

Using Neural Networks for Rapid Switching Between Beam Parameters in an FEL

Auralee Edelen

Fermilab and Colorado State University

Working with: Jonathan Edelen, Sandra Biedron, Stephen Milton, Peter van der Slot

Motivation: Switching Between User Requests

- FEL facilities support a wide variety of scientific endeavors (e.g. *imaging protein structures*¹, *understanding processes like photosynthesis*², *origin of material properties*³)



e.g. the *Linac Coherent Light Source*
(image: lcls.slac.stanford.edu)

[1] J.-P. Colletier, et al., "De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure," *Nature*, vol. 539, pp. 43–47, Sep. 2016.
[2] I. D. Young, et al., "Structure of photosystem II and substrate binding at room temperature," *Nature*, vol. 540, pp. 453–457, Nov. 2016.
[3] M. P. Jiang, et al., "The origin of incipient ferroelectricity in lead telluride," *Nature Communications*, vol. 7, no. 12291, Jul. 2016.

Motivation: Switching Between User Requests

- FEL facilities support a **wide variety of scientific endeavors** (e.g. *imaging protein structures¹, understanding processes like photosynthesis², origin of material properties³*)
- Need to accommodate requests for a **wide variety of photon beam characteristics**



e.g. the *Linac Coherent Light Source*
(image: lcls.slac.stanford.edu)

[1] J.-P. Colletier, et al., "De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure," *Nature*, vol. 539, pp. 43–47, Sep. 2016.
[2] I. D. Young, et al., "Structure of photosystem II and substrate binding at room temperature," *Nature*, vol. 540, pp. 453–457, Nov. 2016.
[3] M. P. Jiang, et al., "The origin of incipient ferroelectricity in lead telluride," *Nature Communications*, vol. 7, no. 12291, Jul. 2016.

Motivation: Switching Between User Requests

- FEL facilities support a **wide variety of scientific endeavors** (e.g. *imaging protein structures¹, understanding processes like photosynthesis², origin of material properties³*)
- Need to accommodate requests for a **wide variety of photon beam characteristics**
- May switch as often as every few days
- Have save/restore settings, but these are discrete, and there can be some drift in the machine



e.g. the *Linac Coherent Light Source*
(image: lcls.slac.stanford.edu)

[1] J.-P. Colletier, et al., "De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure," *Nature*, vol. 539, pp. 43–47, Sep. 2016.
[2] I. D. Young, et al., "Structure of photosystem II and substrate binding at room temperature," *Nature*, vol. 540, pp. 453–457, Nov. 2016.
[3] M. P. Jiang, et al., "The origin of incipient ferroelectricity in lead telluride," *Nature Communications*, vol. 7, no. 12291, Jul. 2016.

Motivation: Switching Between User Requests

- FEL facilities support a **wide variety of scientific endeavors** (e.g. *imaging protein structures¹, understanding processes like photosynthesis², origin of material properties³*)
- Need to accommodate requests for a **wide variety of photon beam characteristics**
- May switch as often as every few days
- Have save/restore settings, but these are discrete, and there can be some drift in the machine
- **Time spent tuning = reduced scientific output for a given operational budget**



e.g. the *Linac Coherent Light Source*
(image: lcls.slac.stanford.edu)

[1] J.-P. Colletier, et al., "De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure," *Nature*, vol. 539, pp. 43–47, Sep. 2016.
[2] I. D. Young, et al., "Structure of photosystem II and substrate binding at room temperature," *Nature*, vol. 540, pp. 453–457, Nov. 2016.
[3] M. P. Jiang, et al., "The origin of incipient ferroelectricity in lead telluride," *Nature Communications*, vol. 7, no. 12291, Jul. 2016.

Motivation: Switching Between User Requests

- FEL facilities support a **wide variety of scientific endeavors** (e.g. *imaging protein structures¹*, *understanding processes like photosynthesis²*, *origin of material properties³*)
- Need to accommodate requests for a **wide variety of photon beam characteristics**
- May switch as often as every few days
- Have save/restore settings, but these are discrete, and there can be some drift in the machine
- **Time spent tuning = reduced scientific output for a given operational budget**

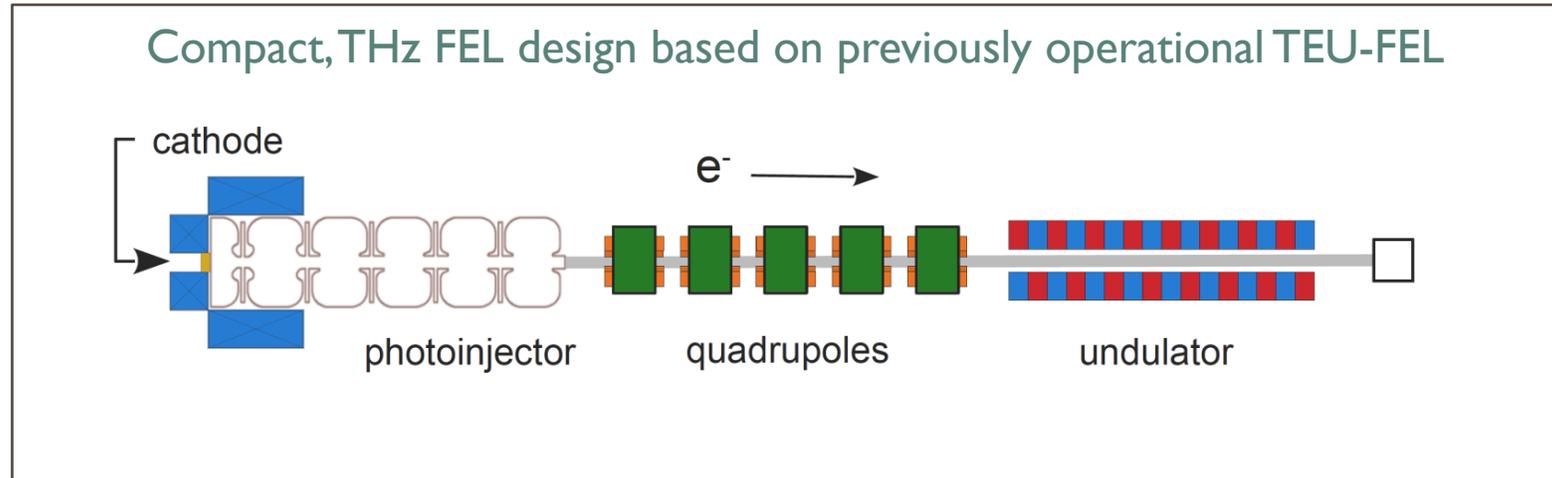


e.g. the *Linac Coherent Light Source*
(image: lcls.slac.stanford.edu)

Would be nice to have a tool that can quickly give suggested settings for a given photon beam request, is valid globally, and can adapt to changes over time

[1] J.-P. Colletier, et al., "De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure," *Nature*, vol. 539, pp. 43–47, Sep. 2016.
[2] I. D. Young, et al., "Structure of photosystem II and substrate binding at room temperature," *Nature*, vol. 540, pp. 453–457, Nov. 2016.
[3] M. P. Jiang, et al., "The origin of incipient ferroelectricity in lead telluride," *Nature Communications*, vol. 7, no. 12291, Jul. 2016.

Starting Smaller: A Case Study

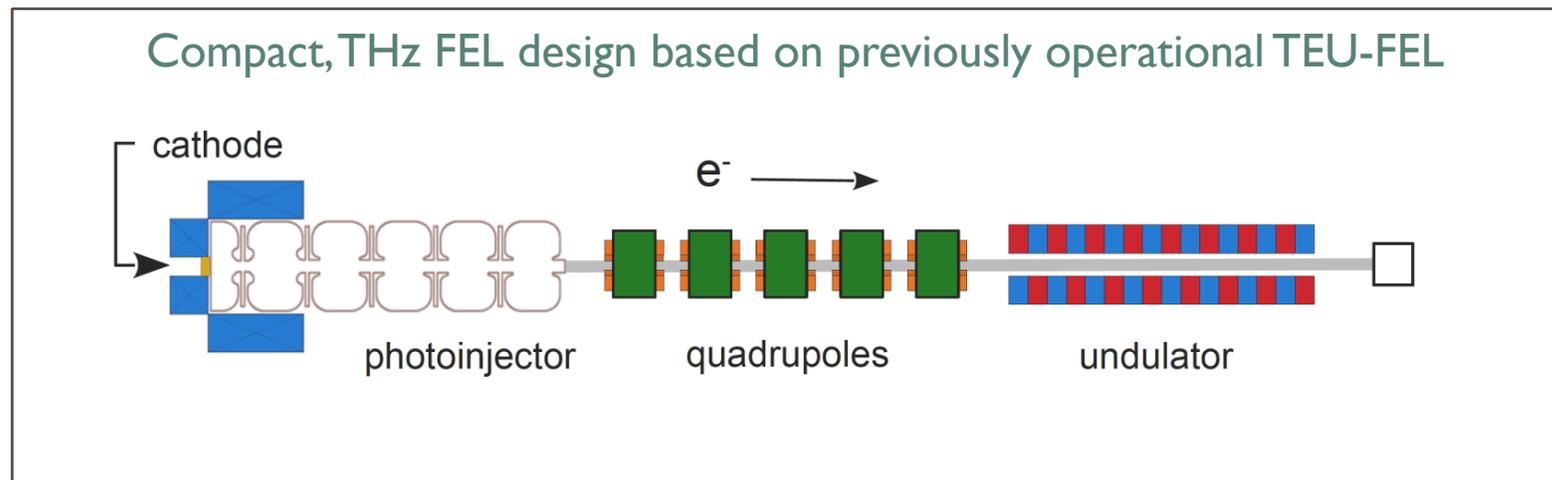


3 – 6 MeV electron beam
200 – 800 μm photon beam

Previously operated at University of Twente in the Netherlands

Was going to be re-built at CSU:
have simulation from design studies

Starting Smaller: A Case Study



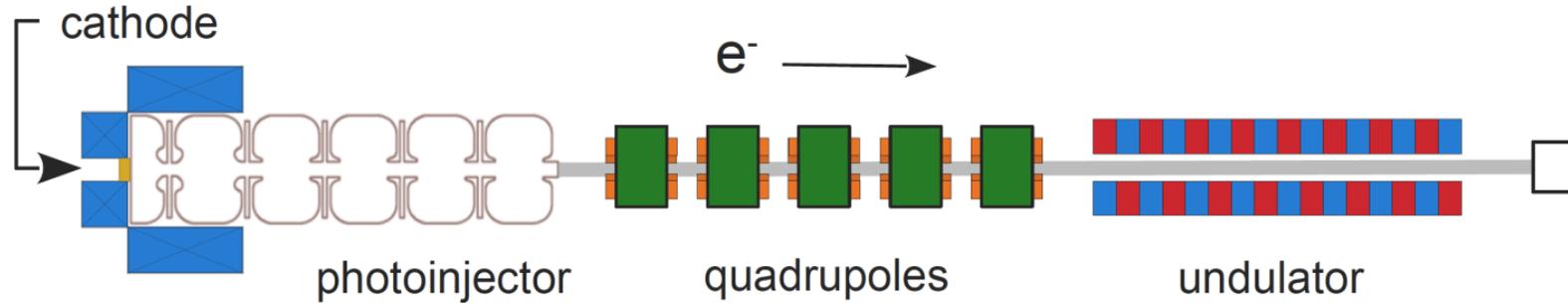
3 – 6 MeV electron beam
200 – 800 μm photon beam

