# Accelerating HEP theory with ML models

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### Why talk about machine learning?

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#### because

- it is an essential set of algorithms for building models in science,
- fast development of new tools and algorithms in the past years,
- nowadays it is a requirement in experimental and theoretical physics,
- large interest from the HEP community: IML, conferences, grants.

### When apply machine learning in theoretical physics?

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when:

- Ambiguous choices.
- Lack of information.

- Interpolation, sampling.
- Performance acceleration.

### Machine learning algorithms

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• Supervised learning: regression, classification, ...





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- Unsupervised learning: clustering, dim-reduction, ...



#### **Unsupervised learning**



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- Unsupervised learning: clustering, dim-reduction, ...
- Reinforcement learning: real-time decisions, ...



#### **Reinforcement learning**



### ML in HEP

Some remarkable examples are:

- Signal-background detection: Decision trees, artificial neural networks, support vector machines.
- Jet discrimination:

Deep learning imaging techniques via convolutional neural networks.

• HEP detector simulation:

Generative adversarial networks, e.g. LAGAN and CaloGAN.



### Some examples of ML in HEP theory

#### Supervised learning:

- The structure of the proton at the LHC\*
- Theoretical prediction and combination
- Monte Carlo reweighting techniques\*
- BSM searches and exclusion limits
- Generative models (GANs)\*

#### **Unsupervised learning:**

- Clustering and compression
- Density estimation and anomaly detection
- Monte Carlo integration\*

#### **Reinforcement learning:**

Jet grooming\*



## **ML** and Parton Density functions

### Parton density functions

The **parton** model was introduced by Feynman in 1969 in order to characterize **hadrons** (*e.g.* protons and neutrons) in QCD processes and interactions in high energy particle collisions.



Partons are quarks and gluons characterized by a probability density functions of its nucleon momentum.

### Perturbative calculations

#### The Feynman Parton Model





- Photon probes the proton by striking a free massless "parton" (quark, gluon) that carries a fraction x of its parent proton.
- Value of x is fixed by final-state kinematics.
- Cross-section proportional to probability  $q_i(x)$  of finding parton of species i with momentum-fraction x in target proton.

### Perturbative QCD





- The Parton Model is the first order of a perturbative expansion
- PDFs are not calculable: reflect non-perturbative physics of confinement.
- **PDFs** are **essential** for a **realistic computation** of any particle physics **observable**, *σ*, thanks to the factorization theorem

$$\sigma = \hat{\sigma} \otimes f,$$

where the elementary hard cross-section  $\hat{\sigma}$  is convoluted with f the PDF.

• Can be proven rigorously using the OPE (Wilson expansion).

Factorization theorem is applied to several processes:



PDFs are extracted by comparing theoretical predictions to real data.

#### Parton density functions

- PDFs are **necessary** to determine theoretical predictions for **signal/background** of experimental **measurements**.
  - e.g. the Higgs discovery at the LHC:



### **PDF** uncertainties

PDF determination requires a sensible estimate of the **uncertainty**, and not only the central value, so not a well researched topic in ML.

CERN Yellow Report 4 (2016)



PDF uncertainties are a **limiting** factor in the accuracy of theoretical predictions for several processes at LHC.

 $\Rightarrow$  Need of **precise** PDF determination and **uncertainty** estimate.

#### Parton density functions

#### Historical examples of the first PDF models:



#### where

- PDFs are very simple functional forms (polynomials).
- PDFs are constrained by few data points and low order theory.
- No uncertainties are provided.
- No cross-validation methods are implemented.

#### Parton density functions

**Possible improvement:** use ML in PDF determination. **NNPDF** (Neural Network PDFs) created **10 years ago**.



### Why ML in PDFs determination?

 PDFs are essential for a realistic computation of hadronic particle physics observable, σ, thanks to the factorization theorem, e.g. in pp collider:

$$\underbrace{\sigma_X(s, M_X^2)}_{Y} = \sum_{a, b} \int_{x_{\min}}^1 dx_1 dx_2 \underbrace{\hat{\sigma}_{a, b}(x_1, x_2, s, M_X^2)}_{X} f_a(x_1, M_X^2) f_b(x_2, M_X^2),$$

where the elementary hard cross-section  $\hat{\sigma}$  is convoluted with f the PDF.

