Imperial College London

SCHOOL OF DATA ANALYSIS

SLAC

UNIVERSITY OF OXFORD

Black-box optimisation with Local Generative Surrogates

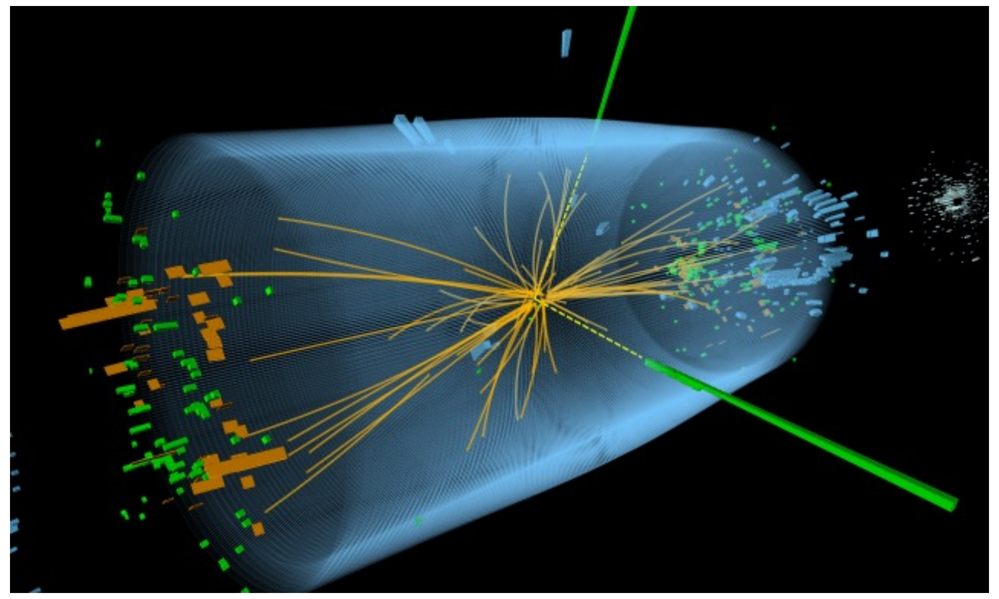
April 2023

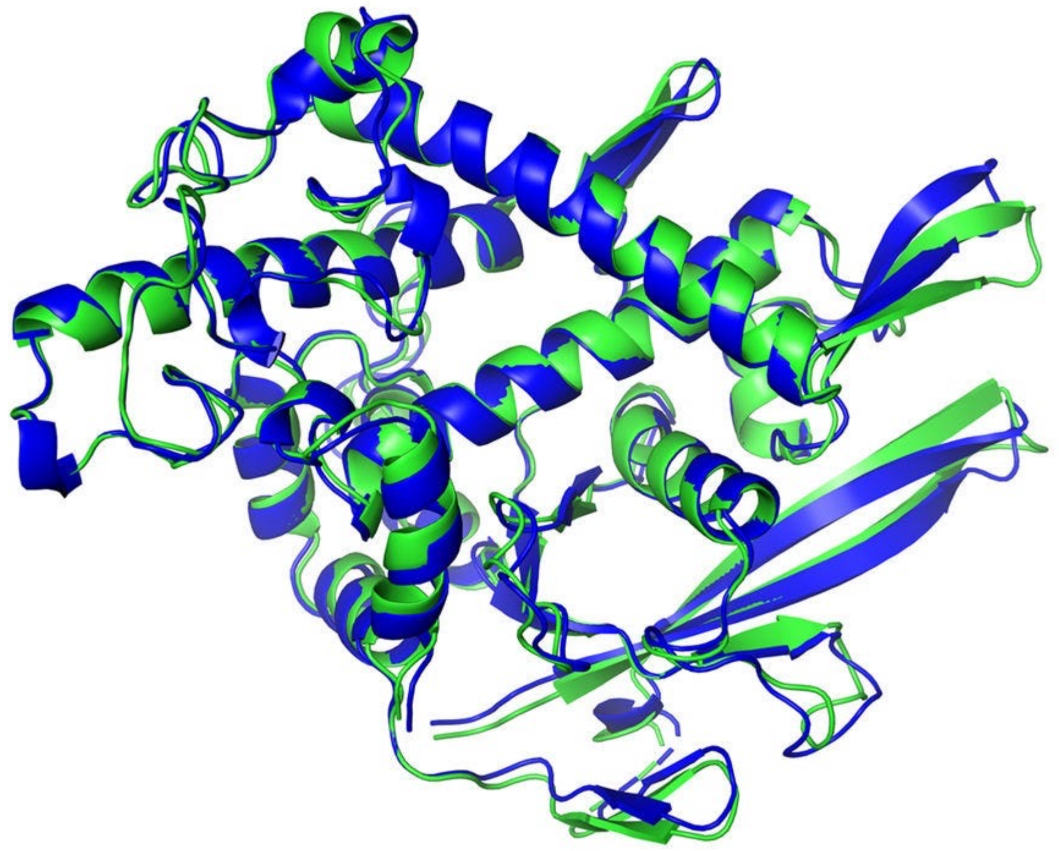
Sergey Shirobokov

In NeurIPS 2020:
Black-box optimization with Local Generative Surrogates
S.Shirobokov*, V.Belavin*, M.Kagan, A. Ustyuzhanin, A.G. Baydin

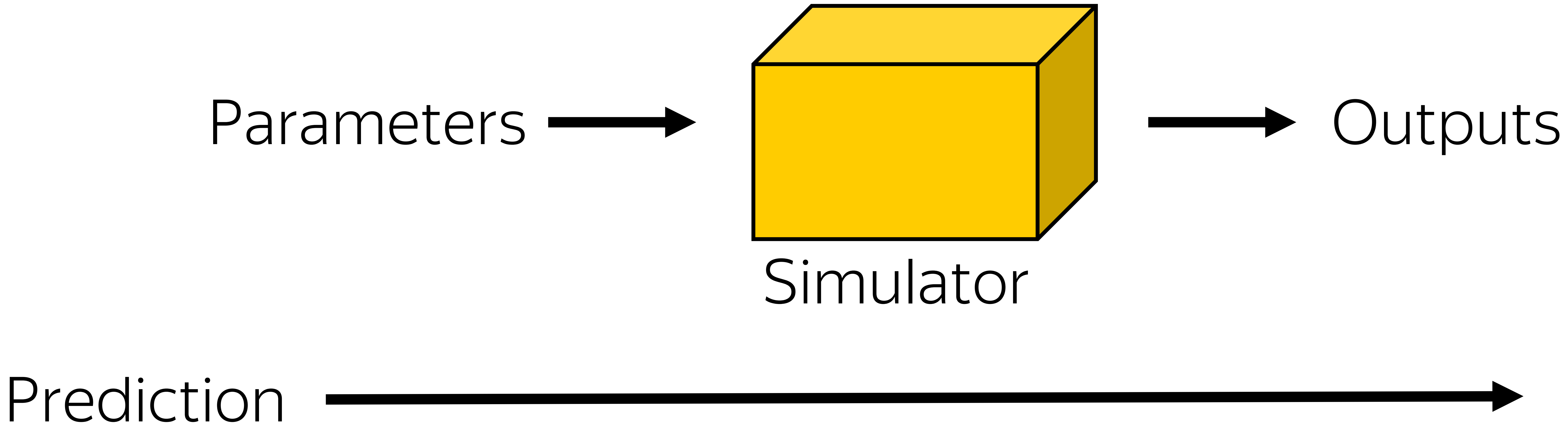
Simulators

- High energy physics
- Drug discovery
- Weather predictions
- Vehicle control
- Hardware
- Material science





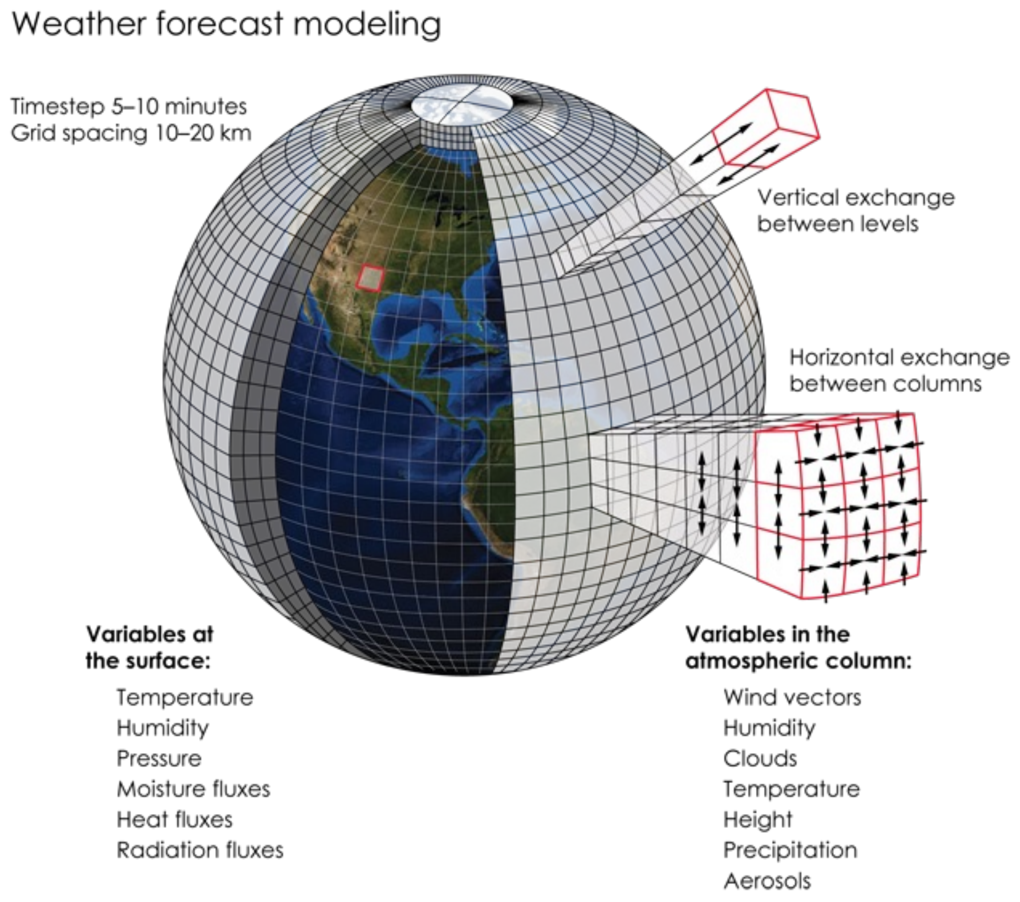
Simulators

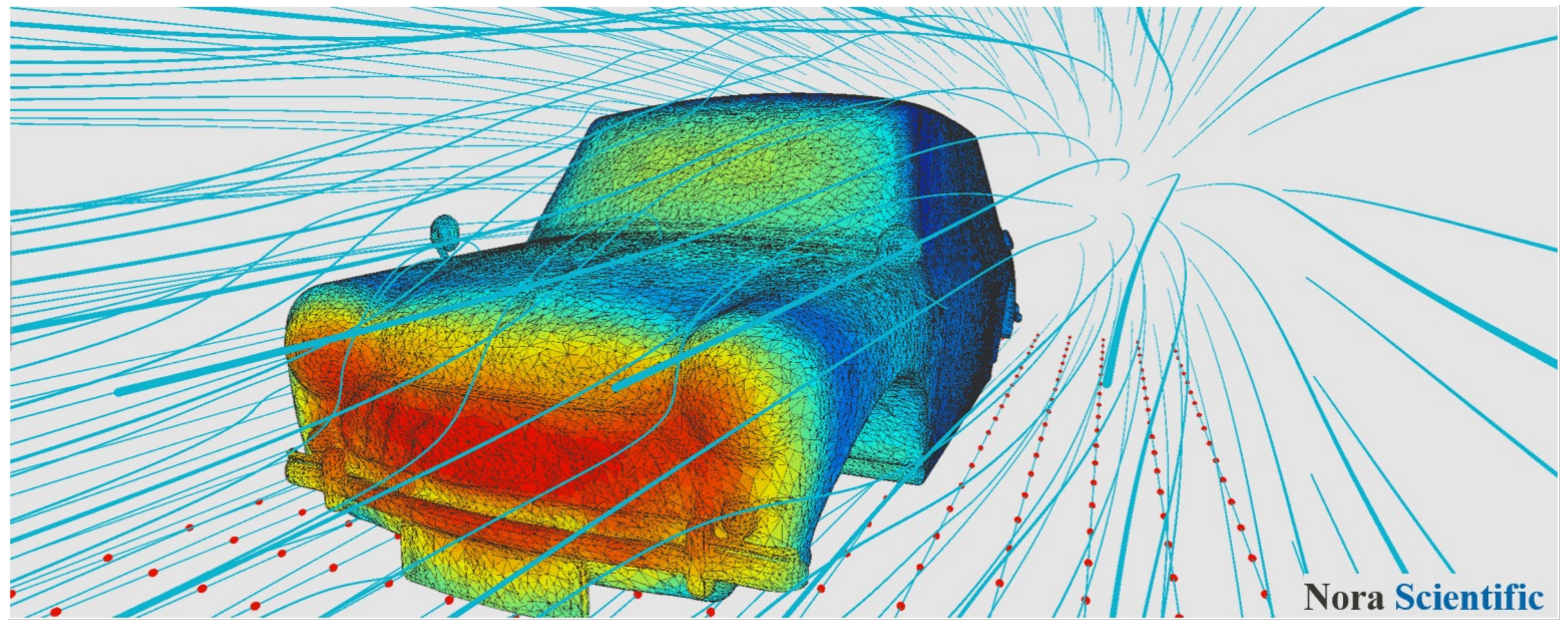


Parameters → Simulator → Outputs

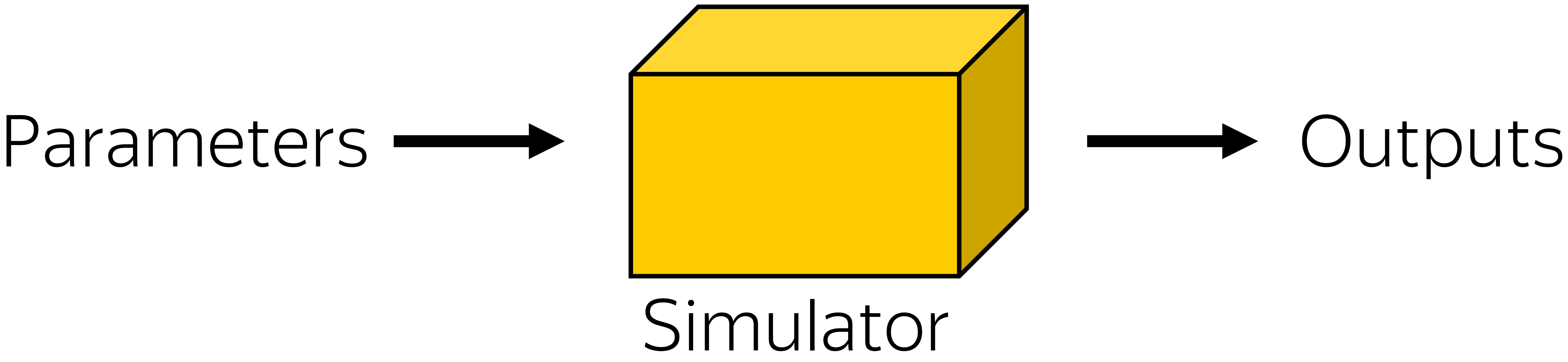
Prediction →

- Simulation of a (stochastic) system
- Output samples from a distribution





Simulators



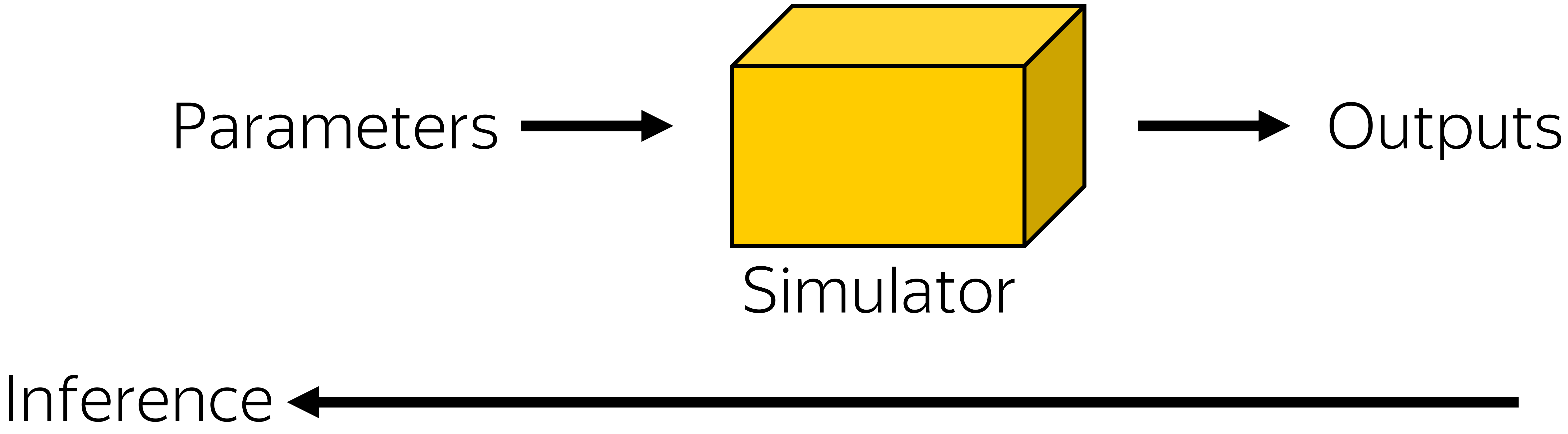
Prediction

- Simulation of a (stochastic) system
- Output samples from a distribution

Inference

- Find parameters that explain observed data
- Perform optimisation w.r.t to the parameters
- Solve inverse problem

Simulators

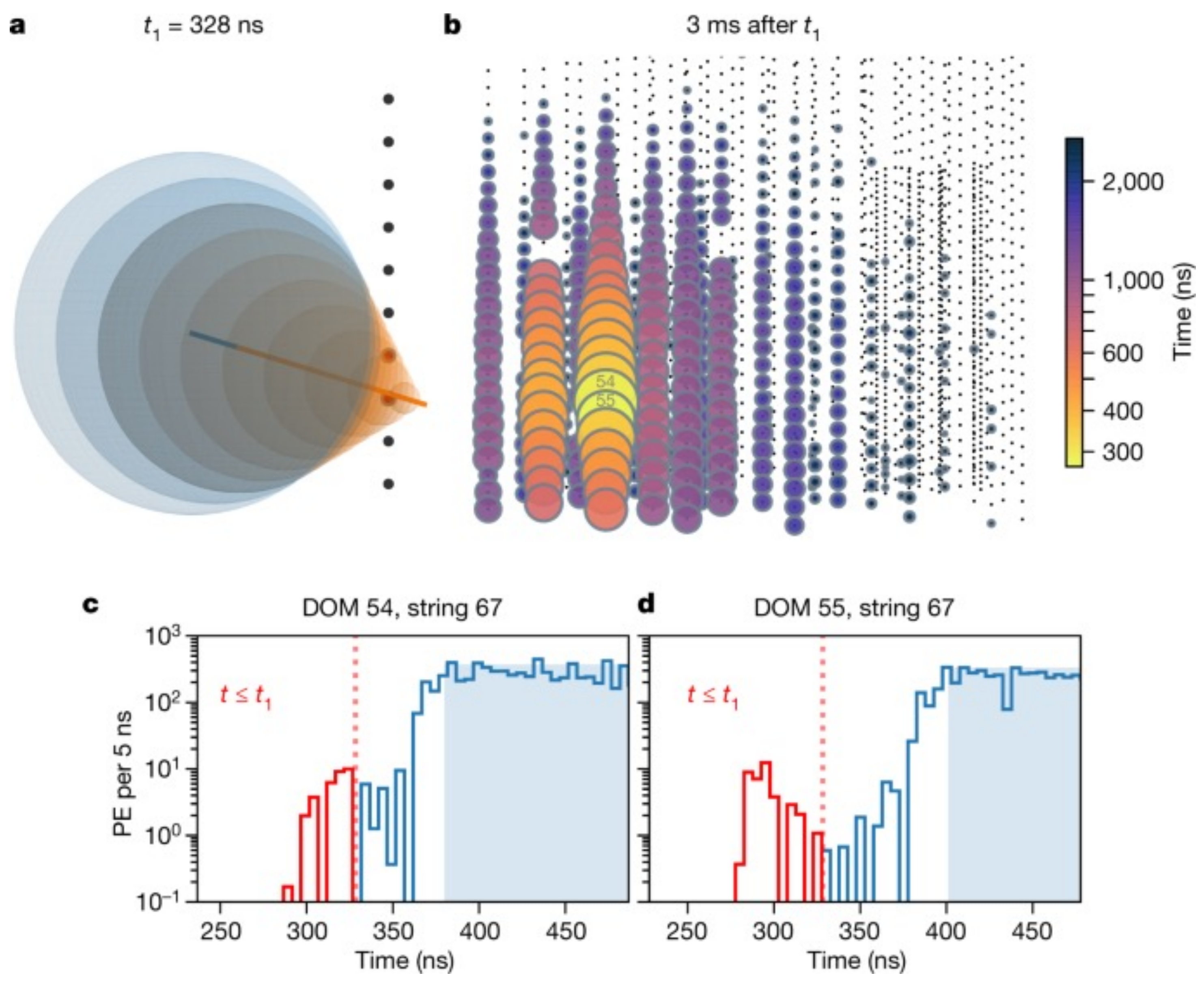


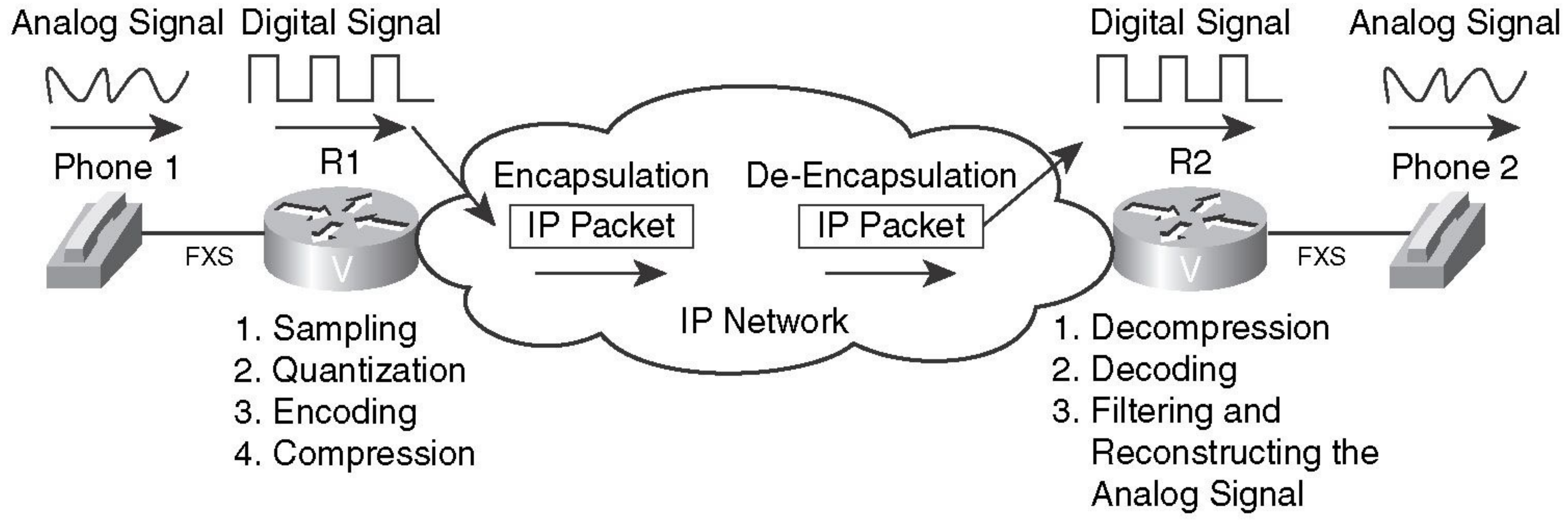
Parameters

Simulator

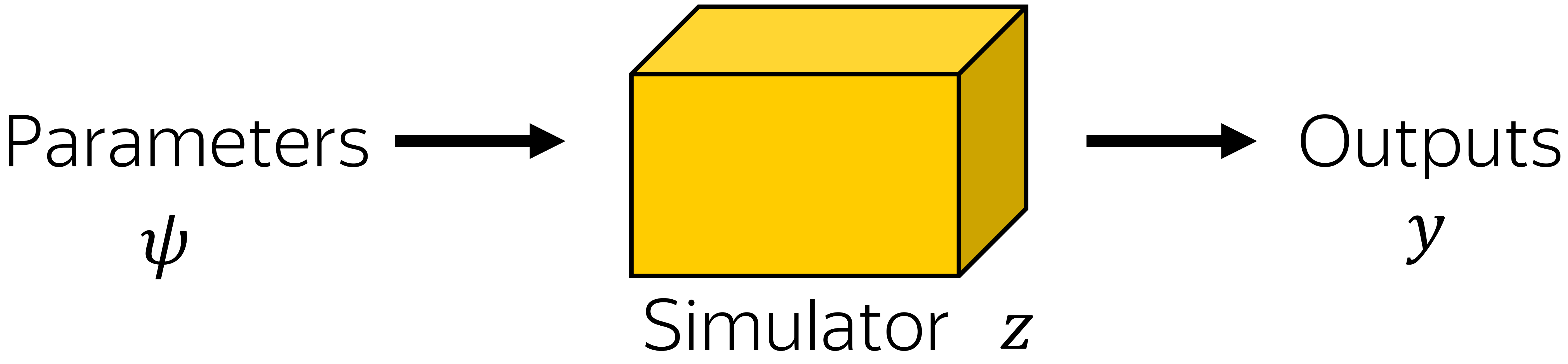
Outputs

Inference





Simulator-based optimisation



Parameters ψ → Simulator z → Outputs y

Prediction →

$$y, z, \psi \sim p(y, z, \psi)$$

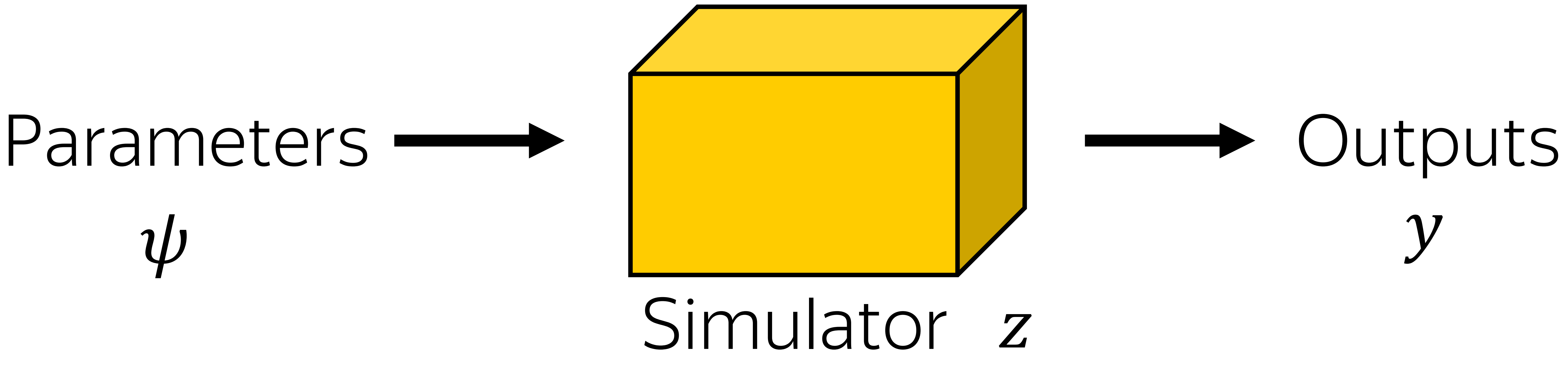
Observe: $y \sim p(y|\psi) = \int p(y, z|\psi) dz$

Inference ←

Likelihood: $p(y|\psi) = \int p(y, z|\psi) dz$

Posterior: $p(\psi|y) = \frac{p(y|\psi)\, p(\psi)}{p(y)}$

Simulation-based Inference problem



Parameters ψ

Simulator z

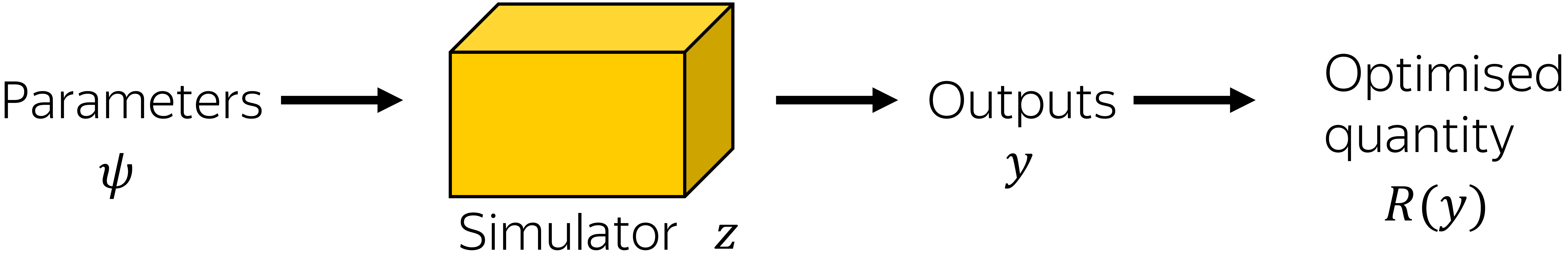
Outputs y

- Observe: $y_{det} \sim p(y_{det}|\psi_{true})$
- Can generate: $y_{sim} \sim p(y_{sim}|\psi)$

$$p(\psi|y) = \frac{p(y|\psi)\,p(\psi)}{p(y)}$$

- Find:
  - MLE estimate ψ_{MLE} of ψ_{true} → requires $p(y|\psi)$
  - Posterior: $p(\psi|y_{det})$ → requires $p(y|\psi)$
- A variety of methods exists to solve this problem
  ABC, Neural networks-based solutions

Simulator optimisation problem



Parameters ψ → Simulator z → Outputs y → Optimised quantity $R(y)$

Prediction →

$$y, z, \psi \sim p(y, z, \psi)$$

Observe: $y \sim p(y|\psi) = \int p(y, z|\psi) dz$

Can compute/observe a function $R(y)$

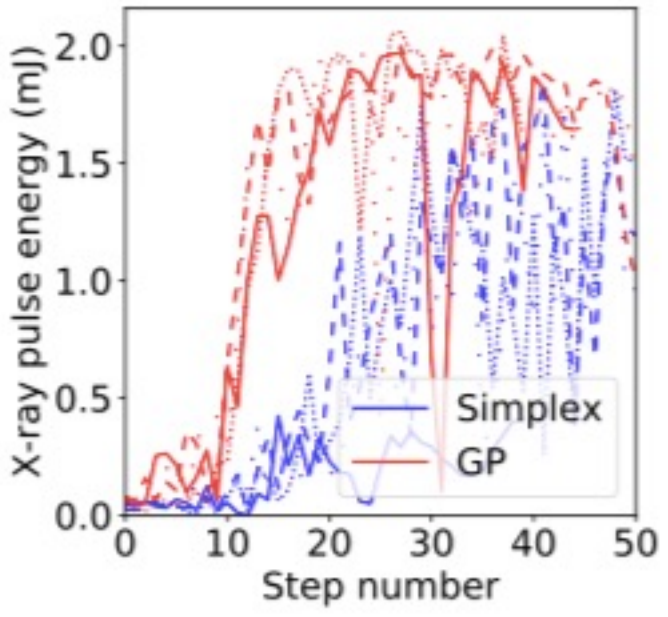
Inference ←

$$\psi_{opt} = \mathrm{argmin}_{\psi} R(y)$$

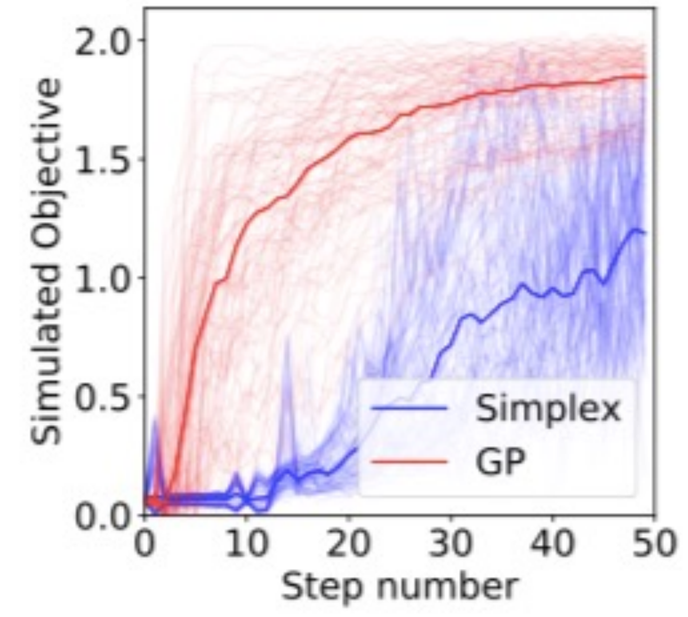
- Not interested in MLE or a posterior

Simulators optimisation

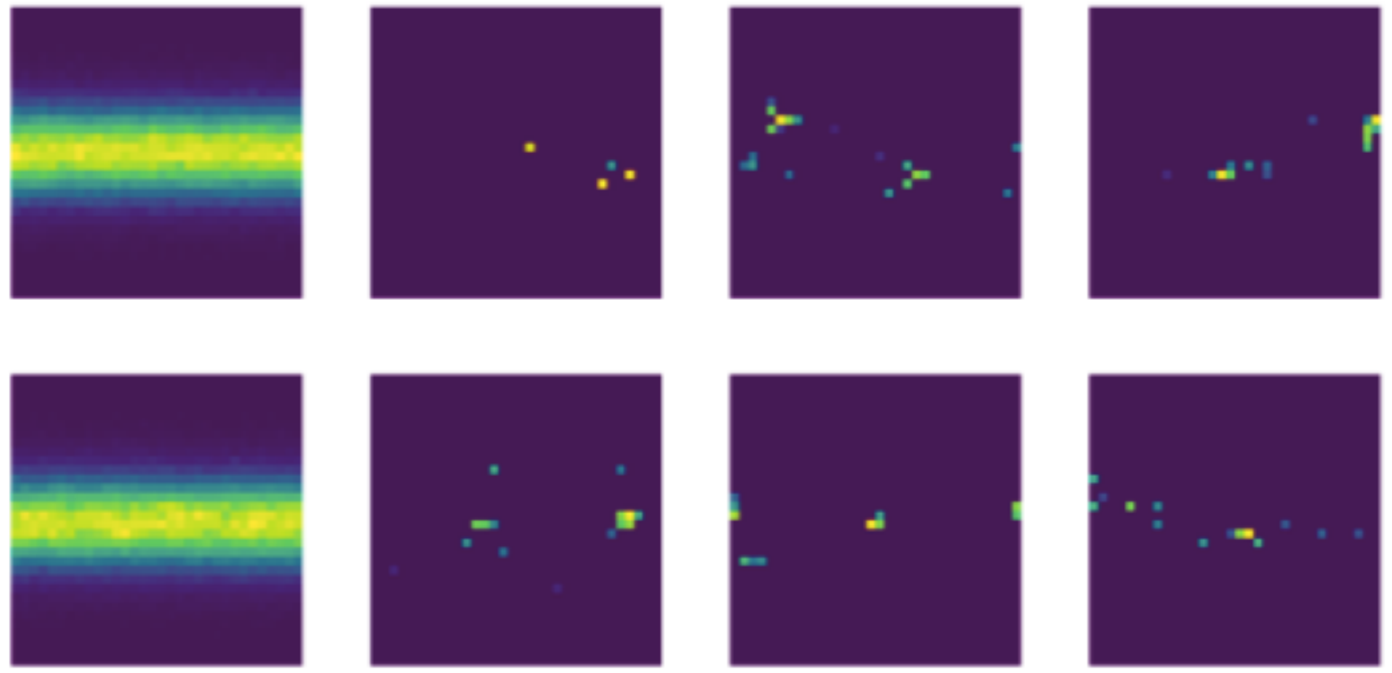
- Traffic scenes generation
- Control of the accelerator
- High Energy Physics
- Hardware



