Bayesian Target-Vector Optimization for Efficient Parameter Reconstruction

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Optical metrology: the inverse problem

Problems in optical metrology often **inverse problems**

- Results of experimental measurement $\boldsymbol{y}^*$
- Parameterized model $\boldsymbol{f}(\boldsymbol{p})$ of measurement process (e.g. using FEM)
- Find model parameters $\boldsymbol{p}^*$ that explain measurement results

$$\text{Minimize} \quad \chi^2(\boldsymbol{p}) = \sum_i^N \left(\frac{y_i^* - f_i(\boldsymbol{p})}{\eta_i} \right)^2$$

$\rightarrow$ Minimization algorithm

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Requirements for minimization schemes

- Can handle the discrete results of measurement and model
  - E.g. Levenberg-Marquardt
- Uses available resources sparingly (forward model may be expensive)
  - E.g. methods that use surrogate models (Kriging, GPR, BO)

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Combining both aspects:

Bayesian target vector optimization[1,2]

- Least-square minimization in a Bayesian optimization framework
  - ✓ Responsible use of resources
  - ✓ Direct use of each data channel

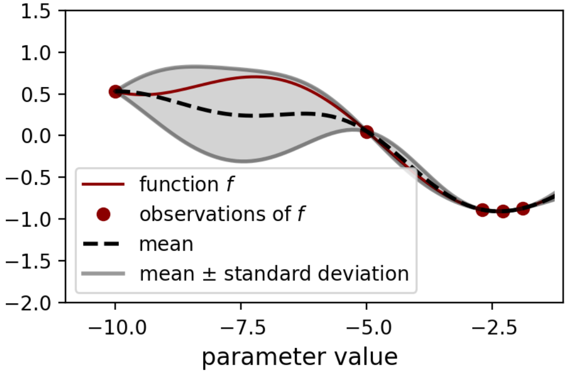
[1] Uhrenholt and Jensen, PMLR (2019)

[2] Plock, et al., Adv. Theory Simul. 5, 2200112 (2022)

Bayesian Optimization, least-square problems, and a new approach

Bayesian optimization fundamentals

- Sequential optimization methods
- Use model observations to create surrogate model (Gaussian process (GP) regression)
- GP completely specified by
  - Mean function $m(\boldsymbol{p})$ (often just m_0)
  - Covariance kernel function $k(\boldsymbol{p}, \boldsymbol{p}')$
  - Model observations



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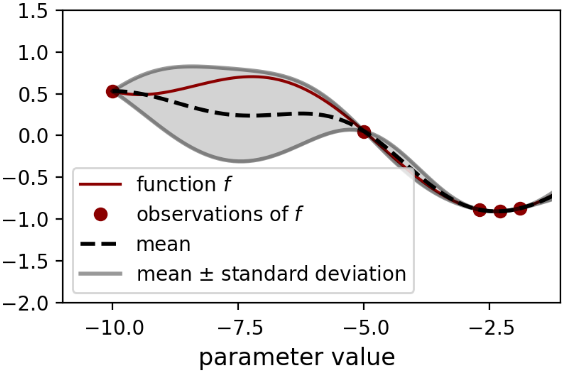

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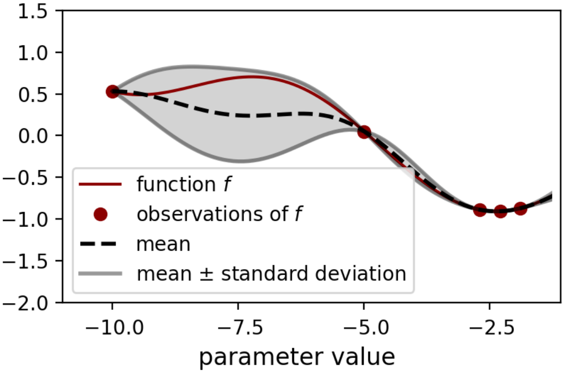
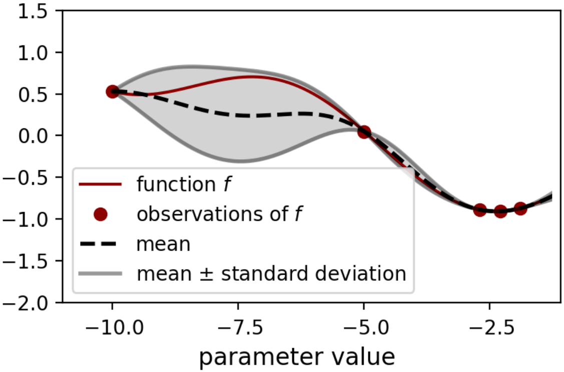


