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Technical University of Munich

Near-optimal noise control in derivative-free stochastic optimization

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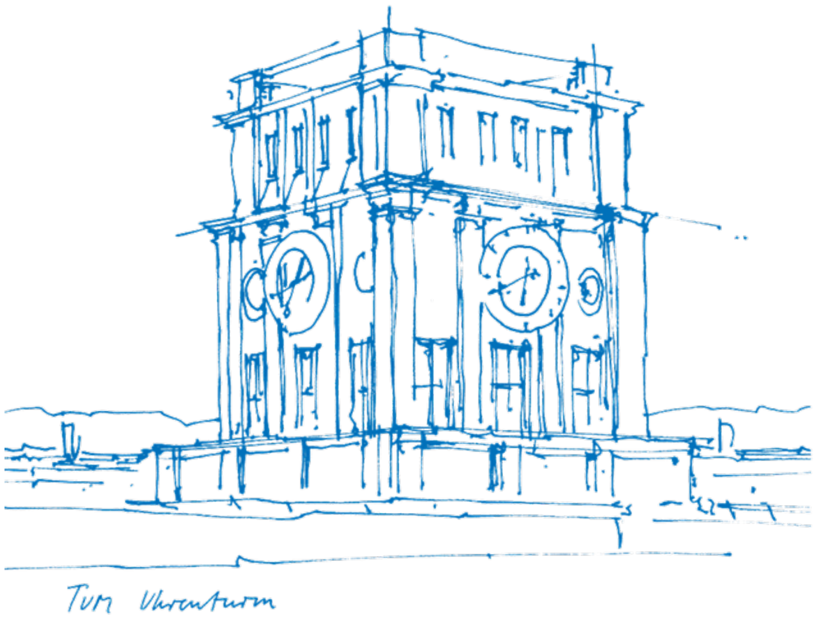


ICCOPT

H 2033:

Derivative-free optimization under uncertainty (Part II)

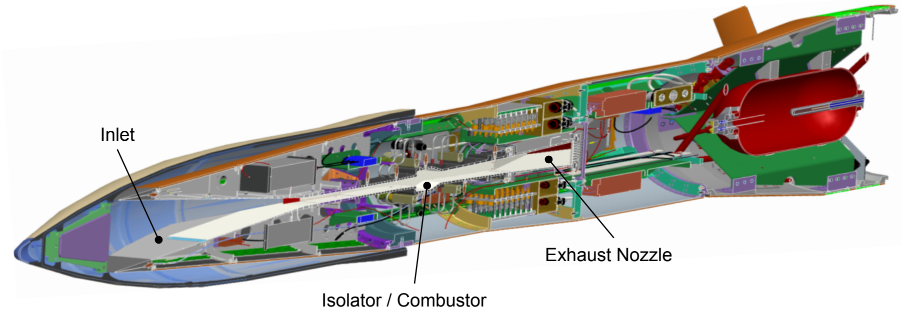
Berlin, Aug. 7th, 2019

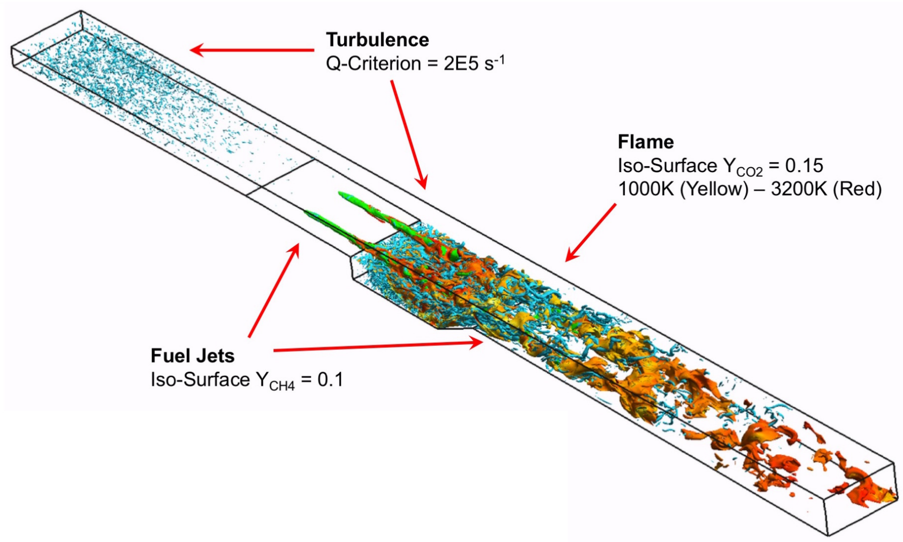
Motivation: Design optimization of a SCRAMJET

Provided by Sandia National Laboratories

- No rotating elements for compression
- Air compressed dynamically
- Supersonic mixture and combustion
- (Some) challenges:
  - Low throughput time vs. mixture and self-ignition
  - Compressibility effects
  - Stable combustion for constant thrust
- [Javier Urzay, 2018]:

  The challenge of enterprising supersonic combustion in scramjet is [...] as difficult as lighting a match in a hurricane.





SNOWPAC

SNOWPAC [1]

~~Robust~~ Stochastic optimization problem statement

- Find **robust** solution with respect to uncertainty
- Using measures of robustness $\mathscr{R}$, e.g. $\mathbb{E}, \mathbb{V}$, CVaR.
- E.g., weigh expected gain vs. confidence: $\max \mathbb{E} - \lambda \mathbb{V}^{\frac{1}{2}}$

$$\mathscr{R}^*_{\omega} = \mathscr{R}(\mathbf{x}^*, \omega) = \min_{\mathscr{R}^c(\mathbf{x},\omega)\leq 0} \mathscr{R}^f(\mathbf{x}, \omega)$$

[1] F. Augustin, Y. Marzouk, A trust-region method for derivative-free nonlinear constrained stochastic optimization. 2017

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Stochastic optimization problem statement

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Features of SNOWPAC:

0. **Extension of NOWPAC**: Derivative-free nonlinear constraint optimization method using trust-regions (deterministic)

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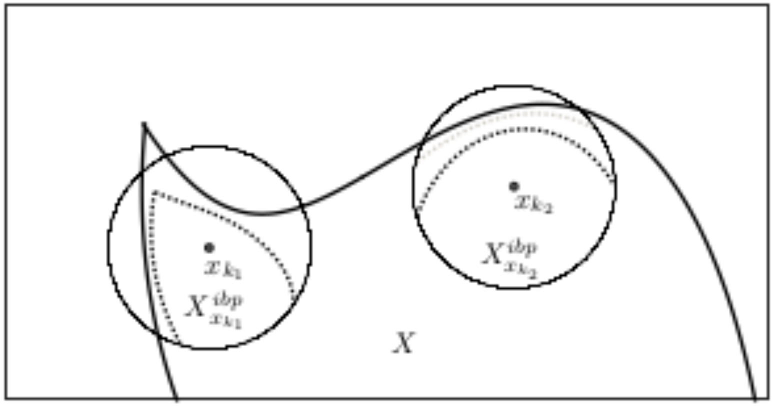
Derivative-free optimization using NOWPAC [2]

- **Non-intrusive optimization** framework
- **Trust region approach** for nonlinearly-constrained DFO
- Build **fully linear surrogate models** of objective and constraints
- Find improved designs by **minimizing surrogate models**



Inner Boundary Convexification

- New way of **handling constraints using an inner boundary path**
  - The inner boundary path is an additive convex function to the constraints
- Global **convergence to a first-order locally optimal design**

[2] F. Augustin, Y. Marzouk, NOWPAC: A path-augmented constraint handling approach for nonlinear derivative-free optimization. 2014

SNOWPAC [1]

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Features of SNOWPAC:

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1. **Estimate robustness measures**: Use sampling, e.g. $\mathcal{R}^f_\omega = \mathbb{E}[f_\omega(\mathbf{x})] \approx R^f = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}, \theta_i) + \varepsilon_N$

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   NEW: Leverage multilevel estimators.

