



DAVIDSON



Machine learning techniques
to map from experimental cross sections to
QCD theory parameters

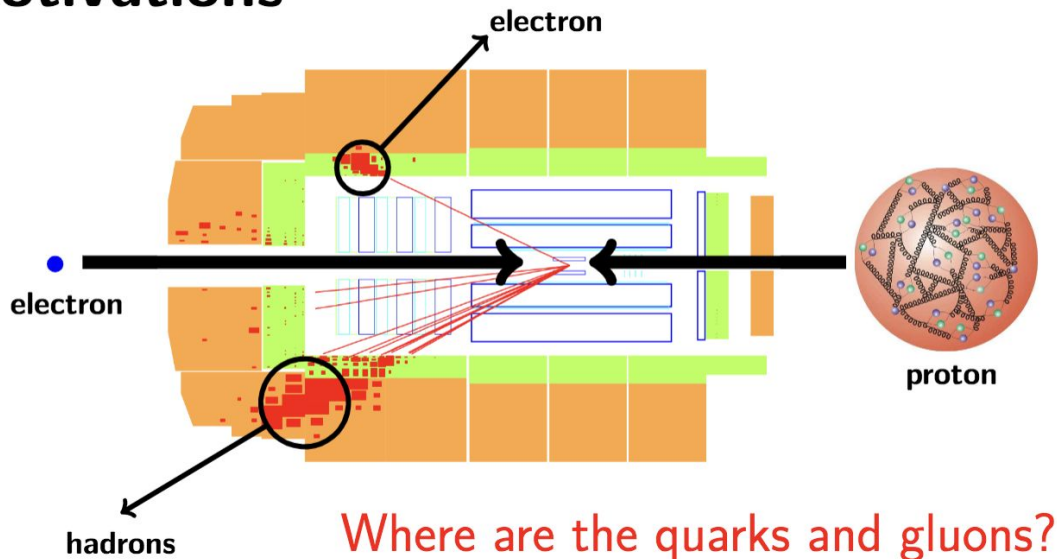
Eleni Tsitinidi



What is QCD

Quantum Chromodynamics (QCD) is the theory that pertains to quark-gluon interactions and the strong force, particularly as components of hadrons.

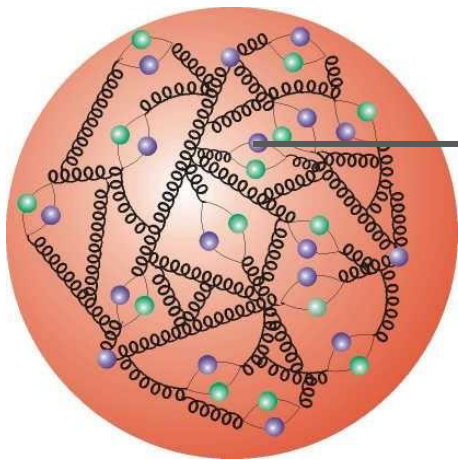
Motivations



Quarks and gluons
cannot be measured
directly

Picture: Nobuo Sato

PDF function : How are quarks and gluons distributed? (number density)



k

$$x = \frac{k}{P}$$

Momentum fraction

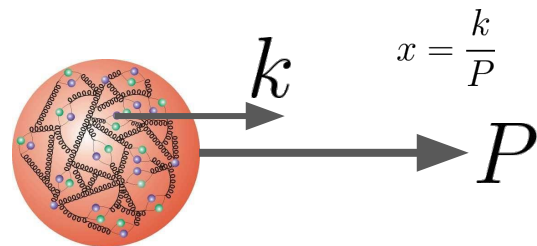
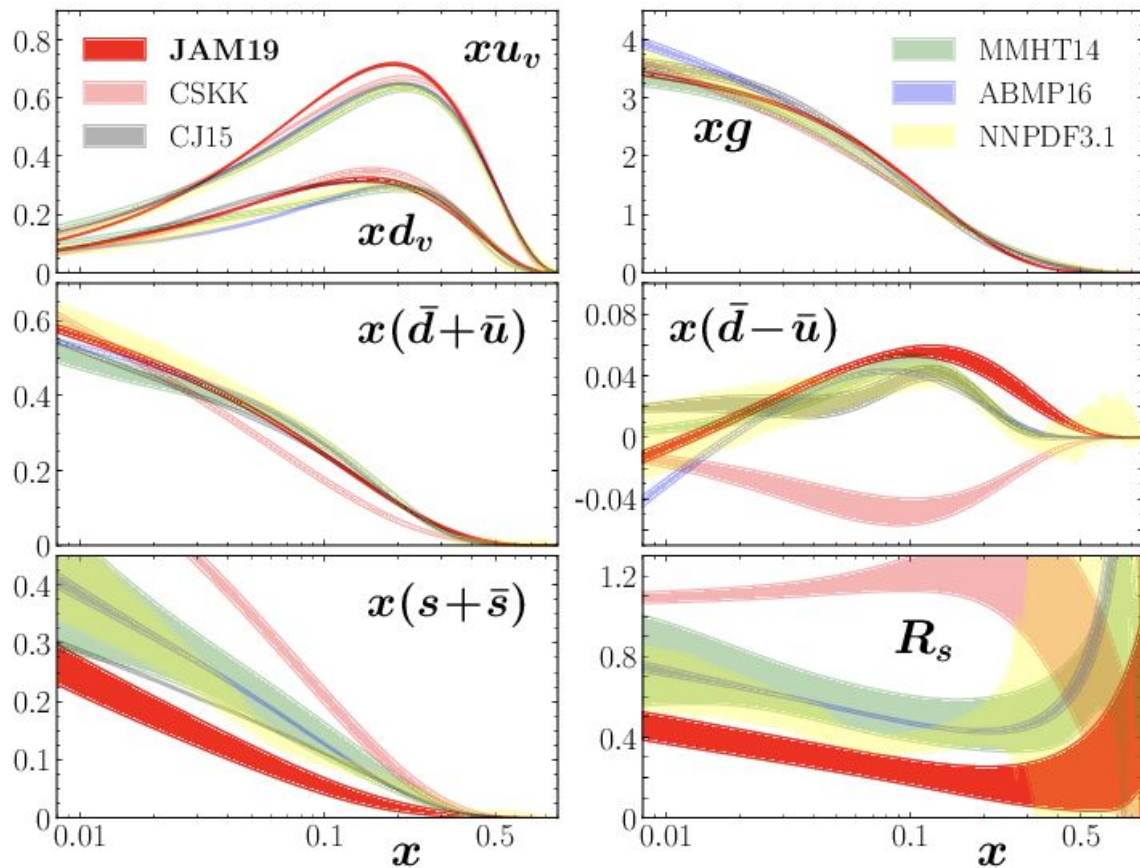
P