•  $f_i(x_1, M_X^2)$  is the PDF of parton *i* carrying a fraction of momentum *x* at scale  $M \Rightarrow$  needs to be learned from data.

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- $f_i(x_1, M_X^2)$  is the PDF of parton *i* carrying a fraction of momentum *x* at scale  $M \Rightarrow$  needs to be learned from data.
- Constraints come in the form of convolutions:

$$X \otimes f \to Y$$

- Experimental data points is ~5000  $\rightarrow$  not a big data problem
- Data from several process and experiments over the past decades
  ⇒ deal with data inconsistencies

The NNPDF (Neural Networks PDF) implements the Monte Carlo approach to the determination of a global PDF fit. We propose to:

- 1. reduce all sources of theoretical bias:
  - no fixed functional form
  - possibility to reproduce non-Gaussian behavior
  - $\Rightarrow$  use Neural Networks instead of polynomials
- 2. provide a sensible estimate of the uncertainty:
  - uncertainties from input experimental data
  - minimization inefficiencies and degenerate minima
  - theoretical uncertainties

 $\Rightarrow$  use MC artificial replicas from data, training with a GA minimizer

3. Test the setup through closure tests

The total number of data points for the default PDF determination is

- 4175 at LO, 4295 at NLO and 4285 at NNLO.
- 7 physical processes from 14 experiments over ~30 years (deal with data inconsistencies)
- few data points at high and low x (deal with extrapolation)
- range of 5 and 7 orders of magnitude per PDF evaluation arguments  $(x,Q^2)$



Can we reduce the PDF input size? Yes, thanks to DGLAP:

$$f_i(x_\alpha, Q^2) = \Gamma(Q, Q_0)_{ij\alpha\beta} f_j(x_\beta, Q_0^2)$$

We remove the  $Q^2$  dependence from PDF determination thanks to the DGLAP evolution operator  $\Gamma.$ 

$$f(x,Q^2) \rightarrow f(x,Q_0^2) := f(x)$$

- Precompute the DGLAP operator for all data points
- Apply the operator to the partonic cross section
- Store the results and perform fast convolutions

In NNPDF theoretical predictions are stored in **APFELgrid** tables:

$$\sigma = \sum_{i,j}^{n_f} \sum_{\alpha,\beta}^{n_x} W_{ij\alpha\beta} f_i(x_\alpha, Q_0^2) f_j(x_\beta, Q_0^2)$$

In comparison to a typical ML problem, a PDF fit

- requires a statistically sound uncertainty estimate
- is a regression problem but complex dependence on PDFs
- must satisfy physical constrains:
  - $f(x) \rightarrow 0$  for  $x \rightarrow 1$  (continuity)
  - sum rules:

$$\sum_{i=1}^{n_f} \int_0^1 dx \, x f_i(x) = 1, \qquad \int_0^1 dx \, (u(x) - \bar{u}(x)) = 2$$

$$\int_0^1 dx \left( d(x) - \bar{d}(x) \right) = 1, \quad \int dx \left( q(x) - \bar{q}(x) \right) = 0, \ q = s, b, t$$

### **PDF** parametrizations

• Early models:

$$f_i(x) = A \cdot x^{\alpha} (1-x)^{\beta}$$

- parameters are chosen based on Hessian minimization approach
- Can a simple model provide a reliable uncertainty estimate?
- Can it deal with data inconsistencies?