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Multilevel error estimator for SNOWPAC

Generic MLMC estimators:

- Mean:

$$\mathbb{E}[Q] \approx \hat{Q}_L = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left(Q_\ell^{(i)} - Q_{\ell-1}^{(i)} \right)$$

- Variance:

$$\mathbb{V}[Q] = \sum_{\ell=0}^{L} \mathbb{E}\left[(Q_\ell - \mathbb{E}[Q_\ell])^2 - (Q_{\ell-1} - \mathbb{E}[Q_{\ell-1}])^2 \right] = \sum_{\ell=0}^{L} \mathbb{E}[P_\ell^2] - \mathbb{E}[P_{\ell-1}^2]$$

$$\approx \quad s_{ML}^2 \quad = \sum_{\ell=0}^{L} (\widehat{P_\ell^2} - \widehat{P_{\ell-1}^2}), \quad \text{where} \quad \hat{P}_\ell^2 = \frac{1}{N_\ell - 1} \sum_{i=1}^{N_\ell} \left(Q_\ell^{(i)} - \hat{Q}_\ell \right)^2.$$

- Standard deviation:

$$\sqrt{\mathbb{V}[Q]} \approx \sqrt{s_{ML}^2}$$

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- Standard deviation:

$$\sqrt{\mathbb{V}[Q]} \approx \sqrt{s_{ML}^2}$$

$\Rightarrow$ Multilevel estimators for $\mathbb{E}$, $\mathbb{V}$ and $\sqrt{\mathbb{V}}$.

Multilevel error estimator for SNOWPAC

Generic MLMC error estimators:

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$$\mathbb{V}[\hat{Q}_L] = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \mathbb{V}[\hat{Y}_l]$$

- Variance s_{ML}^2:

$$\mathbb{V}[s_{ML}^2] = \sum_{\ell=0}^{L} \mathbb{V}[\widehat{P_\ell^2}] + \mathbb{V}[\widehat{P_{\ell-1}^2}] - 2\mathrm{Cov}(\widehat{P_\ell^2}, \widehat{P_{\ell-1}^2})$$

$$\text{where} \quad \mathbb{V}[\widehat{P_\ell^2}] = \frac{1}{N_\ell}\left(\mu_{4,\ell} - \mathbb{V}[Q_\ell]^2\right) + \frac{2}{N_\ell(N_\ell - 1)} \mathbb{V}[Q_\ell]^2$$

- Standard deviation $\sqrt{s_{ML}^2}$:

$$SE(s_{ML}^2) \approx \frac{1}{2\sqrt{s_{ML}^2}} \sqrt{\mathbb{V}[s_{ML}^2]}$$

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- Mean $\hat{Q}_L$:

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- Variance s^2_{ML}:

$$\mathbb{V}[s^2_{ML}] = \sum_{\ell=0}^{L} \mathbb{V}[\widehat{P^2_\ell}] + \mathbb{V}[\widehat{P^2_{\ell-1}}] - 2\mathrm{Cov}(\widehat{P^2_\ell}, \widehat{P^2_{\ell-1}}) = (\frac{\varepsilon_N}{2})^2$$

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$\Rightarrow$ Multilevel error estimators for $\mathbb{E}$, $\mathbb{V}$ and $\sqrt{\mathbb{V}}$.

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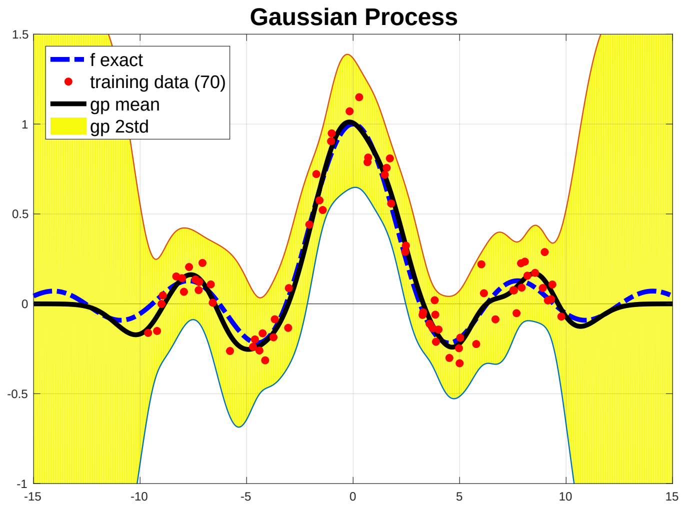
SNOWPAC – Gaussian process surrogate

- **Use black box evaluations** to build global Gaussian process surrogates
- **Probabilistic estimator:**
  - GP mean: $\mu_{GP}(\mathbf{x}) = \mathbf{k}_{x\mathbf{X}}[\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_{\mathbf{n}}^{\mathbf{2}}\mathbf{I}]^{-1}\mathbf{R}$
  - GP variance: $\sigma_{GP}^2(\mathbf{x}) = k_{xx} - \mathbf{k}_{x\mathbf{X}}[\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_{\mathbf{n}}^{\mathbf{2}}\mathbf{I}]^{-1}\mathbf{k}_{\mathbf{X}x}$



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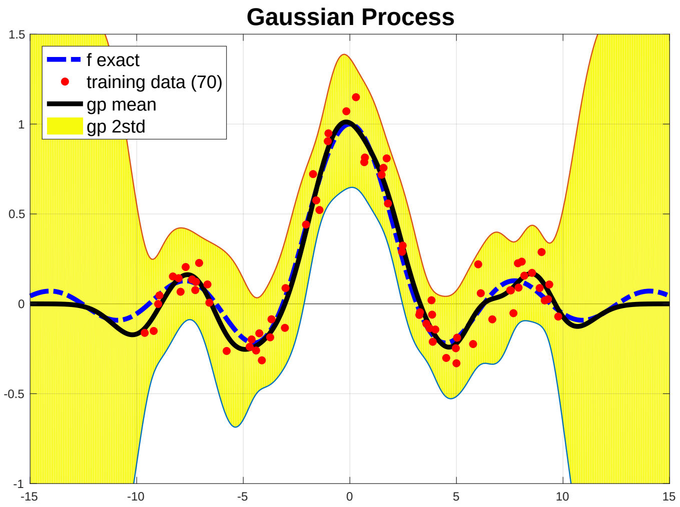
- **Replace noisy black box evaluations by GP mean**:

$$\tilde{R} = \alpha \cdot \mu_{\mathrm{GP}} + (1-\alpha) \cdot R_\omega$$



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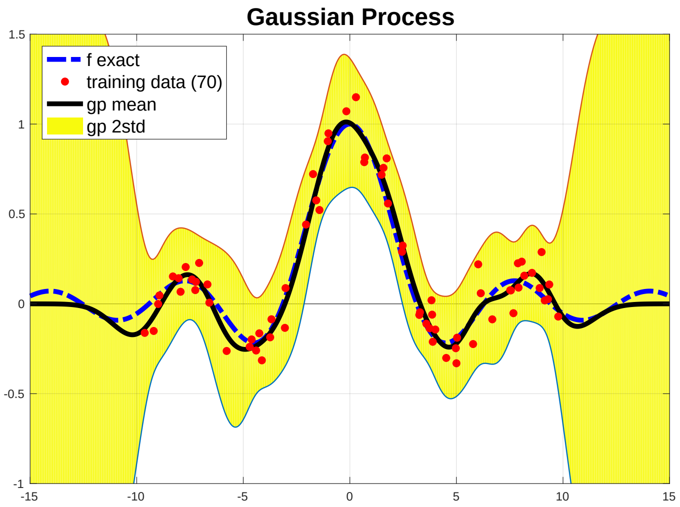

