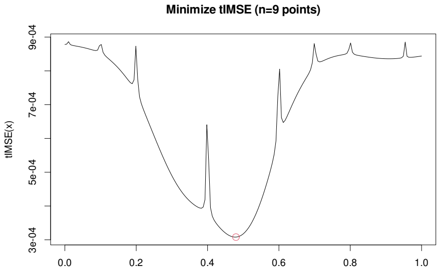




targeted IMSE - Example

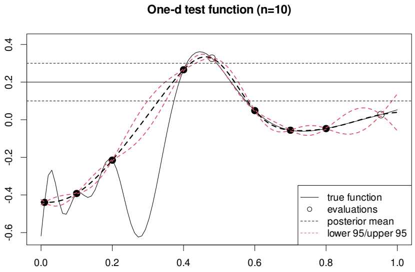
Initial design $n = 7$, add 10 points.

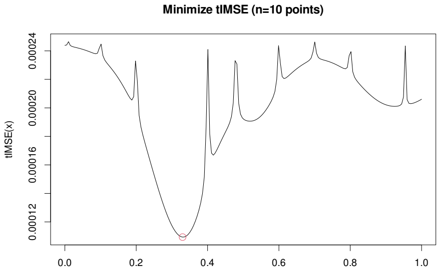




targeted IMSE - Example

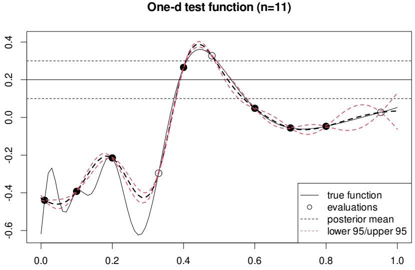
Initial design $n = 7$, add 10 points.

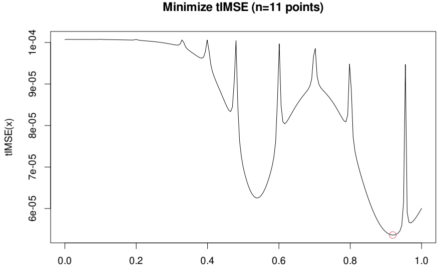




targeted IMSE - Example

Initial design $n = 7$, add 10 points.





targeted IMSE - Example

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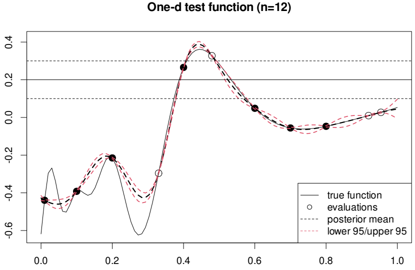
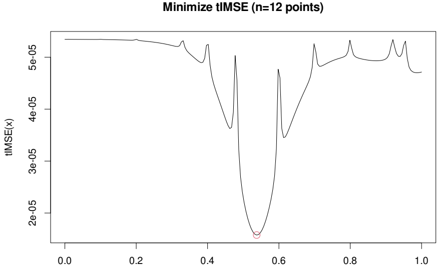
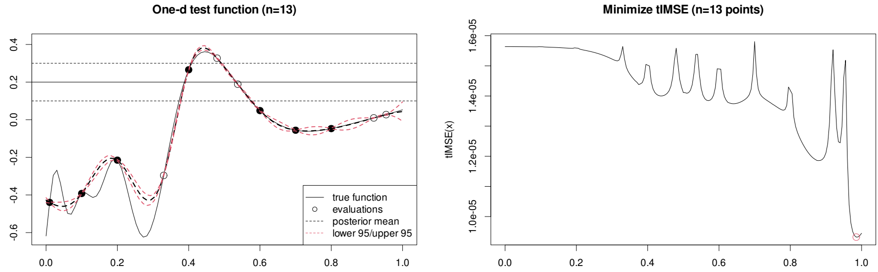




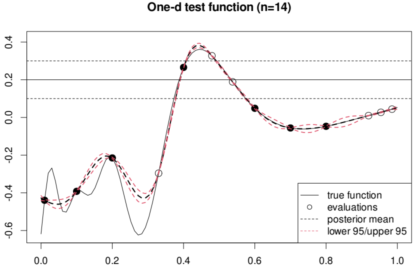
targeted IMSE - Example

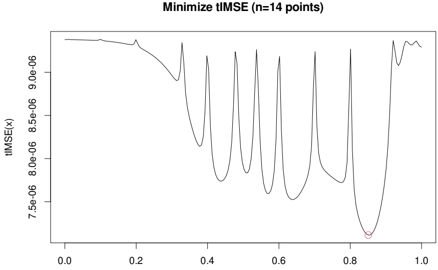
Initial design $n = 7$, add 10 points.



targeted IMSE - Example

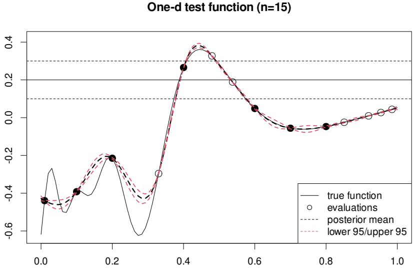
Initial design $n = 7$, add 10 points.

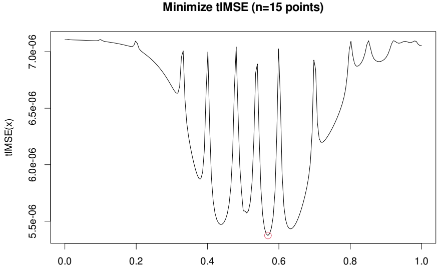




targeted IMSE - Example

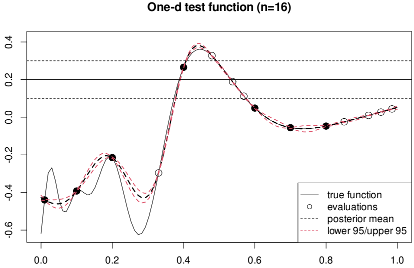
Initial design $n = 7$, add 10 points.

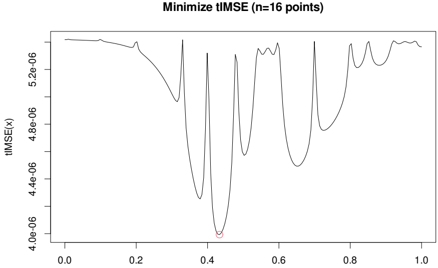




targeted IMSE - Example

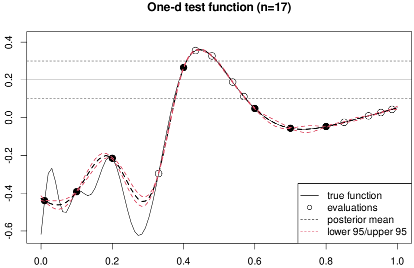
Initial design $n = 7$, add 10 points.

