Neural-Network-based Surrogate Simulator for Particle Accelerator with High Dimensional Control Settings

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Wednesday 6th November 2024

Motivations

Surrogate models : from aggregate to 6D

- Models are good for reproducing beam aggregate properties (size, emittance, Edep, ...)
- aggregates could be insufficient to get all properties of a beam
- by definition, full beam reconstruction gets all the beam properties
- 6D beam as input for a new simulation
- Full 6D beam helps to better understand disturbed beam
- helps to better understand the beam halo
- better understand collective effects

Where to learn

- Large machines mean a very large amount of data
- Why not slice a machine
- in each slice, reconstruct 6D beam
- could help in transfer learning
- could help in fault detection and machine drift
- problem of multi-task learning

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Multi-Layer Perceptron: A First Model

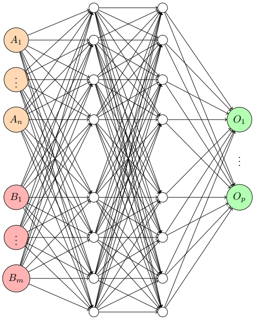

Figure: MLP as a surrogate model of a Linac

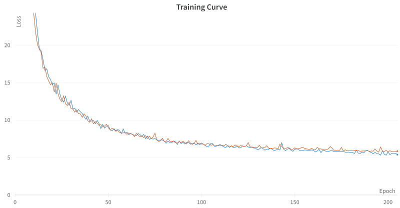

Figure: Training Curve

Multi Layer Perceptron

- Stack all inputs and outputs
- 10k simulations sampling $\mathcal{A}$ and $\mathcal{B}$
- Minimization of the L2 loss

Physics-aware: Cutting the non-causal links

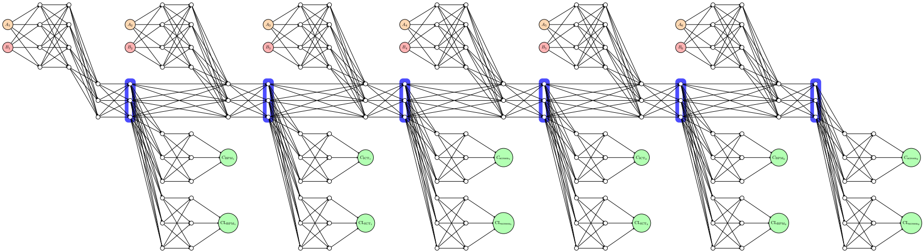

Figure: LinacNet with 6 modules corresponding to 6 diagnostic stations on the Linac

LinacNet

- Split input and output according to their position in the Linac
- Neural Network Architecture reflecting a Linac architecture
- Each Module models one Diagnostic (could be real or virtual)

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PointNet as a Beam Representation Network

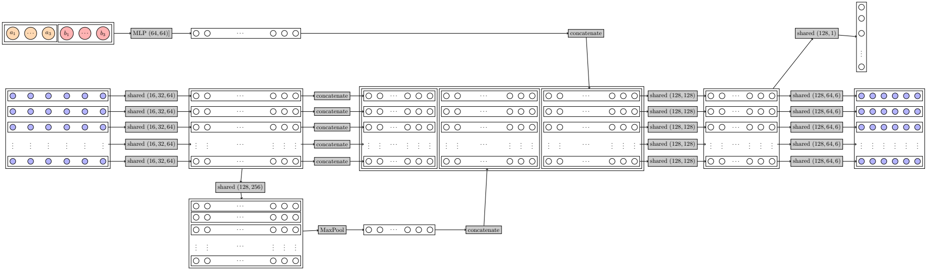

Figure: One module of ThomNet

ThomNet

- Track the full distribution of particles
- Inspired by Qi et al., "PointNet: Deep Learning on Point Sets for 3D Classification and Segmentation" (CVPR 2017)

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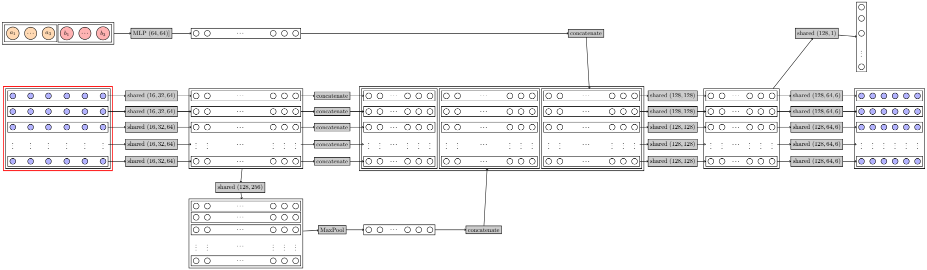

