Inference-Aware Neural Optimisation (INFERNO)

ML-INFN Meeting

Pablo de Castro, Tommaso Dorigo,
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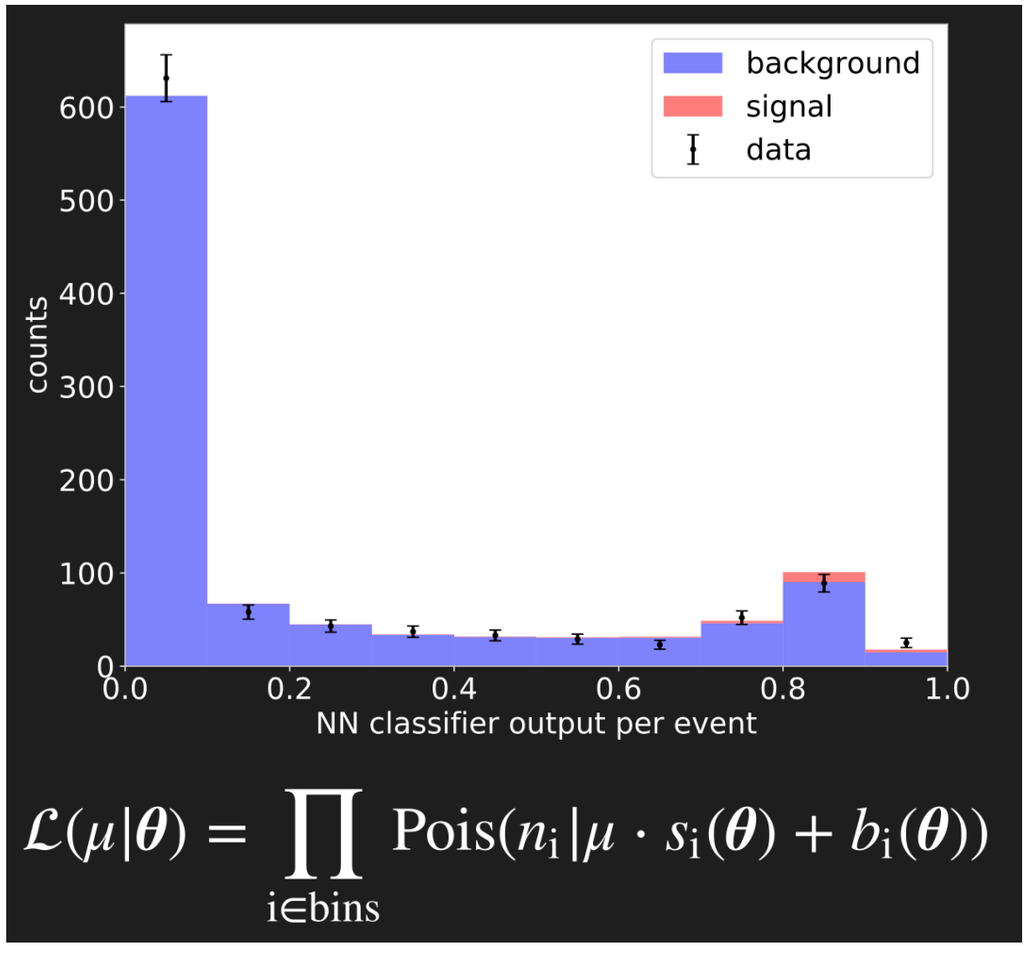
Problem Statement

Our data is high dimensional.
How do we choose the best summary statistics for the inference of the parameter of interest?

Classical approach in HEP

- **Signal vs. background classification** with simulated samples by minimizing **Binary Cross-Entropy** of **Neural Networks** to approximate the optimal Likelihood Ratio

- Inference with **histograms** by building binned non-parametric **Poisson counts likelihood**