Previously operated at University of Twente in the Netherlands

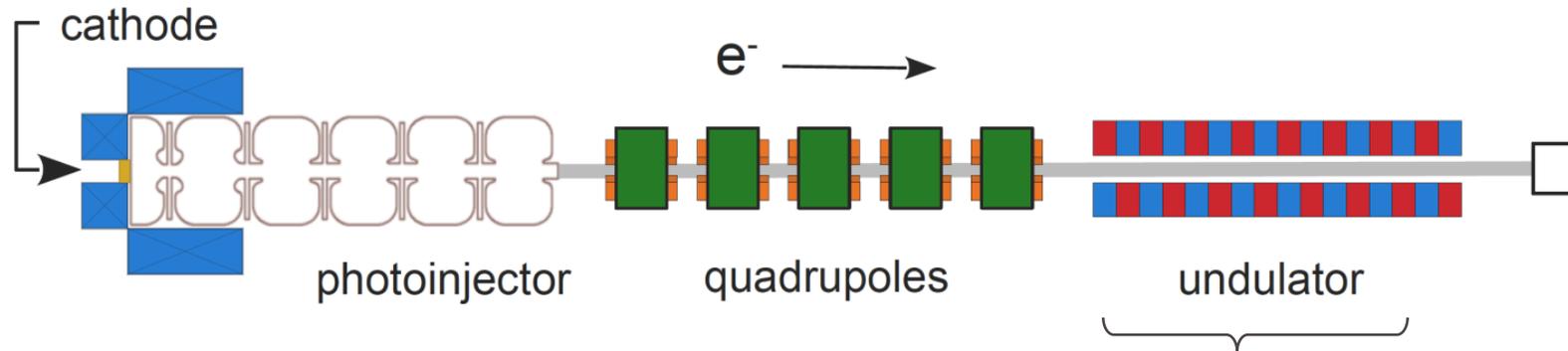
Was going to be re-built at CSU:
have simulation from design studies

This is an appealing system for an initial study because it has a **small number of machine components**, yet it exhibits **non-trivial beam dynamics**.

How to get the right wavelength?



How to get the right wavelength?



FEL output is related to beam parameters at the entrance of the undulator

Roughly speaking:

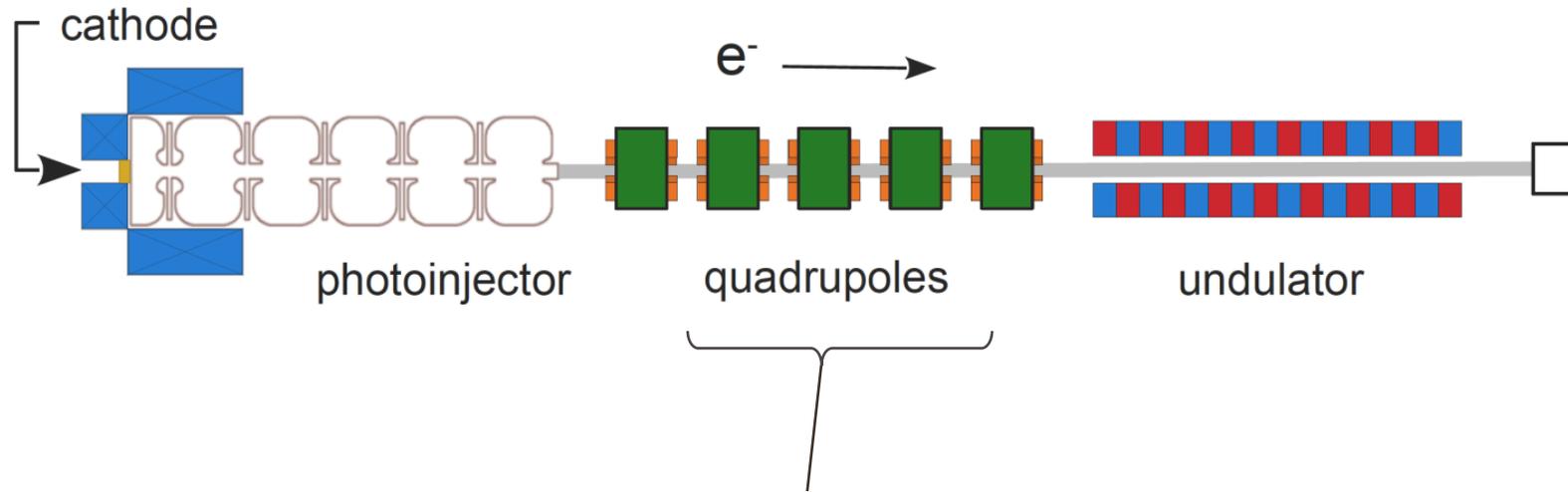
- Beam **energy** determines FEL wavelength
- Beam **size** (β) and **divergence** (α) need to be set to minimize beam losses
- Beam **emittance** (ε) impacts FEL gain
- $\alpha, \beta, \varepsilon$ are defined in the position-momentum phase space of the beam

simple analytic case:

$$\lambda_r = \frac{\lambda_u}{2\gamma^2} \left(1 + \frac{K^2}{2} \right)$$

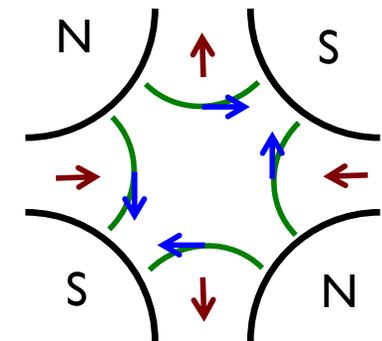
(in reality the FEL process is more complicated)

How to get the right wavelength?



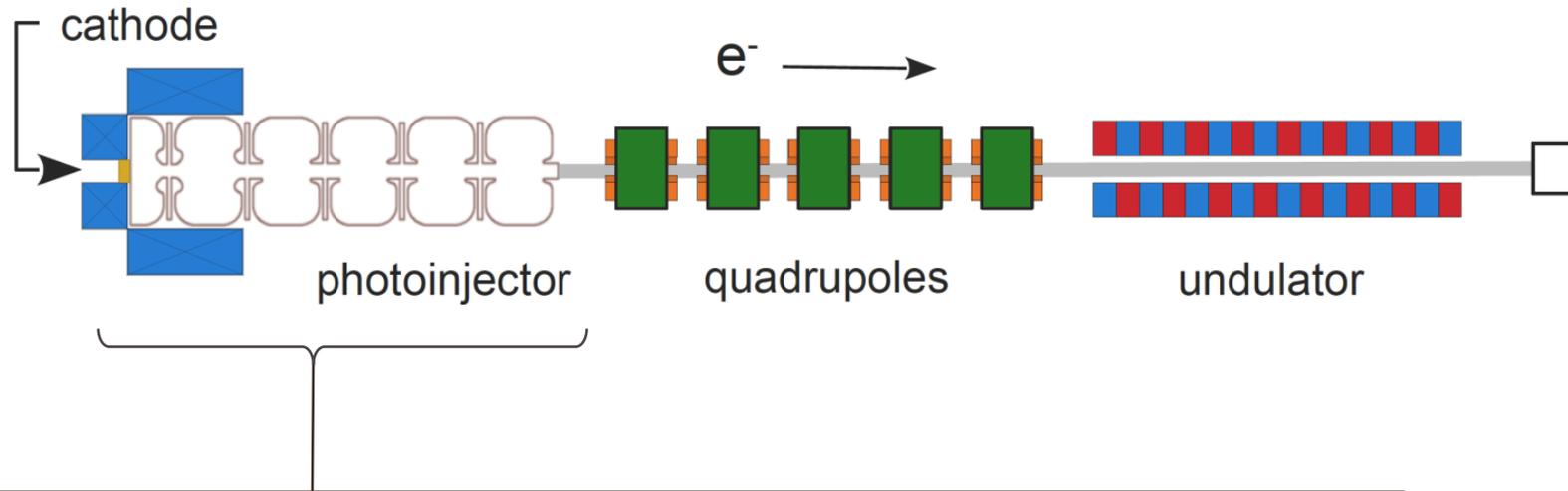
Quadrupole electromagnets are used to match the beam into the undulator

- Focus in one transverse plane and defocus in the other
- A pair provides net focusing
- In principle only affects α, β
(but beam self-fields can thwart this \rightarrow also affects ε)



 force on beam
 B field

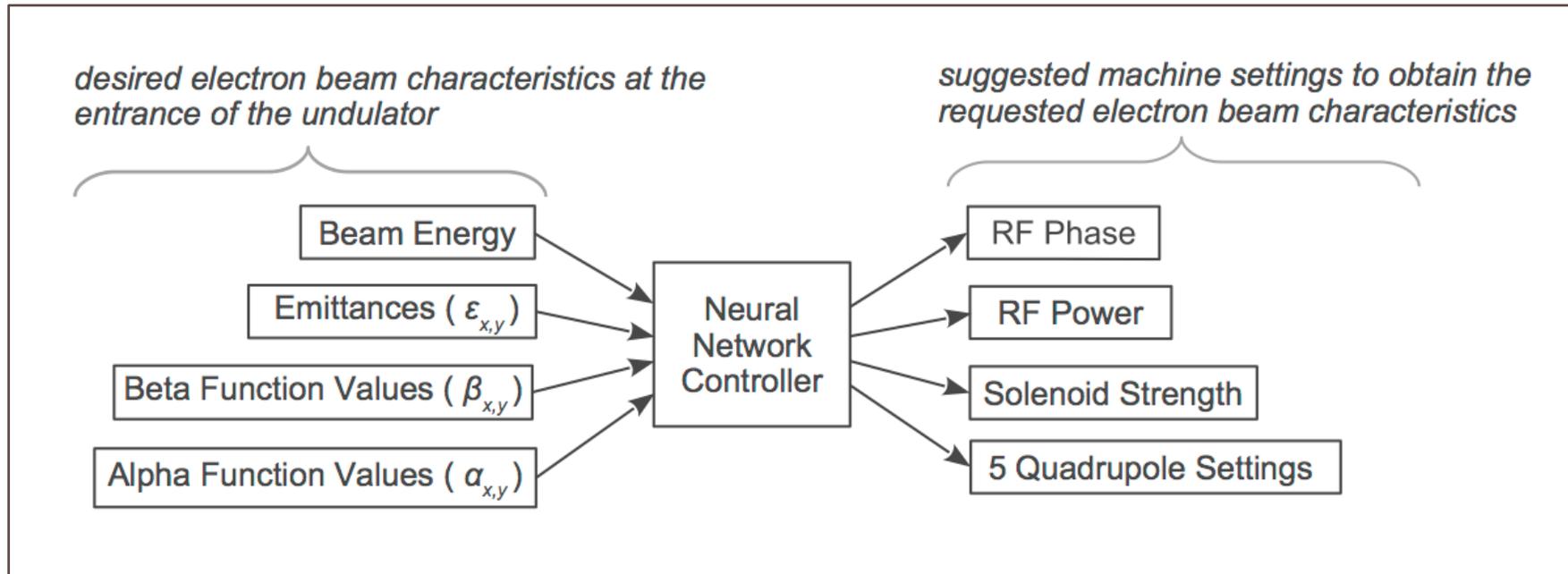
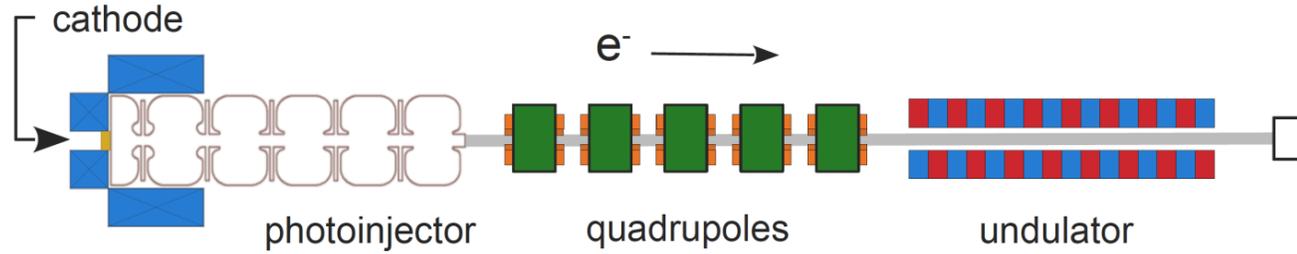
How to get the right wavelength?