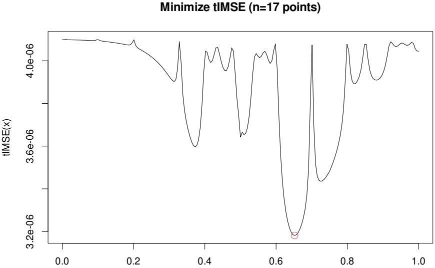




targeted IMSE - Example

Initial design $n = 7$, add 10 points.





The measure of excursion as proxy

Consider now the problem of estimating the set

$$\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \geq t\}.$$

Bayesian approach: f is a realization of a GP $(Z_\mathbf{x})_{\mathbf{x} \in D}$, then $\Gamma^\star$ is a realization of $\Gamma = \{\mathbf{x} \in D : Z_\mathbf{x} \geq t\}$

Interesting feature: measure of the set

Finite measure μ on D, a proxy for the set is $\alpha = \mu(\Gamma^\star)$,
For Γ (random), estimate it with

$$\widehat{\alpha} = \mathbb{E}_n[\mu(\Gamma)] = \int_D p_n(\mathbf{u})\mu(d\mathbf{u})$$

Uncertainty: variance of excursion volume

Uncertainty on $\widehat{\alpha} = \mathbb{E}_n[\mu(\Gamma)]$ can be measured with $\mathrm{var}_n[\mu(\Gamma)]$

$$\mathrm{var}_n[\mu(\Gamma)] = \mathbb{E}_n[\left(\int_D \mathbf{1}_\Gamma(\mathbf{u}) - p_n(\mathbf{u})\mu(d\mathbf{u})\right)^2]$$

$$\leq \mu(D)\mathbb{E}_n[\int_D (\mathbf{1}_\Gamma(\mathbf{u}) - p_n(\mathbf{u}))^2 \mu(d\mathbf{u})]$$

$$\leq \mu(D)\int_D p_n(\mathbf{u})(1 - p_n(\mathbf{u}))\mu(d\mathbf{u})$$

Uncertainty measures

$H_n^\Gamma = \int_D p_n(\mathbf{u})(1 - p_n(\mathbf{u}))\mu(d\mathbf{u})$, integrated Bernoulli variance;

$H_n^{(\alpha)} = \mathrm{var}_n[\mu(\Gamma)]$, variance of excursion volume.

Criterion: integrated Bernoulli variance

The integrated Bernoulli variance uncertainty naturally provides a criterion for a sequential design

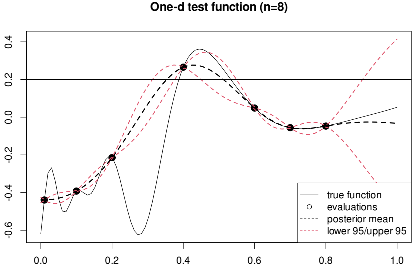
$$
\begin{aligned}
J_n^{\Gamma}(\mathbf{x}) &= \mathbb{E}_n[H_{n+1}^{\Gamma} | \mathbf{x}_{n+1} = \mathbf{x}] \\
&= \mathbb{E}_n\left[\int_D p_{n+1,\mathbf{x}_{n+1}}(\mathbf{u})(1 - p_{n+1,\mathbf{x}_{n+1}}(\mathbf{u}))\mu(d\mathbf{u}) \mid \mathbf{x}_{n+1} = \mathbf{x}\right] \\
&= \int_D \Phi_2\left(\begin{pmatrix} a(\mathbf{u}) \\ -a(\mathbf{u}) \end{pmatrix}; \begin{pmatrix} c(\mathbf{u}) & 1 - c(\mathbf{u}) \\ 1 - c(\mathbf{u}) & c(\mathbf{u}) \end{pmatrix}\right)\mu(d\mathbf{u})
\end{aligned}
$$

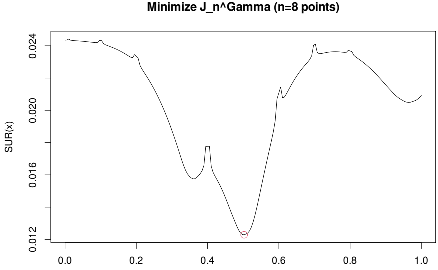
where $a(\mathbf{u}) = \frac{m_n(\mathbf{u}) - t}{\sqrt{k_{n+1}(\mathbf{u})}}$, $c(\mathbf{u}) = k_n(\mathbf{u})/k_{n+1}(\mathbf{u})$.

Bect, J., Ginsbourger, D., Li, L., Picheny, V., and Vazquez, E. (2012). *Sequential design of computer experiments for the estimation of a probability of failure.* Stat. Comput., 22 (3):773–793.

Integrated Bernoulli variance

Initial design $n = 7$, add 10 points.





Integrated Bernoulli variance

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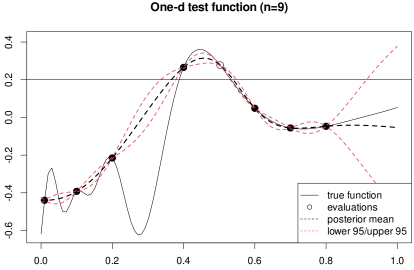

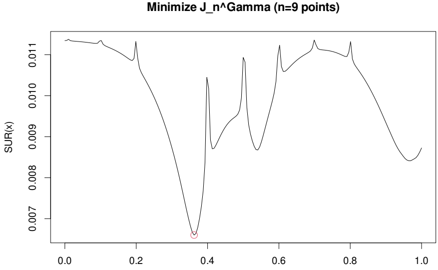

Integrated Bernoulli variance

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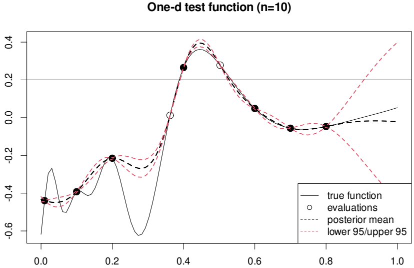

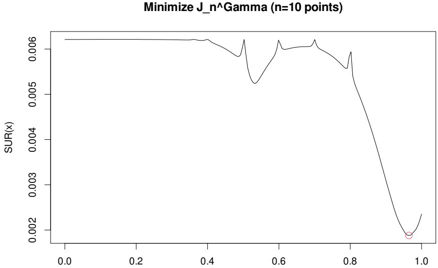

Integrated Bernoulli variance

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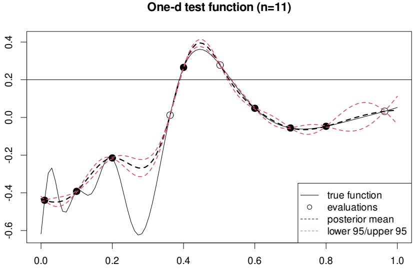