Bayesian optimization fundamentals

- GP predicts $\hat{f}(\boldsymbol{p}) \sim \mathcal{N}(\mu(\boldsymbol{p}), \sigma^2(\boldsymbol{p}))$ for all $\boldsymbol{p} \in \mathcal{X}$
- *Acquisition function* uses $\mu(\boldsymbol{p})$ and $\sigma^2(\boldsymbol{p})$
- Finds useful points in parameter space to achieve goal of optimization



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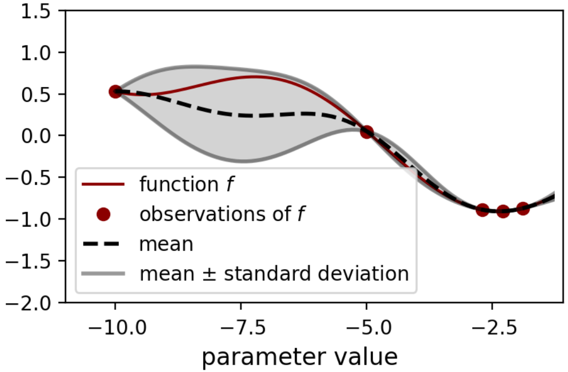
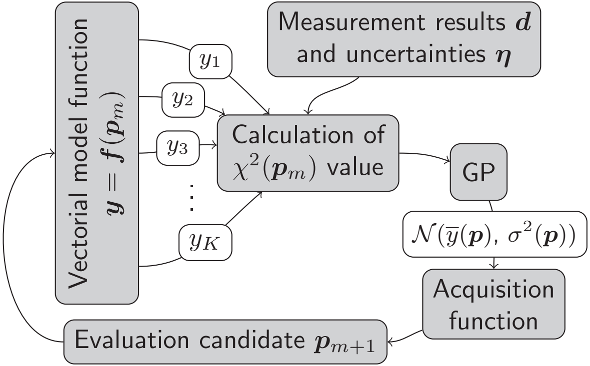


Least-squares using a conventional Bayesian optimization scheme



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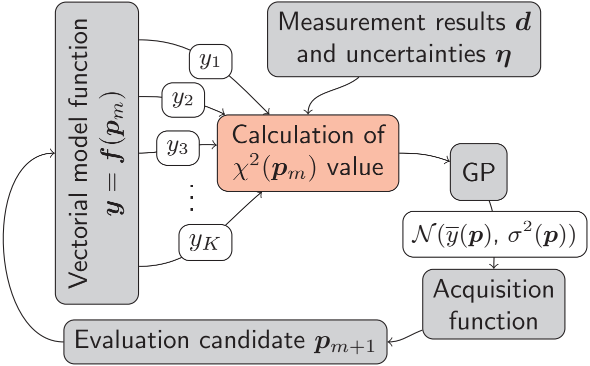