Photoinjector determines initial beam properties and accelerates the beam

- Electrons generated via photoelectric effect (laser incident on cathode)
- Beam energy dominated by RF power setting (acceleration in cavity)
- Solenoid compensates for strong beam self-fields (improves emittance)
- Bucking coil minimizes magnetic field on the cathode (improves emittance)

End goal: get the right beam parameters at the undulator entrance



First: Learn a Model from Physics-Based Simulation

Simulation in PARMELA

- Standard particle tracking code (numerical)
- Includes beam self-fields (computationally expensive)
- Load EM field maps for cavities, solenoid, bucking coil

First: Learn a Model from Physics-Based Simulation

Simulation in PARMELA

- Standard particle tracking code (numerical)
- Includes beam self-fields (computationally expensive)
- Load EM field maps for cavities, solenoid, bucking coil
- Unfortunately: distribution restricted, source code not available, and compiled for windows → *couldn't just run a lot of interactions with controller on a cluster*

First: Learn a Model from Physics-Based Simulation

Simulation in PARMELA

- Standard particle tracking code (numerical)
- Includes beam self-fields (computationally expensive)
- Load EM field maps for cavities, solenoid, bucking coil
- Unfortunately: distribution restricted, source code not available, and compiled for windows → *couldn't just run a lot of interactions with controller on a cluster*

Decided to **learn a neural network model from simulation**:

- *faster-executing than physics-based simulation*
- *can update with measured data*
- *would be nice to have a differentiable model*

First: Learn a Model from Physics-Based Simulation

Simulation in PARMELA

- Standard particle tracking code (numerical)
- Includes beam self-fields (computationally expensive)
- Load EM field maps for cavities, solenoid, bucking coil
- Unfortunately: distribution restricted, source code not available, and compiled for windows → *couldn't just run a lot of interactions with controller on a cluster*

Decided to **learn a neural network model from simulation**:

- *faster-executing than physics-based simulation*
- *can update with measured data*
- *would be nice to have a differentiable model*

More broadly: machine time is expensive, mistakes can be costly, and simulations don't always match the machine well

- *Sample efficiency matters a lot (both with slow sim and machine)*
- *Learning a machine model using simulation results and updating it with existing measurements can aid controller development*

First: Learn a Model from Physics-Based Simulation

Simulation in PARMELA

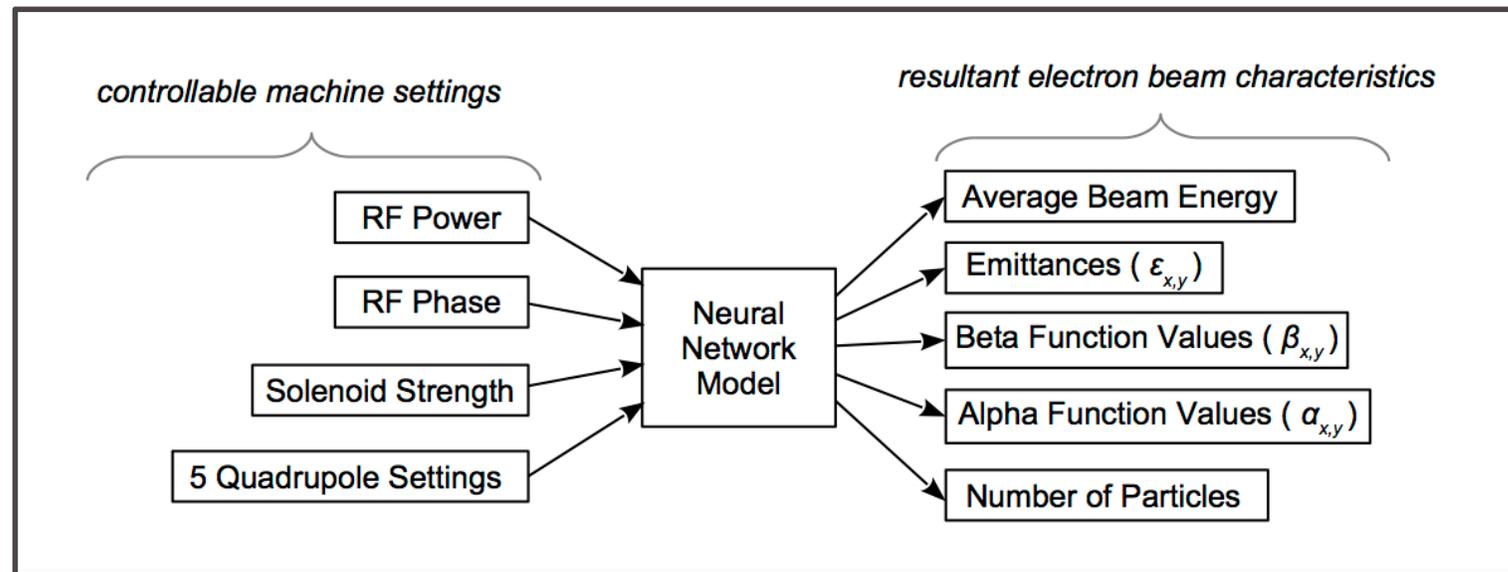
- Standard particle tracking code (numerical)
- Includes beam self-fields (computationally expensive)
- Load EM field maps for cavities, solenoid, bucking coil
- Unfortunately: distribution restricted, source code not available, and compiled for windows → *couldn't just run a lot of interactions with controller on a cluster*

Decided to **learn a neural network model from simulation**:

- *faster-executing than physics-based simulation*
- *can update with measured data*
- *would be nice to have a differentiable model*

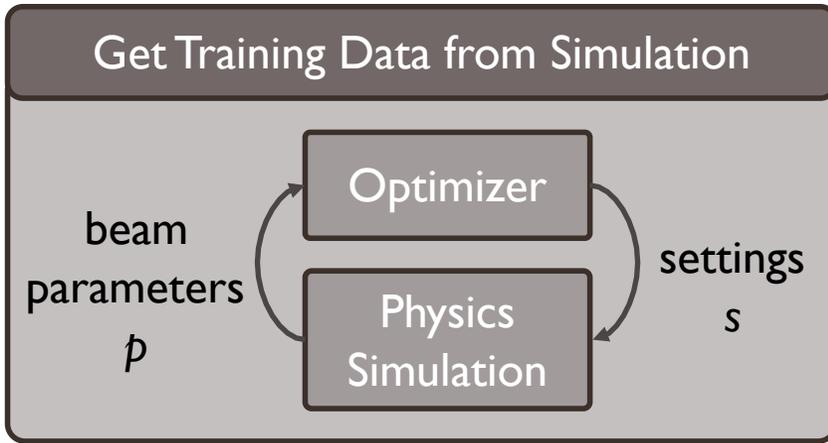
More broadly: machine time is expensive, mistakes can be costly, and simulations don't always match the machine well

- *Sample efficiency matters a lot (both with slow sim and machine)*
- *Learning a machine model using simulation results and updating it with existing measurements can aid controller development*



Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

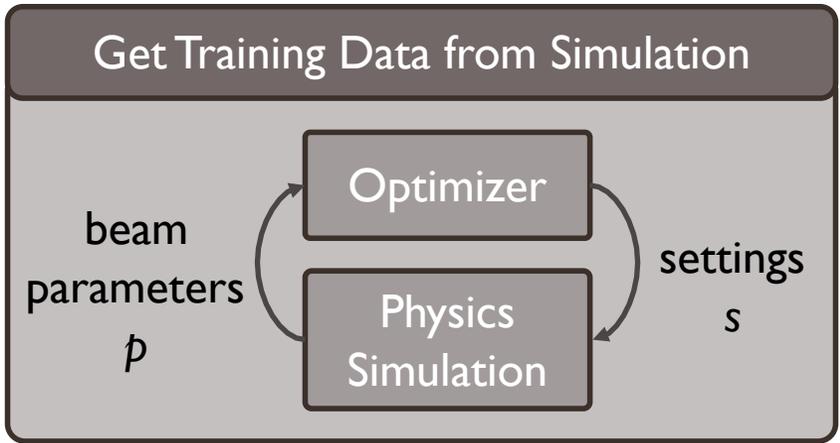
Noisy data + tuning around roughly optimal settings