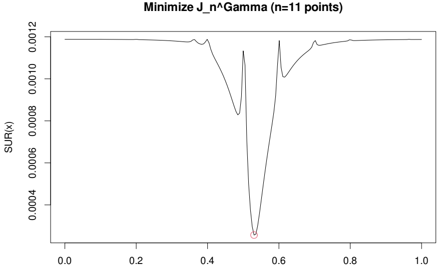

Integrated Bernoulli variance

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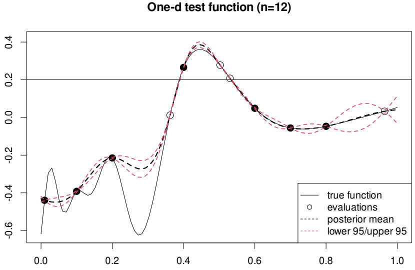

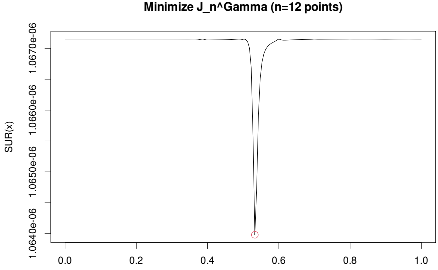

Integrated Bernoulli variance

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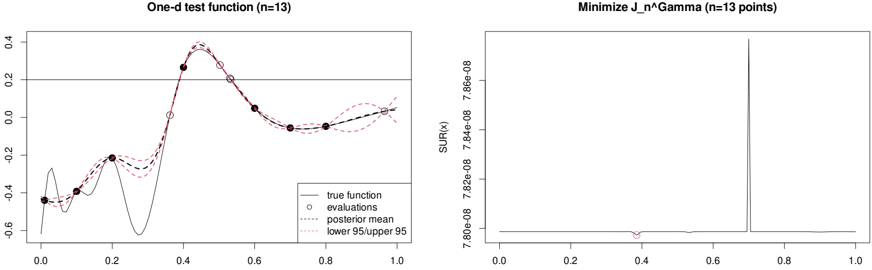

Integrated Bernoulli variance

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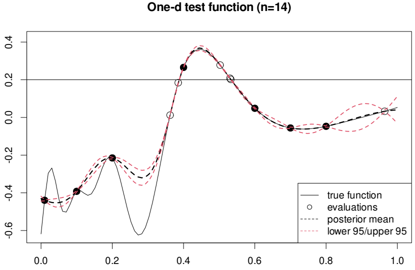

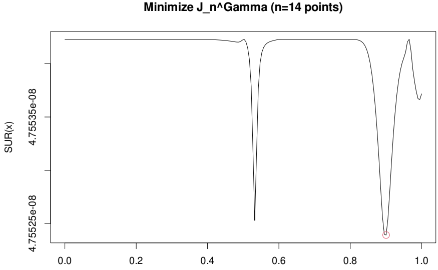

Integrated Bernoulli variance

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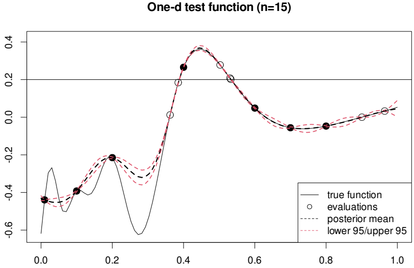

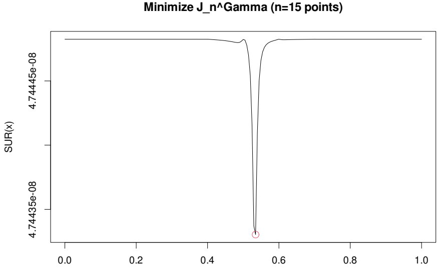

Integrated Bernoulli variance

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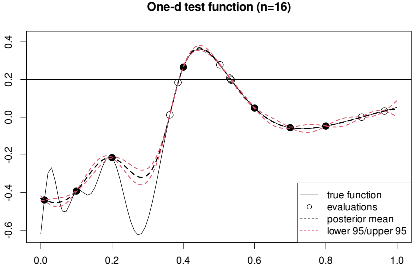

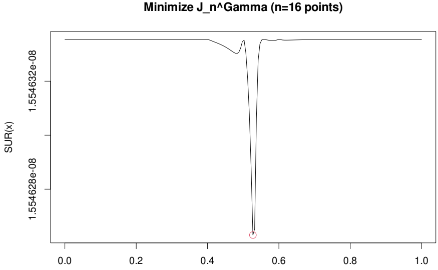

Integrated Bernoulli variance

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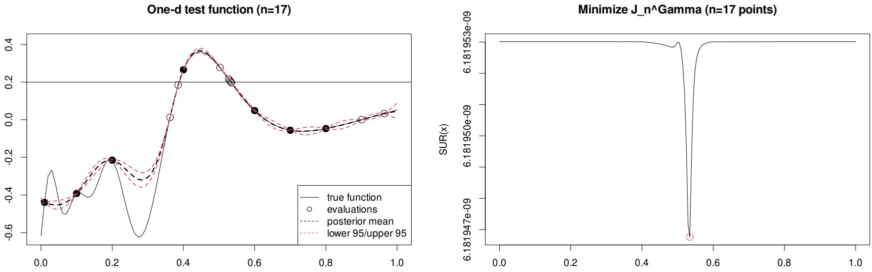


Criterion: variance of excursion volume

The variance of the excursion volume also defines a criterion

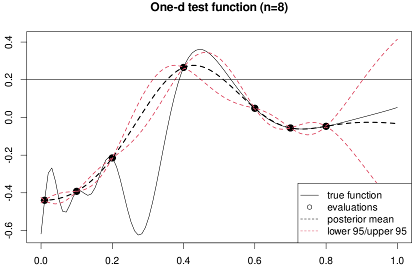
$$
\begin{aligned}
J_n^{(\alpha)}(\mathbf{x}) &= \mathbb{E}_n[H_{n+1}^{(\alpha)} | \mathbf{x}_{n+1} = \mathbf{x}] \\
&= \mathbb{E}_n\left[\mathrm{var}_{n+1}[\mu(\Gamma)] \mid \mathbf{x}_{n+1} = \mathbf{x}\right] \\
&= \gamma_n - \int_{D\times D} \Phi_2\left(\begin{pmatrix} a(\mathbf{u}_1) \\ a(\mathbf{u}_2) \end{pmatrix}; \begin{pmatrix} c(\mathbf{u}_1) & d(\mathbf{u}_1, \mathbf{u}_2) \\ d(\mathbf{u}_1, \mathbf{u}_2) & c(\mathbf{u}_2) \end{pmatrix}\right) \mu(d\mathbf{u}_1)\mu(d\mathbf{u}_2)
\end{aligned}
$$

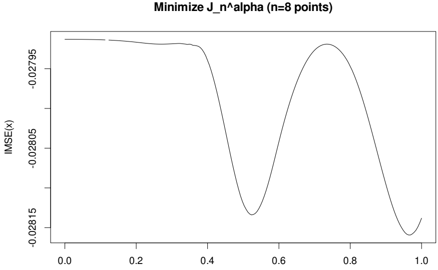
where $a(\mathbf{u}) = \frac{m_n(\mathbf{u}) - t}{\sqrt{k_{n+1}(\mathbf{u})}}$, $c(\mathbf{u}) = k_n(\mathbf{u})/k_{n+1}(\mathbf{u})$,
$d(\mathbf{u}_1, \mathbf{u}_2) = k_n(\mathbf{u}_1, \mathbf{x}_{n+1}) k_n(\mathbf{u}_2, \mathbf{x}_{n+1}) / k_n(\mathbf{x}_{n+1}, \mathbf{x}_{n+1})$

Chevalier, C., Bect, J., Ginsbourger, D., Vazquez, E., Picheny, V. and Richet, Y. (2013). *Fast parallel kriging-based stepwise uncertainty reduction with application to the identification of an excursion set.* Technometrics, 56 (4):455–465.