(c) Live 12 quadrupole optimization



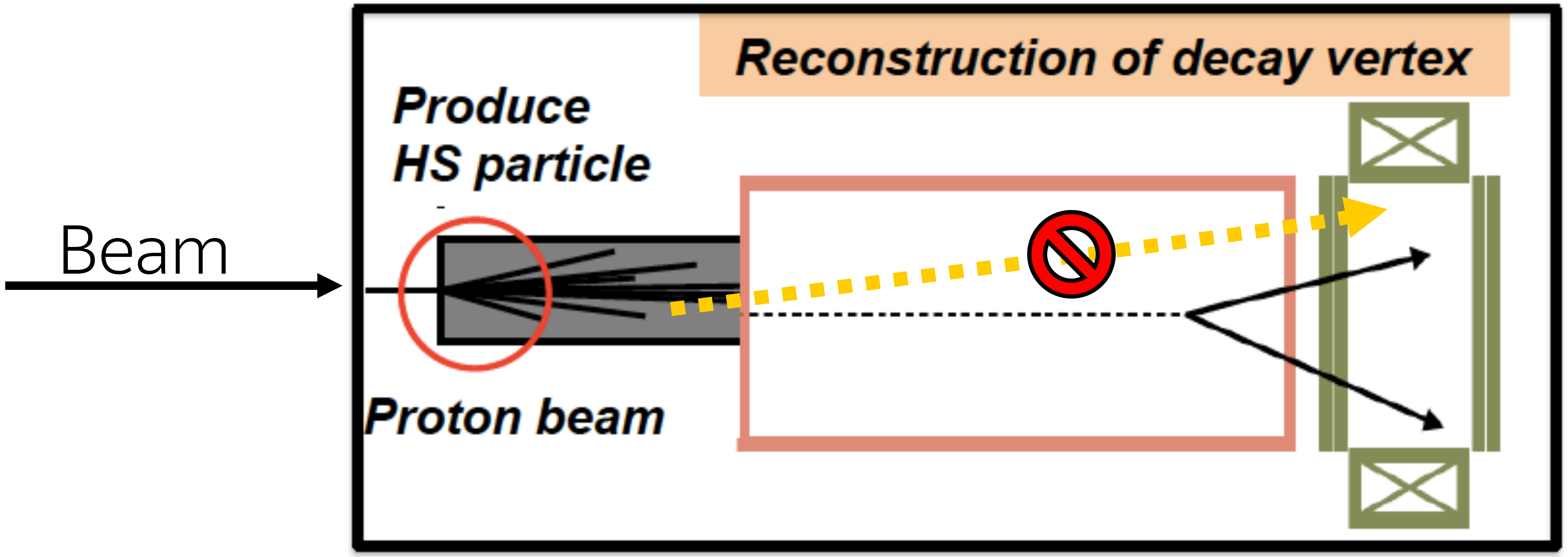
(d) Simulated 12 quadrupole optimization



Examples: 1810.02513, 1610.06151, 1909.05963, 1707.07113

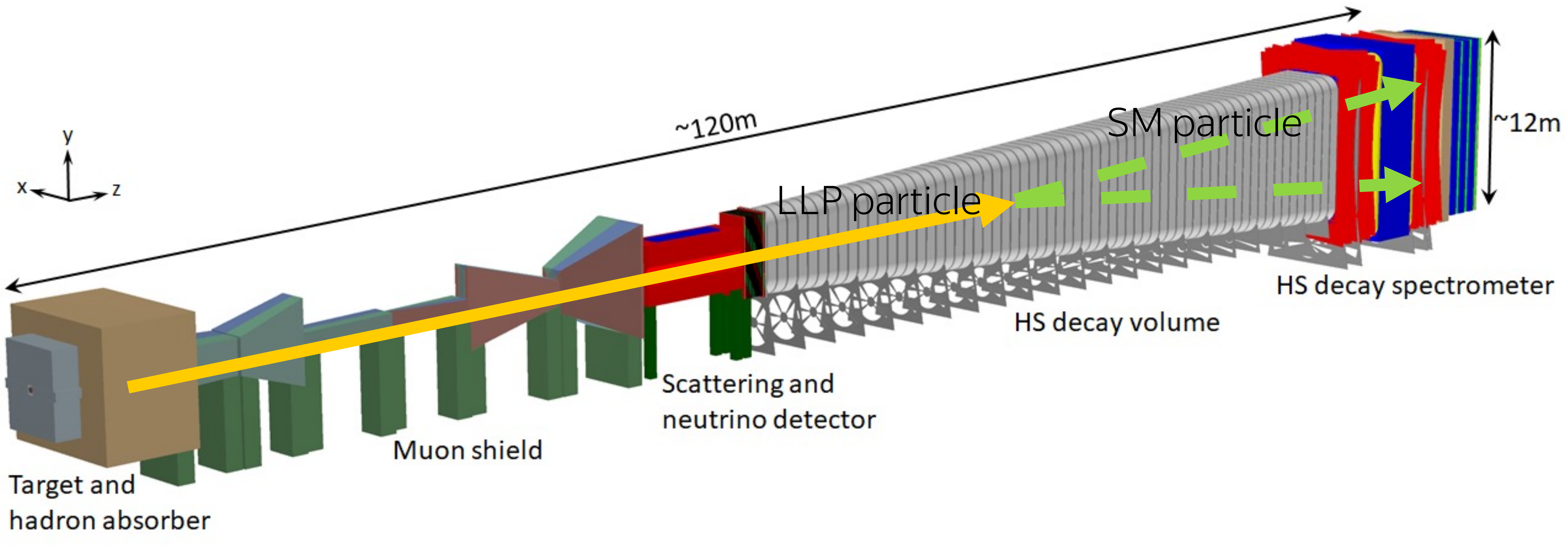
Motivation. HEP experiment

- Particle experiment at CERN
- 400 GeV/c proton beam
- Beam dump
- Hidden or LLP particles(signal), i.e. Dark Matter
- Background(muons)
- Goal: Detect signal, remove background



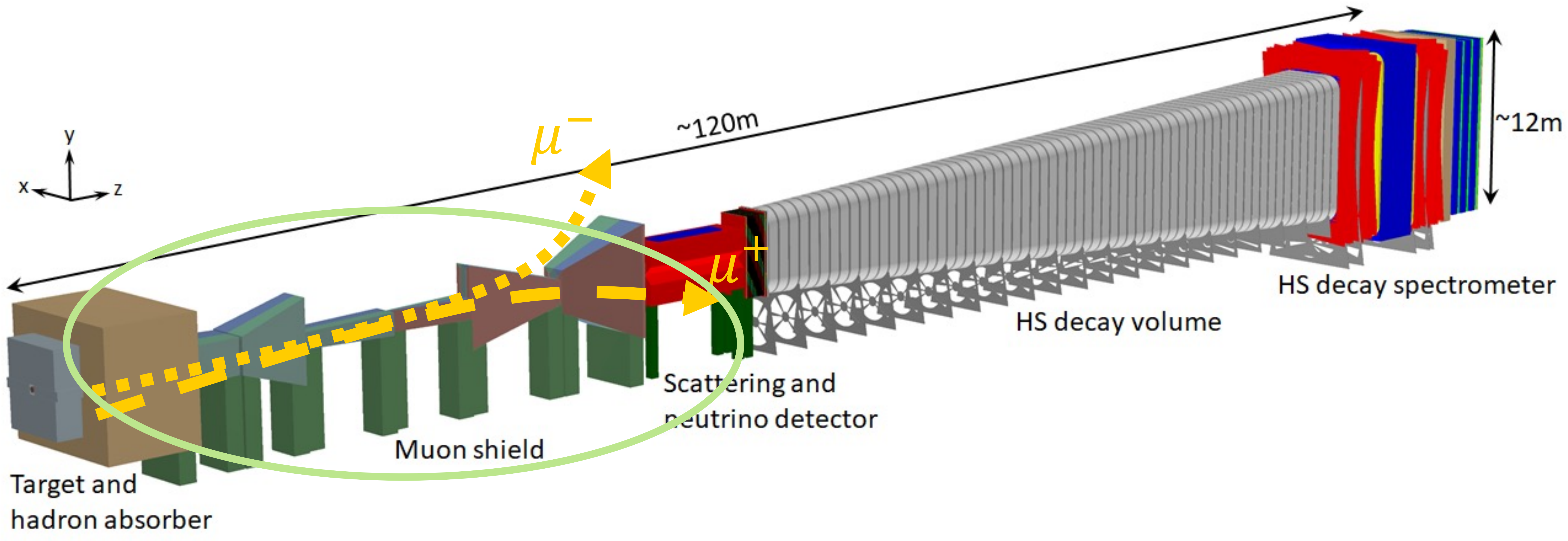
SHiP experiment

SHiP Technical proposal
1504.04956



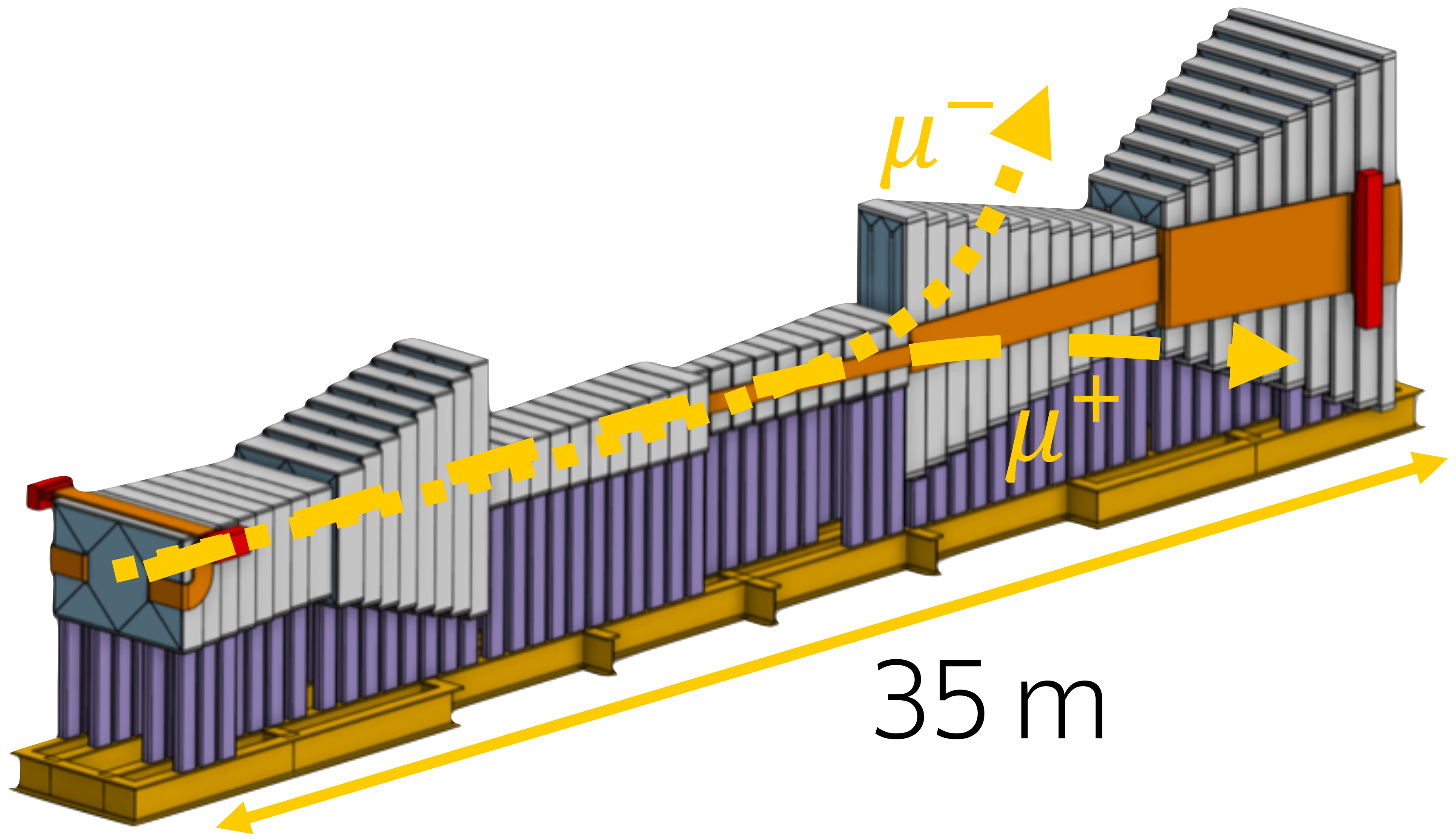
- Can detect very weakly coupled long-lived particles via decay or DM via scattering
- Planned zero background experiment

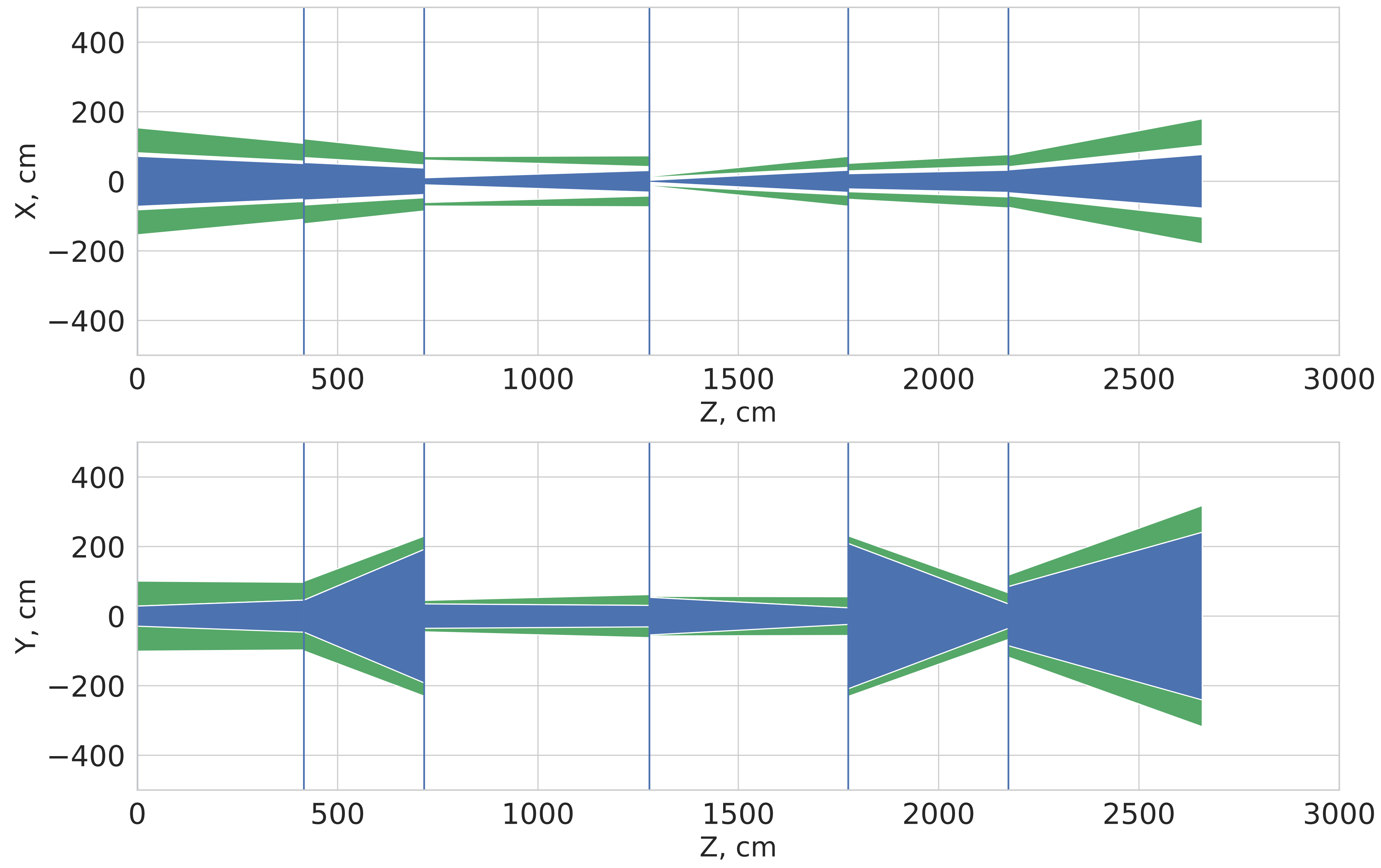
SHiP background



- 10^{11} muons/spill is produced inside the target
- Reduce background rate by six orders of magnitude
- Optimise the shield for the best physics performance and cost

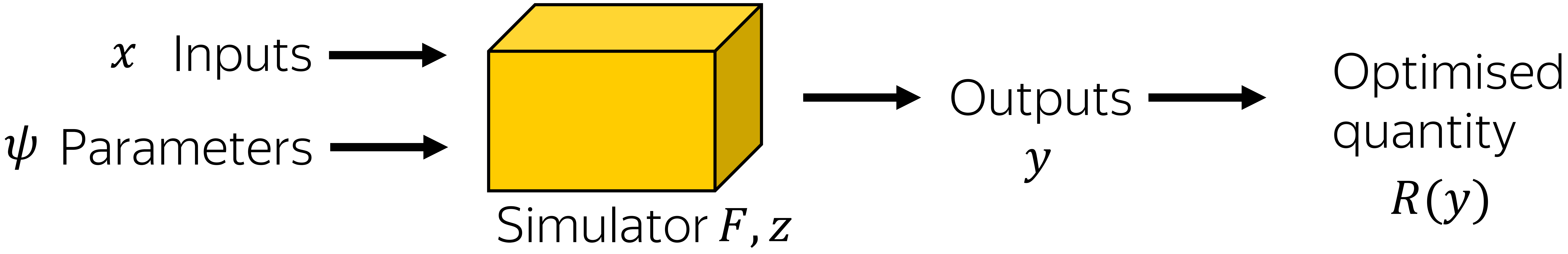
SHiP muon shield





- Optimise parameters to reduce number of muons in the detector
- GEANT4 simulates muons propagation through the shield
- Shield is characterised by 42 parameters
- *Very slow to simulate data points → hard to generate large samples*

Simulator optimisation problem



- x – muon kinematics
- ψ – geometry of the shield
- F – is the GEANT4 simulator
- y – observations: output of the simulator
- $R(y)$ - objective function

Want to find:

$$\psi_{opt} = \text{argmin}_{\psi} E_y\, [R(y)]$$

Observe samples:

$$y = F(x, \psi, z)$$

Stochastic black-box simulator

- F – random variable:

$$y = F(x, \psi, z) \leftrightarrow y \sim p(y|x;\psi)$$

z – latent variable

- F – black-box

$p(y|x;\psi)$ is not known

Can only sample from p

- How to optimise?

$$\psi_{opt} = \mathrm{argmin}_{\psi} E_y\,[R(y)]$$

Stochastic black-box optimisation

$$\text{argmin}_{\psi}\, E_y[R(y)] = \text{argmin}_{\psi} \int R(y)\, \boxed{p(y|x;\psi)}\, q(x) dx\, dy$$

Intractable

How can the optimisation be performed in such case?

- Bypass the estimation of $p(y|x;\psi)$
- Compute $\nabla_{\psi} E_y[R(y)] \rightarrow \nabla_{\psi} p(y|x;\psi)$

Existing black-box optimisation methods

Gradient based:

- Numerical differentiation
- Score function estimation (REINFORCE)

Alternatives:

- Bayesian optimisation
- Evolutionary strategies

Proposed by us:

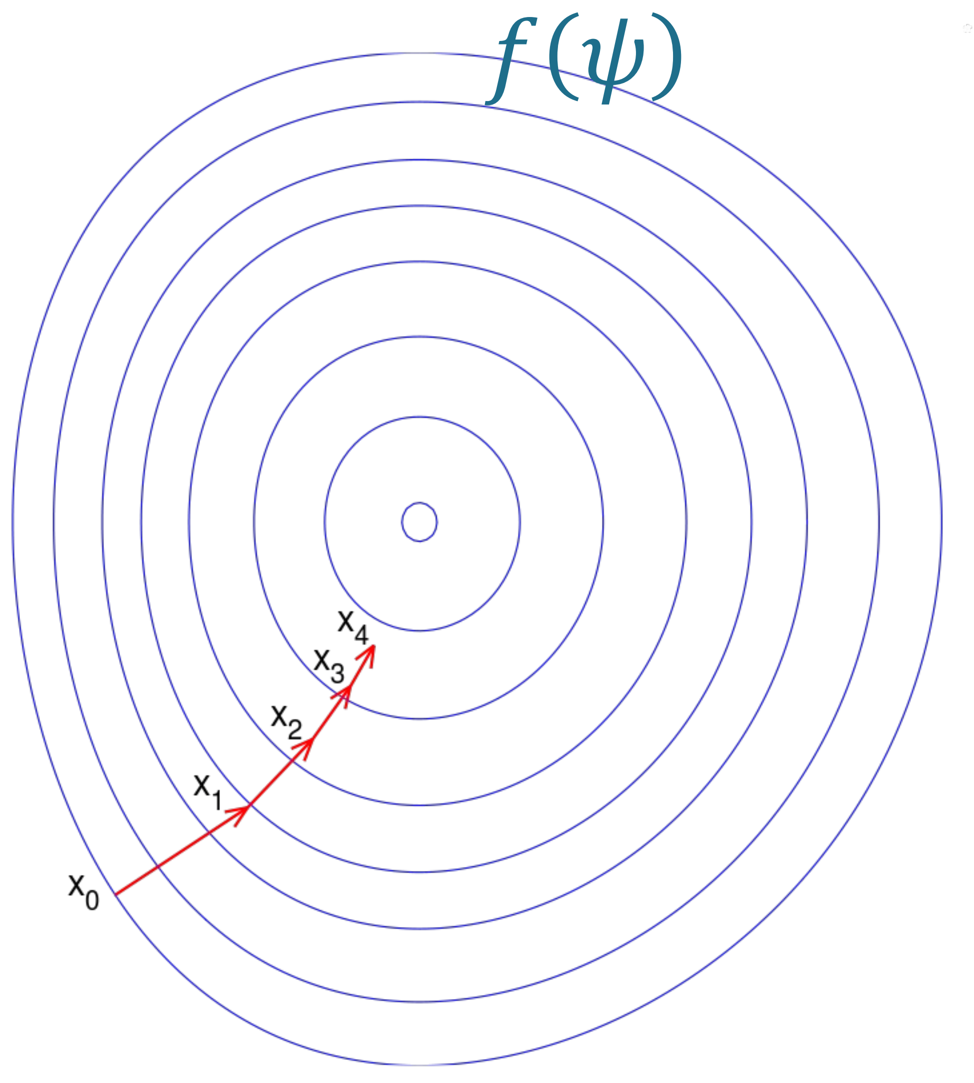
- Local Generative Surrogate optimisation

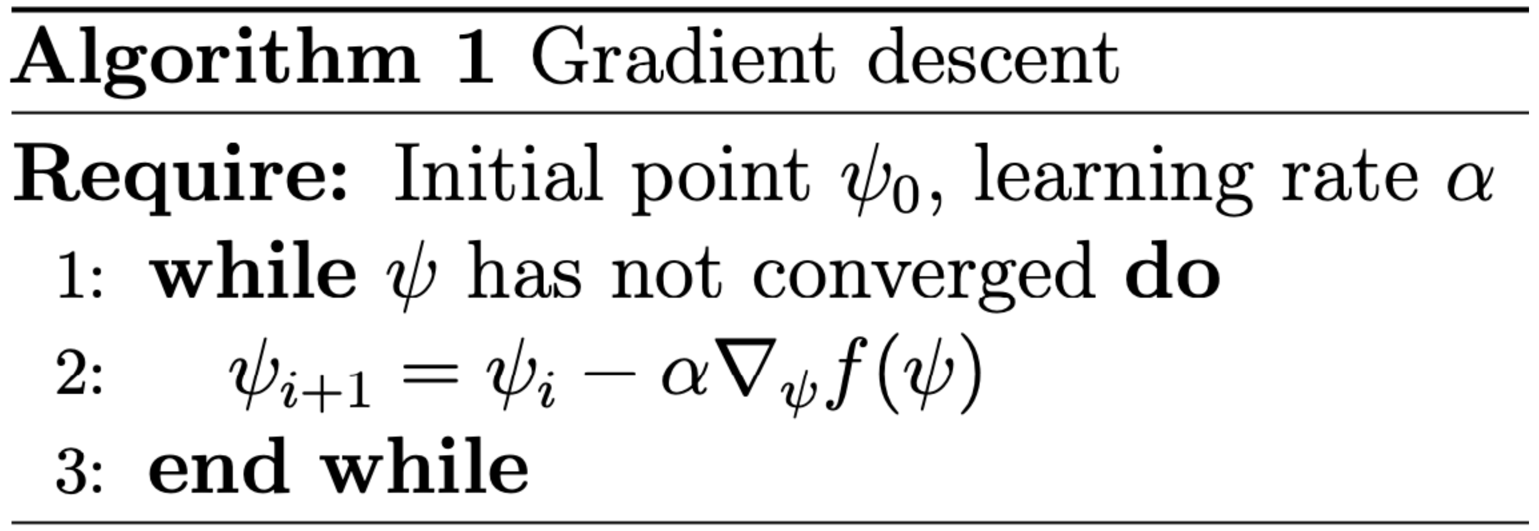
Gradient descent

- Goal: $\mathrm{Argmin}_{\psi}\, f(\psi)$.
- Solution: $\nabla_{\psi} f(\psi) = 0$,
- Method: gradient descent

$$\psi_{t+1} = \psi_t - const * \nabla_{\psi} f(\psi)$$

- Problem: $\nabla_{\psi} f(\psi)$ can NOT be computed





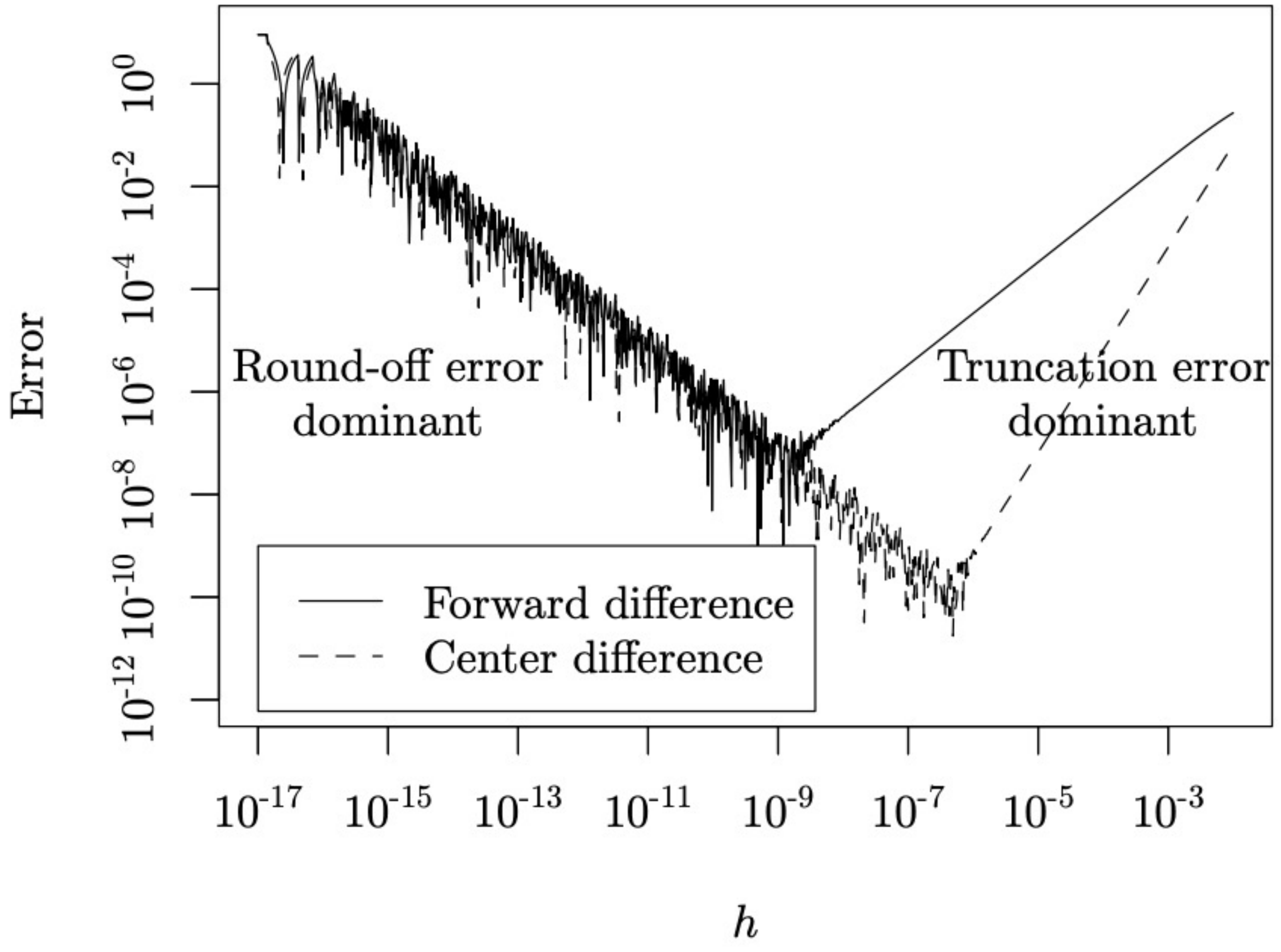
Algorithm 1 Gradient descent

```
Require: Initial point $\psi_0$, learning rate $\alpha$
while $\psi$ has not converged do
    $\psi_{i+1} = \psi_i - \alpha \nabla_{\psi} f(\psi)$
end while
```

How to estimate $\nabla_{\psi} f(\psi)$?

Numerical differentiation

$\nabla_\psi f(\psi) \approx \frac{f(\psi+h)-f(\psi)}{h}$, h – step size



- May have numerical instabilities
- Require $O(d)$ evaluation of f. $\psi \in \mathbb{R}^d$
- Can be challenging to apply with stochastic functions
- Perform linear interpolation

Score function estimator

- Often called as REINFORCE gradient estimation
- Remember our objective function:

$$f(\psi) = E_y\left[R\left(y_\psi\right)\right] = \int R(y)\, p(y|x;\psi) q(x) dx\, dy,$$

- Introduce distribution over ψ: $\psi \sim p(\psi|\mu)$
- $f(\psi)$ is now stochastic. We want to optimise $E_{\psi \sim p(\psi|\mu)}\,[f(\psi)]$

$$\nabla_\psi f(\psi) \approx \nabla_\mu E_{\psi \sim p(\psi|\mu)}\,[f(\psi)]$$

- How can we compute $\nabla_\mu E_{\psi \sim p(\psi|\mu)}[f(\psi)]$?

