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UNCERTAINTY-QUANTIFIED MACHINE MODEL CONSTRUCTION FROM NONLINEAR ORBIT RESPONSE USING PHYSICS-INFORMED GAUSSIAN PROCESSES

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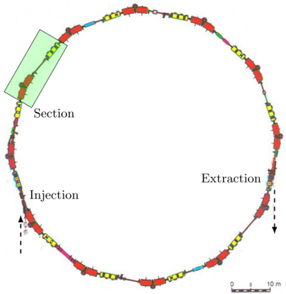
April 9, 2025

MACHINE MODEL OF SYNCHROTRON

Idea: Construct effective machine model of synchrotron



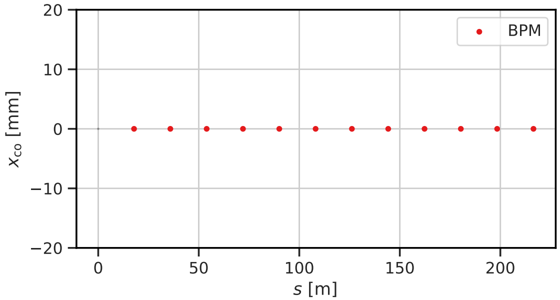
As an example: Heavy-ion synchrotron SIS18 located at GSI-Fair

- 12-fold symmetry
- Bending dipoles in red
- Quadrupoles in yellow

Image: Rahul Singh, “Tune measurement at GSI SIS-18: Methods and applications”, PhD thesis

MOTIVATION

Simulations: Synchrotron SIS18



Deviation **at the BPMs** (Beam Position Monitors):

- Is zero here
- Minimized by standard closed orbit (co) correction method
  (e.g. Singular Value Decomposition based)

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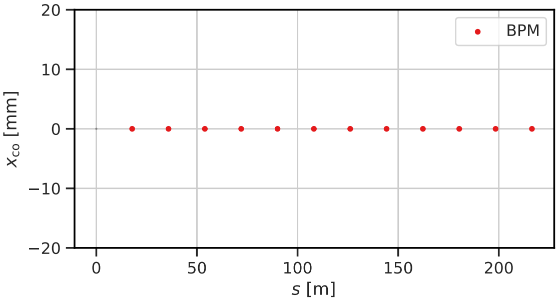

Deviation **at the BPMs** (Beam Position Monitors):

- Is zero here
- Minimized by standard closed orbit (co) correction method (e.g. Singular Value Decomposition based)

→ What does the closed orbit look like?

MOTIVATION

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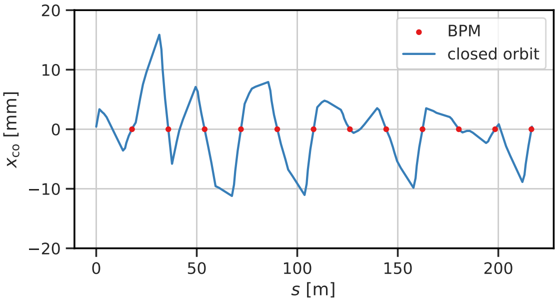

Distorted closed orbit:

- Is zero at BPMs
- Caused by dipole-like errors (e.g. quadrupole misalignment)

Remaining closed orbits with RMS=0 at BPMs

MOTIVATION

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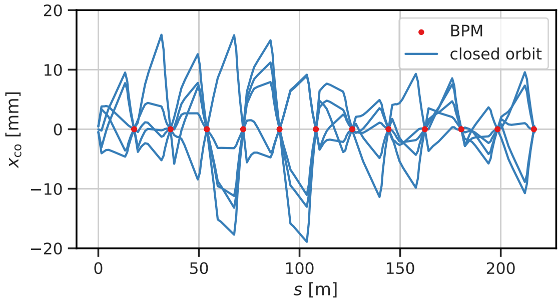


