Charting proton structure (and beyond) with deep learning

Juan Rojo
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Machine Learning for High Energy Physics seminar
Radboud University Nijmegen
Zoom, 11/03/2021

Outline

- A crash course on **proton structure**
- The Neural Network approach to **parton distributions**
- Deep learning for **Effective Field Theory** analyses
- Deep learning for data analysis in **Electron Microscopy**

A Crash Course on Proton Structure

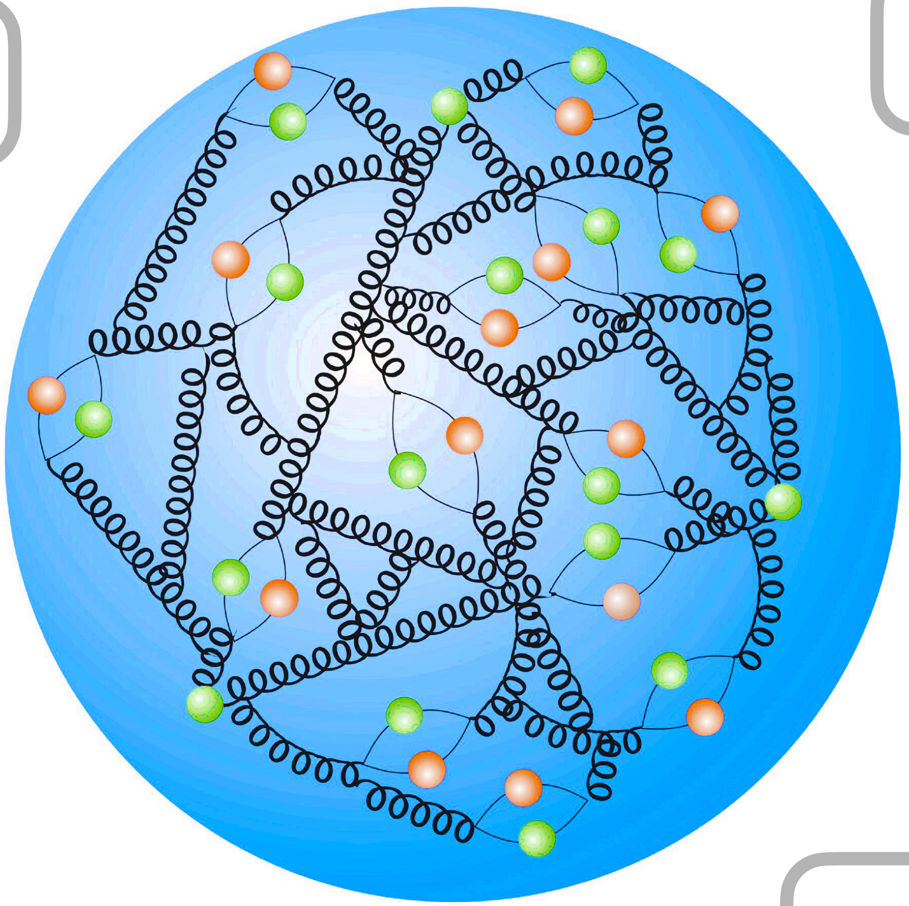
for more info see Gao, Harland-Lang, Rojo *Physics Reports* (2021)

The many faces of the proton

QCD bound state of **quarks** and **gluons**

Origin of mass?

Origin of spin?



Gluon-dominated matter?

3D imaging?

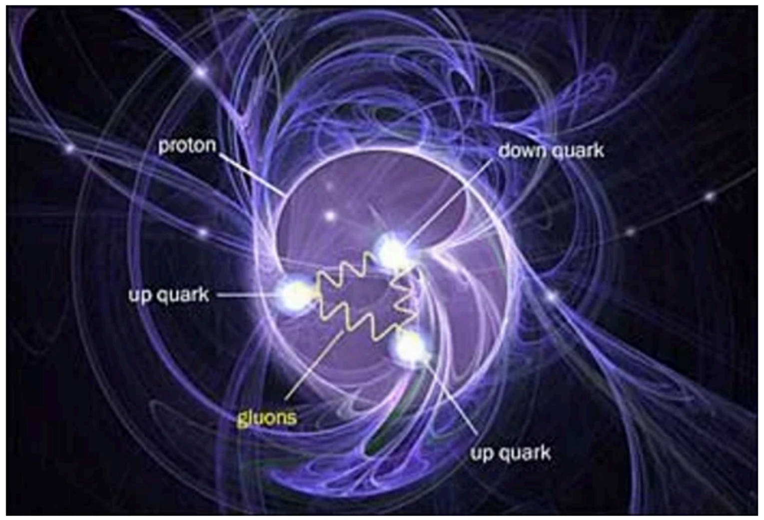
Heavy quark content?

Nuclear modifications?

The proton in the spotlight

THE SCIENCES

Proton Spin Mystery Gains a New Clue



Non-zero gluon polarisation

Scientific American (2014)

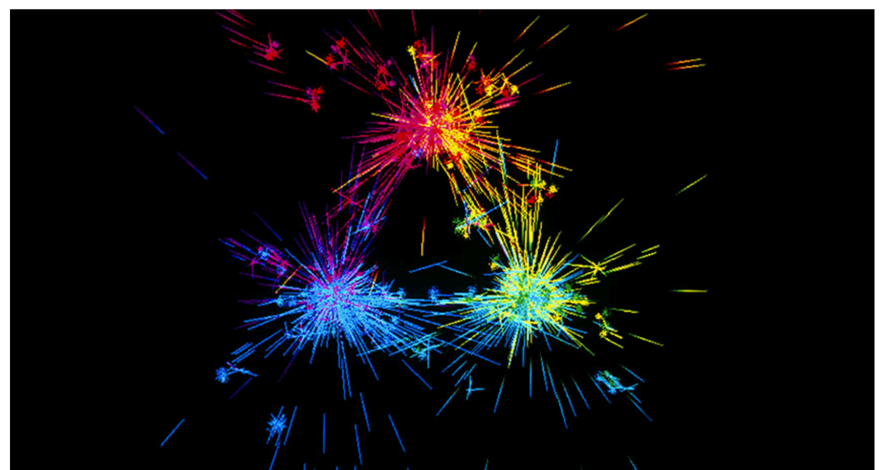
Nucleon pressure

NEWS PARTICLE PHYSICS

The inside of a proton endures more pressure than anything else we've seen

For the first time, scientists used experimental data to estimate the pressure inside a proton

BY EMILY CONOVER 1:18PM, MAY 16, 2018



FEELING THE PRESSURE Extreme pressures are found within the proton, scientists report. The proton contains three particles called quarks (illustrated) as well as gluons, which hold the particle together.

Science News (2018)

After 40 years of studying the strong nuclear force, a revelation

This was the year that analysis of data finally backed up a prediction, made in the mid 1970s, of a surprising emergent behaviour in the strong nuclear force

BFKL dynamics

The Guardian (2017)

The proton keeps surprising us as an endless source of **fundamental discoveries**

The proton in the spotlight

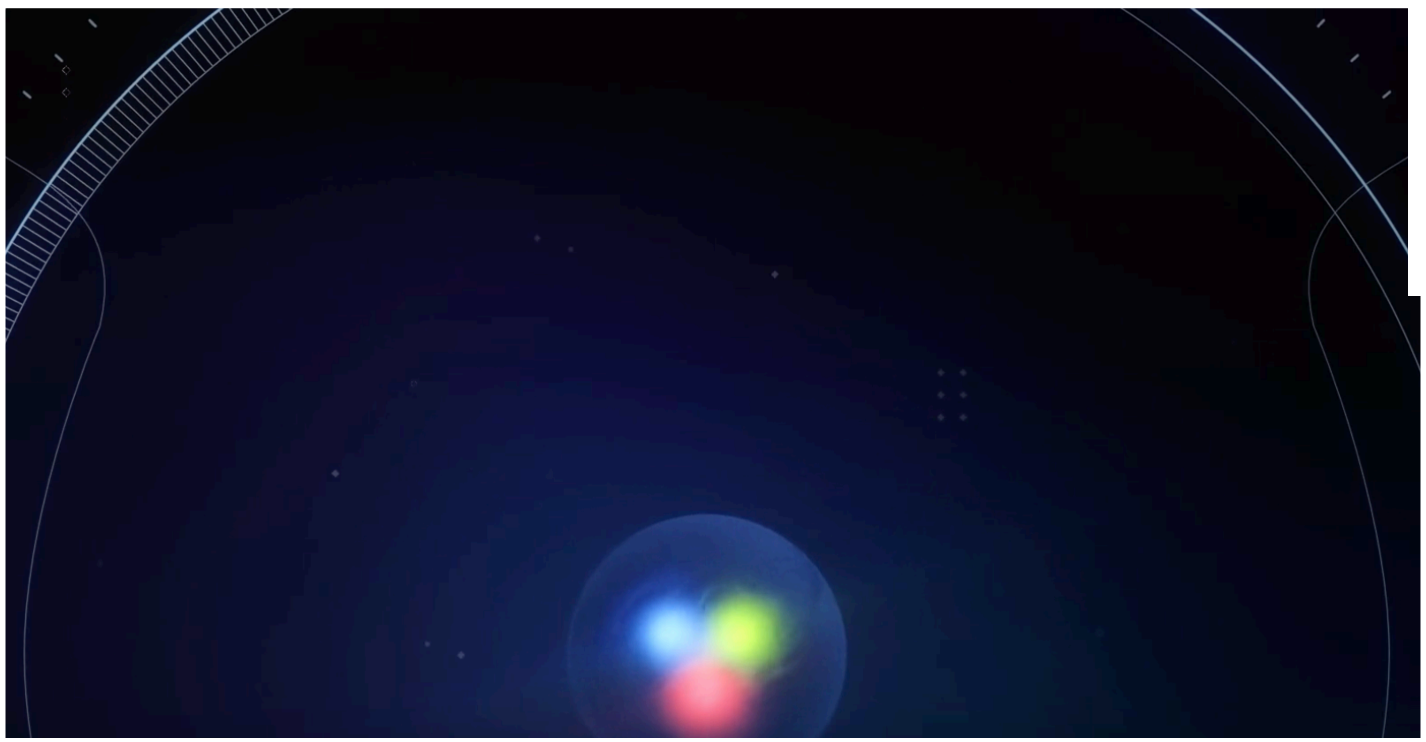
QUANTUM PHYSICS

Decades-Long Quest Reveals Details of the Proton's Inner Antimatter

27

Twenty years ago, physicists set out to investigate a mysterious asymmetry in the proton's interior. Their results, published today, show how antimatter helps stabilize every atom's core.

Proton antimatter asymmetry



deVolkskrant

Onthuld: de bizarre wereld in het binnenste van protonen, bouwstenen van alles om ons heen

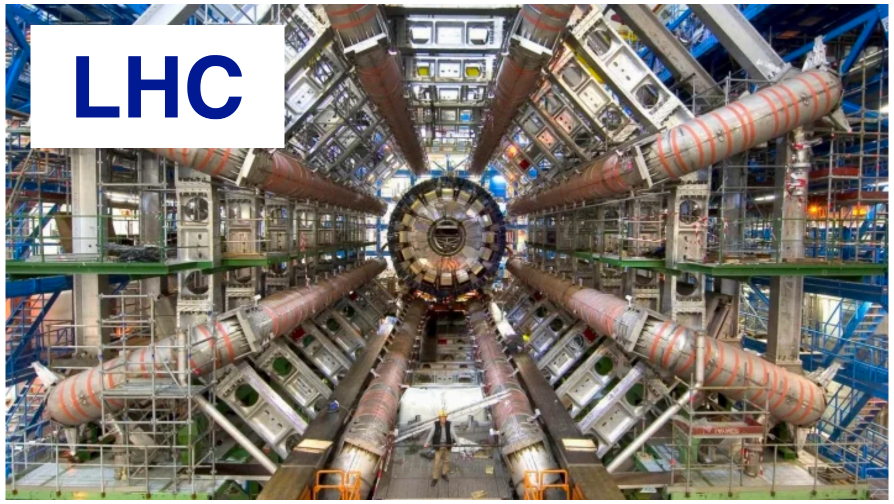
Ze zitten in alles, van onze lichamen tot het broodje dat je bij de lunch eet: protonen. Natuurkundigen beschrijven deze week hoe in het binnenste van die deeltjes een wereld heerst die zó bizar is dat het twintig jaar kostte om hem in kaart te brengen.

George van Hal 25 februari 2021, 19:19

Nature + Quanta, Volkskrant, New Scientist … (2021)

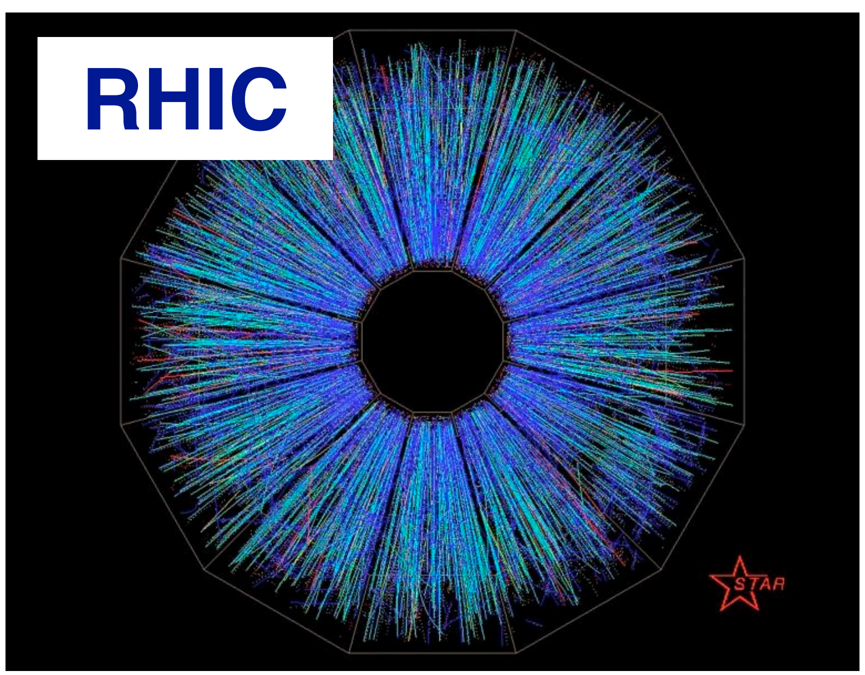
The proton keeps surprising us as an endless source of **fundamental discoveries**

From colliders to the cosmos



New **elementary particles** beyond the **Standard Model?**

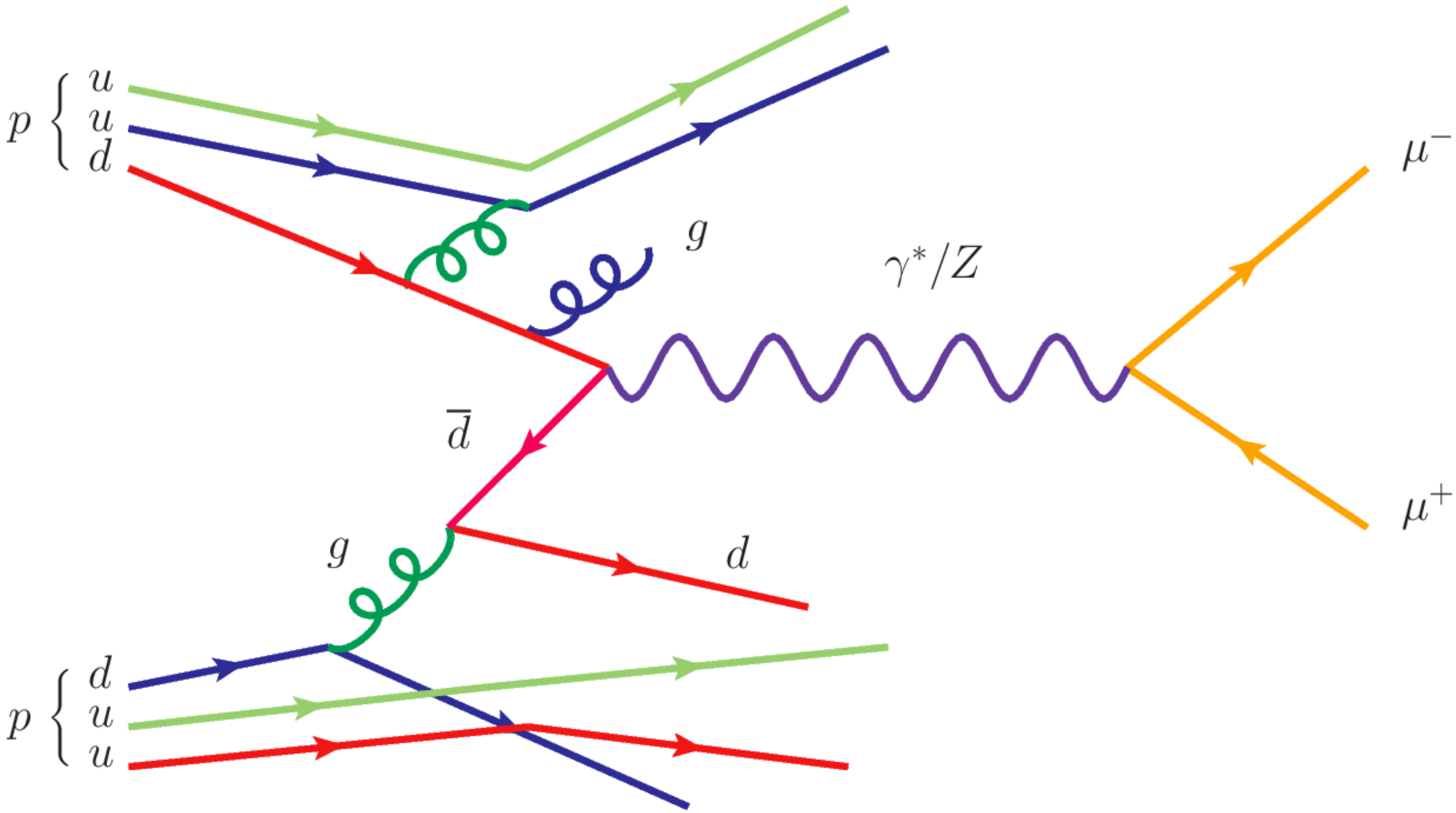
Origins and properties of **cosmic neutrinos**?