$$f_i(x) = \lim_{\Delta x \rightarrow 0} \frac{N_{i,x}}{\Delta x}$$

Parton distribution functions (PDFs)

Number of partons of type "i" in an interval x and $x+dx$

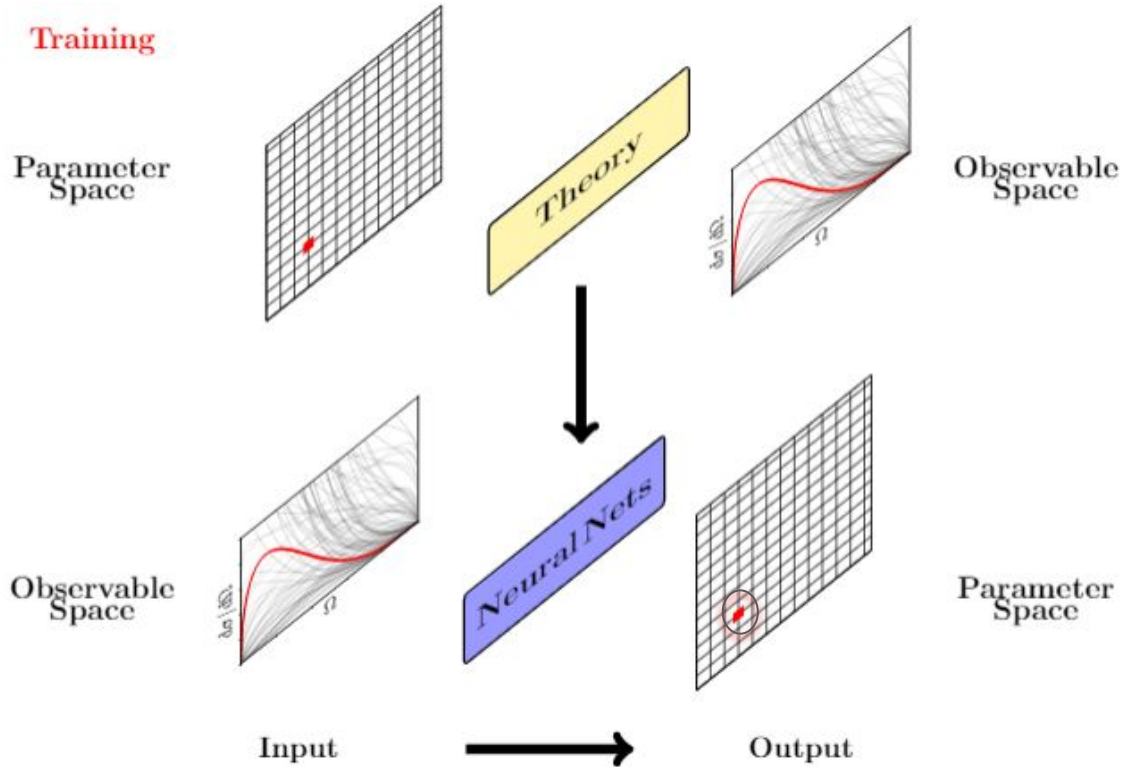
PDF extracted from experimental data



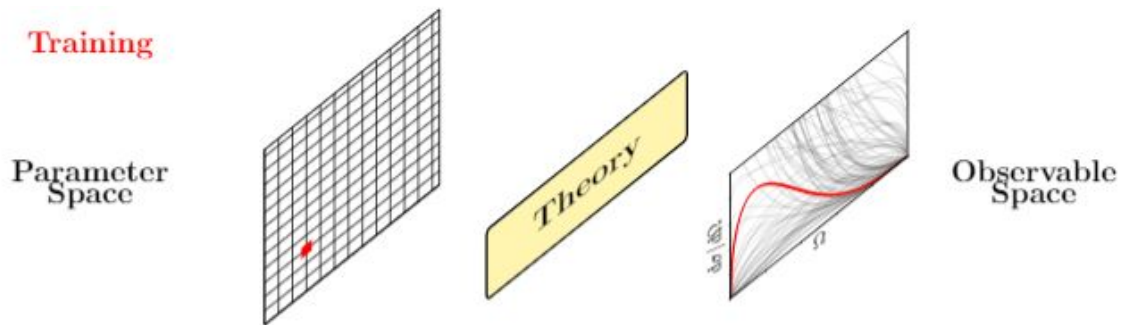
$$u_v = u - \bar{u}$$

$$d_v = d - \bar{d}$$

Initial problem - Multiple Solutions



Jefferson Lab Angular Momentum (JAM) workflow



JAM model



How JAM tunes the parameters

Experimental data

Experimental statistical uncertainties