- **Replace noise estimate by**:

b) Heuristic: $\tilde{\varepsilon} = \alpha \cdot 2\sigma_{\mathrm{GP}}(\mathbf{x}) + (1-\alpha) \cdot \varepsilon_N$, where $\alpha = e^{-\sqrt{\sigma^2_{\mathrm{GP}}(\mathbf{x})}}$

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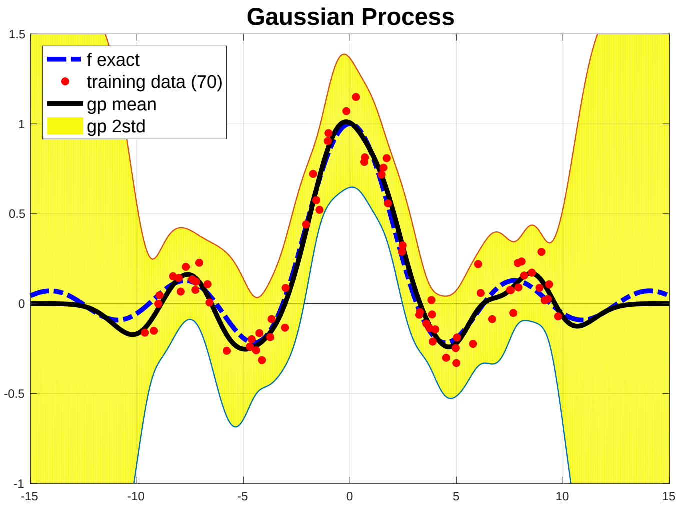

- **Replace noise estimate by**:

NEW a) Analytic: $\tilde{\varepsilon} = 2 \cdot \min_\alpha \text{RMSE}(\tilde{R}),$ where $\alpha = \arg\min_\alpha \text{RMSE}(\tilde{R})$ NEW

b) Heuristic: $\tilde{\varepsilon} = \alpha \cdot 2\sigma_{\text{GP}}(\mathbf{x}) + (1-\alpha) \cdot \varepsilon_N,$ where $\alpha = e^{-\sqrt{\sigma^2_{\text{GP}}(\mathbf{x})}}$

SNOWPAC – Gaussian Process Noise Correction

MSE:

$$\begin{aligned}\text{MSE}_\alpha &= \text{BIAS}(\tilde{R})^2 + \mathbb{V}[\tilde{R}] \\ &= [\alpha(\mu_{GP}[\mathscr{R}] - \mathscr{R}_\omega)]^2 + \alpha^2\mathbb{V}[\mu_{GP}] + (1-\alpha)^2\mathbb{V}[R] + \alpha(1-\alpha)2\text{cov}[\mu_{GP}, R]\end{aligned}$$

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Optimal α:

$$\alpha^* = \frac{\mathbb{V}[R] - \text{cov}[\mu_{GP}, R]}{(\mu_{GP}[\mathscr{R}] - \mathscr{R}_\omega)^2 + \mathbb{V}[\mu_{GP}] + \mathbb{V}[R] - 2\text{cov}[\mu_{GP}, R]}$$

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Optimal estimator:

$$\begin{aligned}\tilde{R} &= \alpha^* \cdot \mu_{\mathrm{GP}} + (1-\alpha^*) \cdot R_\omega \\ \tilde{\varepsilon} &= 2 \cdot \sqrt{\mathrm{MSE}_{\alpha^*}(\tilde{R})}\end{aligned}$$

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- $\mu_{GP}[\mathscr{R}] - \mathscr{R}_\omega = \mathbb{E}[\mu_{GP}] - \mathscr{R}_\omega \approx \mathbb{E}[\mu_{GP}[\hat{R}]] - \mu_{GP}[R]$

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3. **Introduce Gaussian process surrogates**: Mitigate effect of noise ε_N
4. **Only feasible trial points**, i.e. $\mathscr{R}^c_\omega(\mathbf{x}_{k+1}) \leq 0$, **should be accepted**

$\Rightarrow$ Feasibility restoration mode: $\min_{\substack{m_k^c(\mathbf{x})\leq\tau \\ \|\mathbf{x}-\mathbf{x}_k\|\leq\Delta_k}} \sum_{i\in\mathscr{I}} \left(m_k^{c_i}(\mathbf{x})^2 + \lambda_g m_k^{c_i}(\mathbf{x})\right)$

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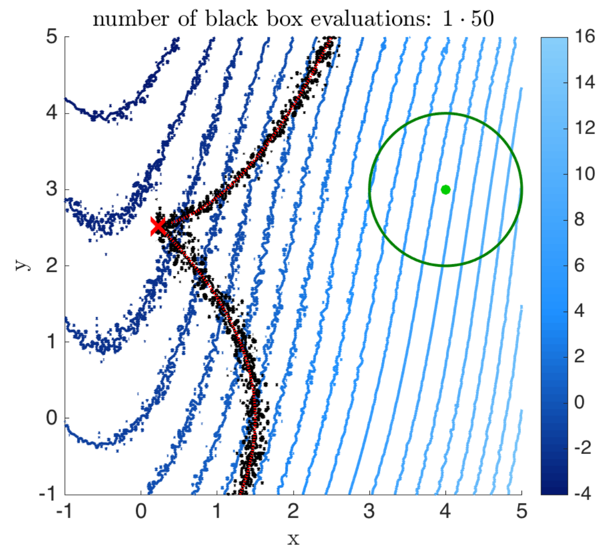
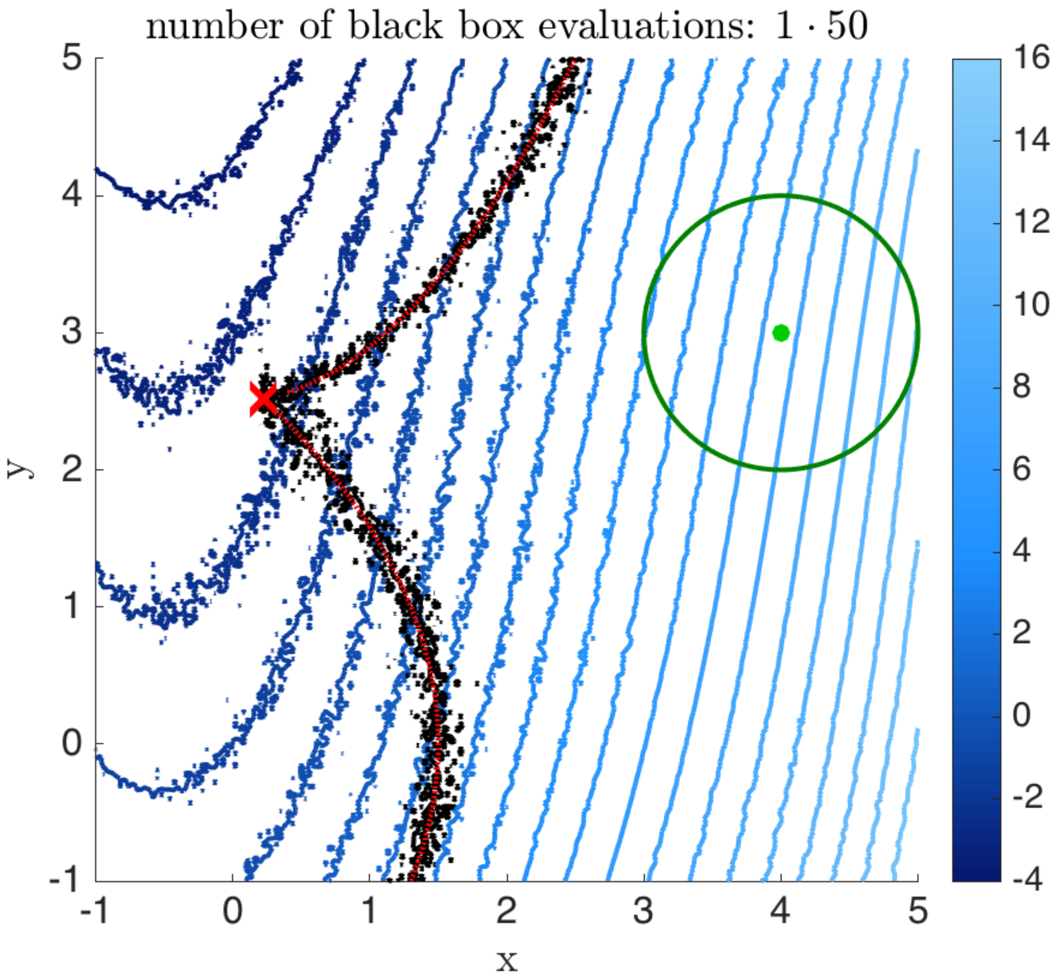
SNOWPAC – Example