Nature of **Quark-Gluon Plasma** in **heavy-ion collisions?**

Parton Distributions

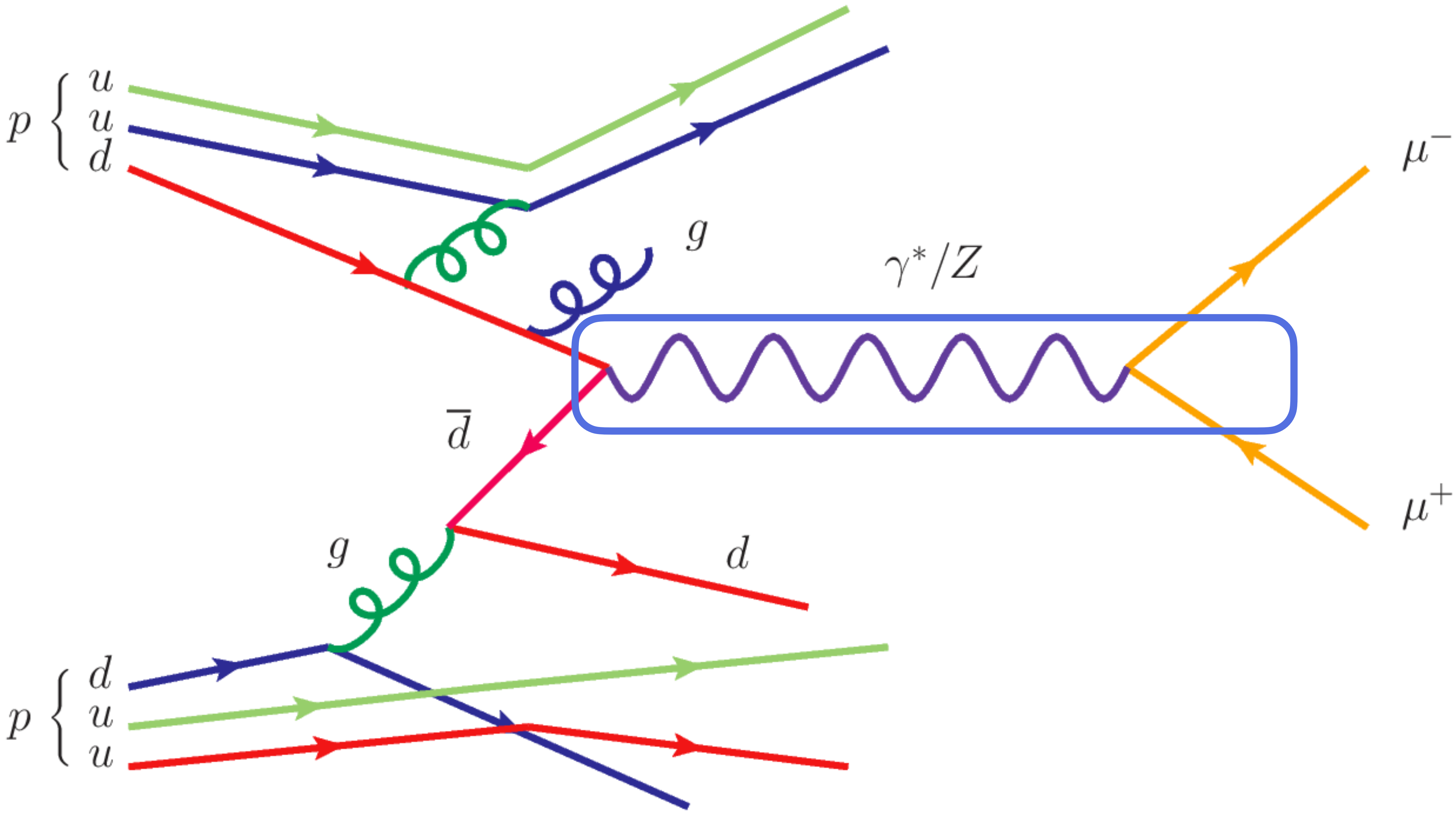
In high-energy **hadron colliders**, such as the LHC, the collisions involve **composite particles** (protons) with **internal structure** (quarks and gluons)



$$\frac{d\sigma(pp \to l^+l^-)}{dm_{ll}} = ?$$

Parton Distributions

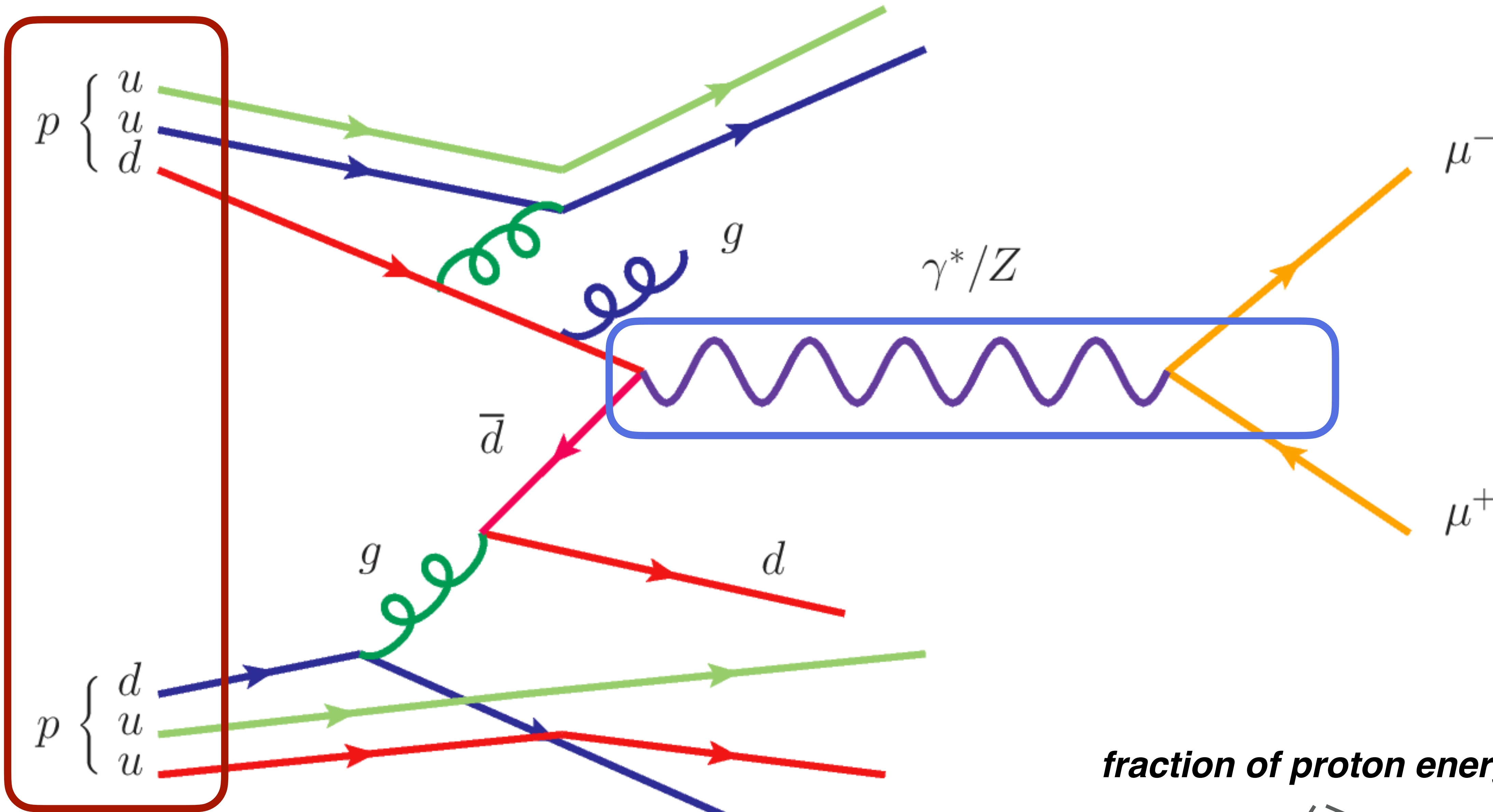
In high-energy **hadron colliders**, such as the LHC, the collisions involve **composite particles** (protons) with **internal structure** (quarks and gluons)



$$\frac{d\sigma(pp \to l^+l^-)}{dm_{ll}} = \frac{d\sigma(q_i\bar{q}_j \to l^+l^-)}{dm_{ll}} \otimes \ldots$$

Parton Distributions

In high-energy **hadron colliders**, such as the LHC, the collisions involve **composite particles** (protons) with **internal structure** (quarks and gluons)

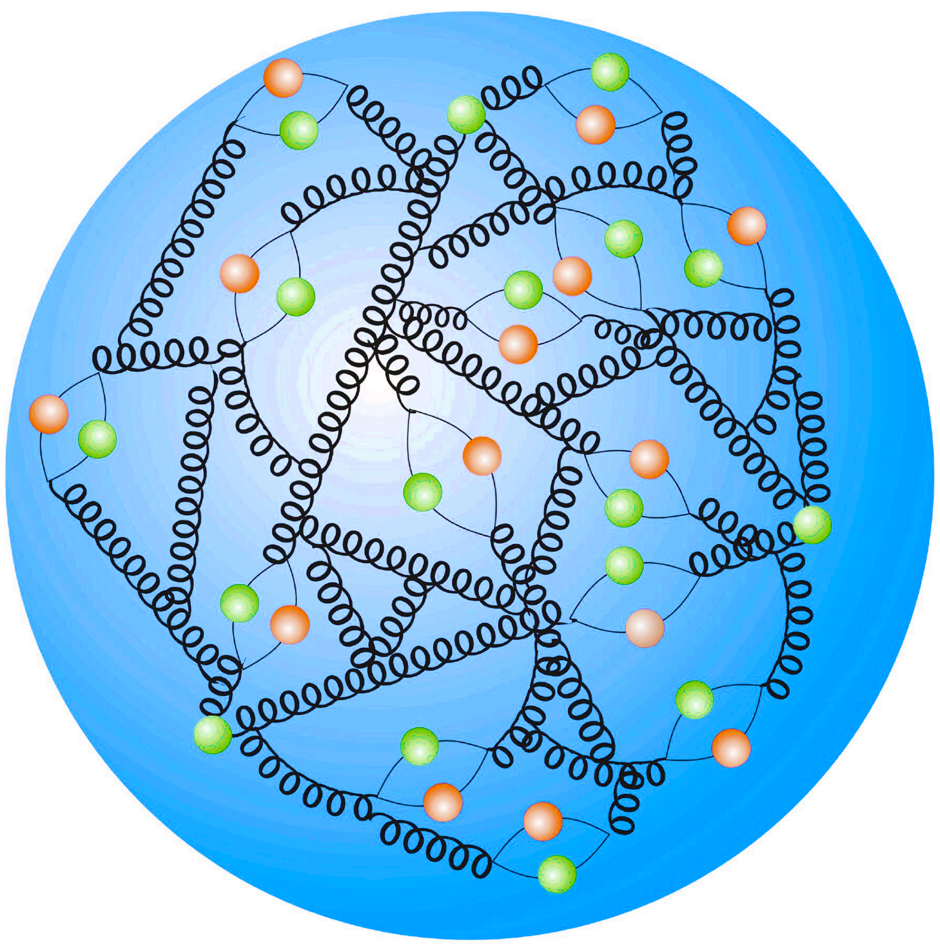


fraction of proton energy

$$\frac{d\sigma(pp \to l^+l^-)}{dm_{ll}} = \frac{d\sigma(q_i\bar{q}_j \to l^+l^-)}{dm_{ll}} \otimes \mathrm{Prob}(q_i, x_1) \otimes \mathrm{Prob}(\bar{q}_j, x_2)$$

Parton Distributions

Proton energy divided among constituents: **quarks** and **gluons**



Parton Distribution Functions (PDFs)

Determine from **data:**

Global QCD analysis

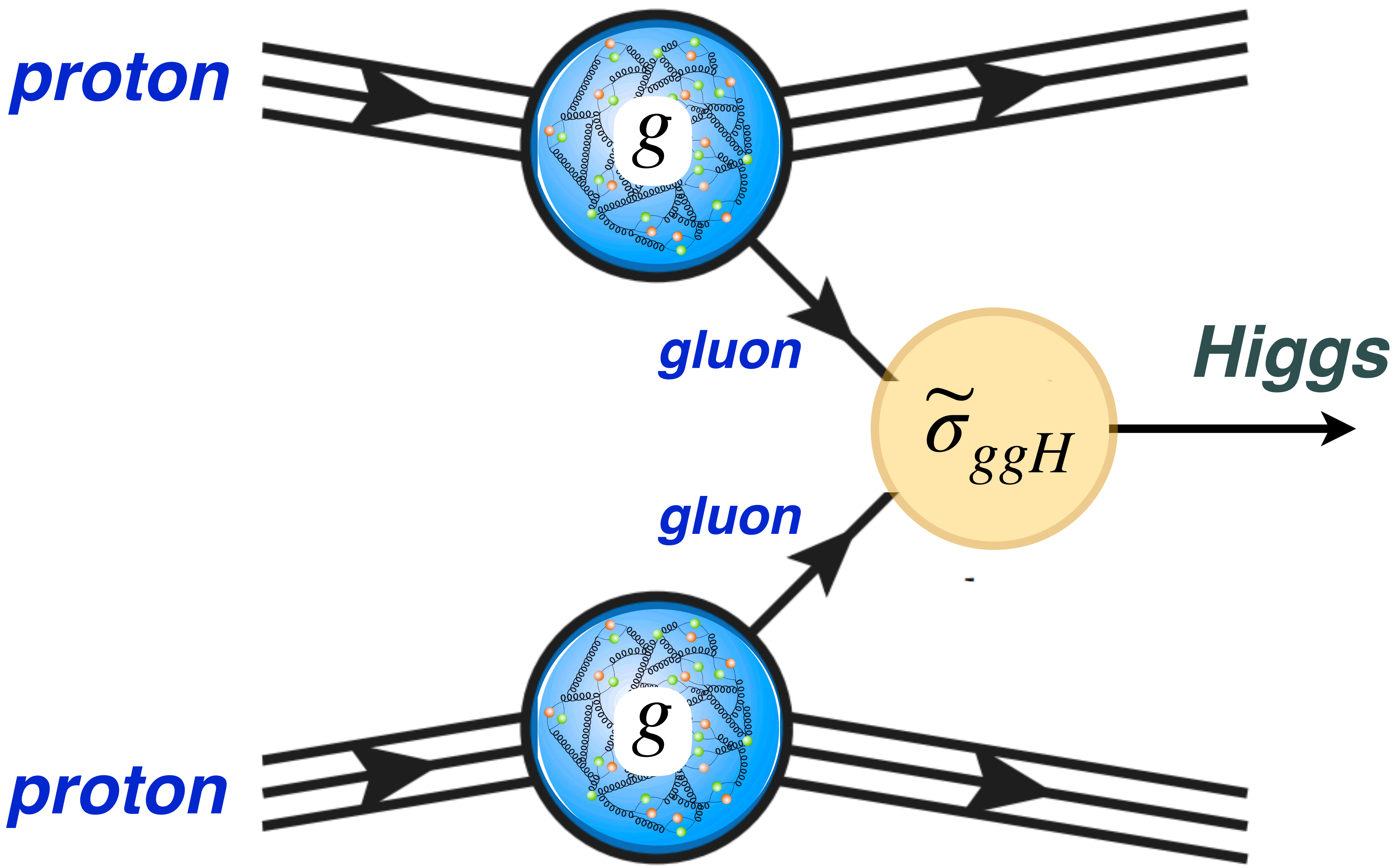
Mass? Spin?
Heavy quark content?
Novel QCD dynamics?

Theoretical predictions for LHC, RHIC, IceCube?

Parton Distributions

$$N_{\mathrm{LHC}}(H) \sim g \otimes g \otimes \tilde{\sigma}_{ggH}$$

Parton Distributions



All-order structure: **QCD factorisation theorems**

Parton Distributions

$$g(x, Q)$$

Probability of **finding a gluon inside a proton**, carrying a fraction ***x*** of the proton momentum, when probed with energy ***Q***

***x*:** fraction of proton momentum carried by gluon

Energy of hard-scattering reaction**:** inverse of resolution length

Dependence on *x* fixed by **non-perturbative QCD dynamics**: extract from experimental data

- **Energy conservation**: momentum sum rule

$$\int_0^1 dx\, x \left(\sum_{i=1}^{n_f} \left[q_i((x, Q^2) + \bar{q}_i(x, Q^2) \right] + g(x, Q^2) \right) = 1$$

- **Quark number conservation**: valence sum rules

$$\int_0^1 dx\, \left(u(x, Q^2) + \bar{u}(x, Q^2) \right) = 2$$

Parton Distributions

$$g(x, Q)$$

Energy of hard-scattering reaction**:** inverse of resolution length

Probability of **finding a gluon inside a proton**, carrying a fraction ***x*** of the proton momentum, when probed with energy ***Q***

x: fraction of proton momentum carried by gluon

Dependence on ***Q*** fixed by **perturbative QCD dynamics**: computed up to $\mathcal{O}\left(\alpha_s^4\right)$

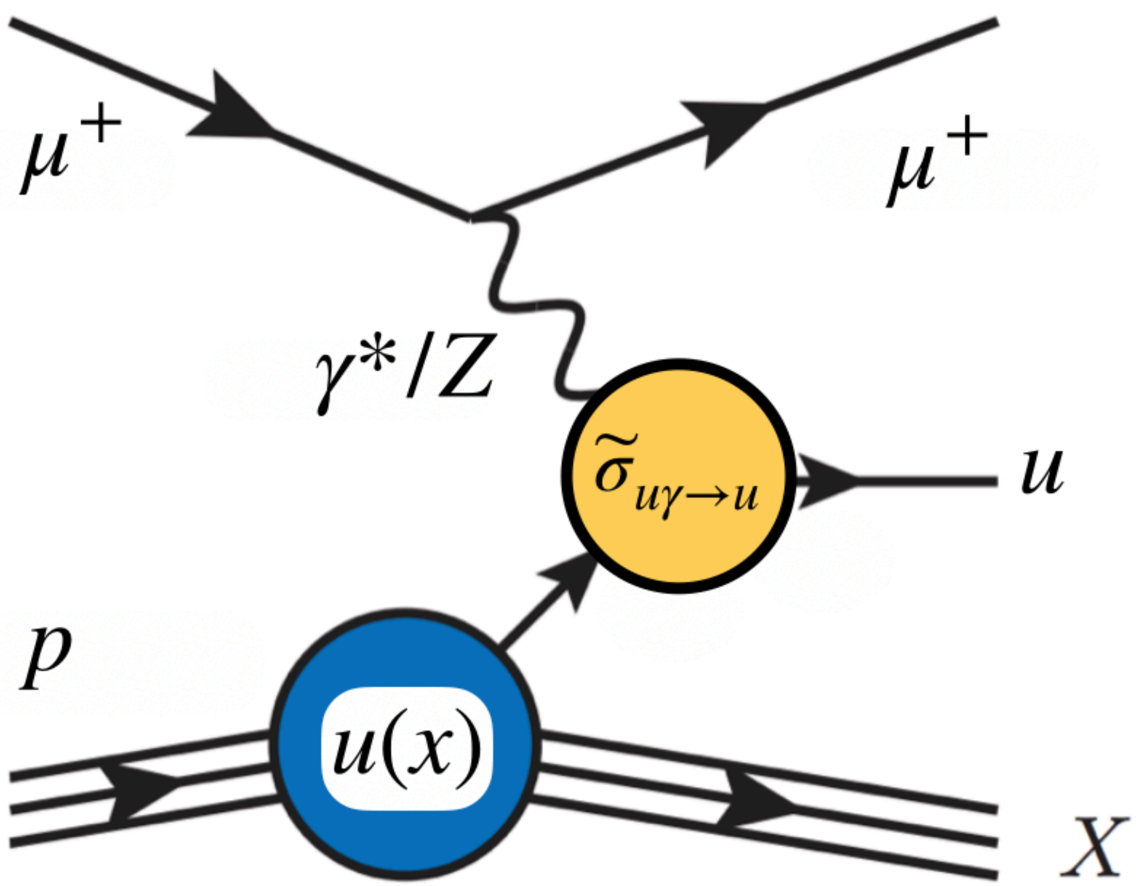
$$\frac{\partial}{\partial \ln Q^2} q_i(x, Q^2) = \int_x^1 \frac{dz}{z} P_{ij}\left(\frac{x}{z}, \alpha_s(Q^2)\right) q_j(z, Q^2)$$

DGLAP *parton evolution equations*

The Global QCD analysis paradigm

QCD factorisation theorems**: PDF universality**

$$\sigma_{l\,p\to\mu\,X} = \widetilde{\sigma}_{u\gamma\to u} \otimes u(x)$$



$$u(x) \simeq \frac{\sigma_{lp\to lX}\ (\text{exp})}{\widetilde{\sigma}_{u\gamma^*\to u}\ (\text{QED theory})}$$

leading-order calculations + only up quark in proton

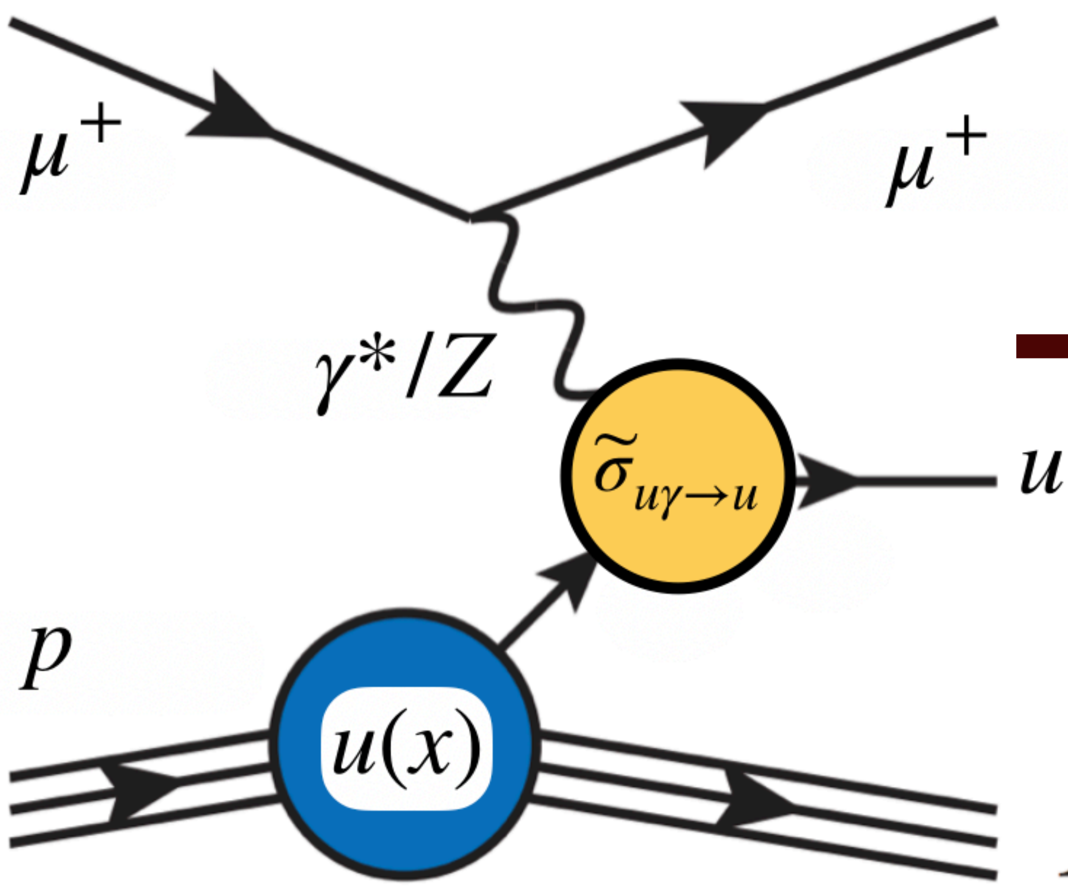
Determine PDFs from ***deep-inelastic scattering****…*