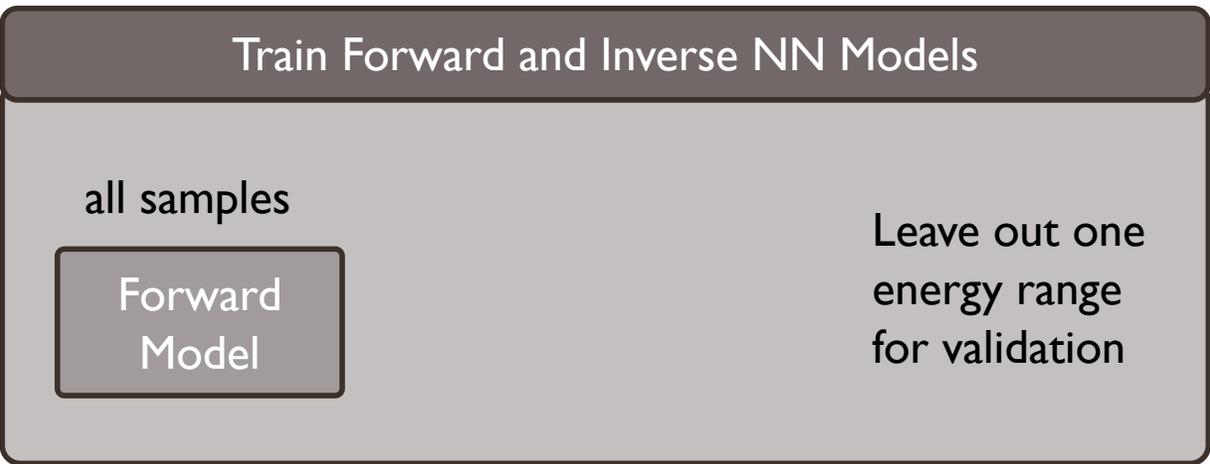
repeat for different target energies

Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

Noisy data + tuning around roughly optimal settings

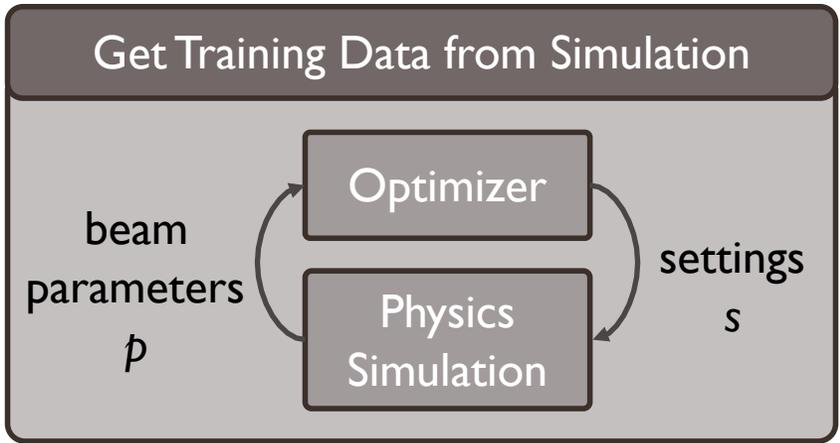


repeat for different target energies

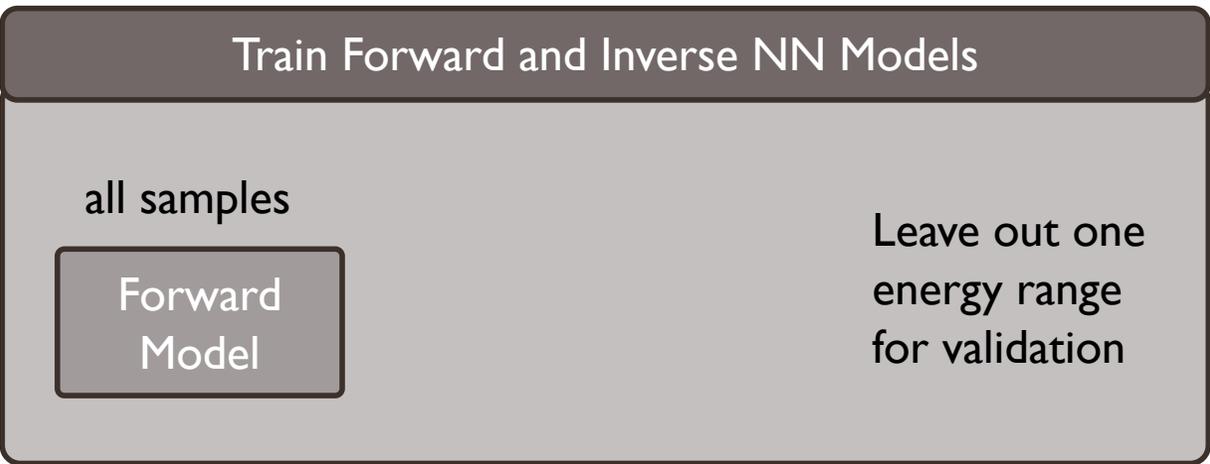


Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

Noisy data + tuning around roughly optimal settings



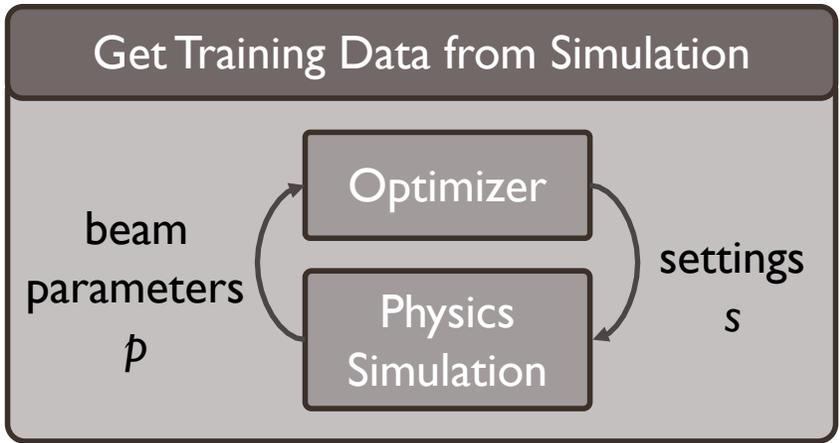
repeat for different target energies



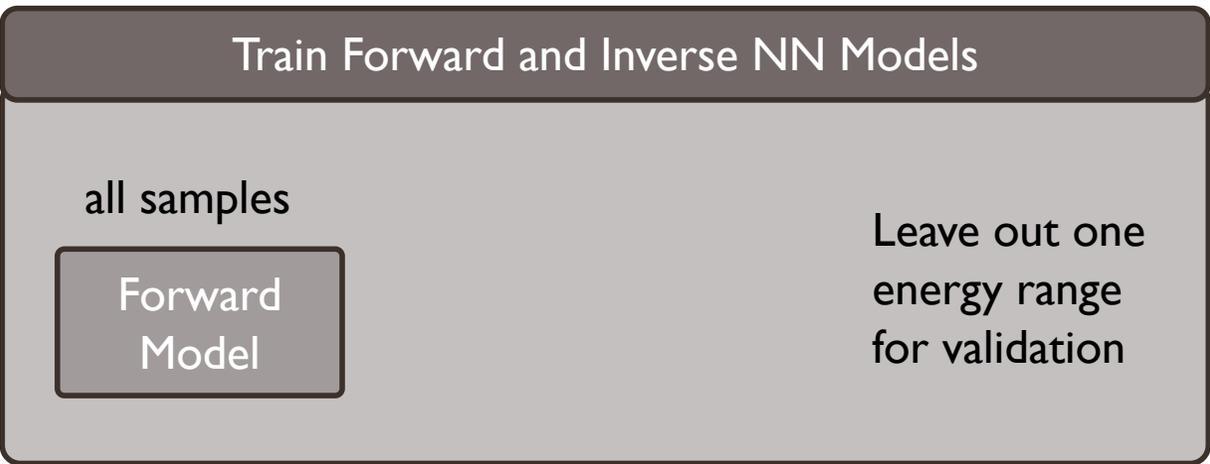
Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

Noisy data + tuning around roughly optimal settings

Bulk beam parameter estimation relies on good statistics → *only train on those outputs when transmission > 90%*



repeat for different target energies

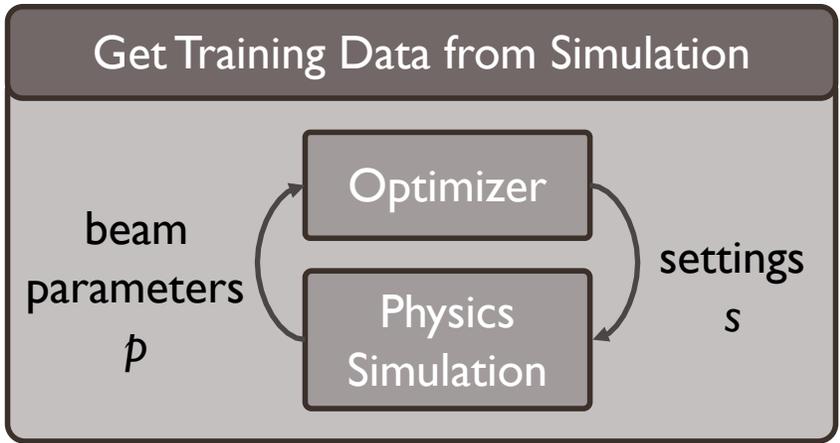


Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

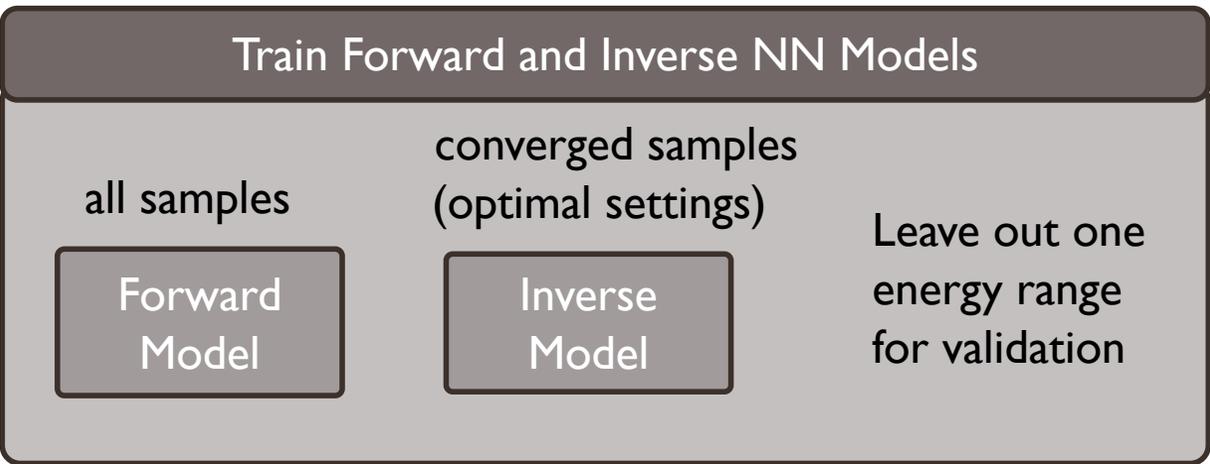
Noisy data + tuning around roughly optimal settings

Bulk beam parameter estimation relies on good statistics → *only train on those outputs when transmission > 90%*