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- NNPDF approach:

$$f_i(x, Q_0) = A \cdot x^{\alpha} (1 - x)^{\beta} N N(x)$$



- fully connected MLP (2-5-3-1)
- two sigmoid hidden layers and linear output layer
- x8 independent PDFs  $\Rightarrow$  296 free parameters

• We minimize the cost function:

$$\chi^{2} = \sum_{ij} (D_{i} - O_{i})\sigma_{i,j}^{-1}(D_{j} - O_{j})$$

- $D_i$  is the experimental measurement for point i
- $O_i$  the theoretical prediction for point  $i \ (= \bar{\sigma} \otimes f)$
- $\sigma_{ij}$  is the covariance matrix between points i and j with corrections for normalization uncertainties
- · supplemented by additional penalty terms for positivity observables

Generate artificial **Monte Carlo** data replicas from experimental data. We perform  $N_{\text{rep}}$  O(1000) fits, sampling pseudodata replicas:

$$D_i^{(r)} \to D_i^{(r)} + \text{chol}(\Sigma)_{i,j} \mathcal{N}(0,1), \quad i, j = 1...N_{\text{dat}}, r = 1...N_{\text{rep}}$$

We obtain  $N_{\rm rep}$  PDF replicas. No assumptions at all about the Gaussianity of the errors.

### PDF fit example

The procedure delivers a Monte Carlo representation of results:



The central value of observables based on PDFs are obtained with:

$$\langle \mathcal{O}[f] \rangle = \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \mathcal{O}[f_k]$$

### **Optimization algorithm**

The current approach is genetic optimization, based on nodal mutation probabilities and more recently the covariance matrix evolution strategy

$$w \to w + \eta \frac{r_{\delta}}{N_{\text{ite}}^{r_{\text{ite}}}}, \quad \eta = 15, \, r_{\delta} \sim U(-1, 1), \, r_{\text{ite}} \sim U(1, 0)$$

At each iteration, generate 80 mutants and select best mutant.

#### Advantages

- Simple to implement and understand.
- Good dealing with complex analytic behavior.
- Doesn't require evaluating the gradient.

#### Disadvantages

- May not be close to a global minimum.
- Requires many functions evaluations.
- Needs tuning.

## Stopping

We have cross-validation implemented:

- We split data in a training and validation set.
- Training fraction is 50%, different for each replica.
- We perform the GA on the training set for a fixed number of iterations O(30000).
- Stop at the minimum of the validation set, storing the parameters from the replica at that iteration.



#### **Closure tests**

- Assume that the underlying PDF is known, generate data, fluctuations around the prediction of the true PDF.
- Perform a fit and compare to underlying PDF.
- Check that the results are consistent.



#### W and Z production cross-sections at LHC 13 TeV



NNPDF3.1 have smaller PDF uncertainties than NNPDF3.0.

#### Higgs production cross-sections



Higgs production: WH associate production



Higgs production: ZH associate production



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# Towards deep learning PDFs
#### **Challenges:**

- How to increase fit performance speed?
  - faster fits  $\Rightarrow$  more fits
- How can we tune/learn the methodology?
  - select the best model for our data/theory

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Solution  $\Rightarrow$  move towards deep learning

- in terms software/technology
- in terms of **methodology**

PDF determination is a supervised learning problem thus we need to provide review for the following sectors:



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## The n3fit model



#### New features:

- Python/C++ implementation using TensorFlow
- Modular approach  $\Rightarrow$  easier and faster development
- Can vary all aspects of the methodology

## Performance benefits - time per replica



#### **Benefits**

- · Gain on speed and efficiency, less CPU hours for a fit
- Usage of new technologies  $\rightarrow$  hardware, libraries
- Usage of gradient descent optimization methods

 $\Rightarrow$  Possibility to learn and tune the methodology

# Learning the methodology

## How to determine the best methodology?



#### Perform hyperoptimization scans:

Neural Network	Fit options	
Number of layers (*)	Optimizer (*)	
Size of each layer	Initial learning rate (*)	
Dropout	Maximum number of epochs (*)	
Activation functions (*)	Stopping Patience (*)	
Initialization functions (*)	Positivity multiplier (*)	

- Optimize figure of merit: validation  $\chi^2$
- Use bayesian updating (hyperopt)

# The overfitting problem

Using validation set  $\chi^2$ :



The choice of the right figure of merit is important:

- **NNPDF** wiggles  $\rightarrow$  finite size , goes away as  $N_{\rm rep}$  grows
- N3PDF wiggles → overfitting, correlations training-validation data!