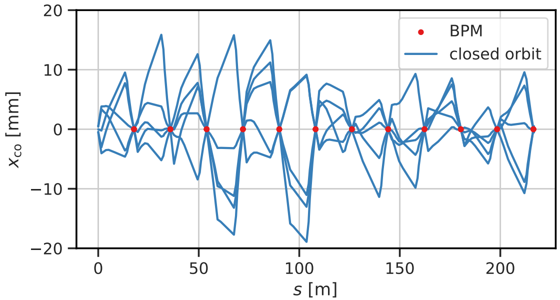
Distorted closed orbit:

- Is zero at BPMs
- Caused by dipole-like errors (e.g. quadrupole misalignment)
- Different quadrupole misalignment results in a different closed orbit

Remaining closed orbits with RMS=0 at BPMs

MOTIVATION

Simulations: Synchrotron SIS18



Remaining closed orbits with RMS=0 at BPMs

Distorted closed orbit:

- Is zero at BPMs
- Caused by dipole-like errors (e.g. quadrupole misalignment)
- Different quadrupole misalignment results in a different closed orbit

→ Develop a closed orbit model **everywhere** with uncertainty quantification from orbit response measurements

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MOTIVATION

Example for application of co model: Beamsteering at septum

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MOTIVATION

Example for application of co model: Beamsteering at septum

- Use e.g. YASP (Yet Another Steering Program) to predict closed orbit in beetween BPMs
- Use prediction to calculate steering

→ Only **one** underlying MAD-X model

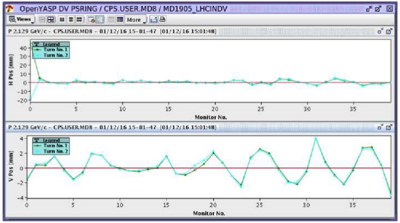

Image: Fuchsberger, Kajetan and others, “Operational Experience during the LHC Injection Tests”

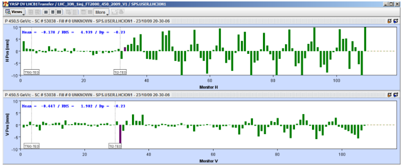

Image: Serluca, M. and Aumon, S., and Efthymiopoulos, I. “The (7,7) Optics at CERN PS”

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MOTIVATION

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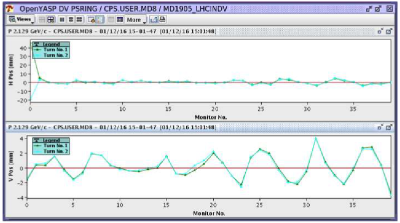

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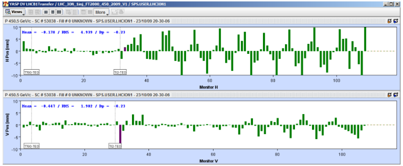

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- We do not exactly know the position of the closed orbit → Use uncertainty

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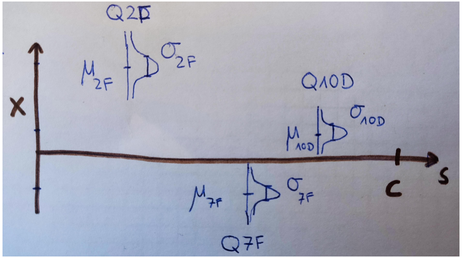
IDEA

A closed orbit model with intrinsic uncertainty quantification

- Constructed from orbit response measurements
- Uses physics-informed Gaussian Process (GP) model
- Hyperparameters: Distribution of quadrupole misalignment
- Build on top of stochastic ensemble of MAD-X (simulation software) lattices

Sketch:



DOF: Quadrupole misalignment

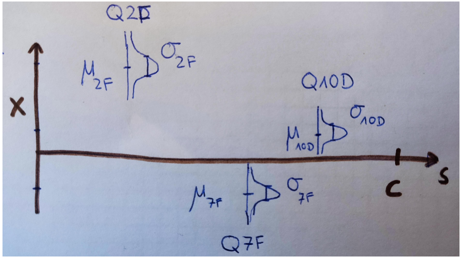
IDEA

A closed orbit model with intrinsic uncertainty quantification

- Constructed from orbit response measurements
- Uses physics-informed Gaussian Process (GP) model
- Hyperparameters: Distribution of quadrupole misalignment
- Build on top of stochastic ensemble of MAD-X (simulation software) lattices
- Beam physics: How to infer knowledge in between BPMs?