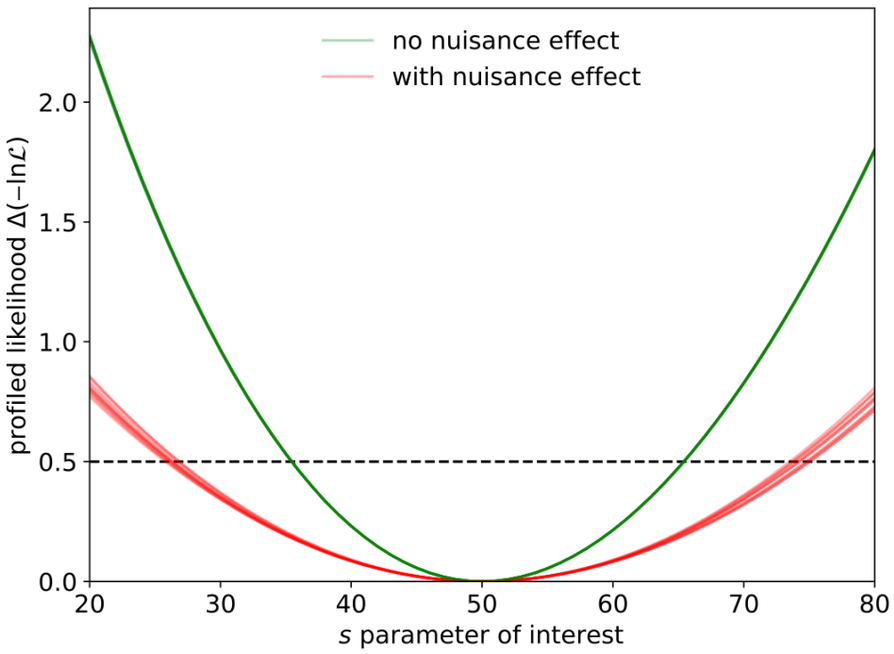
Problem Statement

Our data is high dimensional.
How do we choose the best summary statistics for the inference of the parameter of interest?

- Problem: **simulations** are **imperfect** → lack of knowledge for inference accounted by additional **nuisance parameters**

- Neglecting nuisance parameters in the training process leads to **larger** measurement **uncertainties**

- **Upper limit** of ML usefulness in LHC analyses



Idea: include nuisance parameters in the loss function of a Neural Network and directly minimize variance of POI

INFERNO

Overview

- **Inference-Aware Neural Optimization** developed by **Pablo de Castro** and **Tommaso Dorigo:** P. de Castro Manzano, T. Dorigo, “INFERNO: Inference-Aware Neural Optimization”, Comp. Phys. Commun. 244 (2019) 170; https://doi.org/10.1016/j.cpc.2019.06.007

- **Objective**: optimize statistical **inference** in the presence of **nuisance parameters** by learning non-linear **summary statistics** with neural networks via minimization of an **inference-motivated loss**

- Code written in **TF 1.x** (https://github.com/pablodecm/paper-inferno) → key elements reproduced in **TF 2.x** (https://github.com/llayer/inferno)

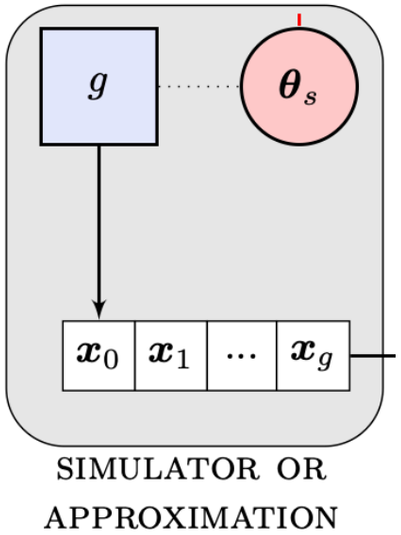
Summary statistics with INFERNO

- “Standard HEP summary statistics” **histograms** are not differentiable → **softmax** as differentiable approximation

- **Nuisance parameters approximated** by changes of mixture coefficients, translations of a subset of features, or conditional density ratio re-weighting → restricted to **likelihood-free inference** problems

$$\hat{s}_i(D;\phi) = \sum_{x \in D} \frac{e^{f_i(x;\phi)/\tau}}{\sum_{j=0}^{b} e^{f_j(x;\phi)/\tau}}$$

Algorithm



Algorithm 1 Inference-Aware Neural Optimisation.

Input 1: differentiable simulator or variational approximation $g(\boldsymbol{\theta})$.
Input 2: initial parameter values $\boldsymbol{\theta}_s$.
Input 3: parameter of interest $\omega_0 = \theta_k$.
Output: learned summary statistic $\boldsymbol{s}(D; \boldsymbol{\phi})$.