Experimental systematic uncertainties

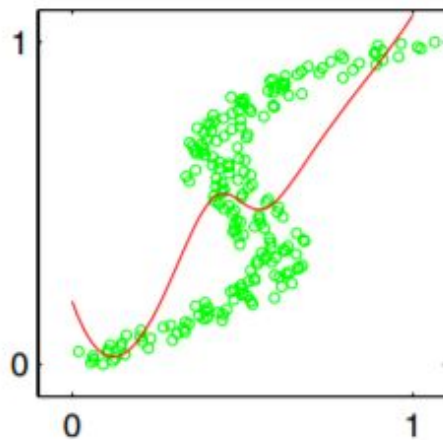
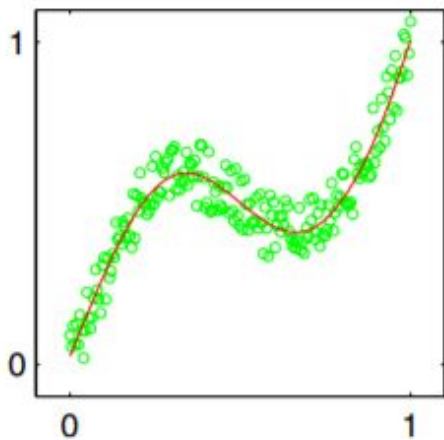
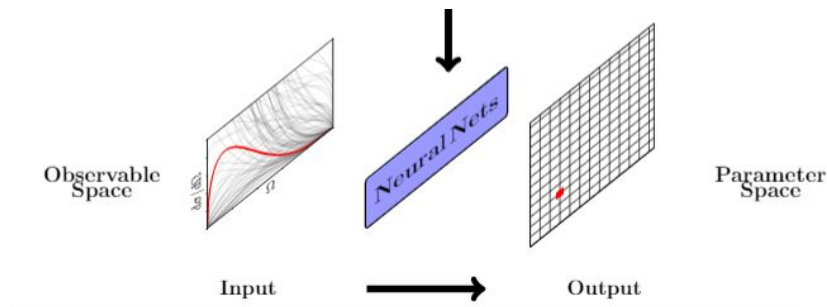
Theory model

parameters

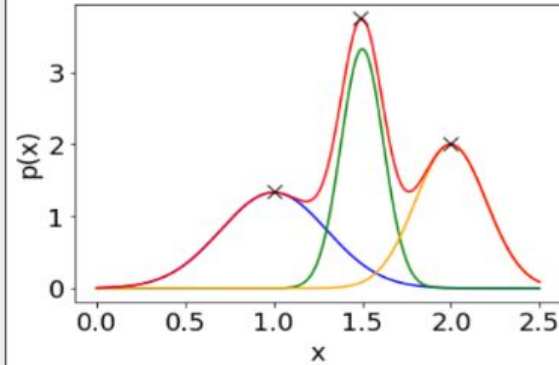
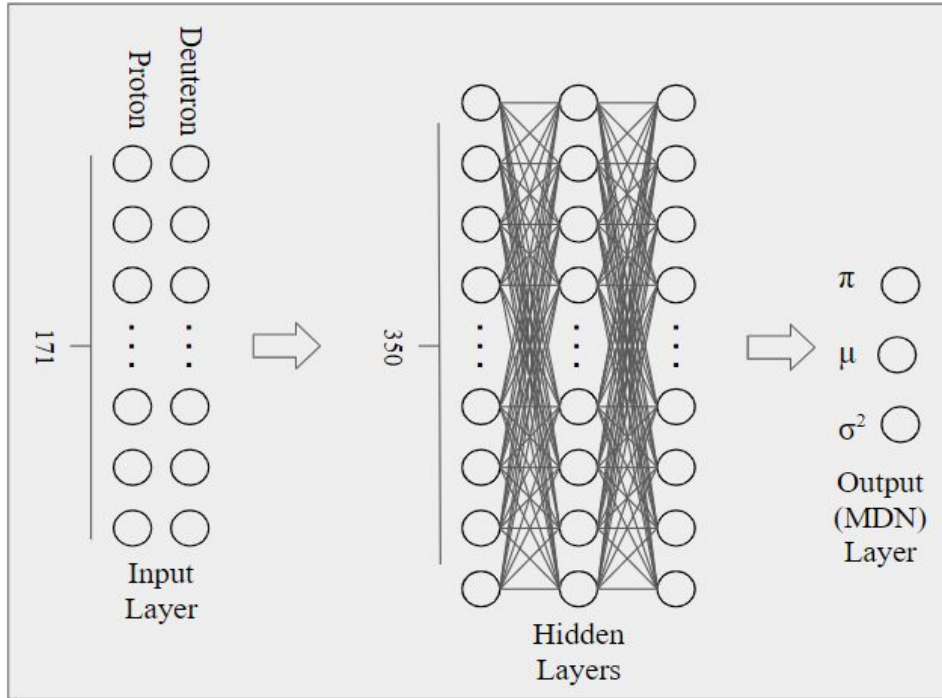
Loss function

$$\chi^2(\mathbf{a}, \text{data}) = \sum_{e,i} \left(\frac{d_{e,i} - \sum_k r_{e,k} \beta_{e,k,i} - t_{e,i}(\mathbf{a}) / N_e}{\alpha_i} \right)^2 + \sum_k r_{e,k}^2 + \left(\frac{1 - N_e}{\delta N_e} \right)^2 \quad (16)$$

