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Automation of accelerator tuning with safety constraints using Bayesian Optimisation

LMU seminar – 28.01.2022



- PACMAN
- (beamline) optimisation
- optimisation GUI
- Examples PSI
 - SwissFEL
 - HIPA
 - PiE1 MIXE
- Practicalities & Next steps
- Conclusions







- PACMAN (Particle Accelerators & Machine Learning) project
- Swiss Data Science Center (SDSC), the École Polytechnique Fédérale de Lausanne (EPFL), CERN, ETH-Z and PSI
- Particle accelerators are complex facilities that produce and handle large amounts of data
- The project target is to explore the possibilities to use machine learning to improve the performance of particle accelerators
- March 2019 June 2021



Why automate beamline tuning?

- Time-consuming repetitive task for operators
- (potentially) faster
 - Quick iterations, no dead time
 - Can change many parameters at once
 - Evaluate noise
- (potentially) safer
 - No "human" mistakes
 - Can supervise all safety constraints simultaneously



Optimisation at HIPA and SwissFEL

HIPA

- HIPA beam power (1.3 MW) limited to the beam losses
 - Reduce damage and activation
- Optimisation is now mostly done empirically
- Large potential for automated optimisation and surrogate model construction
 - No accurate and fast physics model available
 - Needs to be *safe*

SwissFEL

- Goal: Optimise the FEL pulse intensity
 - -> Many Photons = Happy Users
- Challenges:
 - Manual tuning is time consuming & inefficient
 - Use many knobs (~40)
 - Don't drive the machine into the wall...
 - Exponential dependence of FEL output on many, coupled machine parameters
- ML experts from ETHZ suggested Bayesian Optimisation
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- The work is supported by the Swiss National Science Foundation under grant 200020_159557





Why Bayesian Optimisation?

Human Optimisation

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• Life-long learning

- Experience
- Limited working memory
- (relatively) Slow decisions

Numerical Optimisation

- Bulk learning
- Cannot estimate uncertainty
- Juggle many things at once
- Fast decisions

EHzürich



Learning & Adaptive Systems



Why Bayesian Optimisation?

Bayesian Optimisation

- Life-long-learning
- Experience
- Limited working memory
- (relatively) Slow decisions

- Bulk learning
- Cannot estimate uncertainty
- Juggle many things at once
- Fast decisions

ETH zürich



Learning & Adaptive Systems



Bayesian Optimisation

- Bayesian Optimisation: flexible, data-driven approach for global optimisation with noisy feedback.
- Fit a statistical regression model of the data, typically a gaussian process.
- On each iteration the model looks for evaluation points that reduce the uncertainty of the unknown target function.



Approximating true function with more data



Safe Bayesian Optimisation



- X are evaluation points, for each evaluation point the performance (e.g. FEL pulse energy) is measured and the model is updated
- Additionally, the safety function (e.g. losses recorded by various detectors) is evaluated and its model is also updated → taking into account the uncertainties of the safety function this defines the safe-set marked in green
- Combines both exploration and exploitation



SwissFEL example



 Orange crosses are expanding steps, blue crosses are exploitation steps, red dashed line marks safe-set boundaries, contour plot shows model of the performance function (modeled with Gaussian processes)



Optimisation GUI

- Server application
 - Python
 - Optimiser runs on a server
 - client GUI through REST API
- Status data in EPICS
- Additional algorithms
 - Extremum seeking (CMA-ES)
 - Nelder Mead (Simplex)
 - Line Scan
 - Easy to implement more
- Few settings
- Machine related beam checks (e.g. good-flags from the feedbacks, beam detection)
- Live plotting & analysis
- Accelerator independent
 - used at SwissFEL, HIPA, PiE1





- Possible to pause
 - Load different results
 - Set machine to these states
- Resume