Taken from https://arxiv.org/pdf/1806.04743.pdf

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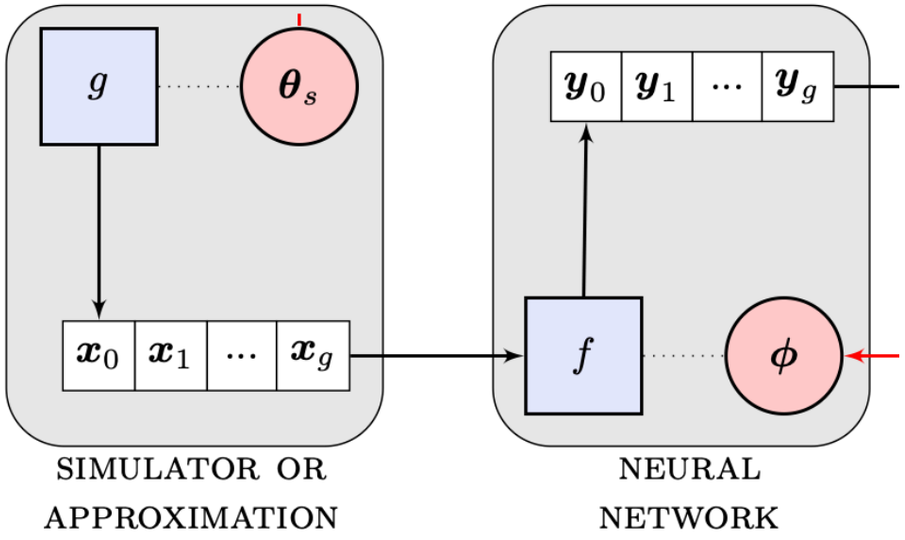

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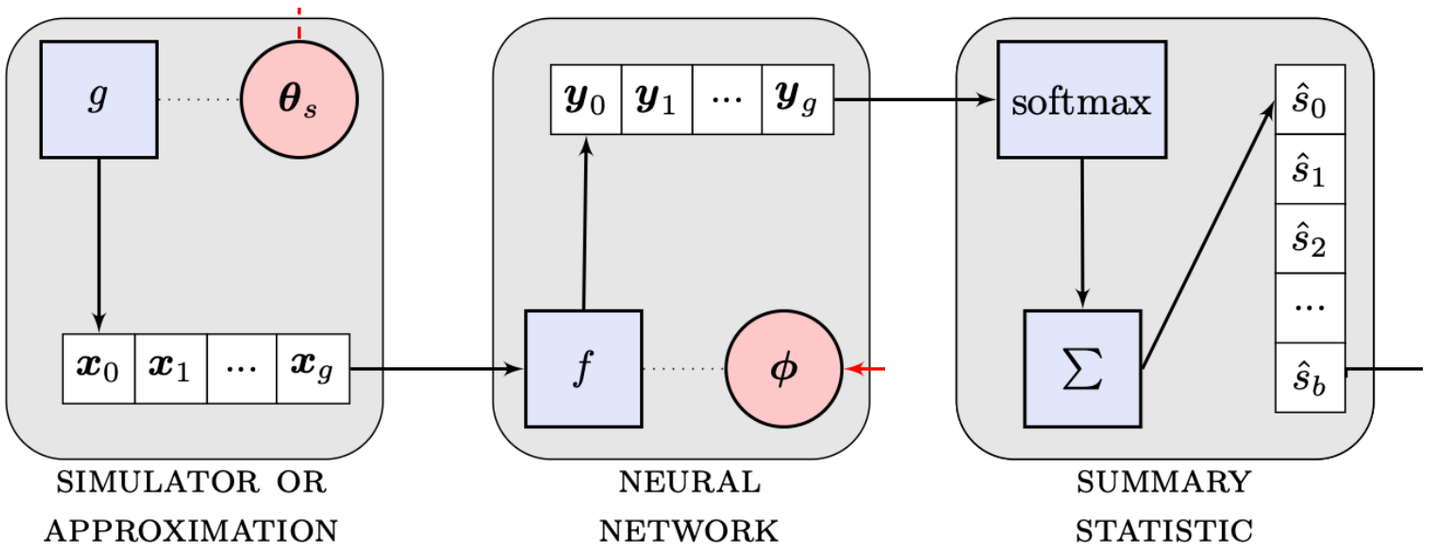

