AI/ML for Design (10/Oct/2022)
Session Summary

(Wouter Deconinck & Evaristo Cisbani)

- Max Balandat – MOO Tutorial
- Karthik Suresh – Adaptive experimentation in EIC
- Benjamin Nachman – AI-driven detector design
- Elena Fol – ML in LHC
- Todd Satogata – AI/ML for Accelerator Design

Max Balandat / Multi Objective Optimization (tutorial)

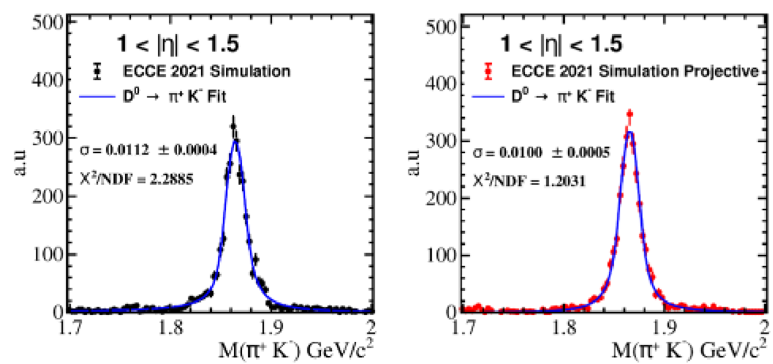
- Ingredients:
  - Several parameters >10 that define the potential design space
  - Constrains on parameters
  - Multiple Objectives to be optimize (either minimized or maximized) → require time-consuming computation
- Adopted Approach
  - Parallel Bayesian Optimization of vector based black-box functions, with Expected Hypervolume Improvement → superior sample-efficiency → find the Pareto frontier of optimal trade-offs
- Implementation
  - BoTorch (Bayesian Optimization on top of PyTorch)
    https://botorch.org/tutorials/multi_objective_bo
    Ax (Adaptive Experimentation Platform) recommended for scheduling, storage, high-level APIs

M.B. / MOO
Limitations, Hints and Beyond

Limitations / Hints	Beyond Limitation, R&D, Advanced Features
Scalability • model fitting is $O(n^3)$ with Gaussian Process surrogate (n = data points) • statistical efficiency and model quality degrade with larger number of parameters • hypervolume is super-polynominal in number of objectives	High dimensional MOBO • SAASBO: for high-dimensional problems where few pars have large influence → sparsity-inducing prior + Markov Chain Monte Carlo inference • MORBO: multi-objective trust Region BO for efficient scaling of high number of evaluation points
Regions of interest of the objective functions • proper settings improve efficiency	
Noisy data (intrinsic tolerances, environmental variations ...) • provide to model helps optimization	Noisy data • MARS: Modified value-at-risk approximation based on Random scalarizations
Numerical precision • double precision is reccomended to mitigate ill-conditioned linear systems	Mixing Discrete and Continuos parameters • probabilistic reparameterization by optimizing discrete variable over a probability distribution

Karthik Suresh / Adaptive experimentation in EIC (an overview)

- Practical implementation of MOO + GEANT4 in ECCE tracker design
  - design parameters ~ 10
  - constrains ≥3 (hard + soft), no (GEANT4) overlaps
  - objective functions: momentum, (projected) angular resolutions, tracking reconstruction ability
  - validation: compare achieved performance with “baseline” and post-hoc reconstructed physics observables
  - exploit existing software libraries based on Multi-Objective Evolutionary Algorithm and Bayesian Optimization (MOEA and MOBO)

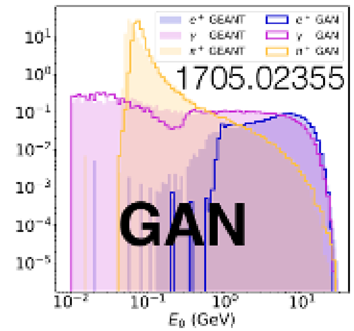


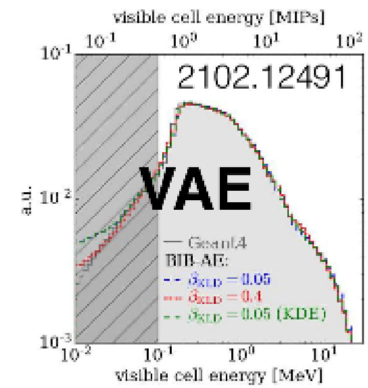
- migration from ECCE to ePIC software framework ongoing