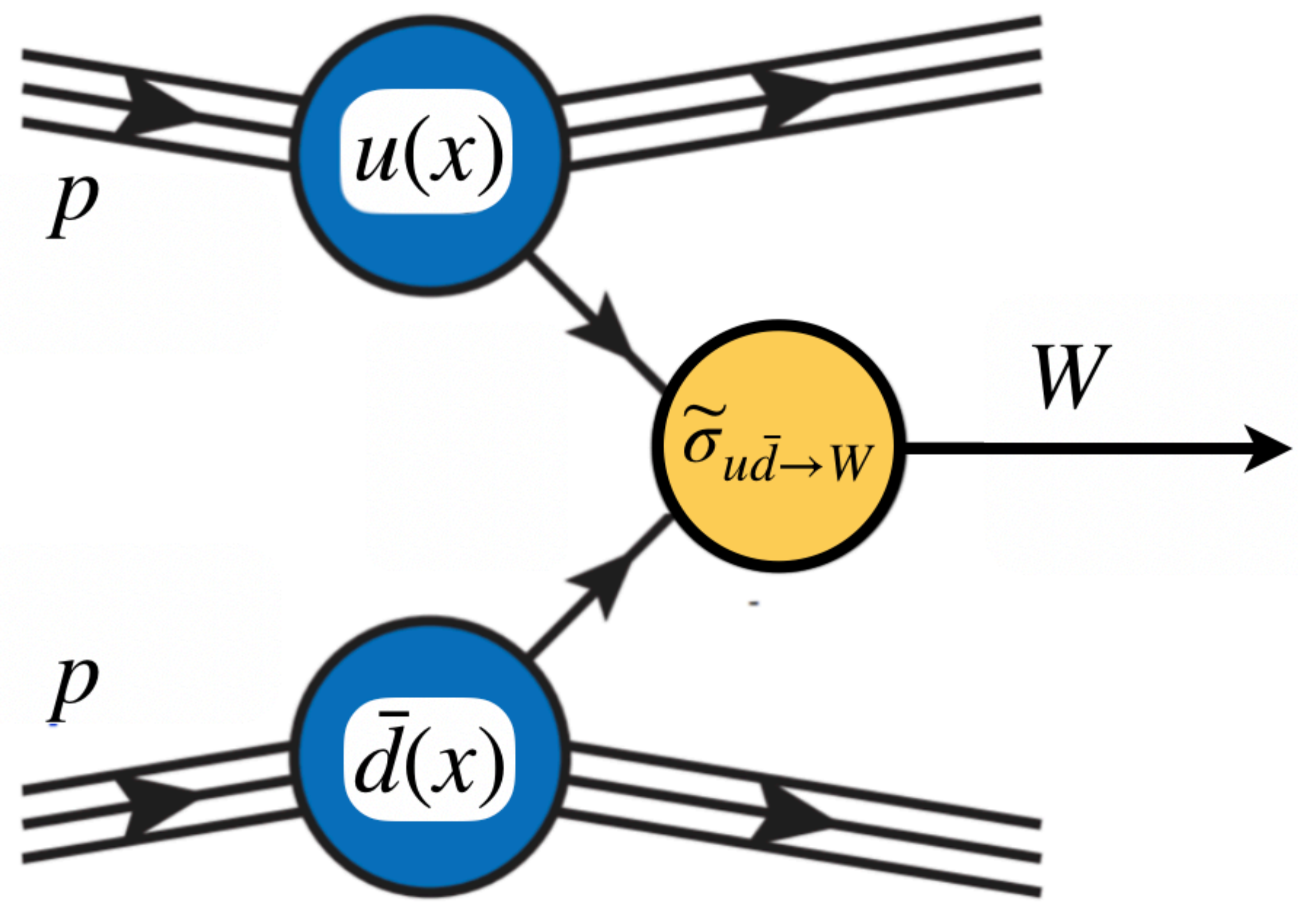
in general: introduce a parametrisation for the PDFs and fit their parameters from data

The Global QCD analysis paradigm

QCD factorisation theorems**: PDF universality**

$$\sigma_{l\,p\to\mu\,X} = \widetilde{\sigma}_{u\gamma\to u} \otimes u(x) \;\rightarrow\; \sigma_{p\,p\to W} = \widetilde{\sigma}_{u\bar{d}\to W} \otimes u(x) \otimes \bar{d}(x)$$

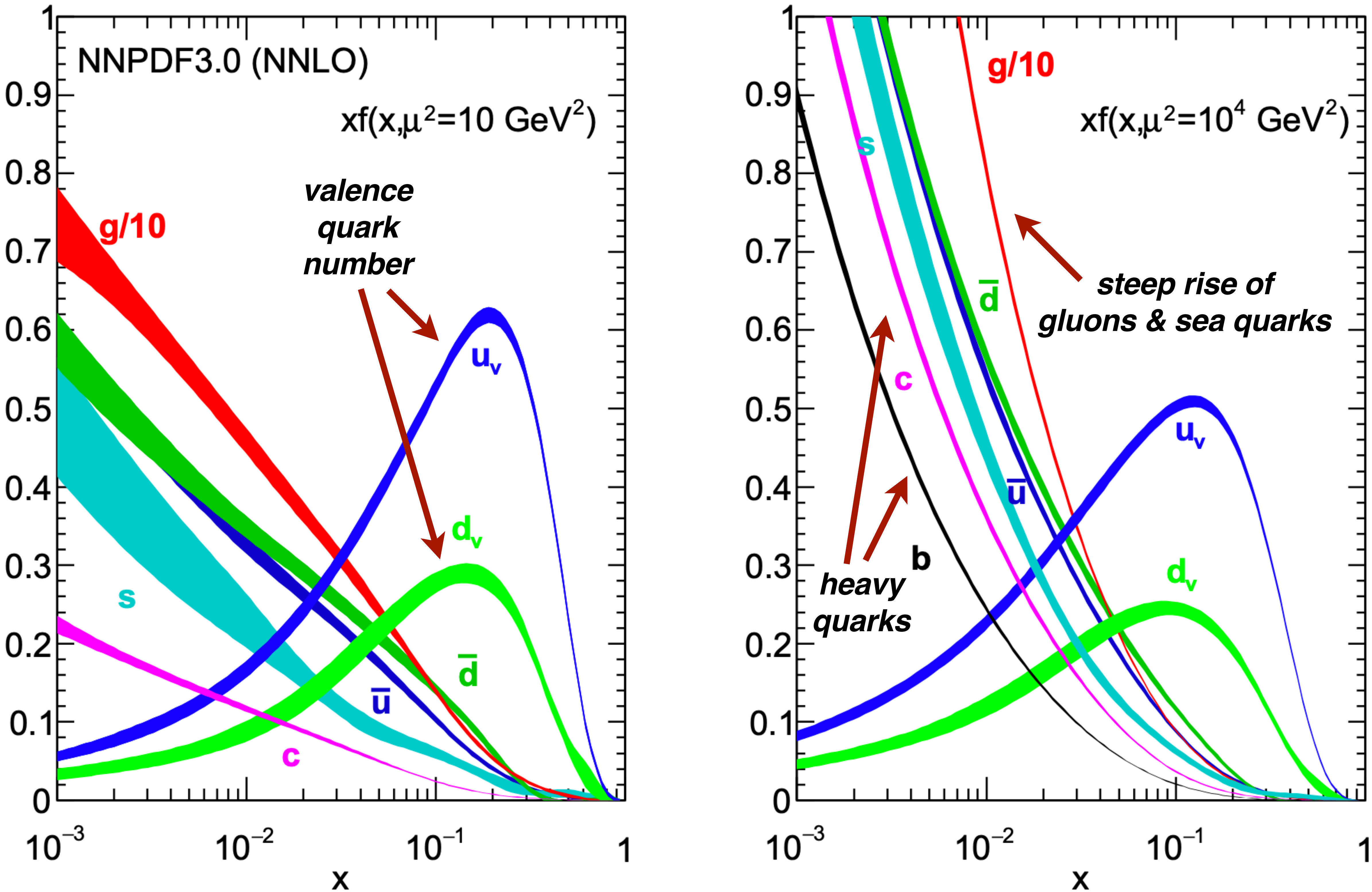




*Determine PDFs from **deep-inelastic scattering**…*

*… and use them to compute predictions for **proton-proton collisions***

A proton structure snapshop



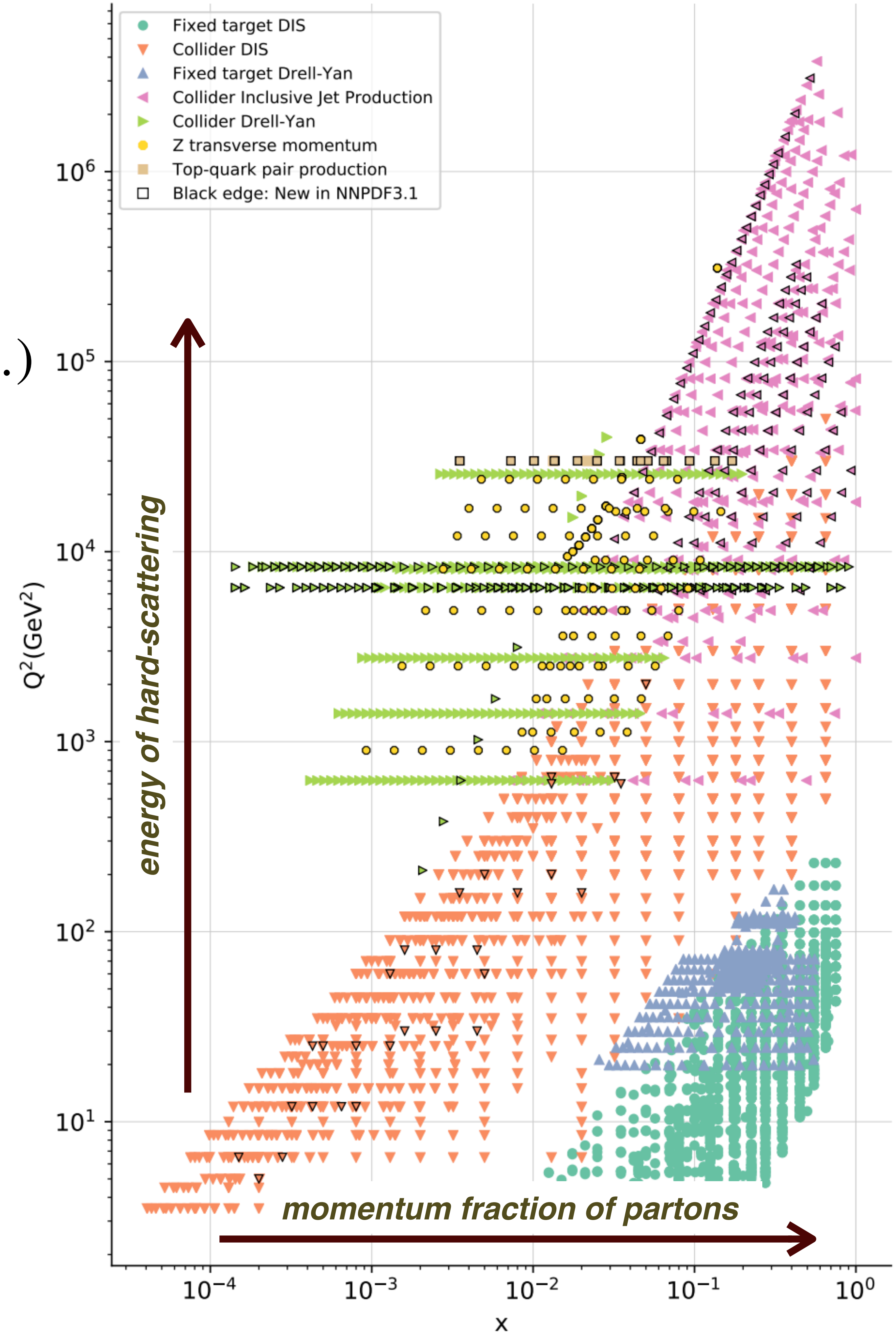
Fitting PDFs

- **Parametrise PDFs at** some low scale Q_0 (around the proton mass, 1 GeV)

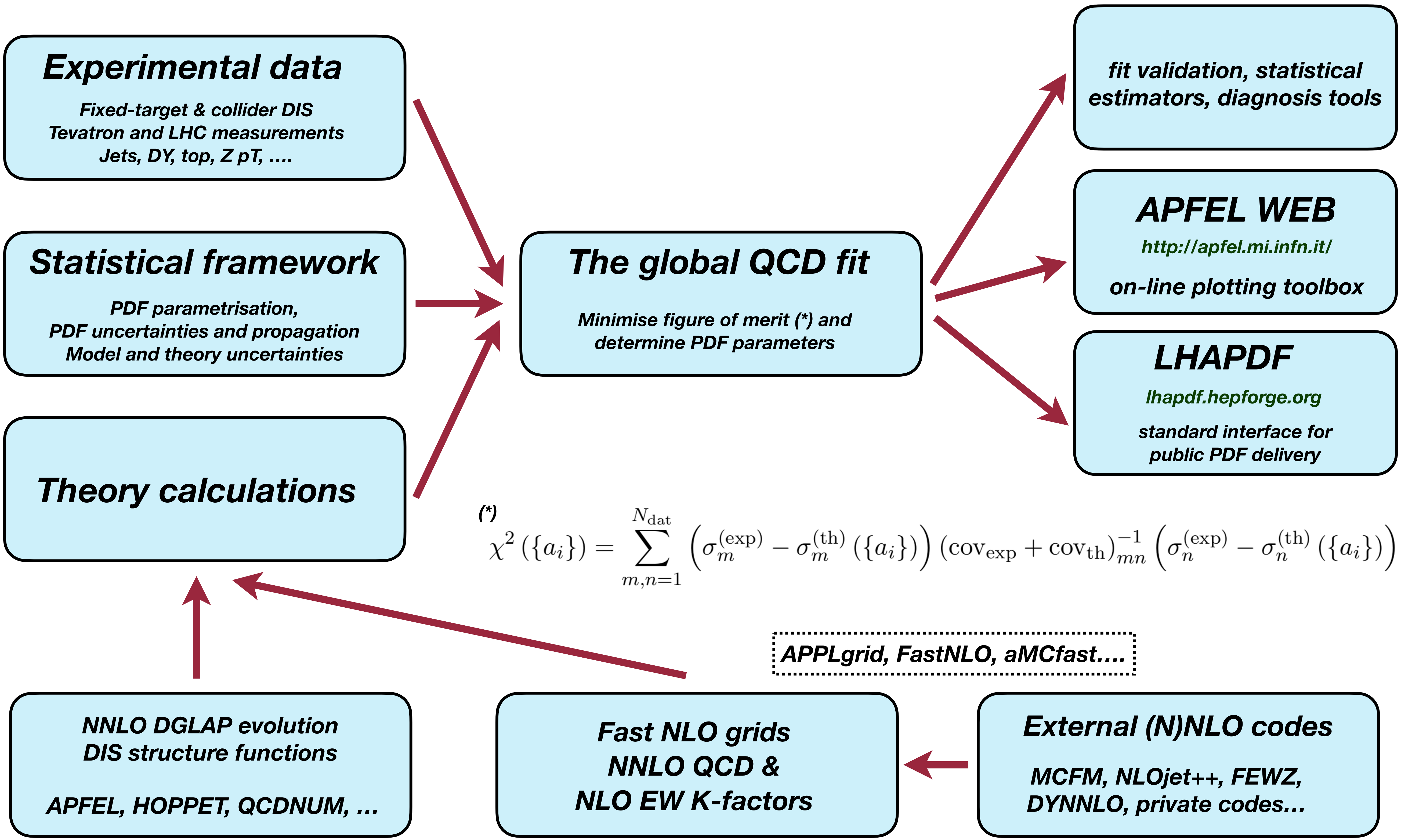
$$g(x, Q_0) \simeq A_g x^{-b_g}(1-x)^{c_g} \times P_g(x, d_g, f_g, \ldots)$$

- Fix some parameters from **theory constraints** (e.g. momentum conservation)
- Extract remaining parameters (+ their uncertainties) from global fit to wide dataset

more than **5000 independent cross-section measurements** from **40 different processes**



The global PDF fit pipeline



(*)

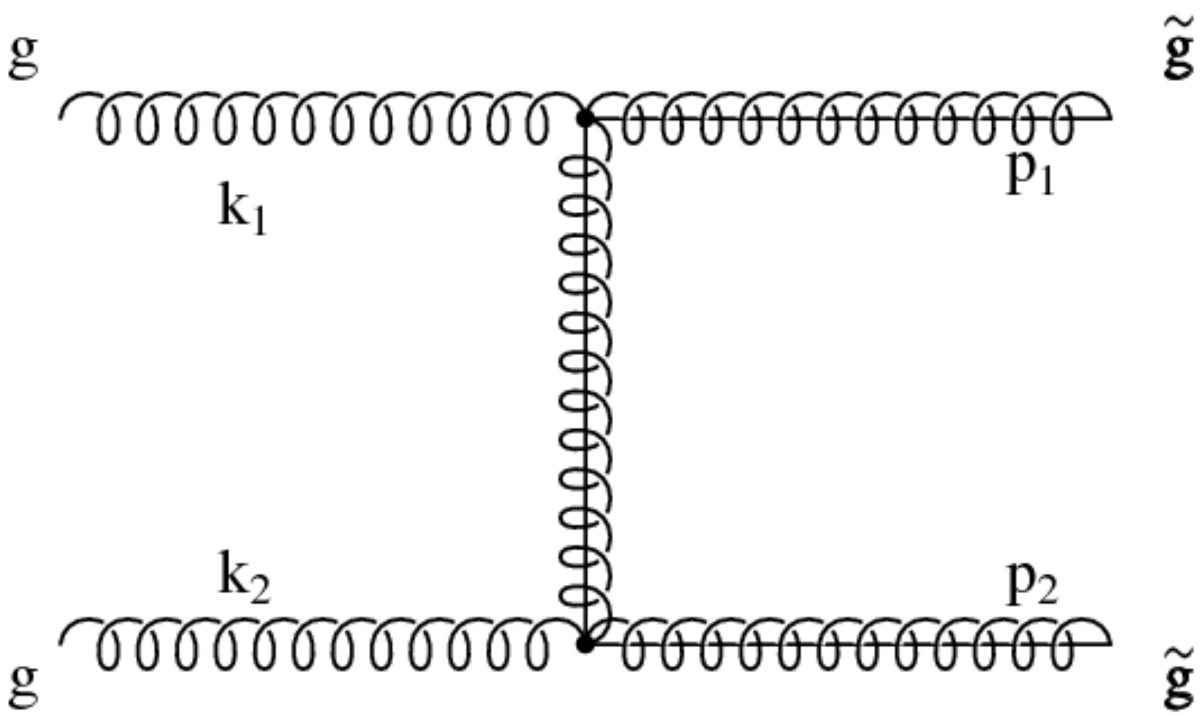
$$\chi^2\left(\{a_i\}\right) = \sum_{m,n=1}^{N_{\rm dat}} \left(\sigma_m^{(\rm exp)} - \sigma_m^{(\rm th)}\left(\{a_i\}\right)\right) \left({\rm cov}_{\rm exp} + {\rm cov}_{\rm th}\right)^{-1}_{mn} \left(\sigma_n^{(\rm exp)} - \sigma_n^{(\rm th)}\left(\{a_i\}\right)\right)$$

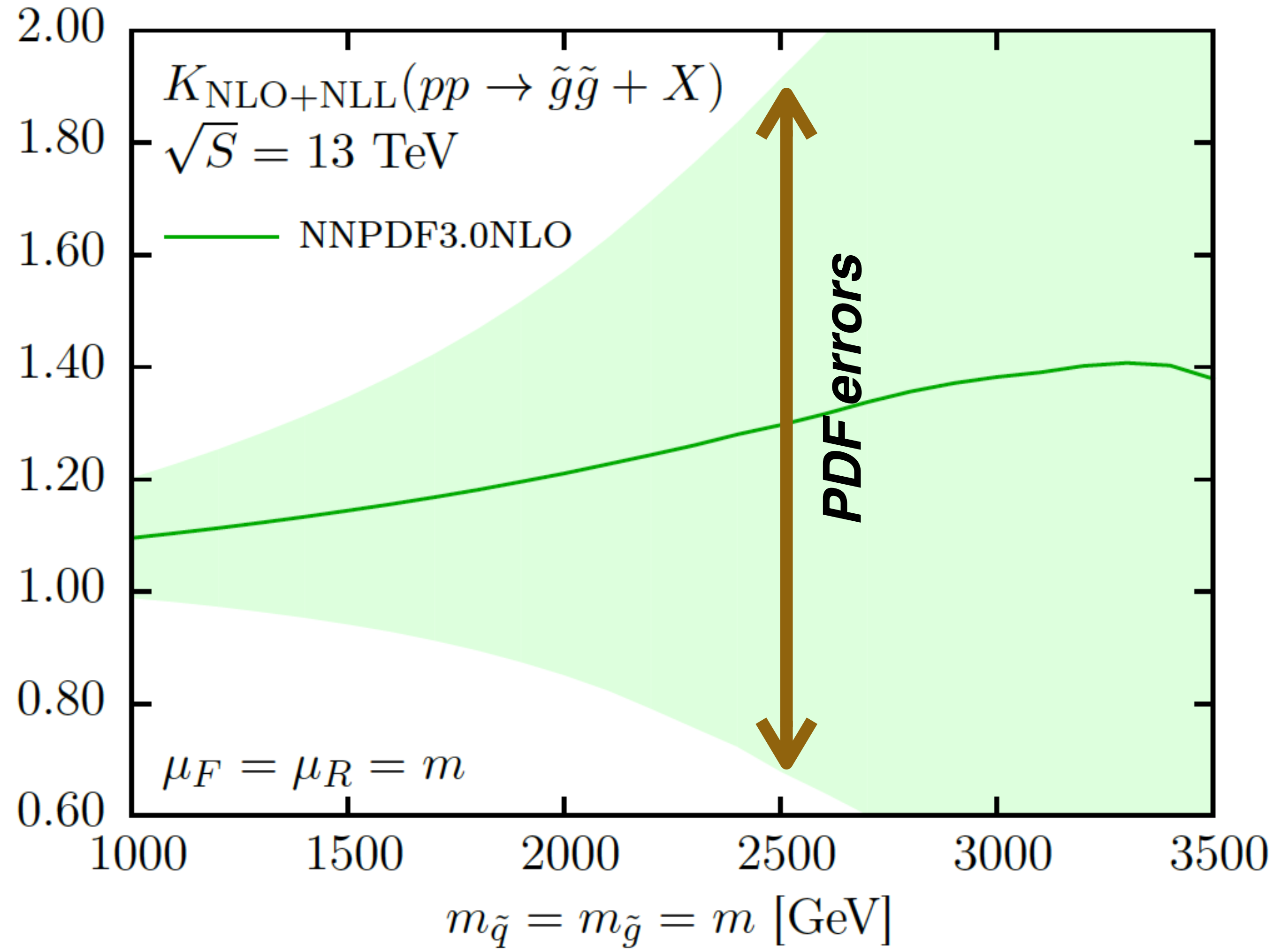
Why do we need better PDFs?