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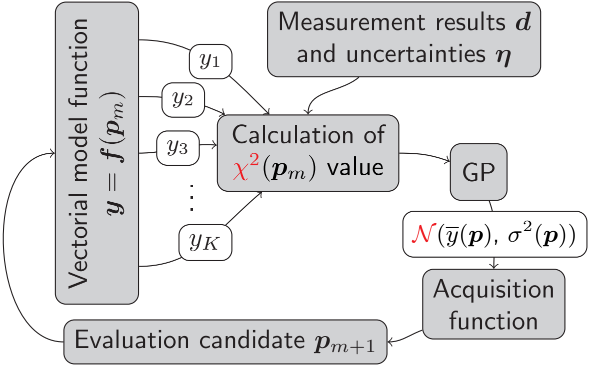
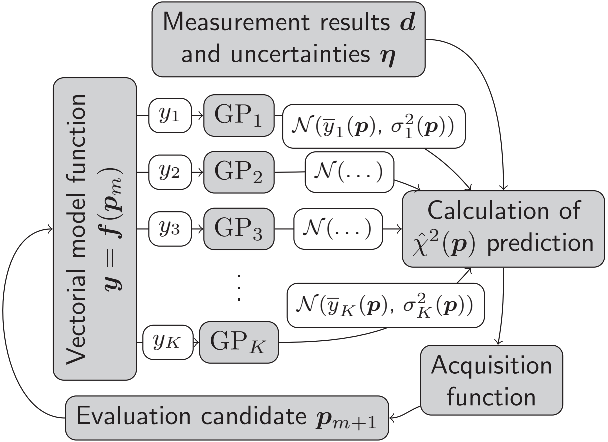


The Bayesian target-vector optimization scheme



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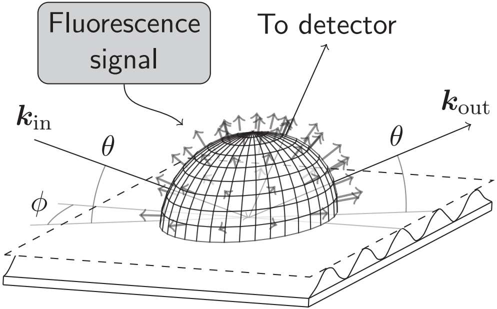
Application of the method

Application of the method: the experimental dataset

- GIXRF (Grazing Incidence XRay Fluorescence)
- Measured at PTB/BESSY



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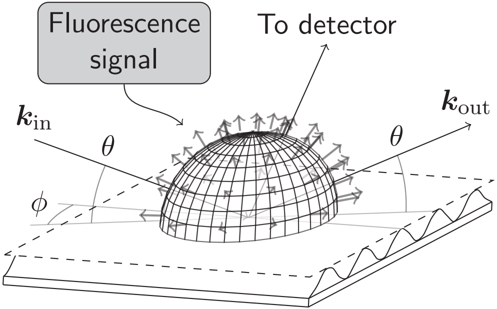

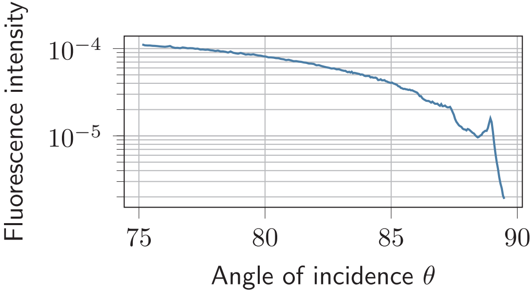

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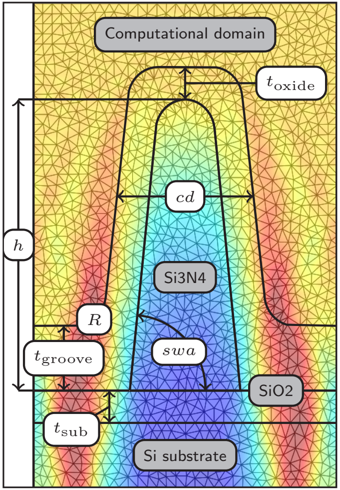
Application of the method: the forward model



- Model created using FEM Maxwell Solver (JCMsuite)
- 10 free parameters
  - 7 geometrical
  - 3 auxiliary