- Another example: CMA-ES
- virtual mode ("virtual EPICS") available for testing

			Pause (VIRT	UAL EPICS)				
Start time: 14:46:24. Step: 65								
Main Channel Config		og						
Algorithm configuration				Optimizer Controls				
Current algorithm	Change algorithm:			DI Resume	e	🗆 s	top	
sfopt.	algorithms.SafeCoc	ordinateLi	neBO	Parameters				
	lengthscale	0.50 🗘		Show parameters:	Best measur	ed 👻	Set	
	constraint lengthscale	0.50 🗘		Name	Value	Differer	nce	
				SARMA01-MOUA060:I-SI	ET 5.2 0).13		
				SARMA01-MQUA140:I-S	ET 4.8 -	0.29		
				SARMA02-MQUA050:I-SI	ET 5.2 C).05		
				SARMA01-MQUA080:I-S	ET 4.9 -	0.18		
				SARMA01-MQUA120:I-S	ET 5.2 C).05		
Tuning Signal: SARFE10 Averages: 10	-PBPG050:HAMP-INTENS	ытү						
Best Predicted Every: 0				Table Plot				
Optimizing: SA		I-SFT	Par	ameters		Target and r	model	
Optimizing: SA	ARMA01-MQUA120:	I-SET	Para	ameters		Target and r	nodel	
Optimizing: SA	ARMA01-MQUA120:	I-SET	Para 5.8	ameters	1	Target and r	nodel	
Optimizing: SA	ARMA01-MQUA120:	I-SET	Para	ameters	ı J	Target and r	nodel	
Optimizing: SA	ARMA01-MQUA120:	I-SET	Para	ameters	1 0.8	Target and r	nodel	
Optimizing: SA	ARMA01-MQUA120:	I-SET	Para	ameters	1 0.8 0.6	Target and r		
Optimizing: SA	ARMA01-MQUA120:	I-SET	Pari	ameters	1 0.8 0.6	Target and r		
Optimizing: SA	ARMA01-MQUA120:	I-SET 5 5	Para 5.8 5.6 5.4	ameters	1 0.8 0.6 0.4	Target and r		
Optimizing: SA	ARMA01-MQUA120:	I-SET 5 5	Para 5.8 5.4 5.2 5		1 0.8 0.6 0.4	Target and r		
Optimizing: SA 1 Target 0.8 Constraints 0.4 O 0.2 O	ARMA01-MQUA120:	I-SET	Para 5.8 5.4 5.2 5 4.8		1 0.8 0.6 0.4 0.2	Target and r		
Optimizing: SA 1 Target 0.6 0.4 0.2 0 - 0.2	ARMAO1-MQUA120:	I-SET	Para 5.8 5.4 5.2 5.4 5.2 5.4 5.2 5.4 5.2 5.4 10 10 10 10 10 10 10 10 10 10 10 10 10		1 0.8 0.6 0.4 0.2	Target and r		
Optimizing: S/ 1 Target 0.6 0.4 0.2 -0.2 -0.4	ARMAO1-MQUA120:	I-SET	Para 5.8 5.4 5.2 5 4.8		1 0.8 0.6 0.4 0.2 0			
Optimizing: SA 1 Target 0.6 Constraint 0.6 - 0.2 - -0.2 - -0.4 -3 -2 -1 -0.4 -3 -2 -1	ARMA01-MQUA120:	I-SET	Para 5.8 5.6 5.4 5.2 5.4 4.8 4.6	ameters	1 0.8 0.6 0.4 0.2 0	Target and r	nodel	



- Easy selection of the parameters (channels) to tune during the optimisation.
- Individual limits can be set for each channel
 - machine check
 - optimisation constraint

Se	Server Logging Help								
	Offline (VIRTUAL EPICS)								
	1ain	Channel Config Machine Config Log							
		PV	Readback PV	Lim Low	Lim Up	Lim Rel			
		channel_config_set_testing (active: 4)							
		SARMA01-MQUA010:I-SET	SARMA01-MQUA010:I-READ	-4.0	7.0				
		SARMA01-MQUA060:I-SET	SARMA01-MQUA060:I-READ			3.0			
		SARMA01-MQUA140:I-SET	SARMA01-MQUA140:I-READ			2.0			
		SARMA02-MQUA050:I-SET	SARMA02-MQUA050:I-READ			3.0			
	~	channel_config_set_testing2 (active: 2)							
		SARMA01-MQUA080:I-SET	SARMA01-MQUA080:I-READ			2.0			
		SARMA01-MQUA120:I-SET	SARMA01-MQUA120:I-READ			3.0			

