# DeepEfficiency <br> arXiv:1809.06101 

Mikael Mieskolainen

IRN Terascale
21/05/2019, Annecy, France


UNIVERSITY OF HELSINKI

## Neural networks - the meta-math-tool for everything?

Example: "Fast Cosmic Web Simulations with GAN networks" (internally a Nash equilibrium type minimax optimization problem)

[Rodriguez et al., ETH Zürich, arXiv:1801.09070, orders of magnitude speed improvement in 2D slices]

Learn the tool: play with GAN in your browser! https://poloclub.github.io/ganlab


Gradients
[Kahng et al., Georgia Tech/Google brain, arXiv:1809.01587]

Example: Neural networks meet holography in "AdS/CFT as a deep Boltzmann machine" (Boltzmann net is Ising model like net)
data $\simeq$ boundary scalar field theory generating functional, hidden network weights $\simeq$ bulk spacetime metric (geometry), the deepest layer $\simeq$ the black-hole horizon

[Hashimoto, Osaka University, arXiv:1903.04951]

## Now this work

[MM, DeepEfficiency, arXiv:1809.06101]

A new way implementing detector fiducial efficiency corrections in higher phase space dimensions, towards optimal measurements

Talk 15 min , so accurate details you can find in the Tensorflow framework based code at
<github.com/mieskolainen>, MIT open source
Try it out, make it better

# Basic HEP Measurement Cross section (differential) 

$$
\frac{N-\langle B\rangle}{\mathcal{E} \times A \times L}
$$

- Events: N, number of measured events after trigger \& selection cuts
- Background: $\langle B\rangle$, expected number of background events
- Integrated luminosity: $L$, van der Meer scan calibration + online tech.
- Acceptance (Geometric): $A \rightarrow 1 \Leftrightarrow$ fiducial measurement, $A \rightarrow 0$, highly non-fiducial (extrapolating)
- Efficiency: $\mathcal{E} \equiv$ number of selected / number of generated within fiducial phase space $\in[0,1]$

In this work, we reformulate the detector efficiency term $\mathcal{E}$ evaluation as a problem of learning a probabilistic function

$$
\mathcal{E}: \mathbb{R}^{D} \rightarrow[0,1]
$$

## Fully differential final state event kinematics in, probability out.

## Before DeepEfficiency

Histograms used in Bills of Mortality (1662) by John Graunt

## Natural and Political OBSERVATIONS

Mentioned in a following INDEX, and made upon the
Bills of Mortality.

B Y
Capt. $70 H N G R A \cup N T$,
Fellow of the Royal Society.
With reference to the Government, Religion, Trade, Growth, Air, Difeafes, and the feveral Changes of the faid CITY.

So I expect histogram bin-by-bin 'counting efficiency corrections' of measurements have been used for centuries.

This is obvious and quite solid ${ }^{1}$, but only if your observable is truly low-dimensional. However, in HEP, observables (differential distributions) are constructed as a function of multidimensional final state kinematics.

[^0]
## Main Problem and

## Solution

The usual way of doing efficiency corrections is to rely on the MC event generator + detector simulation (GEANT). We use GEANT too, but minimize (even get rid of) the event generator dependence by using fully differential final state kinematics.

MC theory dependence: $\mathrm{Bias}^{2}$ can (will) propagate from the event generator (dynamics) if no fully differential treatment, whenever the process $\simeq$ scattering amplitudes + rest cannot be well simulated. For example: transverse momentum low $-p_{t}$ parametrizations, system high $-p_{t}$ ISR shower (MC resummation) uncertainties, QCD color coherence, non-perturbative spin polarization $\sim$ decay angle $(\theta, \varphi)$ dependence e.g.
in QCD spectroscopy...

[^1]
## What people have done to handle this problem?

- Multidimensional histograms, bin over differential kinematics (e.g. system mass, rapidity, transverse momentum), approx $D=3$ practical maximum
- Histograms + Spherical Harmonic Expansions ${ }^{3}$ on top of them - for the angular dependence
- These do not scale to higher dimensions, exponential statistics requirement for histogram hypercells - think about exponential number of binary combinations $=2^{D}$ as a function of $D$, then change binary (2) to some large integer (\# bins) approximating real line, much worse

[^2]
## DeepEfficiency

## Universal Approximator

So, we assume that a wide and deep enough fully connected feed-forward network will work as a universal function approximator and that modern neural network optimization tools can optimize ${ }^{4}$ the network, based on (stochastic) gradient search, with the underlying technique being Reverse Mode Automatic Differentiation (backpropagation as a special case)

Original RMAD: Seppo Linnainmaa, MSc thesis, Helsinki, 1970
For the universal approximator theorems:
Wikipedia, Universal approximation theorem
See also the classic Stone-Weierstrass theorem

[^3]

Figure: Types of neural nets, [Fjodor van Veen], we use the top right $\uparrow$

## Network for Probabilities

To train for probabilities, we need to train (minimize) using cross entropy cost ${ }^{5}$

$$
L=-\frac{1}{|\mathcal{S}|} \sum_{i \in \mathcal{S}}\left[R_{i} \ln \mathcal{E}_{i}+\left(1-R_{i}\right) \ln \left(1-\mathcal{E}_{i}\right)\right]
$$

where $R_{i}$ is simulated selection ( $0=$ lost, $1=$ selected) for the $i$-th event in the sample $\mathcal{S}$ and $\mathcal{E}_{i}$ the network output. We found hyperbolic tangent to work fine as the activation function with 5 hidden layers and $\sim 100$ neurons per layer. Also, we use sigmoid $f(x)=1 /\left(1+e^{-x}\right)$ as the final layer function to get output values in $[0,1]$.