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 $\Rightarrow$  define a proper quality control criterion

# **Cross-Validation vs hyperoptimization**

Define a completely uncorrelated **Test Set** 



Optimize on weighted average of validation and test.

# **Removing overfitting**

#### Using test-validation set $\chi^2$ :



- No overfitting
- Greater stability
- Reduced uncertainties

	DIS only	Global
n3fit (new)	1.10	1.15
nnfit (old)	1.13	1.16

# **Quality control**

# **Chronological fits**

#### Idea:

- Take a pre-HERA dataset
- **2** Perform hyperoptimization
- ❸ Compare predictions to "future" data

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#### **Examples:**



⇒ Results within PDF uncertainty!

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  - Use k partitions in a rotation estimation for the Test Set
  - hyperoptimize the mean value of the Test Set  $\chi^2$



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 $\Rightarrow$  Compatible with our previous Test Set definition.

# Questions?

# ML and jet substructure

# Boosted jets at the LHC

High energy collisions at the LHC  $\Rightarrow$  **boosted objects**:

- particles such as  $W, Z, H, t, \ldots$  are produced with  $p_T^{\text{jet}} \gg m_{\text{jet}}$ ,
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**Problem:** identify hard structure of a jet from radiation patterns. (Jet from W, Z, H, t or QCD?)



# Jet grooming techniques

#### How to identify hard structure of a jet?

- Look at the mass of the jet.
- Remove distortion due to QCD radiation and pileup.

 $\textbf{Grooming goal} \Rightarrow \text{remove unassociated soft wide-angle radiation}.$ 

# Jet grooming techniques

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**Grooming goal**  $\Rightarrow$  remove unassociated soft wide-angle radiation.

# Jet grooming algorithms: modified MassDrop Tagger Dasgupta *et al.*, arXiv:1307.0007 Soft Drop (SD) Larkoski *et al.*, arXiv:1402.2657 Recursive Soft Drop (RSD) Dreyer *et al.*, arXiv:1804.03657





**①** Cast jet as clustering tree with nodes  $\mathcal{T}^{(i)}$  and children nodes a, b.



$$z = \frac{\min(p_{t,a}, p_{t,b})}{p_{t,a} + p_{t,b}}, \quad \Delta_{ab}^2 = (y_a - y_b)^2 + (\phi_a - \phi_b)^2$$



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**③** Evaluate policy ( $\beta$ ,  $z_{cut}$  and  $R_0$  are free parameters):

$$\pi_{\text{RSD}}(s_t) = \begin{cases} 0 & \text{if } z > z_{\text{cut}} \left(\frac{\Delta_{ab}}{R_0}\right)^{\beta} \\ 1 & \text{else} \end{cases}$$



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④ If  $\pi_{RSD}(s_t) = 1 \rightarrow$  remove softer branch and update jet tree, ⑤ If  $\pi_{RSD}(s_t) = 0 \rightarrow$  stop recursion.

#### Goal of this project?

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#### How?

• using Deep Reinforcement Learning (DRL) techniques.

A deep learning approach

#### Input data:

Generate jet events with Monte Carlo. Define a set of possible **states** in a five dimensional box:

$$s_t = \{z, \Delta_{ab}, \phi, m, k_t\}$$

#### Methodology:

Jet grooming is characterized by a policy and a sequential set of actions/cuts, so:

- Train a reinforcement learning agent which learns how to decide which action to take.
- Define an environment reward which motivates the agent to groom efficiently.