→ Exploit nonlinearity caused by sextupoles for chromaticity correction

Sketch:



DOF: Quadrupole misalignment

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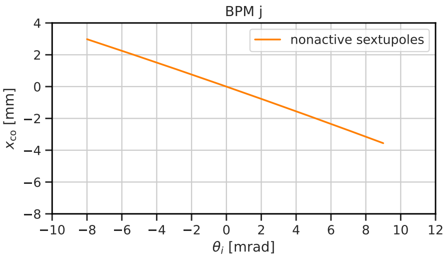
IDEA

Orbit response:



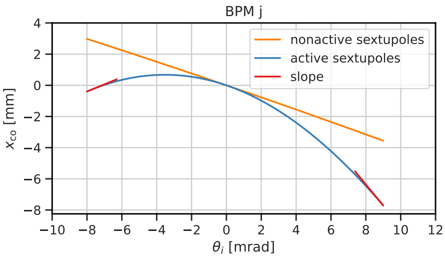
Distortion of the closed orbit:

$$x_{\mathrm{COD}}(s) = \theta \cdot \sqrt{\beta_x(s_0) \cdot \beta_x(s)} \cdot \frac{\cos(|\Delta\psi_x| - \pi Q_x)}{2\sin(\pi Q_x)}$$

- Orbit Response Matrix (ORM = $\Delta x / \Delta\theta$)
- Used by tool LOCO (Linear Optics from Closed Orbits) to fit machine model
- No information in between BPMs: Linear orbit response at BPMs due to kicks

IDEA

Orbit response:



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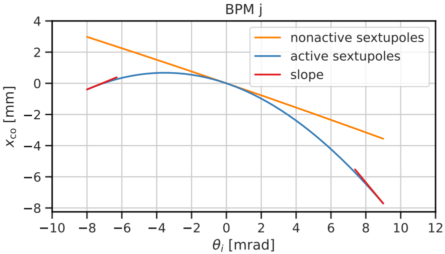

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$\rightarrow$ Crucial ingredient: nonlinearity from sextupoles

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KEY ADVANTAGES

Key advantages of multidimensional GP compared to LOCO (Linear Optics from Closed Orbits - Software to create machine model):

1. Can be more **sample efficient** with an active learning approach than measuring an orbit response matrix
2. Predict the closed orbit with uncertainty in between BPMs
3. Fits a distribution of parameters (dipole-like field errors) which inherently models uncertainty
4. Incorporates of measurement uncertainty from BPM noise

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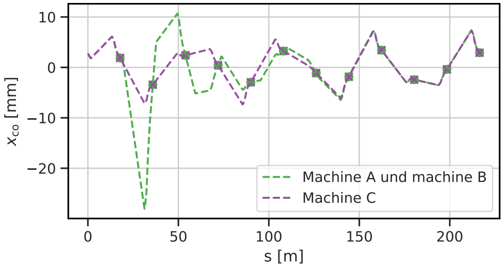
CONTENT

1. Motivation and idea
2. **Is it possible?**
3. Approach and small example
4. Outlook

POSSIBLE?

Is it possible to distinguish two setups of a synchrotron (A vs. C)?