Variance of excursion volume

Initial design $n = 7$, add 5 points.





Variance of excursion volume

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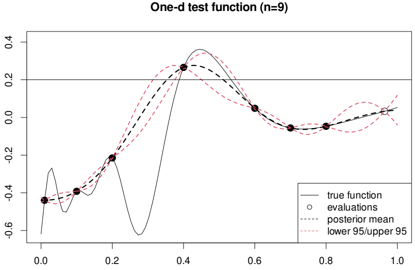
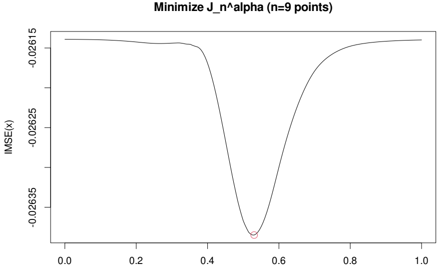
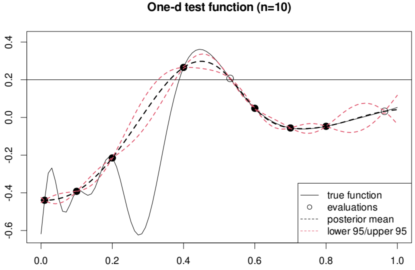
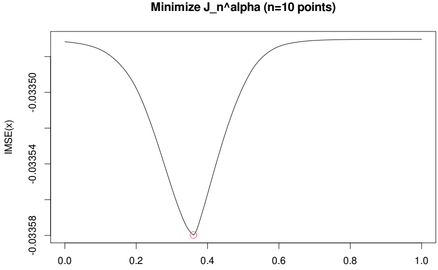




Variance of excursion volume

Initial design $n = 7$, add 5 points.





Variance of excursion volume

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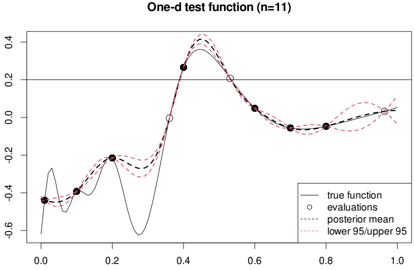

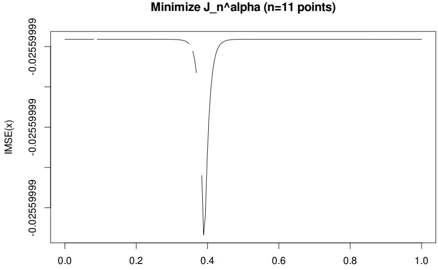

Variance of excursion volume

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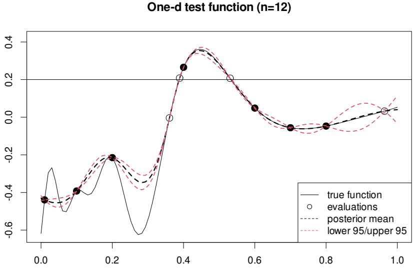

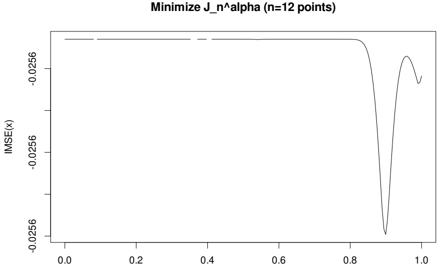

Variance of excursion volume

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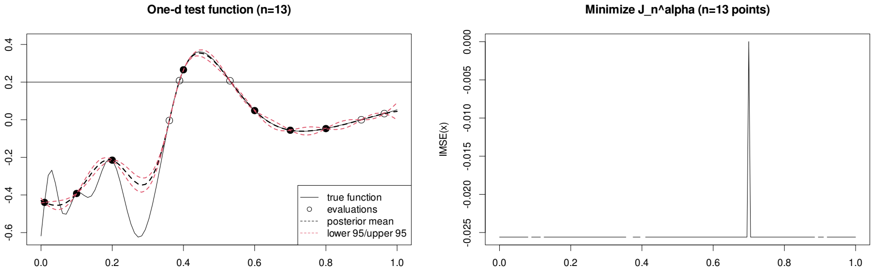
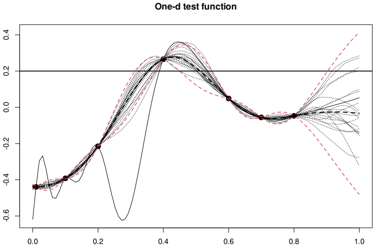


Outline

A prior on the space of functions

Assume: f realization of $(Z_{\mathbf{x}})_{\mathbf{x}\in D}$, Gaussian Random Field (GRF)



Prior: $(Z_{\mathbf{x}})_{\mathbf{x}\in D}$ with

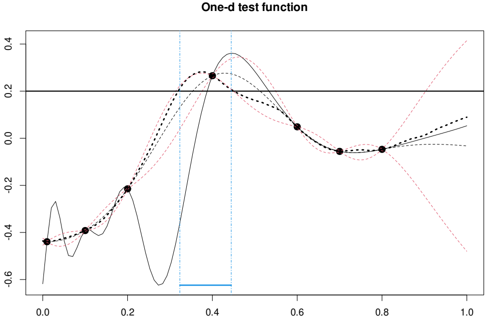
- a.s. continuous paths;
- Matérn covariance kernel k ($\nu = 5/2$);
- constant mean function m.

Given $n = 7$ evaluations $\mathbf{z}_n$ at $\mathbf{X}_n$

We can generate realizations of the **posterior field**.

Distribution of excursion sets

The posterior field induces a posterior distribution on excursion sets.



Note that

- Z continuous paths;
- $[t, +\infty)$ is a closed set.

The set $\Gamma = \{\mathbf{x} \in D : Z_{\mathbf{x}} \geq t\}$ is a random closed set.