Score function estimator

- Remember that: $\nabla_x \log(f(x)) = \frac{\nabla_x f(x)}{f(x)}$ → $\nabla_x f(x) = f(x)\nabla_x \log(f(x))$

$$\nabla_\mu E_{\psi\sim p(\psi|\mu)}[f(\psi)] = \nabla_\mu \int f(\psi)\underline{p(\psi|\mu)}d\psi = \int f(\psi)\underline{\nabla_\mu p(\psi|\mu)}d\psi$$

$$= \int f(\psi)\underline{\underline{p(\psi|\mu)}\nabla_\mu \log(p(\psi|\mu))}d\psi$$

$$= E_{\psi\sim p(\psi|\mu)}\left[f(\psi)\nabla_\mu \log(p(\psi|\mu))\right]$$

- We have an estimate of the gradient!

$$\nabla_\psi f(\psi) \approx E_{\psi\sim p(\psi|\mu)}\left[f(\psi)\nabla_\mu \log(p(\psi|\mu))\right]$$

Score function estimator

- Trick:

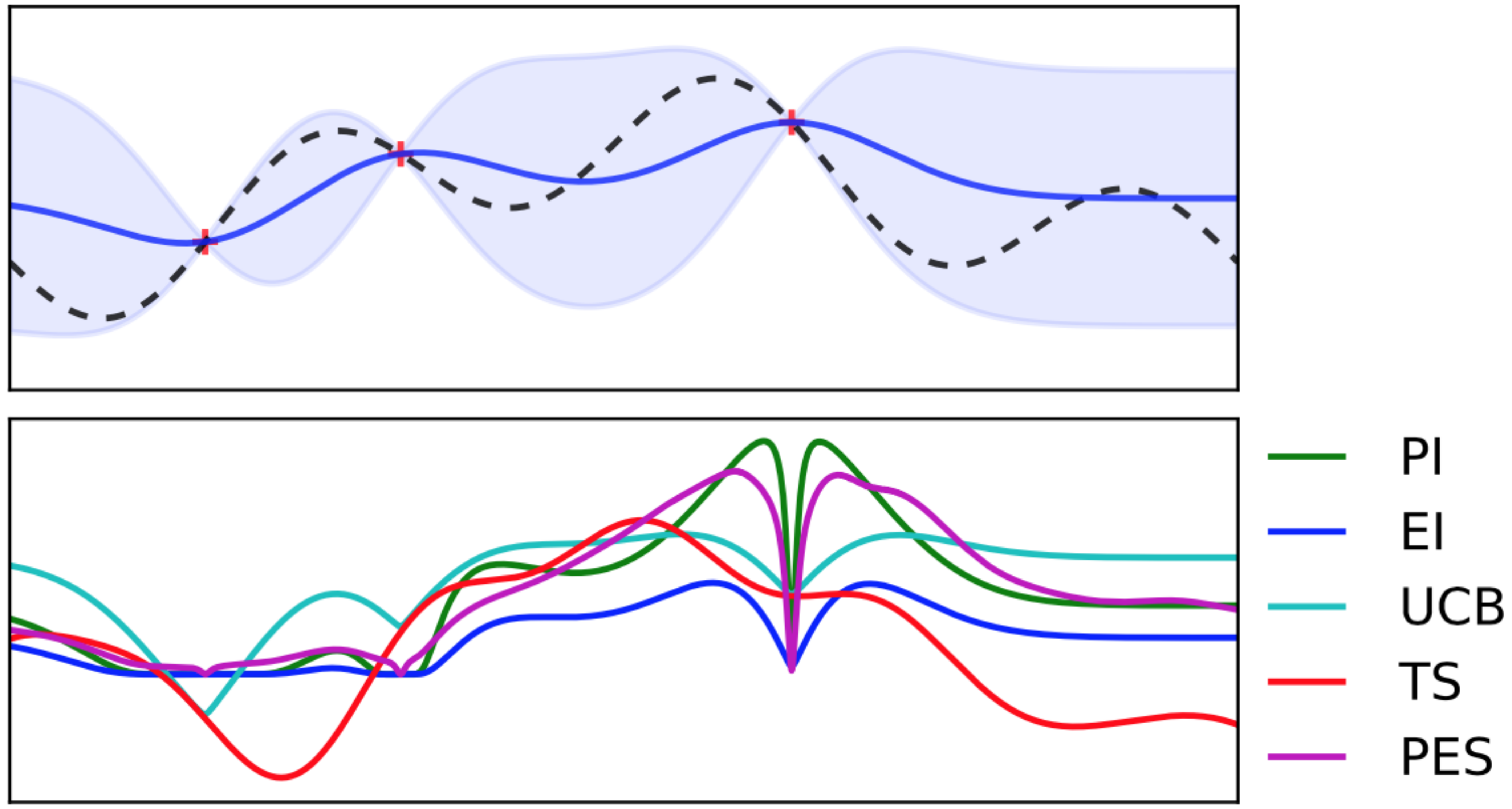
$$\nabla_{\psi} f(\psi) \approx E_{\psi \sim p(\psi|\mu)}\left[\overset{\text{Can evaluate}}{f(\psi)}\,\overset{\text{Can compute}}{\nabla_{\mu}\log(p(\psi|\mu))}\right]$$

- Have high variance[1]
- Require prior distribution over ψ
- Techniques developed to reduce variance[2,3]

But: **Fast to compute**

[1]https://doi.org/10.1007/BF00992696. [2]1711.00123, [3]1810.02513

Bayesian optimisation with Gaussian Processes



- Goal: $\text{argmin}_{\psi} f(\psi)$
- Approximate $f(\psi)$ with surrogate model (GP) → $\mu(\psi)$ and $\sigma(\psi)$
- Chose acquisition function $\beta(\psi)$:
  Set exploration/exploitation of the space
- Evaluates $\beta(\psi)$ → new point ψ' to probe

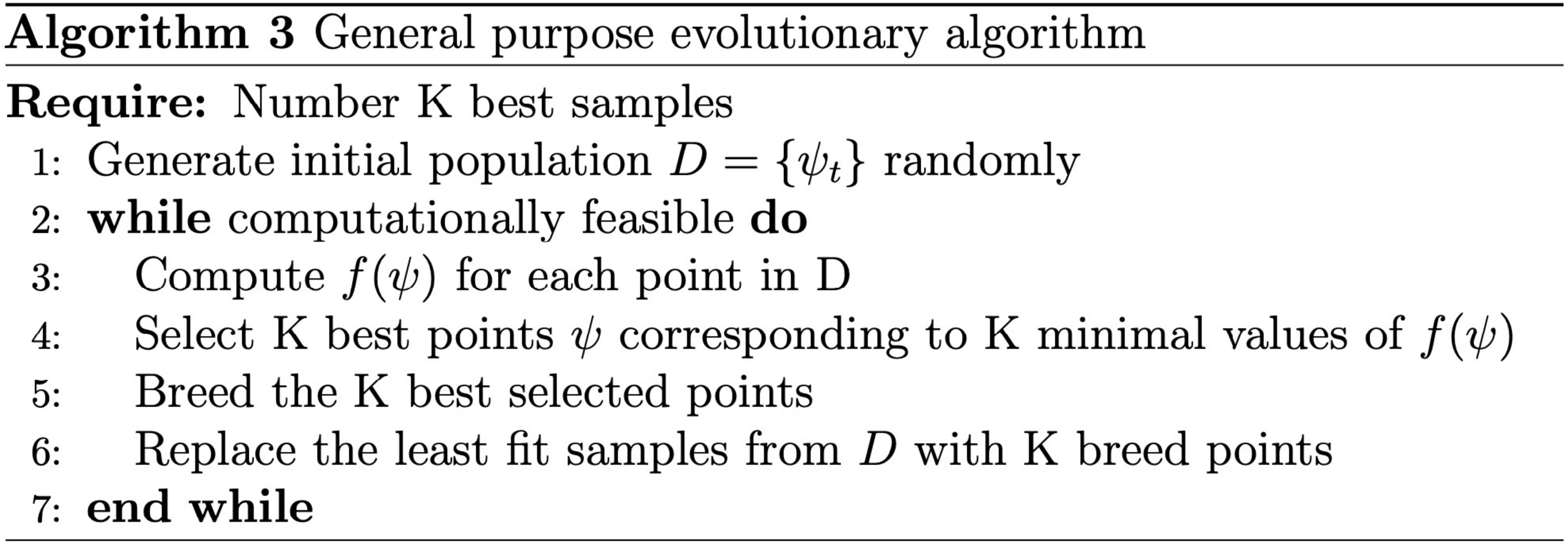
- Benefits:

  - Can potentially find global minima
  - Work with non-differentiable functions

- Drawbacks:

  - Scales as $O(n^3 + n^2 d), n$ – size of the traning set
  - Suffer from curse of dimensionality

Evolutionary strategies



Algorithm 3 General purpose evolutionary algorithm

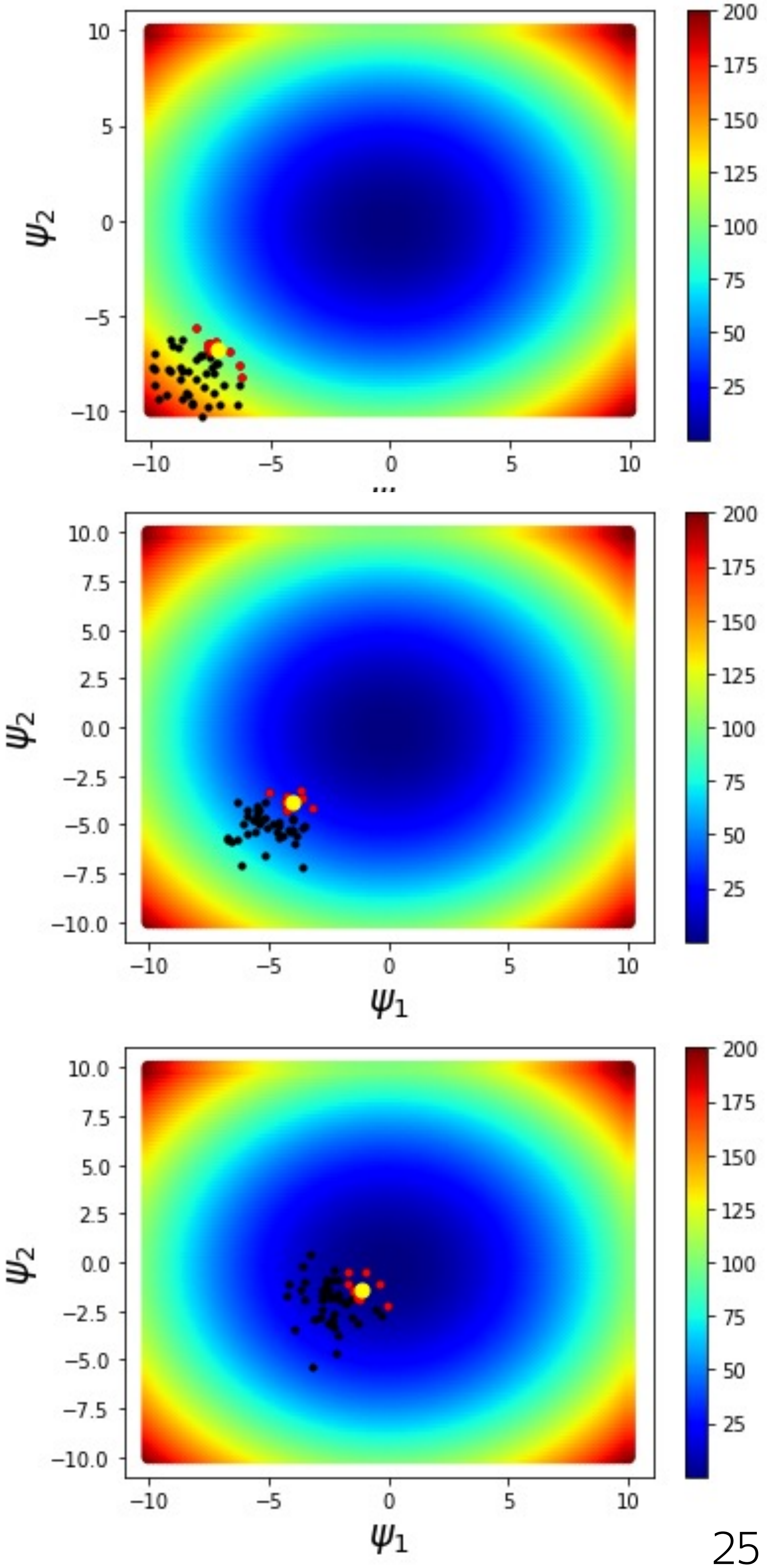
```
Require: Number K best samples
Generate initial population $D = \{\psi_t\}$ randomly
while computationally feasible do
    Compute $f(\psi)$ for each point in D
    Select K best points $\psi$ corresponding to K minimal values of $f(\psi)$
    Breed the K best selected points
    Replace the least fit samples from $D$ with K breed points
end while
```

Evolutionary strategies

- Simple case of Gaussian ES:
  - Set $\theta = (\mu), p_\theta(\psi) = N(\mu, \sigma^2 I)$
  - Sample M values of ψ_i, compute $f(\psi_i)$
  - Select best K values by sorting $f(\psi_i)$
  - Update μ using selected ψ_i

- Usually requires large number of sample M.

- Modifications such as CMA-ES[1] or Guided ES[2] might utilse surrogate gradient information.



[1] http://www.cmap.polytechnique.fr/~nikolaus.hansen/cmaartic.pdf, [2] https://arxiv.org/abs/1806.10230

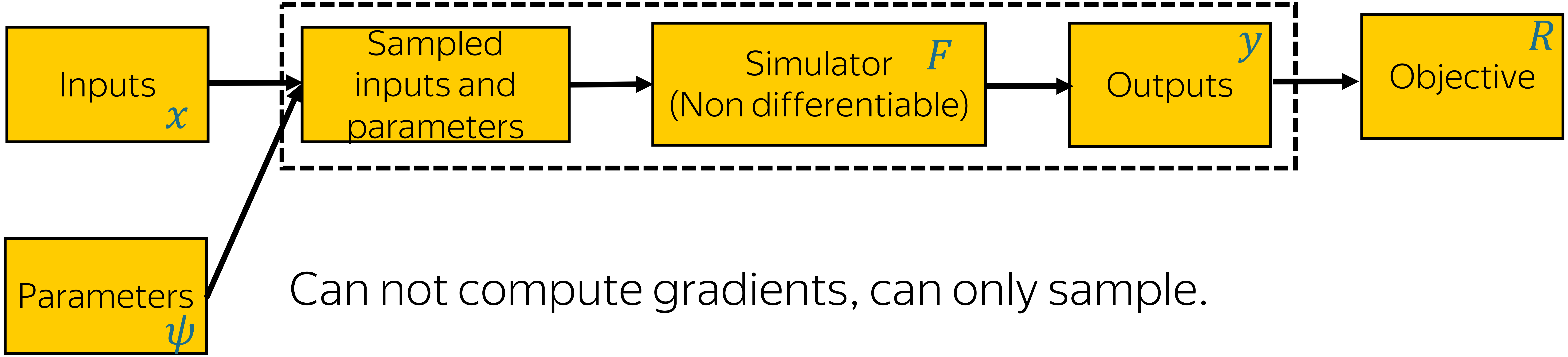
Why to create something new?

- Require frequent simulator calls → computationally expensive
- Require prior distribution or search region
- May not scale well to high dimensions
- Have high variance
- Estimate only first order gradients

We try to solve some of those issues with our method.

Generative surrogates

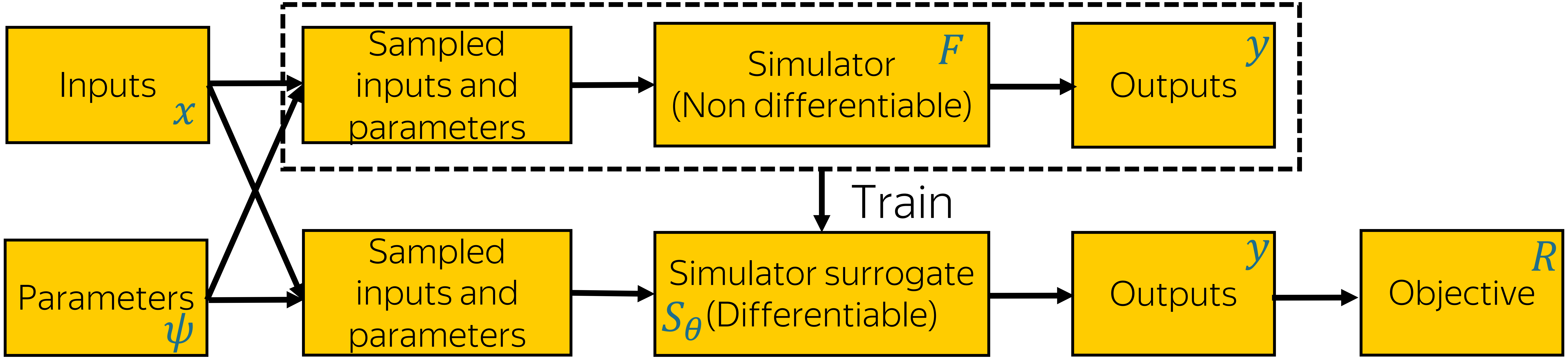
$$E_y[R(y_\psi)] \approx \frac{1}{N}\sum_{i=1}^{N} R(F(x_i;\psi_i))$$



Can not compute gradients, can only sample.

Generative surrogates

$$E_y[R(y_\psi)] \approx \frac{1}{N}\sum_{i=1}^{N} R(F(x_i;\psi_i))$$

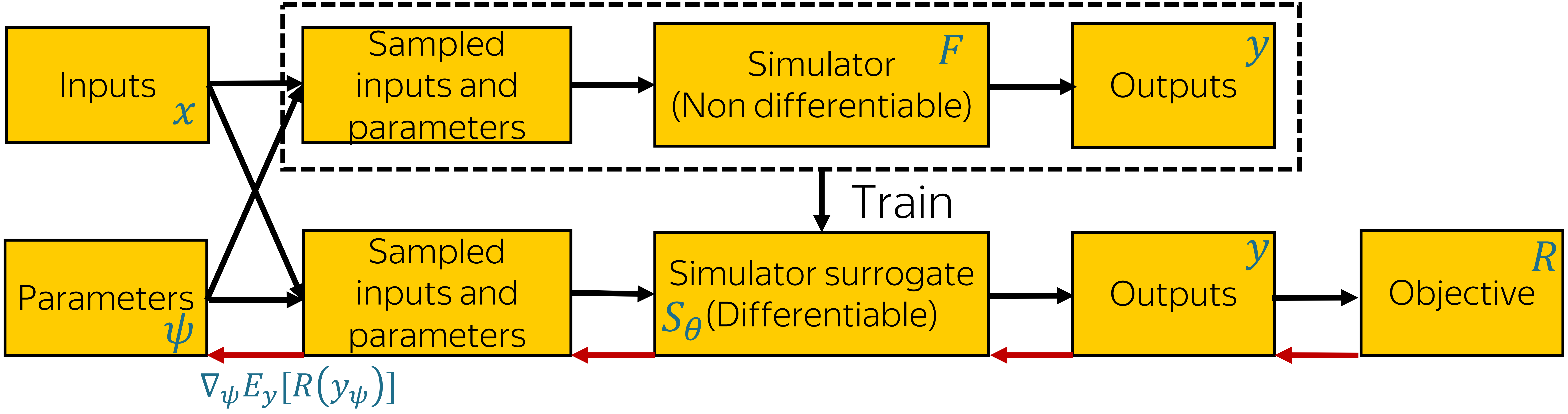


Inputs x
Parameters ψ
Sampled inputs and parameters
Simulator (Non differentiable) F
Outputs y
Train
Sampled inputs and parameters
Simulator surrogate S_θ(Differentiable)
Outputs y
Objective R

$$E_y[R(y_\psi)] \approx \frac{1}{N}\sum_{i=1}^{N} R(S(z_i, x_i;\psi_i))$$

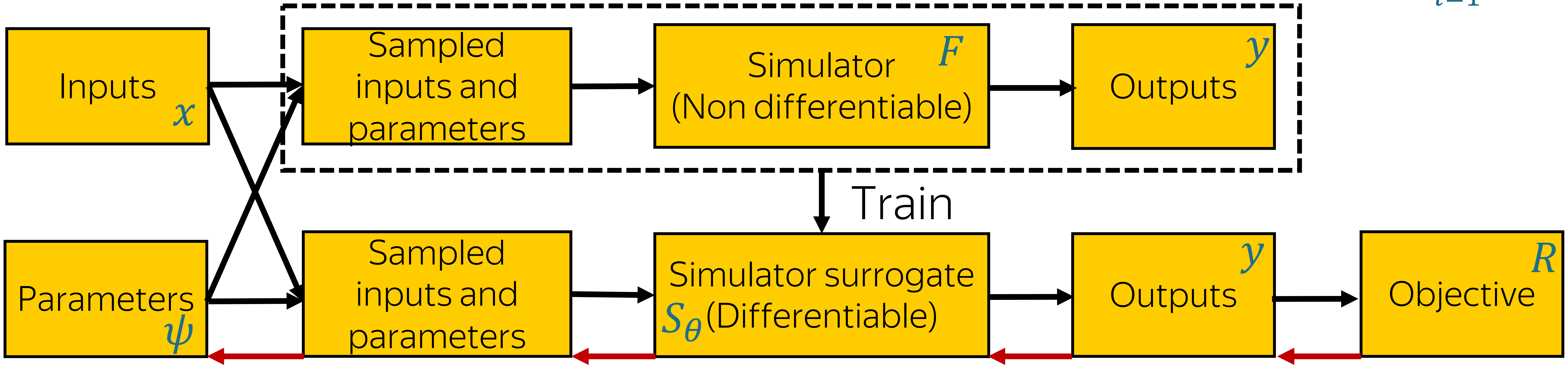
Generative surrogates

$$\nabla_\psi E_y[R(y_\psi)] \approx \frac{1}{N}\sum_{i=1}^{N} \boxed{\nabla_\psi R(F(x_i;\psi_i))} \approx \frac{1}{N}\sum_{i=1}^{N} \boxed{\nabla_\psi R(S(z_i, x_i;\psi_i))}$$



Generative surrogates

$$\sum_{i=1}^{N} \nabla_\psi R\big(S_\theta(z_i, x_i; \psi)\big)$$

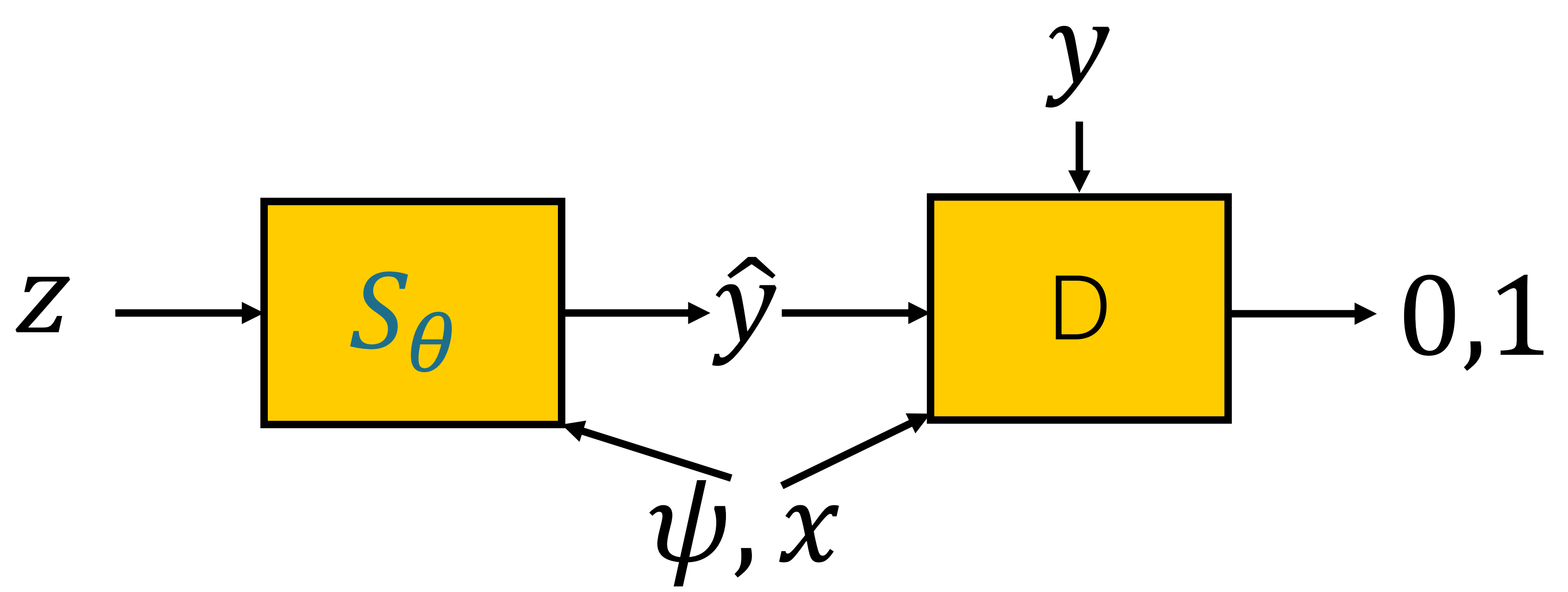

Inputs x
Parameters ψ
Sampled inputs and parameters
Simulator F (Non differentiable)
Outputs y
Train
Sampled inputs and parameters
Simulator surrogate S_θ (Differentiable)
Outputs y
Objective R

- S_θ any conditional deep generative model: GAN, NF, VAE, …
- Once trained produce differentiable samples:

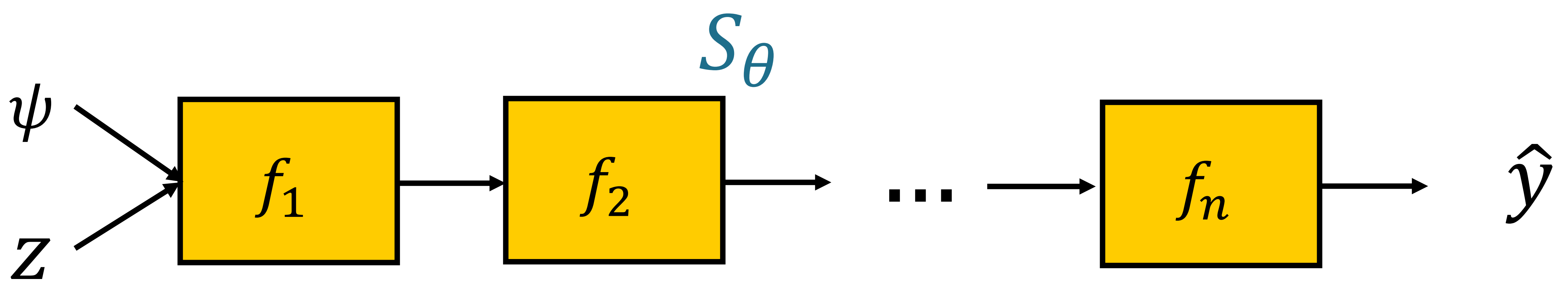
$$\nabla_\psi E_y[R(y)] \sim \sum \frac{\partial\, R}{\partial y_i} \times \boxed{\frac{\partial y_i}{\partial \psi}} = \sum \frac{\partial\, R}{\partial y_i} \times \boxed{\frac{\partial S_\theta}{\partial \psi}}$$

Conditional Generative Networks

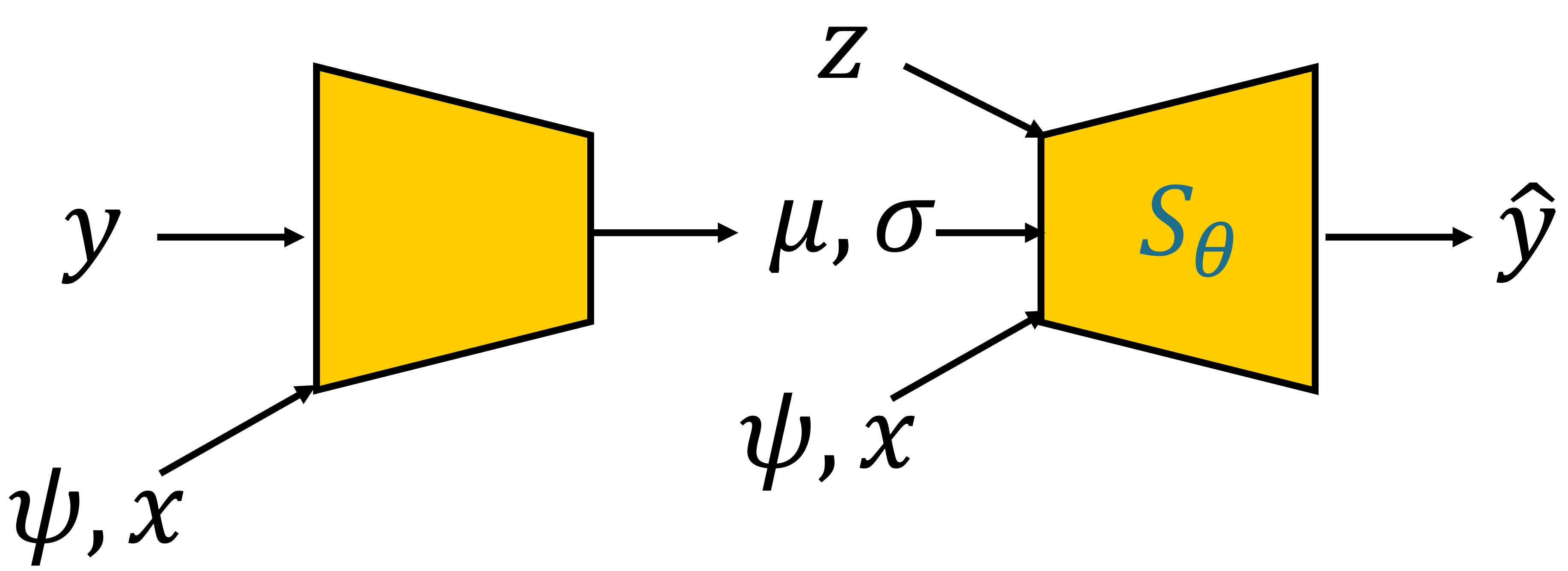
- Generative Adversarial Networks



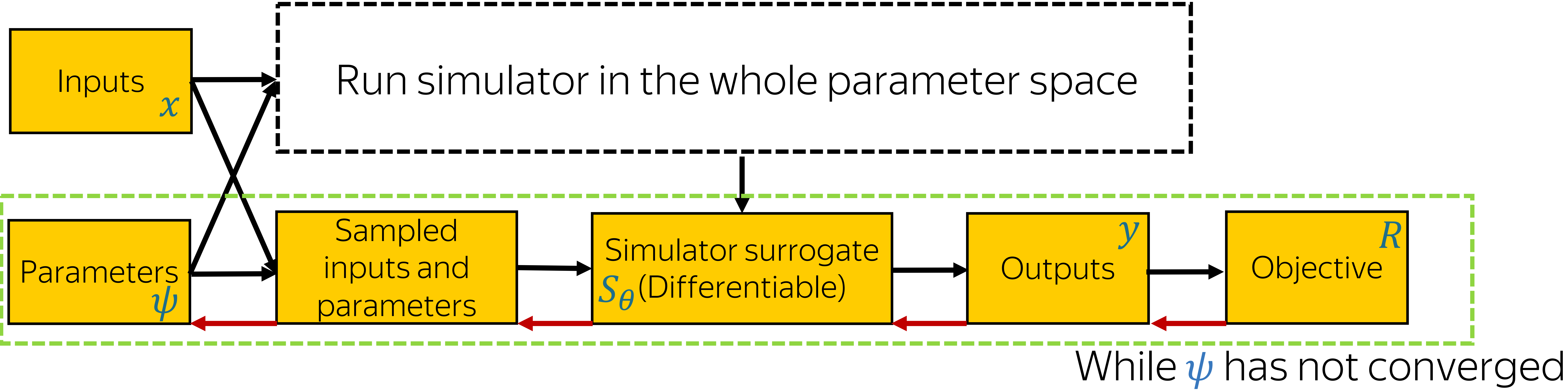
- Normalising flows



- Variational Autoencoders



Generative surrogates: training

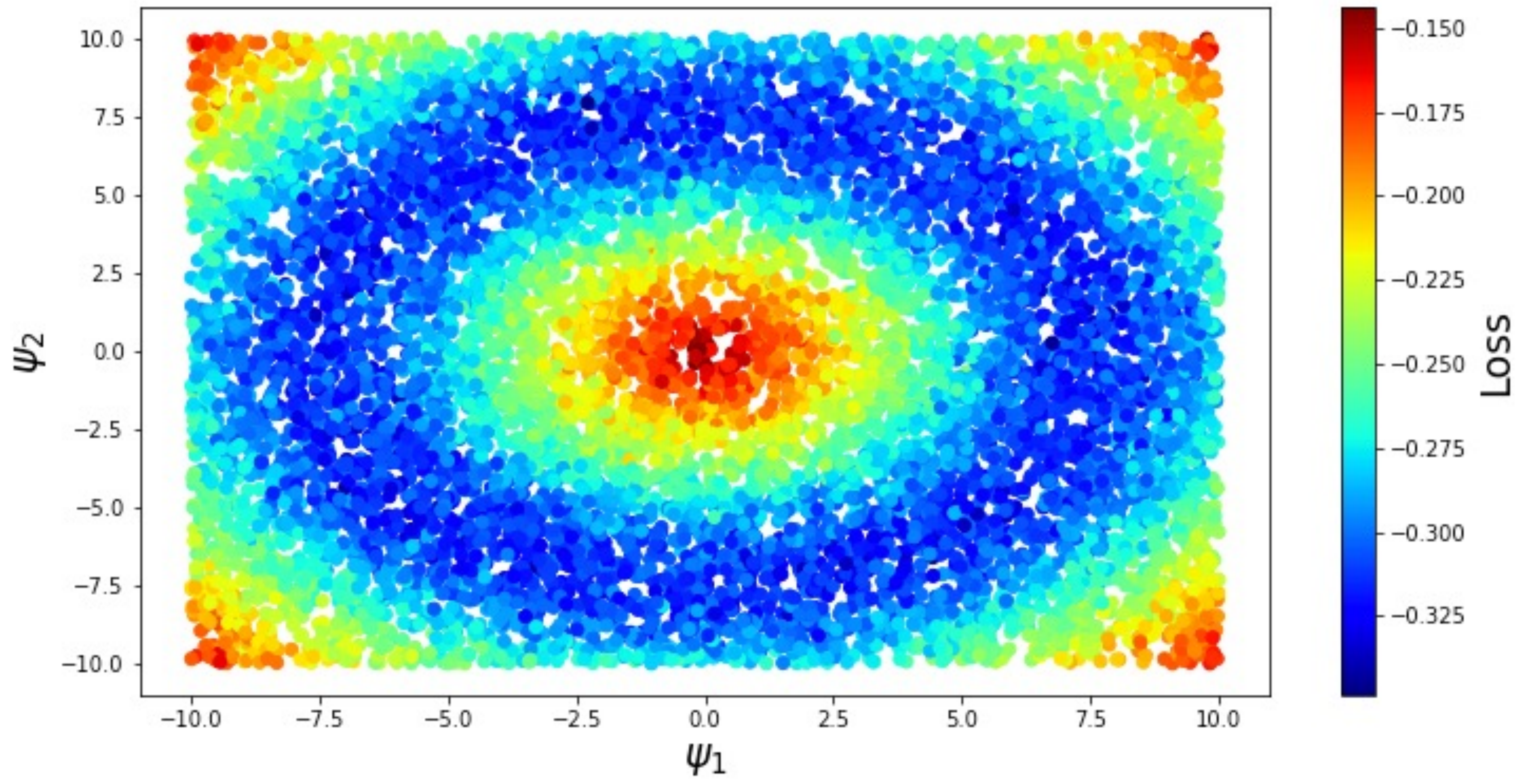

Inputs
x
Run simulator in the whole parameter space
Parameters
ψ
Sampled inputs and parameters
Simulator surrogate S_θ(Differentiable)
Outputs
y
Objective
R
While ψ has not converged