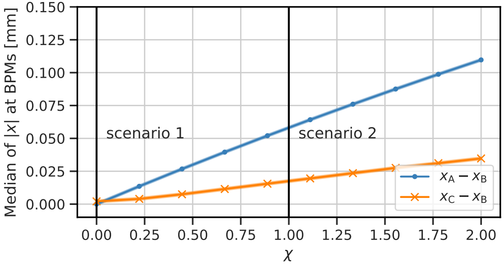


- Machine A: $\mu_{\mathrm{Q2F}} = 5$mm, $\chi = [0...2]$
- Machine B: $\mu_{\mathrm{Q2F}} = 5$mm, $\chi = 0$
- Machine C: $\mu_{\mathrm{Q2F}} = 0$mm, $\chi = [0...2]$

$\chi = 0$, no sextupoles are activated
$\chi = 1$, sextupoles correct natural chromaticity

Simulation closed orbit of machines for $\chi = 0$, corrected + $\Delta\theta_1$

POSSIBLE?



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- Machine B: $\mu_{\mathrm{Q2F}} = 5$mm, $\chi = 0$
- Machine C: $\mu_{\mathrm{Q2F}} = 0$mm, $\chi = [0...2]$

Yes, possible with nonlinear machine:

- Scenario 1: vanishing discrepancy between A and C $\rightarrow$ no distinction of 5mm misalignment possible
- Scenario 2: > 0.04mm median discrepancy between A and C $\rightarrow$ distinction possible!

CONTENT

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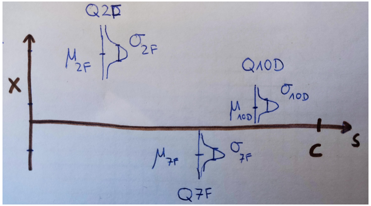
APPROACH: KEY INGREDIENTS

- A GP for every BPM:
  - Input: vector of steerer angles $\vec{\theta} = (\theta_{\text{steerer1}}, \ldots, \theta_{\text{steerer12}})$
  - Output: deviation Δx_{atBPMi}
- Hyperparameters are the Gaussian **distributions** $(\mu_{\text{Q}}, \sigma_{\text{Q}})$ of the misalignments of the quadrupoles (dipoles-like errors)
- Use Monte Carlo (MC) method to sample closed orbits = realizations
- Simulate with MAD-X (simulation tool) the realization to include full beam dynamics around the machine
- **Estimate** kernel (and mean function) via statistics of the realizations [1]

([1] Papers: "Physics-informed kriging: A physics-informed Gaussian process regression method for data-model convergence." by X. Yang, G. Tartakovsky, and A. Tartakovsky)

SMALL EXAMPLE



- Lattice of SIS18 with active sextupoles to correct natural chromaticity ($\chi = 1$)

- "Real" accelerator:
  - $\mu_{\text{Q2F}} = 5$mm,
  - $\mu_{\text{Q7F}} = -2$mm,
  - $\mu_{\text{Q10D}} = 1.3$mm

  $\rightarrow$ returns observations (x_{co} at BPMs)

- Model accelerator: DOF are μ_{Q2F}, μ_{Q7F}, μ_{Q10D}, σ_{Q2F}, σ_{Q7F}, σ_{Q10D}

- Only corrector 7 is varied, all other are set to zero

APPROACH

1. Condition DOF (μ_Q, σ_Q) to set of observation data ✓
   - Establish a model
   - Establish reading out of a kernel functions
   - Find effective way to evaluate Log Marginal Likelihood (LML)
   - Establish optimization of hyperparamters

2. Evaluate closed orbit distribution ✓

3. Choose most promising next input $\vec{\theta}$ with acquisition function

4. Update GP with new data

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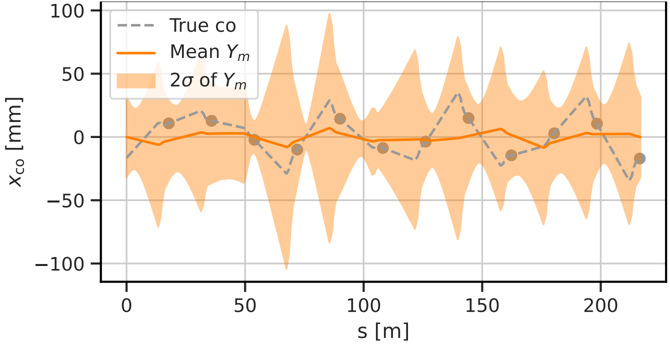
CONTENT