$$\min \mathbb{E}[\sin(x-1+\theta_1)+\sin(\frac{1}{2}y-1+\theta_1)^2]+\frac{1}{2}(x+\frac{1}{2})^2-y$$
$$\text{s.t.} \quad \mathbb{E}[-4x^2(1+\theta_2)-10\theta_3] \quad \leq 25-10y, \theta_i \sim \mathscr{U}(\theta_i|-1,1), i=1,\ldots 4 \tag{1}$$
$$\mathbb{E}[-2y^2(1+\theta_4)-10(\theta_4+\theta_2)] \leq 20x-15, \mathbf{x}^{(0)}=(x^{(0)},y^{(0)})=(4,3).$$

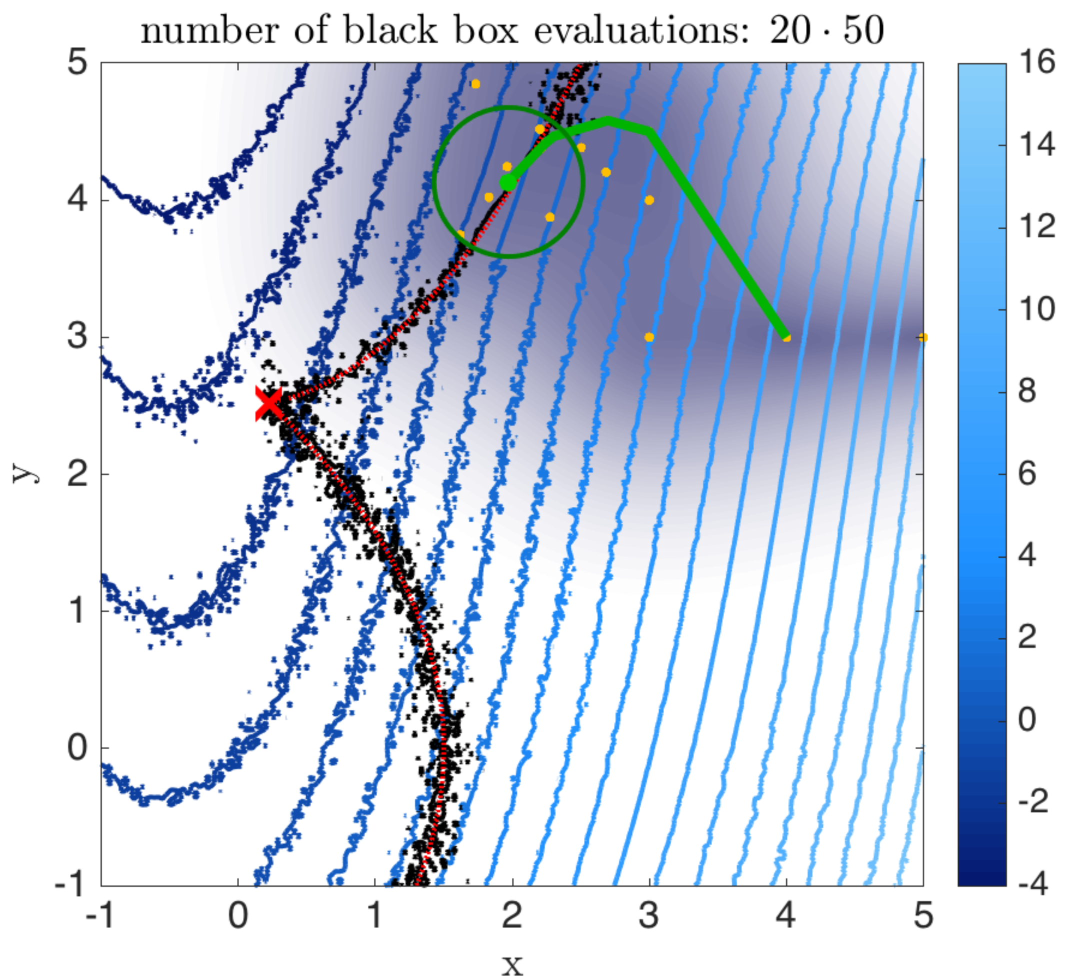


- Locally smoothed black box functions within the trust region
- Optimal design (red cross), exact constraints (red dotted lines)
- Objective (blue lines), constraints (black lines)
- Current design and trust region (green dot and circle)
- GP points (yellow dots), scaling factor γ (gray shade)