Want to use the existing data to initialize control policy → *model not invertible, but can pre-train policy with converged settings*



repeat for different target energies

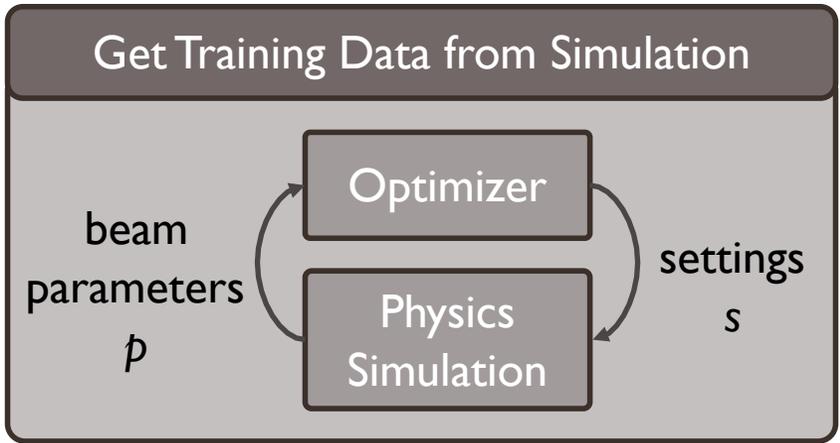


Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

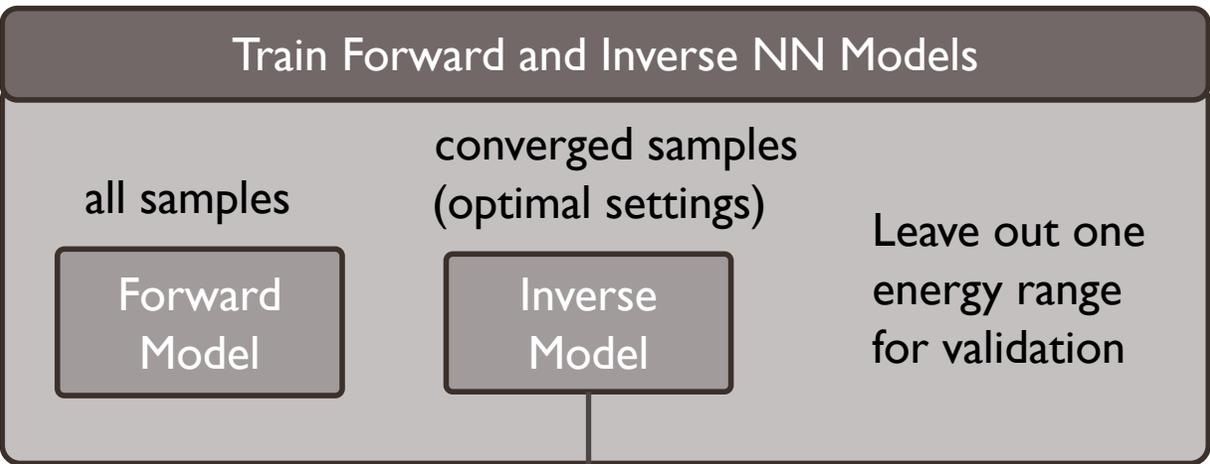
Noisy data + tuning around roughly optimal settings

Bulk beam parameter estimation relies on good statistics → *only train on those outputs when transmission > 90%*

Want to use the existing data to initialize control policy → *model not invertible, but can pre-train policy with converged settings*



repeat for different target energies



Don't always have a good physics-based model for particle accelerators, so what's in the data archive of a real facility?

Noisy data + tuning around roughly optimal settings

Bulk beam parameter estimation relies on good statistics → *only train on those outputs when transmission > 90%*

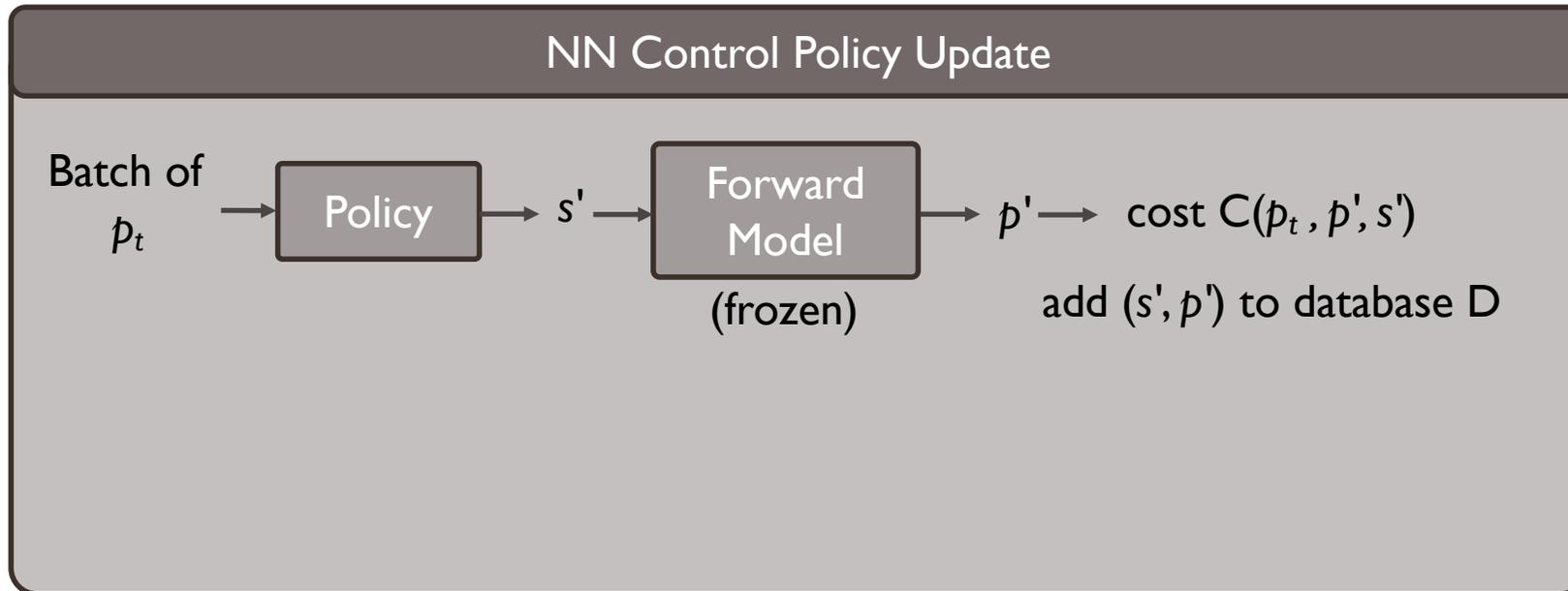
Want to use the existing data to initialize control policy → *model not invertible, but can pre-train policy with converged settings*

Training the Control Policy (v0)

- *First: just want to switch to roughly correct settings*
- *Then, two options: efficient local tuning algorithms we already use, or online model/controller updating*

Training the Control Policy (v0)

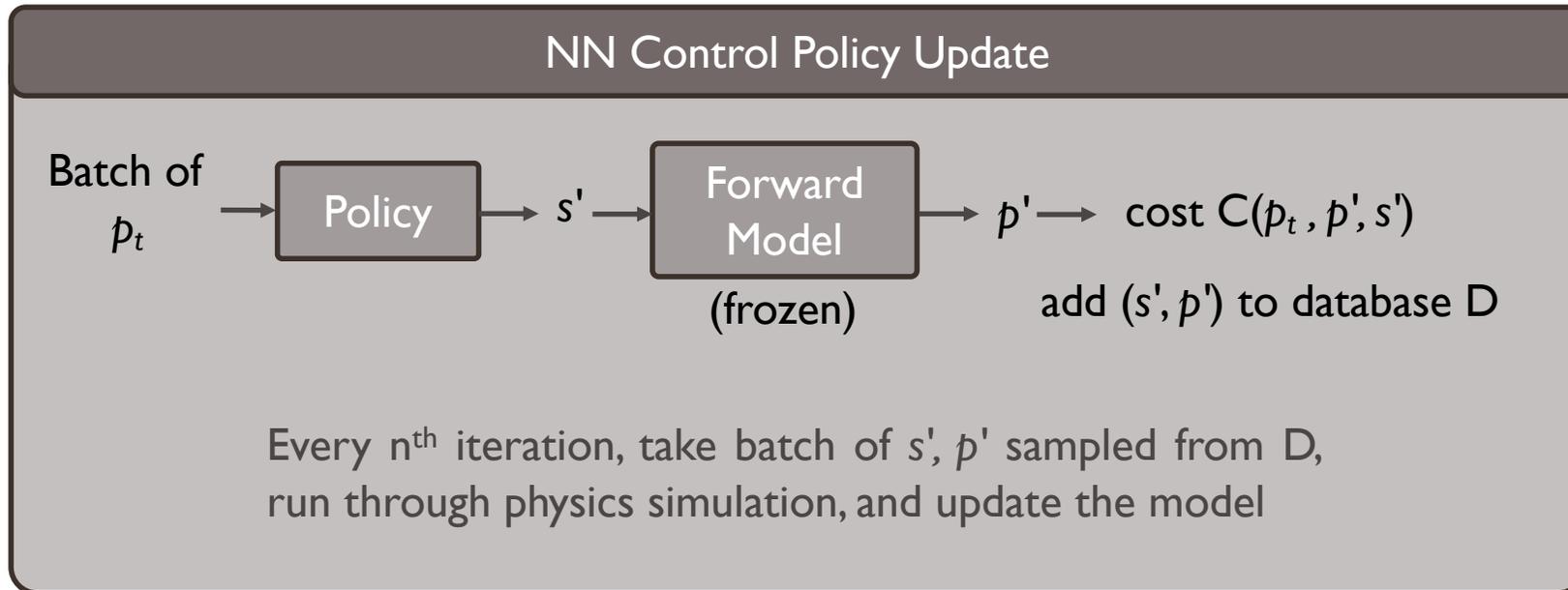
- *First: just want to switch to roughly correct settings*
- *Then, two options: efficient local tuning algorithms we already use, or online model/controller updating*



Cost:
difference between p' and p_t
penalize loss of transmission
penalize higher magnet settings

Training the Control Policy (v0)