Application of the method: Performance measurement

- Comparing Bayesian Target Vector optimization method (BTVO) against ...
  - Levenberg-Marquardt (LM) least-squares (`scipy` implementation)
  - Conventional Bayesian optimization (BO) method
- Determine mean and standard deviation of six optimization runs
- Metric is distance to best reconstruction result $\boldsymbol{p}_{\mathrm{LSQE}}$ in terms of Gaussian reconstruction uncertainties

$$d(\boldsymbol{p}) = \sqrt{\sum_{i}^{N} \left(\frac{p_i - p_{\mathrm{LSQE},i}}{\epsilon_{\mathrm{LSQE},i}} \right)^2}, \quad \epsilon_i \text{ from Jacobian at } \boldsymbol{p}_{\mathrm{LSQE}}$$

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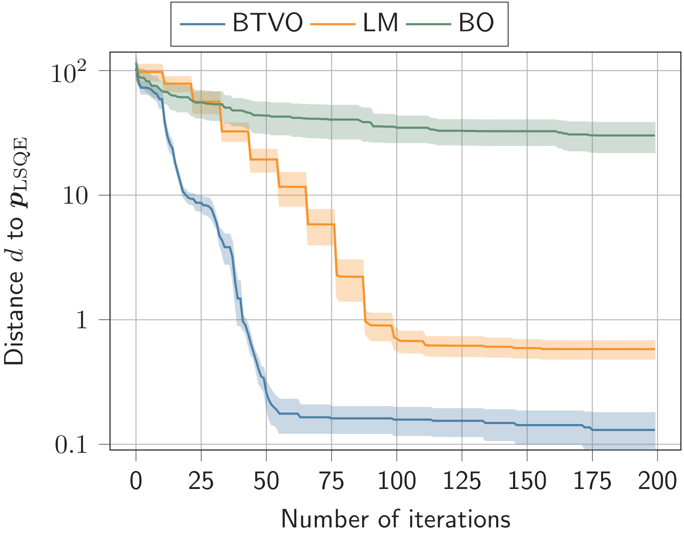
Reconstruction results



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- BTVO and LM reach distance of less than 1 standard deviation
- BTVO outperforms LM: faster and closer to $\boldsymbol{p}_{\mathrm{LSQE}}$

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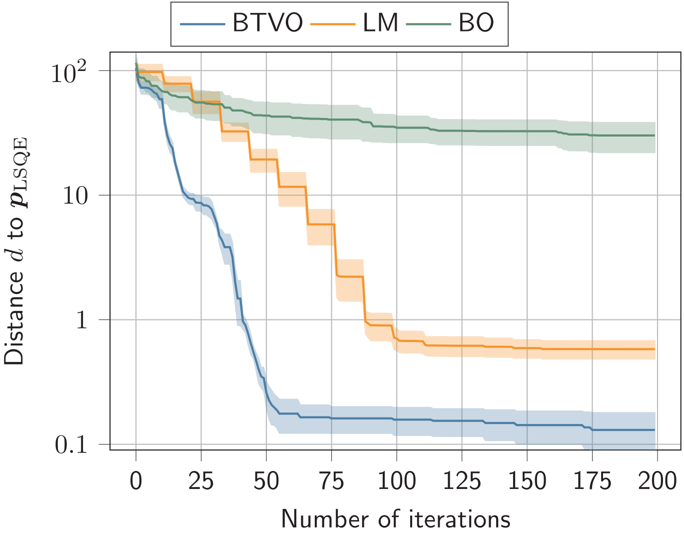

