

Machine Learning for the precision determination of Parton Distribution Functions

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UNIVERSITÀ
DEGLI STUDI
DI MILANO



How to adult...



SHOP FOR A NEW TIE.



MAKE MACARONI



DO CARDIO.



DON'T LET THE EXISTENTIAL
DREAD SET IN.



DON'T LET IT SET IN.



VACUUM THE RUG.

How to be a mature physicist...



Measure Higgs couplings.



Search for WIMPs.



Improve PDFs
determination



DON'T LET THE EXISTENTIAL
DREAD SET IN.



DON'T LET IT SET IN.



Look for strings

Outline

① QCD in a nutshell

- The Standard Model & strong interactions
- Parton Distribution Functions
- Factorization theorem

② Machine Learning

- Motivation for Machine Learning
- Neural Networks & general strategy

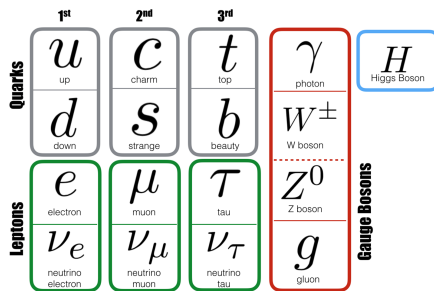
③ The N3PDF project

- The NNPDF methodology
- Operator implementation in TensorFlow
- Results & Conclusions

Quantum Chromodynamics in a nutshell

QCD in a nutshell

The Standard Model



Quantum Field Theory describing physics at the TeV scale

- 1 Fermions composing matter
- 2 Bosons mediating interactions
- 3 Scalar Higgs generating mass

QCD in a nutshell

Explore the strong interactions

How to explore proton's inner structure?

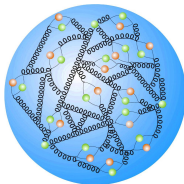
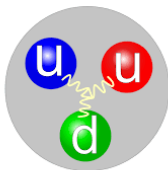


- Point-like projectile on the object \rightarrow DIS
- Smash the two objects \rightarrow LHC physics

"A way to analyze high energy collisions is to consider any hadron as a composition of point-like constituents \rightarrow **partons**" R.Feynman, 1969

QCD in a nutshell

Parton Distribution Functions



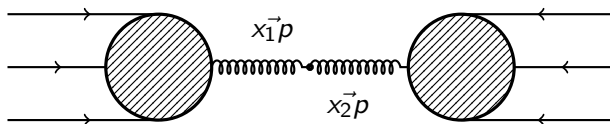
- Hadrons made of partonic objects \longrightarrow non perturbative physics
- Interactions take place only at partonic level

Parton Distribution Functions: probability distribution of finding a particular parton (u, d, ..., g) carrying a fraction x of the proton's momentum

QCD in a nutshell

Factorization theorem

Observables in hadronic events $\rightarrow \sigma$ is hard to compute



Factorize the problem \rightarrow Convolute the **PDFs** with the partonic $\hat{\sigma}_{ij}$

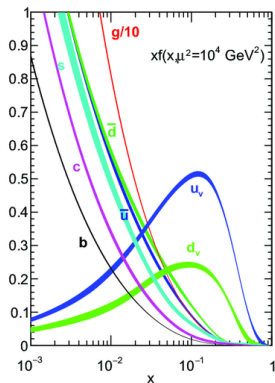
$$\sigma = \int_0^1 dx_1 dx_2 f_{\alpha}(x_1, \mu_F) * f_{\beta}(x_2, \mu_F) * \hat{\sigma}_{\alpha\beta}(\alpha_s(\mu_R), \mu_F)$$

- Partonic $\hat{\sigma}$ can be computed as perturbative series in α_s
- **PDFs** absorb the non perturbative effects, evaluated at μ_F

QCD in a nutshell

What PDFs look like

- Each parton has a different PDF
 $u(x)$, $d(x)$, ..., $g(x)$
- PDFs are not predicted, and can not be measured
- PDFs are **extracted** from data



Machine Learning

Machine learning

A hot topic at IFAE

TITLE: Searches for new phenomena at the LHC using machine-learning techniques

TITLE: Design and performance study of machine learning techniques for the ATLAS experiment event selection at the High-Luminosity LHC

TITLE: Enhanced ATLAS Level-1 trigger capabilities with Artificial-Intelligence regression on Field-Programmable Gate Array architecture.