Inverse problem with standard ML



Model Architecture - Mixture Density Network



Output Layer Interpretation:

$$p(\mathbf{t}|\mathbf{x}) = \sum_{k=1}^K \pi_k(\mathbf{x}) \mathcal{N}(\mathbf{t} | \boldsymbol{\mu}_k(\mathbf{x}), \sigma_k^2(\mathbf{x}))$$

Further architectures

Auto-Encoder Architecture

AE

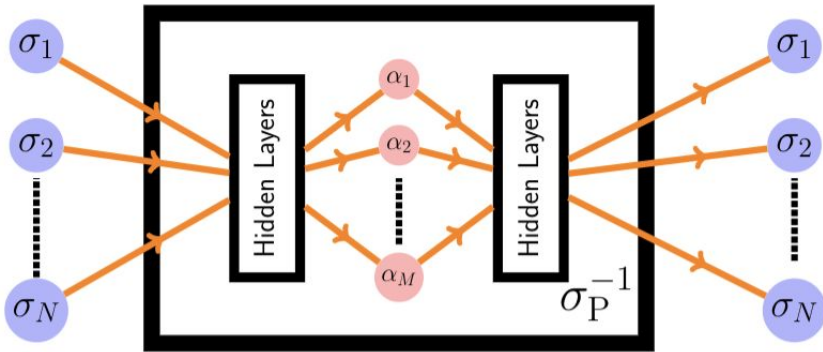


FIG. 3. Inverse mapper based on the parameter supervised autoencoder.

Auto-Encoder with embedded MDN architecture

AEMDN

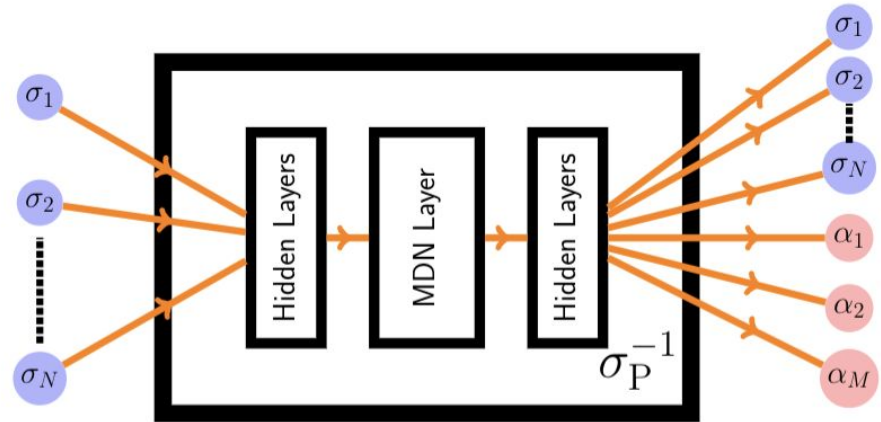


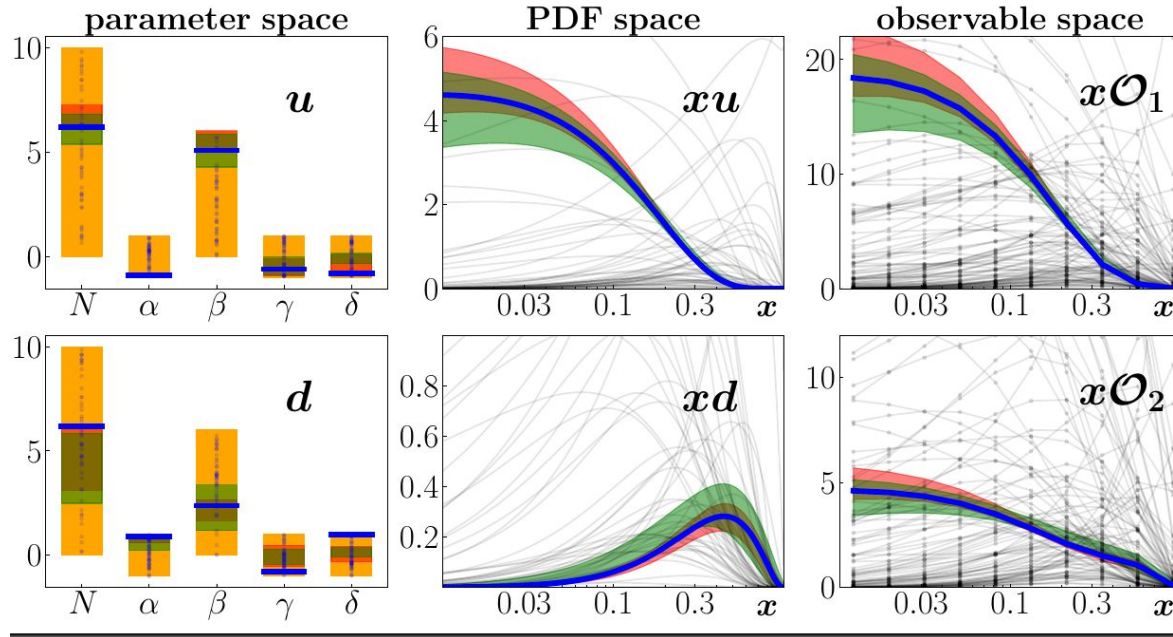
FIG. 4. The parameter supervised autoencoder with the MDN layer.