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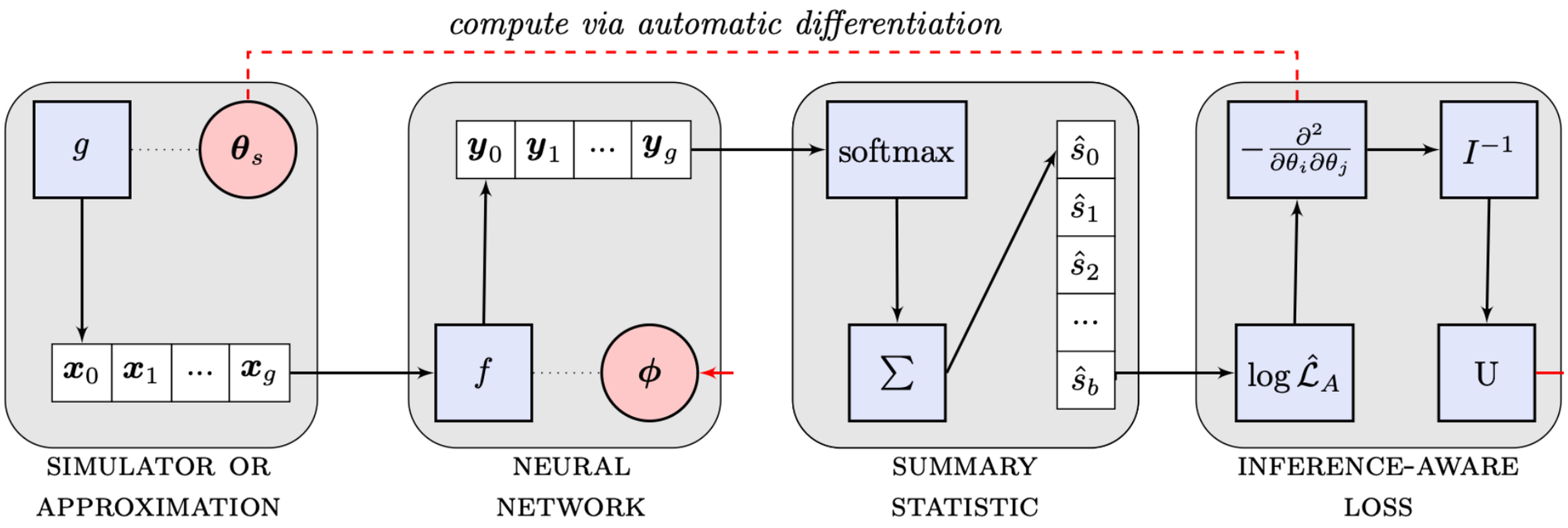

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for $i = 1$ to N **do**
  Sample a representative mini-batch G_s from $g(\boldsymbol{\theta}_s)$.
  Compute differentiable summary statistic $\hat{\mathbf{s}}(G_s; \boldsymbol{\phi})$.
  Construct Asimov likelihood $\mathcal{L}_A(\boldsymbol{\theta}, \boldsymbol{\phi})$.
  Get information matrix inverse $I(\boldsymbol{\theta})^{-1} = \boldsymbol{H}_{\boldsymbol{\theta}}^{-1}(\log \mathcal{L}_A(\boldsymbol{\theta}, \boldsymbol{\phi}))$.
  Obtain loss $U = I_{kk}^{-1}(\boldsymbol{\theta}_s)$.

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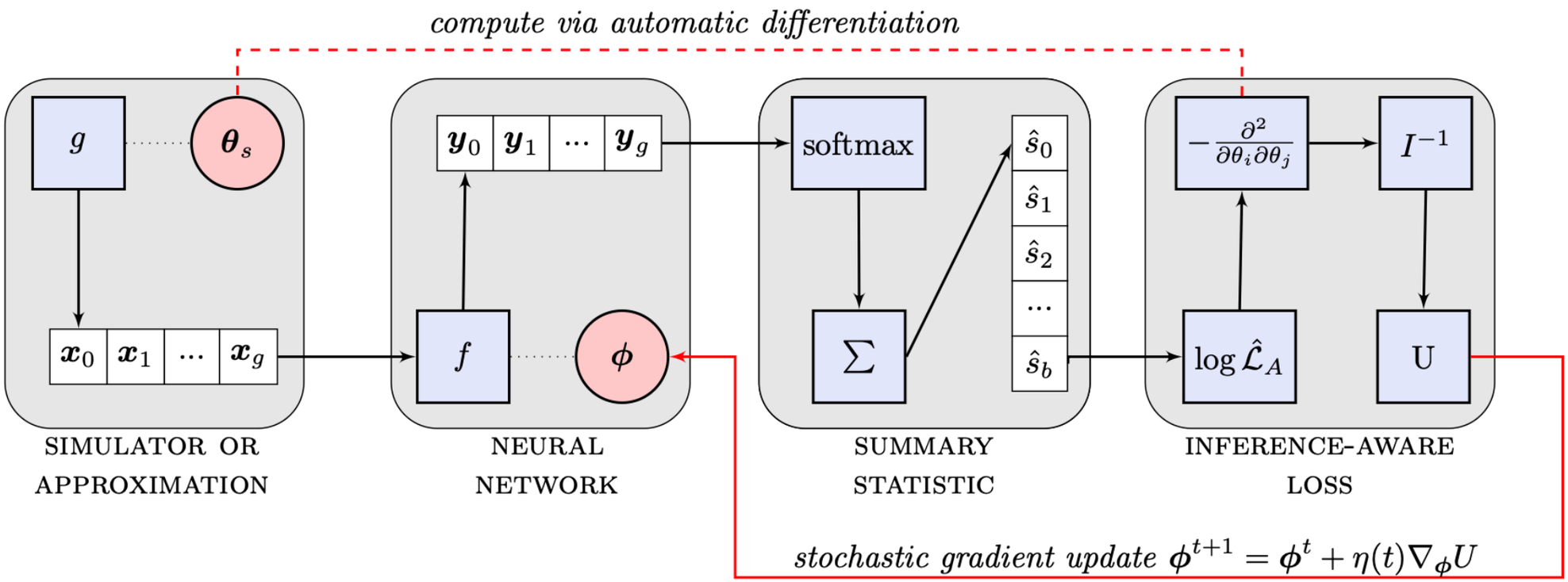