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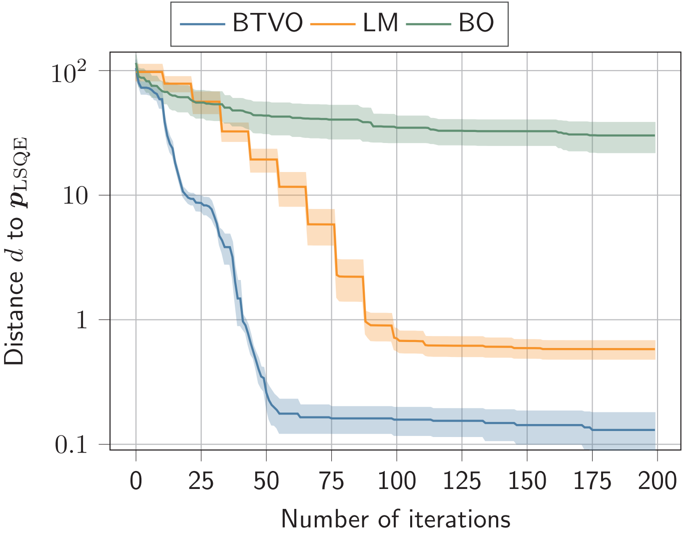

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Parameter uncertainty estimation using MCMC on a trained surrogate model

MCMC with a trained multi output surrogate model

- Markov Chain Monte Carlo (MCMC) often used to determine parameter uncertainties and correlations
- Fitting an error model to the data
- Requires many samples of objective function

- BTVO and BO automatically train surrogate model
- Sampling of surrogate model cheaper than objective function
- Use trained surrogate models as stand-in for objective function

$\rightarrow$ Perform MCMC on trained surrogate model

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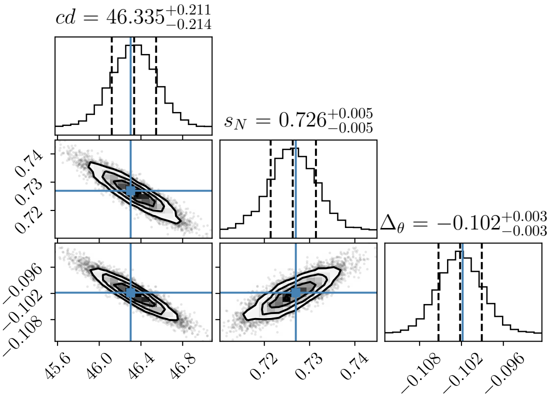
GIXRF MCMC analysis

Applied to GIXRF forward problem[1]

- Reveal correlations between parameters (also discussed in [2])
- MLE and uncertainties confirm optimization reconstruction results



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Summary

- Bayesian Target Vector optimization performs very well
- Manages to outperform a traditional least-square algorithm for the considered parameter reconstruction problem
- Multi-output GP yields fast & inexpensive MCMC option

Thank you for your interest!

Contact: plock@zib.de

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GEFÖRDERT VOM

Bundesministerium
für Bildung
und Forschung

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aufgrund eines Beschlusses
des Deutschen Bundestages

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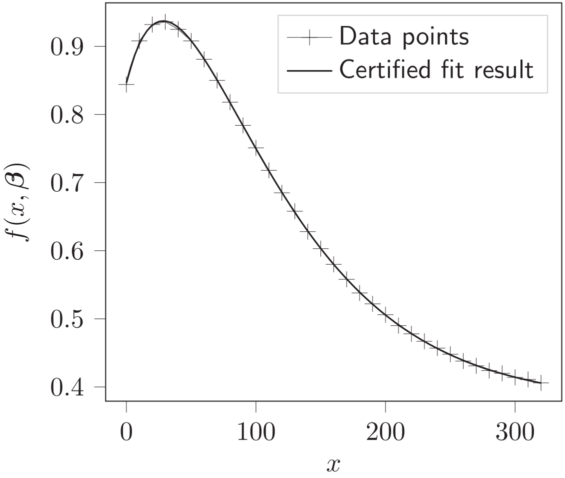
The MCMC demonstration dataset (MGH17)