PDF uncertainties in the production of **New Physics heavy resonances** up to **100%**

Due to limited coverage of the **large Bjorken-*x* region**

gluino-pair production in supersymmetry



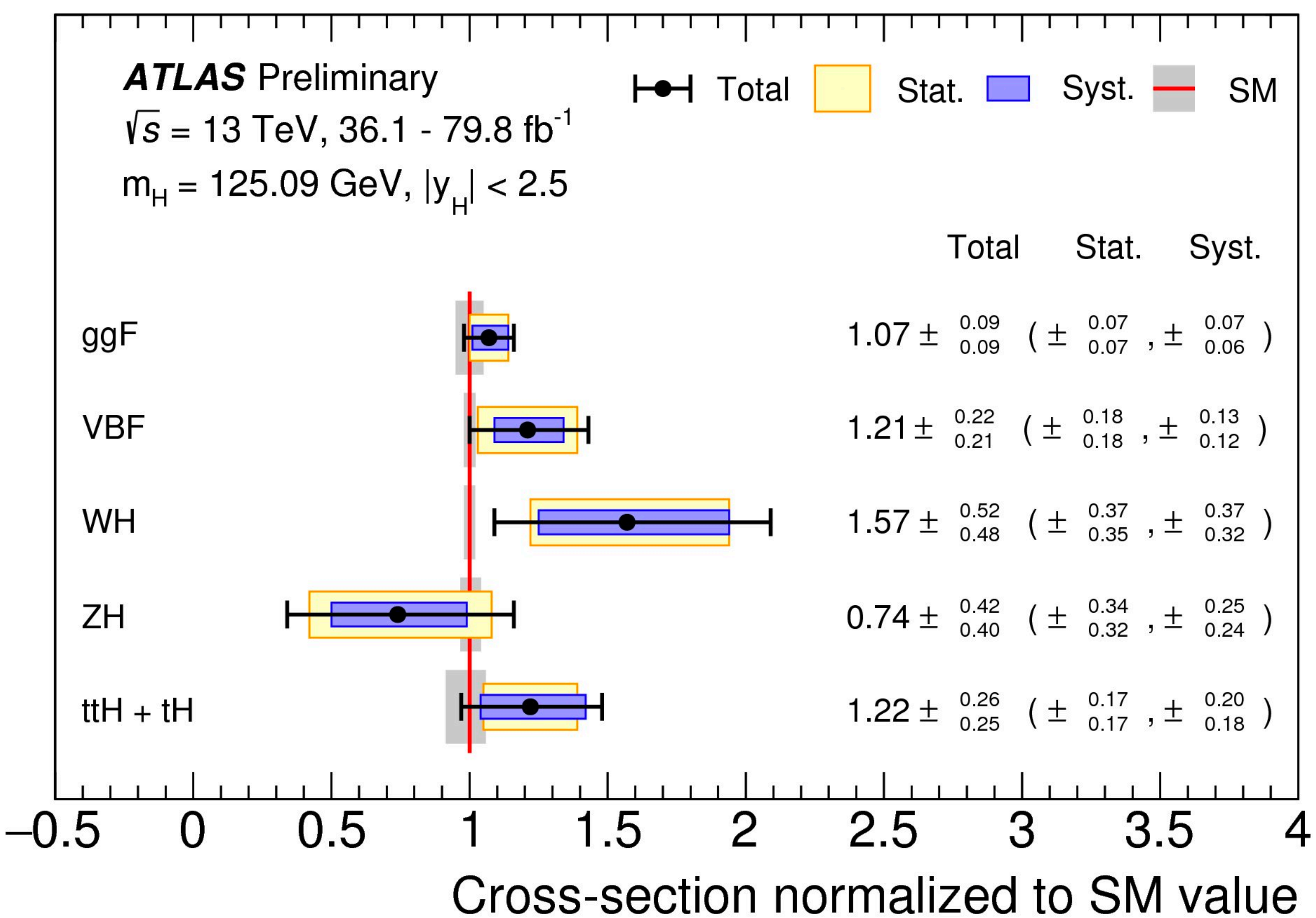


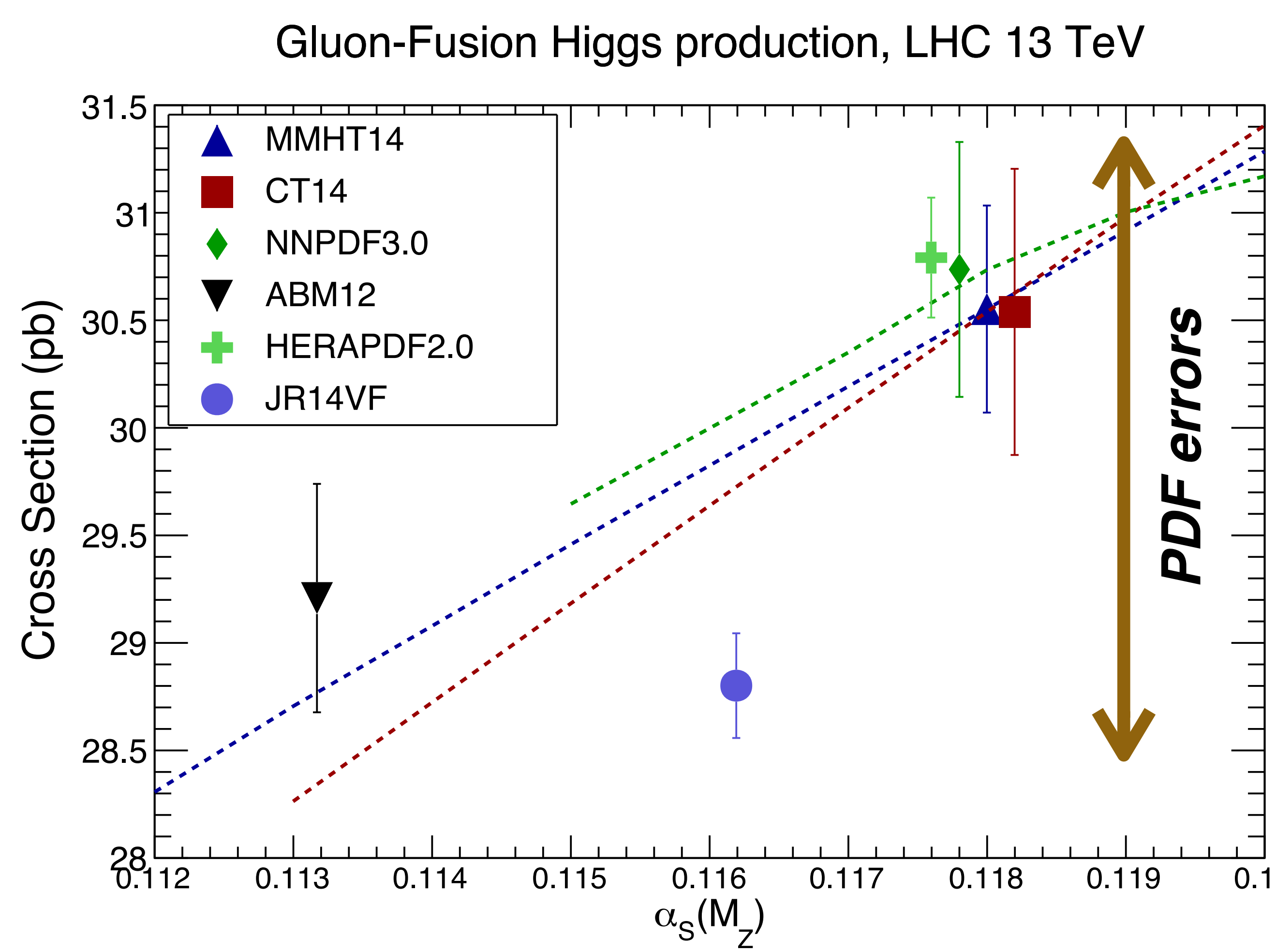
Why do we need better PDFs?

$$\frac{\Delta\sigma_h^{(\mathrm{BSM})}}{\sigma_h^{(\mathrm{SM})}} \simeq \frac{v^2}{\Lambda^2} = \text{few } \% \text{ for } \Lambda = \mathcal{O}(\mathrm{TeV})$$

Higgs coupling measurements **at the few percent level** (and below) are a must for indirect BSM searches

Inclusive Higgs production rates

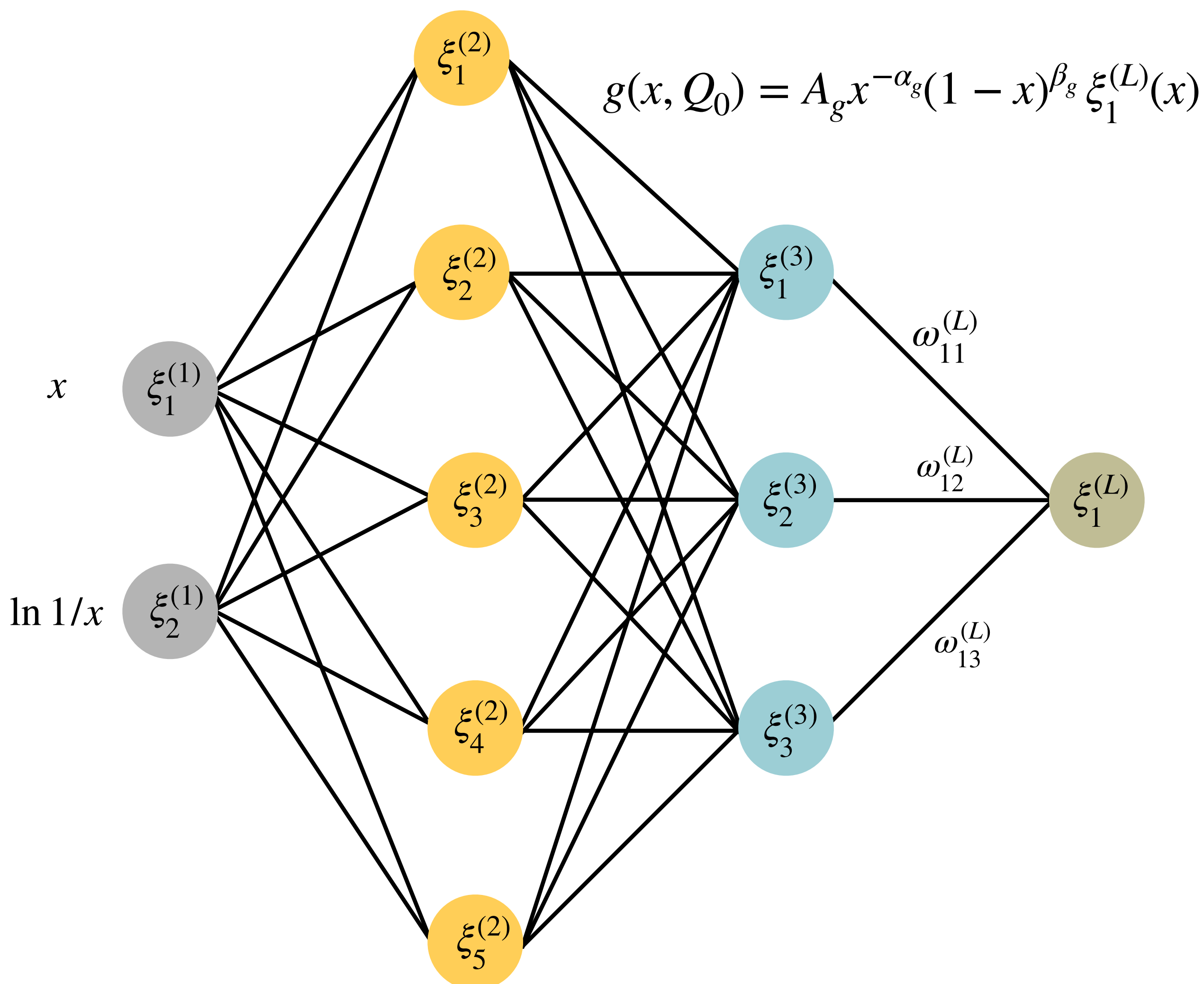




The Neural Network Approach to Proton Structure

http://nnpdf.mi.infn.it/

ML for proton structure



- **Neural Networks** can be used universal unbiased interpolants to **parametrise PDFs**
- Removes model dependence: **unbiased learning** the physical laws from data
- Highly **redundant parametrisation:** identical results if O(10) increase in # free params

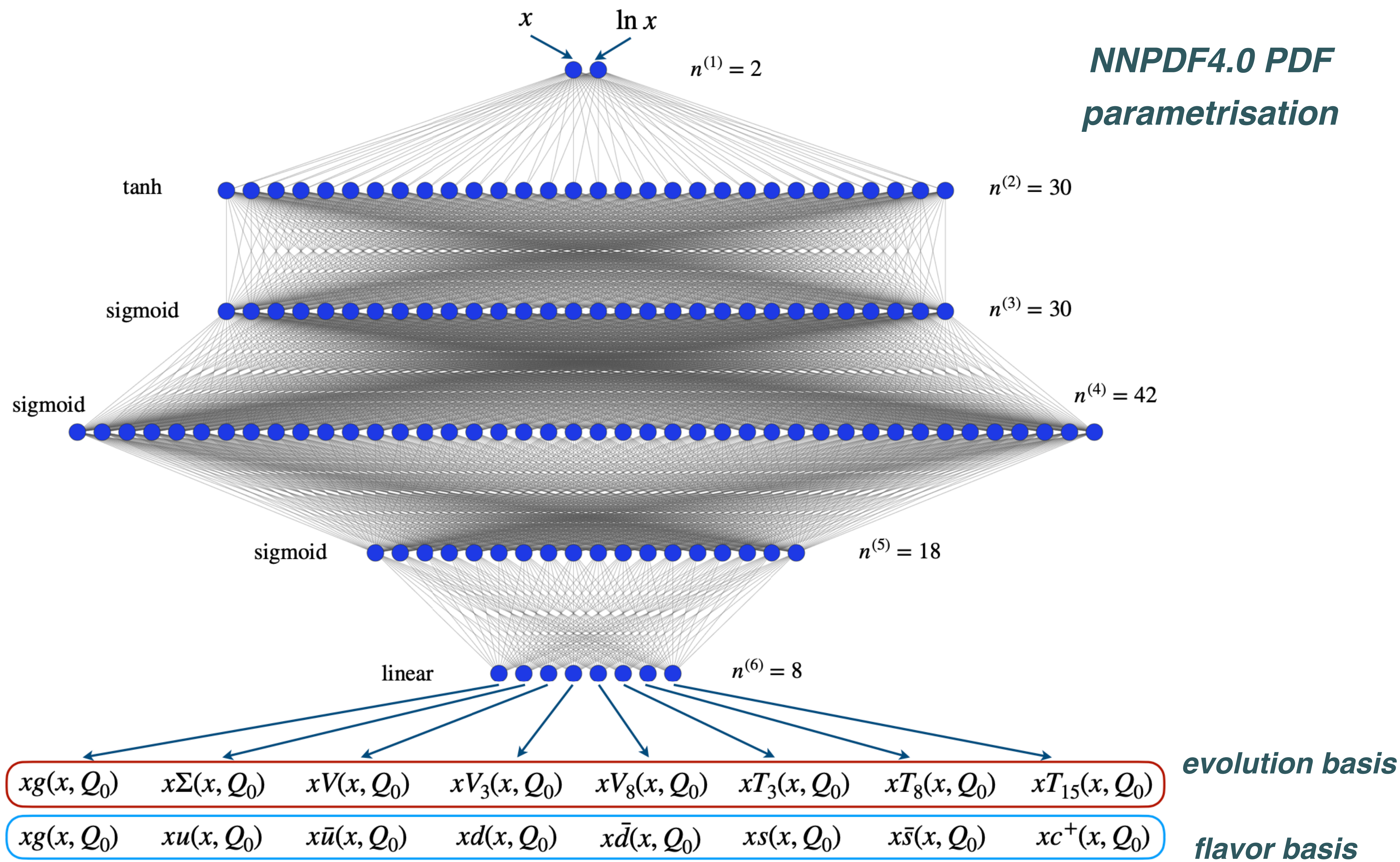
	Proton PDFs	***Nuclear PDFs***
Traditional	$g(x) \simeq x^{-b}(1-x)^c$	$R_g(x, A) \simeq (1 + bx + cx^2) \times A^d$
Neural Nets	$g(x) \simeq \mathrm{NN}(x)$	$R_g(x, A) \simeq \mathrm{NN}(x, A)$

x: *proton's **energy fraction** carried by gluons*

A: *number of protons + neutrons*

ANN-based parametrisation

NNPDF4.0 PDF parametrisation

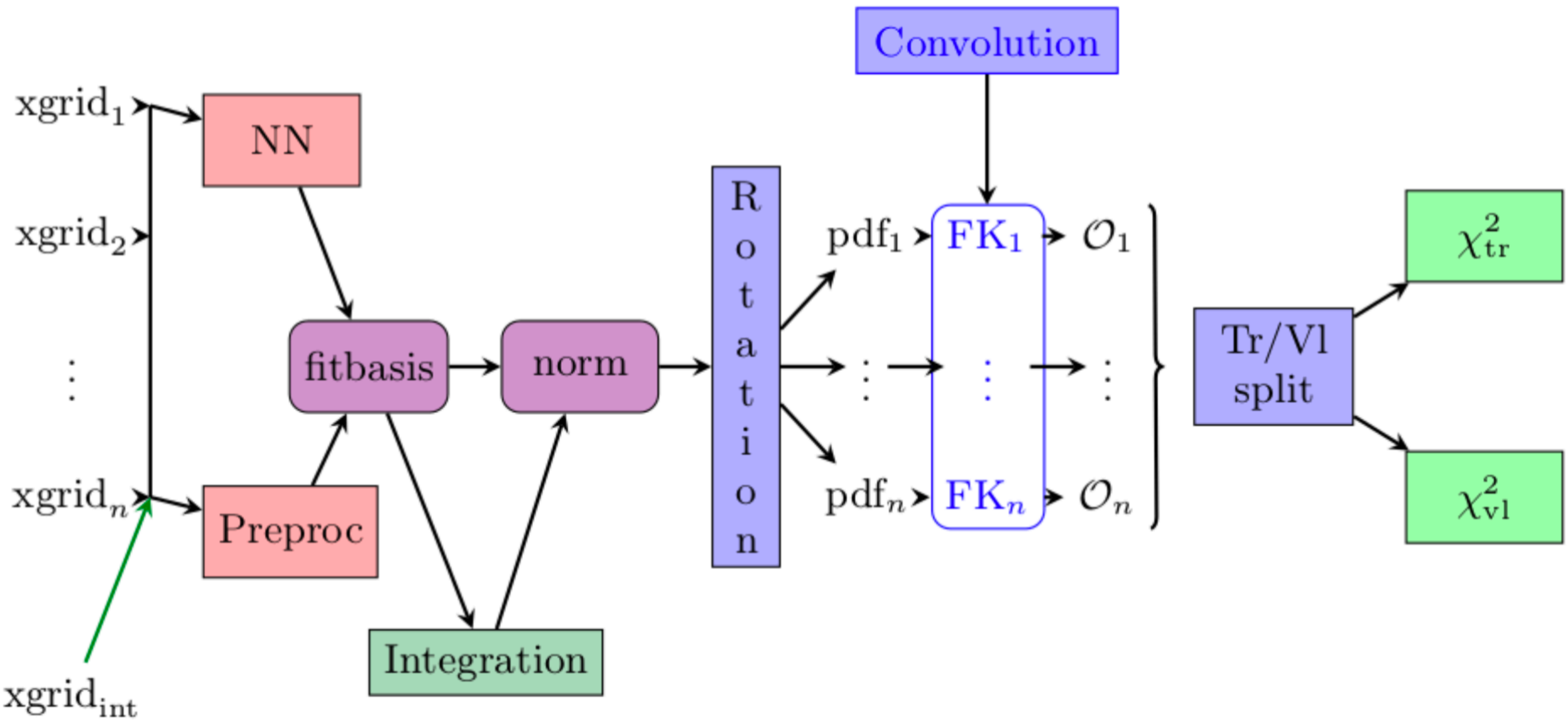


$$f_i(x, Q_0) = x^{-\alpha_i}(1-x)^{\beta_i}\mathrm{NN}_i(x)$$

How do we use ML for PDF fits?