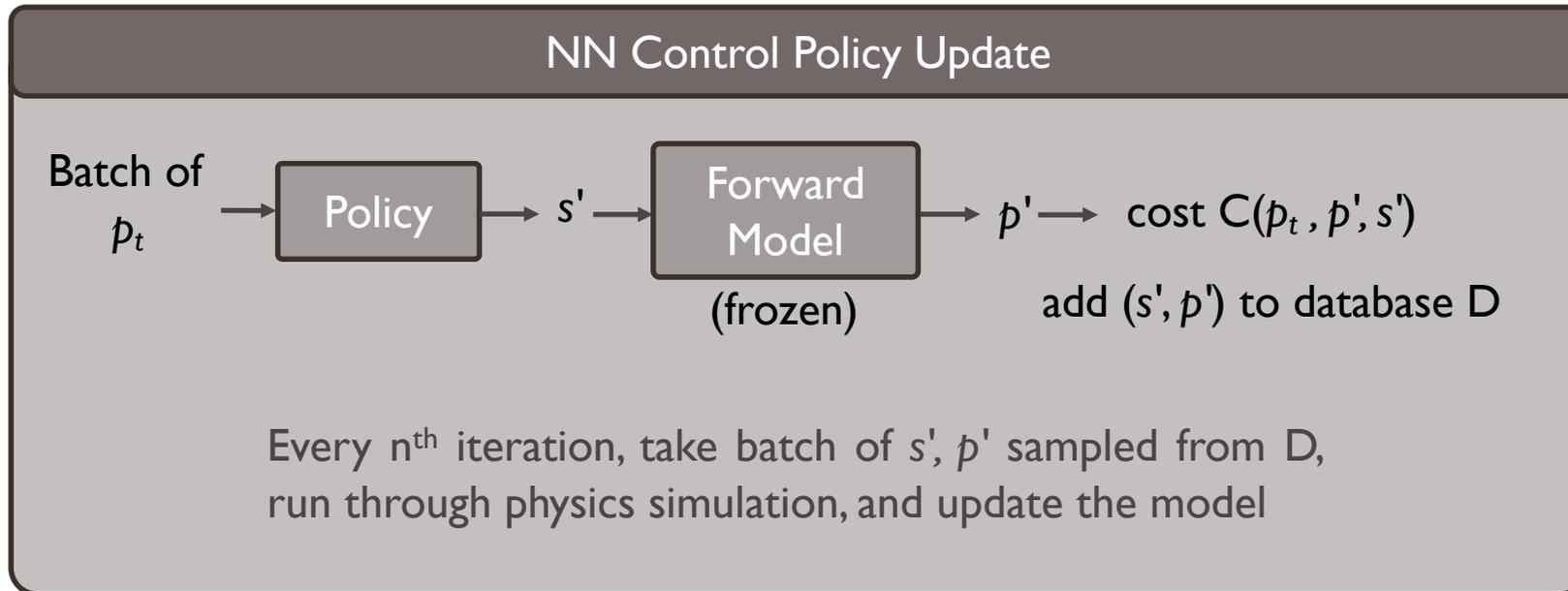
- *First: just want to switch to roughly correct settings*
- *Then, two options: efficient local tuning algorithms we already use, or online model/controller updating*



Cost:
difference between p' and p_t
penalize loss of transmission
penalize higher magnet settings

Training the Control Policy (v0)

- *First: just want to switch to roughly correct settings*
- *Then, two options: efficient local tuning algorithms we already use, or online model/controller updating*



Cost:
difference between p' and p_t
penalize loss of transmission
penalize higher magnet settings

Then test policy directly on simulation

Initial Model and Policy

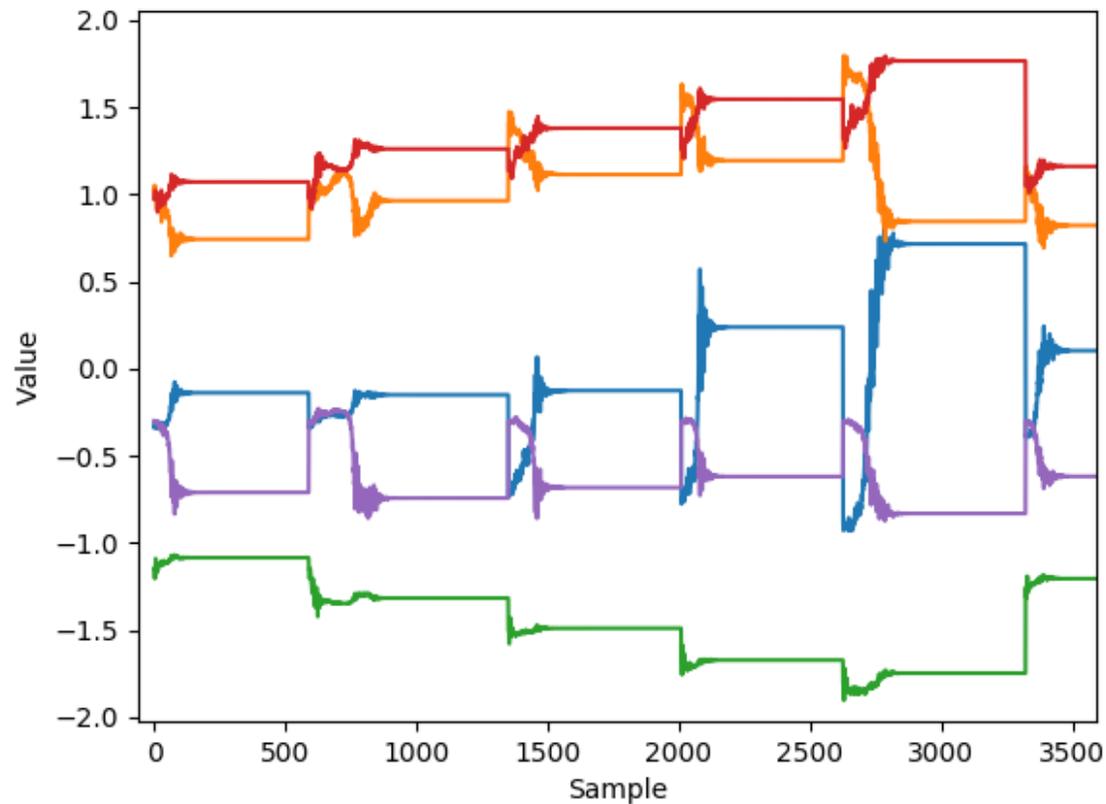
Training data from simulation:

- output from each iteration of Nelder-Mead, L-BFGS
- 12 beam energies between 3.1 – 6.2 MeV (7195 samples)

Initial Model and Policy

Training data from simulation:

- output from each iteration of Nelder-Mead, L-BFGS
- 12 beam energies between 3.1 – 6.2 MeV (7195 samples)

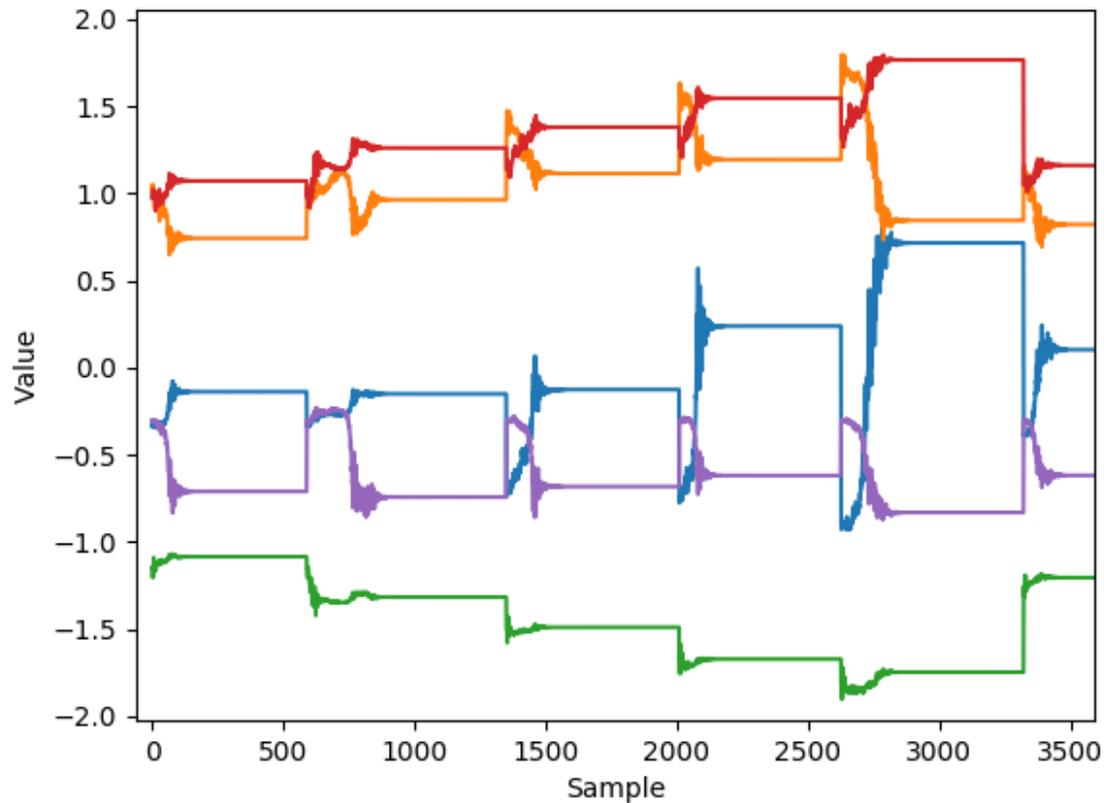


*Example of what the training data looks like
(quads in this case)*

Initial Model and Policy

Training data from simulation:

- output from each iteration of Nelder-Mead, L-BFGS
- 12 beam energies between 3.1 – 6.2 MeV (7195 samples)



*Example of what the training data looks like
(quads in this case)*

Model: 50-50-30-30 tanh nodes in hidden layers

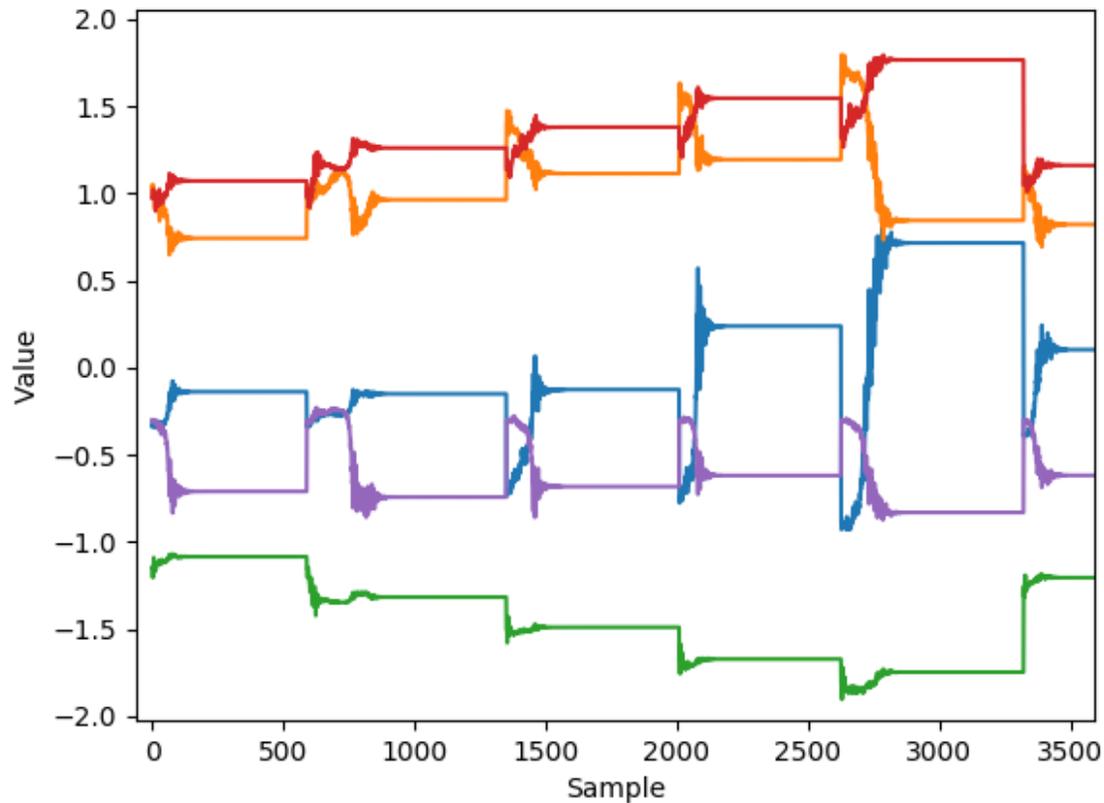
- 8 inputs (*rf power, rf phase, sol. strength, quads*)
- 8 outputs ($\alpha_{xy}, \beta_{xy}, \varepsilon_{xy}, E, N_p$)
- 5.7-MeV run used for validation set