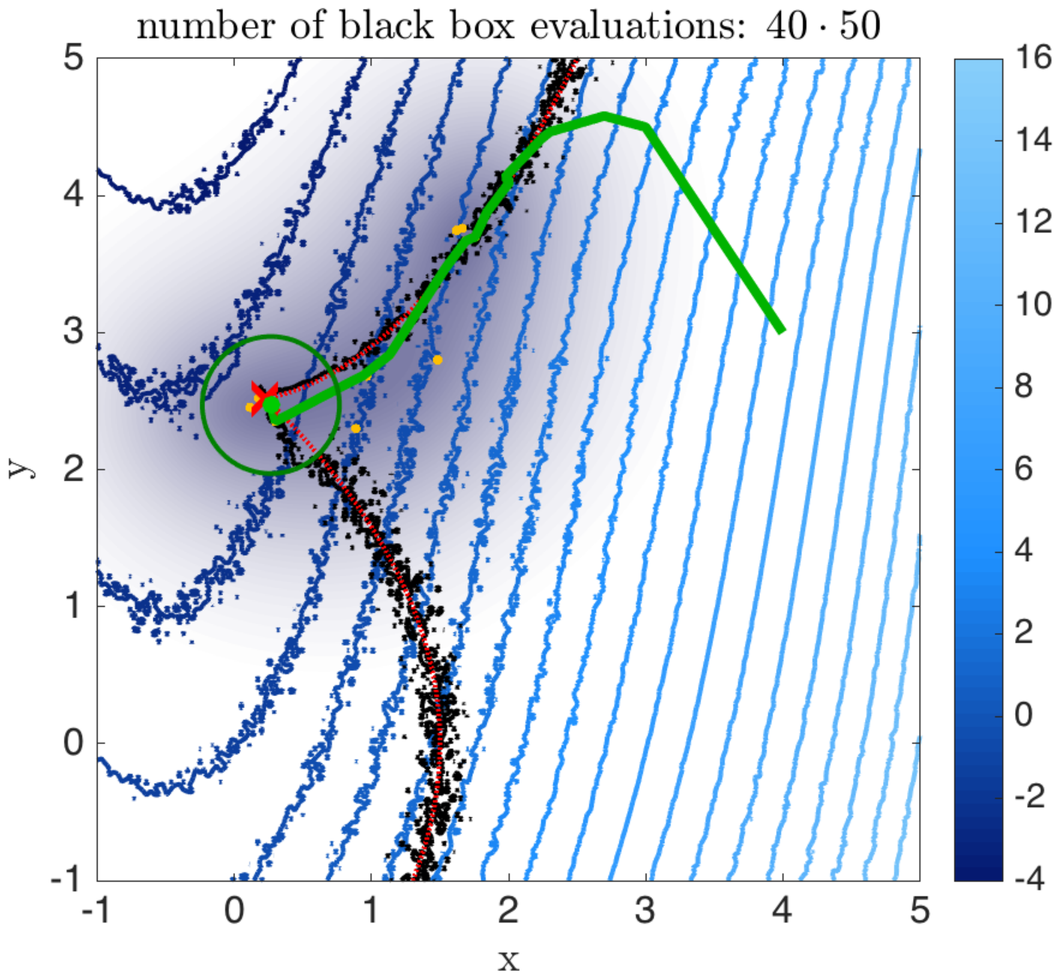
SNOWPAC – Example



SNOWPAC – Example



SNOWPAC – Example



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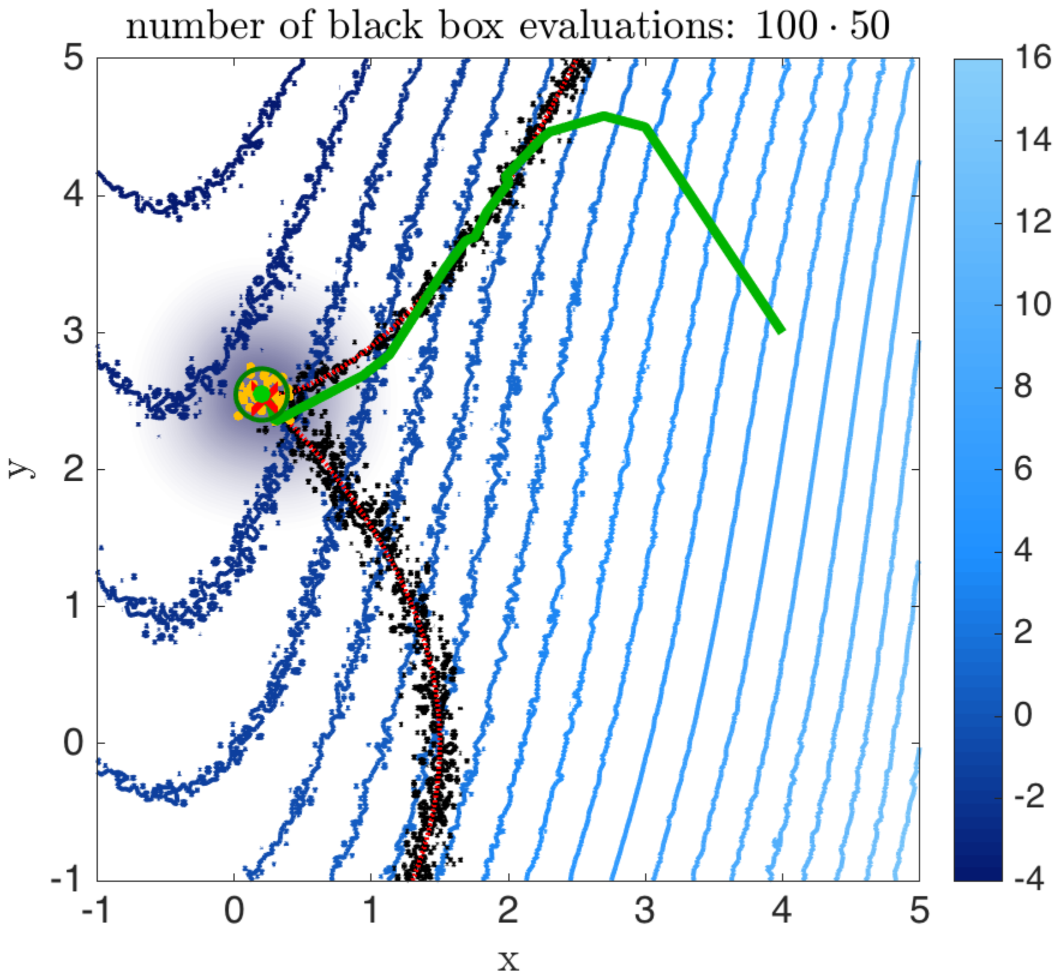
SNOWPAC – Example



Benchmark results

SNOWPAC – Benchmark setup

- Benchmark comparison of performance of SNOWPAC to COBYLA, NOMAD, cBO, SPSA and KWSA
- Use 8 CUTEst benchmark problems with added noise

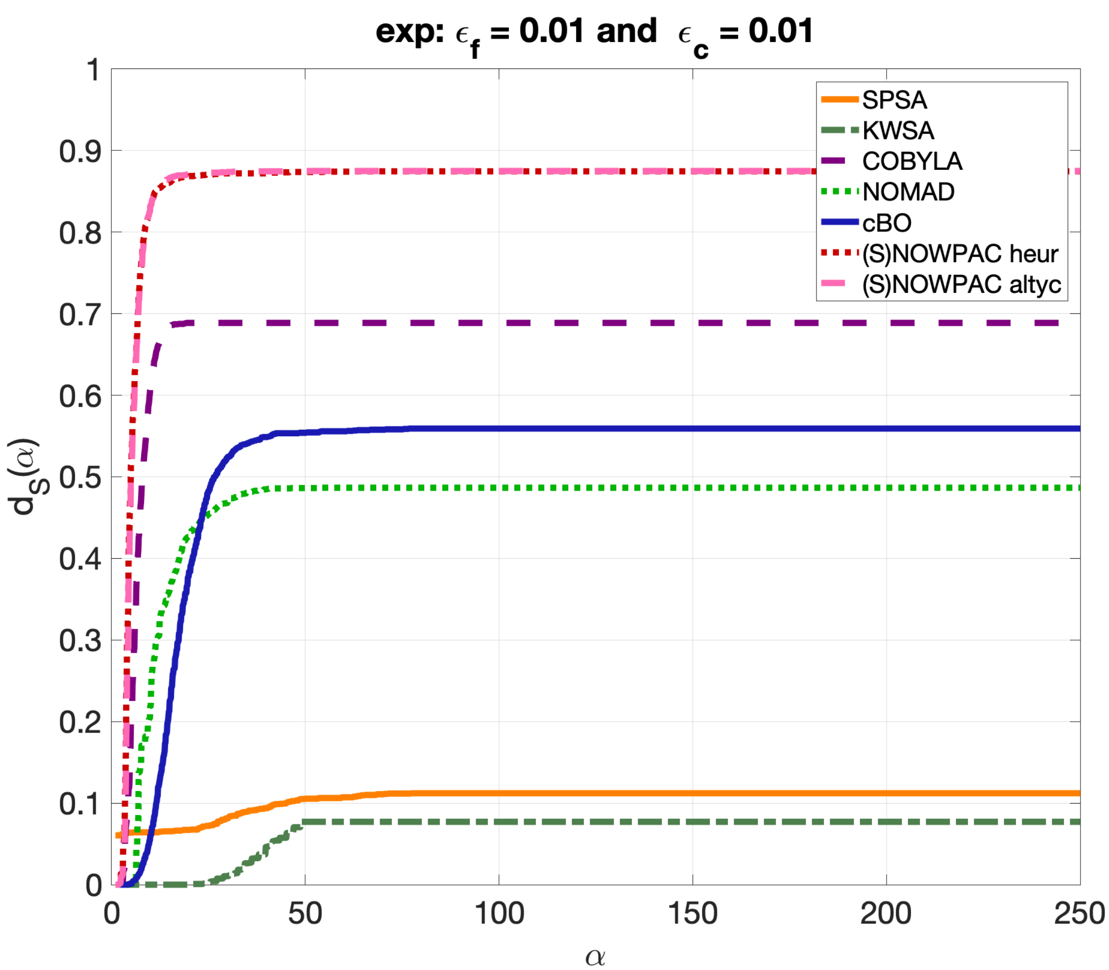
$$\min R_N[f(\mathbf{x}) + \omega_1]$$
$$\text{s.t. } R_N[c_i(\mathbf{x}) + \omega_{2,i}] \leq 0,$$