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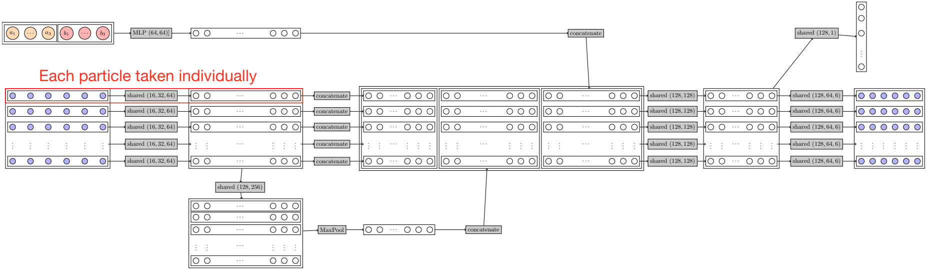

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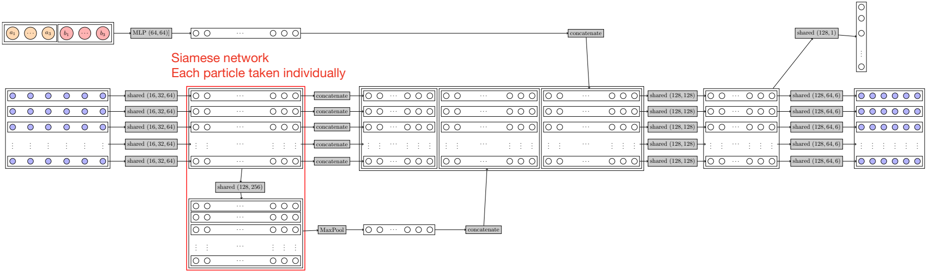

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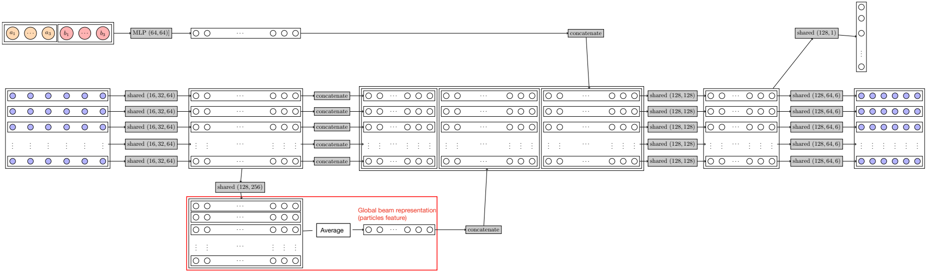

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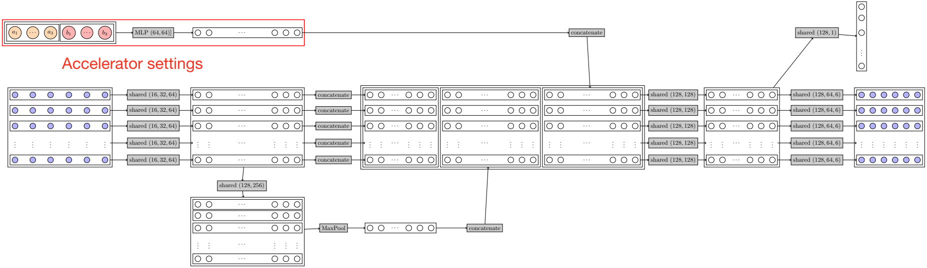

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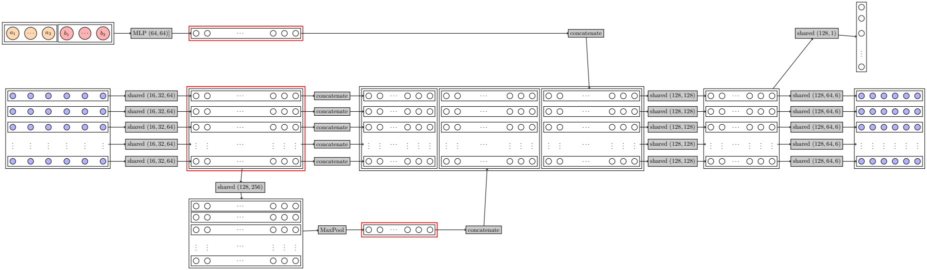