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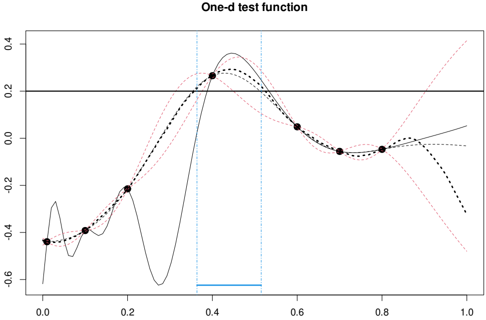

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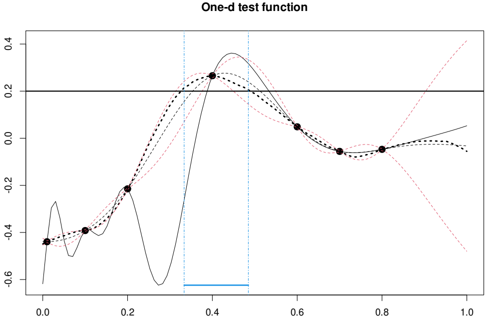

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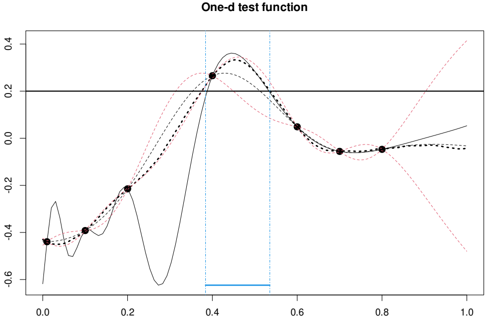

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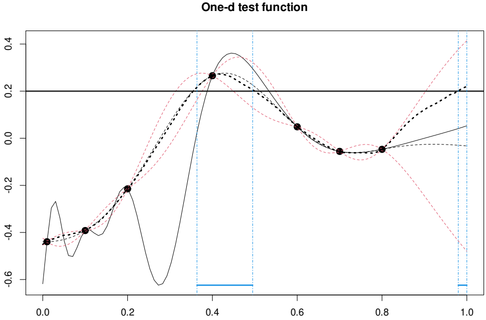

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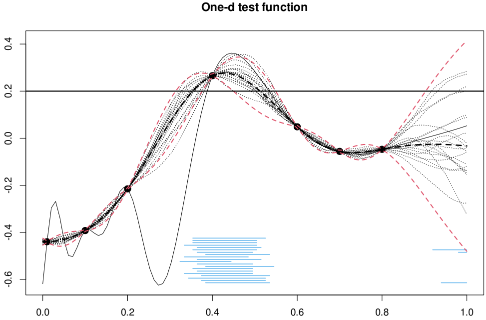

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How to summarize the distribution on sets?

Here we consider **estimates** for Γ^* with

Expectations of random closed sets[1],
in particular *Vorob'ev expectation*.

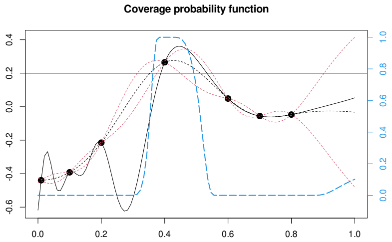
Conservative estimates, based on Vorob'ev quantiles.

1. for more definitions of expectation see Molchanov, I. (2017). Theory of Random Sets. Second edition. Springer.

Vorob'ev quantiles

Recall: posterior **coverage probability function of** Γ

$$p_n(\mathbf{x}) = P_n(\mathbf{x} \in \Gamma) = \Phi\left(\frac{m_n(\mathbf{x}) - t}{\sqrt{k_n(\mathbf{x},\mathbf{x})}}\right)$$



used in volume computation, tIMSE criterion;

p_n creates a family of set estimates $Q_\rho = \{\mathbf{x} \in D : p_n(\mathbf{x}) \geq \rho\}$

high ρ, then points in Q_ρ have high marginal probability.

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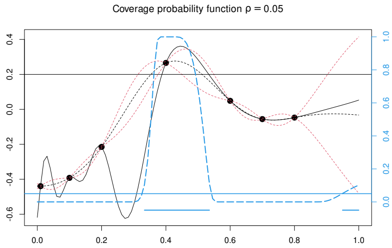

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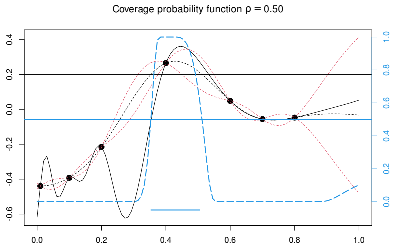

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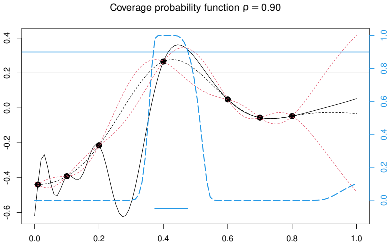

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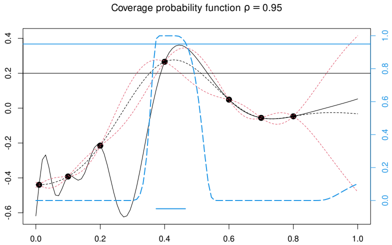

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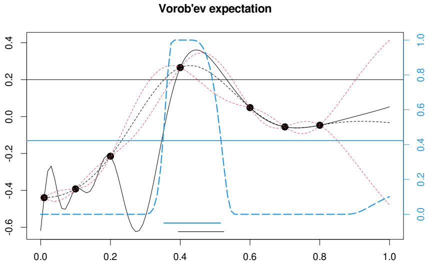
Vorob'ev expectation

From Q_ρ, choose $Q_{\widetilde{\rho}}$ such that $\mu(Q_{\widetilde{\rho}}) = \mathbb{E}[\mu(\Gamma)]$.



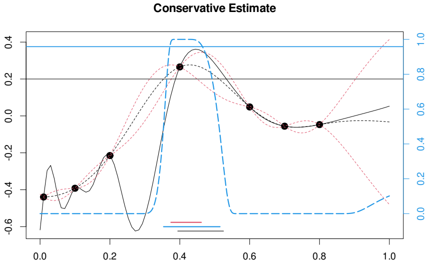
Properties:

- depends on (finite) measure μ;
- generally fast to compute;

Chevalier, C., Ginsbourger, D., Bect, J., and Molchanov, I. (2013). *Estimating and quantifying uncertainties on level sets using the Vorob'ev expectation and deviation with Gaussian process models.* mODa 10.

A **conservative estimate** of Γ^* is

$$C_{\Gamma,n} = Q_{\rho^*} \text{ where } \rho^* \in \arg\max_{\rho \in [0,1]} \{\mu(Q_\rho) : P_n(Q_\rho \subset \Gamma) \geq \alpha\}$$



- joint confidence statement on the set estimate;
- general method based on high dimensional Gaussian approximation

More

A., D., Ginsbourger, D. (2018) *Estimating Orthant Probabilities of High-Dimensional Gaussian Vectors with An Application to Set Estimation*, Journal of Computational and Graphical Statistics, 27:2, 255-267.

How to reduce the uncertainty on set estimate?