  and approximate robustness measures with $N \in \{200, 1000, 2000\}$ samples of

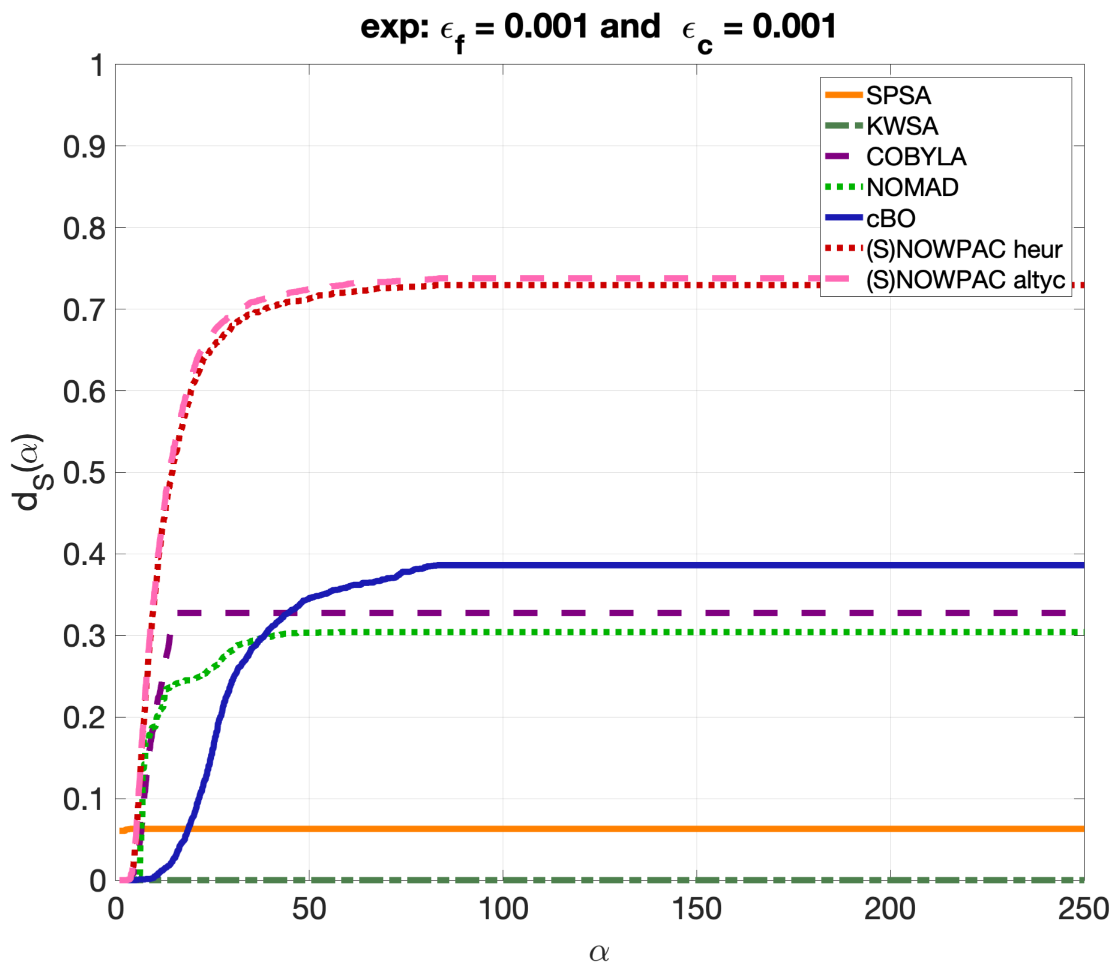
$$\omega_1, \omega_{2,i} \sim \mathscr{U}[-1, 1]$$

- Limit max number of black box evaluations to 250
- Comparison of results from 100 repeated optimization runs
- Use data profile [Moré/Wild2009] to compare performance $d_S(\alpha) = \frac{1}{2400}\left|\left\{p \in \mathscr{P} \, : \, \frac{t_{p,S}}{n_p+1} \leq \alpha\right\}\right|$
  - Based on $|\mathscr{P}| = 8 \cdot 100 \cdot 3 = 2400$ optimization runs

SNOWPAC – Benchmark results



SNOWPAC – Benchmark results



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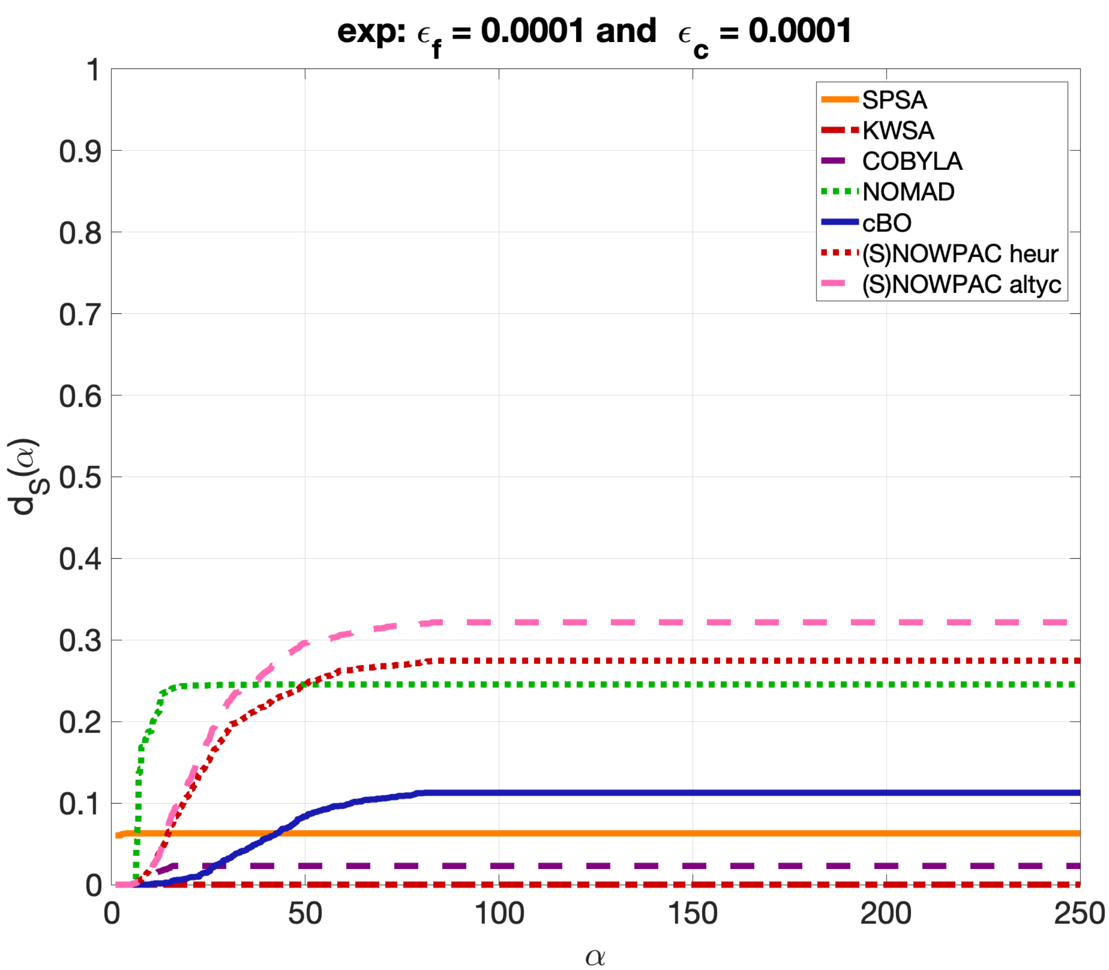
SNOWPAC – Benchmark results