Where $\alpha_1 \dots \alpha_M$ are the actual parameters

Data

| | Simplified model | DIS data |
|---|--|--|
| Cross sections (Observable space) | 171 σ_p 171 σ_n Xsec σ_p and σ_n mimic Fp2 And Fn2 structure functions | 2680 The cross section space is defined by the kinematics of the world's inclusive DIS datasets from SLAC (p,d), BCDMS (p,d), NMC (p,d/p) and HERA (p) |
| Parameters | 10 | 25 |
| Parton Distribution Functions (PDFs) "probability densities" of parton carrying a momentum fraction x at a squared energy scale Q ² | $i = \bar{u}, \bar{d},$ | $i = \bar{u}, \bar{d}, s \text{ and } \bar{s}.$ $i = g, u_v \text{ and } d_v$ And relationships between them |

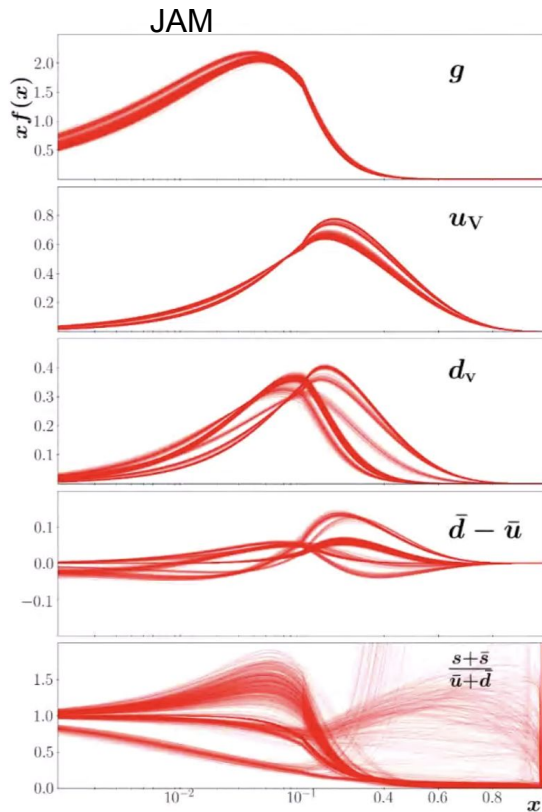
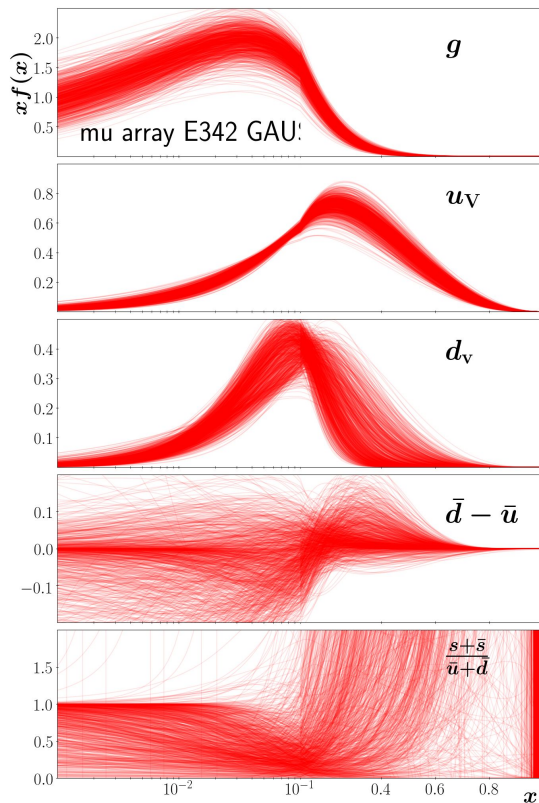
Simplified Model Results



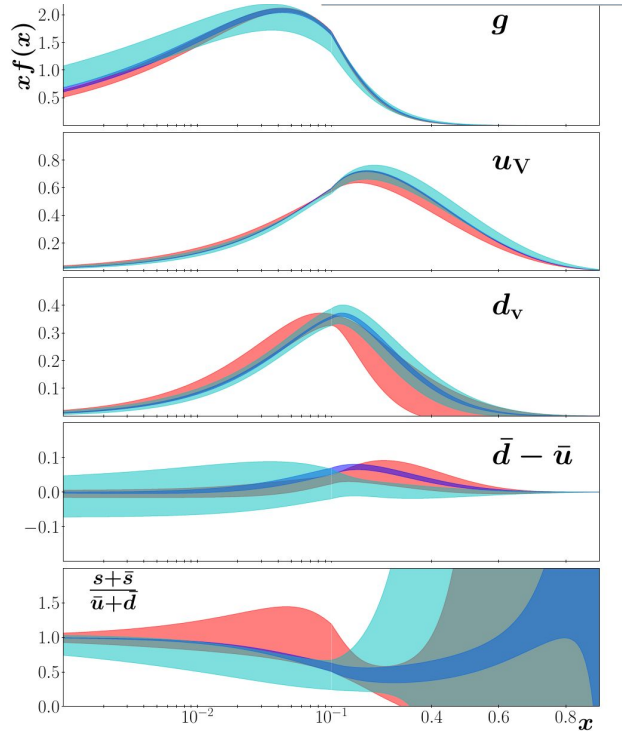
Green=MDN
Red= AE
Blue = JAM
Yellow = full parameter range