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6: Obtain loss $U = I_{kk}^{-1}(\boldsymbol{\theta}_s)$.
7: Update network parameters $\boldsymbol{\phi} \rightarrow \text{SGD}(\nabla_{\boldsymbol{\phi}}U)$.
8: **end for**

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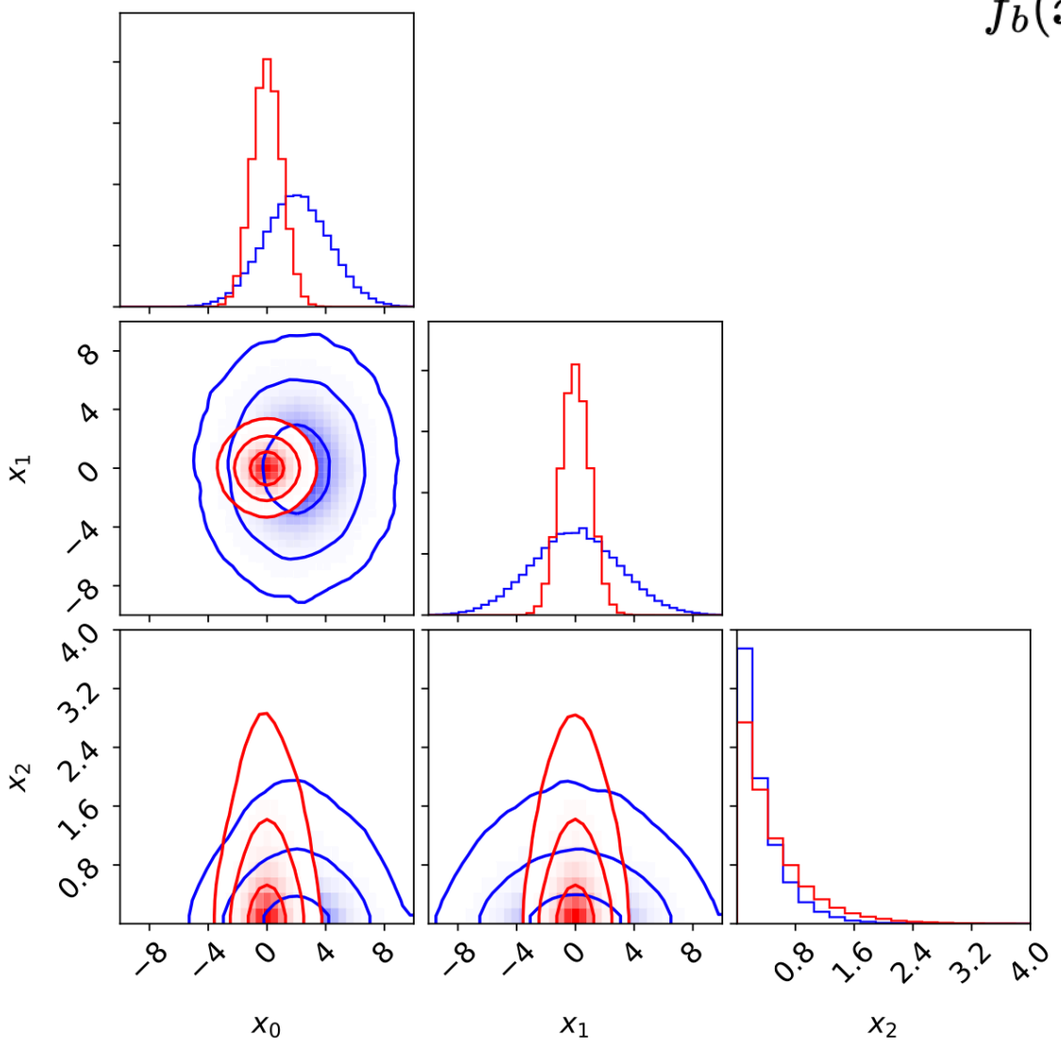
Application to 3D Synthetic Mixture model