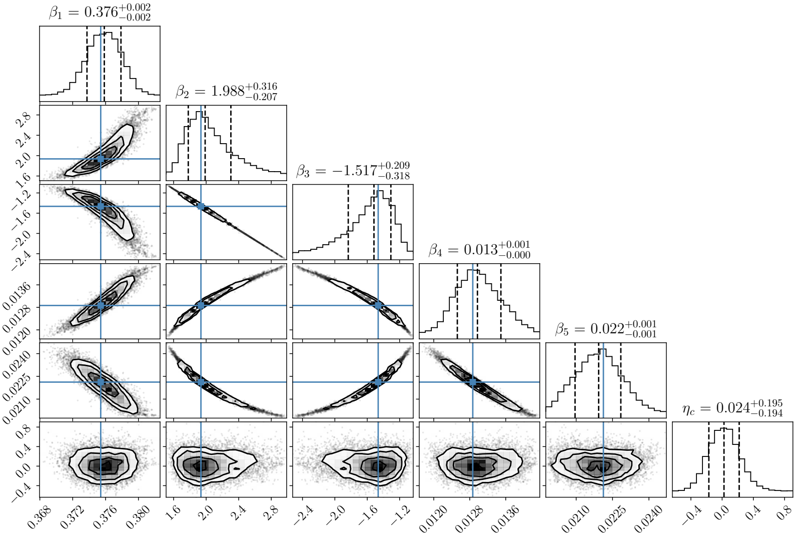


- MGH17 dataset[1] from NIST Standard Reference Database
- 33 discrete data points and 5 free parameters $(\beta_1, \ldots, \beta_5)$

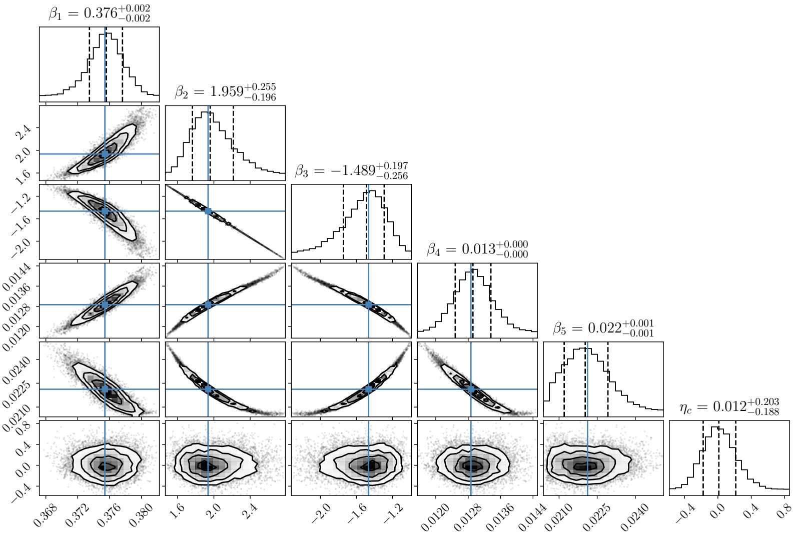
$$f(x,\boldsymbol{\beta}) = \beta_1 + \beta_2 \mathrm{e}^{-x\cdot\beta_4} + \beta_3 \mathrm{e}^{-x\cdot\beta_5}$$

[1] https://www.itl.nist.gov/div898/strd/nls/data/mgh17.shtml

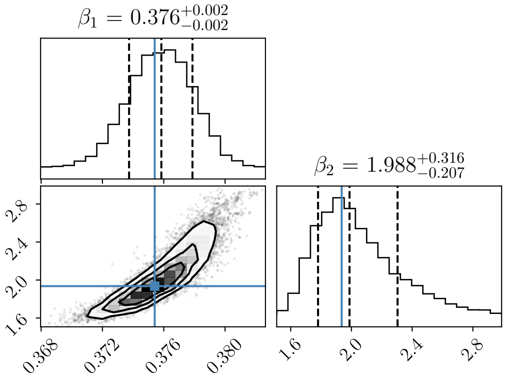
MCMC for MGH17 (50000 obs. of model function / 32 walkers)