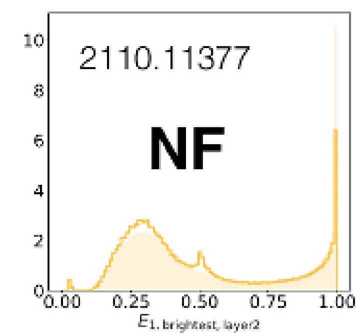
Benjamin Nachman
AI-driven detector design

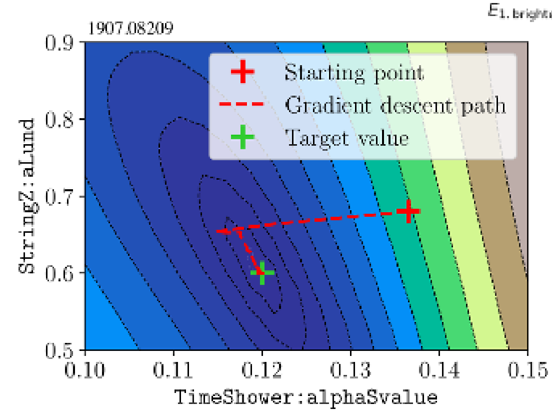
Goal: find best detector parameters given a metric(s) → ML

- Detector Modeling
  - Surrogate models
    - Generative Adversarial Networks
    - Variational Autoencoders
    - Normalizing Flows
  - Differentiable Simulation $\text{sim}(\mu_0 + \epsilon) \approx \text{sim}(\mu_0) + \frac{\partial \text{sim}}{\partial \mu}\epsilon$
- ML-based optimization:
  - Gradient descend
- Calorimetry application in progress









Todd Satogata / AI/ML for Accelerator Design (an overview)

- Computer optimization methods and AI/ML applications for Accelerator Physics in use since forever
- Some AI/ML Challenges
  - Computational complexity
  - Dealing with highly “pervasive” Coulomb interactions
  - Interesting beam dynamics problems are mainly non-linear
  - Many tradeoffs: cost↔performance↔technical challenges ↔R&D efforts
- Snowmass21 Accelerator Modelling Community White Paper
  - focuses on Accelerator modeling (design) priorities/strategies
  - provide reccomendations for next generation accelerator modeling
- Impact of AI/ML on EIC accelerator design questionable

T.S. / AI/ML for Accelerator Design

(an overview)

- Some ongoing AI/ML approaches:
  - Multi-Objective Genetic Algorithm regurlarly used for component optimization (e.g. SRF gun)
    - Require human intervention near parametric singularities;
    - many different codes/approaches
  - Virtual/Digital Twin
    - Inexpensive generation of dataset; online modeling; operator training
    - WP: can explore larger parameter space with possibility of design innovative particle accelerators in the future
- Very recent advances may impacting in Accelerator Design
  - Fundamental Algorithm Improvements, e.g. in computational linear algebra
  - Nonlinear/Chaotic system forecasting → accelerator surrogate models → initial nolinear design

Elena Fol / ML in LHC Optics Control

(maximize luminosity → control β)

Application	Approach	Advantage
Detection of Instrumentation Faults	Anomaly detection by Isolation Forest (decision-tree) Algorithm	detection of unexplored hardware and electronics problems in BPMs
Predict Optimal settings	Decision Tree/Random Forest	save operation time; LHC upgrade study: model is able to apply corrections in single iteration with $\Delta\beta/\beta$ <2%
De-noising of beam measurements	Autoencoder NN to denoise (simulated) data	improvement measurement quality; possibility to reconstruct phase advance in faulty BPMs locations
Virtual Diagnostics	Reconstruct optics observables without direct measurements by supervised learning with linear regression model	potential speed-up of machine commissioning

✓ **Paving the way for new studies currently being in progress:**

- Optics corrections for High Luminosity – LHC upgrade (Reinforcement Learning)
- Exploring more complex optics error sources in the LHC: coupling corrections
- Improving Dynamic Aperture estimates using clustering
- **Optimizing the design of future colliders (Ionisation Cooling channel for a muon collider).**

Sparse outcomes from Q/A

- AI/ML applications in physics (and any other field) involve new multidisciplinary expertises and need to reconsider dissemination and dedicated positions in the research physics teams
- AI/ML is not a universal tool; it should be applied when/where appropriate and other “traditional” approaches are not adequate/less performing
- AI/ML approaches are not generally accepted as engineering tools yet; need efforts to move toward this direction
- EIC can take advantage of AI applications for control, commissioning, monitoring and operation of accelerators (and should consider these opportunities during design)
- R&D on AI/ML for EIC design does not match current funding framework (and project timing)
- Socialogical aspects behind optimization – individual design vs collaboration process