- Deep neural networks as **universal unbiased interpolants**
- Automated **hyper-parameter optimisation** (NN architecture, minimiser, theory constraints, training time,….)
- **Monte Carlo sampling** for faithful uncertainty estimate and propagation (data errors, model errors, theory errors, …)
- Broad range of **minimisers**: SGD w. backpropagation, genetic algorithms, CMA-ES
- **GANs** to improve efficiency of **PDF compression** and **reweighting methods**
- New methods to detect **over-learning** and under-fitting beyond cross-validation
- Deploying **GPUs** to parallelize tasks and reduce CPU time
- Optimisation of NN training time (release fits take several weeks running on hundreds of cores)

ML-based PDFs



Complete restructure of the NNPDF fitting framework: enhanced modularity that dramatically improves its flexibility, in particular to exploit **external ML libraries** *eg* Keras, TensorFlow, …

ML-based PDFs

Convolution

brute-force calculation

convolution with hard-scattering matrix element

$$N(p+\mathrm{Pb}\to\pi+X)\propto\sum_{i,j,k=u,d,g,\dots}^{n_f}\int dx_1\int dx_2\int dz\,\widetilde{\sigma}_{ij\to k+X}(x_1,x_2,z,Q)\Big(f_i(x_1,Q,1)\,f_j(x_2,Q,A_{\mathrm{Pb}})\,f_{k\to\pi}(z,Q,A_{\mathrm{Pb}})\Big)$$

DGLAP evolution from Q_0

$$f_i(x,A,Q)=\sum_{j=u,d,g,\dots}^{n_f}\int dQ'\int dz\,\Gamma_{ij}(x/x',Q'/Q_0)\,f_j(x',A,Q_0)$$

NN outputs

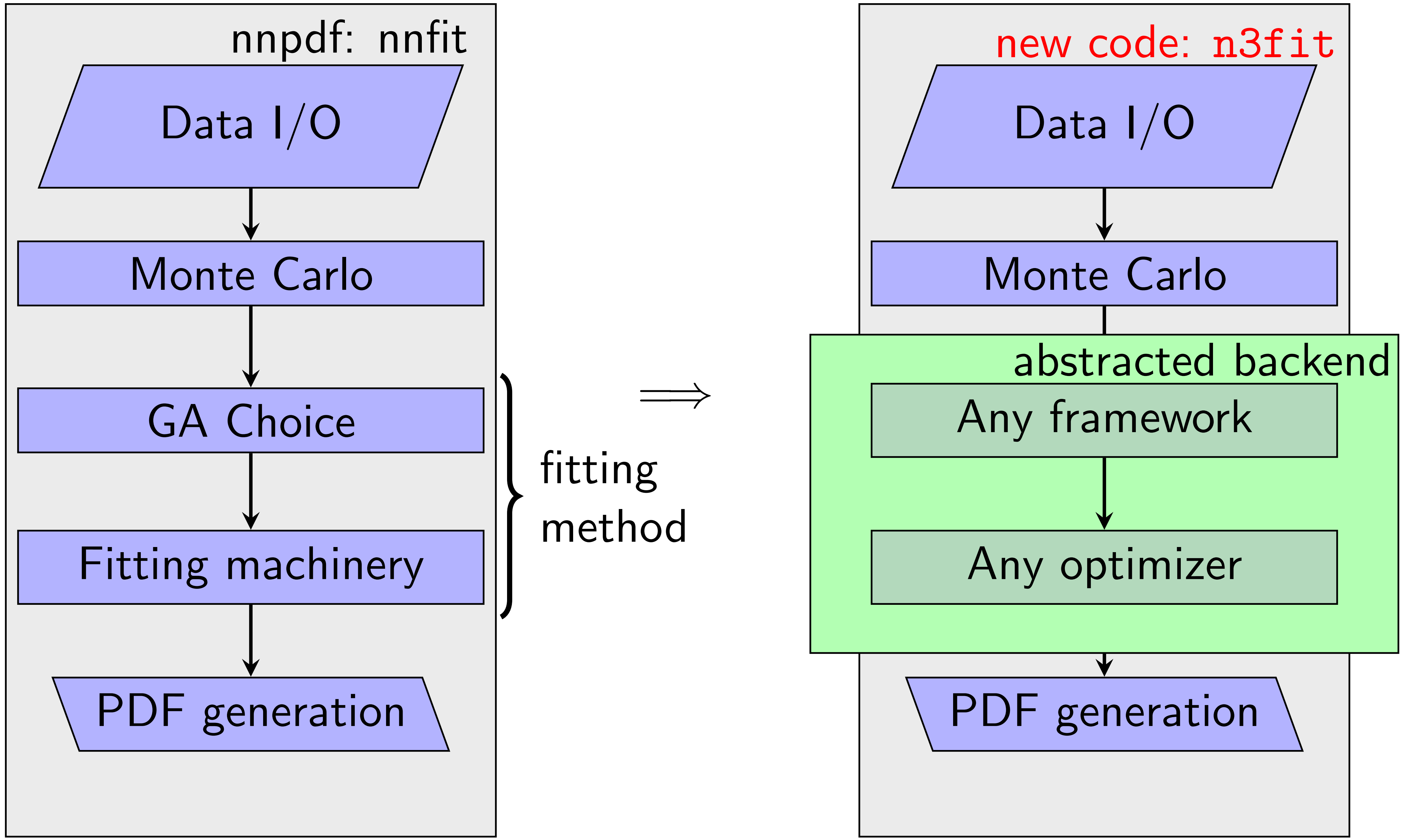
via grid interpolation (NNPDF method)

$$N(p+\mathrm{Pb}\to\pi+X)\propto\sum_{m,n,p=1}^{n_x}\sum_{i,j,k}^{n_f}\left(\mathbf{FK}_{m,n,p,i,j,k}\right)\times\Big(f_i(x_m,Q_0,1)\,f_j(x_n,Q_0,A_{\mathrm{Pb}})\,f_{k\to\pi}(z_p,Q_0,A_{\mathrm{Pb}})\Big)$$

sum over x,z grids *sum over flavour*

Complete restructure of the NNPDF fitting framework: enhanced modularity that dramatically improves its flexibility, in particular to exploit **external ML libraries** *eg* Keras, TensorFlow, …

ML-based PDFs



Complete restructure of the NNPDF fitting framework: enhanced modularity that dramatically improves its flexibility, in particular to exploit **external ML libraries** *eg* Keras, TensorFlow, …

Hyper optimisation

In most Machine Learning applications, the model has several parameters which are typically **adjusted by hand** (trial and error) rather than algorithmically:

- Network architecture: number of layers of neurons per layer, activation functions, …
- Choice of minimiser (which of the Gradient Descent variants?)
- Learning rate, momentum, memory, size of mini-batches, ….
- Regularisation parameters, stopping, dropout rate, patience, …

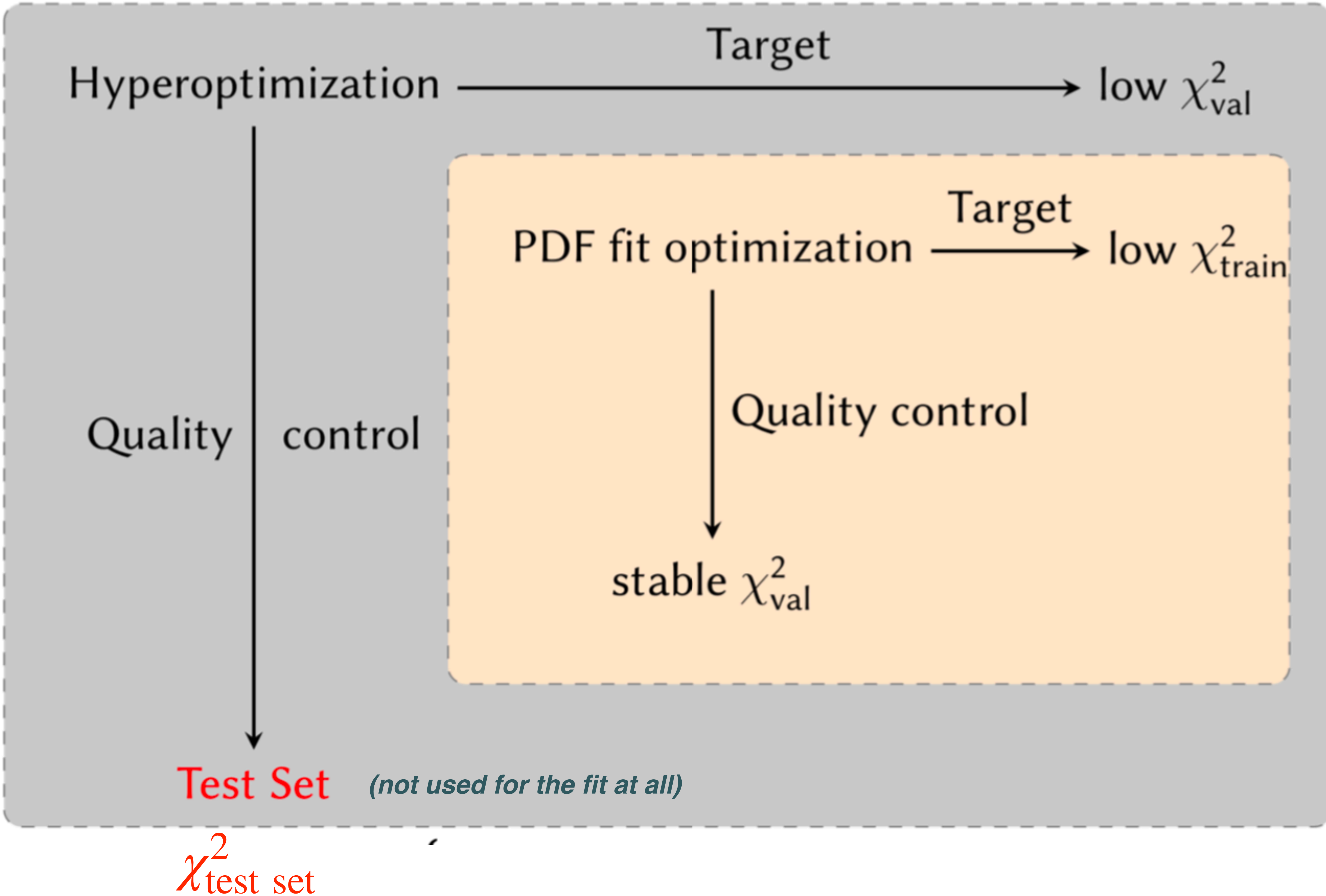
one can avoid the need of subjective choice by means of **an hyperoptimisation procedure**, where all model and training/stopping parameters are determined algorithmically

Such hyperoptimisation requires introducing a **reward function** to grade the model. Note that this is different from the **cost function:** the latter is optimised separately model by model (e.g. for each NN architecture) while the former compares between all optimised models

e.g. cost function $C = E_{\rm tr}$

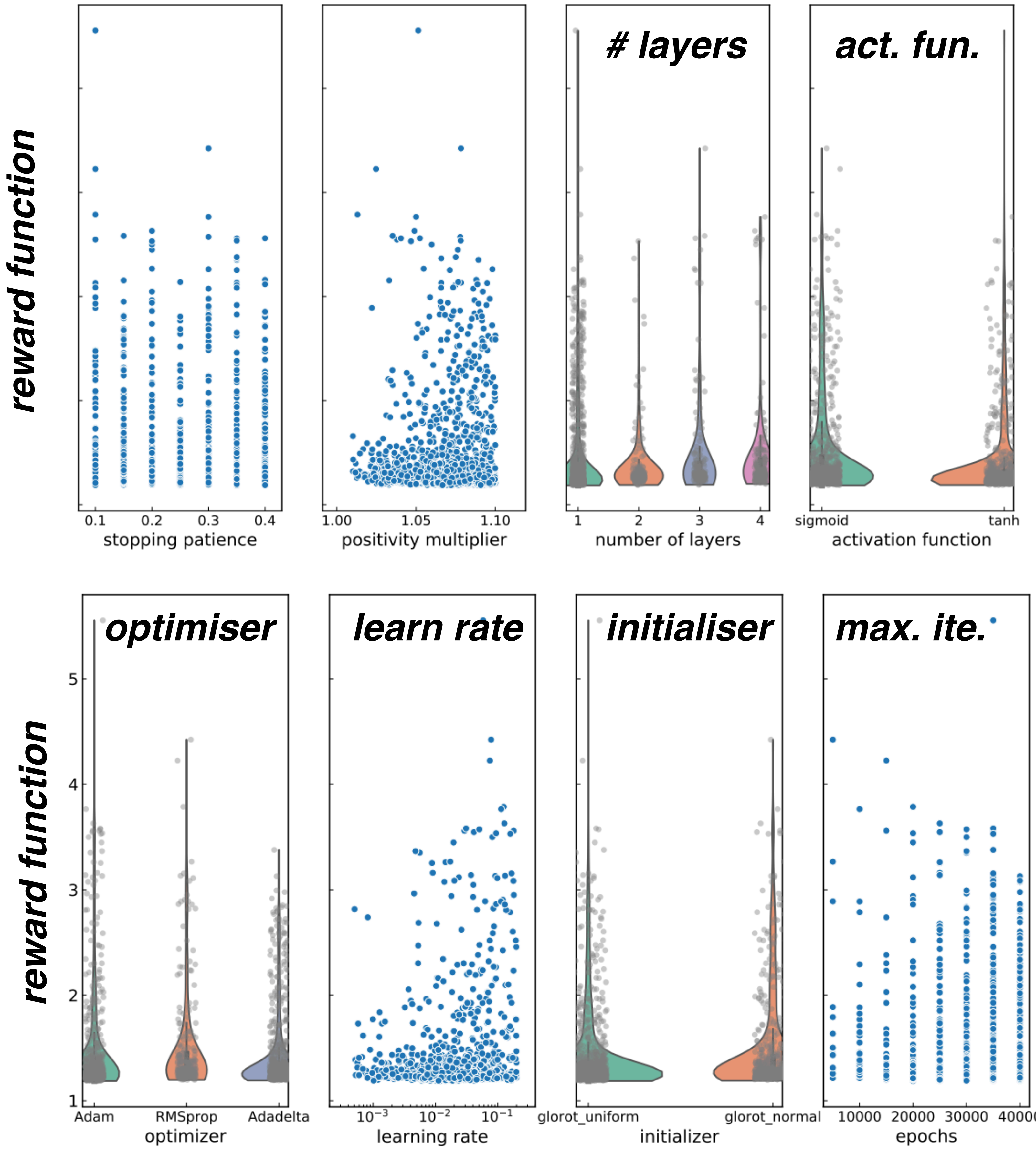
reward function $R = \frac{1}{2}\left(E_{\rm val} + E_{\rm test}\right)$

Hyper optimisation



Hyper optimisation

- In a hyperparameter scan one can compare the performance of **hundreds or thousands** of parameter combinations
- Some choices are **discrete** (type of minimiser, # of layers) others are **continuous** (learning rate)
- One can also **visualise** which choices are more crucial and which ones less important
- The violin plots are the **KDE-reconstructed probability distributions** for the hyper-parameters

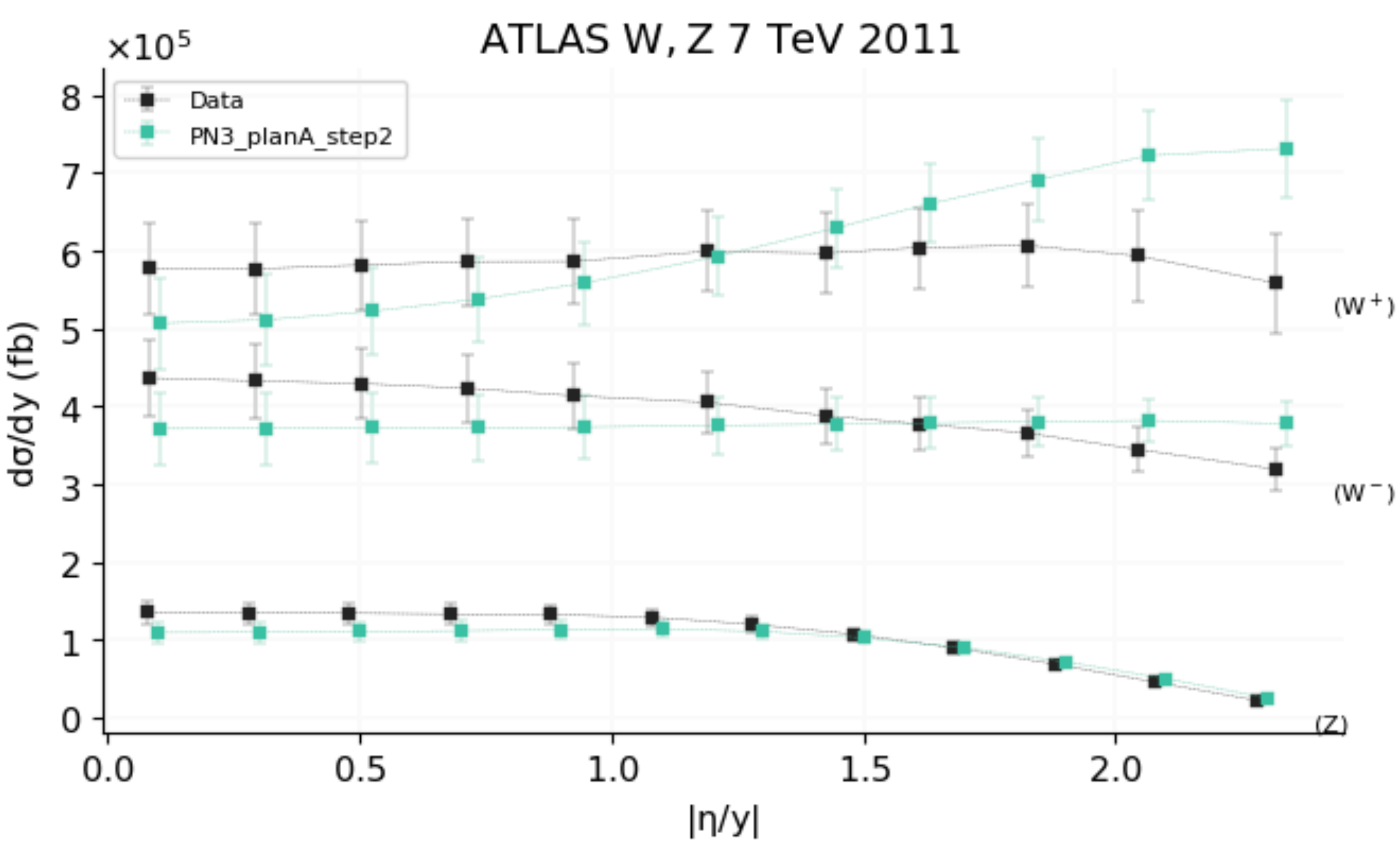


AI & forecasting tests

- Crucial aspect of ML methods, beyond describing existing data, is to **generalise to future data**
- Train PDFs on **pre-HERA** and **pre-LHC data**, and then **forecast** for all data available now
- Include in this exercise PDF errors in the **χ^2 definition**

		n3fit pre-hera		nnfit pre-hera	
		ndata	χ^2/ndata	ndata	χ^2/ndata
HERACOMB	Total	1145	1.135	1145	1.089
ATLAS	Total	360	0.9744	360	0.9443
CMS	Total	409	0.9699	409	0.9200
LHCb	Total	85	1.195	85	1.008
Total	Total	2215	1.055	2215	1.013

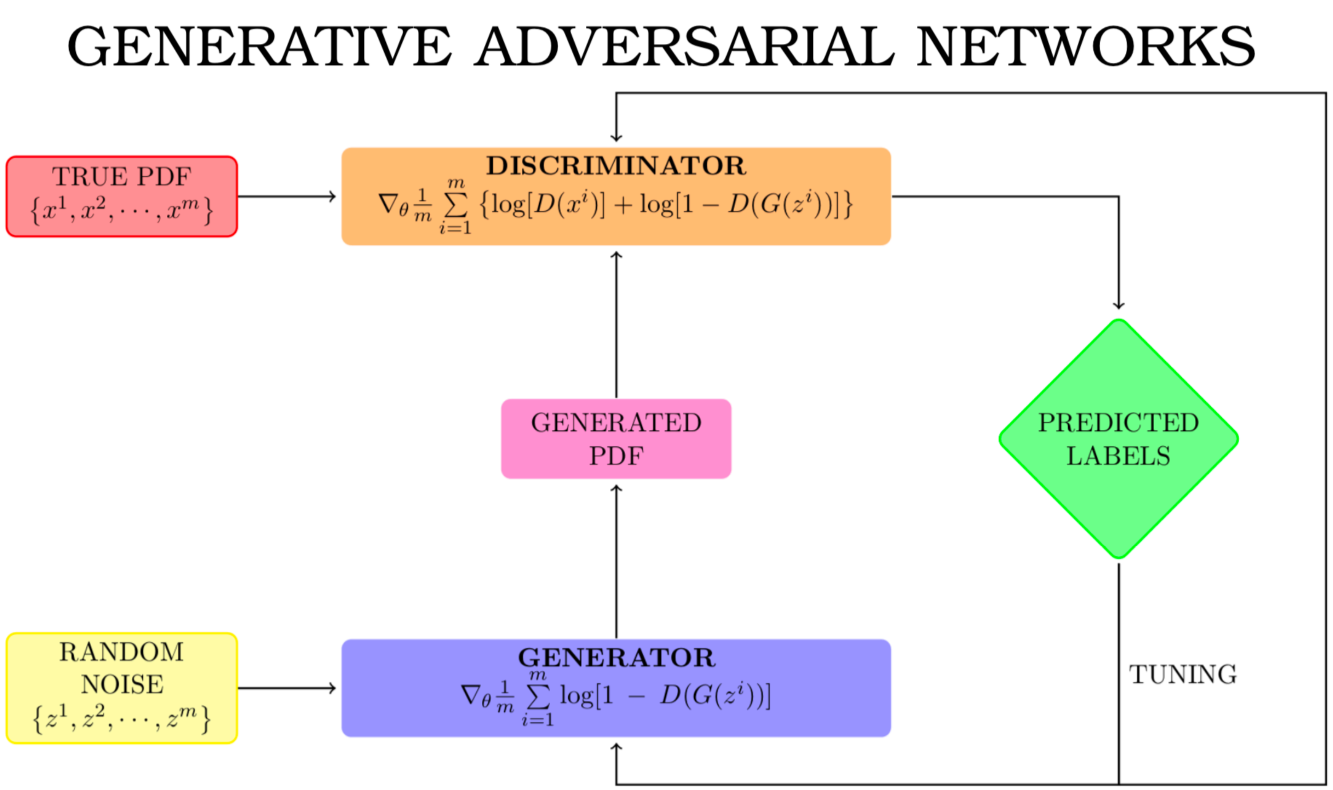
2215 data points not used to train the NN model!