Reload Channel List



- Beam limits are checked before moving to the next step
 - Stability conditions
- Possible to investigate and go back to each previous step

Server Logging Help							
Scruci Logging risp		Offline (VIRTUAL EPIC	S)			
			Not running	5/			
Main Channel Config	Machine Config	Log					
Beam Check Configuration					Acquisition Config		
Check PV Values:					Method	maximize_pv	-
	P		Lower Limit	Upper Limit 📤	Tuning Signal (PV):	50:HAMP-INTENSI	
SARMA01-MQUA010:I-R	EAD		1648.0	0.3	Averages:		
SARMA01-MQUA060:I-R	EAD			0.3	Read Frequency (Hz):	100.00	
SARMA01-MQUA080:I-R	EAD			0.3	Best Predicted Every:		
SARBD01-DBPM040:Q1					Readonly		
SARFE10-OPSH044:PLC	_CLOSE						
SARFE10-PBPG050:HAM	IP-INTENSITY						
SARFE10-PBPG050:HAM	IP-INTENSITY-CAL						
SARMA01-MQUA120:I-R	EAD						
SARMA01-MQUA140:I-R	EAD						
SARMA02-MQUA050:I-R	EAD						
SARMA02-MQUA120:I-R	EAD						
SARUN01-DBLM065:B1	_LOSS_MPS_REL_L1						
SARUN03-DBLM030:B1	_LOSS_MPS_REL_L1						





- Variants:
 - C(oord)-LineBO: Find each parameter target optimum individually.
 - A(scent)-LineBO: Move each parameter to find the "best-direction" and then search for the best point in that direction.
 - *-Loc: "Localised" Maximum step size is 10% of the available range.
 - CMA-ES: Similar to swarm optimisation.
 - Does not have safety constraints.
 - Standard well developed global optimisation evolutionary algorithm.
 - Used here as baseline to compare the rest of the method



- Objective: Minimize combined losses (M4HIPA:VERL:2)
 - weighted average of 60 loss monitors
- Tuning Parameters: 5-16 Quadrupole Magnets
- Constraints: About 200 loss monitors with individual warning levels
- Beam checks:
 - Beam on
 - Orbit feedbacks stable
- Effective control rate: ~ 5 seconds / step



- Low Intensity with manually detuned machine
- 5 parameters



- safe variants competitive
- non-safe methods create interlocks (violate constraints)
 - proves constraints are working



- High intensity
- 16 parameters



• Also competitive and safe at high current



- Localised option (Maximum step size is 10% of the available range)
 - faster to set
 - at HIPA we don't set parameters instantly
 - quicker for feedbacks to stabilise
 - similar solution









- Objective: Shot by shot FEL intensity
- Tuning Parameters (39): Quadrupole Magnets, Beam position, Undulator settings
- Constraints:
 - Lower bound on intensity
 - Loss monitors
- Effective control rate: ~ 0.5 seconds / step







Bayesian Optimisation shows best result





• Constraint on minimum energy improves average and even optimum



- Elemental composition analysis with negative muons
 - non-destructive and depth sensitive
 - Implant muons at different depths by selecting muon energy





- probe scanned at several layers
 - different muon momenta about every hour
 - —> tuning manually every hour(!)
- Objective: muon rate (ZPIE1CNT:INP3)
 - average rate —> reduce exploration
- Parameters: 20 quads, magnets and spin rotator (same as in setpoint)
 - 'ASY51:SOL:2', 'ASL51:SOL:2', 'ASK51:SOL:2', 'SPIN2:SOL:2', 'QSN54:SOL:2', 'QSN55:SOL:2', 'QSN56:SOL:2', 'QTH51:SOL:2', 'QTH52:SOL:2', 'QTB51:SOL:2', 'QSL51:SOL:2', 'QSL52:SOL:2', 'QSL53:SOL:2', 'QSL54:SOL:2', 'QSE51:SOL:2', 'QSE52:SOL:2', 'QSN51:SOL:2', 'QSN52:SOL:2', 'QSN53:SOL:2'
- Constraints: none
 - Could set a minimum muon rate as constraint
- Machine checks
 - Beam on (MHC4 current monitor > 1800)