- Generate ψ on the grid
- S_θ is trained *once* in the *whole* space of parameters ψ

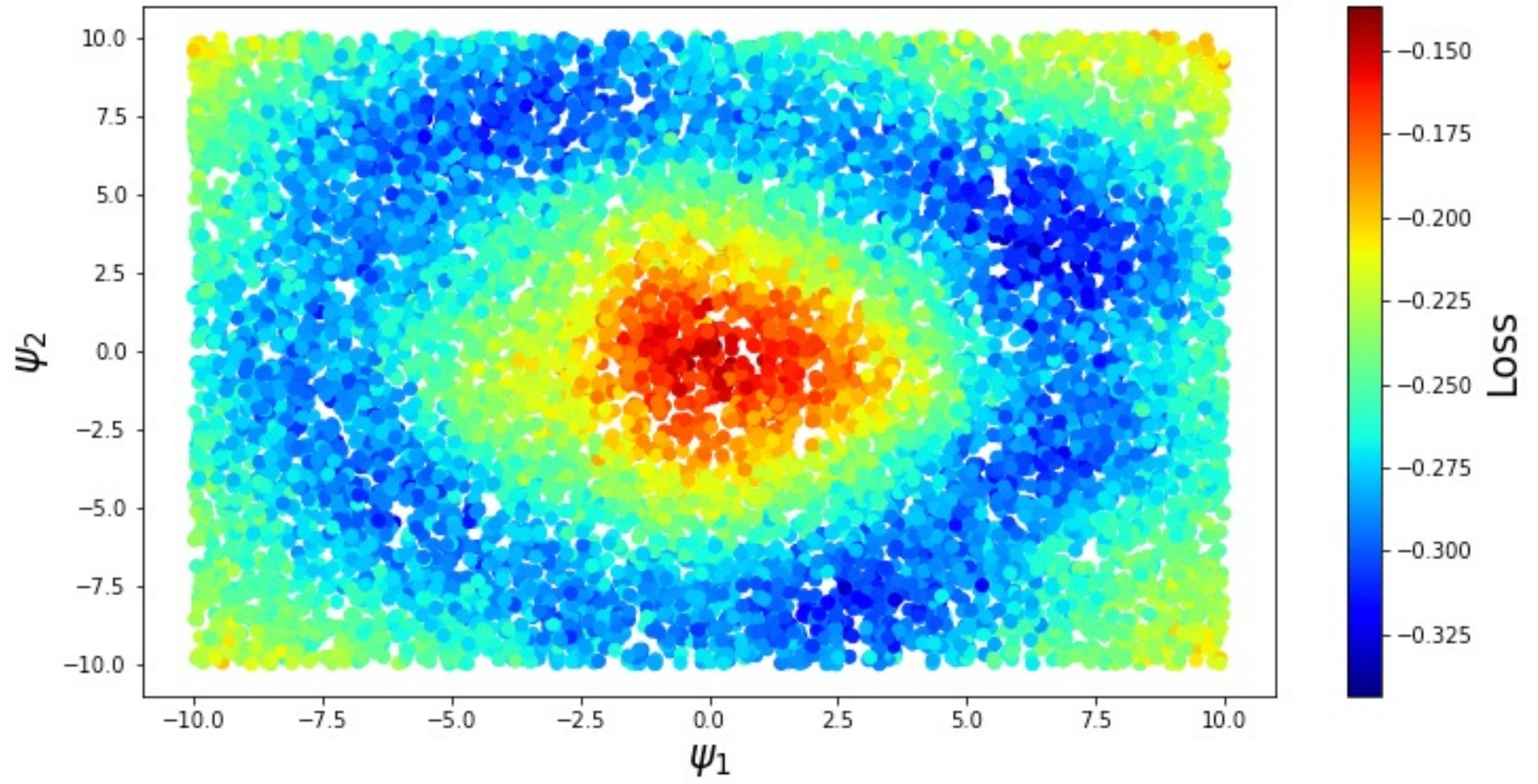
$$\psi_{t+1} = \psi_t - const * \frac{1}{N}\sum_{i=1}^{N} \nabla_\psi R(S(z_i, x_i; \psi_i))$$

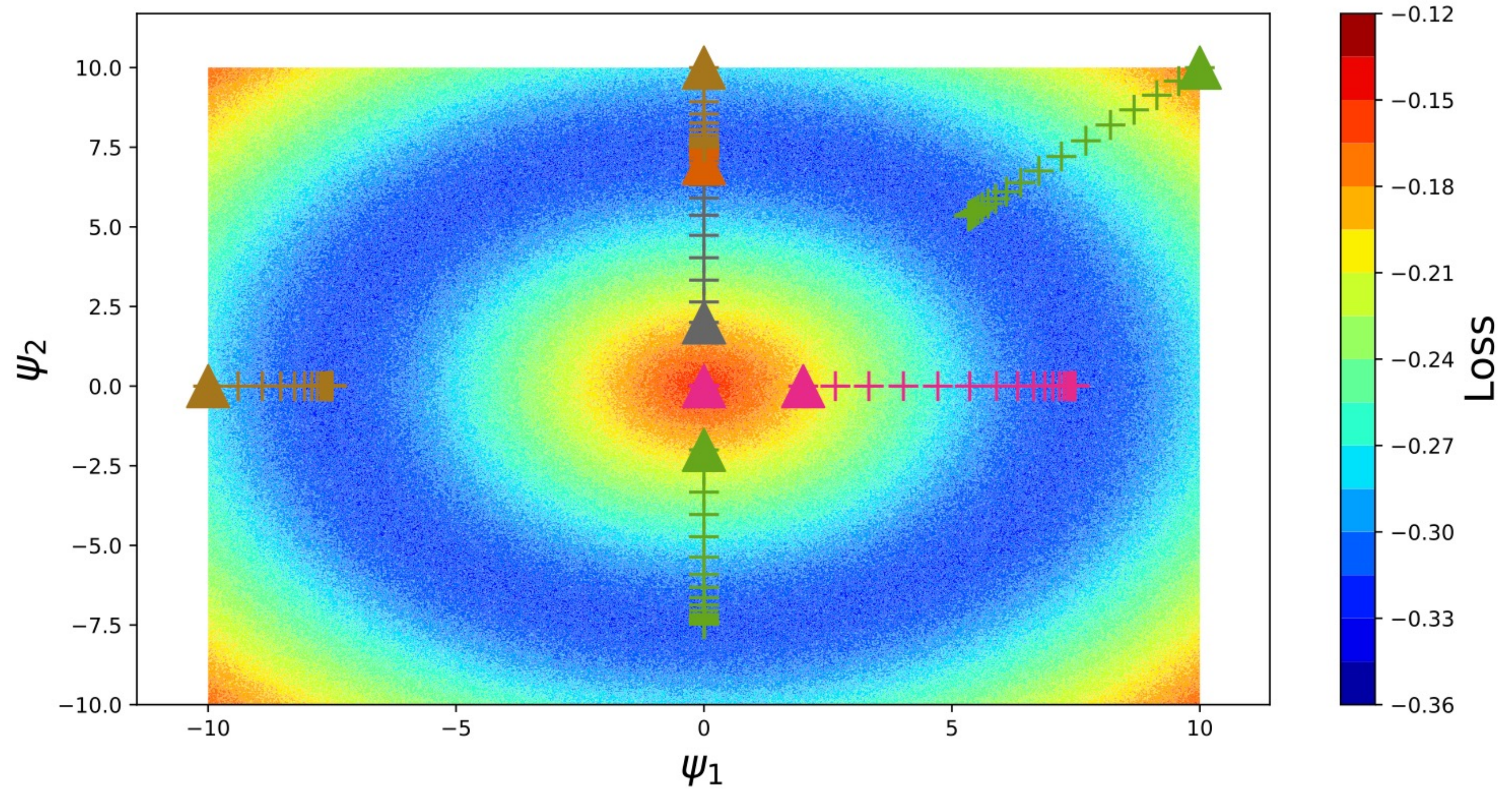
Generative surrogates: toy example

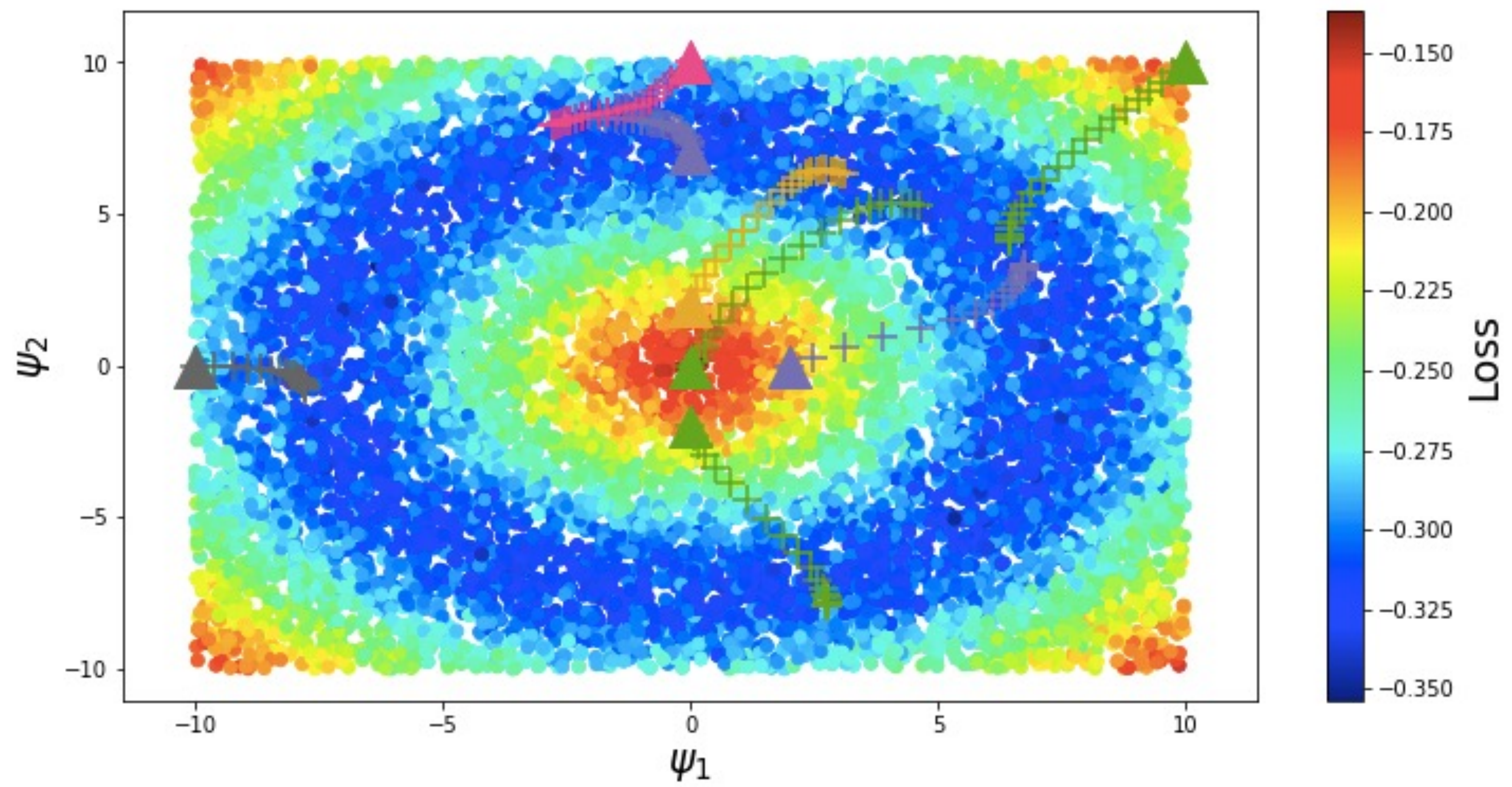
Simulator loss



GAN loss

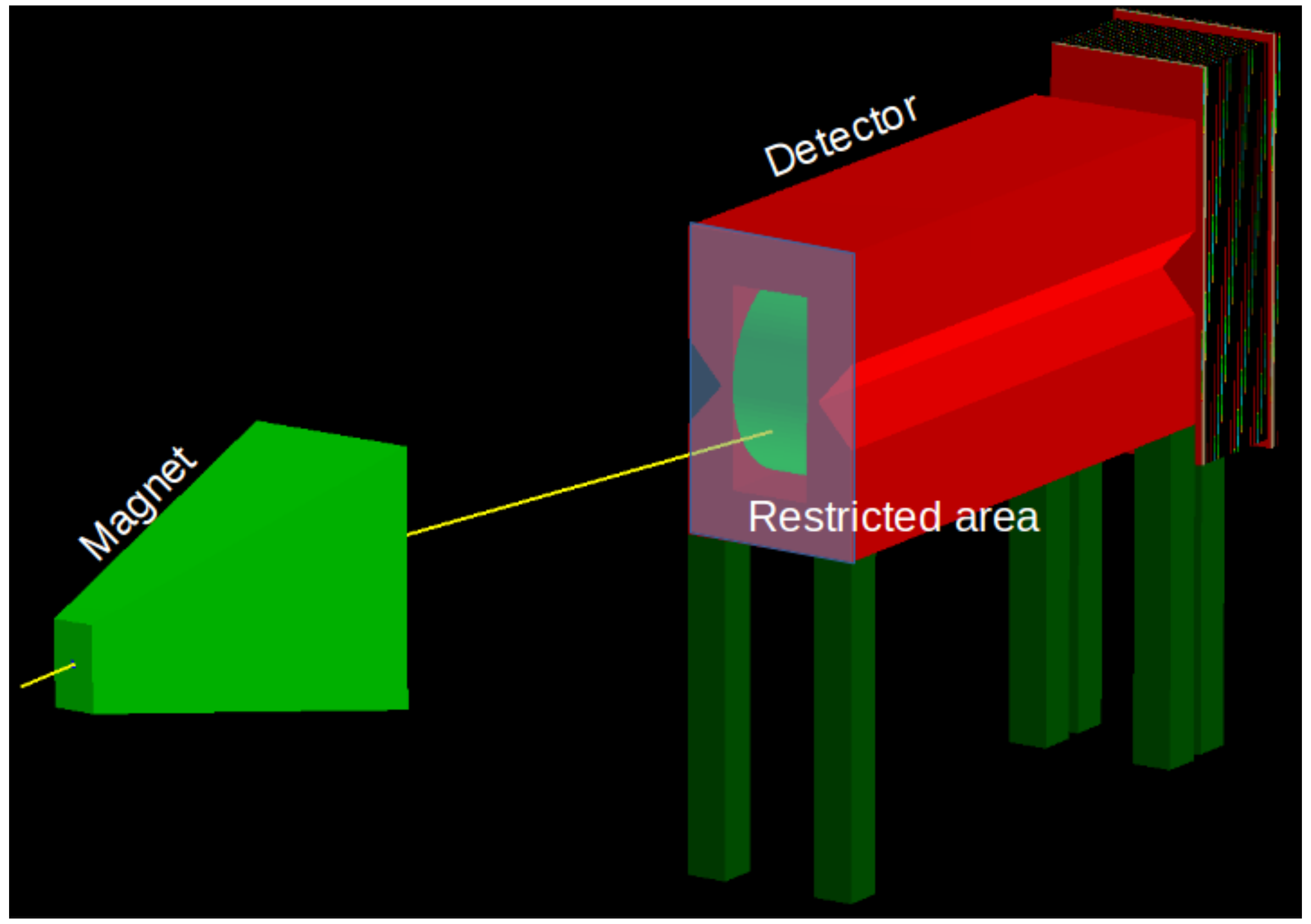




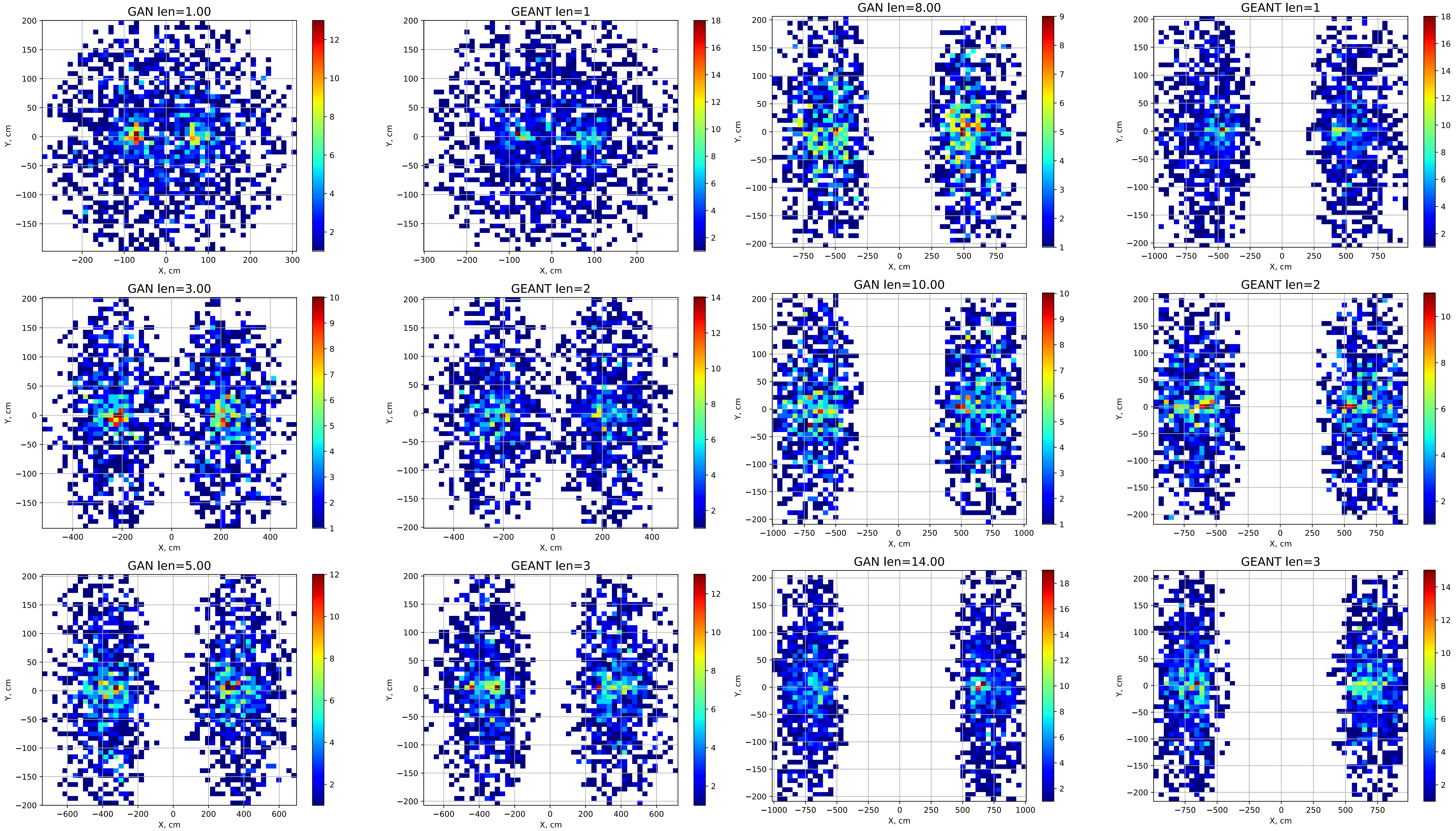


Generative surrogates: physics toy example

$\psi \in \mathbb{R}^1$



GAN Simulator GAN Simulator

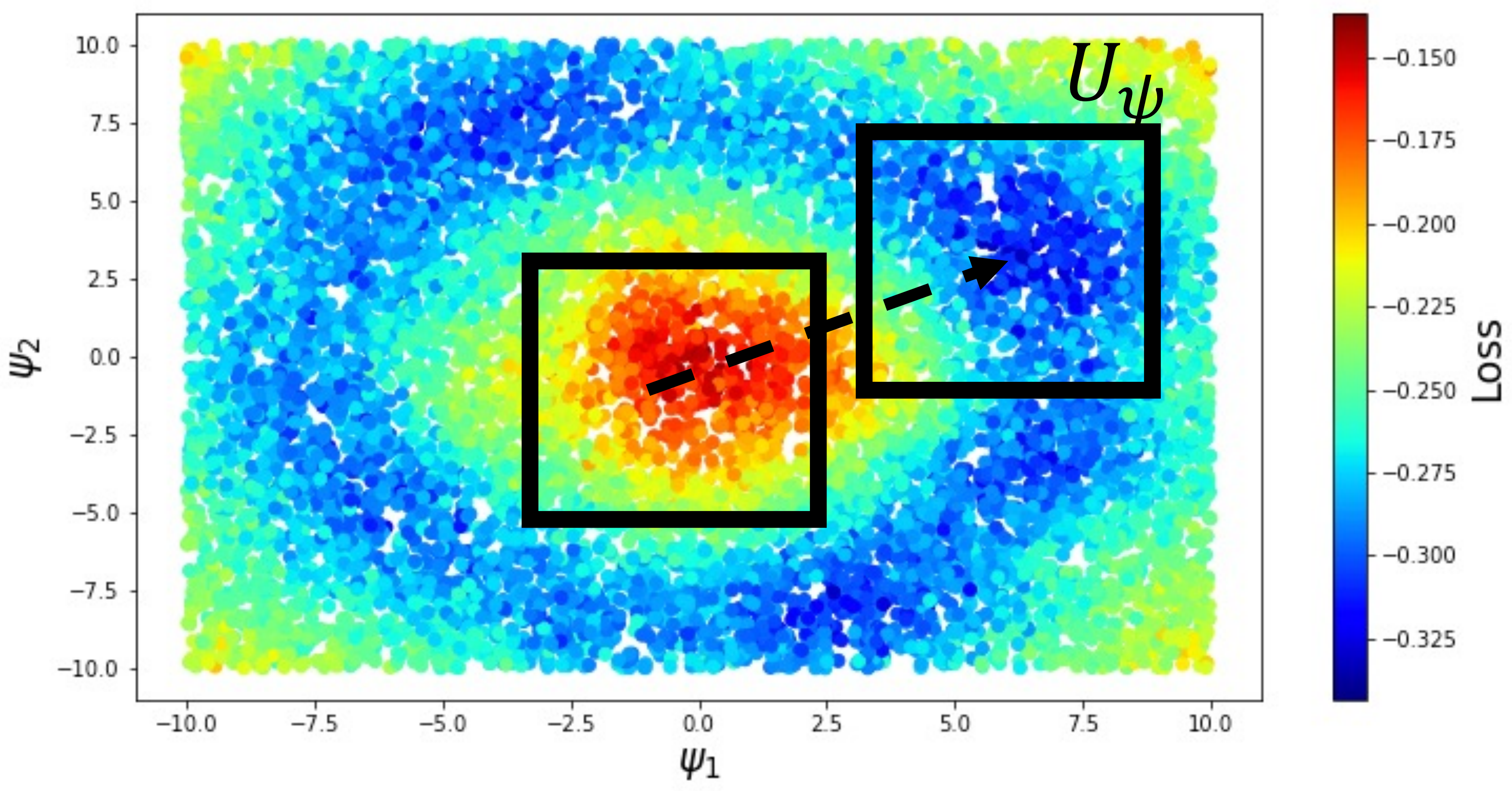


There is no locality...

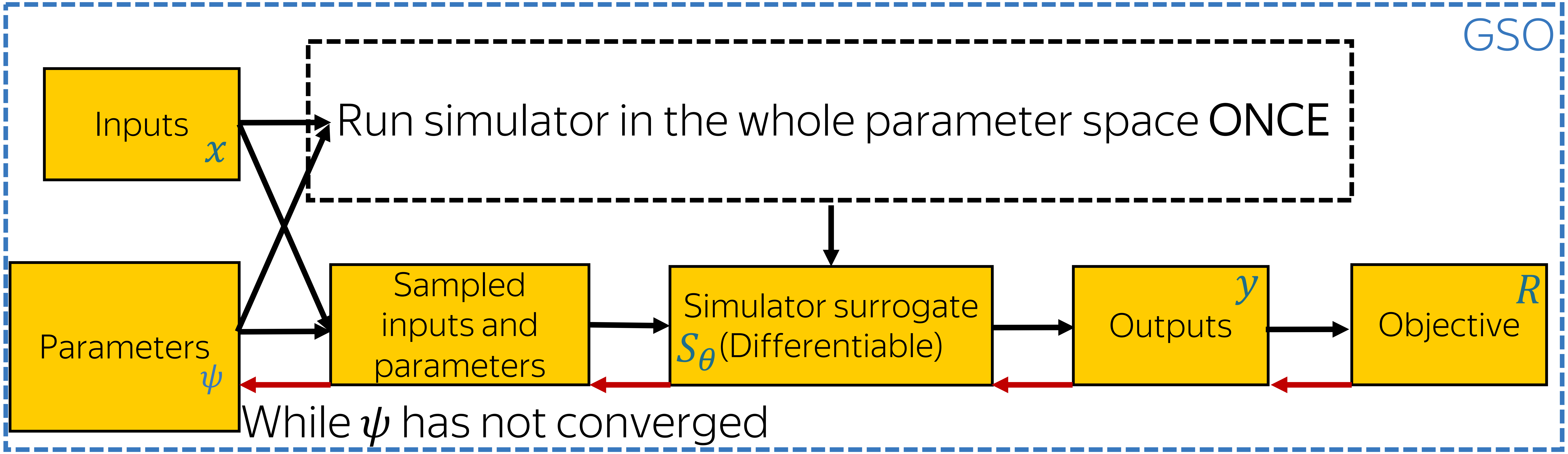
S_θ is trained in the whole ψ space:

- Curse of dimensionality
- Number of samples scales exponentially with dimension d: $\left(\frac{L}{\Delta}\right)^d$
- Generative models do not extrapolate well

Need to impose locality in the ψ space

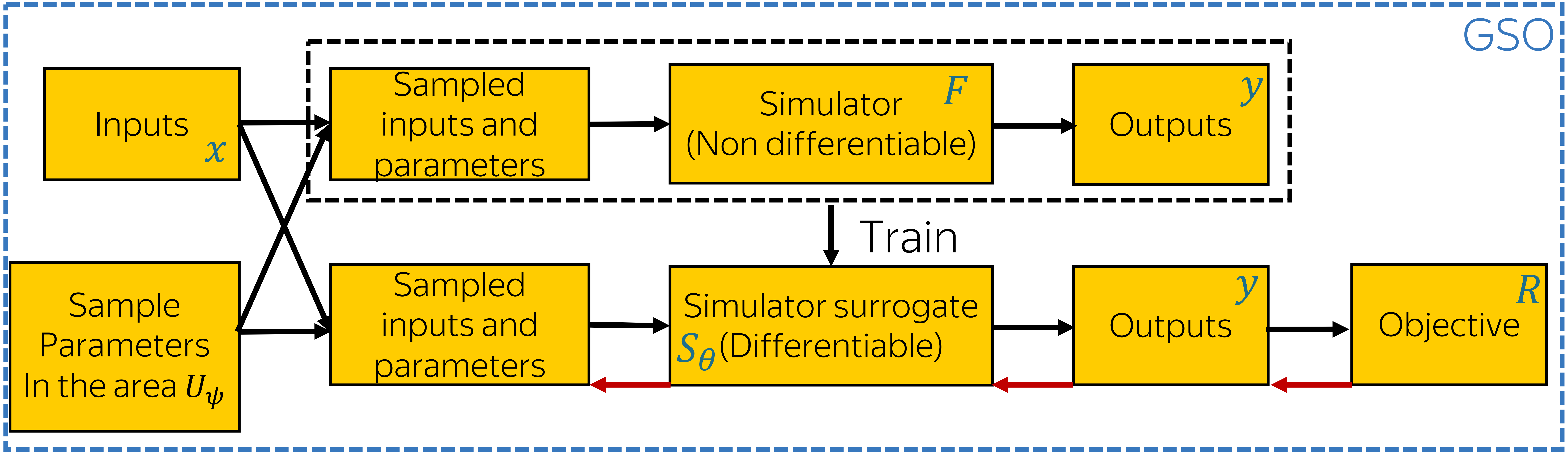


Local Generative Surrogates (L-GSO)


GSO
Inputs x
Run simulator in the whole parameter space ONCE
Parameters ψ
Sampled inputs and parameters
Simulator surrogate S_θ (Differentiable)
Outputs y
Objective R
While ψ has not converged

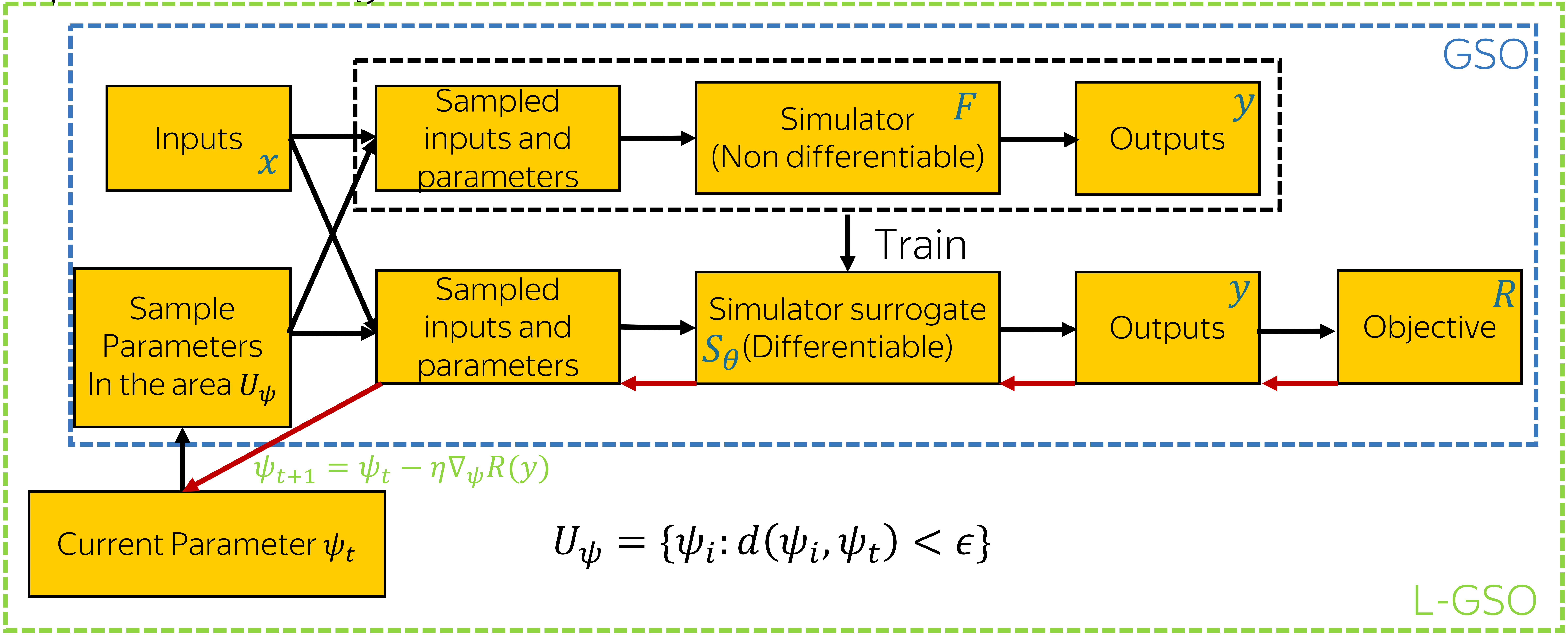
Local Generative Surrogates (L-GSO)

While ψ has not converged do:

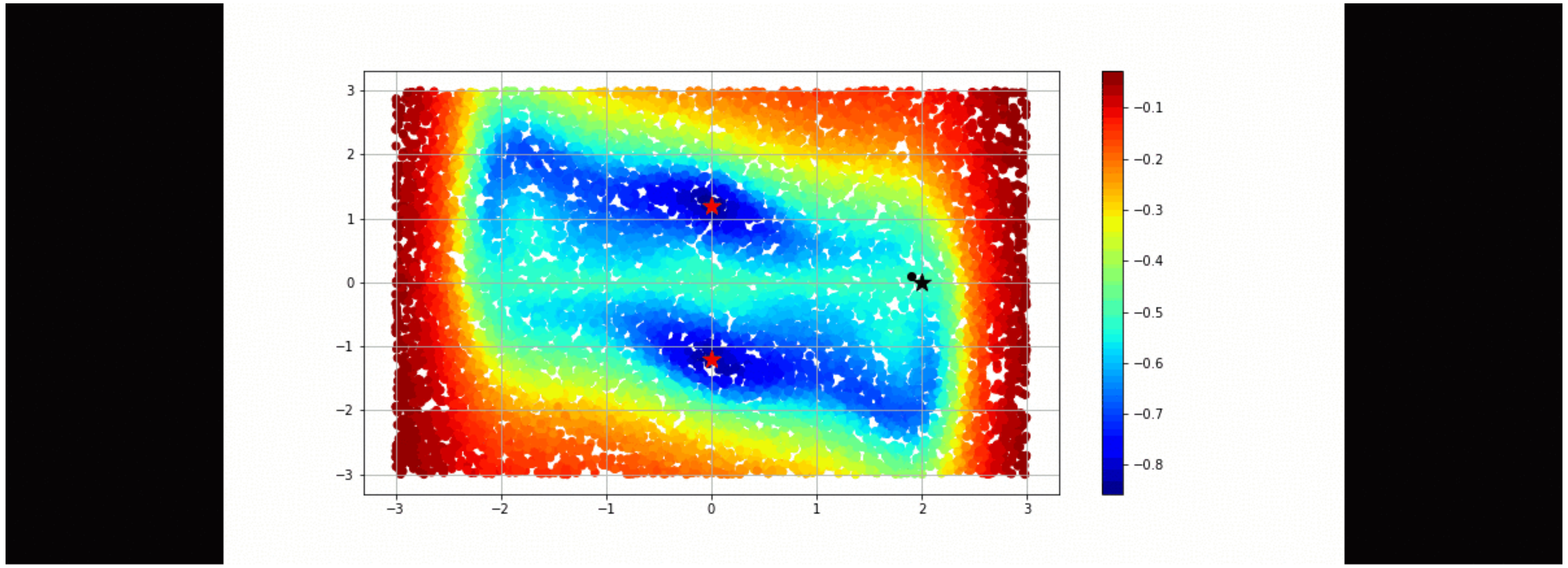

GSO
Inputs x
Sampled inputs and parameters
Simulator F (Non differentiable)
Outputs y
Train
Sample Parameters In the area U_ψ
Sampled inputs and parameters
Simulator surrogate S_θ (Differentiable)
Outputs y
Objective R

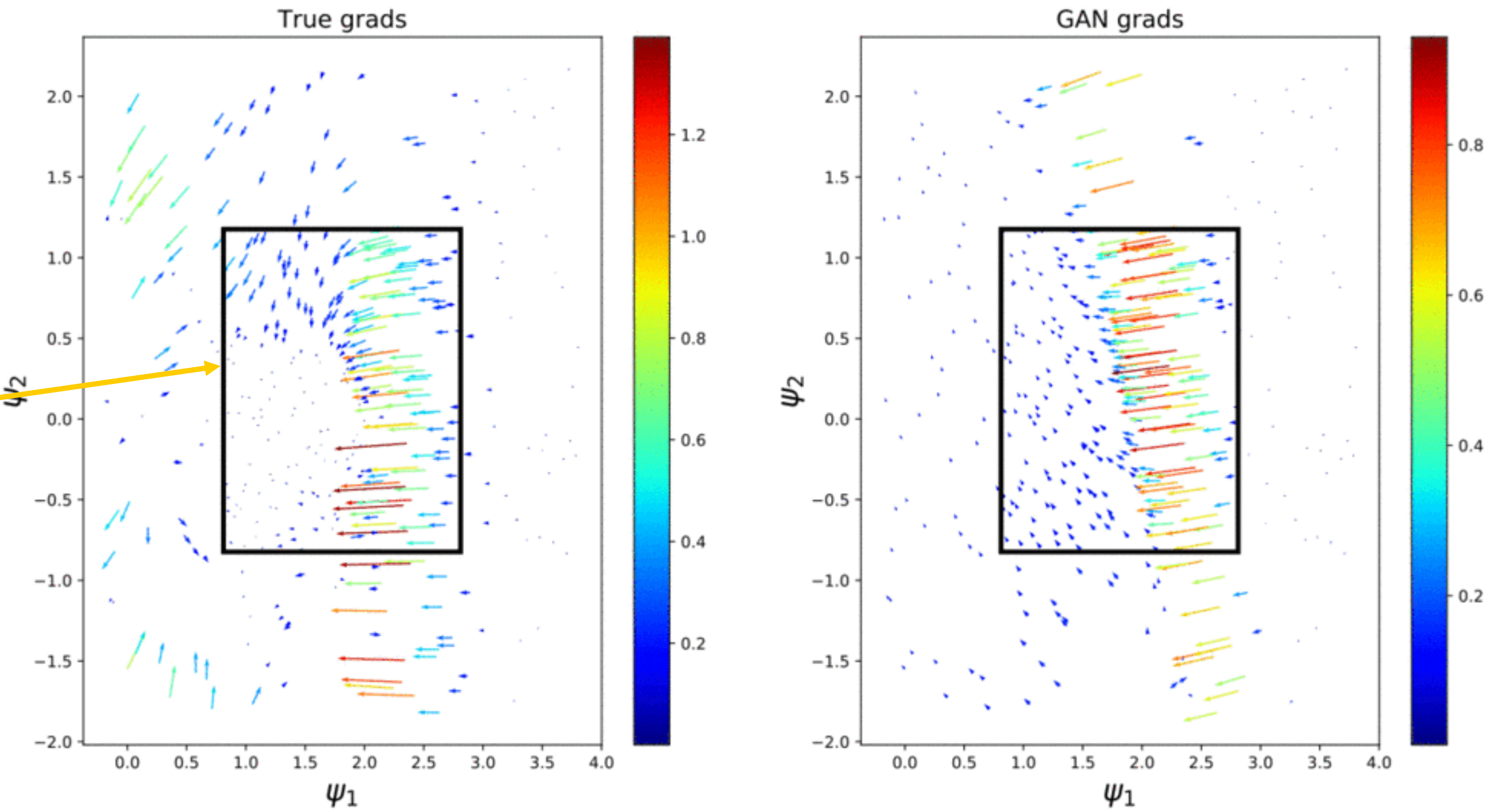
Local Generative Surrogates (L-GSO)

While ψ has not converged do:


GSO
Inputs x
Sampled inputs and parameters
Simulator (Non differentiable) F
Outputs y
Train
Sample Parameters In the area U_ψ
Sampled inputs and parameters
Simulator surrogate S_θ (Differentiable)
Outputs y
Objective R
$\psi_{t+1} = \psi_t - \eta \nabla_\psi R(y)$
Current Parameter ψ_t
$U_\psi = \{\psi_i : d(\psi_i, \psi_t) < \epsilon\}$
L-GSO

Local Generative Surrogates (L-GSO)





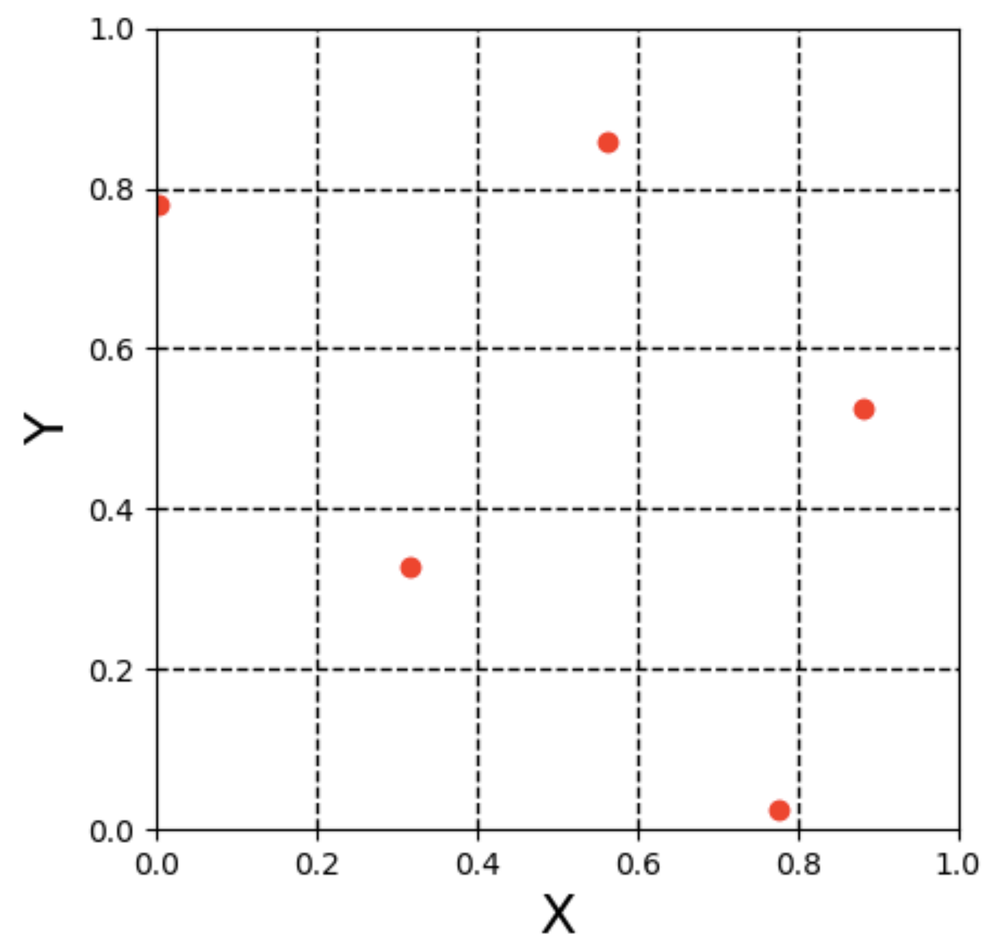
U_ψ where the surrogate is trained

Gradients are well estimated in the local area

Link:https://doi.org/10.6084/m9.figshare.9944597.v3

What is U_ψ?

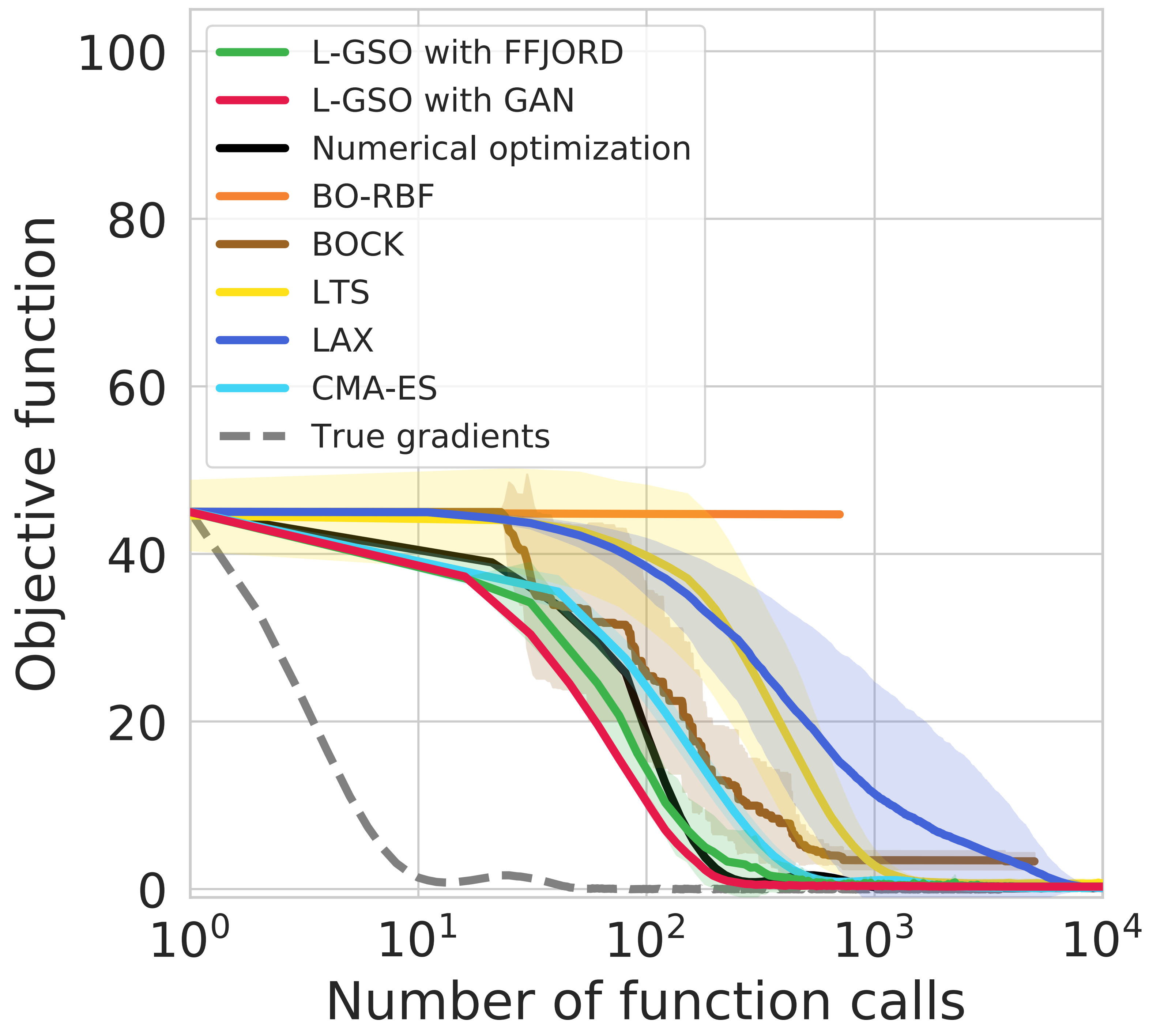
- $U_\psi = \{\psi_i\colon |\vec{\psi}_t - \vec{\psi}_i| < \epsilon\}$
- Fill U_ψ with Latin Hypercubes sampling
- ϵ is fixed
- Select ϵ: $E[|R(y_{\psi+\epsilon})$ - $R\left(y_{\psi-\epsilon}\right)|\,] > Var\left[R\left(y_\psi\right)\right]$



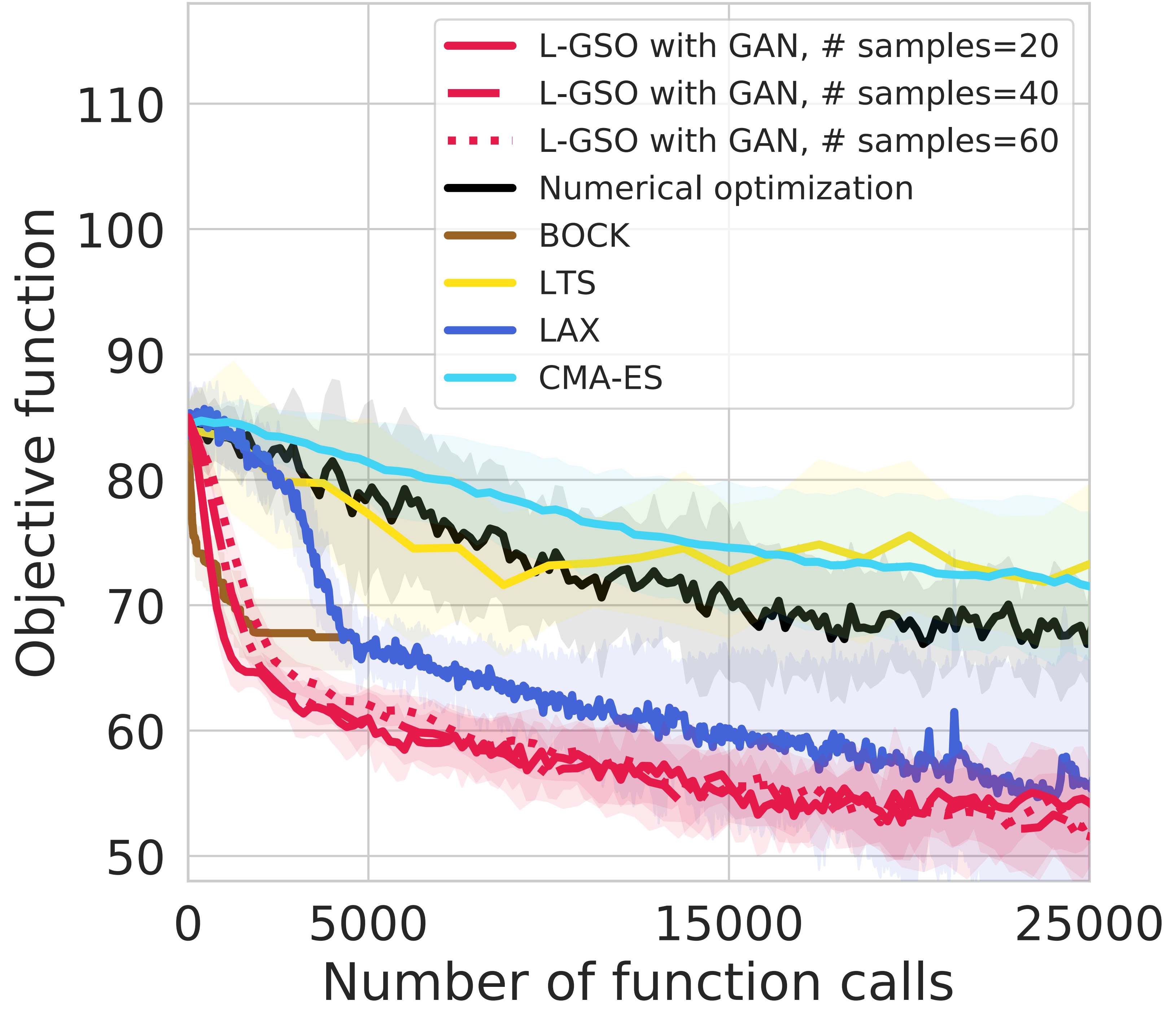
Toy Experiments

- 4 toy problems
- Various dimensions
- Degenerate parameters
- Costly simulator call
- Compare in:
  - number of calls
  - attained minimum

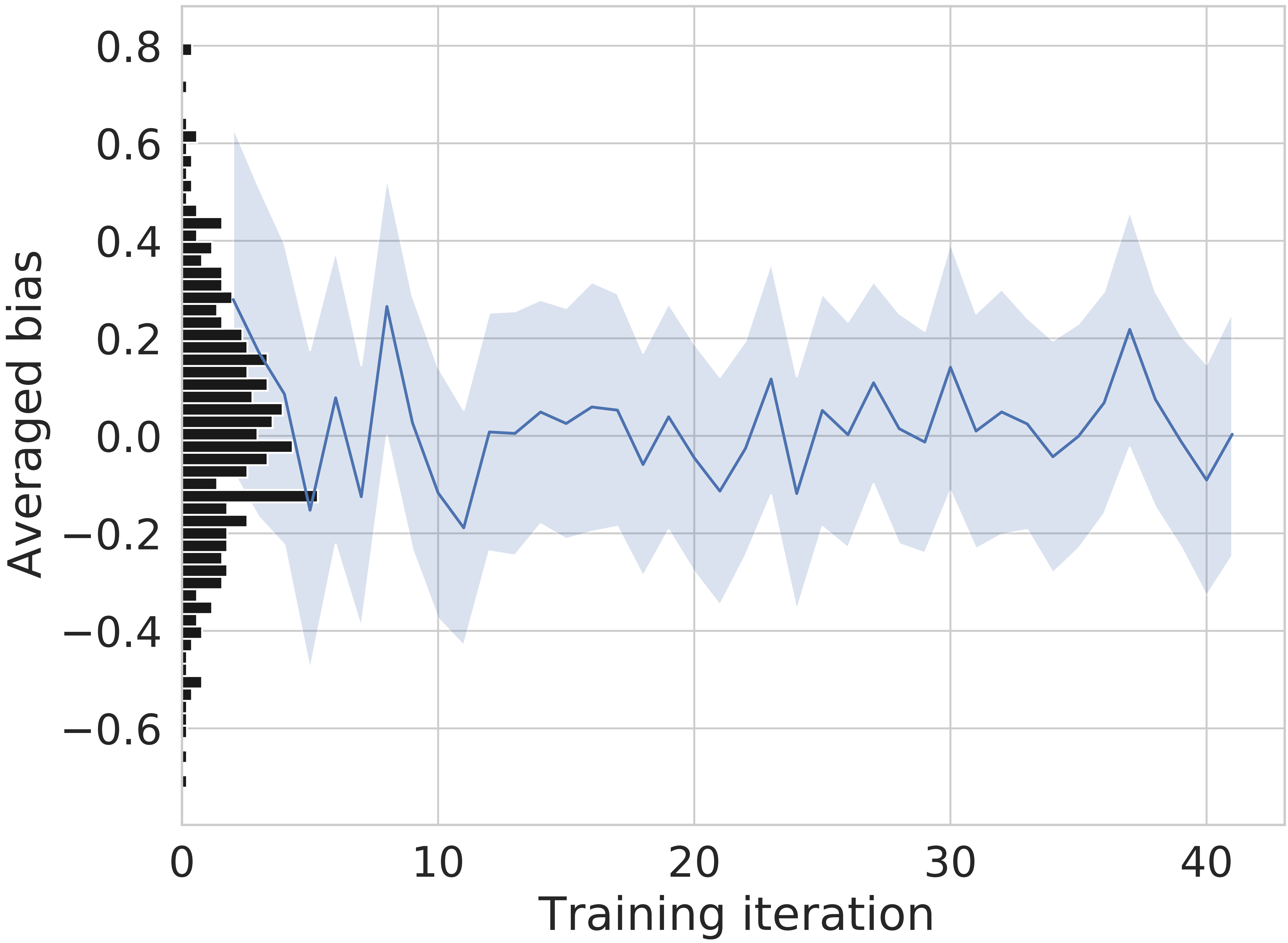
Rosenbrock problem
10-dim

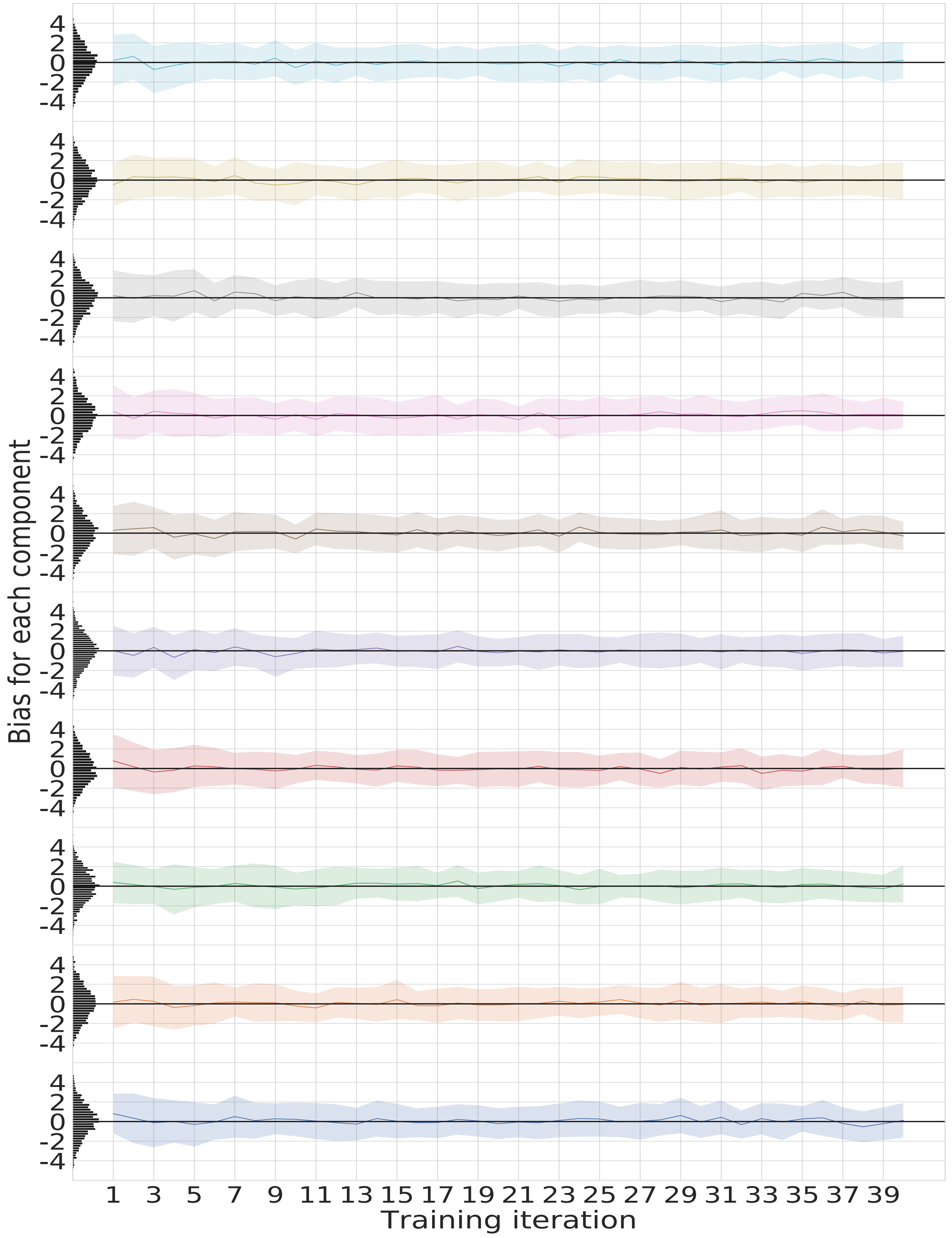


Neural Networks weights
optimisation
91-dim



L-GSO bias





$$Bias_t = \nabla_{\psi|\psi_t} R(y_\psi) - \nabla_{\psi|\psi_t} R(\bar{y})$$

- No bias observed for L-GSO

SHiP: Shield optimisation

Muon kinematics, including start coordinate

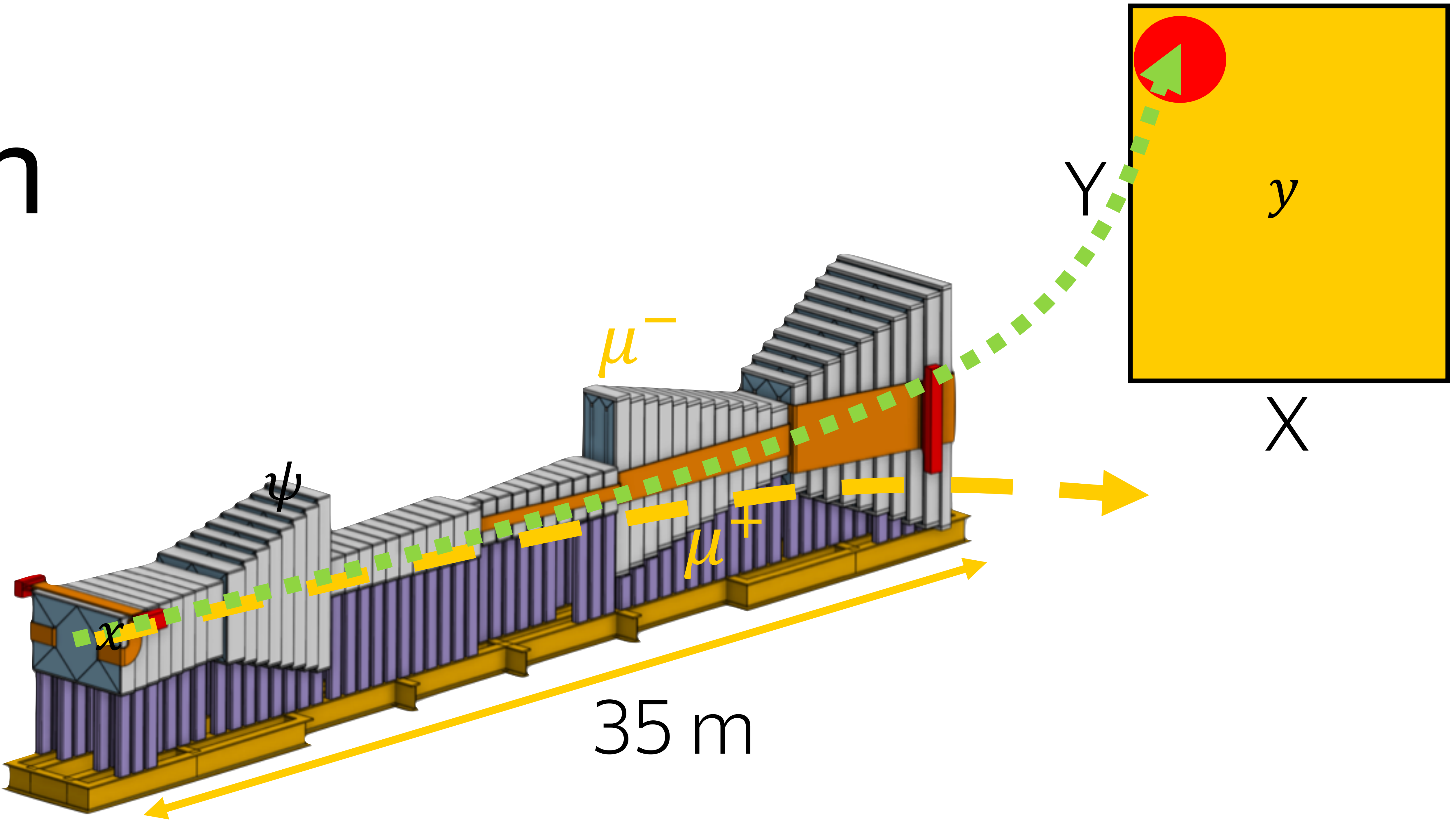
$$x = \{P, \phi, \theta, Q, \boldsymbol{C}\}, X \in \mathbb{R}^7$$