Uncertainty function(s):

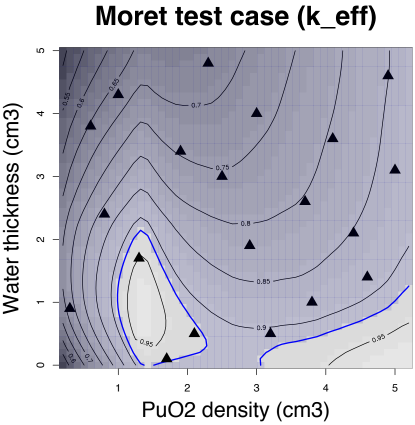
$$H_n(\rho) = \mathbb{E}_n[\mu(\Gamma \Delta Q_{n,\rho})], \quad \Gamma \Delta Q_{n,\rho} = \Gamma \setminus Q_{n,\rho} \cup Q_{n,\rho} \setminus \Gamma,$$
$$H_n^{\mathrm{T2}}(\rho_n^\alpha) = \mathbb{E}_n[\mu(\Gamma \setminus Q_{n,\rho_n^\alpha})],$$

For each uncertainty function, we define the following **SUR criteria**

$$J_n(\mathbf{x}) = \mathbb{E}_n[H_{n+1}(\rho) \mid X_{n+1} = \mathbf{x}] = \mathbb{E}_{n+1}[\mu(\Gamma \Delta Q_{n+1,\rho}) \mid X_{n+1} = \mathbf{x}]$$
$$J_n^{\mathrm{T2}}(\mathbf{x}) = \mathbb{E}_n[H_{n+1}^{\mathrm{T2}}(\rho_n^\alpha) \mid X_{n+1} = \mathbf{x}] = \mathbb{E}_{n+1}[\mu(\Gamma \setminus Q_{n+1,\rho_n^\alpha}) \mid X_{n+1} = \mathbf{x}],$$

More

Example: IRSN test case



Test case:

- $\mathrm{k_{eff}}$ function of $\mathrm{PuO_2}$ density and $\mathrm{H_2O}$ thickness, $D = [0.2, 5.2] \times [0, 5]$;
- $\mathrm{k_{eff}}$ continuous, expensive to evaluate;
- $n = 20$ observations (black triangles);

Objective: estimate $\Gamma^\star = \{\mathbf{x} \in D : f(\mathbf{x}) \leq t\}$ and evaluate the uncertainty of the estimate.

GRF model: m constant, k Matérn ($\nu = 5/2$), MLE for hyper-parameters.

Acknowledgements: Yann Richet, Institut de Radioprotection et de Sûreté Nucleaire.

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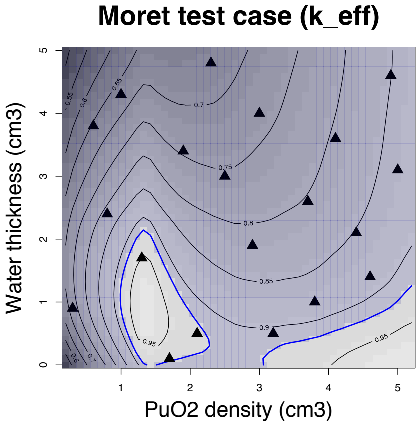

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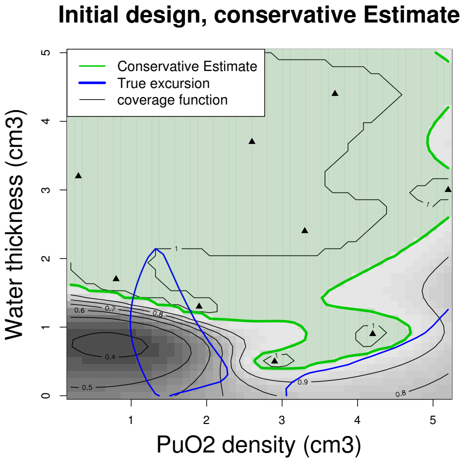
Example: type II uncertainty



Criterion: $J^{\mathrm{T2}}_{n+q}(\mathbf{x}_q) = \mathbb{E}_n[\mu(\Gamma \setminus Q_{n+1,\rho_n^\alpha}) \mid \mathbf{X}_{n+q} = \mathbf{x}_q]$,

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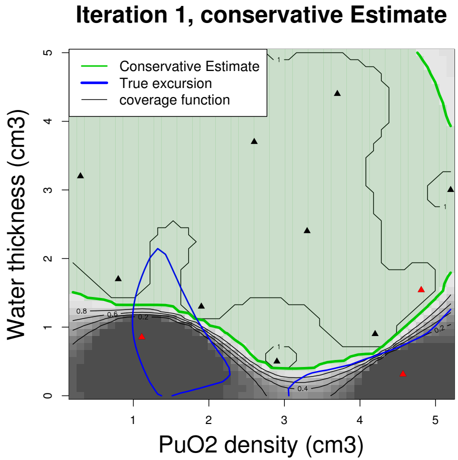

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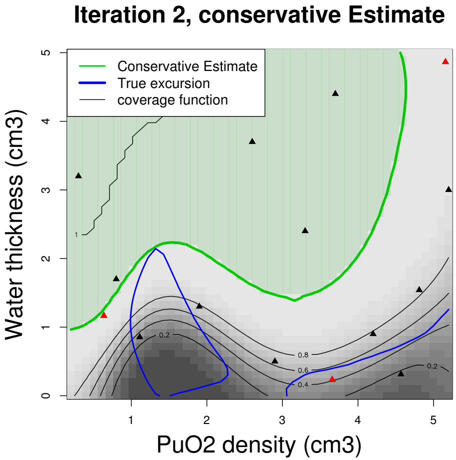

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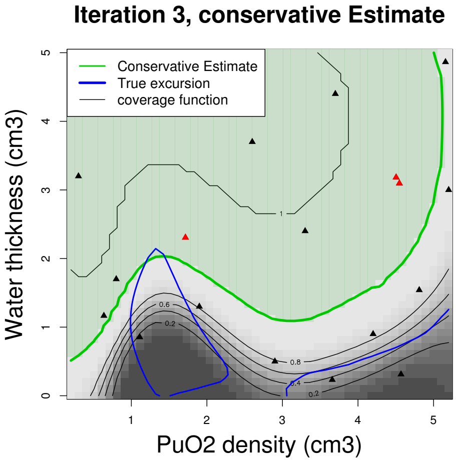

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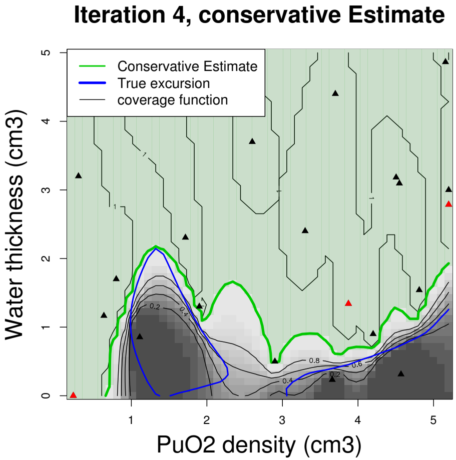