Results DIS

Multiple Solutions

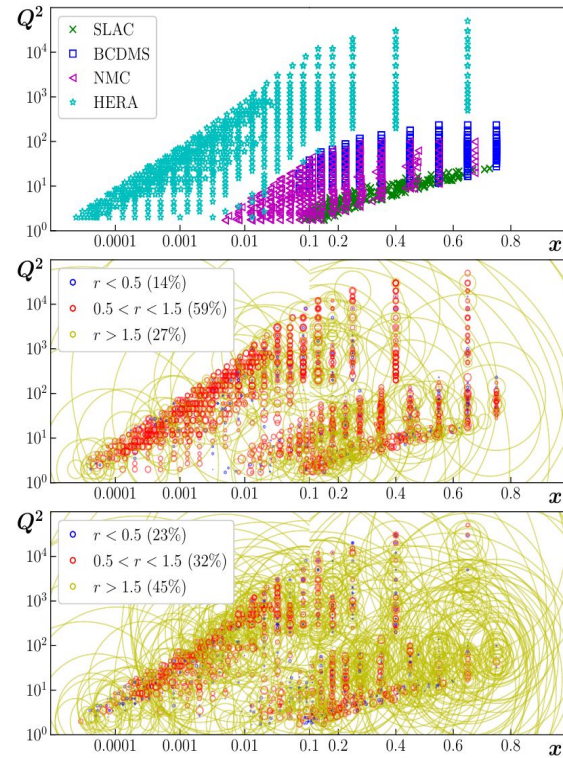


Average and Error Plot



Cyan= MDN
Red= Jam
Blue = AE

Chi² plot need less yellow circles and more points



$$r = \frac{\chi_{\text{ML}}^2(x, Q^2)}{\chi_{\text{JAM}}^2(x, Q^2)}$$

FIG. 8. **Upper panel:** Kinematics of inclusive DIS global data sets. **Middle panel:** χ^2 ratio to JAM from the PSA predictions. **Lower panel:** χ^2 ratio to JAM from the MDN predictions.

Taking a step back

- While the results were promising, it was important for us to understand how **applicable** the model would be to universal fits.
- What happens when we have a **different number of free parameters**
- **Which parameters** can be effectively predicted in using our methods.
- What happens when we **shrink or expand the trained kinematic region**?

Answering those questions

Hyperbox coverage search :

Working up from 10% of the hyperbox of entire experimental kinematic space

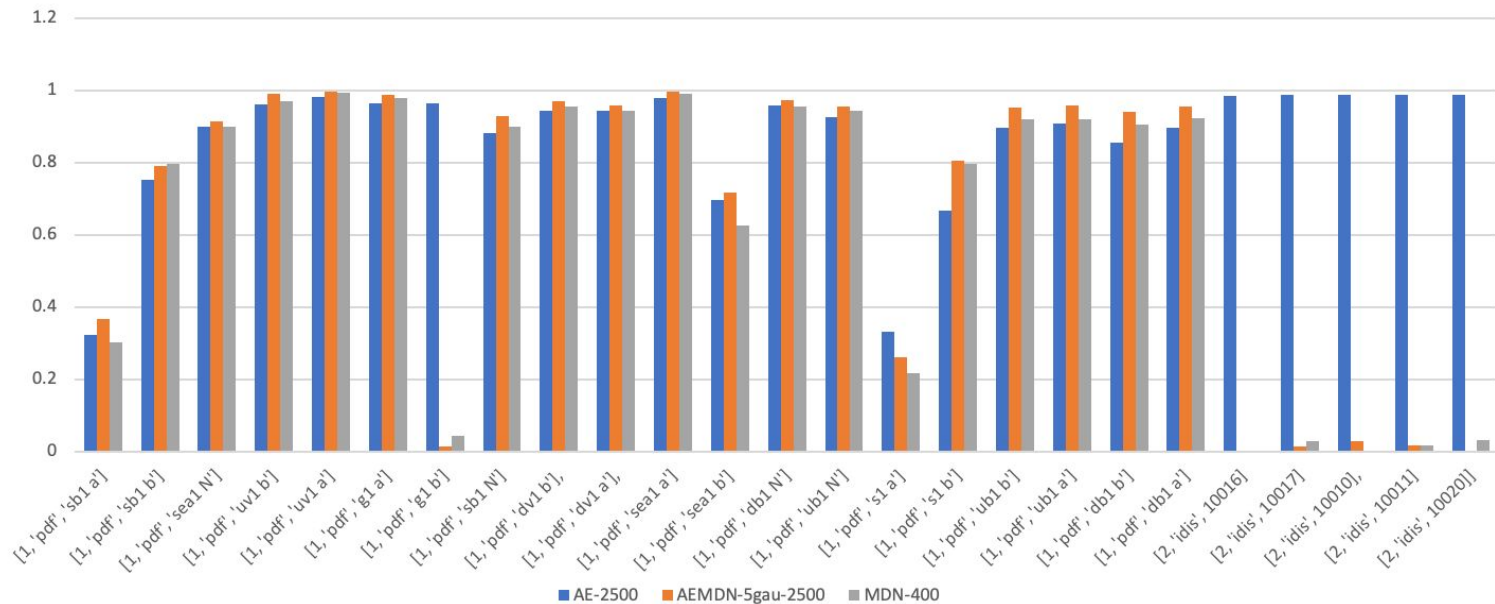
Parameter Search:

Working up from 2 to 25 free theoretical parameters

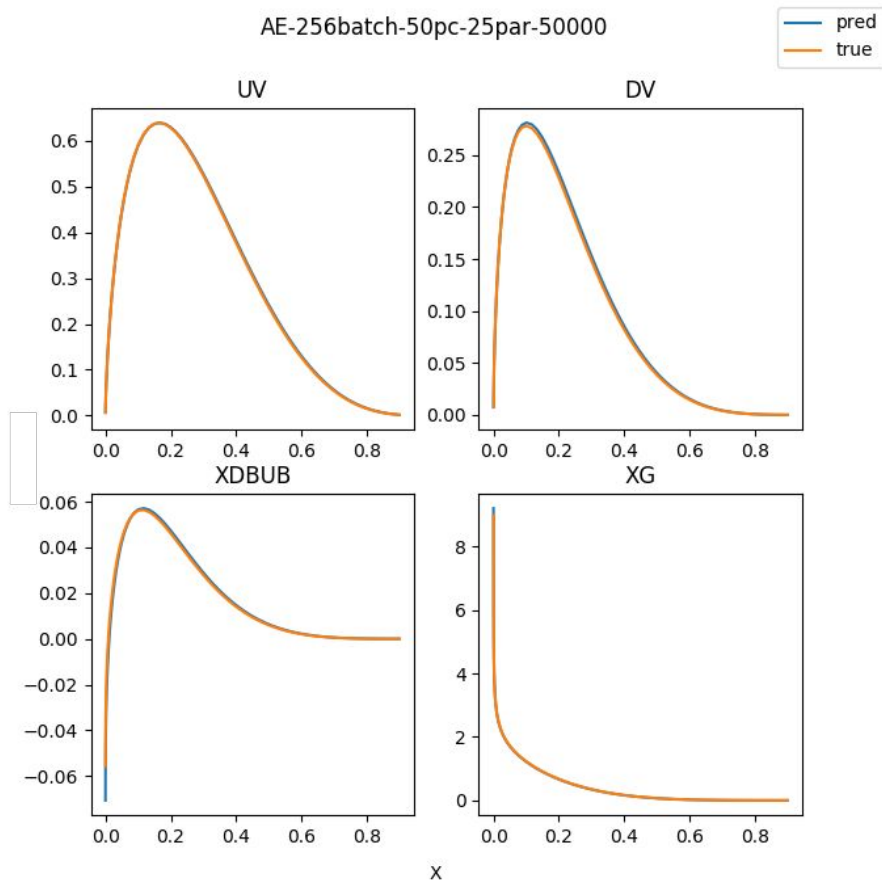
Some initial exploration on 10% of the hyperbox

| No params | Model Architecture | Chi2 |
|-----------|-------------------------|-------|
| 2 | Auto Encoder | 1.041 |
| 2 | Mixture Density Network | 1.20 |
| 2 | AEMDN | 1.066 |
| 10 | Auto Encoder | 1.037 |
| 10 | Mixture Density Network | 2.14 |
| 10 | AEMDN | 1.041 |

Pearson Correlation



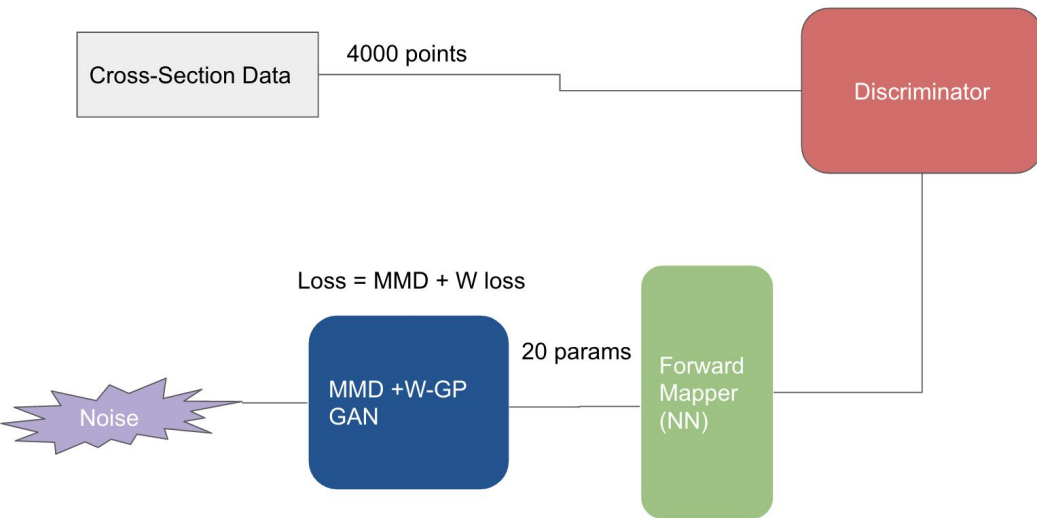
Blind Test Result given one JAM solution -AE



| % coverage | No params | Model Architecture | Chi2 |
|------------|-----------|--------------------|-------|
| 75 | 20 | AutoEncoder | 1.049 |
| 50 | 25 | AutoEncoder | 1.173 |

This semester -- Honors Thesis

GAN for data generation



Preliminary Results

| Experiment | Points | $\chi^2/npts$ |
|-----------------------|--------|---------------|
| SLAC (p) | 222 | 2.69 |
| BCDMS (p) | 348 | 2.09 |
| NMC (p) | 274 | 3.52 |
| HERA II NC e+ (1) (p) | 402 | 2.72 |
| HERA II NC e+ (2) (p) | 75 | 2.29 |
| HERA II NC e+ (3) (p) | 259 | 1.06 |
| HERA II NC e+ (4) (p) | 209 | 1.22 |
| HERA II NC e- (p) | 159 | 2.16 |
| HERA II CC e+ (p) | 39 | 2.27 |
| HERA II CC e- (p) | 42 | 1.66 |
| SLAC (d) | 231 | 5.15 |
| BCDMS (d) | 254 | 2.83 |
| NMC (d/p) | 174 | 1.00 |