1. Motivation and idea
2. Is it possible?
3. **Approach and small example**
   - Number of observation data
   - Influence position of steerer
   - Influence noise on observations
4. Outlook

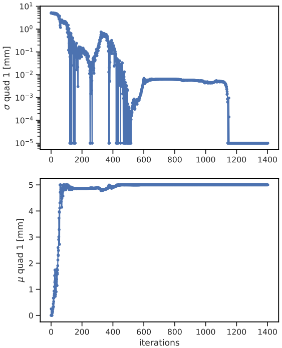
BEFORE CONDITIONING

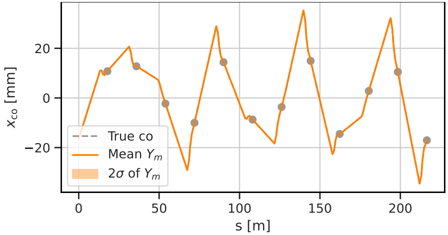


- Conditioning DOF
- Set initial value to zero misalignment
- Compare to true closed orbit

OBSERVATION DATA SET OF 4 VALUES θ

3 DOF: $\mu_{\mathrm{Q2F}} = 5$mm, using only steerer 7





- Use only steerer 7
- Use **four** values of theta

→ For this setup four values are sufficient to reduce the uncertainty

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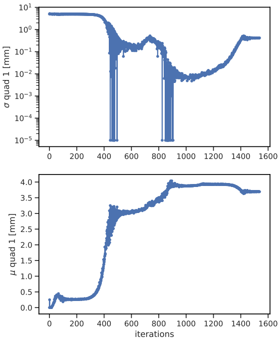
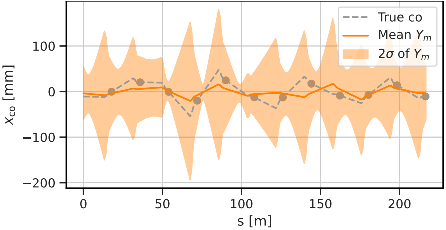
OBSERVATION DATA SET OF 2 VALUES θ

3 DOF: $\mu_{\mathrm{Q2F}} = 5$mm, using only steerer 7





- Use only steerer 7
- Use two values of theta

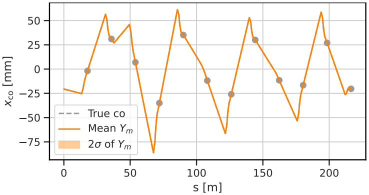
$\rightarrow$ For 3 DOFs more values are needed

INFLUENCE POSITION OF STEERER

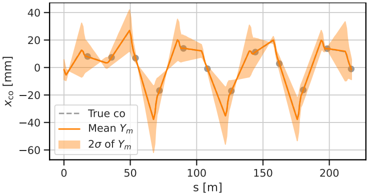
3 DOF ($\mu_{\mathrm{Q2F}} = 5$mm, $\mu_{\mathrm{Q7F}} = -2$mm, $\mu_{\mathrm{Q10D}} = 1.3$mm), using 4 observation values

After conditioning:

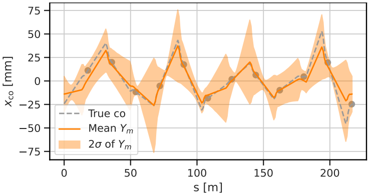
Steerer 7:



Steerer 1:



Steerer 11:



Steerer 11: Phase advance between steerer and quadrupole with DOF is unfavorable

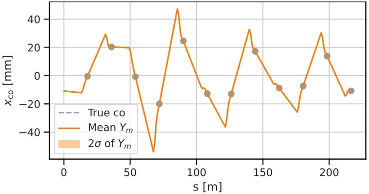
$\rightarrow$ Choose the appropriate steerer: To reduce uncertainty σ_{Q}