MLMC Results

Problem statement

Objective:

$$f(x) = \begin{cases} (x-2)^2 & \text{if } x \leq 3 \\ 2\log(x-2)+1 & \text{if } x > 3 \\ x \in [0,6] \end{cases}$$

Constraint:

$$g_{det}(x) = \frac{2.log(1.5)}{2.5}x + 1. - \frac{2.log(1.5)}{2.5}$$
$$g_H(x,\xi) = g_{det}(x) + \xi^3$$
$$g_L(x,\xi) = g_{det}(x) + A\xi^3, \xi \sim \mathscr{U}(-0.5, 0.5)$$

OUU:

$$\min_x f(x)$$

Mean:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)]$

Push back:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)] + 3\sigma[g_H(x,\xi)]$

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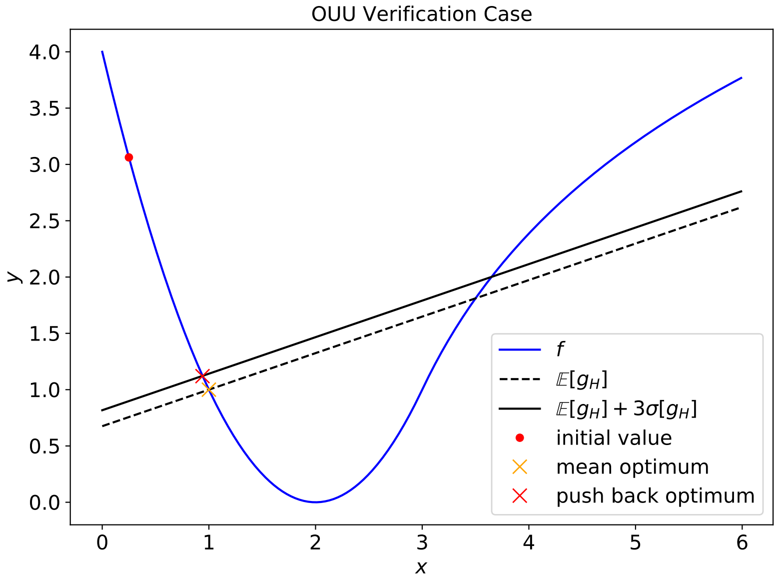

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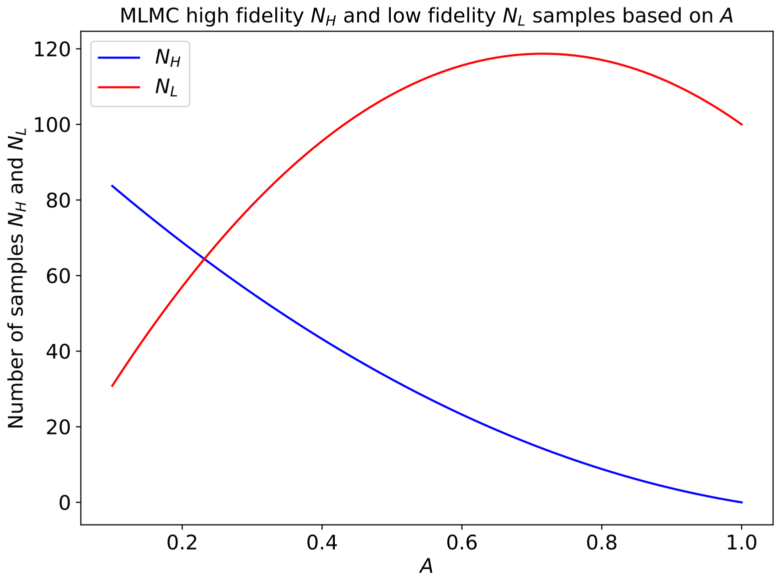

Results

Mean:

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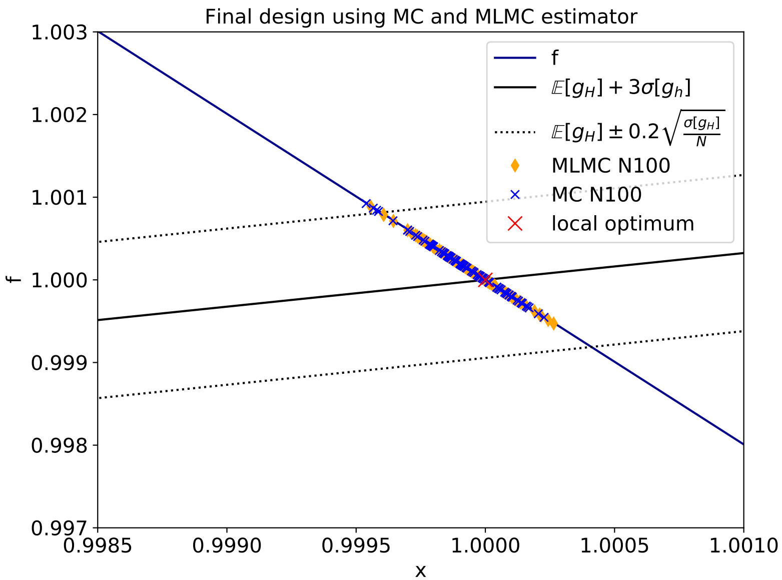

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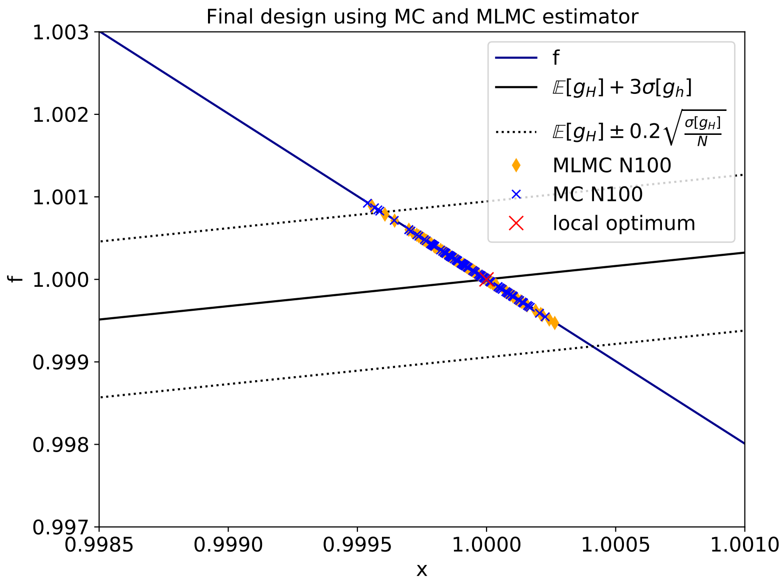