Bulk beam parameter estimation relies on good statistics
→ *only train on those outputs when transmission > 90%*

Initial Model and Policy

Training data from simulation:

- output from each iteration of Nelder-Mead, L-BFGS
- 12 beam energies between 3.1 – 6.2 MeV (7195 samples)



*Example of what the training data looks like
(quads in this case)*

Model: 50-50-30-30 tanh nodes in hidden layers

- 8 inputs (*rf power, rf phase, sol. strength, quads*)
- 8 outputs ($\alpha_{xy}, \beta_{xy}, \varepsilon_{xy}, E, N_p$)
- 5.7-MeV run used for validation set

Bulk beam parameter estimation relies on good statistics

→ *only train on those outputs when transmission > 90%*

First study: focus on target α, β for a given energy

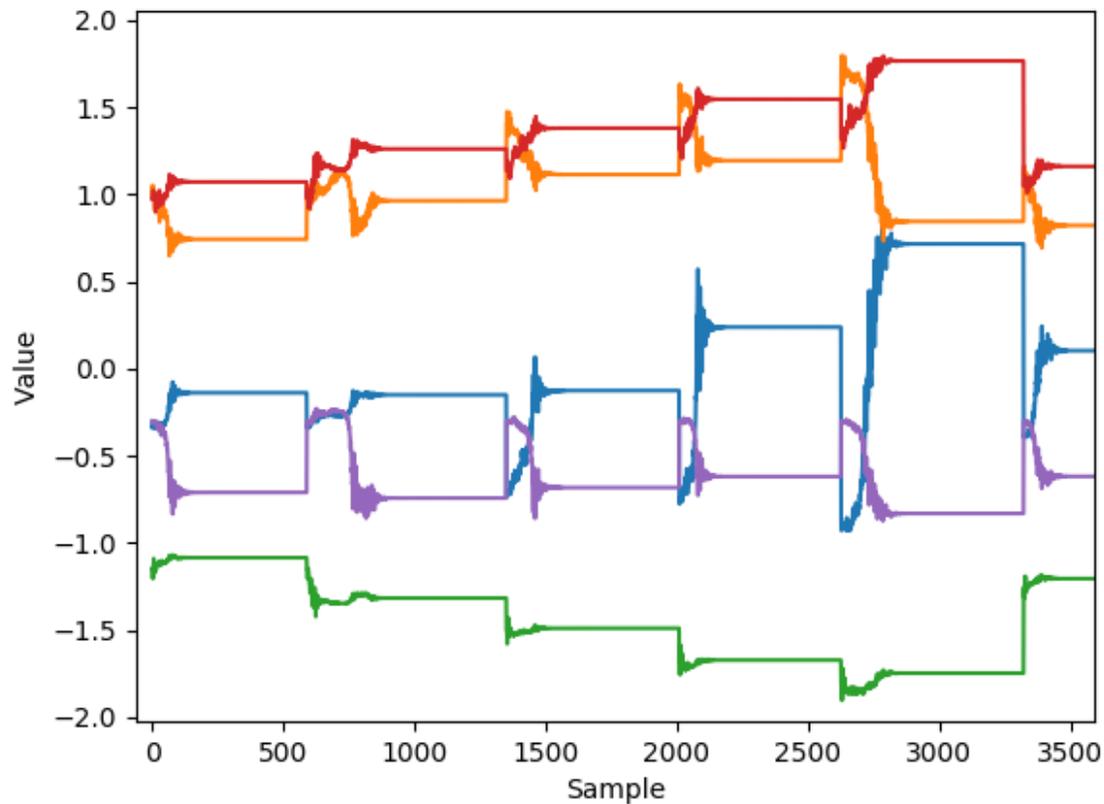
→ *don't allow variation in gun settings beyond known optima*

→ *exclude emittance in cost*

Initial Model and Policy

Training data from simulation:

- output from each iteration of Nelder-Mead, L-BFGS
- 12 beam energies between 3.1 – 6.2 MeV (7195 samples)



*Example of what the training data looks like
(quads in this case)*

Model: 50-50-30-30 tanh nodes in hidden layers

- 8 inputs (*rf power, rf phase, sol. strength, quads*)
- 8 outputs ($\alpha_{xy}, \beta_{xy}, \varepsilon_{xy}, E, N_p$)
- 5.7-MeV run used for validation set

Bulk beam parameter estimation relies on good statistics

→ *only train on those outputs when transmission > 90%*

First study: focus on target α, β for a given energy

→ *don't allow variation in gun settings beyond known optima*

→ *exclude emittance in cost*

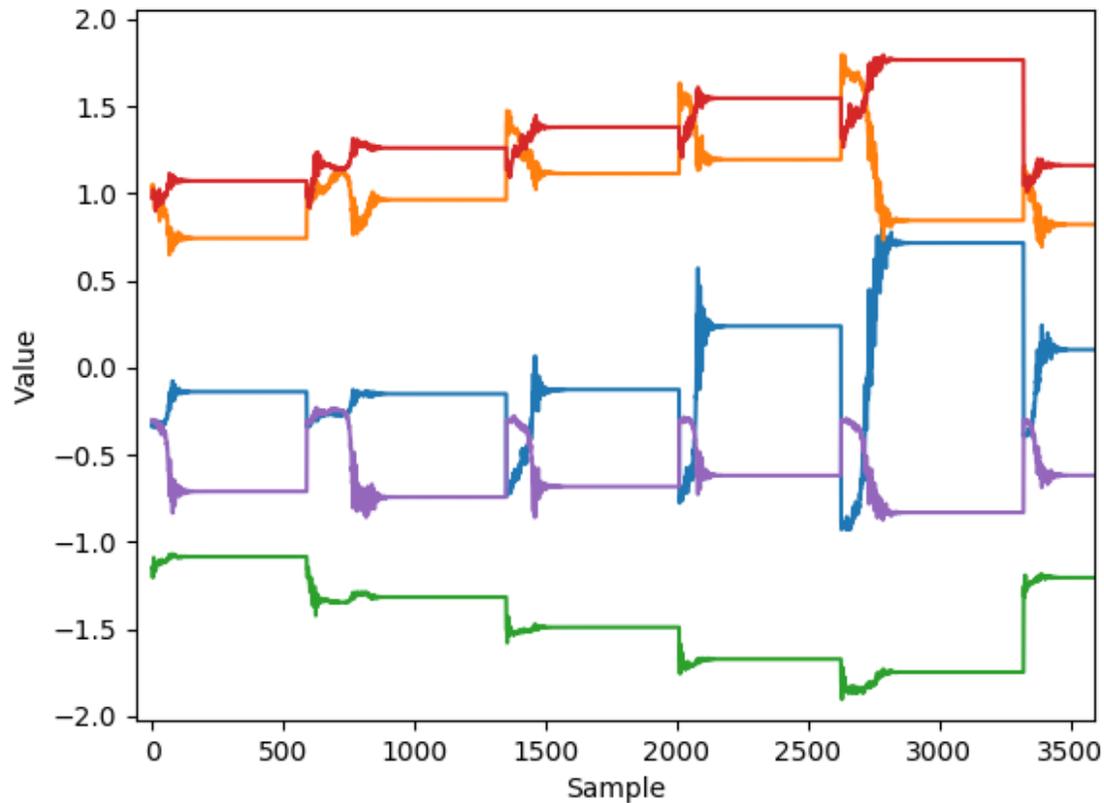
Policy: 30-30-20-20 tanh nodes in hidden layers

- inputs/outputs opposite the above (except N_p)
- random target energies, $\alpha_{xy} = 0, \beta_{xy} = 0.106$
- exclude 4.8 – 5.2 MeV range for validation

Initial Model and Policy

Training data from simulation:

- output from each iteration of Nelder-Mead, L-BFGS
- 12 beam energies between 3.1 – 6.2 MeV (7195 samples)



Example of what the training data looks like
(quads in this case)

Model: 50-50-30-30 tanh nodes in hidden layers

- 8 inputs (*rf power, rf phase, sol. strength, quads*)
- 8 outputs ($\alpha_{xy}, \beta_{xy}, \varepsilon_{xy}, E, N_p$)
- 5.7-MeV run used for validation set

Bulk beam parameter estimation relies on good statistics

→ only train on those outputs when transmission > 90%

First study: focus on target α, β for a given energy

→ don't allow variation in gun settings beyond known optima

→ exclude emittance in cost

Policy: 30-30-20-20 tanh nodes in hidden layers

- inputs/outputs opposite the above (except N_p)
- random target energies, $\alpha_{xy} = 0, \beta_{xy} = 0.106$
- exclude 4.8 – 5.2 MeV range for validation

- weights/biases updated with AdaMax
- batch size of 200
- implemented in Theano and lasagne

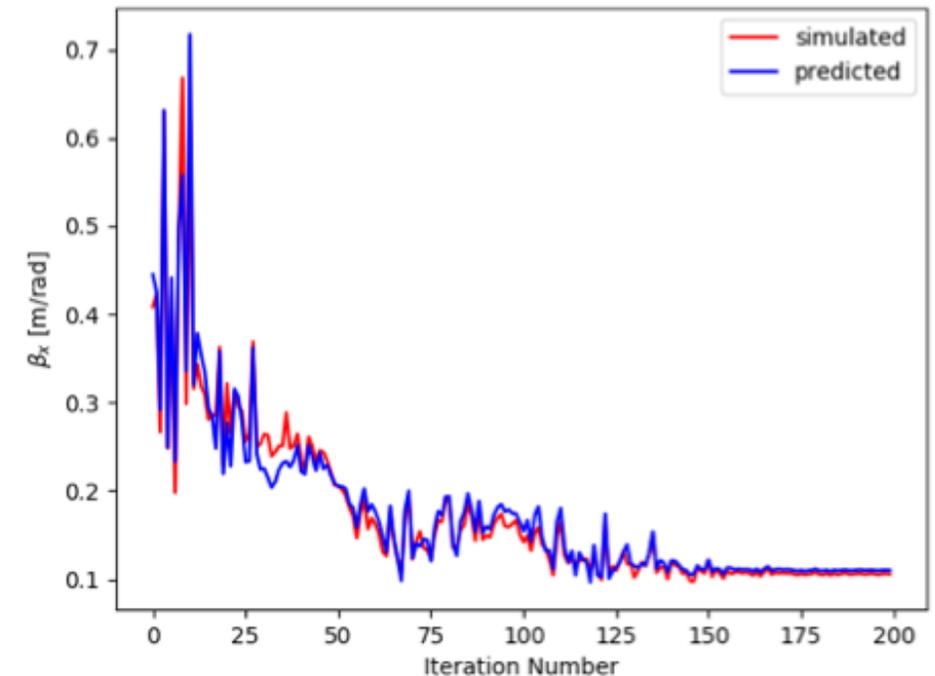
Initial Model and Policy Performance

First study: focus on target Twiss parameters and don't allow variation in gun settings beyond known optima