INFLUENCE OBSERVATION NOISE

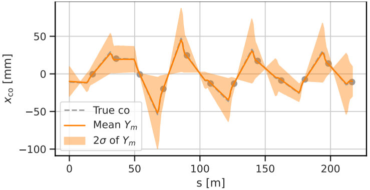
3 DOF ($\mu_{\text{Q2F}} = 5$mm, $\mu_{\text{Q7F}} = -2$mm, $\mu_{\text{Q10D}} = 1.3$mm), using steerer 7, using 4 observation values, Gaussian distributed noise

After conditioning:

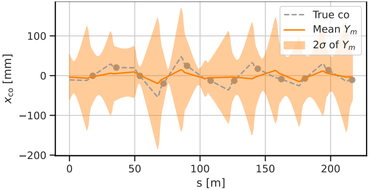
$\sigma_{\text{noise}} = 0.1$mm:



$\sigma_{\text{noise}} = 0.3$mm:



$\sigma_{\text{noise}} = 0.7$mm:



→ For observation noise at BPMs less than 0.1mm the uncertainty can be reduced to exactly model the closed orbit

SUMMARY AND OUTLOOK

We have:

- Established a model
- Conditioned DOF $(\mu_{\mathrm{Q}}, \sigma_{\mathrm{Q}})$ to set of observation data
- Established reading out of a kernel functions
- Found effective way to evaluate Log Marginal Likelihood (LML)
- Established optimization of hyperparameters
- Evaluate closed orbit distribution

Future work:

- Choose most promising next input $\vec{\theta}$ with acquisition function $\rightarrow$ Bayesian Inference

Outlook:

- Use developed multidimensional GP model with ensemble of MADX lattices for different applications than CO

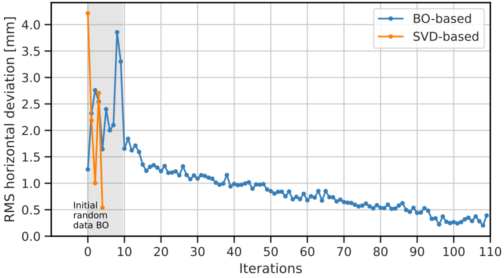
BACKUP

BEAM TIME RESULTS AT SIS18

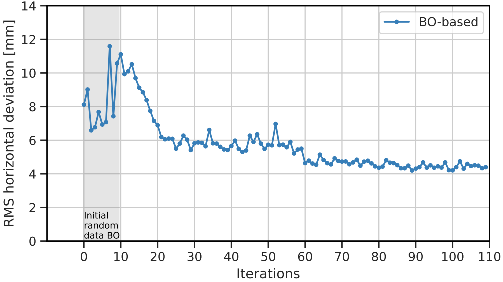
Masters's thesis: Reduce closed orbit deviation at BPMs of SIS18

- Use Gaussian Processes and Bayesian Optimization (BO)
- Compare to conventional method (based on Singular Value Decomposition (SVD))

Standard optics:

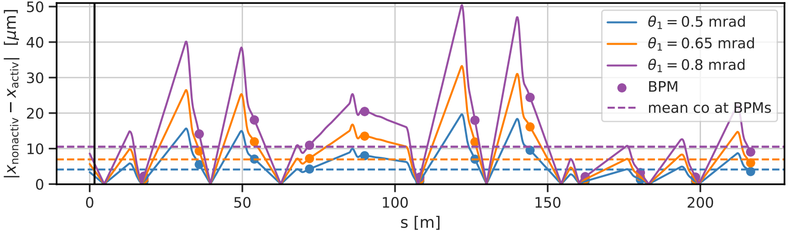


Challenging optics:



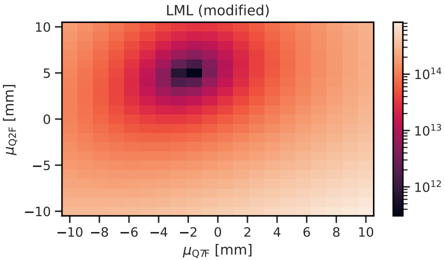
DIFFERENCE OF THE CLOSED ORBITS

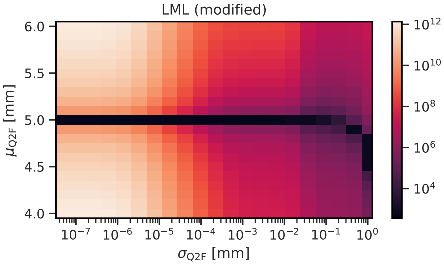
Absolute difference of closed orbits for activated $(x_{\text{activ}}, \chi_x = 1)$ and non-activated $(x_{\text{nonactiv}}, \chi_x = 0)$ sextupoles in μm



- One-turn measurement has up to 100 μm (Conrad), to achieve 3μm at 1kHz revolution frequency: Averaging over 1000 turns $(100/\sqrt{M} = 100/\sqrt{1000} \approx 3.2)$
- For $3\sigma \approx 10\mu$m, steerer angles has to be at least ± 0.8 mrad

TOPOLOGY OF LML





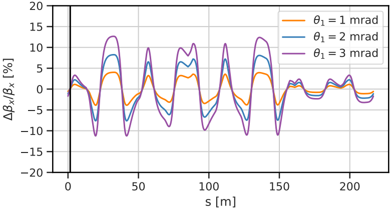
Log marginal likelihood (LML) with $\mathbf{K}$=Covariance matrix:

$$\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}) = -\frac{1}{2}\mathbf{y}^T\mathbf{K}^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K}| - \frac{N}{2}\log(2\pi)$$

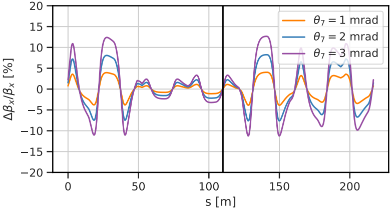
BETA BEATING

Horizontal beta beating for steerer 1 and 7 for different values (1, 2, and 3 mrad), while the sextupole strengths are set to achieve $\chi = 1$

Steerer 1:



Steerer 7:



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- Influence of steerer depends on position

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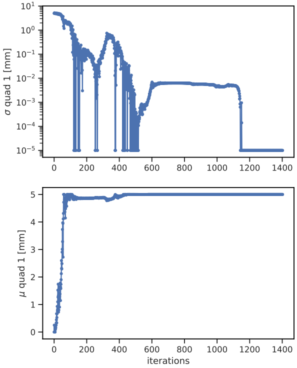
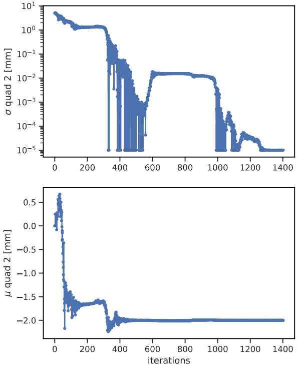
CONDITIONING DOF