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Model

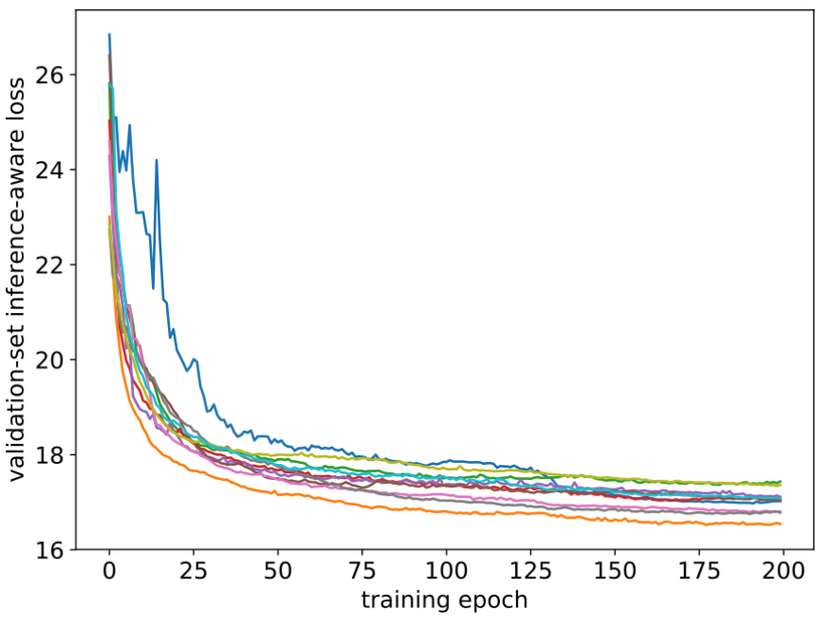
$$f_b(\boldsymbol{x}|r,\lambda) = \mathcal{N}\left((x_0,x_1)\,\middle|\,(2+r,0),\begin{bmatrix}5 & 0\\ 0 & 9\end{bmatrix}\right) Exp(x_2|\lambda)$$

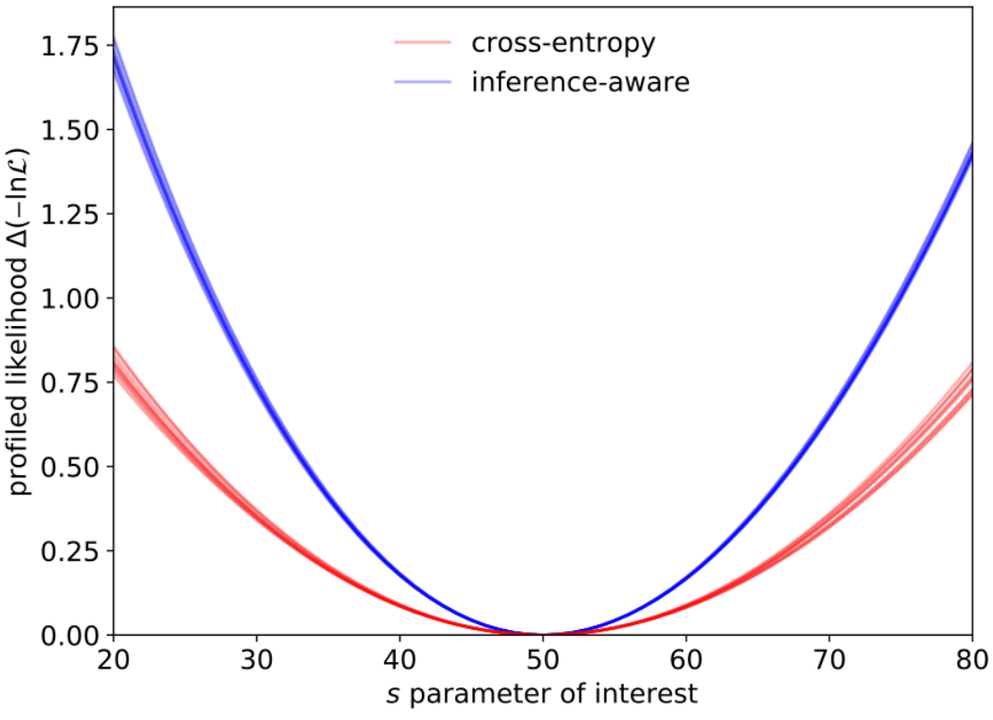
$$f_s(\boldsymbol{x}) = \mathcal{N}\left((x_0,x_1)\,\middle|\,(1,1),\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\right) Exp(x_2|2)$$

$$p(\boldsymbol{x}|\mu,r,\lambda) = (1-\mu)f_b(\boldsymbol{x}|r,\lambda) + \mu f_s(\boldsymbol{x})$$

- 3D Mixture model: 2D Multivariate Normal and 1D Exponential
- Signal distribution is fully specified
- Background distribution depends on the parameters r (shift of the 2D Normal mean) and λ (rate of the exponential)

Results for the synthetic model





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Comparison of inference with INFERNO summary statistics and classical binary cross-entropy summary statistics

- **Confidence intervals** considerably **narrower** with INFERNO than those using BCE and closer to those expected when using the true model
- **Improvement** over standard classification increases with **more nuisance parameters**
- The inference-aware summary statistics learnt for $\boldsymbol{\theta}_S$ work well when $\boldsymbol{\theta}_{true} \neq \boldsymbol{\theta}_S$ in the range of variation explored.