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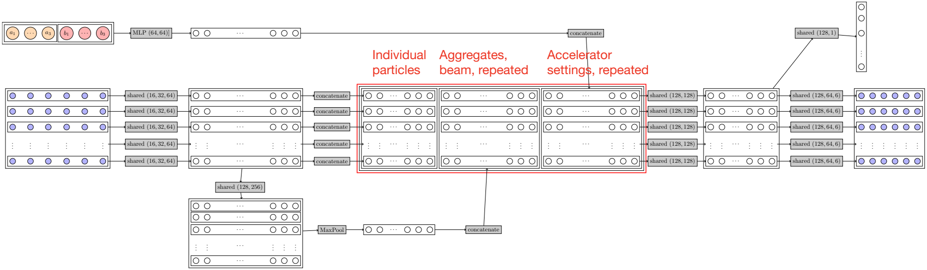

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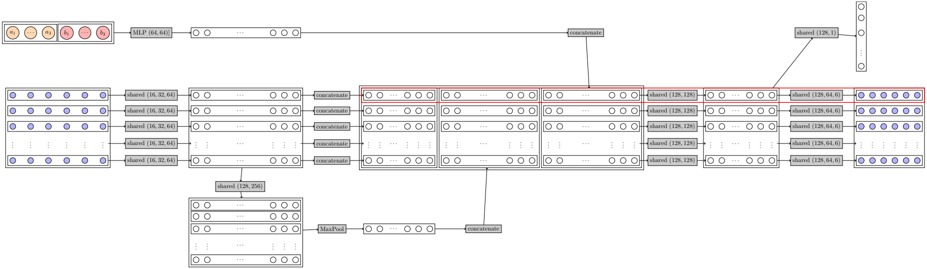

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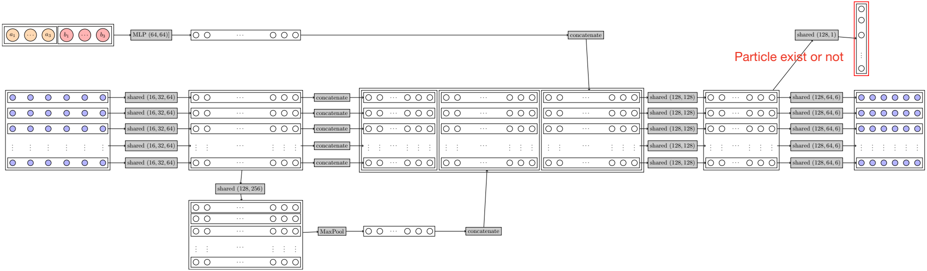

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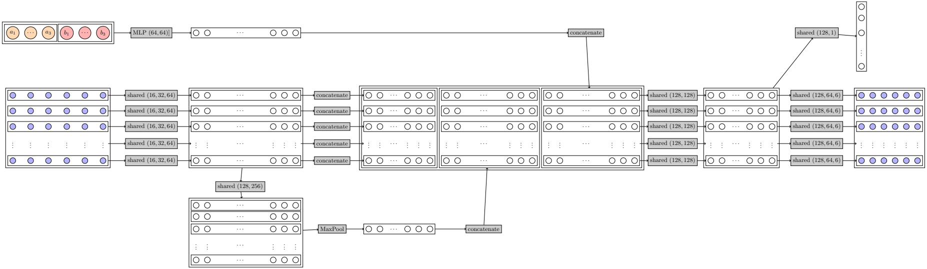

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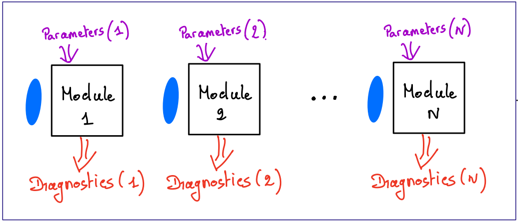
Accelerator as a sequence of modules



- We divide our accelerator in a sequence of sub-parts
- Each part could contain controls / measurements (real or virtual)
- Learning a full machine could be complicated, costly