TITLE: Unraveling New Physics effects in rare B decays using Neural Networks

Machine learning

What is Machine Learning?

- 1 A subset of Artificial Intelligence (AI) algorithms
- 2 Used to solve *complex* tasks like classification and regression
- 3 Rely on comparison with data → **Learning**



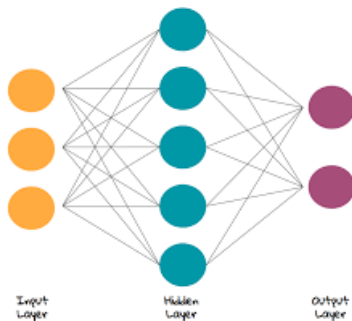
Machine learning

Building a ML model



Machine learning

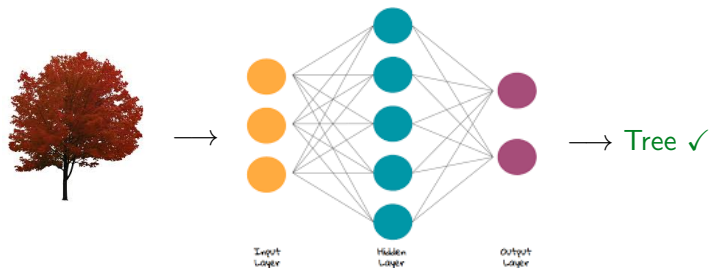
Building a ML model



- 1 Turn the input set into an array and build a **random** prediction
- 2 Compare with truth and compute a **Loss** function
- 3 Update the parameters in a specific way

Machine learning

Building a ML model



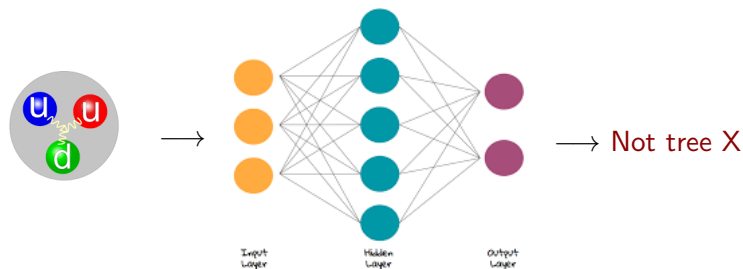
Machine learning

Building a ML model



Machine learning

Building a ML model



Machine learning

Building a ML model



Machine Learning

Loss function

$$Loss = \underbrace{\begin{pmatrix} y_1^{true} \\ y_2^{true} \\ \vdots \\ y_n^{true} \end{pmatrix}}_{y_{true}} - \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{y_{pred}}$$

- 1 Compute a loss function

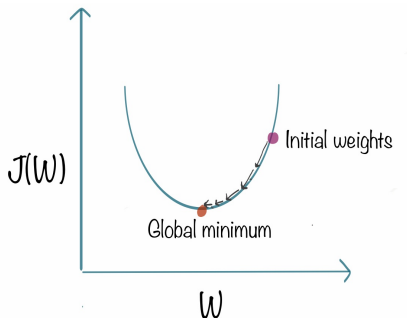
$$L = \sum_{i=1}^N (y_i^{true} - y_i^{pred})^2$$

- 2 Perfect prediction will mean $L = 0$

Machine Learning

Loss function

- 1 Loss is a function of weights and bias $L = L(w, b)$
- 2 Compute gradient $\nabla_{w_{ij}} L$ to look for the minimum of L