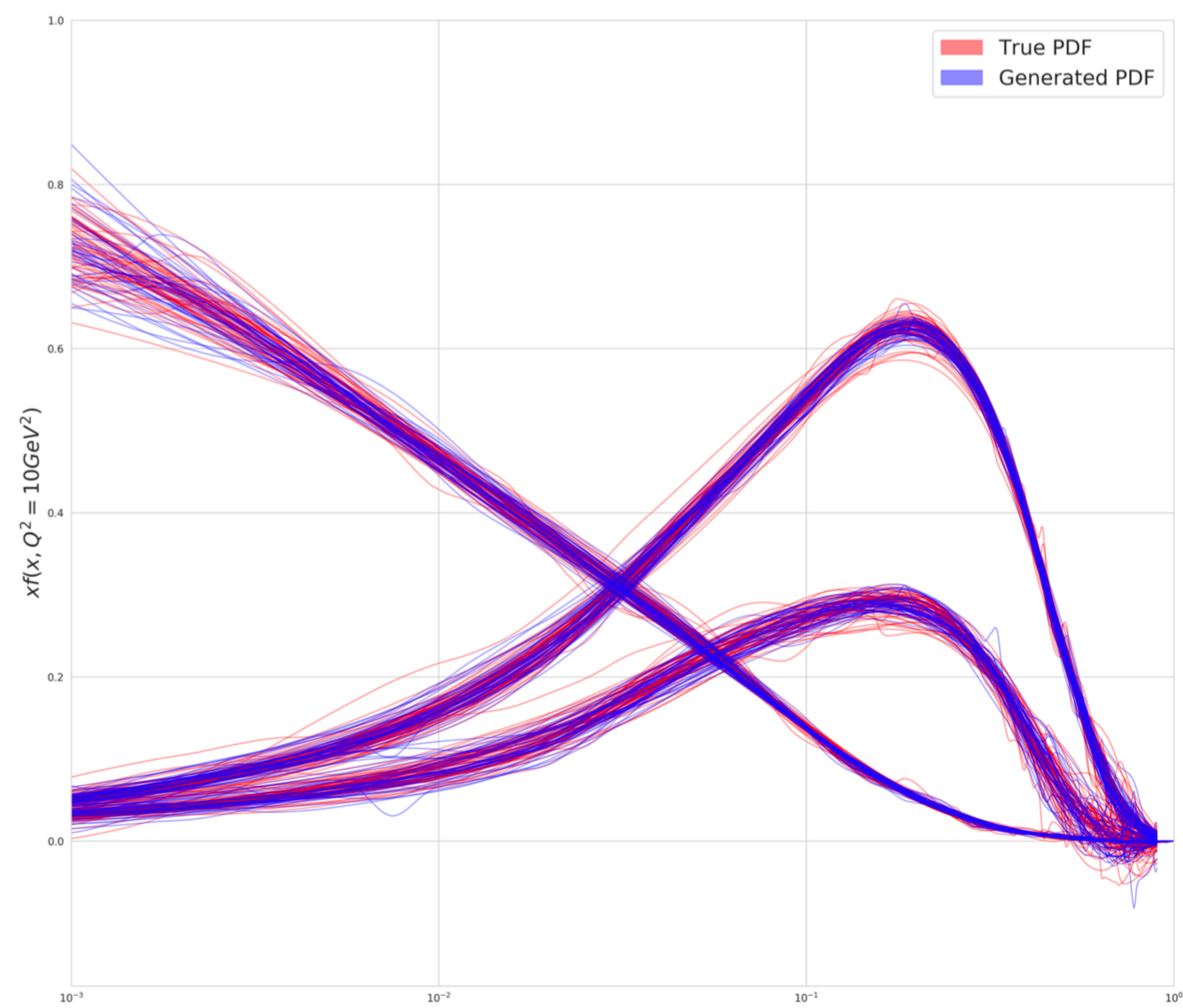


- Training PDFs on only old fixed-target DIS and DY datasets, the extrapolation to ``future" data is fully satisfactory: **χ^2_{new} =1**
- Test succesful both with 3.1 and 4.0 methodologies: in both cases the PDF uncertainties are **faithfully estimated,** with 4.0 being **more accurate** than 3.1

GANs for PDF fits

- Even with all the n3fit speedups, producing large samples of PDF replicas still time-consuming
- Solution: produce new PDF fit replicas using **Generative Adversarial Networks**
- While no additional information is being added, such method can be applied to many cases with a very large $\mathbf{N_{rep}}$ is beneficial, such as **Bayesian reweighting studies**



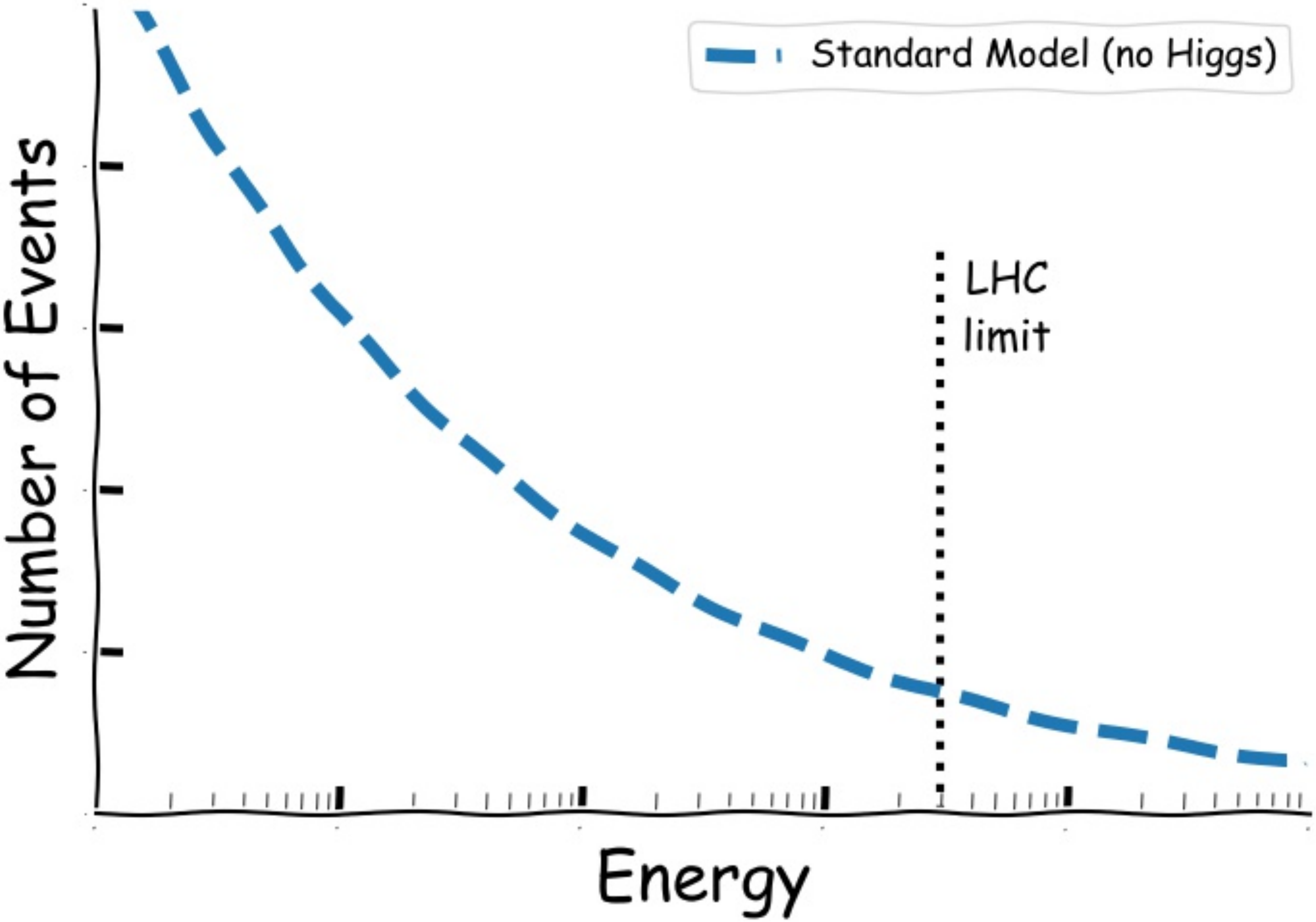


Deep Learning for Effective Field Theories

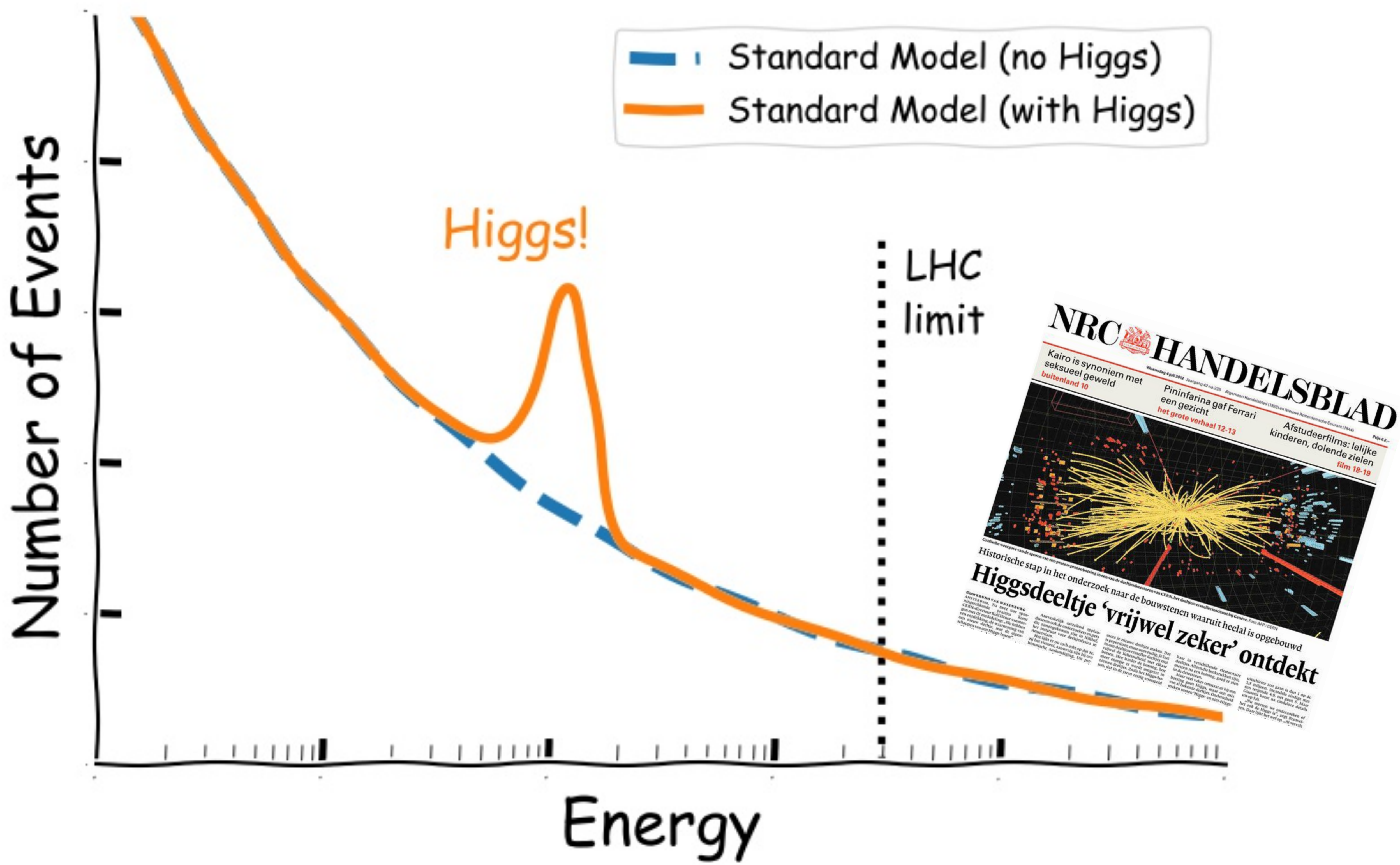
based on Chen et al., arXiv:2007.10356

+ ter Hoeve & Rojo, work in progress

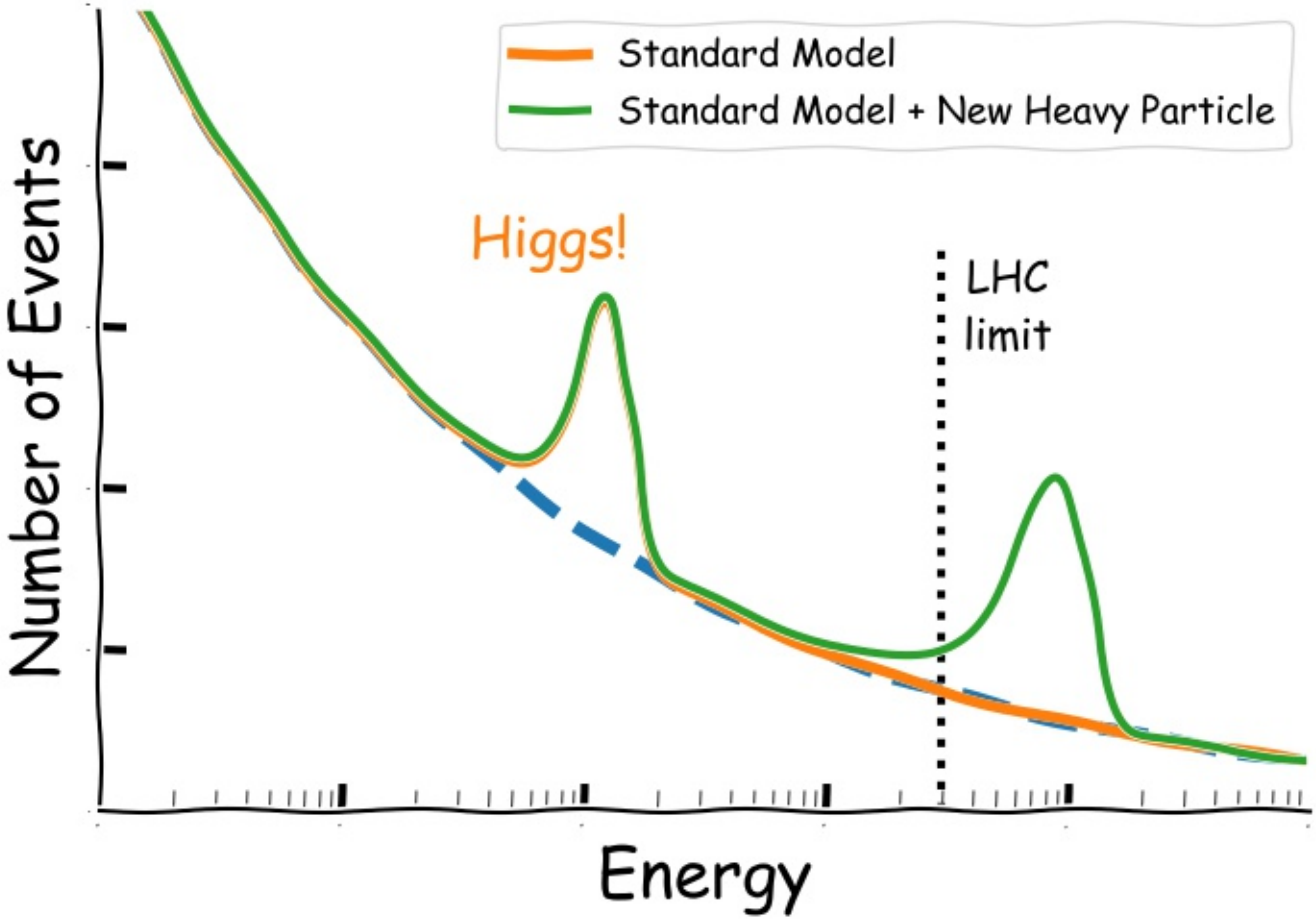
Hunting for New Physics



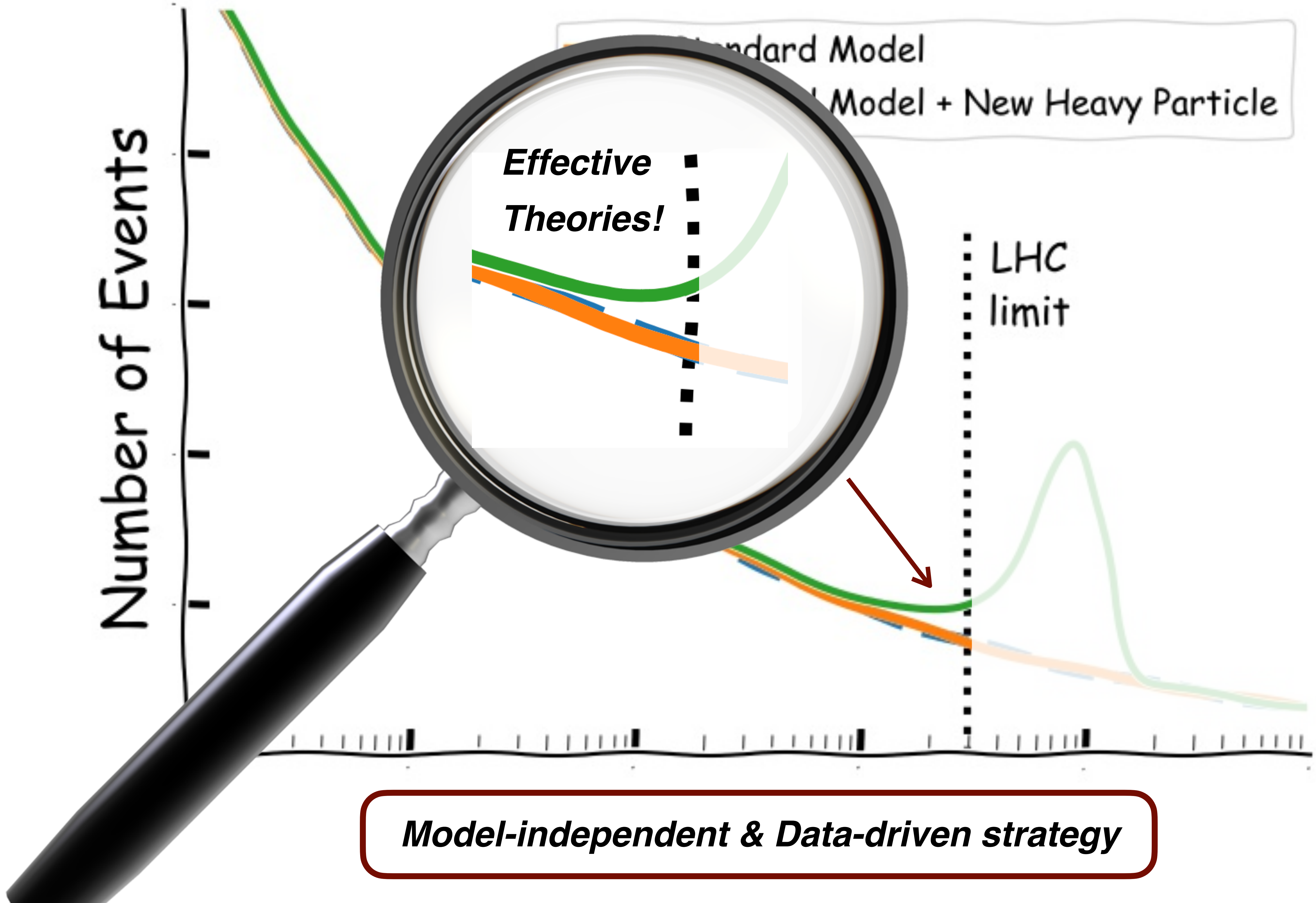
Hunting for New Physics



Hunting for New Physics



Hunting for New Physics



Model-independent & Data-driven strategy

The Standard Model as an Effective Theory

Assemble a New Standard Model from the **bottom up!**

The **Standard Model Effective Field Theory (SMEFT):**

more than 2000!

$$\Big(\text{Standard Model}\Big) + \sum_k c_k \times \Big(\text{New Interaction}\Big)_k$$

extract from data

complete basis spanning space of New Physics theories

rich variety of signals!

constrain **all SMEFT interactions** from a global dataset

The Standard Model as an Effective Theory

Assemble a New Standard Model from the **bottom up!**

The **Standard Model Effective Field Theory (SMEFT):**

$$\mathscr{L}_{\rm SMEFT} = \mathscr{L}_{\rm SM} + \sum_{d=5}^{\infty} \sum_{i=1}^{N_d} \frac{c_i^{(d)}}{\Lambda^{d-4}} \mathcal{O}_i^{(d)}$$

more than 2000!

known physics

extract from data

complete basis spanning space of New Physics theories

rich variety of signals!