Summary of Model Performance

Parameter	Train MAE	Train STD	Train Max	Val. MAE	Val. STD	Val. Max
α_x [rad]	0.018	0.042	0.590	0.067	0.091	0.482
α_y [rad]	0.022	0.037	0.845	0.070	0.079	0.345
β_x [m/rad]	0.004	0.009	0.287	0.008	0.012	0.130
β_y [m/rad]	0.005	0.011	0.357	0.012	0.017	0.189

Example of Model Performance on Validation Set



Initial Model and Policy Performance

First study: focus on target Twiss parameters and don't allow variation in gun settings beyond known optima

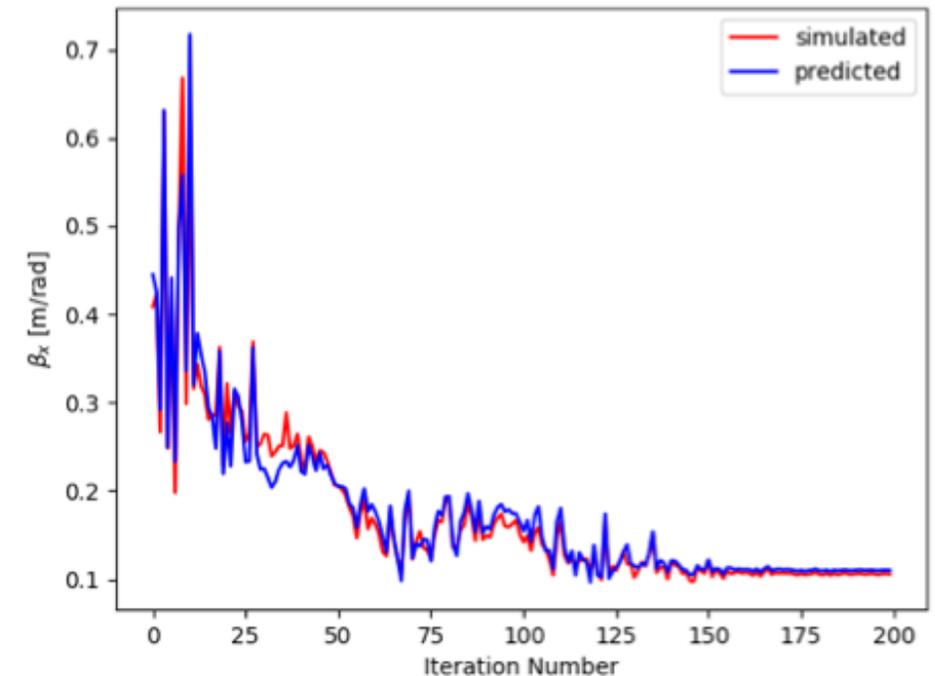
Summary of Model Performance

Parameter	Train MAE	Train STD	Train Max	Val. MAE	Val. STD	Val. Max
α_x [rad]	0.018	0.042	0.590	0.067	0.091	0.482
α_y [rad]	0.022	0.037	0.845	0.070	0.079	0.345
β_x [m/rad]	0.004	0.009	0.287	0.008	0.012	0.130
β_y [m/rad]	0.005	0.011	0.357	0.012	0.017	0.189

Controller ability to reach $\alpha_{x,y} = 0$ and $\beta_{x,y} = 0.106$ in **one iteration**

Parameter	Train MAE	Train STD	Train Max	Val. MAE	Val. STD	Val. Max
α_x [rad]	0.012	0.075	0.011	0.046	0.063	0.141
α_y [rad]	0.013	0.079	0.012	0.045	0.064	0.140
β_x [m/rad]	0.008	0.004	0.006	0.006	0.023	0.008
β_y [m/rad]	0.014	0.011	0.011	0.011	0.069	0.038

Example of Model Performance on Validation Set



Initial Model and Policy Performance

First study: focus on target Twiss parameters and don't allow variation in gun settings beyond known optima

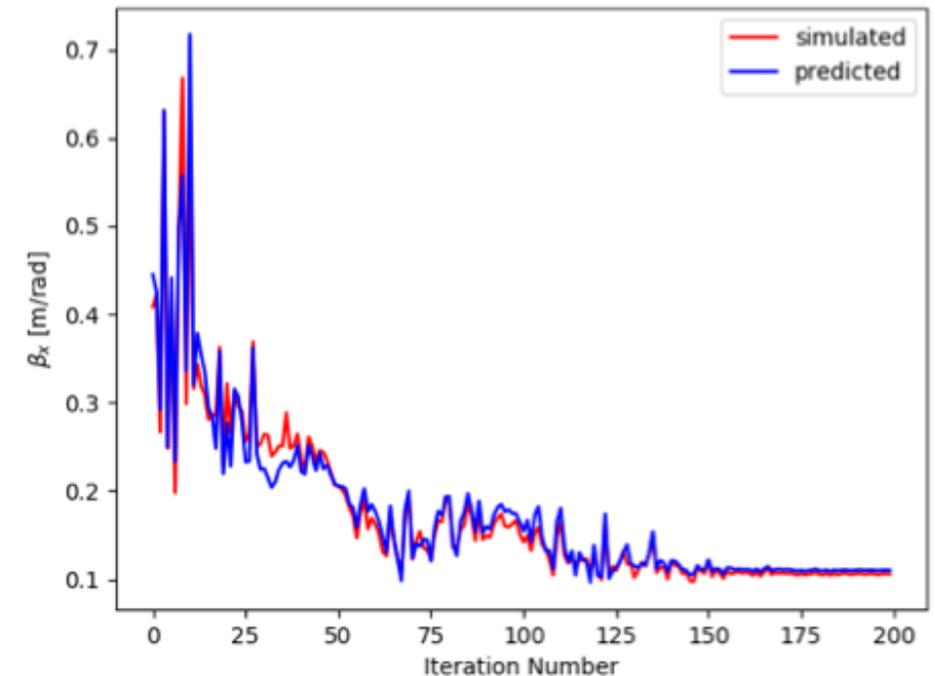
Summary of Model Performance

Parameter	Train MAE	Train STD	Train Max	Val. MAE	Val. STD	Val. Max
α_x [rad]	0.018	0.042	0.590	0.067	0.091	0.482
α_y [rad]	0.022	0.037	0.845	0.070	0.079	0.345
β_x [m/rad]	0.004	0.009	0.287	0.008	0.012	0.130
β_y [m/rad]	0.005	0.011	0.357	0.012	0.017	0.189

Controller ability to reach $\alpha_{x,y} = 0$ and $\beta_{x,y} = 0.106$ in **one iteration**

Parameter	Train MAE	Train STD	Train Max	Val. MAE	Val. STD	Val. Max
α_x [rad]	0.012	0.075	0.011	0.046	0.063	0.141
α_y [rad]	0.013	0.079	0.012	0.045	0.064	0.140
β_x [m/rad]	0.008	0.004	0.006	0.006	0.023	0.008
β_y [m/rad]	0.014	0.011	0.011	0.011	0.069	0.038

Example of Model Performance on Validation Set

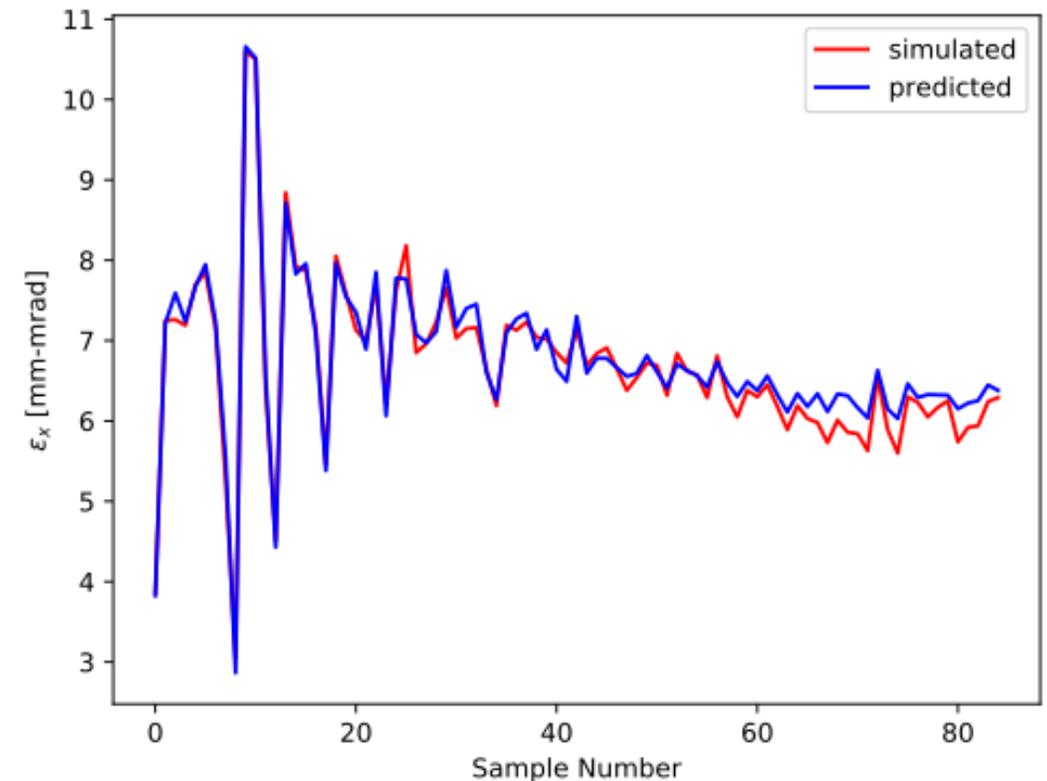


What this means: for a given energy, the controller will immediately reach the desired beam size to within about 10% and the beam will be close to a waist, requiring minimal further tuning (assuming no drift...)

Presently working on the next steps for the complete study

- Including minimization of emittance + more freedom with injector settings
 - *Requires finer start-to-end adjustments, so more simulation data was needed*
 - *Larger network needed to capture relationships accurately in model*
- Need to see how well it does with machine drift
 - *e.g. deviation between settings and real values, deviation in responses*
- Need to compare with other methods
 - *Online optimization methods used in accelerators*
 - *Try comparing with some model-free RL benchmarks (e.g. TRPO)*
- Have plans for trying this approach on an operational machine
- Other tweaks:
 - *Specify change in setting rather than setting*
 - *Weights of cost function should be tuned*

Example of Model Performance on Validation Set



Conclusion

- *Initial study for fast switching between beam energies while preserving α , β looks encouraging*
- *Continuing with more complete study*
- *Will be interesting to see how this might scale to a larger accelerator system*