Machine Learning

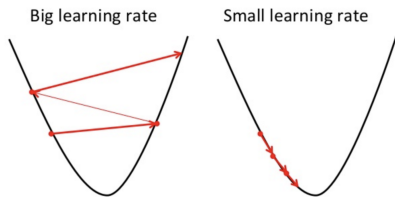
Update rule

Update the parameters of the network following the gradient descend

$$w_{ij} \longrightarrow w_{ij} - \alpha \nabla L$$

$$b_i \longrightarrow b_i - \alpha \nabla L$$

Where α is the learning rate



The N3PDF project

Machine Learning for the precision determination of PDFs

The N3PDF project

The NNPDF methodology

Factorize the problem \longrightarrow Convolute the PDFs with the partonic $\hat{\sigma}_{ij}$

$$\sigma = \int_0^1 dx_1 dx_2 f_{\alpha}(x_1, \mu_F) * f_{\beta}(x_2, \mu_F) * \hat{\sigma}_{\alpha\beta}(\alpha_s(\mu_R), \mu_F)$$

- Partonic $\hat{\sigma}_{\alpha\beta}$ is computed perturbatively. Hadronic σ is measured.
- Use a Neural Networks to generate (*fit*) the PDFs
- Generate a vector of observables σ_N to be compared with data

$$\sigma_N = \sum_{i,j,\alpha,\beta} f_{\alpha}(x_i) f_{\beta}(x_j) \hat{\sigma}_{Nij\alpha\beta}$$

The N3PDF project

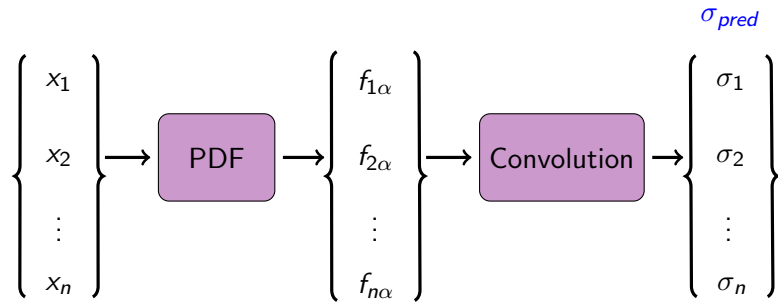
General structure of n3fit



- Use TensorFlow and Keras to determine the PDFs
- See paper by S.Carraza - J.Cruz-Martinez
"Towards a new generation of parton densities
with deep learning models",
<https://arxiv.org/abs/1907.05075>

The N3PDF project

General structure of n3fit

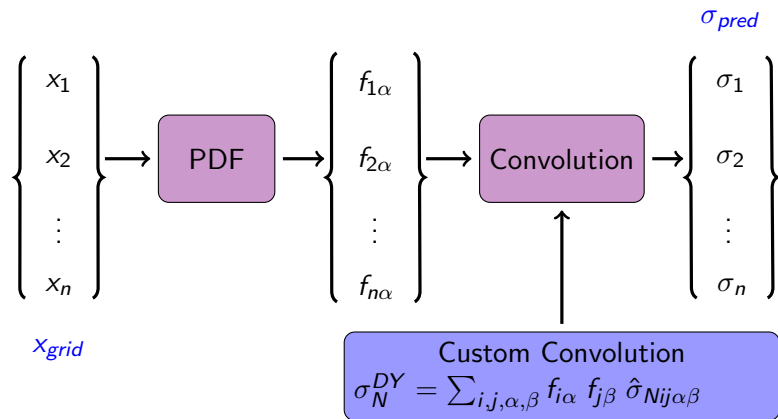


x_{grid}

- 1 Build a NN to compute σ_{pred} observables from a grid x_i
- 2 Compute χ^2 loss function by comparing with data
- 3 Update values of PDF \rightarrow Fit

The N3PDF project

Operator implementation



- 1 TF relies in symbolic computation \rightarrow High memory usage
- 2 Implement c++ operator replacing the convolution

Results

Checking computation

DIS:

	TensorFlow	Custom	Ratio
Convolution	1.9207904	1.9207904	1.0000000
	2.4611666	2.4611664	0.9999999
	1.3516952	1.3516952	1.0000000
Gradient	1.8794115	1.8794115	1.0000000
	1.505316	1.505316	1.0000000
	2.866085	2.866085	1.0000000