[^4]
## How to use

Arbitrary efficiency corrected distributions (1D, 2D, profile...) of observables $\mathcal{O}$ can be constructed with ${ }^{6}$.

$$
\frac{d N}{d \mathcal{O}}=h_{\mathcal{O}}(\{\vec{p}\}) \odot[\mathcal{E}(\{\vec{p}\})]^{-1},
$$

where $h_{\mathcal{O}}$ is a probability distribution estimator operator, such as a (bin width $\Delta \mathcal{O}$ normalized) histogram. The point-wise operator $\odot$ is defined as an integral (sum) over the event sample, event weight $\mathcal{E}(\{\vec{p}\})$ from the trained network.

```
In ROOT ~ for ( i over data event sample ) {
    weight_i = network(kinematics_i);
    histObsA->Fill( observableA(kinematics_i), 1.0/weight_i );
    histObsB->Fill( observableB(kinematics_i), 1.0/weight_i ); ...
}
```

> ${ }^{6}$ Inverse weighting known as Horvitz-Thompson estimator in statistics. Efron's bootstrap re-sampling may be used for statistical uncertainties.


Figure: Non-linear detector visible in 6D-network event weights $\mathcal{E}(=w)$ versus pion track pseudorapidity $\eta$. Setup described in the paper.


Figure: 6D-Network output weight $\mathcal{E}(=w)$ statistics example.

Generated


Reconstructed


Ratio: Reconstructed / Generated


DeepEfficiency-6D


Ratio: DeepEfficiency-6D / Generated


Figure: [GENERATED, RECONSTRUCTED, INVERTED]: 6D-Network inversion in terms of single pion track $(\eta, \phi)$. Stripes propagate from the inactive regimes of the inner most silicon detector layer. Train sample size $<10$ million events. Quite solid inversion of sharp discontinuities.


Figure: 6D-Network inversion of low-mass $K^{+} K^{-}$exclusive QCD diffraction events with $\chi^{2} /$ bin $=1.2$. Train sample size $<10$ million events. Fiducial domain: kaon $p_{t}>0.15 \mathrm{GeV},|\eta|<0.9$.


Figure: 6D-Network inversion of low-mass $\pi^{+} \pi^{-}$exclusive QCD diffraction events with $\chi^{2} / \operatorname{bin}=0.8$. Train sample size $<10$ million events. Seemingly easy case, differentially flat observable within selected fiducial domain: pion $p_{t}>0.15 \mathrm{GeV},|\eta|<0.9$.

## POSITIVE FEATURES

© Maximally MC event generator independent efficiency corrections due to high dimensional inversion $\Rightarrow$ can use even pure phase space generator (to illustrate the point, in practise not smart/possible always)
A Can take highly complicated experimental correlations into account, such as complex trigger etc.
© Arbitrary observables can be efficiency corrected

## NEGATIVE FEATURES

■ Practical performance is limited, of course, by the MC sample sizes, network structure etc.
■ Pure acceptance holes inside the fiducial domain need to taken into account with an additional algorithm, cannot divide null by 0

## UNIVERSAL

- Bias-Variance tradeoff theorem; no free lunch (in general)

Bias: over/undershooting the efficiency correction differentially
Variance: anomalous fluctuations in the efficiency correction weights give fluctuations in observables

# After DeepEfficiency 

## Unsolved Neural Theory

(Riemannian geometry, statistical mechanics, information theory, topology, new math needed?)

- There is no really deep (useful) theory of generic deep neural networks - thus, the optimality claims here are formal, of course - relying on the universal approximator lemma \& 'neural engineering'
- Depth vs width (series vs parallel), type of non-linearity, architecture (feed-forward, convolution, recursive loops ...), gradient descent methods
- How to use Vapnik-Chervonenkis dimension: 'the theoretical capacity of a statistical learning algorithm' in practise?


# Unsolved Algorithms for Theory and Experiment 

- Detector bias/resolution unfolding in higher dimensions $\mathbb{R}^{D} \rightarrow \mathbb{R}^{D}$ (quite difficult), related to super-resolution etc.
- Efficient high dimensional Monte Carlo integration and event generation, beyond VEGAS, multichanneling and hand-engineered Jacobians. For work towards solving this, see: Bendavid, arXiv:1707.00028; better in Müller et al, arXiv:1808.03856
- Neural Scattering Amplitudes (think about GAN-like generator networks). Use for probing theory landscapes beyond Lagrangian descriptions and perturbation theory more powerful re-visit of the 1960's S-matrix era?


## Conclusions

A new efficiency inversion algorithm for precision fiducial measurements using fully differential (multidimensional) final state kinematics
$\Rightarrow$ can be used also with likelihood analyses such as the matrix element method, (fast) simulations, replacing other efficiency parametrizations

Full code at <github.com/mieskolainen>


[^0]:    ${ }^{1}$ Your problem may extend to include heavy unfolding/deconvolution type of corrections of detector resolution/bias, algorithmically since 1970's.

[^1]:    ${ }^{2}$ Usually handled by dumping into systematics by varying the event generators (even if they use in essence the same model...).

[^2]:    ${ }^{3}$ You find this expansion algorithm in my GRANIITTI engine, <github.com/mieskolainen/graniitti>

[^3]:    ${ }^{4}$ Difficult non-convex optimization problem

[^4]:    ${ }^{5}$ Basically, this is an extension of Logistic Regression, both well known in machine learning.