#### **Reinforcement learning**



# Choosing an DRL agent

#### Which agent?

 $\mathsf{Deep}\ Q\operatorname{\mathsf{-Network}}\to \mathsf{off}\operatorname{\mathsf{-policy}} \text{ and discrete action space}.$ 

A deep neural network maximizes the action-value quality function:

$$Q^{*}(s,a) = \max_{\pi} \mathbb{E} \left[ r_{t} + \gamma r_{t+1} + \gamma^{2} r_{t+2} + \dots | s_{t} = s, a_{t} = a, \pi \right]$$

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#### A simple example:

Playing ATARI games with DRL from Minh et al., arXiv:1312.5602, Nature'15:


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In practice we implement the DRL framework using:

- Python  $\in$  (Keras-RL, TensorFlow, OpenAI Gym, hyperopt)
- Public code available at https://github.com/JetsGame

# Environment

# Defining a jet grooming game:

Game score  $\Rightarrow$  reward function (next slides)

### Environment

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#### Game environment:

- 1 Initialize list of all trees for training.
- **2** Each episode starts by randomly selecting a tree and adding its root to a priority queue (ordered in  $\Delta_{ab}$ ).
- Each step removes first node from priority queue, then takes action on removal of soft branch based on s<sub>t</sub>.
- After action, update kinematics of parent nodes, add current children to priority queue, and evaluate reward.
- Episode terminates once priority queue is empty.



We construct a reward function based on two components:

$$R(m, a_t, \Delta, z) = R_M(m) + \frac{1}{N_{\mathrm{SD}}} R_{\mathrm{SD}}(a_t, \Delta, z)$$

so the DQN agent is motivated to:

- improve jet mass resolution  $\Rightarrow$  increase  $R_M$ ,
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The mass reward is defined using  
a Cauchy distribution:  
$$R_M(m) = \frac{\Gamma^2}{\pi \left(|m - m_{\text{target}}|^2 + \Gamma^2\right)}$$



# **Reward function**

The Soft-Drop reward is defined as

$$\begin{aligned} R_{\rm SD}(a_t, \Delta, z) &= a_t \min\left(1, e^{-\alpha_1 \ln(1/\Delta) + \beta_1 \ln(z_1/z)}\right) \\ &+ (1+a_t) \max\left(0, 1 - e^{-\alpha_2 \ln(1/\Delta) + \beta_2 \ln(z_2/z)}\right), \end{aligned}$$

so the DQN agent is motivated to:

- remove wide-angle soft radiation
- keep hard-collinear emissions



### What about background events?

Potential mass bias for background events  $\Rightarrow$  use multi-level training:

• add to the training set signal and background samples  $\Rightarrow$  500k W/QCD jets simulated with Pythia 8

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In the background case, the mass reward term is changed to:

$$R_M^{\rm bkg}(m) = \frac{m}{\Gamma_{\rm bkg}} \exp\left(-\frac{m}{\Gamma_{\rm bkg}}\right)$$



#### Free parameters to be determined:

- DQN architecture  $\Rightarrow$
- Reward parameters  $\Rightarrow$
- Learning parameters  $\Rightarrow$

(layers, nodes, activations, ...)  $(\alpha_{1,2}, \beta_{1,2}, z_{1,2}, \Gamma)$ (optimizer, learning rate, ...)

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#### How?

Use distributed asynchronous hyperparameter optimization  $\Rightarrow$  hyperopt.

**①** Create a validation set with 50k signal (W) and background (QCD) jets.

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  - the median  $w_{\mathrm{med}}$  in that interval.

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- Reward parameters  $\Rightarrow$
- Learning parameters  $\Rightarrow$

( $\alpha_{1,2}, \beta_{1,2}, z_{1,2}, \Gamma$ ) (optimizer, learning rate, ...)

### How?

Use distributed asynchronous hyperparameter optimization  $\Rightarrow$  hyperopt.

- **①** Create a validation set with 50k signal (W) and background (QCD) jets.
- 2 Derive groomed jet mass distribution from validation set and determine:
  - window  $(w_{\min}, w_{\max})$  containing 60% of signal distribution,
  - the median  $w_{\mathrm{med}}$  in that interval.