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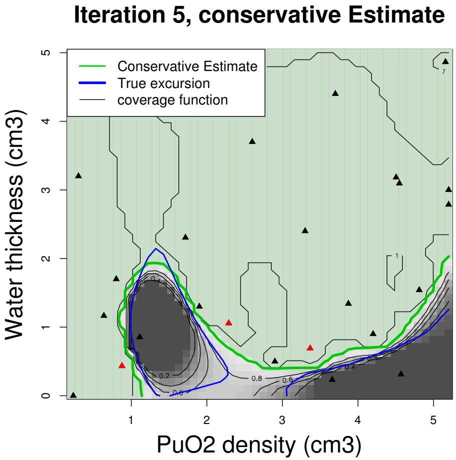

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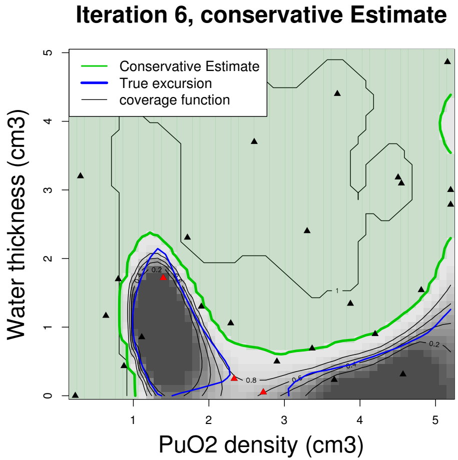

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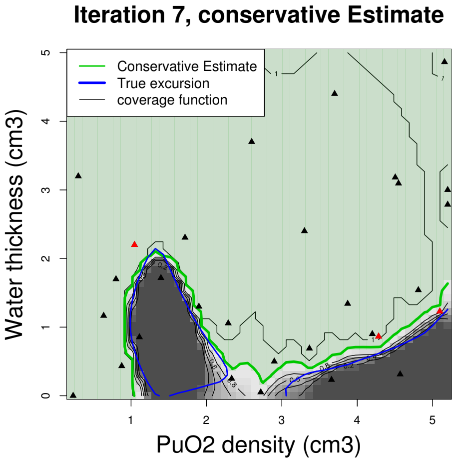

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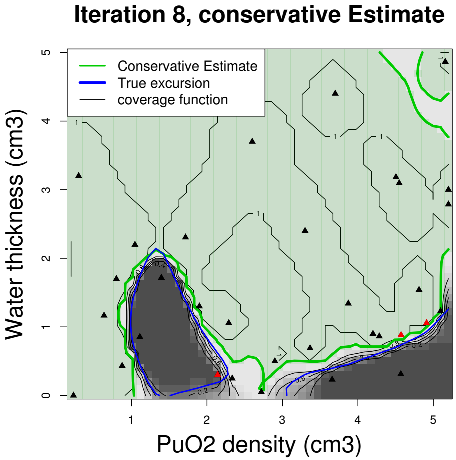

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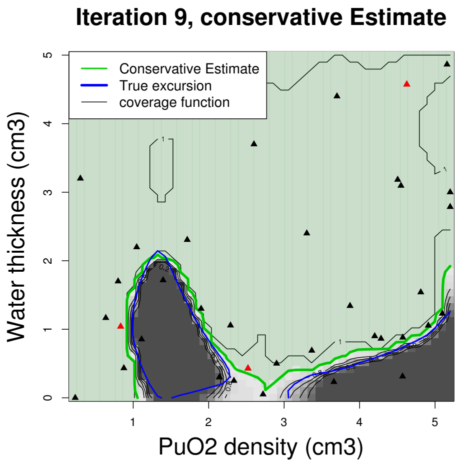

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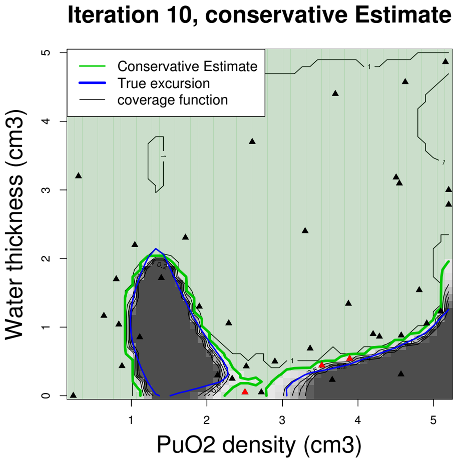

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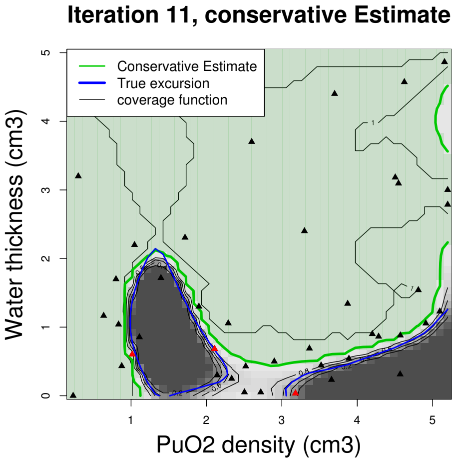

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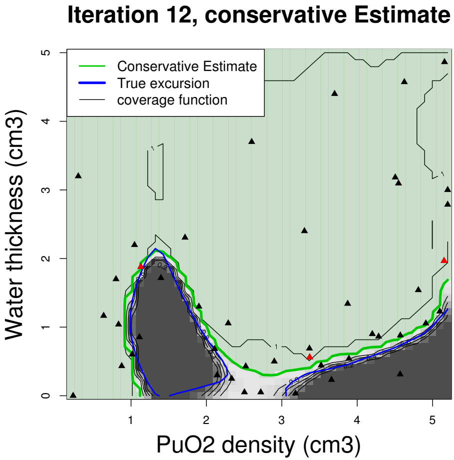

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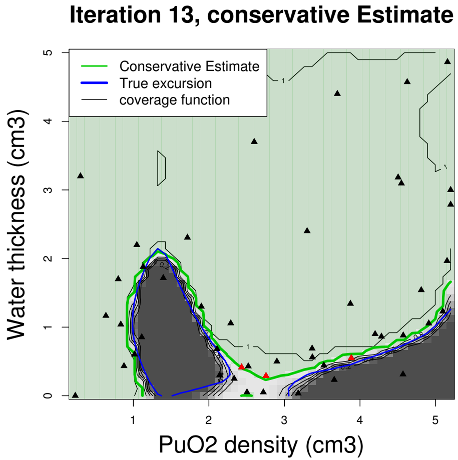

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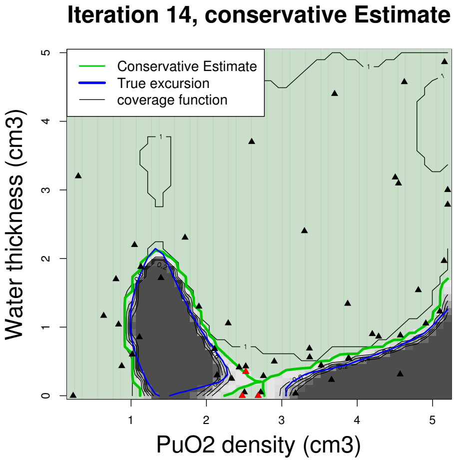