Output: coordinates of the muon hit

$$y = \{X, Y\}, y \in \mathbb{R}^2$$

Optimised parameters: shield geometry

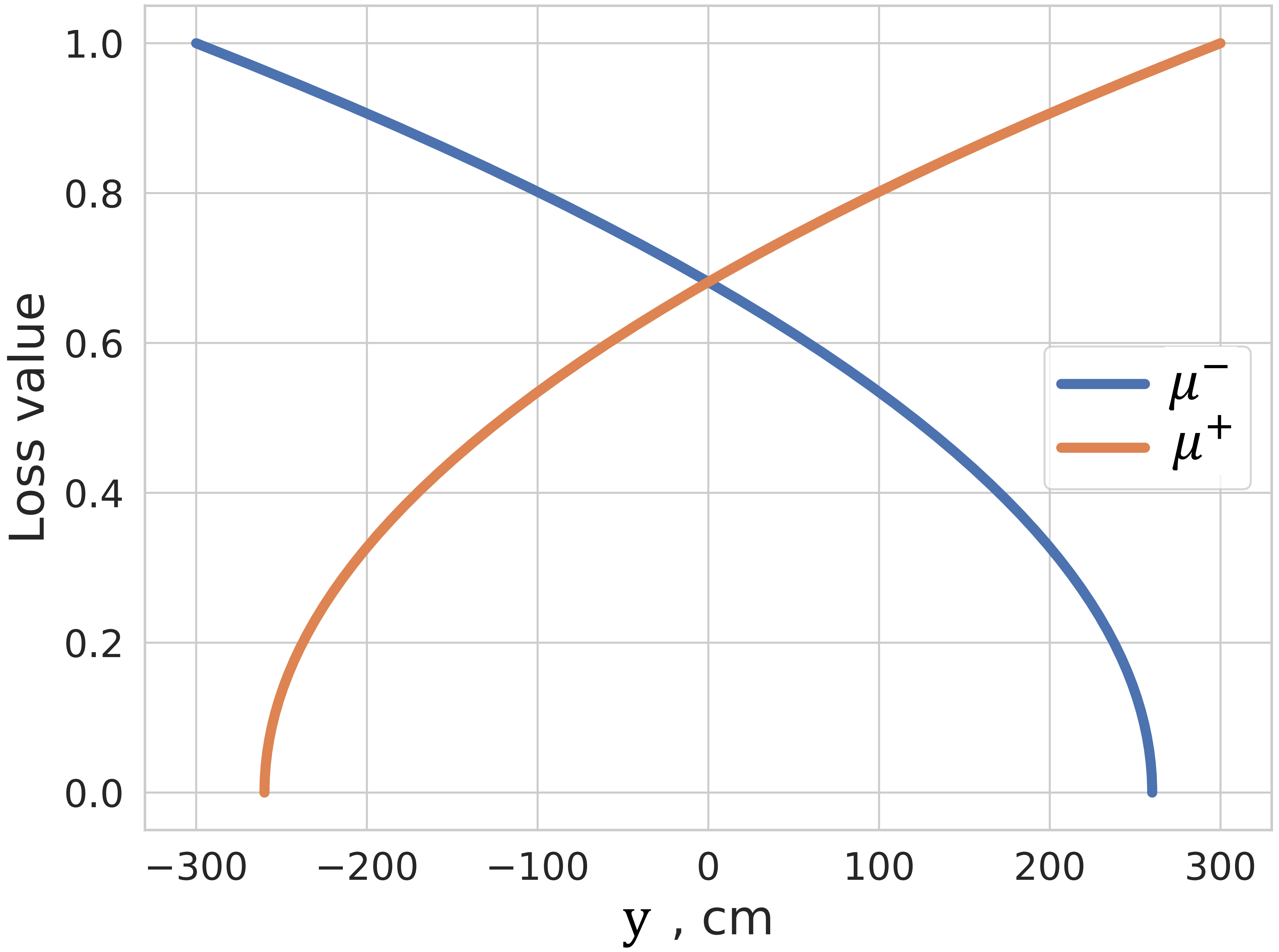
$$\psi \in \mathbb{R}^{42}$$



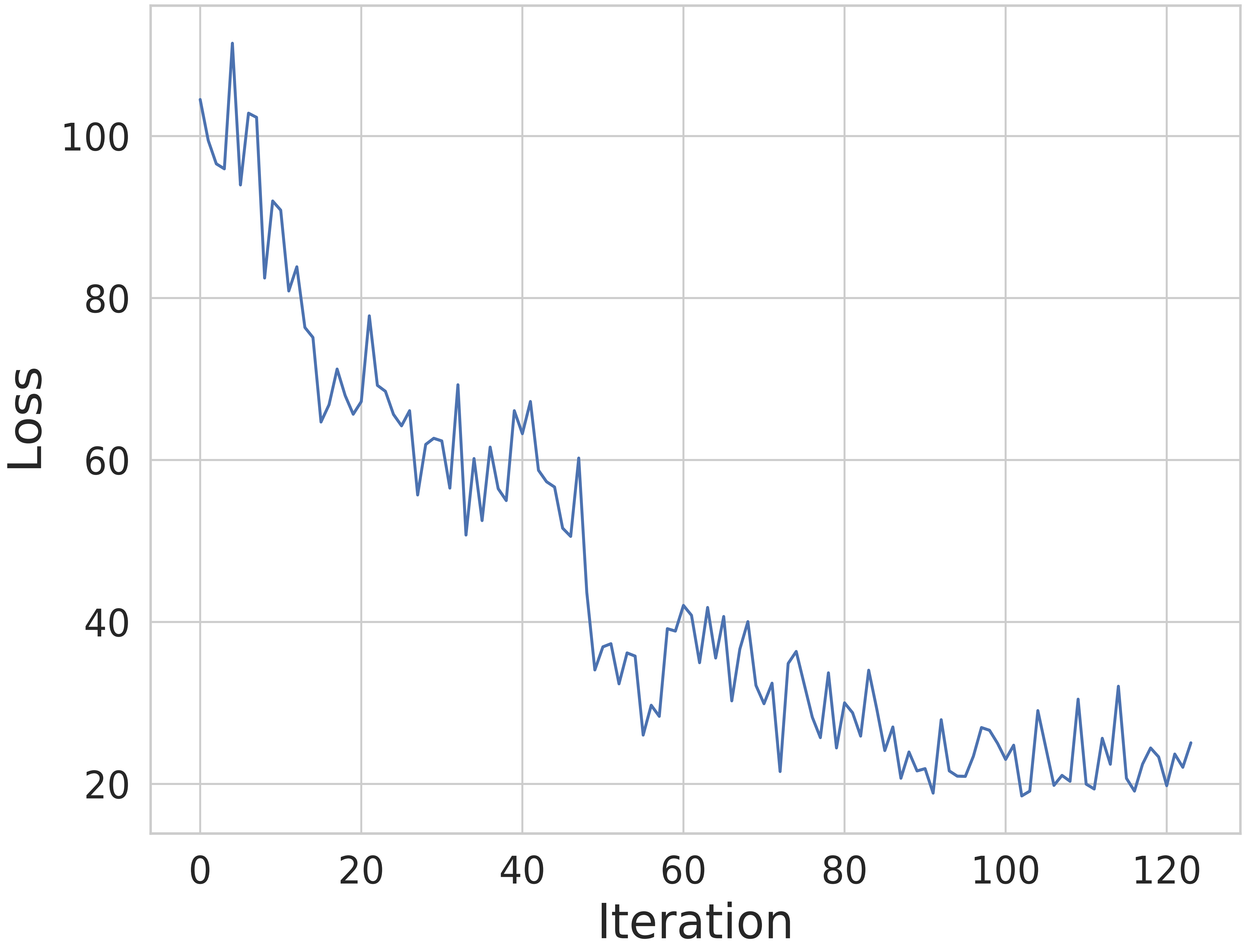
Objective function

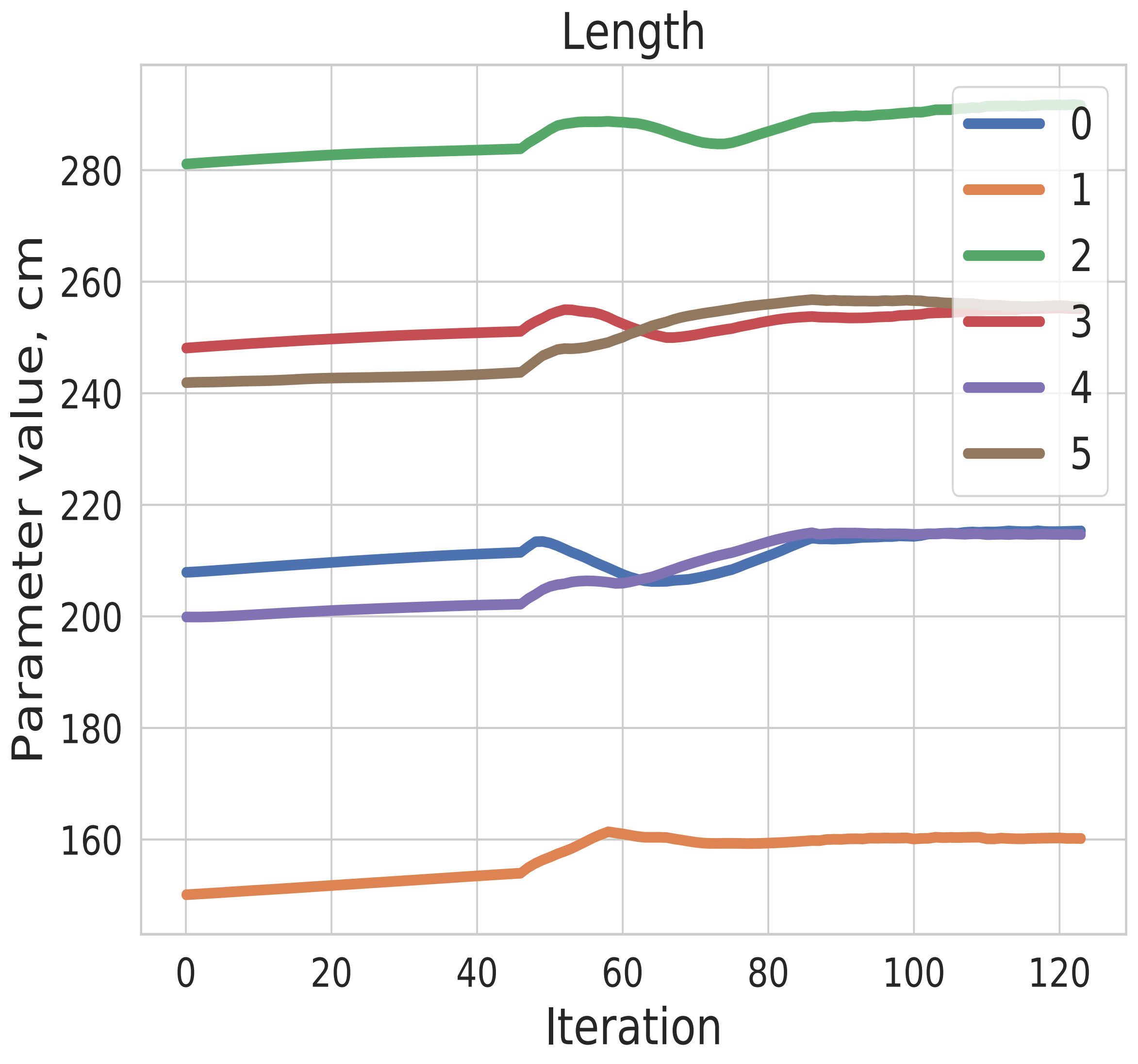
$$R(y; \alpha) = \mathbf{1}_{Q=-1}\sqrt{(\alpha_1 - (y + \alpha_2))/\alpha_1} + \mathbf{1}_{Q=1}\sqrt{(\alpha_1 + (y - \alpha_2))/\alpha_1}$$

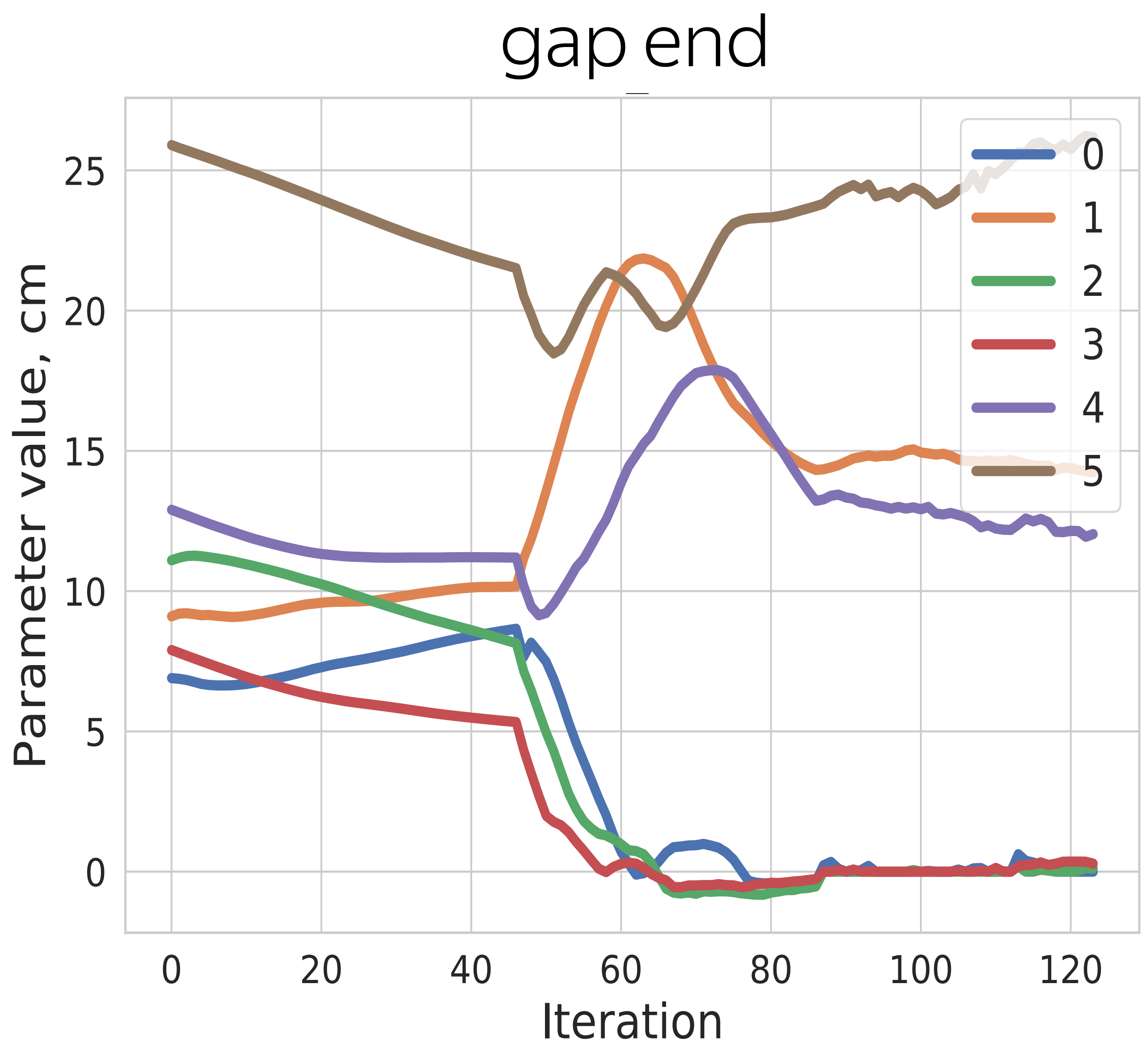
Was previously optimised with BO

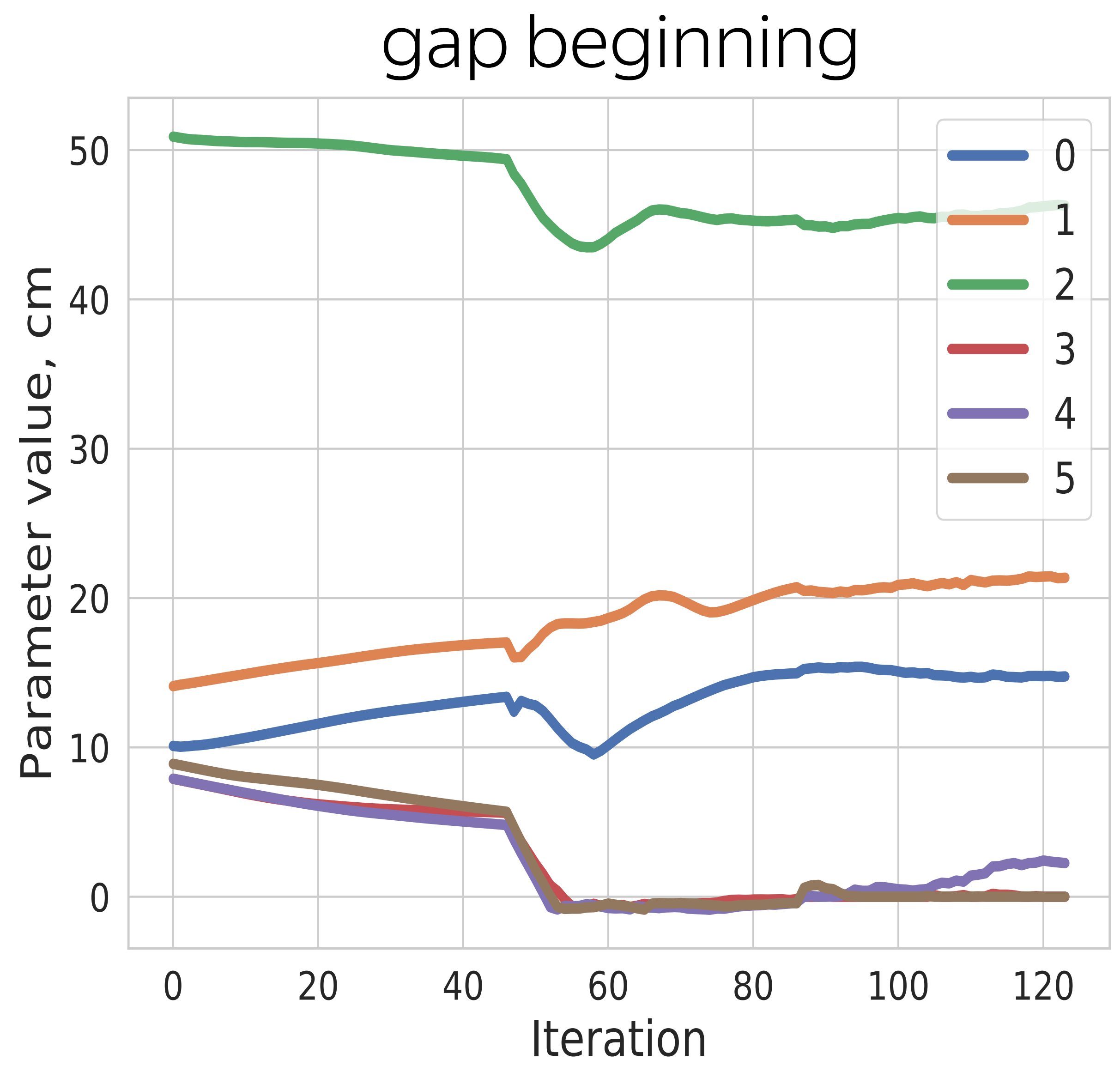


SHiP: Parameter changes





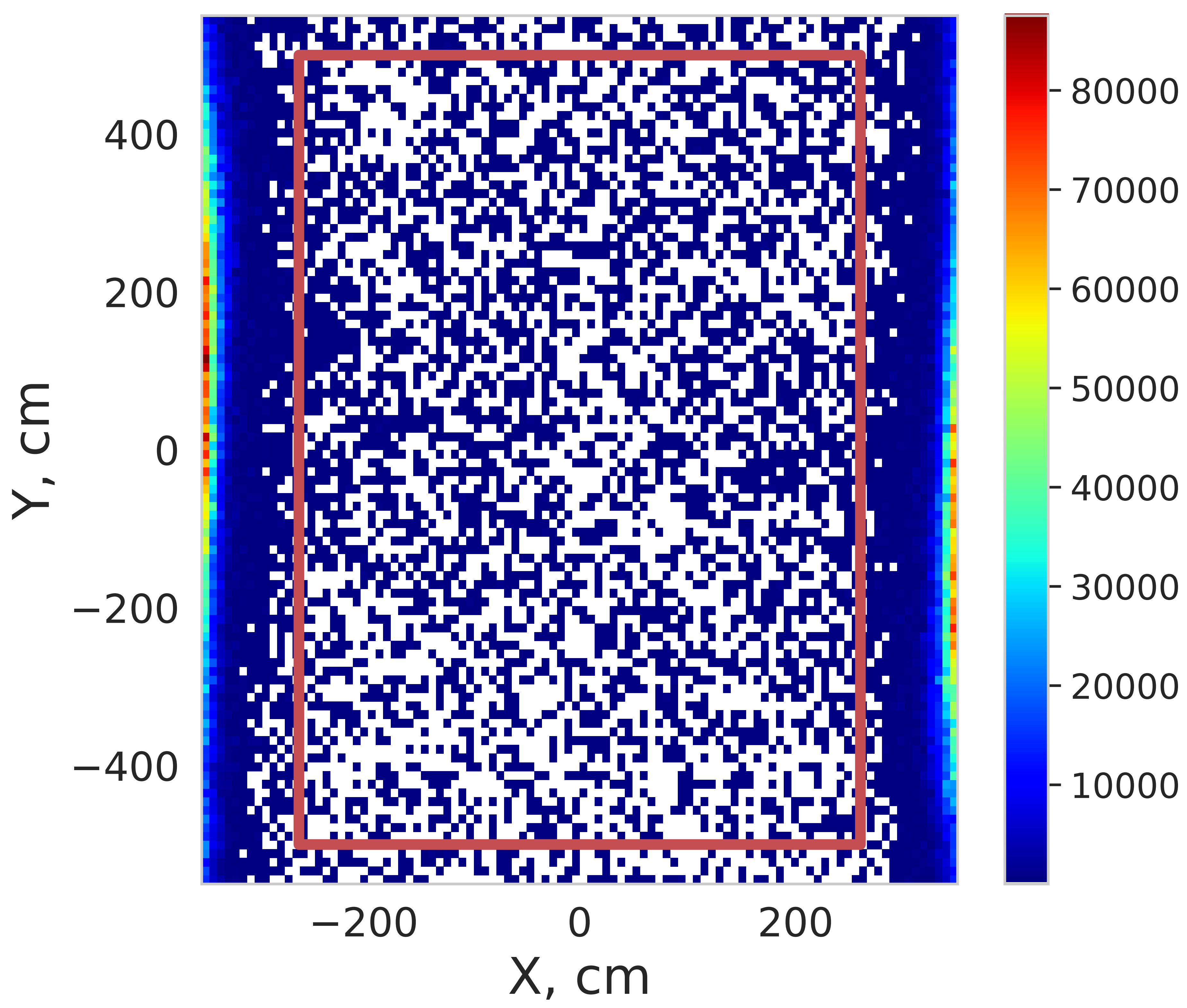




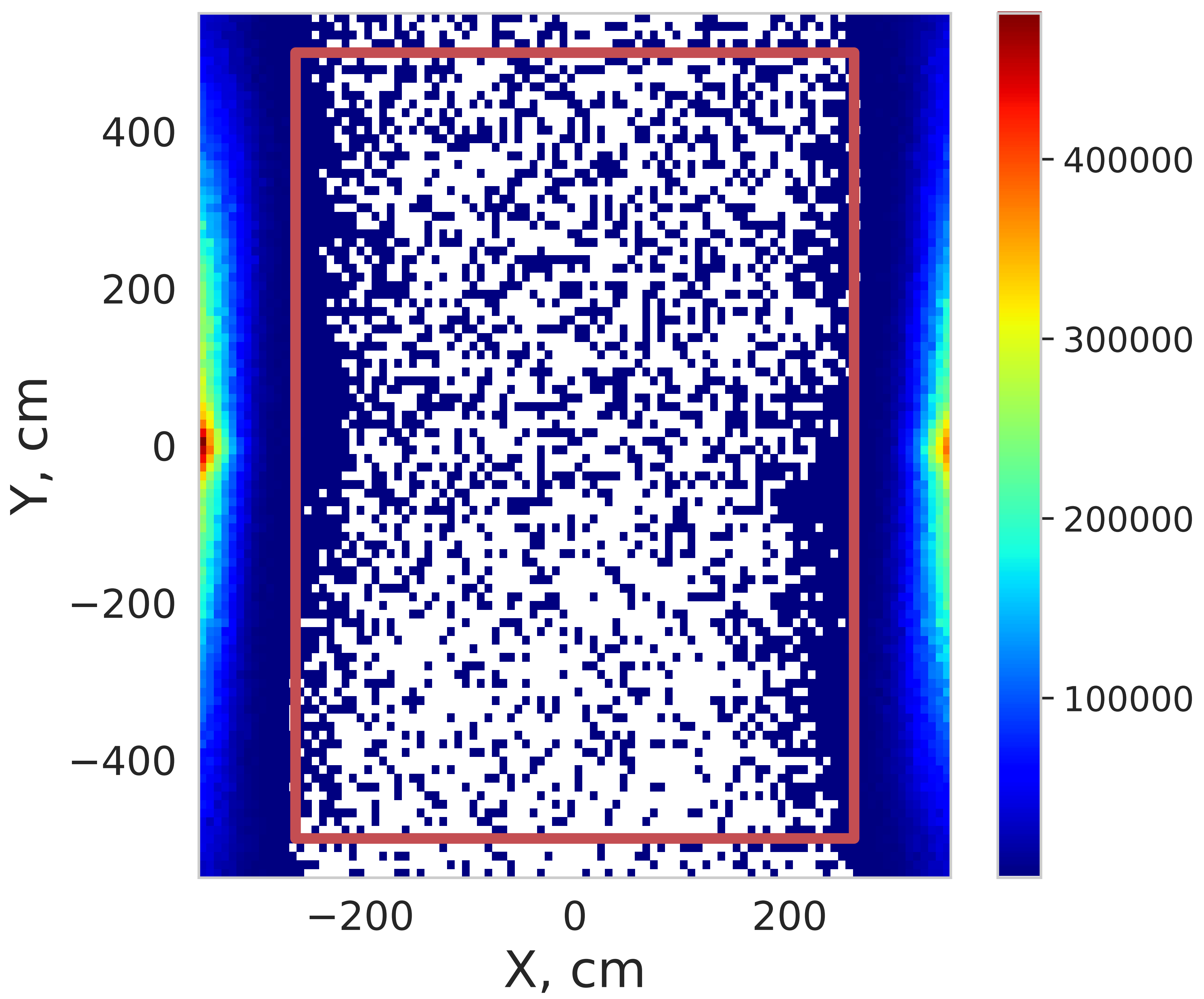
Continuous changes of the parameters: might give some insights about physics!

SHiP: shield optimisation comparison

Previous optimum(BO)



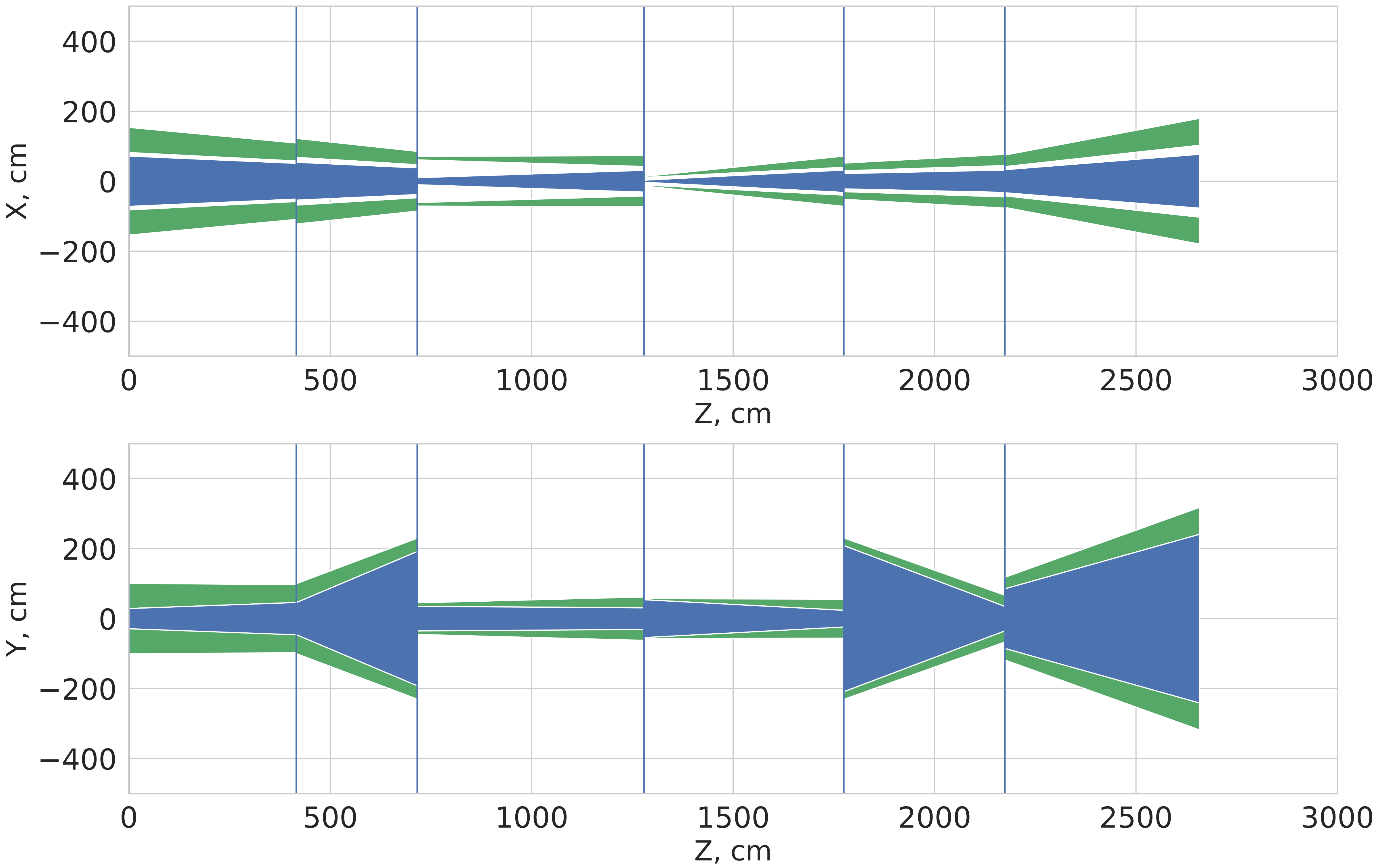
New optimum(L-GSO)



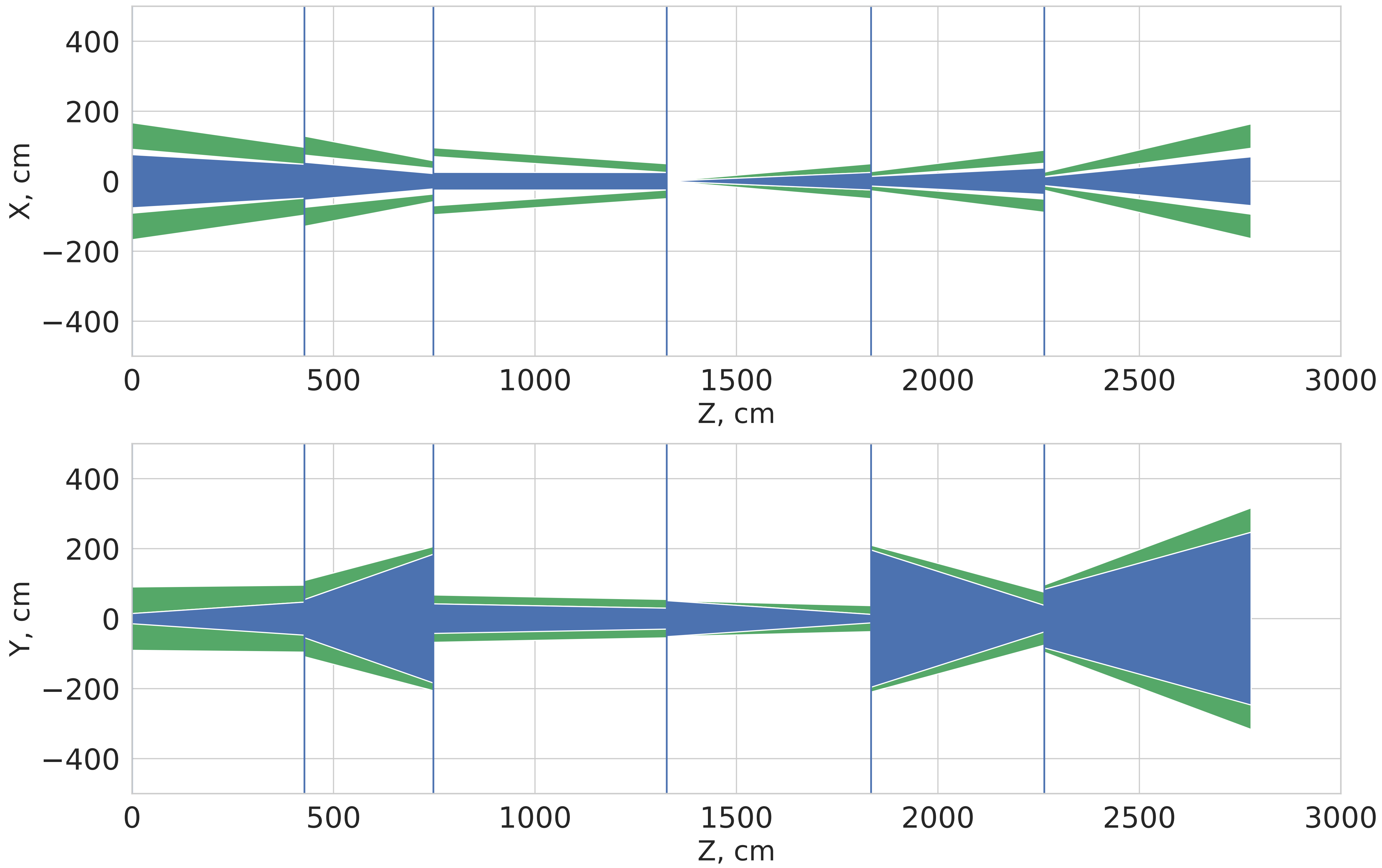
Method	Loss	Shield length (m)	Magnet weight (kt)
L-GSO	~ 2200	33.39	1.05
Bayesian opt.	~ 3000	35.44	1.27

SHiP: shield geometry change

Initial shape



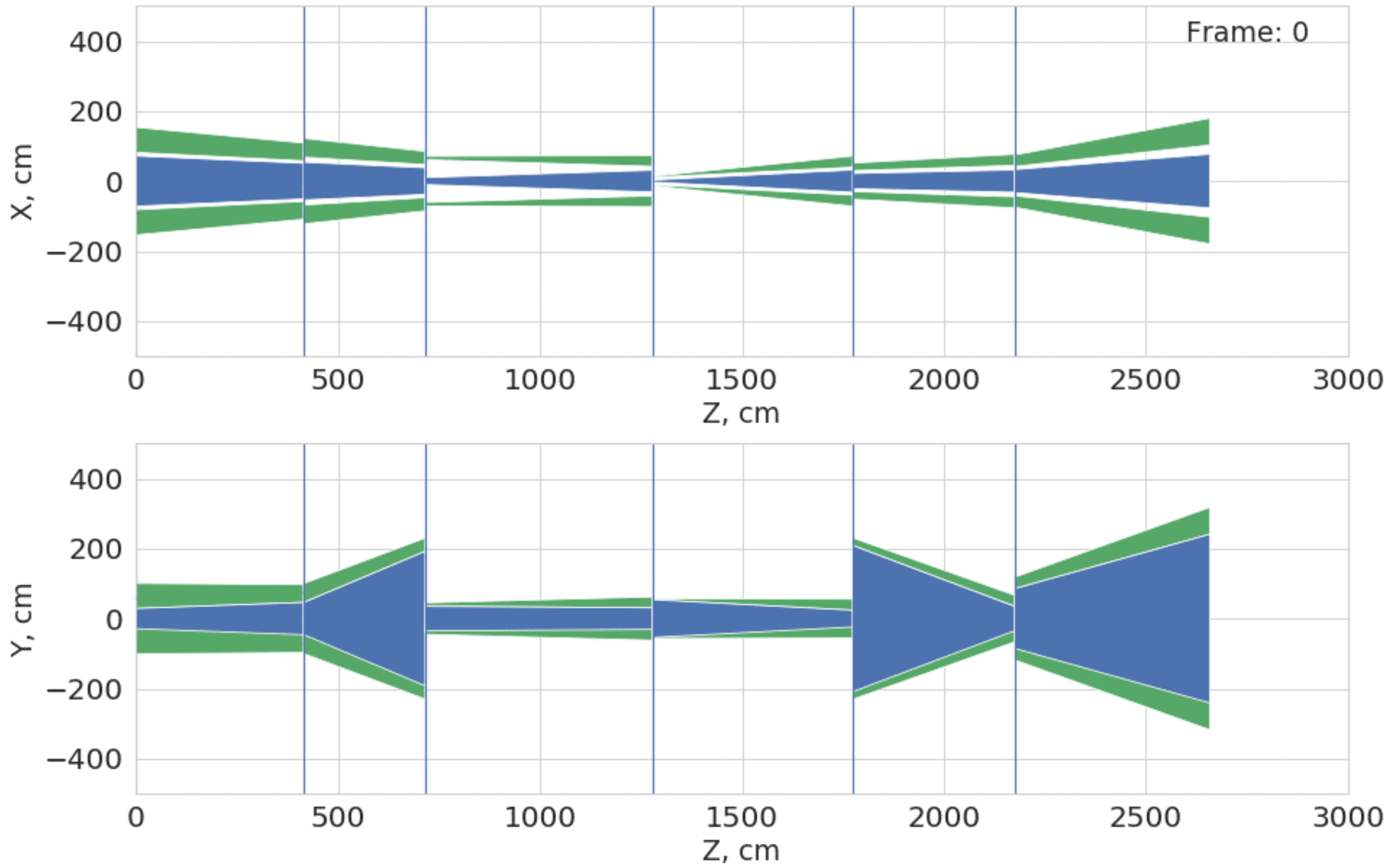
Final shape



Animation of the optimisation: https://doi.org/10.6084/m9.figshare.11778684.v1

SHiP: shield geometry change

Animation



Conclusion

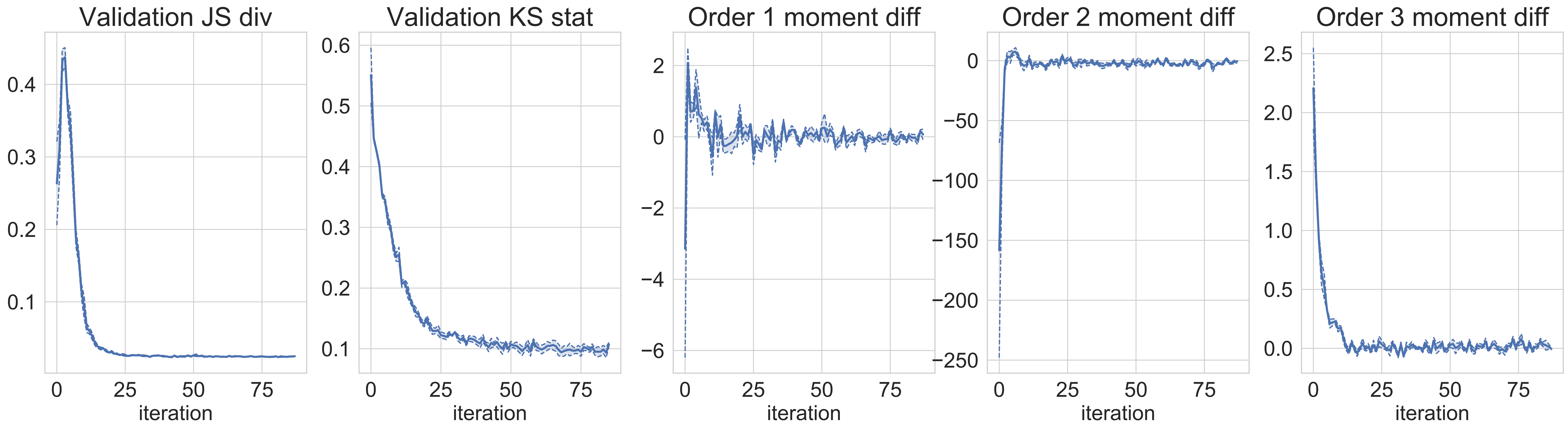
- Overview of black-box optimisation methods / problem formulation
- Present novel optimisation approach: L-GSO
- Excel:
  - Parameters lie on a low-dimensional manifold
  - Simulator call is costly
- Empirically low variance
- Attained better minima than Bayesian optimisation in HEP problem

