

ML enhanced optimal detector design

François Fleuret, Tobias Golling, Jan Kieseler, Stephen Mulligan, Atul Sinha, Kinga Anna Wozniak

> CHIPP AI/ML & computing workshop 19.06.2024

RECONSTRUCTION

RECONSTRUCTION 144

 \rightarrow We want x and x[^] to be 'close'

RECONSTRUCTION

- \rightarrow We want x and x[^] to be 'close'
- \rightarrow Developing detector with physics task in mind \rightarrow impacts 'closeness'

RECONSTRUCTION

- \rightarrow We want x and x[^] to be 'close'
- \rightarrow Developing detector with physics task in mind \rightarrow impacts 'closeness'
- \rightarrow Different options for detector design \rightarrow giving different δ

RECONSTRUCTION

- \rightarrow We want x and x[^] to be 'close'
- \rightarrow Developing detector with physics task in mind \rightarrow impacts 'closeness'
- \rightarrow Different options for detector design \rightarrow giving different δ
- ➔ resource demanding & not differentiable wrt design

RECONSTRUCTION

- \rightarrow We want x and x^{\land} to be 'close'
- \rightarrow Developing detector with physics task in mind \rightarrow impacts 'closeness'
- \rightarrow Different options for detector design \rightarrow giving different δ
- ➔ resource demanding & not differentiable wrt design

Fast assessment of design with local surrogate model

To assess detector design i for task j, simulation + reconstruction has to be developed

- resource demanding
- \rightarrow not differentiable wrt design
- \rightarrow High complexity (pixels, hits, ...)

- For a set of designs ${D^{(i)}}$, each parametrized by a $\theta^{(i)}$, we want to find design that minimizes δ between the true and reconstructed x
- Need differentiability wrt θ
- Idea: Replace Simulation + Reco by a local ML Surrogate Surrogate conditioned on local θ Once trained, can provide a direction for optimization

Local surrogate setup

Gives access to $p(\delta | \theta, x) \rightarrow a$ scalar which encompasses sim+reco process Which δ to pick?

Mutual information (MI): proxy for δ truth vs measurement

Information theoretic metric: $\mathrm{MI}(A,B)\equiv H(A)-H(A|B)$

= average reduction in uncertainty about A when observing B=b

= average amount of information that B conveys about A

$$
\min\delta(x,\hat x)\sim\max \text{MI}(x,\hat x)
$$

Strengths of MI:

- Tells us if information is conserved during sim+reco process
- Captures non-linear dependencies
- X is multidimensional

 \rightarrow MI able to cover large part of phase space

 \rightarrow MI able to cover multiple tasks at once \rightarrow δ can be multi-task

Drawback: Must be recomputed for each design and inputs

Data & Studies

- Geant4 simulation of calorimeter
- Study single particle shot orthogonally at detector (50K)
- Two types of layers: absorber (cheap, lost info) & scintillator (expensive, yields info)
- Particles: photons and hadrons
- Recovering energy deposited
- θ = layer count, layer thickness
- Task: energy resolution and particle ID

Mutual information: # layers vs particle ID

- MI score for set of designs
- $Design θ = number of layers in detector$
- Tasks: ID of particle

K x Y: energy deposited in each layer

Individual contribution informs pid discrimination until deposit saturation

Accumulation dilutes positional information of deposit (early/late)

Surrogate: scintillator and absorber thickness

- Design θ = thicknesses of absorber and scintillator
- Metric δ = energy accuracy

Surrogate: scintillator and absorber thickness

- Design $θ =$ thicknesses of absorber and scintillator
- Metric δ = energy accuracy

re-initialized bumpy model w/o transfer learning

refined smooth transfer learning model

Transfer Learning Hypothesis:

Surrogate is able to map out local θ landscape across design tests

Conclusion

Problem:

development of detector involves simulation + reconstruction

 \rightarrow resource demanding

Solution:

- Surrogate model which maps out local design parameter space and allows for detector optimization
- Mutual information as a viable metric to encompass high-dimensional complex

First promising results applying solution to typical HEP tasks

Surrogate: Scintillator and Absorber Thickness

Applicable to more complex multi-layer problems

Absorbers minimized

Scintillators maximized with decreasing intensity

 $\frac{1}{2}$, $\frac{1$

Smooth refined model evolution

Mutual Information - The Theory

$$
\mathrm{MI}(X,Y)\equiv H(X)-H(X|Y)
$$

H … entropy

Equivalent to Kullback-Leibler divergence between the joint distribution and the product of the marginals

$D_{KL}(P(X,Y)||P(X) \otimes P(Y))$

Mutual Information Estimation with DNNs

[Mine: Mutual Information Neural Estimation](https://arxiv.org/abs/1801.04062)

Donsker-Varadhan dual representation of D_{Kl}

$$
D_{\mathrm{KL}}(U\,||\,V)=\sup_{T:\Omega\rightarrow\mathbb{R}}\mathbb{E}_U[T]-\log(\mathbb{E}_V[e^T])
$$

For a class of functions T for which the expectations are finite

 $=$ > Chose T to be parametrized by a neural network $\left|T_{\theta}\right|$

$$
D_{\mathrm{KL}}(P(X,Y)\,||P(X)\otimes P(Y))=\sup_{\theta\in\Theta}\mathbb{E}_{P_{XY}}[T_{\theta}]-\log(\mathbb{E}_{P(X)\otimes P(Y)}[e^{T_{\theta}}])
$$

MI Model - architecture

X, Y … input random variables

Π … permutation

 $P(X,Y) \sim \text{NN}(X,Y)$ $P(X) \otimes P(Y) \sim \text{NN}(X, \Pi(y \in Y))$