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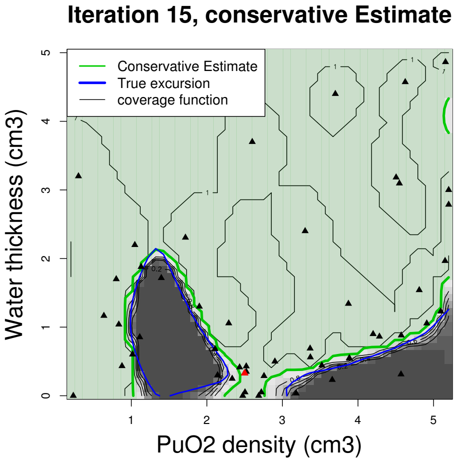

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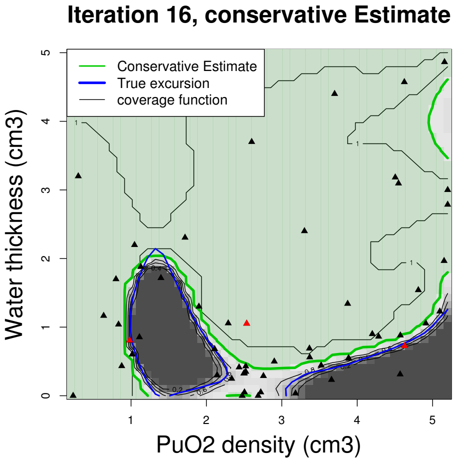

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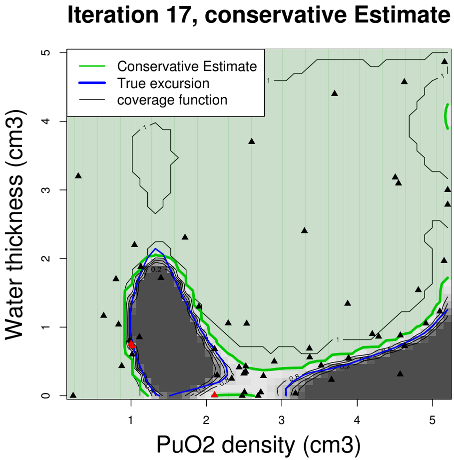

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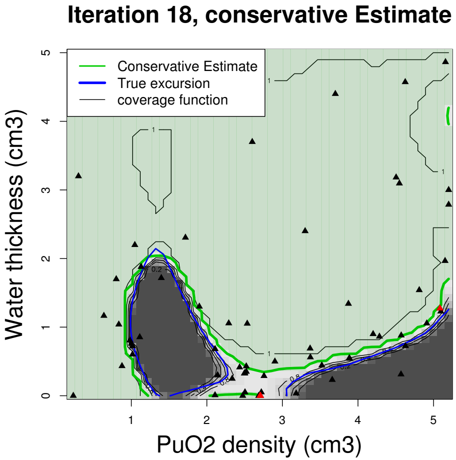

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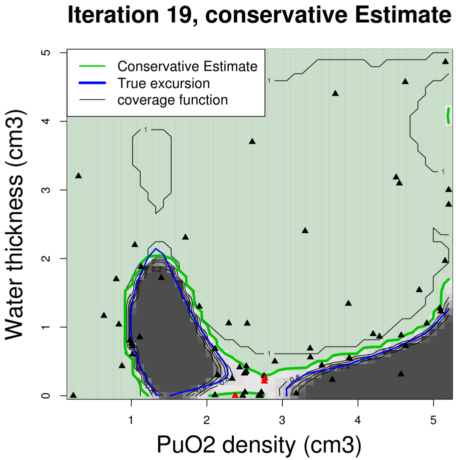

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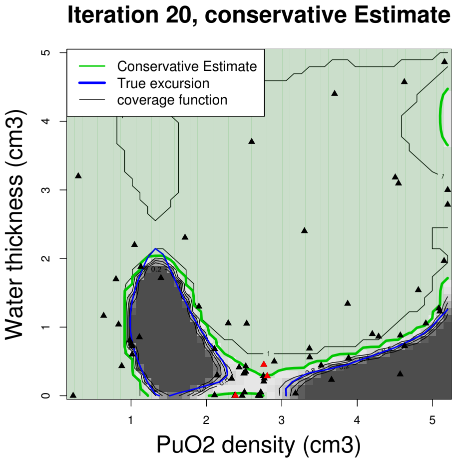

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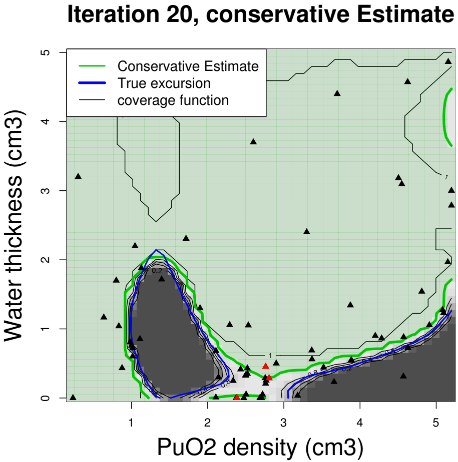


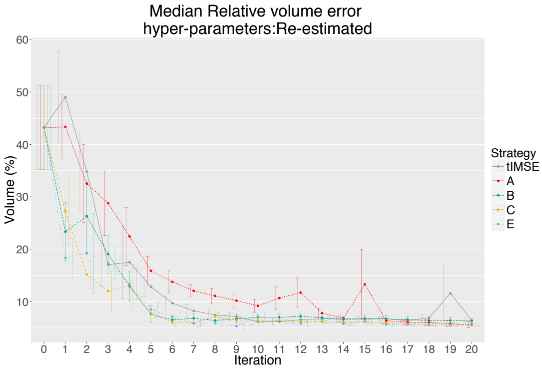
$n = 60$ new evaluations;

Next evaluation chosen in order to minimize criterion $J_n^{\mathrm{T}2}$;

Volume of updated CE: 21.30 (true excursion: 22.04, initial estimate: 18.10)

Comparison with state-of-the-art

IRSN test case: m constant, k Matérn ($\nu = 5/2$).



$n_0 = 10$ initial points;

$q = 3$ points per iteration;

Relative error with respect to 50×50 evaluation grid.

Strategy	Criterion
tIMSE	target=0.92
A	$J_n(\cdot; \rho_n)$, $\rho_n = 0.5$
B	$J_n(\cdot; \rho_n^*)$, $\alpha = 0.95$
C	$J_n^{\mathrm{MEAS}}(\cdot; \rho_n^*)$, $\alpha = 0.95$
E	$J_n^{\mathrm{T2}}(\cdot; \rho_n^*)$, $\alpha = 0.95$

A, D., Ginsbourger, D., Chevalier, C., Bect, J. and Richet, Y. (2021). *Adaptive Design of Experiments for Conservative Estimation of Excursion Sets.* Technometrics, 63:1, 13-26.

Thanks for your attention!

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