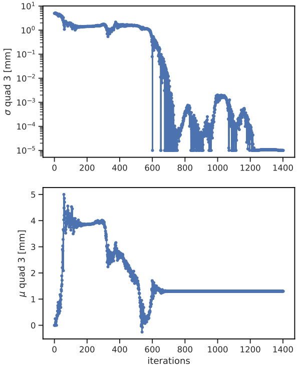
$\mu_{\mathrm{Q2F}} = 5\mathrm{mm}$



$\mu_{\mathrm{Q7F}} = -2\mathrm{mm}$



$\mu_{\mathrm{Q10D}} = 1.3\mathrm{mm}$



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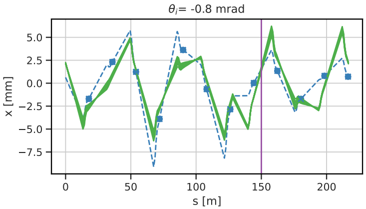
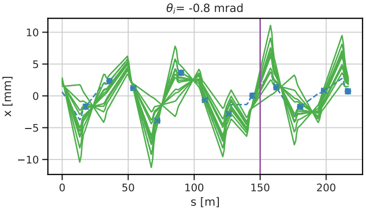
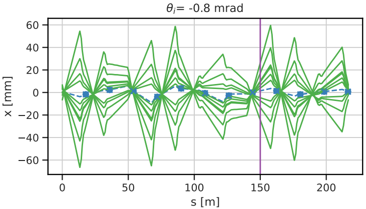
MISALIGNMENT QUADRUPOLE 2F



$\sigma_{\text{quad}} = 6\text{e} - 5\text{m}$



$\sigma_{\text{quad}} = 6\text{e} - 4\text{m}$



$\sigma_{\text{quad}} = 6\text{e} - 3\text{m}$

Only for the 2nd foc quadrupole, σ_{quad} is varied, μ_{quad} is fixed. σ_{co} depends on σ_{quad} as we expected.

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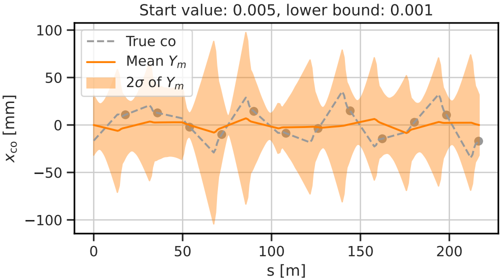
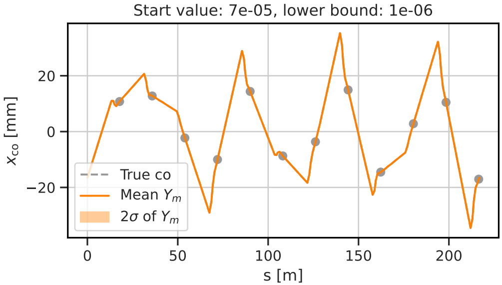
CLOSED ORBIT MODEL

Before Optimization:



After Optimization:



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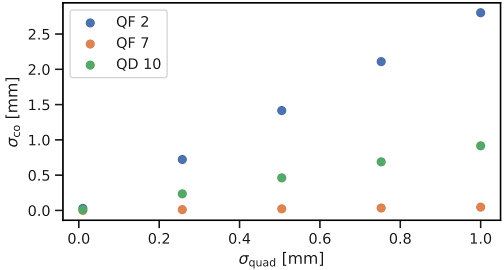
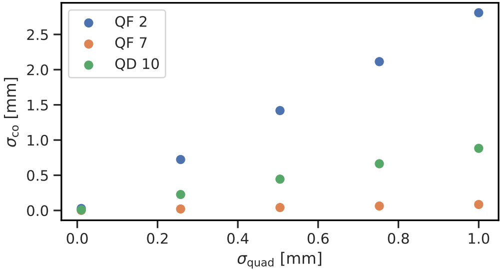
INFLUENCE σ_{quad} ON σ_{co}

Evaluated at s = 150m, number realizations M = 100



$\theta_i = -8\text{mrad}$



$\theta_i = 2\text{mrad}$

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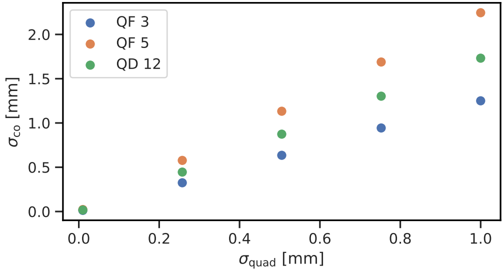
INFLUENCE σ_{quad} ON σ_{co}

Evaluated at s = 150m, number realizations M = 100



$$\theta_i = -8\text{mrad}$$