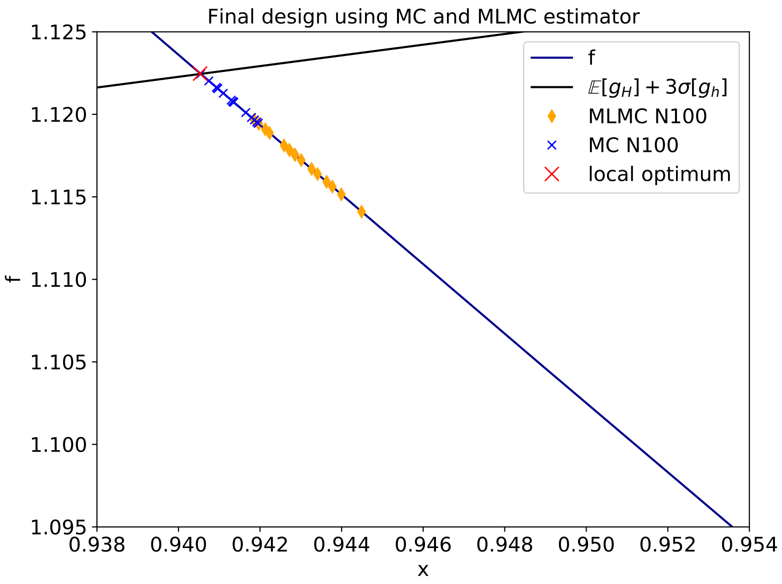

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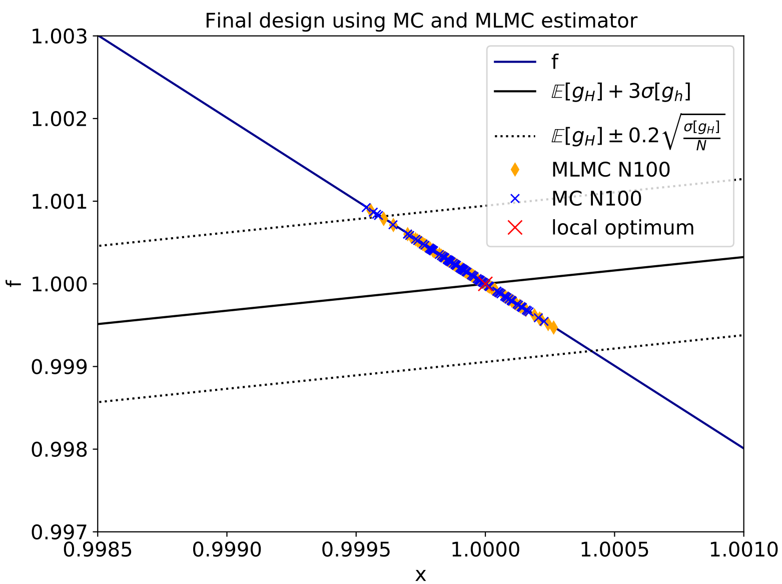

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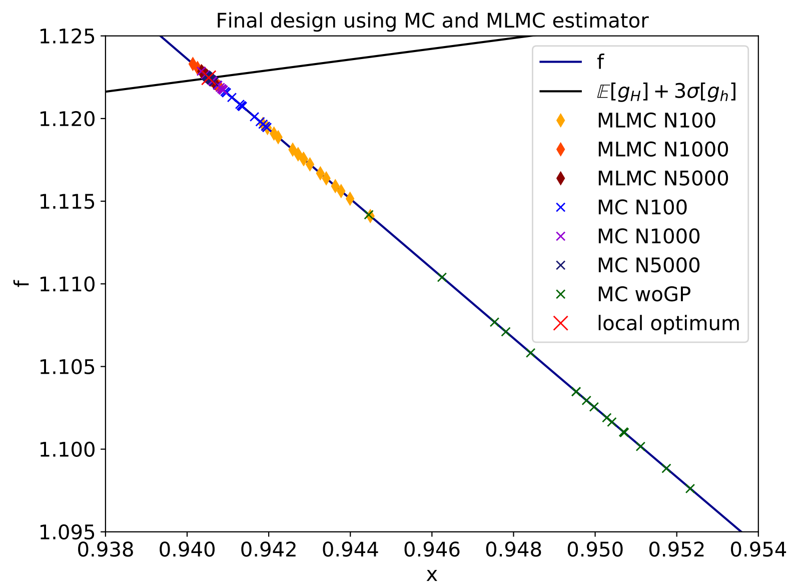

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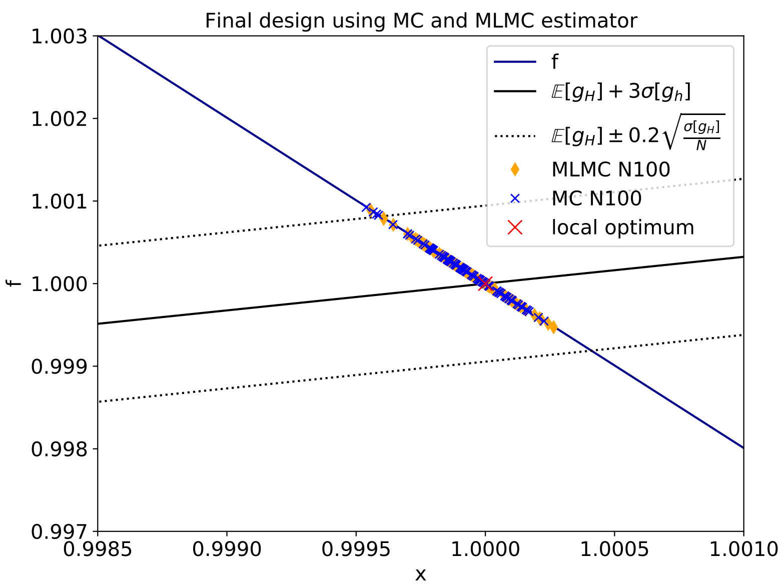

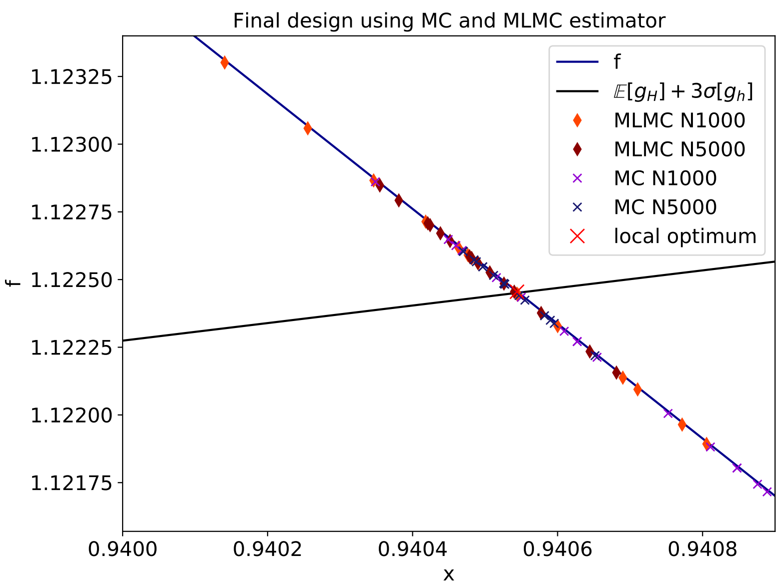

Summary:

- **NOWPAC** – Derivative-free trust region methods for constrained nonlinear optimization
- **SNOWPAC** – Stochastic derivative-free optimization using Gaussian process surrogates

$\Rightarrow$ New analytic approach for noise reduction

- **DAKOTA** – Design Analysis Kit for Optimization and Terascale Applications

$\Rightarrow$ New standard error estimates for MLMC used in **SNOWPAC**.

Future work and open questions:

- Alternatives for surrogate model (e.g. RBF surrogates)
- Mixed integer optimization (e.g. for NN HP optimization)
- New developments for Gaussian process surrogates (e.g. non-stationary kernels)
- MLMC and MC behavior for benchmark problem

Links:

- SNOWPAC: https://github.com/snowpac/snowpac
- Dakota: dakota.sandia.gov

References:

- F. Augustin, Y. Marzouk, A trust-region method for derivative-free nonlinear constrained stochastic optimization. 2017
- GG, FM, X. Huan, C. Safta, YM, H. Najm, ME, Progress in scramjet design optimization under uncertainty using simulations of the HIFiRE configuration. AIAA 2019