MCMC for MGH17 (50000 obs. of surrogate model / 32 walkers)



MCMC for MGH17 (side by side comparison)



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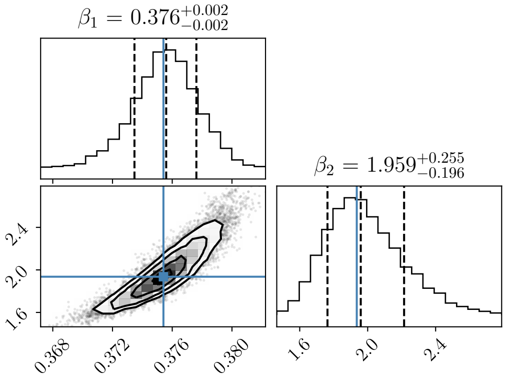
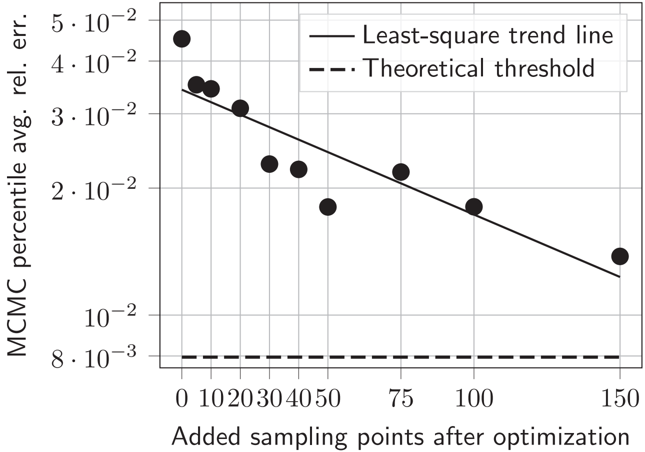


Using surrogate model.

GP MCMC convergence



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- Add data points around the least-square minimum
- Surrogate becomes more accurate
- Measure convergence by looking at percentiles
- Relative error of percentile positions decreases with added data points

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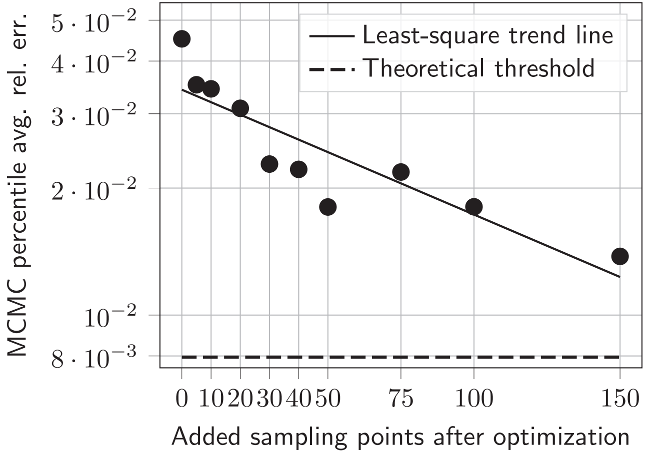

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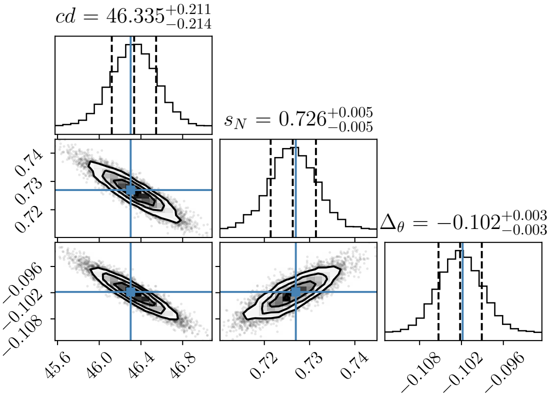

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