Results

Checking computation

Hadronic:

	TensorFlow	Custom	Ratio
Convolution	8.142365	8.142366	1.0000001
	8.947762	8.947762	1.0000000
	7.4513326	7.4513316	0.9999999
Gradient	18.525095	18.525095	1.0000000
	19.182995	19.182993	0.9999999
	19.551006	19.551004	0.9999999

Results

Memory saving

Hadronic only:

	TensorFlow	Custom Convolution	Diff
Virtual	17.7 GB	13.8 GB	3.9 GB
RES	12.1 GB	8.39 GB	3.2 GB

Global:

	TensorFlow	Custom Convolution	Diff
Virtual	23.5 GB	19.7 GB	3.8 GB
RES	18.4 GB	12.5 GB	5.9 GB

"Towards hardware acceleration for parton densities estimation",
<https://arxiv.org/abs/1909.10547>

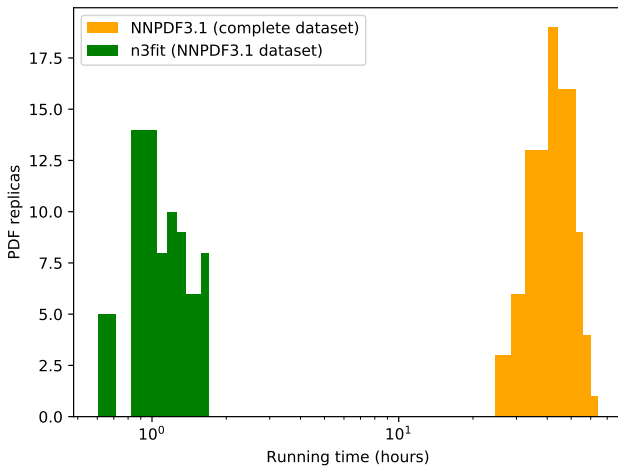
Summary & Conclusions

- ① PDFs are required to have accurate predictions in high energy physics
- ② ML provides a new way of determine the PDFs
- ③ Operator implementation leads to memory saving by taking full control on the computation

Thank you!



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Back up

TF computation of the gradient

- 1 Computing gradient of the χ^2 loss with respect to all parameters of the network.

$$\nabla \chi^2 \longrightarrow \frac{\partial \chi^2}{\partial x_i}$$

- 2 TF requires the gradient with respect to any operation in the model.

$$\frac{\partial \chi^2}{\partial x_i} = \frac{\partial \chi^2}{\partial \mathbf{Op}} \frac{\partial \mathbf{Op}}{\partial f_{\mu\nu}} \cdots \frac{\partial f_{\mu\nu}}{\partial x_i}$$

- 3 TF does not know the structure of **Op**. Compute manually the gradient $\frac{\partial \mathbf{Op}}{\partial f_{\mu\nu}}$ and implement it in the TF framework.

Back up

Manual computation of the gradient

- 1 From the expression of the output:

$$\mathbf{Op} \equiv y_N = \sum_{i,j,\alpha,\beta} f_\alpha(x_i) f_\beta(x_j) \hat{\sigma}_{Nij\alpha\beta}$$

- 2 Gradient of the output with respect to the PDFs:

$$\begin{aligned} \frac{\partial y_N}{\partial f_{\mu\nu}} &= \frac{\partial}{\partial f_{\mu\nu}} \sum_{i,j,\alpha,\beta} f_{i\alpha} f_{j\beta} \hat{\sigma}_{Nij\alpha\beta} \\ &= \sum_{i,j,\alpha,\beta} (\delta_{\mu i} \delta_{\nu \alpha} f_{\beta j} + \delta_{\mu j} \delta_{\nu \beta} f_{\alpha i}) \hat{\sigma}_{Nij\alpha\beta} \\ &= \sum_{j,\beta} f_{j\beta} \hat{\sigma}_{N\mu j \nu \beta} + \sum_{i,\alpha} f_{i\alpha} \hat{\sigma}_{Ni \mu \alpha \nu} \end{aligned}$$