Benchmarks

- Several inference problems are considered based on the 3D benchmark mixture model
- Systematic comparison, shows that **INFERNO** clearly **outperforms any classifier** (even optimal Bayes) when nuisance parameters are relevant

Table 1: Expected uncertainty on the parameter of interest s for each of the inference benchmarks considered using a cross-entropy trained neural network model, INFERNO customised for each problem and the optimal classifier and likelihood based resuls.

	Benchmark 0	Benchmark 1	Benchmark 2	Benchmark 3	Benchmark 4
NN classifier	$14.99^{+0.02}_{-0.00}$	$18.94^{+0.11}_{-0.05}$	$23.94^{+0.52}_{-0.17}$	$21.54^{+0.27}_{-0.05}$	$26.71^{+0.56}_{-0.11}$
INFERNO 0	$\mathbf{15.51^{+0.09}_{-0.02}}$	$18.34^{+5.17}_{-0.51}$	$23.24^{+6.54}_{-1.22}$	$21.38^{+3.15}_{-0.69}$	$26.38^{+7.63}_{-1.36}$
INFERNO 1	$15.80^{+0.14}_{-0.04}$	$\mathbf{16.79^{+0.17}_{-0.05}}$	$21.41^{+2.00}_{-0.53}$	$20.29^{+1.20}_{-0.39}$	$24.26^{+2.35}_{-0.71}$
INFERNO 2	$15.71^{+0.15}_{-0.04}$	$16.87^{+0.19}_{-0.06}$	$\mathbf{16.95^{+0.18}_{-0.04}}$	$16.88^{+0.17}_{-0.03}$	$18.67^{+0.25}_{-0.05}$
INFERNO 3	$15.70^{+0.21}_{-0.04}$	$16.91^{+0.20}_{-0.05}$	$16.97^{+0.21}_{-0.04}$	$\mathbf{16.89^{+0.18}_{-0.03}}$	$18.69^{+0.27}_{-0.04}$
INFERNO 4	$15.71^{+0.32}_{-0.06}$	$16.89^{+0.30}_{-0.07}$	$16.95^{+0.38}_{-0.05}$	$16.88^{+0.40}_{-0.05}$	$\mathbf{18.68^{+0.58}_{-0.07}}$
Optimal classifier	14.97	19.12	24.93	22.13	27.98
Analytical likelihood	14.71	15.52	15.65	15.62	16.89

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Future of INFERNO

Applications

- Application of INFERNO to a real world CMS analysis
- Optimizations of detector designs
- Development of a common package across experiments

Computational needs

- Training and optimization needs powerful GPUs
- Data preprocessing and ML will benefit from Spark / Kubernetes clusters
- Ideally move entirely to cloud computing

Summary

- INFERNO shows promising performance on toy problems

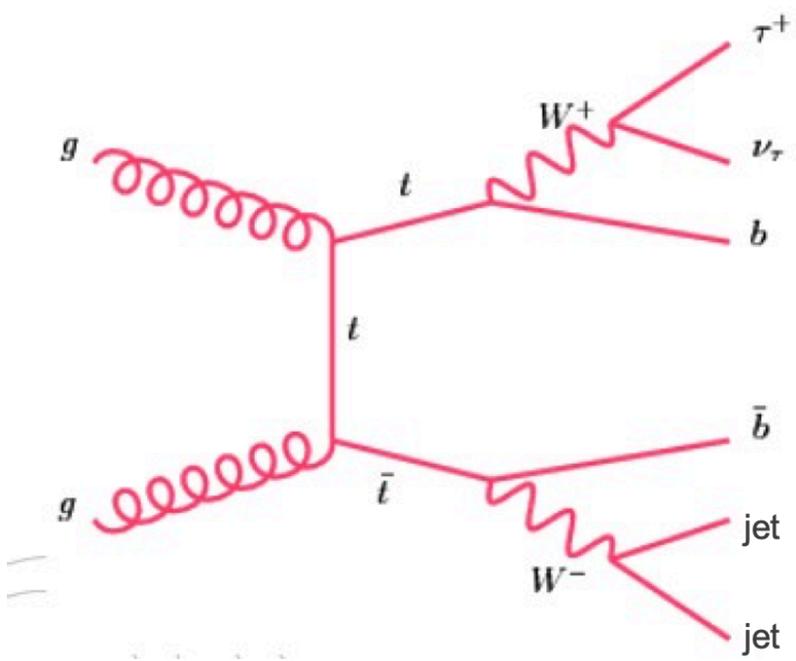
- Several advanced applications of INFERNO are planned / have started