- Tested 13 December 2021 w Lars Gerchow
- First try: CoordinateLine (one parameter line scan)



- Slow noisy progress
 - Too many evaluations per line scan
- Sometimes signal went down
 - Noise parameters might have set wrong
 - Too much exploration?
- CoordinateLine slow with many parameters that are not orthogonal



MIXE - PiE1 - AscentLine

- AscentLine (multiple parameters at once)
 - Steady constant increase, even small increases after one hour
- Note that expected muon rate dependent on muon energy
- NelderMead also promising result
 - More testing needed





- Every problem unique
 - Algorithms and parameters should be benchmarked for optimal results
- Results stored
 - Analysis framework available (Jupyter notebook)
- Similar tools exist (OCELOT DESY, SLAC)
- Possible improvements
 - Installation tricky
 - More automatisation
 - Operator is still needed
 - More robust
 - CPU usage and memory usage large
 - especially for long optimisation runs

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Example configuration - PiE1

```
    api

    pie1.yaml

sfopt.environment:
  tuning signal pv: ZPIE1CNT:INP3
  outlier level: 3.0
  outlier detection: true
  num repetitions: 10
sfopt.interface:
  set_max_trials: 600
  set tolerance: 0.05 # sets tolerance of difference of SOL to IST value
  frequency: 10.0 # machine read/set interval time
sfopt.checks:
  min_value_pvs:
    MHC4:IST:2: 1800.

    algorithm ascent-linebo.yaml

algorithm.gp:
  beta: 1.
  noise std: 40.0
  kernel: rbf
  scale: 4000.0
  bias: 40.0
  lengthscale: 0.3
algorithm.constraint_gp:
  beta: 1.
  noise std: 0.1
  kernel: matern52

    algorithm neldermead.yaml

algorithm.nelder mead:
  contraction factor: 0.8
  initial stepsize: 0.1
  restart threshold: 0.0
  adaptive: True

    config

    channel config set.txt

pv,lim low,lim high,lim rel,wait const,wait linear,wait min,wait max,active,step size
ASY51:SOL:2,,,0.5,,,,1,
ASL51:SOL:2,,,0.5,,,,1,
ASK51:SOL:2,,,0.5,,,,1,
SPIN2:SOL:2,,,10.0,,,,1,
QSN54:SOL:2,,,2.0,,,,1,
```



- Experiments planned end April (HIPA startup commissioning phase)
 - Systematic algorithm comparison
- MIXE First two weeks of May



Conclusions & References

- Ready to use powerful automated tool
 - Very flexible
 - <u>https://gitlab.psi.ch/ext-kirschner_j/swissfel-opt</u>
- Results shown on several beamlines
- More tests in planning at PiE1 MIXE
- Please contact me if interested
- Papers:
 - Tuning Particle Accelerators with Safety Constraints using Bayesian Optimization Phys. Rev. Accelerator and Beams (2022)
 - Bayesian optimisation for fast and safe parameter tuning of SwissFEL FEL 2019
 - <u>Adaptive and Safe Bayesian Optimization in High Dimensions via One-</u> <u>Dimensional Subspaces - ICML 2019</u>
- Presentation:
 - <u>Bayesian Optimization for Safe & Efficient FEL Tuning at SwissFEL & Loss</u> <u>Optimisation at HIPA , N. Hiller, OWLE seminar (2020)</u>



Wir schaffen Wissen – heute für morgen

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- Lars Gerchow (NUM)
- Nicole Hiller (GFA-operation)





CMA-ES Algorithm

- Covariance Matrix Adaptation Evolution Strategy.
- Similar to swarm optimization.
- Does not have safety constraints, we used a very small step size.