**③** Define  $f_{\text{bkg}}$  the fraction of groomed background sample  $(w_{\min}, w_{\max})$ :

$$\mathcal{L} = \frac{1}{5}|w_{\text{max}} - w_{\text{min}}| + |m_{\text{target}} - w_{\text{med}}| + 20f_{\text{fkg}}$$



# Results

Reward evolution during the training of the GroomRL for W bosons and top quarks:

- improvement during the first 300k epochs,
- stability after 300k epochs.



Parameters	Value
m <sub>target</sub>	$80.385~{\rm GeV}$ or $173.2~{\rm GeV}$
$s_t$ dimension	5
reward	Cauchy
Г	2  GeV
$(lpha_1,eta_1,\ln z_1)$	(0.59, 0.18, -0.92)
$(lpha_2,eta_2,\ln z_2)$	(0.65, 0.33, -3.53)
$1/N_{\rm SD}$	0.15
multi-level training	Yes
$\Gamma_{\rm bkg}$	$8 { m GeV}$
$1/N_{\rm bkg}$	1.8 or 1.0
$p_{ m bkg}$	0.48  or  0.2
learning rate	$10^{-4}$
Dueling NN	Yes
Double DQN	No
Policy	Boltzmann
$N_{\rm epochs}^{\rm max}$	500K
Architecture	Dense
Dropout	0.05
Layers	10
Nodes	100
Optimizer	Adam

TABLE I: Final parameters for GroomRL, with the two values of  $m_{\rm target}$  corresponding to the W and top mass.

















### **Optimal** GroomRL model for W jets

#### GroomRL-W tested on QCD, W and Top jet data



TABLE II: Size of the window containing 60% of the W mass spectrum, and median value on that interval.

## **Optimal** GroomRL model for W jets

#### GroomRL-Top tested on QCD, W and Top jet data



TABLE II: Size of the window containing 60% of the W mass spectrum, and median value on that interval.

# Lund jet plane density



#### Lund jet plane before and after applying GroomRL

Inspecting  $(\ln 1/\Delta_{ab}, \ln k_t) \Rightarrow$  soft and wide-angle radiation removed.

# Towards transfer learning in HEP

Some ideas towards the "transfer learning" concept:

**①** Generalize models trained on specific data to new datasets.

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• Generalize models trained on specific data to new datasets.

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  - e.g. CycleGANs
- S Models that propagate higher-order correction to lower order.
  - e.g. reweighting

#### [arXiv:1909.01359]

#### CycleGAN learns unpaired image-to-image mapping functions.



## Reinterpreting events with CycleGANs

Use CycleGAN to transform between two different jet datasets, e.g.

- parton-level simulation  $\leftrightarrow$  detector-level simulation
- $\bullet \ W \text{ jet } \leftrightarrow \mathsf{QCD} \text{ jet }$

Transformed events in good agreement with true sample.



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Use neural nets to adjust unknown higher-order resummation terms.

Use NLO-matched single-top + jet (STJ) from the POWHEG-MINLO formalism:

$$d\sigma_{\mathcal{M}} = \Delta(y_{12}) \left[ d\sigma_{\rm NLO}^{\rm STJ} - \Delta(y_{12}) |_{\bar{\alpha}_S} d\sigma_{\rm LO}^{\rm STJ} \right]$$

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**Solution:** fix at NNLL, fit  $A_2$  with a Neural Network-based tuning of degrees of freedom, and test universality at 8 TeV.

$$\ln \delta \Delta(y_{12}) = -2 \int_{y_{12}}^{Q_{bt}^2} \frac{dq^2}{q^2} \bar{\alpha}_S^2 \mathcal{A}_2(\Phi) \ln \frac{Q_{bt}^2}{q^2}$$

### MINLO *t*-channel single-top plus jet



# Accelerating MC with ML tools

# VEGAS integration algorithm and tensorflow

ML frameworks such as TensorFlow can help theoretical computations.

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- Distributed computation across multiple hardware accelerators.

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### Example: VegasFlow [arXiv:1909.01359]

Monte Carlo integration using Vegas algorithm and TensorFlow code.



# Thanks for your attention!