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The Standard Model as an Effective Theory

Assemble a New Standard Model from the **bottom up!**

The **Standard Model Effective Field Theory (SMEFT):**

$$\sigma_{\rm SMEFT} = \sigma_{\rm SM} + \sum_{i=1}^{N_6} \frac{c_i}{\Lambda^2}\sigma_i^{(\rm eft)} + \sum_{i,j=1}^{N_6} \frac{c_i c_j}{\Lambda^4}\widetilde{\sigma}_{ij}^{(\rm eft)}$$

known physics

extract from data

rich variety of signals!

constrain **all SMEFT interactions** from a global dataset

Matching

Energy

Full Theory

$$\phi\ (m_\phi)\,,\ \Phi\ (M_\Phi)$$

$$\mathscr{L}_{\rm int} = \lambda_3 \phi^2 \Phi$$

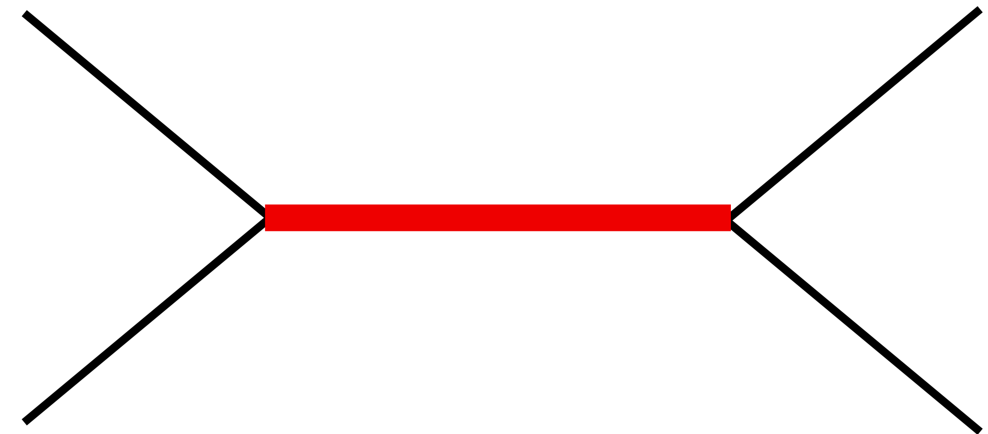
$$E \simeq M_\Phi \gg m_\phi$$

Effective Theory

$$\phi\ (m_\phi)$$

$$\mathscr{L}_{\rm int} \supset c_4(\lambda, M_\Phi)\phi^4$$

$$\phi + \phi \to \Phi \to \phi + \phi$$



Matching

Energy

Full Theory

$$\phi\ (m_\phi)\,,\ \Phi\ (M_\Phi)$$

$$\mathscr{L}_{\text{int}} = \lambda_3 \phi^2 \Phi$$

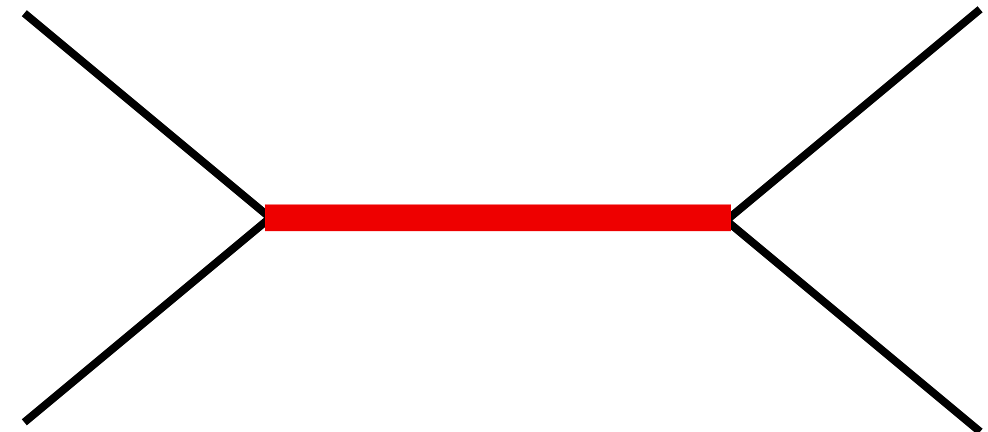
$$E \simeq M_\Phi \gg m_\phi$$

Effective Theory

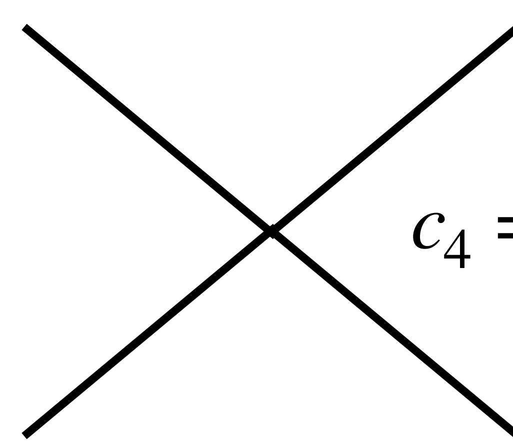
$$\phi\ (m_\phi)$$

$$\mathscr{L}_{\text{int}} \supset c_4(\lambda, M_\Phi)\phi^4$$

$$\phi + \phi \to \Phi \to \phi + \phi$$



$$\phi + \phi \to \phi + \phi$$



$c_4 = \lambda_3^2 / M_\Phi^2$

Low-energy parameters sensitive to ultraviolet dynamics!

Statistically optimal observables for EFT fits

- **Goal**: find the optimal bounds on the EFT coefficients
- **Neyman-Pearson lemma:** the most powerful test at fixed size between two *simple* hypotheses is the (log) likelihood ratio
- However, in EFT problems the likelihood ratio is analytically intractable

$$\lambda(\mathcal{D}) \equiv \log \frac{\mathcal{L}(H_1|\mathcal{D})}{\mathcal{L}(H_0|\mathcal{D})}$$

- **Solution:** use a deep learning model to parametrise the extended likelihood ratio

SM hypothesis

Number of events

$$\boxed{\lambda(\mathcal{D}) \equiv \log \frac{\mathcal{L}(H_1|\mathcal{D})}{\mathcal{L}(H_0|\mathcal{D})} = \mathrm{N}(\mathrm{X}|H_0) - \mathrm{N}(\mathrm{X}|H_1) - \sum_{i=1}^{\mathcal{N}} \log \frac{d\sigma_0(x_i)}{d\sigma_1(x_i)}}$$

Extended likelihood ratio

EFT hypothesis (null)

Expected number of events under the SM

Cross section ratio

Statistically optimal observables for EFT fits

- Exploit **quadratic dependence** of the EFT cross-sections in its coefficients

$$d\sigma_0(x;c) = d\sigma_1(x)\,\left\{[1 + c\,\alpha(x)]^2 + [c\,\beta(x)]^2\right\}$$

EFT differential cross section

final-state kinematics

SM differential cross section

Quadratic dependence on *c* and positivity constraint

- Can be generalised to any number of Wilson coefficients

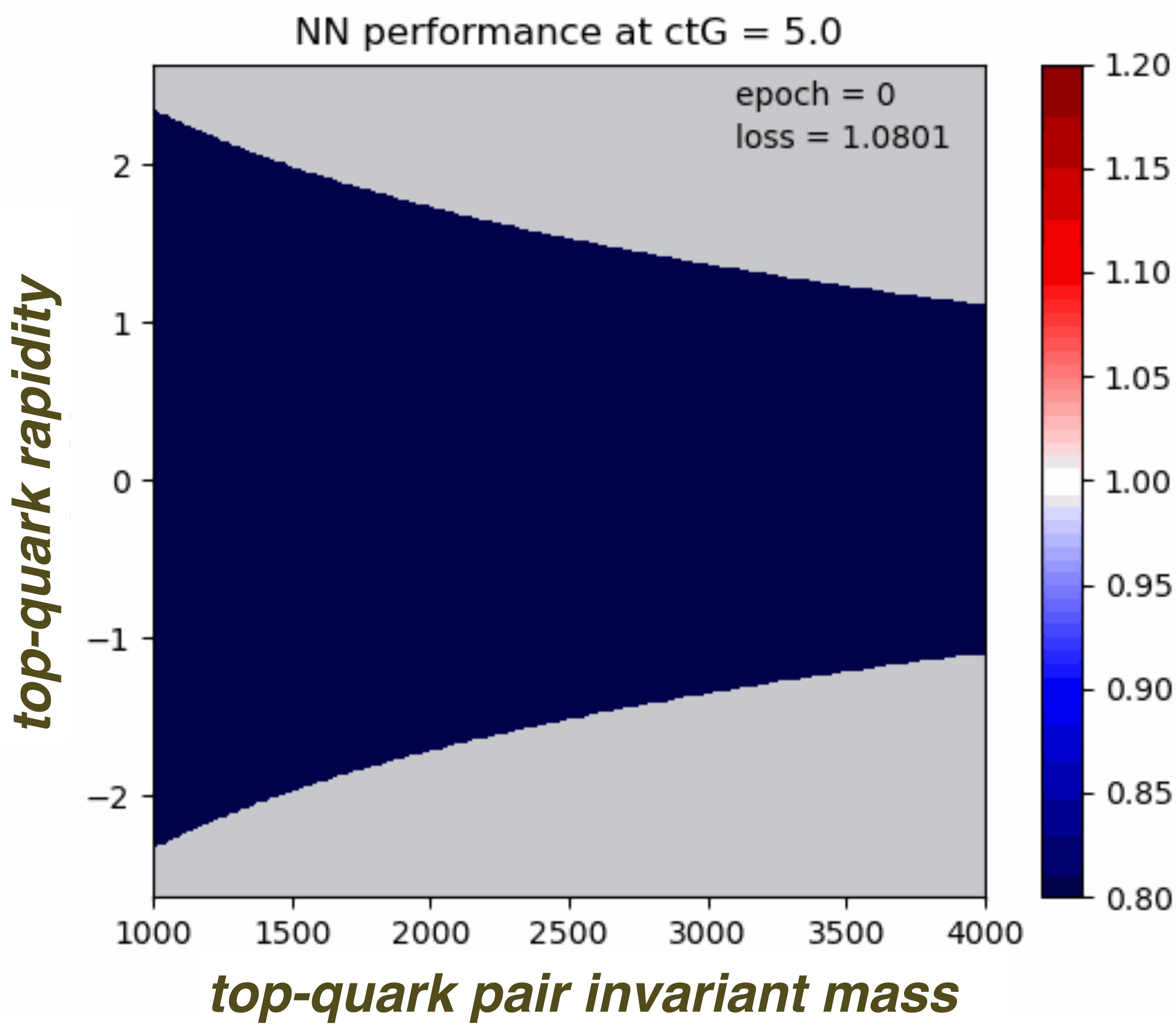
$$d\sigma_0(x,c) = d\sigma_1(x)\left[1 + \sum_{i=i}^{n_{\rm op}} c_i\alpha_i(x) + \sum_{j\geq i}^{n_{\rm op}} c_ic_j\beta_{ij}(x)\right]$$

input: final-state kinematics
output: DNNs

- Train **deep neural networks** on Monte Carlo (ideally, real) data to parametrise the likelihood ratio and use it to construct statistically optimal EFT observables

Statistically optimal observables for EFT fits

- Toy model: (stable) top quark pair production at 14 TeV
- Validate **NN-based likelihood ratio** with **analytical calculation**



$$\frac{d\sigma_0(y_t, m_{t\bar{t}}, c_{tG})\,|_{\rm DNN}}{d\sigma_0(y_t, m_{t\bar{t}}, c_{tG}\,|_{\rm exact}}$$

Reconstructing **2D likelihood** takes a few minutes

now working on **scaling up to *N* operators and fully differential processes**

Deep Learning for Electron Microscopy

ML4HEP meets Electron Microscopy

Ultramicroscopy 222 (2021) 113202

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Charting the low-loss region in electron energy loss spectroscopy with machine learning

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ABSTRACT

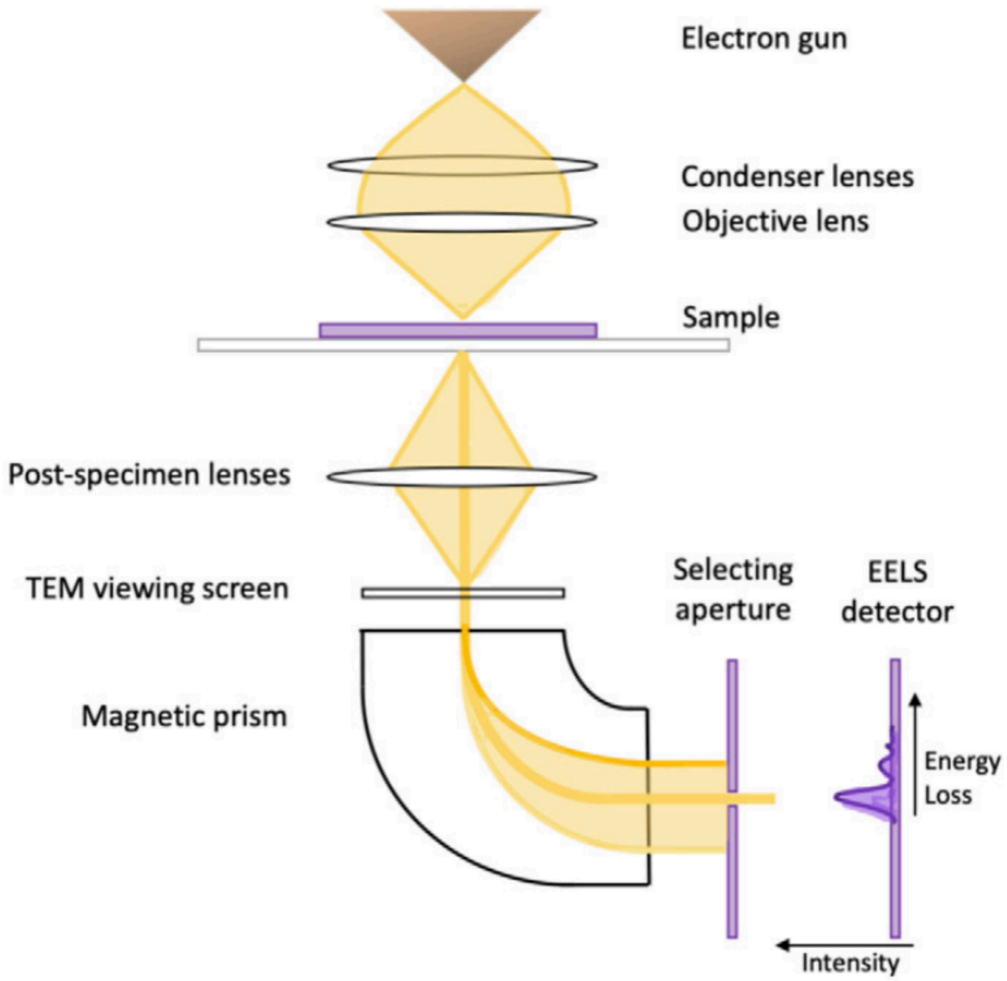
Exploiting the information provided by electron energy-loss spectroscopy (EELS) requires reliable access to the low-loss region where the zero-loss peak (ZLP) often overwhelms the contributions associated to inelastic scatterings off the specimen. Here we deploy machine learning techniques developed in particle physics to realise a model-independent, multidimensional determination of the ZLP with a faithful uncertainty estimate. This novel method is then applied to subtract the ZLP for EEL spectra acquired in flower-like WS_2 nanostructures characterised by a 2H/3R mixed polytypism. From the resulting subtracted spectra we determine the nature and value of the bandgap of polytypic WS_2, finding $E_{BG} = 1.6^{+0.3}_{-0.2}$ eV with a clear preference for an indirect bandgap. Further, we demonstrate how this method enables us to robustly identify excitonic transitions down to very small energy losses. Our approach has been implemented and made available in an open source Python package dubbed `EELSfitter`.

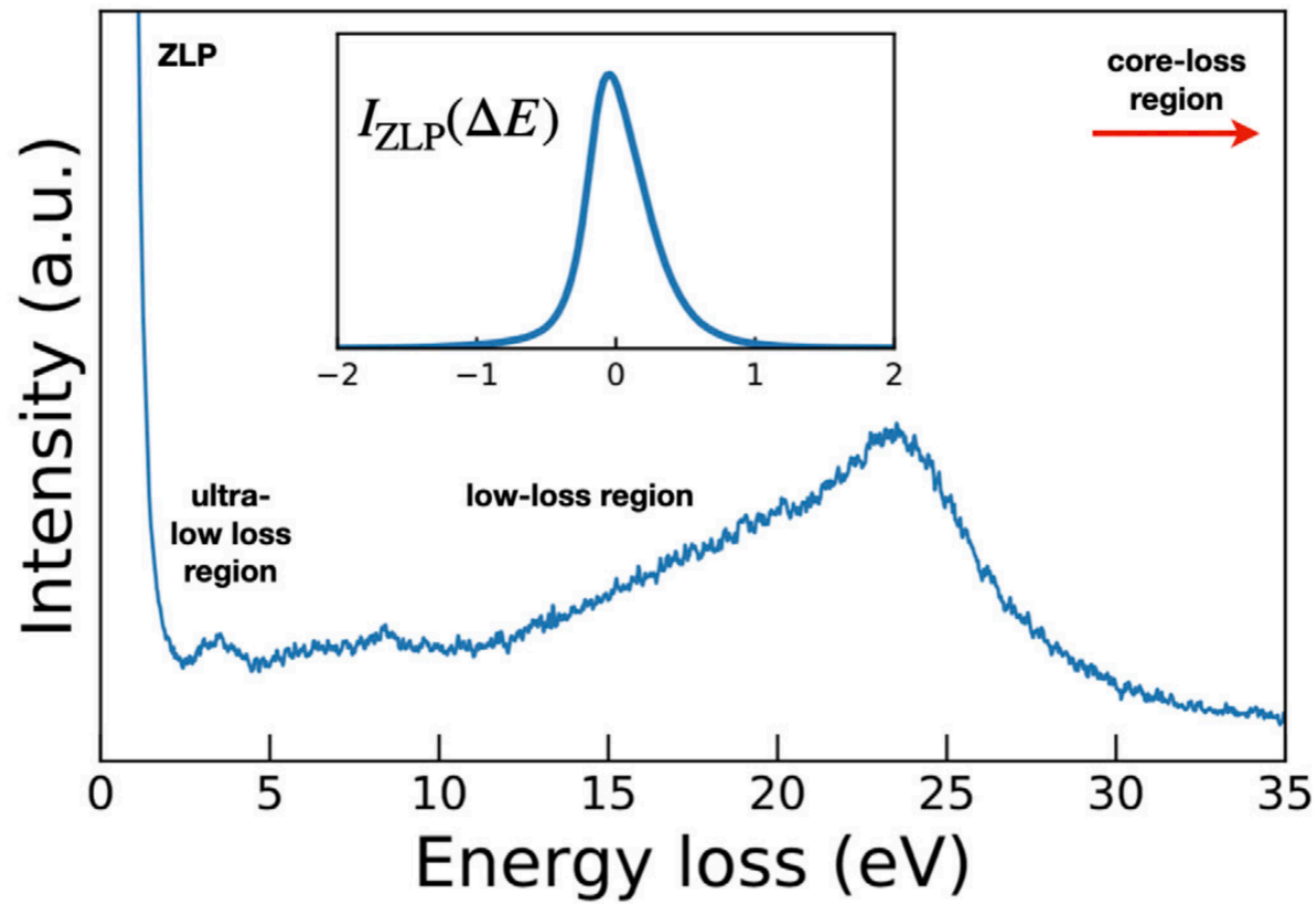
Roest, van Heijst, Maduro, Rojo, Conesa-Boj, *Ultramicroscopy* (2021)

van Heijst, Mukai, Okunishi, Hashiguchi, Maduro, Roest, Rojo, Conesa-Boj, *Annalen der Physiek* (2021)