Future work:

- Implementation of trust-region methods
- Combination of BO and surrogate gradients

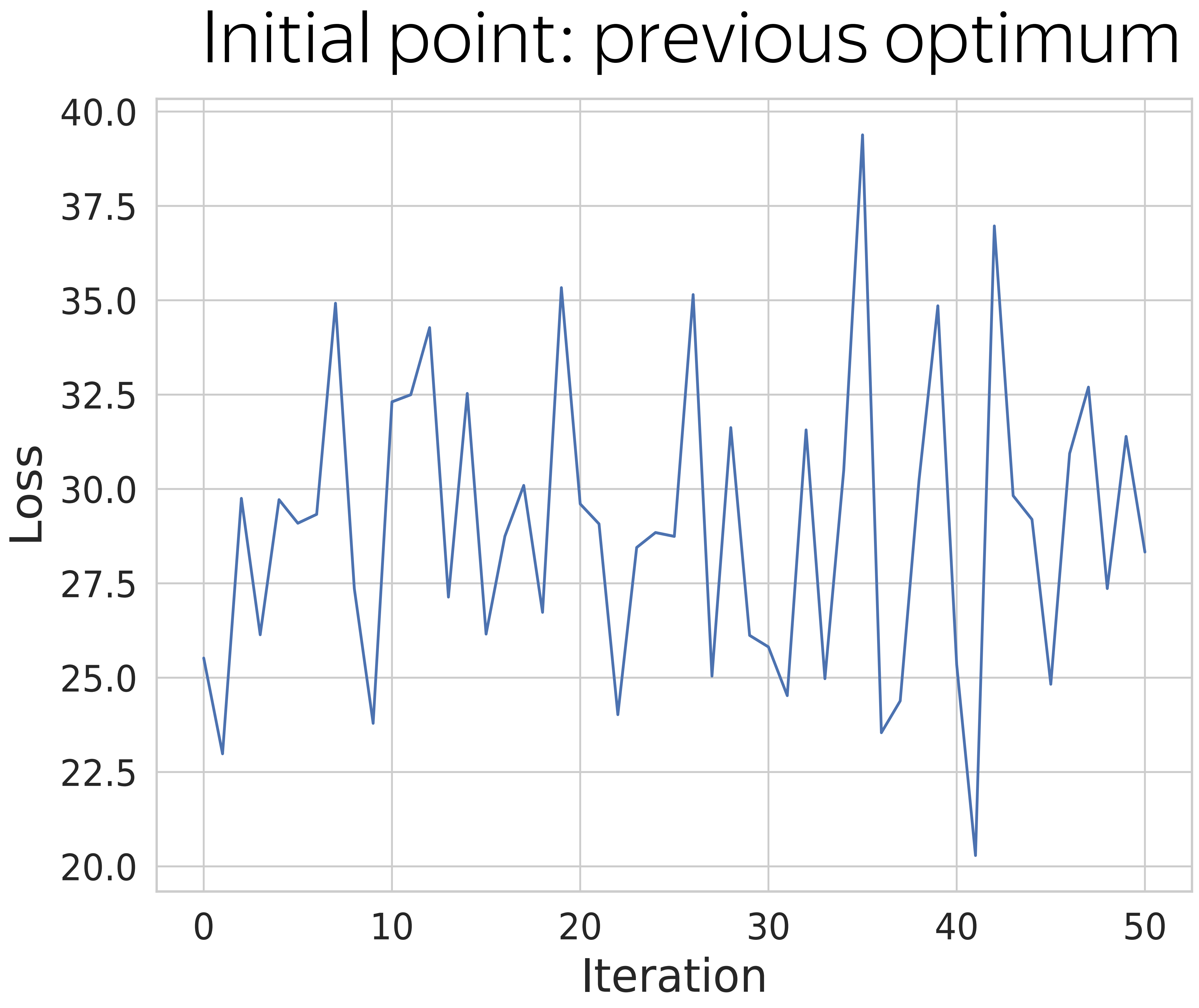
Backup

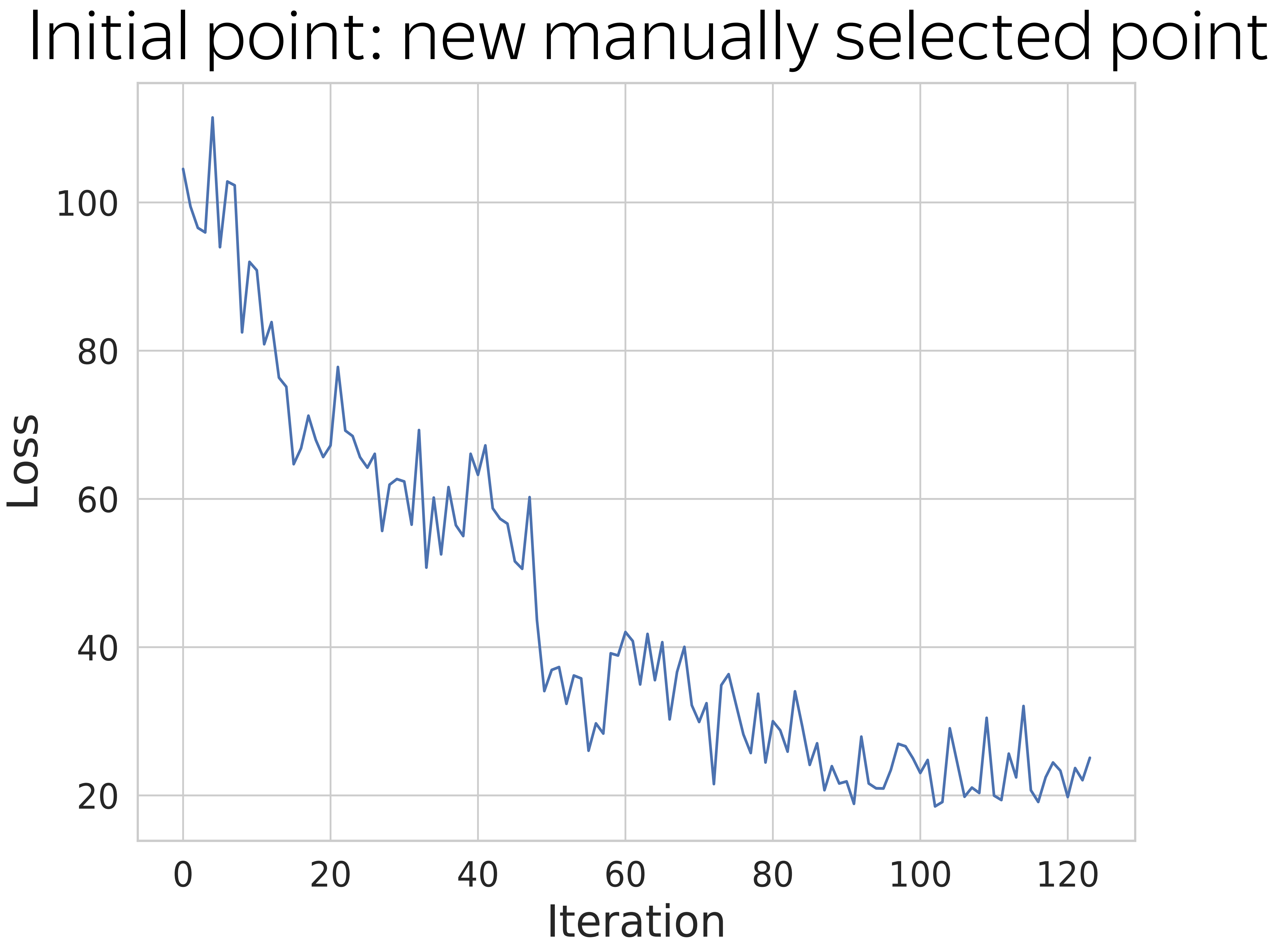
Monitoring of model performance



- Monitor various metrics between train distribution and sampled distribution
- Abort optimisation in case of divergence
- Adjust hyper parameters

SHiP: Shield optimisation

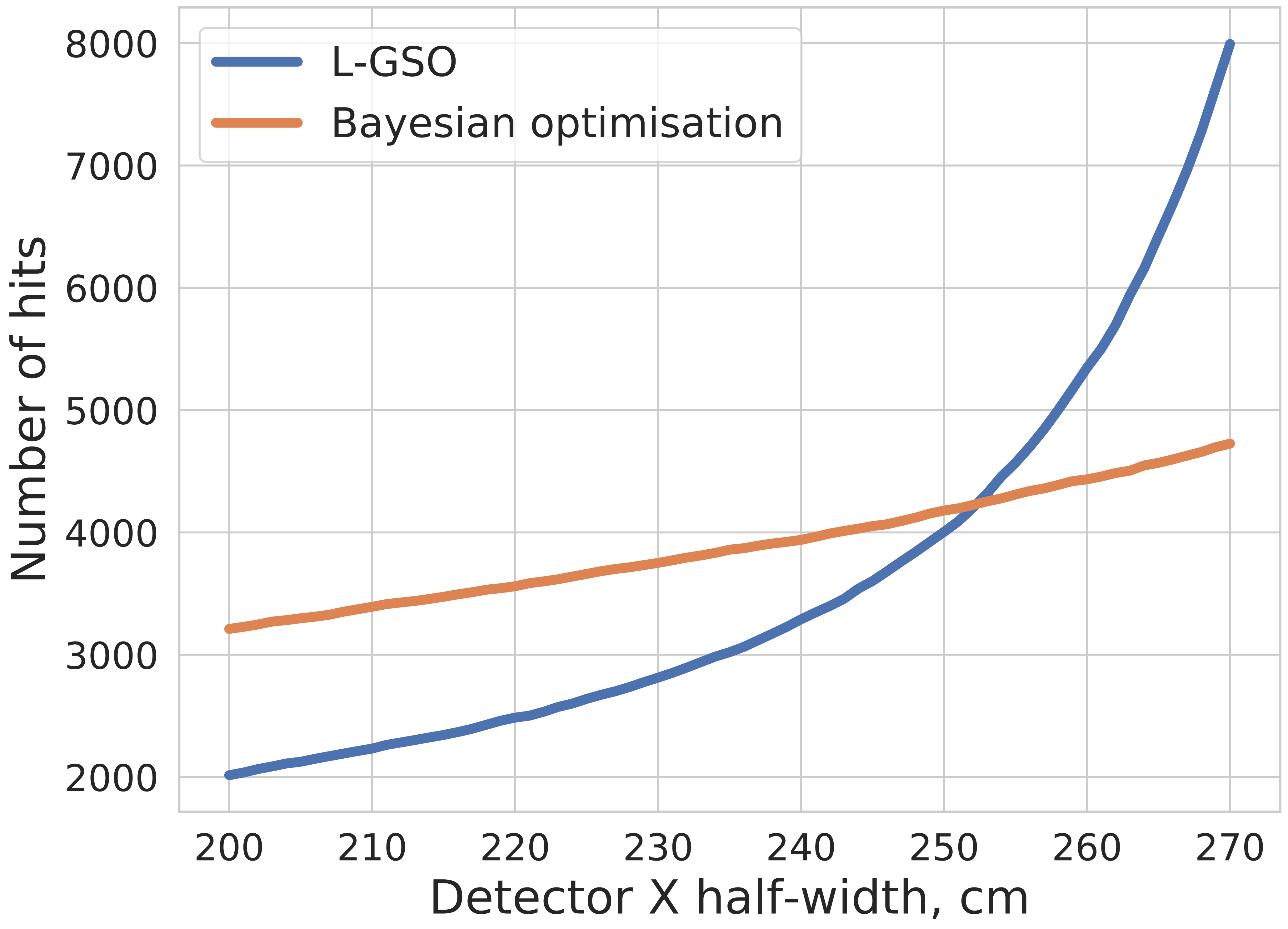




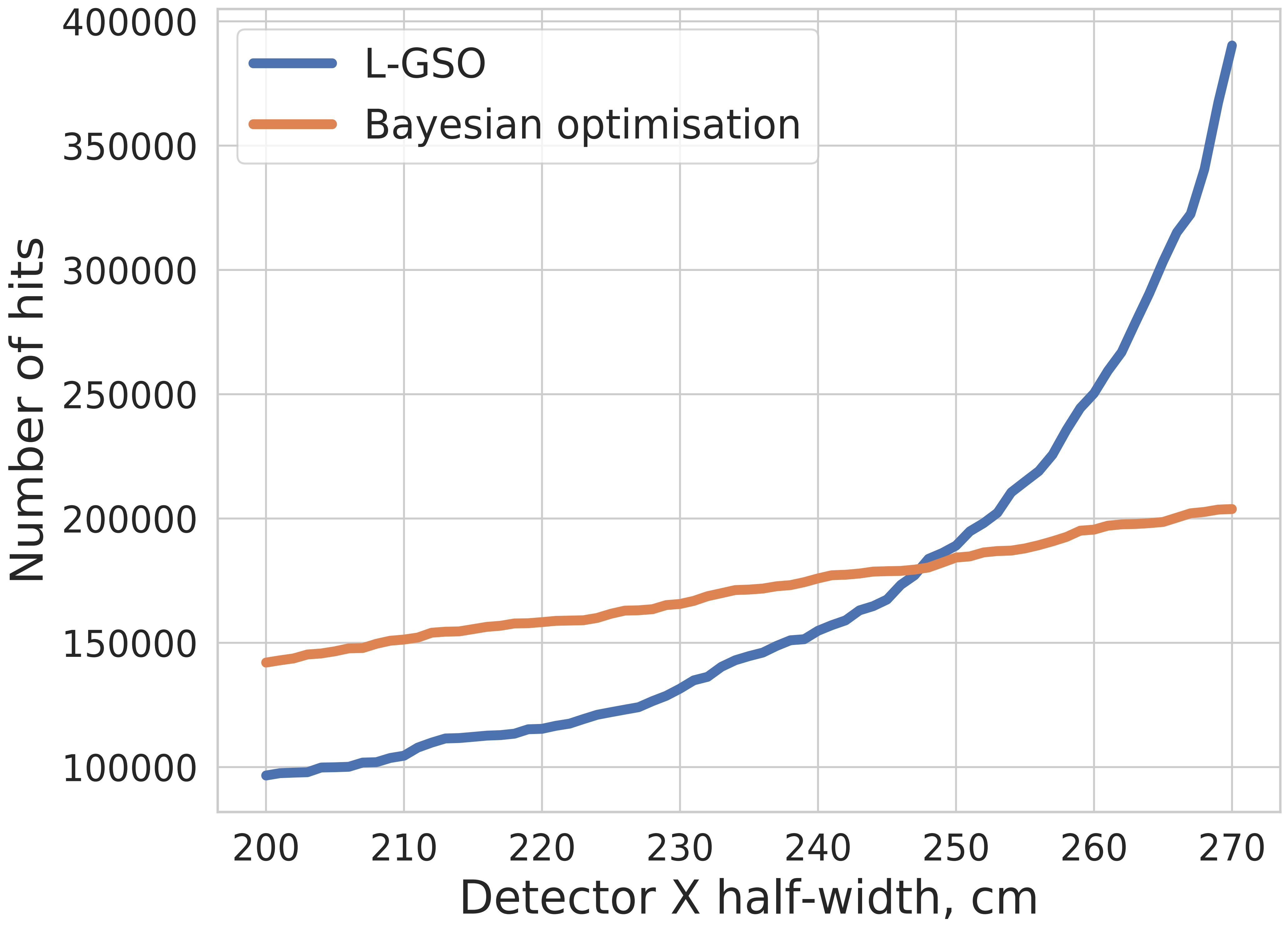
Is it the same optimum?

Shield optimization: comparison

Number of hits(unweighted)

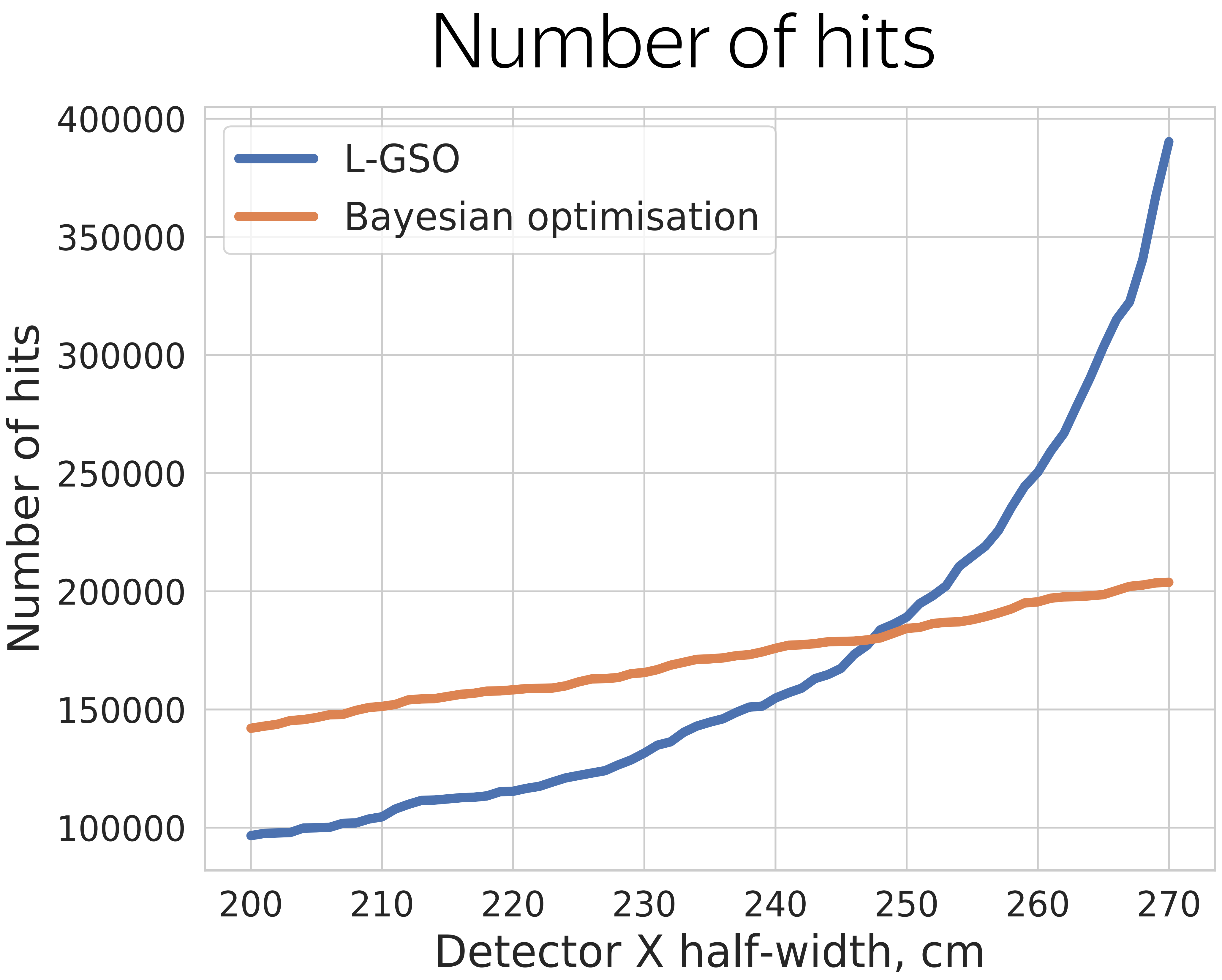


Number of hits(weighted)

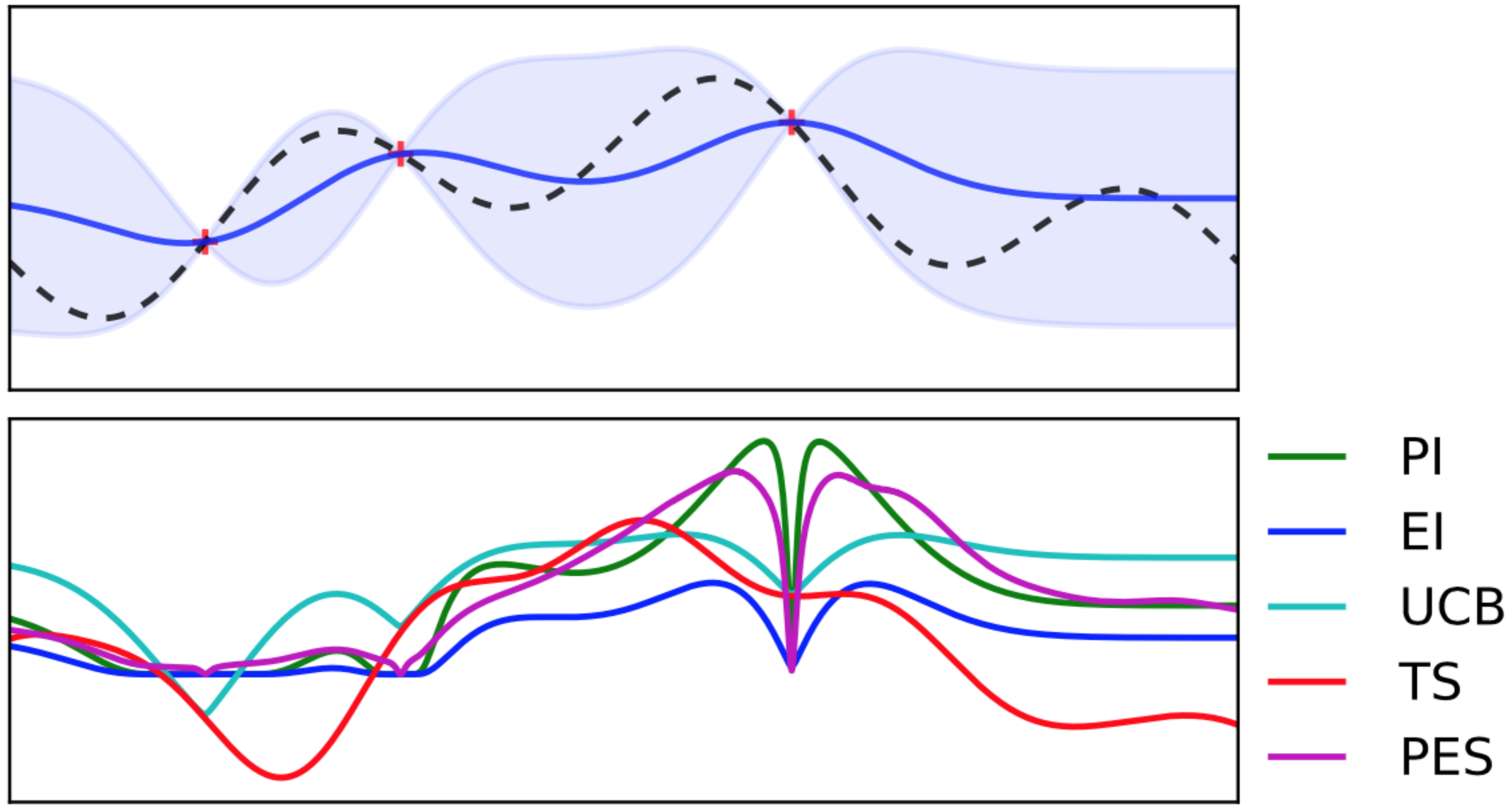


SHiP: shield optimisation comparison

- L-GSO is very sensitive to the optimised parameter changes



Bayesian optimisation with Gaussian Process



$$y_i = f_i + \epsilon, \qquad \epsilon \sim N(0, \sigma_{obs}^2)$$

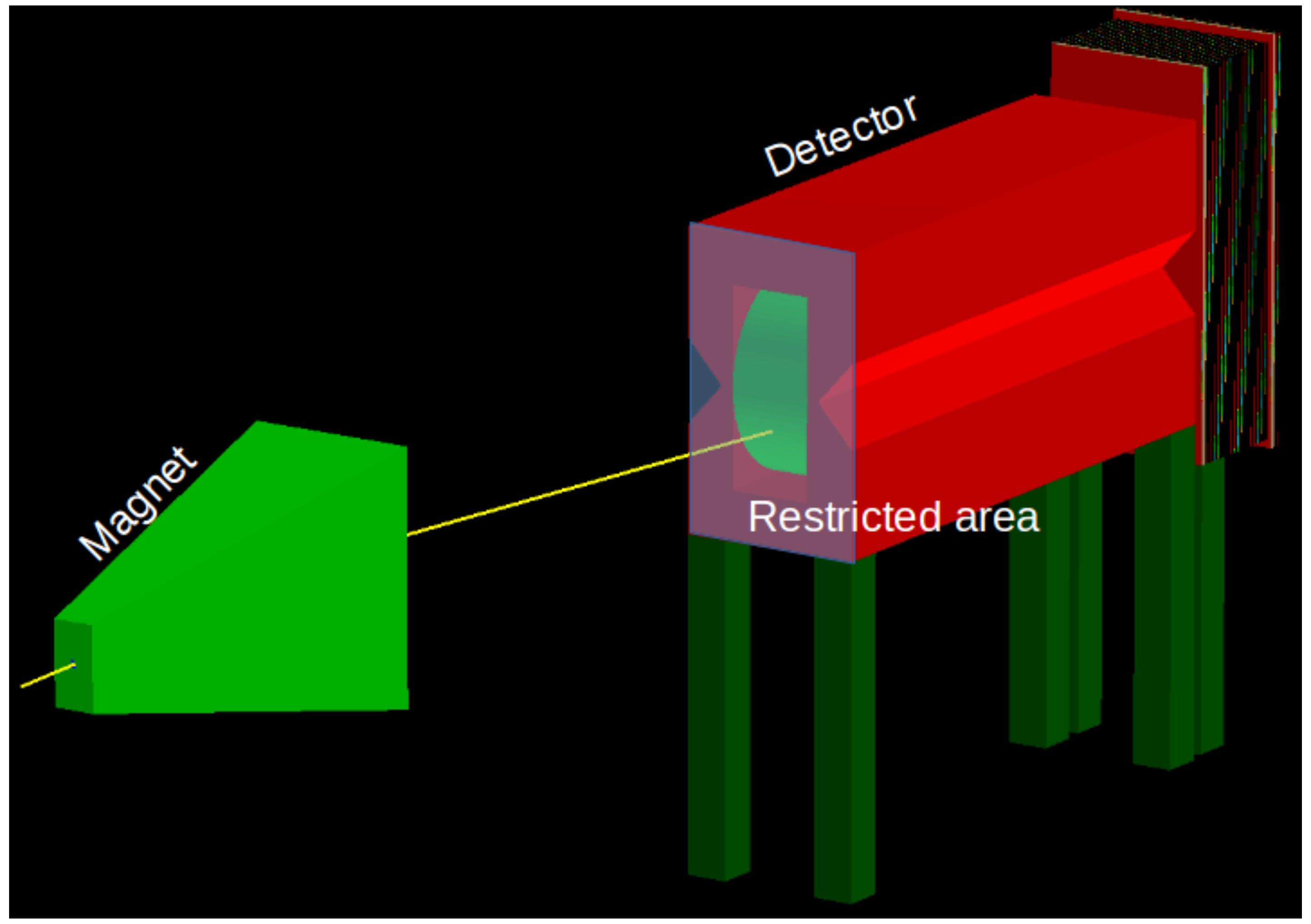
$$\mu(x_* \,|D) = K_{*D}\left(K_{DD} + \sigma_{obs}^2 I\right)^{-1} \boldsymbol{y}$$

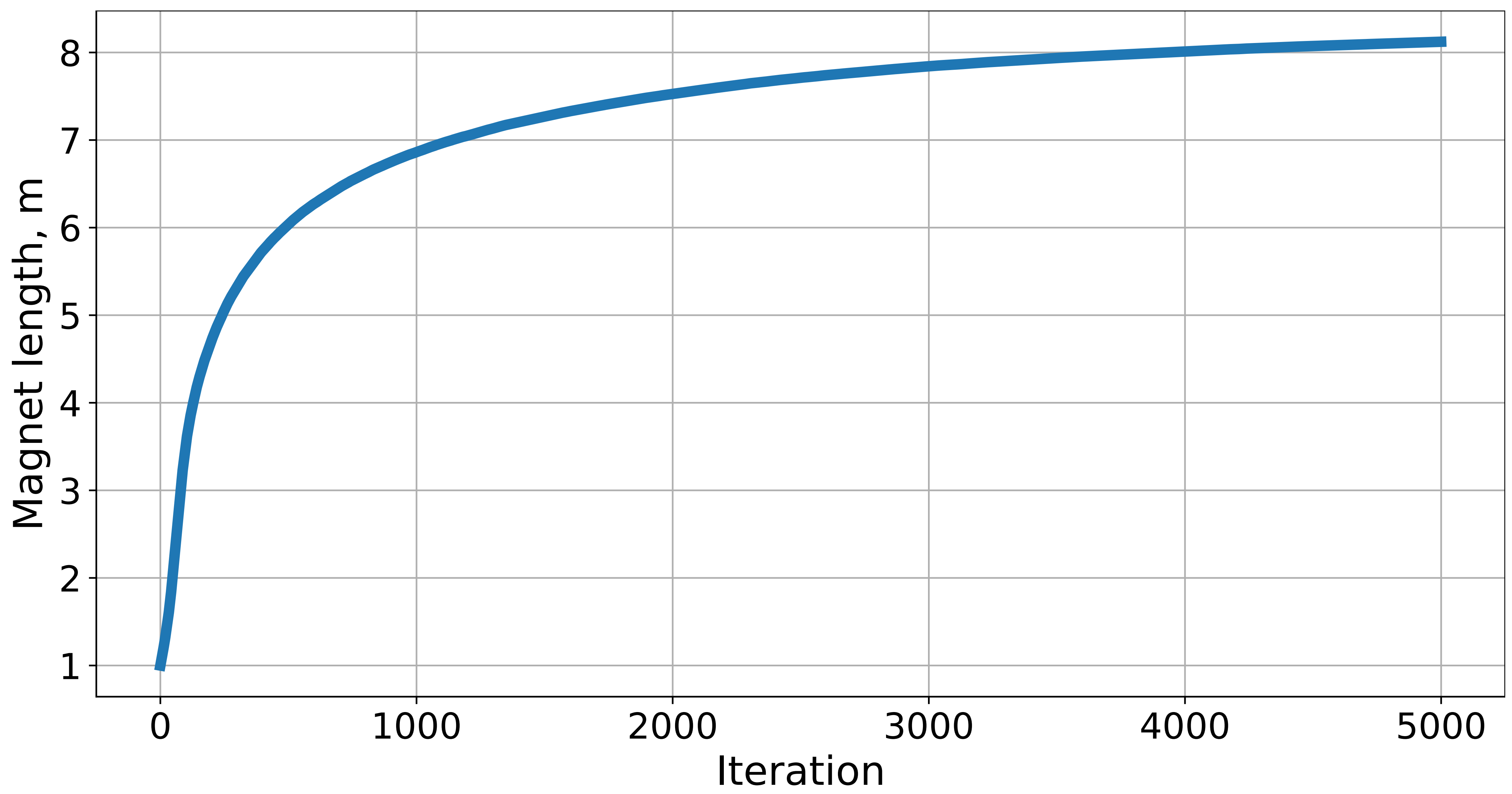
$$\sigma^2(x_* \,|D) = K_{**} - K_{*D}\left(K_{DD} + \sigma_{obs}^2 I\right)^{-1} K_{*D}^T$$