Good for

- transfer to a real machine
- optimize : could be done by part / module
- Retrain locally due to drift in the data
- Address larger machines

Sequential Network as a Multi-Objective Optimization

- General question in machine learning
- how to learn a sequence of models, tasks ?
- Could be heterogeneous : classification, regression, etc
- Conflicting between modules could deteriorate the global loss

- Independent Errors : $Err_{i,i+1}\left(d_i, d_{i+1}, a; \theta\right) = l\left(f_{i,i+1}\left(d_i, a; \theta\right), d_{i+1}\right)$
- End-to-End Errors : $Err_{0,i}\left(d_0, d_i, a; \theta\right) = l\left(f_{0,i}\left(d_0, a; \theta\right), d_i\right)$

Scalarization of the Multi-Objective Loss

$$\mathcal{L}_w\left(d, a; \theta\right) = \sum_{i=1}^{N} w_{i-1,i} Err_{i-1,i}\left(d_{i-1}, d_i, a; \theta\right) + w_{0,i} Err_{0,i}\left(d_0, d_i, a; \theta\right)$$

One example of learning a sequence : MGDA[1]

- Dynamic weighting of the module that moderates conflicting loss between modules

$$w^* = \arg\min_{w} \mathcal{L}_w, \qquad w > 0, \qquad \sum_{i=1}^{N} w_{i-1,i} + w_{0,i} = 1$$

Properties

- Common descent direction to all objectives
- Stop when encountering a Pareto-invariant point

[1] Sener and Koltun, "Multi-Task Learning as Multi-Objective Optimization".

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Numerical Results

The best model achieves results comparable with the diagnostic station accuracy.

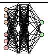
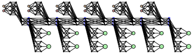
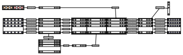
Architecture	BPM	ICT	YAG	ICT	BPM	YAG
FeedForward 	$776\mu m$	$1084\mu m$	$1692\mu m$	$1106\mu m$	$1261\mu m$	$1554\mu m$
LinacNet 	$198\mu m$	$254\mu m$	$541\mu m$	$618\mu m$	$719\mu m$	$913\mu m$
ThomNet 	$\mathbf{178\mu m}$	$\mathbf{134\mu m}$	$\mathbf{247\mu m}$	$\mathbf{224\mu m}$	$\mathbf{258\mu m}$	$\mathbf{336\mu m}$

Table: MAE of the position. The accuracy of the BPM is $\sim 100\mu m$

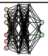
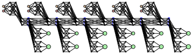
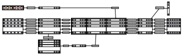
Architecture	BPM	ICT	YAG	ICT	BPM	YAG
FeedForward 	$176pC$	$177pC$	$167pC$	$91pC$	$91pC$	$91pC$
LinacNet 	$28pC$	$28pC$	$29pC$	$34pC$	$34pC$	$35pC$
ThomNet 	$\mathbf{8pC}$	$\mathbf{9pC}$	$\mathbf{9pC}$	$\mathbf{8pC}$	$\mathbf{8pC}$	$\mathbf{8pC}$

Table: MAE of the charge. The accuracy of the ICT is $\sim 10pC$

Distributions

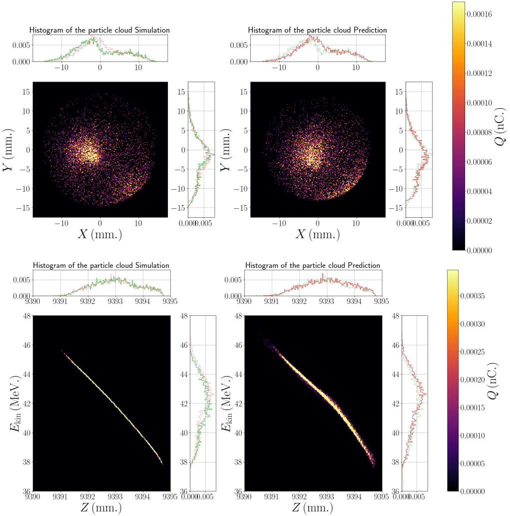


Figure: Comparison between the projection of the simulated beam (left) and predicted beam (right) on the transverse and longitudinal space.

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Perspectives

Results

- Reflecting the physical constraints in the neural architecture speeds up the training and gives better results
- Precision of the same orders as the diagnostics installed on ThomX

Challenges

- Training of a modular model
- Performance for the optimization task to be tested

Questions?