- Need for powerful hardware

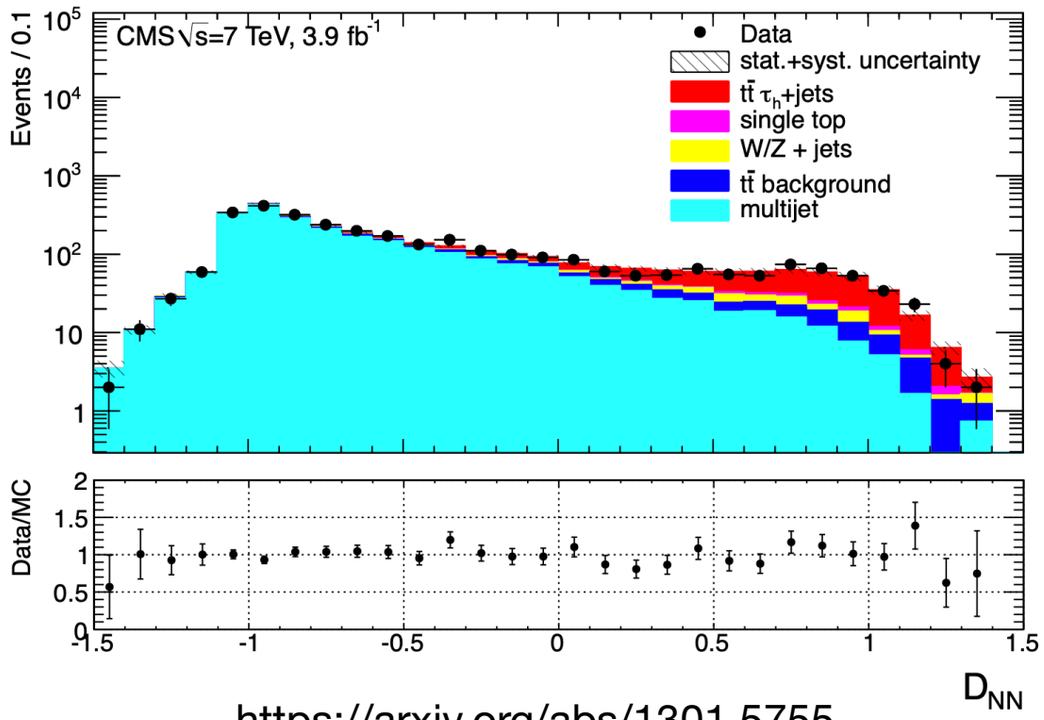
BACKUP

Top pair cross section with CMS open data

TOP-11-004 - Top pair cross section in tau+jets



σ(tt) = 152 ± 12 (stat.) ± 32 (syst.) ± 3 (lum.) pb



https://arxiv.org/abs/1301.5755

- Replication of full TOP-11-004 with CMS open data including systematics
- Relevant 2011 legacy samples available for Data and MC
- Analysis dominated by systematic uncertainties and uses a ANN with TMVA
- Simple analysis, but can be made more challenging by analyzing more decay channels

Status: implemented basic framework to analyze CMS open data with full systematic uncertainties

Recent related work on differentiable analysis

Work by S. Wunsch et. al (CMS)

- **Optimal statistical inference** in the presence of **systematic uncertainties** using neural network optimization based on **binned Poisson likelihoods** with **nuisance parameters** (https://arxiv.org/abs/2003.07186)

- **Idea**: construct binned Poisson Likelihood by using **histograms** and **approximate the gradient** of the bin function by the **derivative of a Gaussian** → avoids the softmax approximation

Work by N. Simpson, L. Heinrich et. al (ATLAS)

- **Idea**: optimize neural networks with **differentiable profile likelihood** in the loss function via **fixed-point differentiation** → allows to directly **optimize CLs limits**

- Library ***neos*** based on autodiff library **JAX** and library **FAX** for differentiating fixed point problems in JAX

https://github.com/pyhf/neos

HSF activity for differentiable analysis

- New **HSF activity** for differential analysis related to various HEP problems **across experiments**

- Discussion channel for the community on gitter