Postmes, Brokkelkamp, van Heijst, ter Hoeve, Maduro, Rojo, Conesa-Boj, *in preparation*

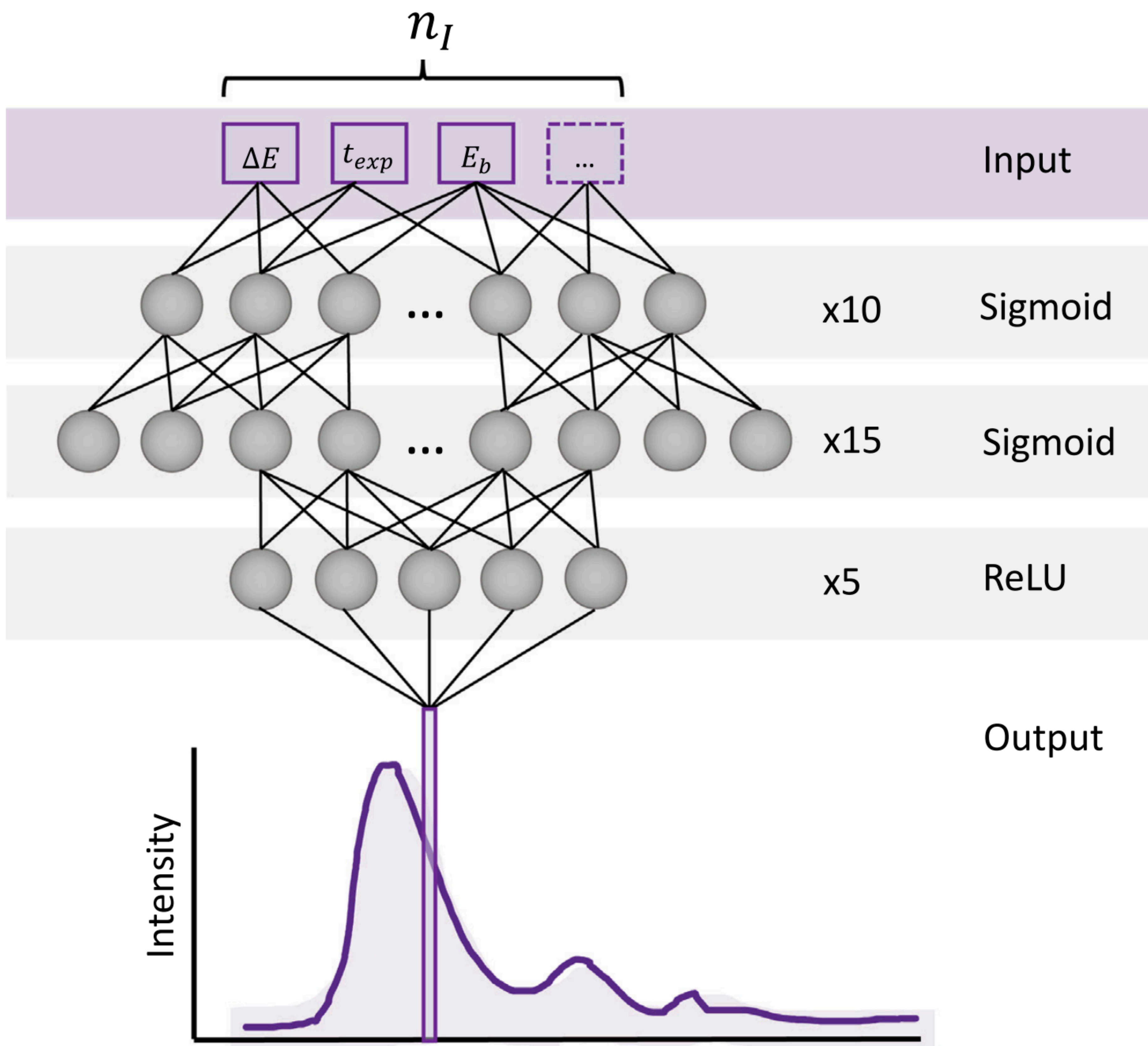
Background subtraction in EM



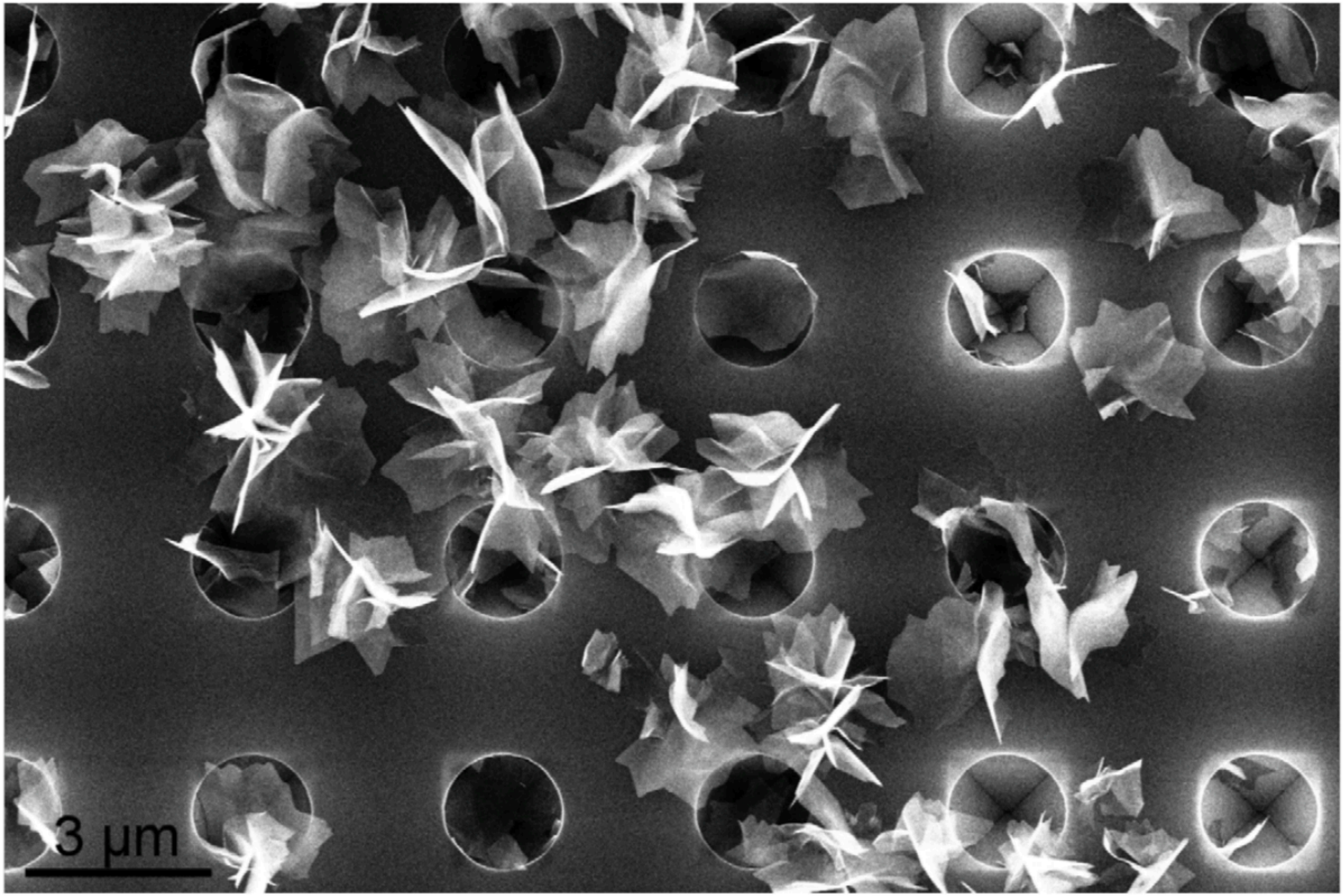


- Electron energy-loss spectroscopy (EELS) measurements affected by **huge background** at low-energy losses: complicates *e.g.* interpretation of material properties
- **Solution:** treat these backgrounds as the PDFs: **parametrise then from data using ANNs** and subtract them in an unbiased, model-independent manner

An ANN model for EELS backgrounds

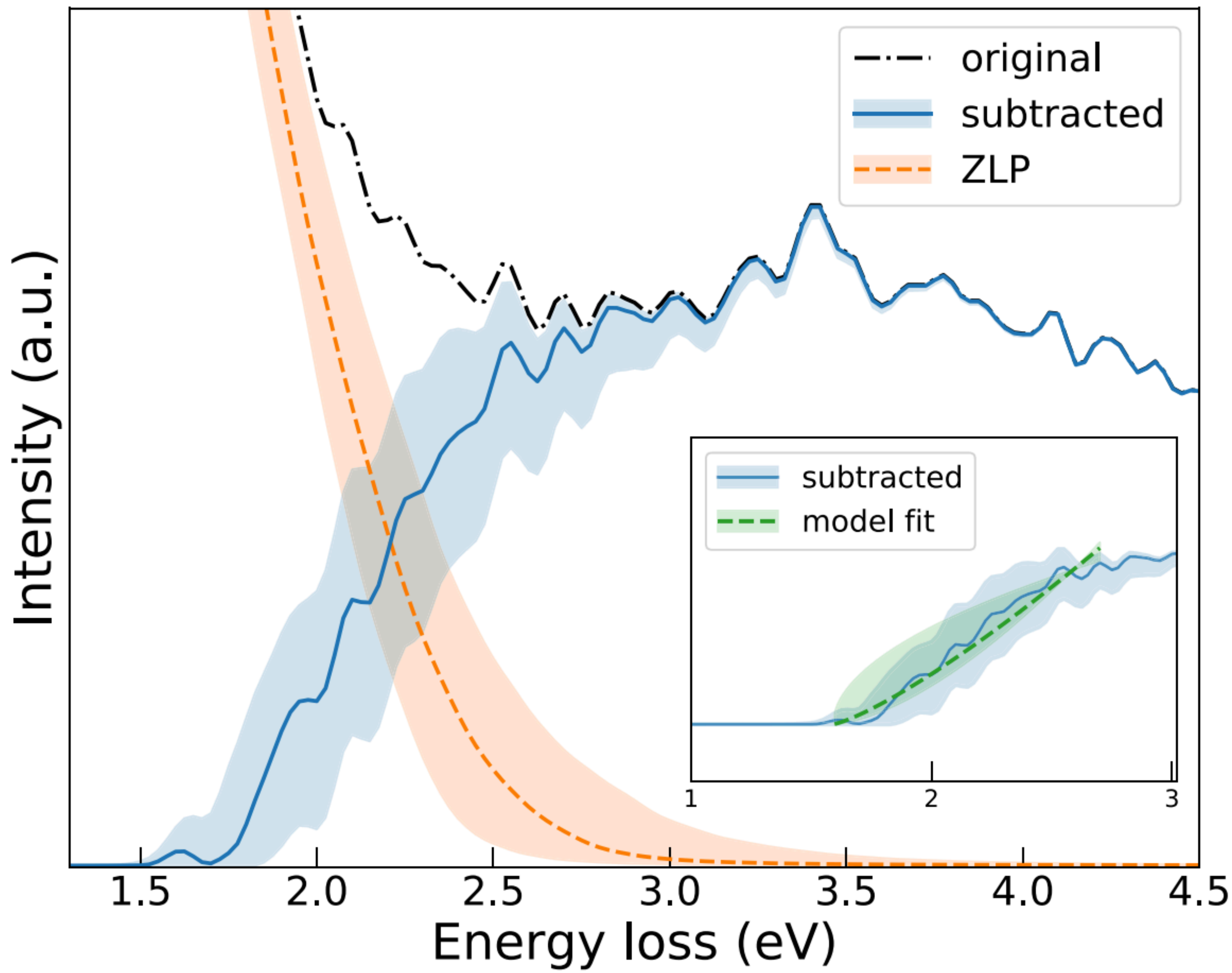


WS_2 Nanoflowers



Deploy this ML method to characterise local electronic properties of **nano-structured quantum materials**: in this case, nanoflowers built upon **2D materials**

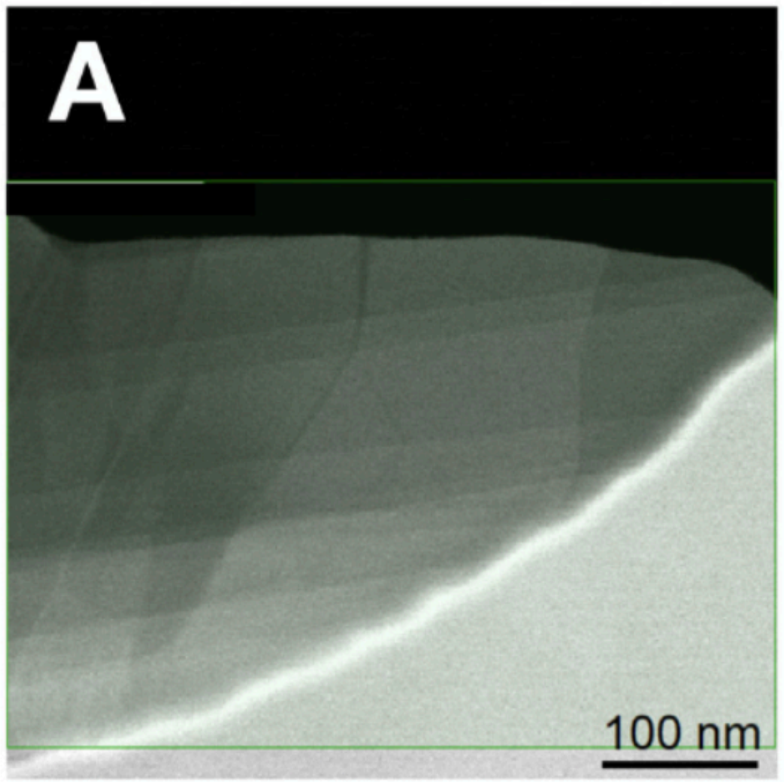
Bandgap determination

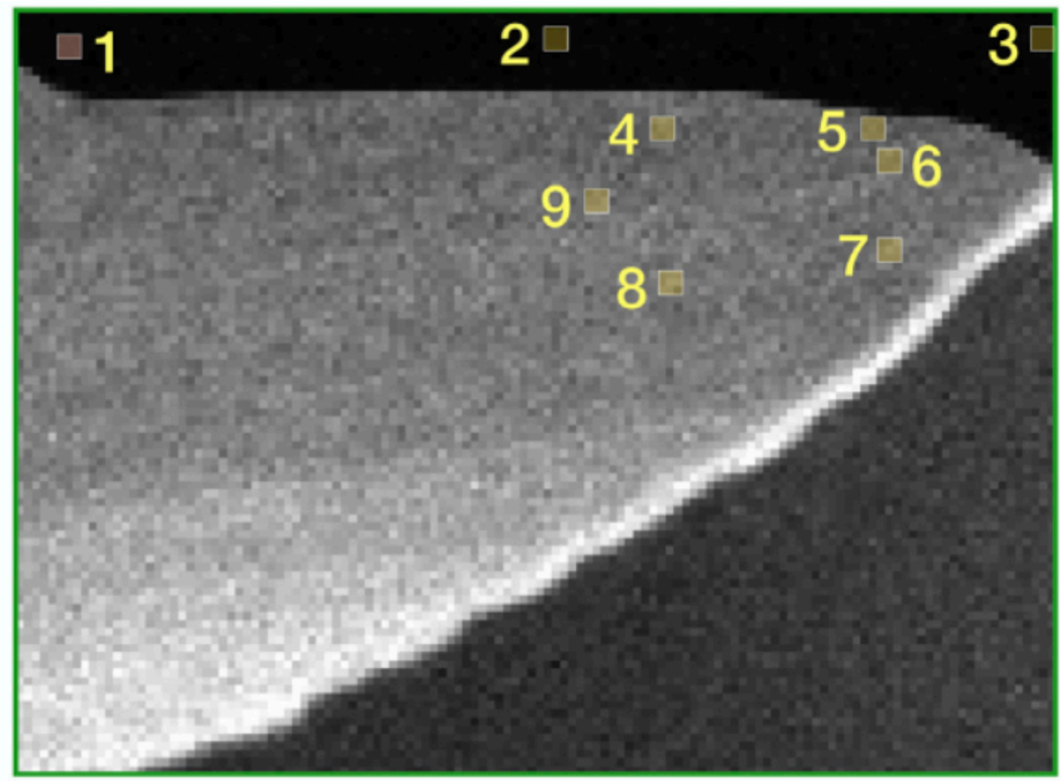


For the first time, we determine the **bandgap** of 3R/2H polytypic WS_2

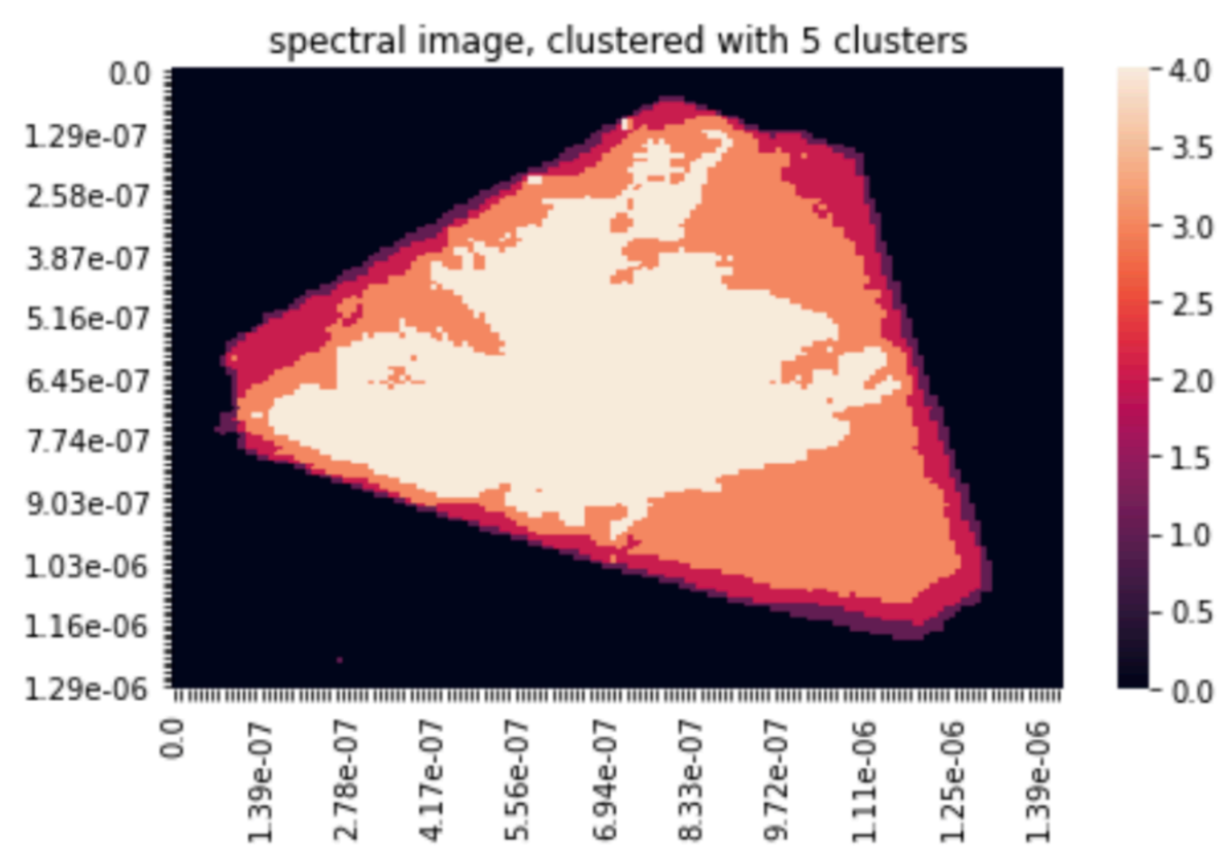
$$E_{\mathrm{BG}} = 1.6^{+0.3}_{-0.2}\,\mathrm{eV}\,, \quad b = 1.3^{+0.3}_{-0.7}\,.$$

Big Data in Electron microscopy





- ☑ Each EELS spectral image contains **O(1M) individual spectra**
- ☑ Use **unsupervised** learning to cluster them and them deep learning to extract automatically all physical information
- ☑ Bandgap values, thickness, dielectric function, plasmons, excitons ….



Summary

The accurate determination of the **quark and gluon structure of the proton** is an essential ingredient for **LHC phenomenology** and **beyond**

- Deep-learning methods allow a **robust, bias-free interpretation of precision hard-scattering data** and make possible a deeper understanding of proton structure

- Many hurdles need to be overcome: long training times, choice of hyperparameters, avoiding overfitting, unbalanced training …

- The same deep learning strategies can be used in the context of **EFT fits** to parametrise multi-dimensional likelihoods and design optimally sensitive observables

- Ditto for data analysis in electron microscopy: bringing **HEP methods to quantum material physics** opens many avenues for new studies in quantum nanoscience