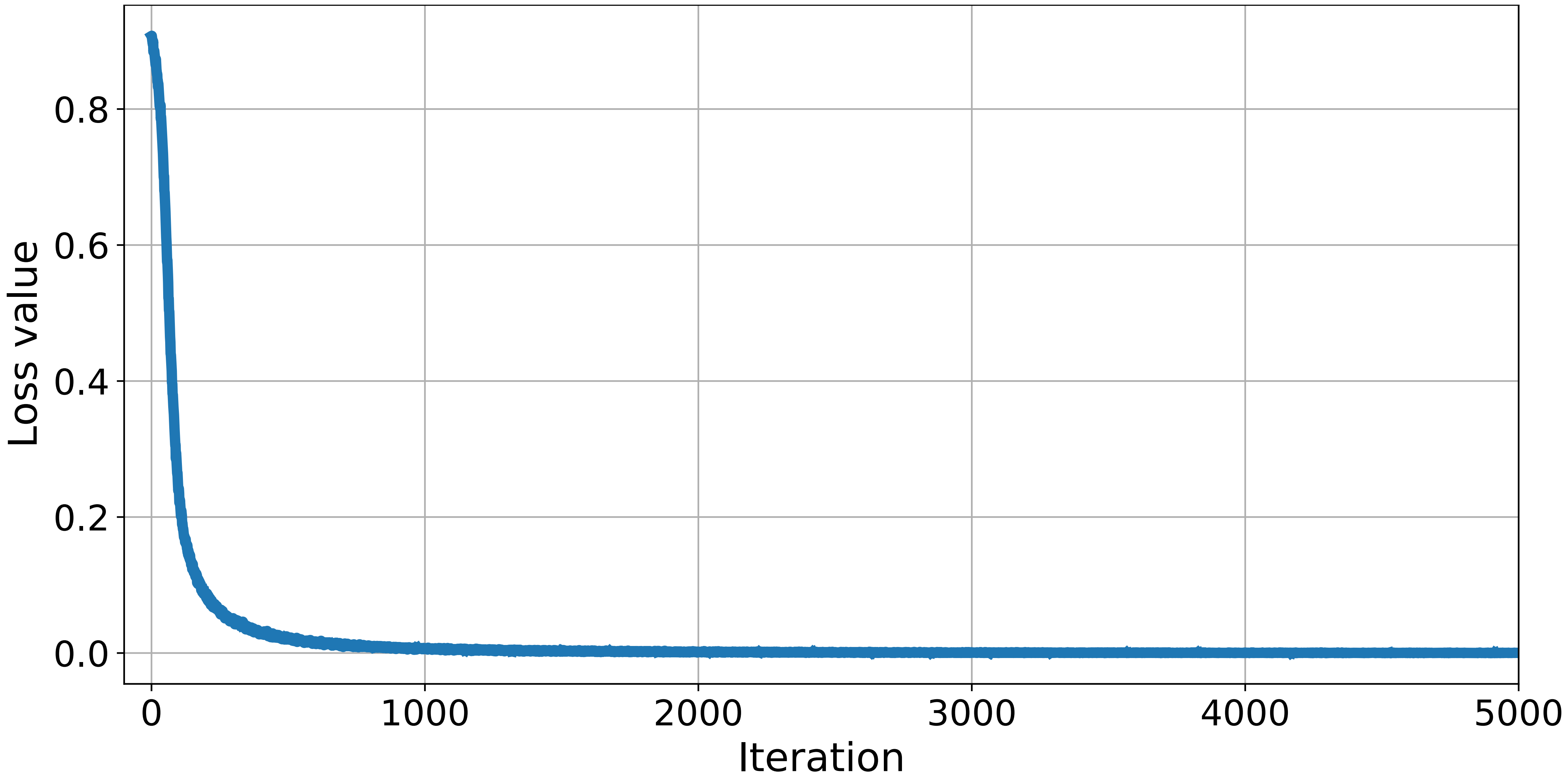
- Optimise $\mathbf{argmin}_\psi f(\psi)$
- Approximates $f(\psi)$ with probabilistic model
- Provide mean μ and variance σ
- Maximise surrogate acquisition function $\alpha(x)$.
  Example: UCB $\alpha(x) = -\mu_*(x) + \eta\, \sigma_*(x)$

Generative surrogates: physics toy example

$\psi \in \mathbb{R}^1$







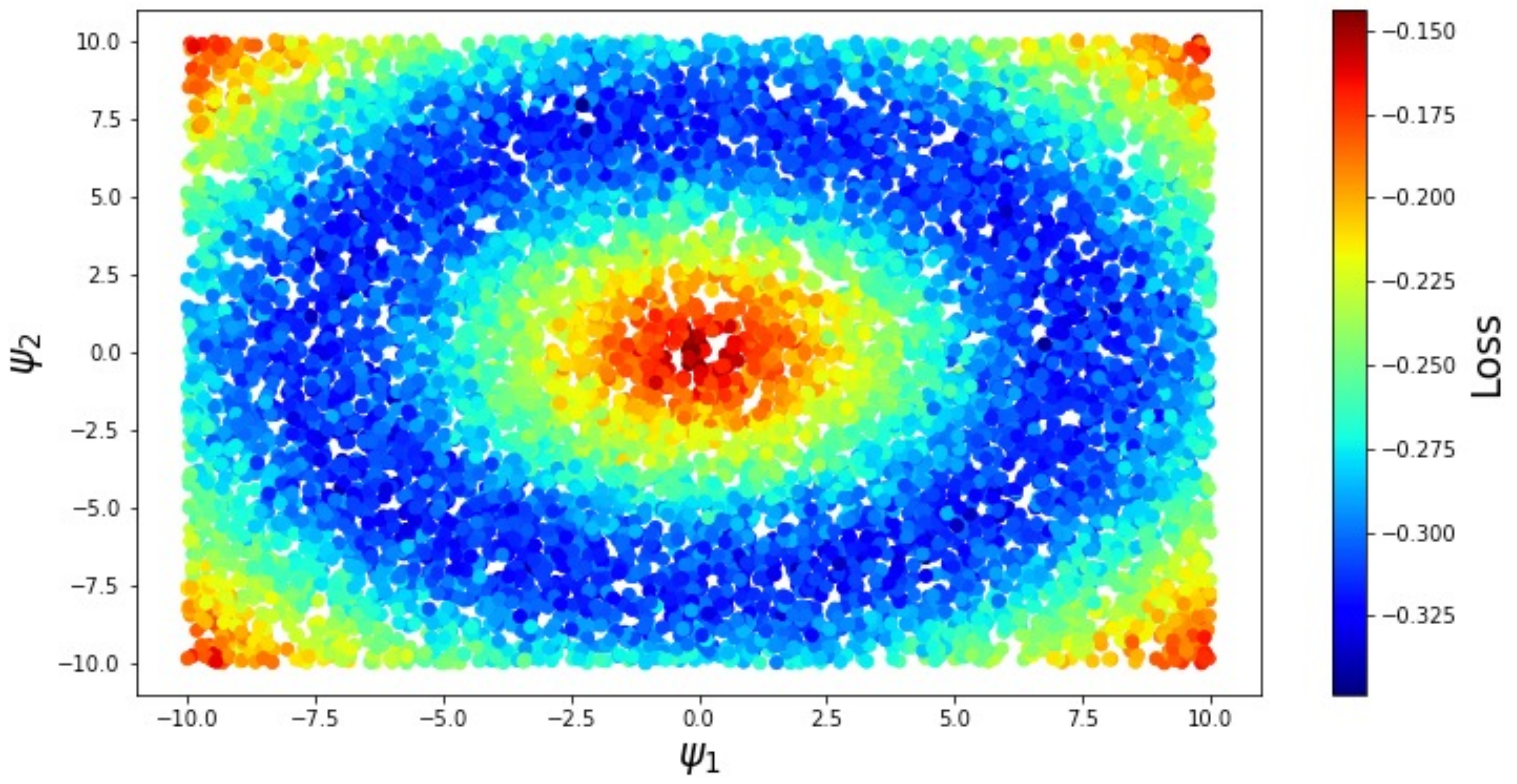
Generative surrogates: toy example

$$x \sim U(-10,10), x_{latent} \sim N(x,1), \psi \in \mathbb{R}^2$$

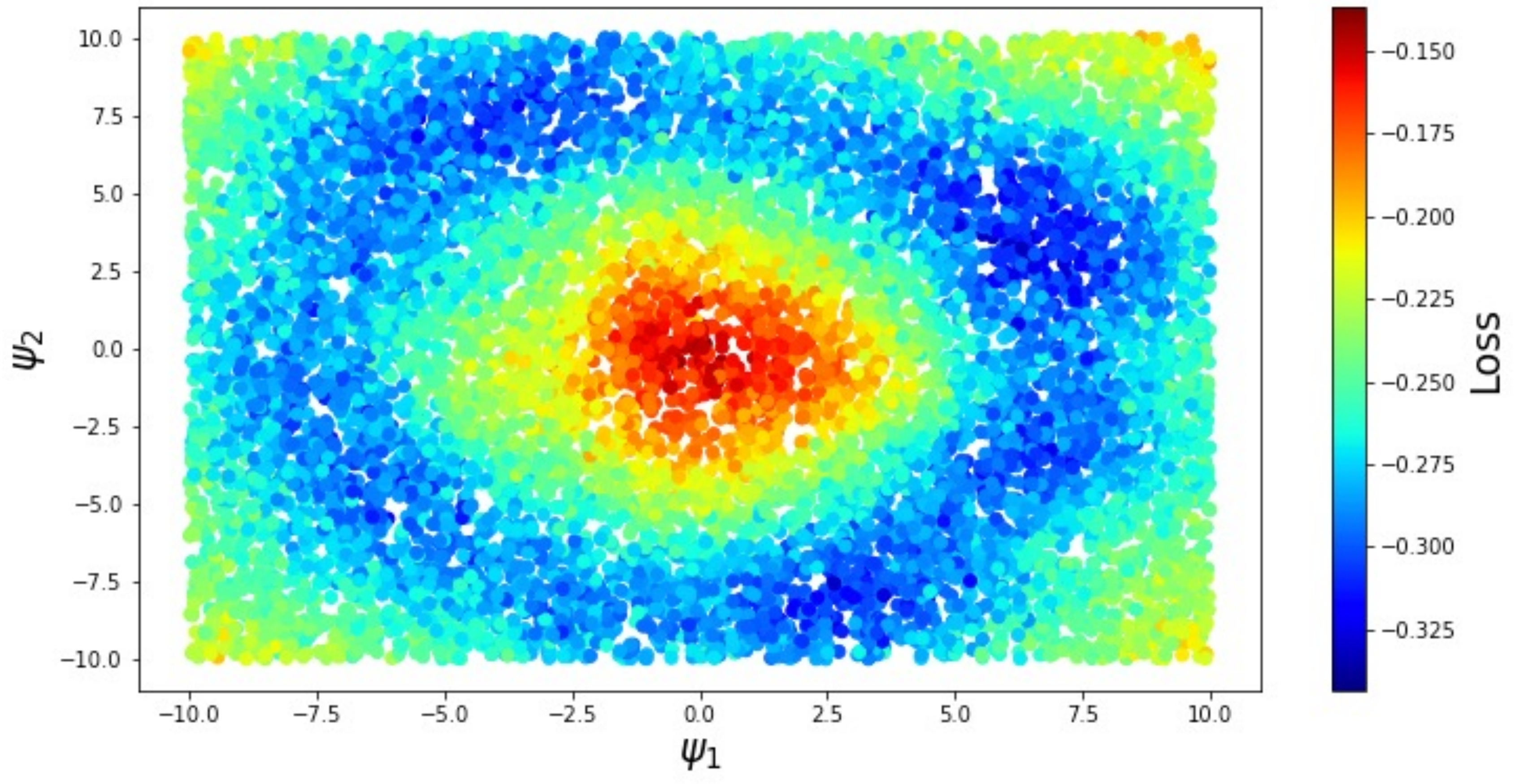
$$y \sim N(\left|\left|\psi\right|\right|_{L_2} + x_{latent}, 0.1 + 0.5\,|x_{latent}|)$$

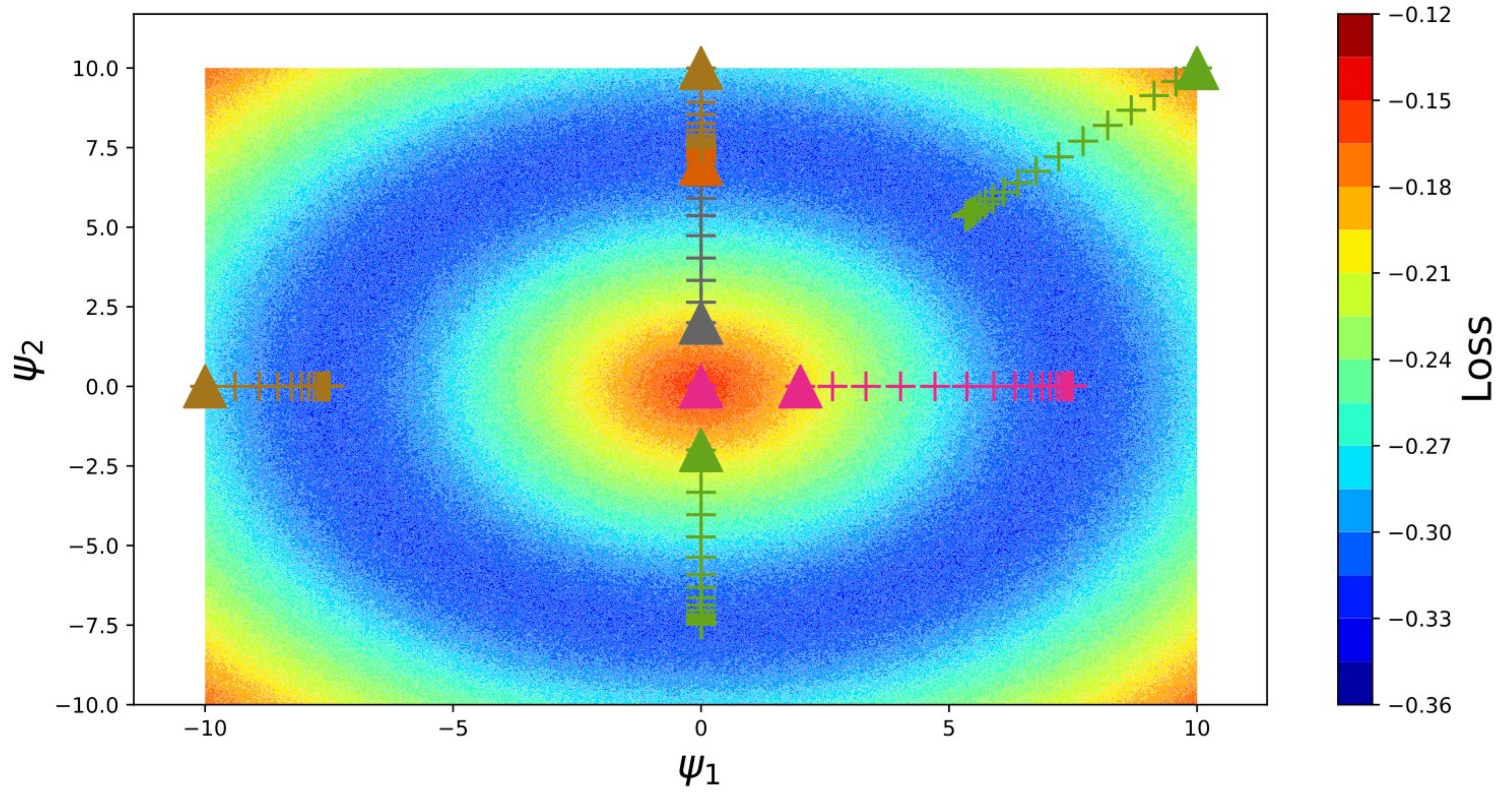
$$R(y) = \sigma(y\ - 10) - \sigma(y\ - 5)$$

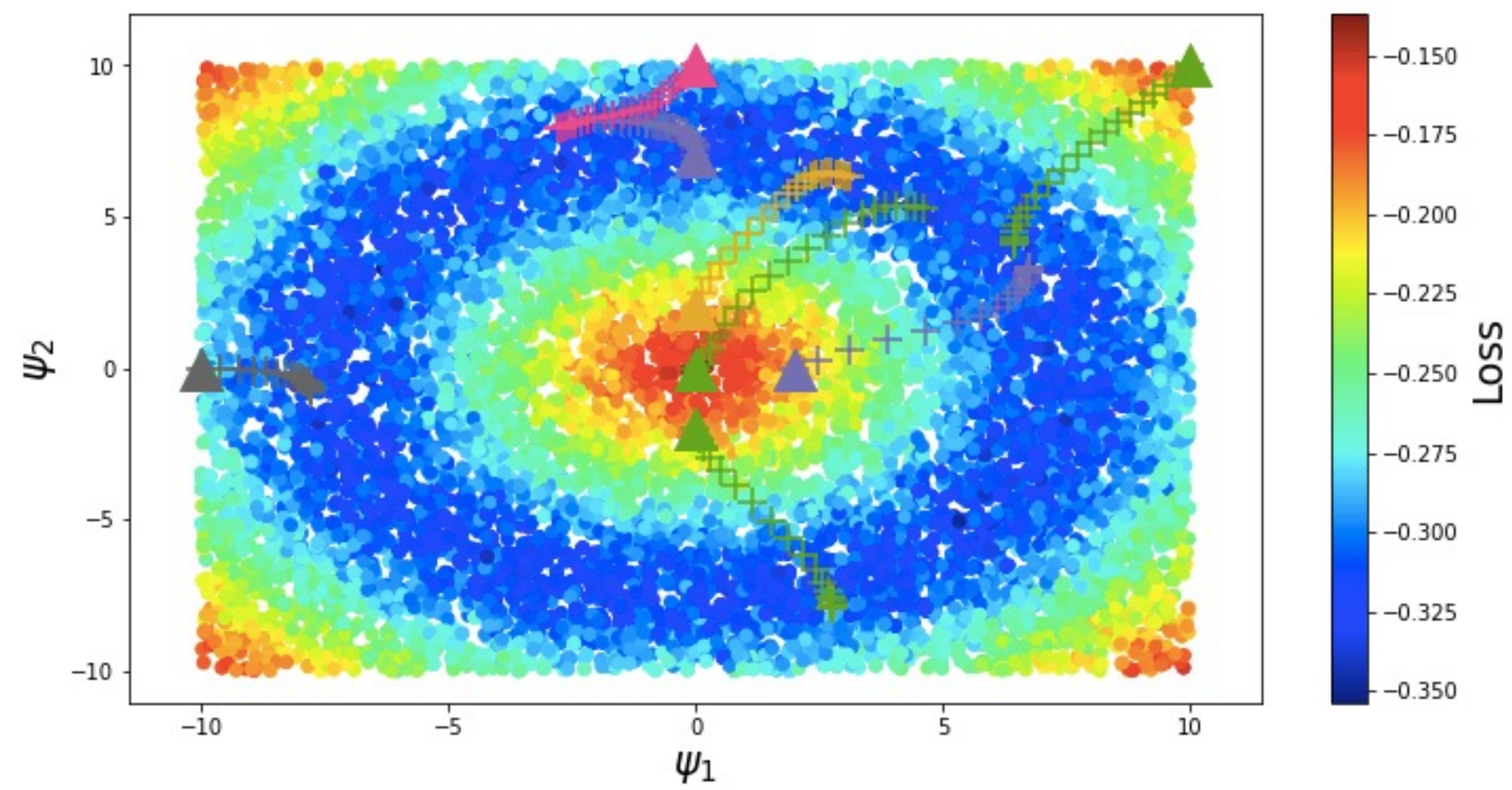
Simulator loss



GAN loss







Toy Experiments

- We run experiments on a set of toy problems, simple ones and with effective dimensions.

- We want to compare L-GSO with other algorithms in small and large dimensional problems.

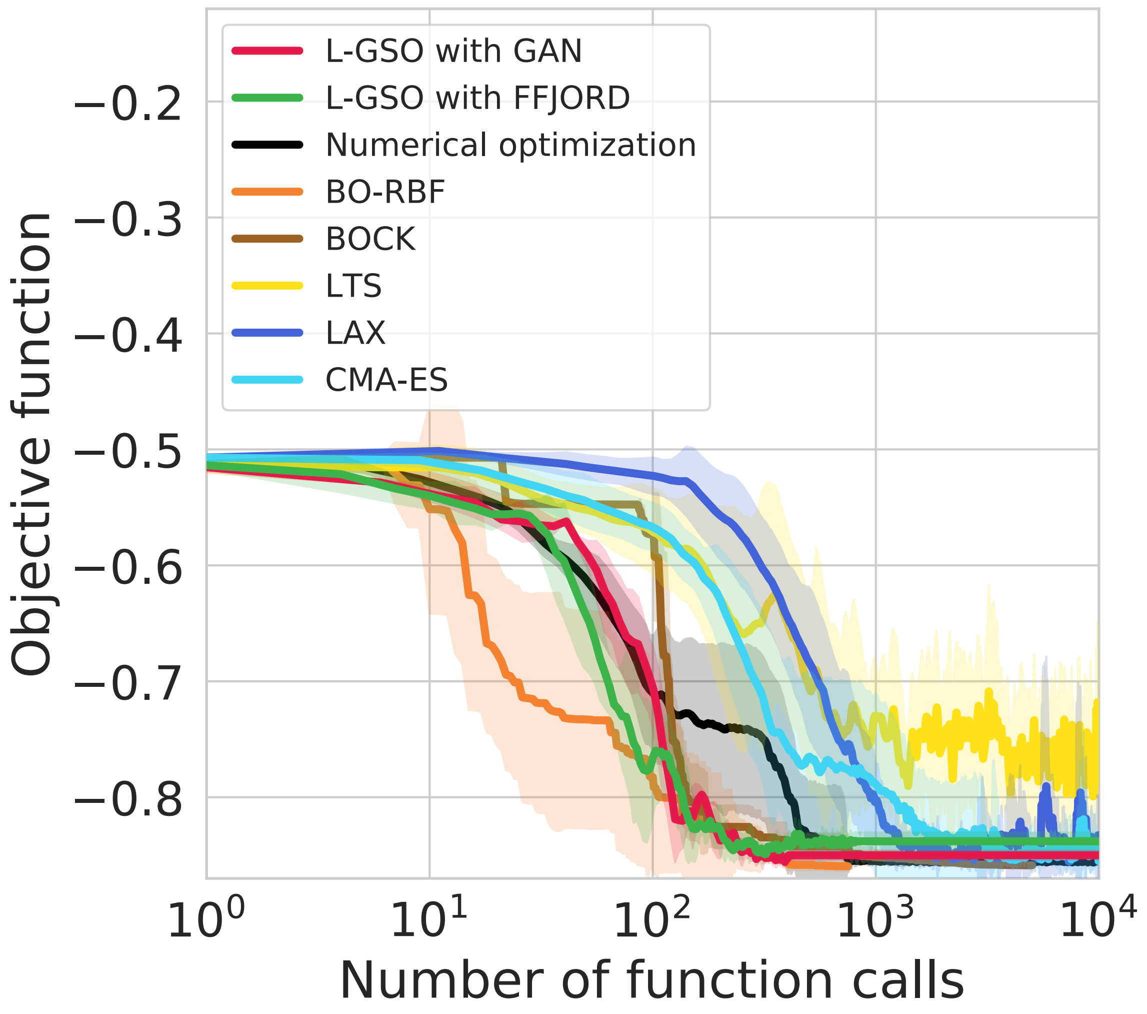
- We want to understand the effect of projecting parameters on the submanifold, as it is often the case in real life.

- We compare results in term of number of simulator calls and attained minima.

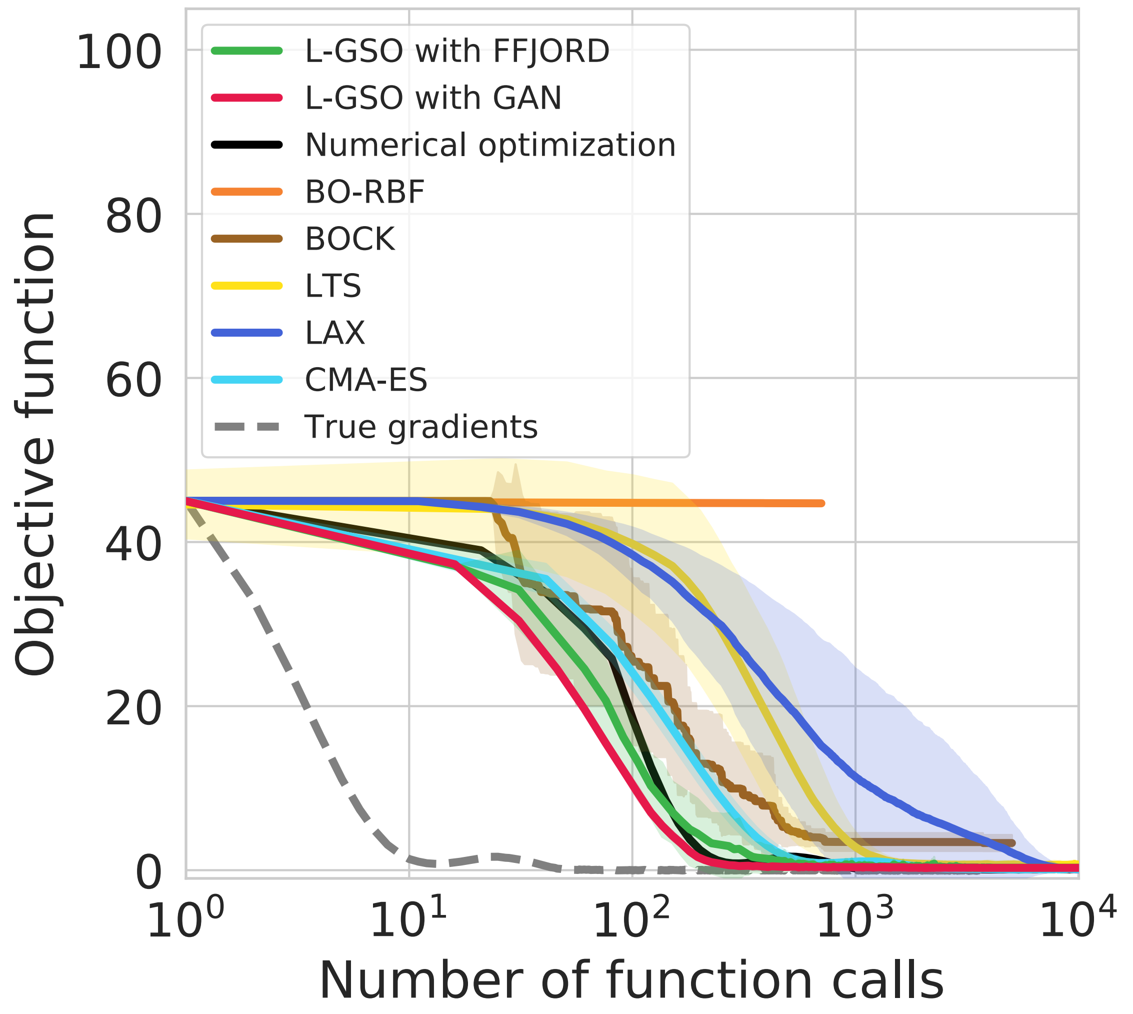
- We assume that a call to a simulator dominates the optimisation time

Toy Experiments

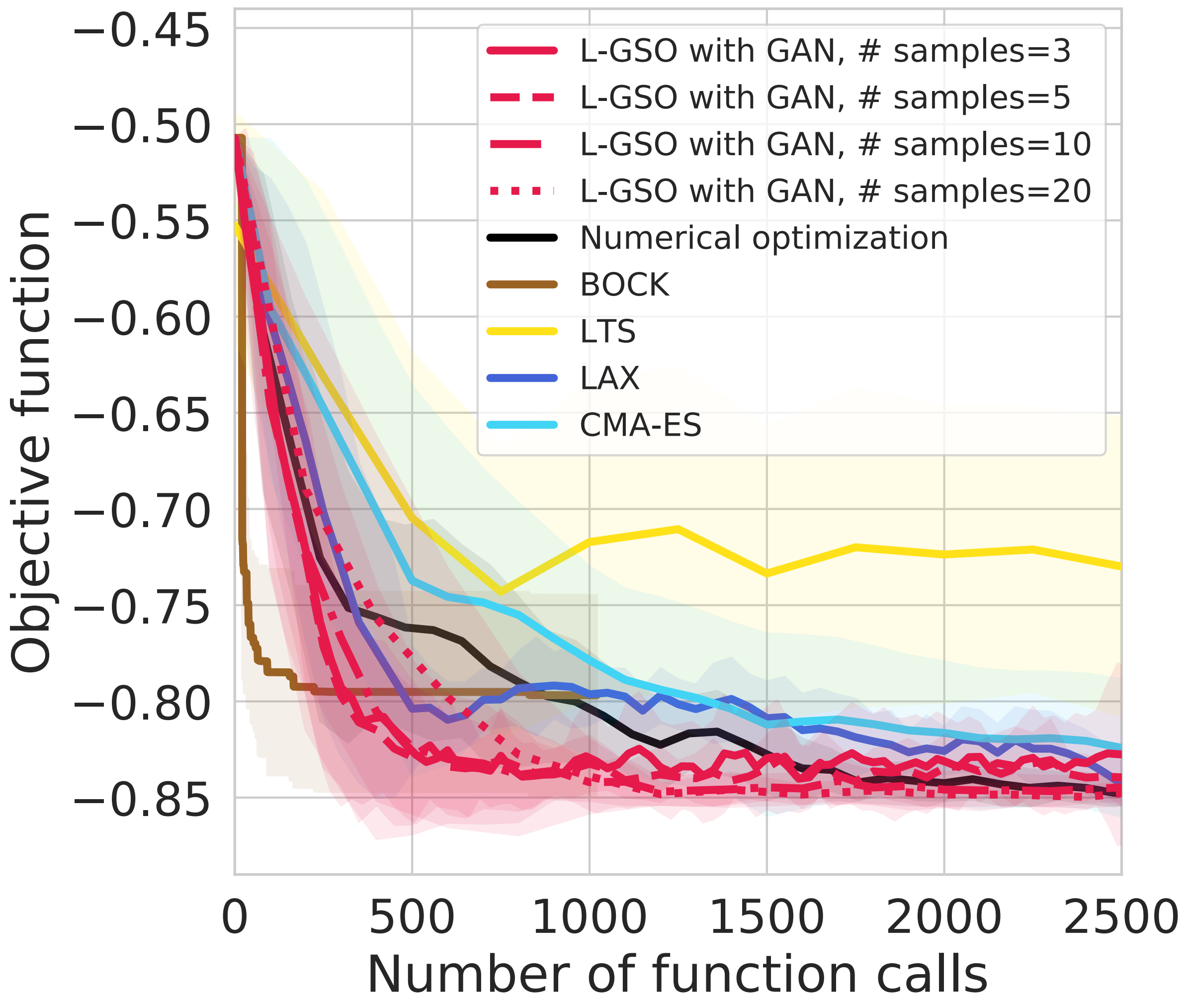
Three-Hump problem
2-dim



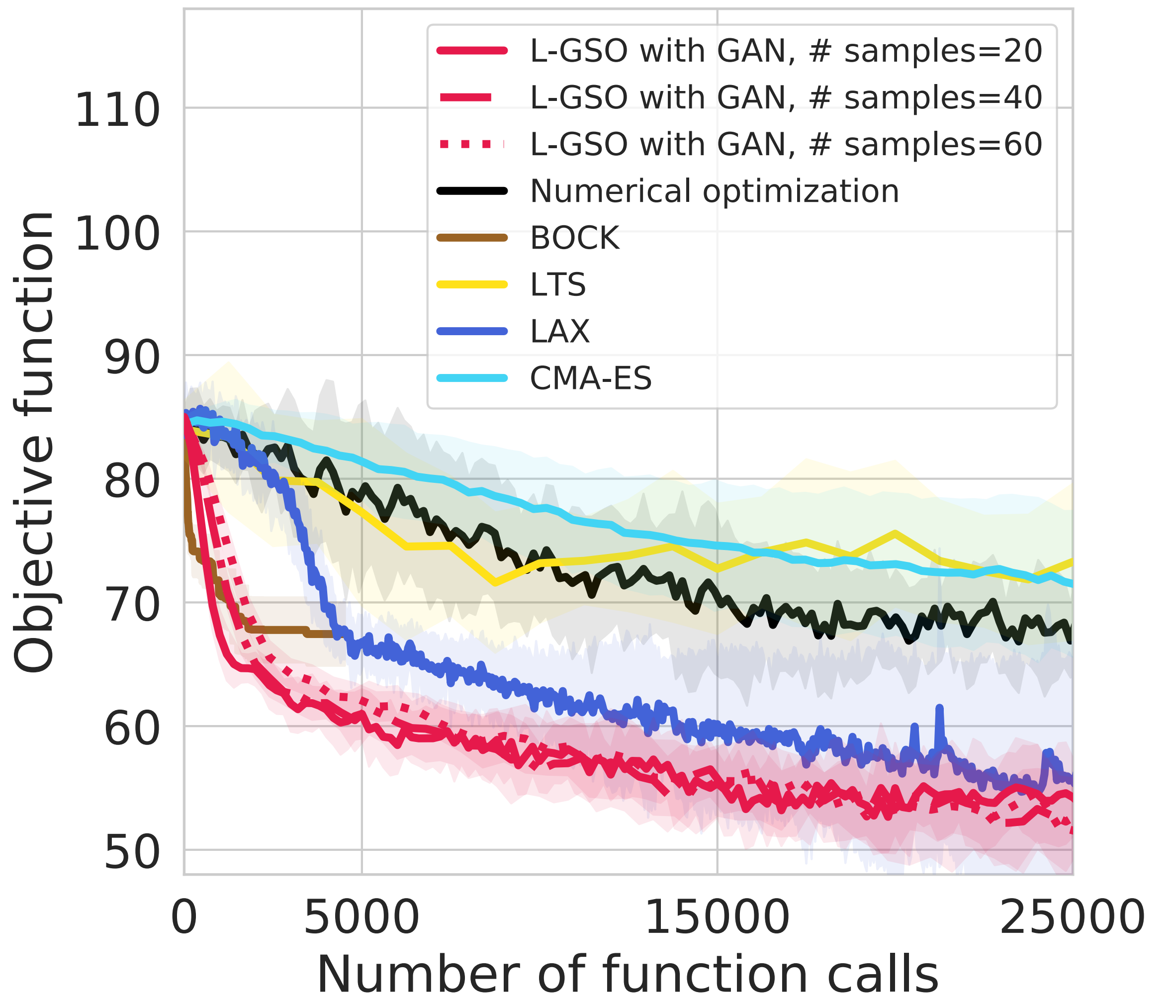
Rosenbrock problem
10-dim



Nonlinear Three-Hump
problem,
40-dim



Neural Networks weights
optimisation
91-dim



- L-GSO comparable to **all** baselines in low-dim problems in the speed of convergence
- L-GSO **outperforms all** baselines in a high-dim setting when parameters lie on a lower dimensional manifold.
- L-GSO has lower variance in resulting objective function value than other methods