DAVIDSON

Thank you

Dr Raghu Ramanujan Meg Houck

Dr Michelle Kuchera Rida Shahid

Eleni Tsitinidi



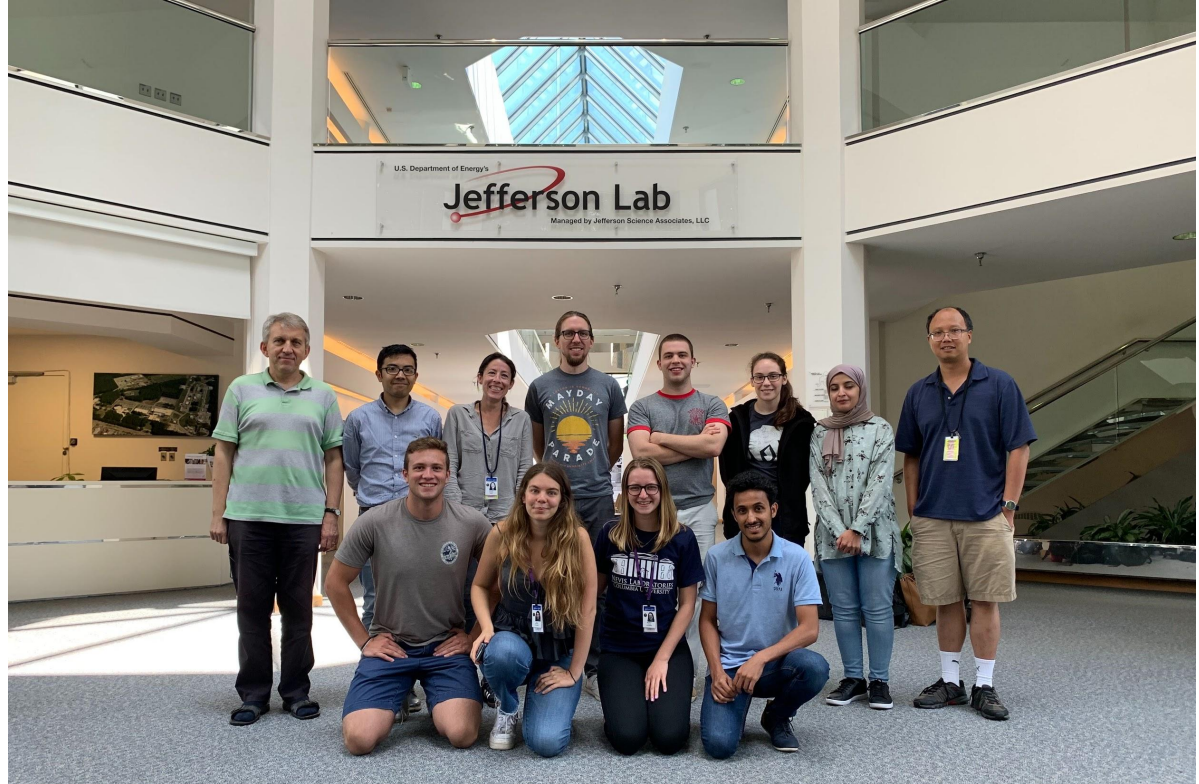
Jefferson Lab
Thomas Jefferson National Accelerator Facility

Dr Nobuo Sato Dr Wally Melnitchouk



Dr Yaohang Lee

Yasir Alanazi Manal Almaeen



Extra slides

Final model Architectures

| Architectures | | |
|------------------------------------|------------------------------------|-----------------------------------|
| AE | MDN | AEMDN |
| IN: Original Shape (Cross Section) | Original Shape $\ Tanh\ KR : 0.01$ | Original Shape |
| Dense $\ 500\ Relu$ | Dense $\ 500\ -$ | Dense $\ 500\ Relu$ |
| Dense $\ 300\ Relu$ | Dense $\ 500\ Tanh\ KR : 0.01$ | Dense $\ 250\ Tanh$ |
| Dense $\ 100\ Relu$ | Dropout $\ 0.2$ | Dropout $\ 0.05$ |
| Dense $\ 25\ -$ | Dense $\ 100\ Sigmoid\ KR : 1E-5$ | Dense $\ 100\ Sigmoid\ KR : 1E-3$ |
| Dense $\ 100\ Relu$ | OUT: MDN Layer $\ 25$ | MDN Layer $\ 25$ |
| Dense $\ 300\ Relu$ | | Dense $\ 100\ Tanh\ KR : 1E-5$ |
| Dense $\ 500\ Relu$ | | Dense $\ 500\ Relu$ |
| OUT: Original Shape | | Original Shape |
| Mean Squared Error | MDN Mixture Loss | [MDN Mixture Loss, MSE] |
| | 3 Gaussians | 5 Gaussians |
| LR $1E - 5$ | LR $1E - 5$ | LR $1E - 5$ |
| Batch 256 | Batch 1024 | Batch 256 |

The data DIS

Dimensions

2680

Cross sections

$$f_i(x, \mu_0) = \frac{N_i x^{\alpha_i} (1-x)^{\beta_i}}{B(2 + \alpha_i, \beta_i + 1)} \quad i = \bar{u}, \bar{d}, s \text{ and } \bar{s}.$$

$$f_i(x, \mu_0) = \frac{N_i x^{\alpha_i} (1-x)^{\beta_i}}{B(2 + \alpha_i, \beta_i + 1)} + \frac{N_S x^{\alpha_S} (1-x)^{\beta_S}}{B(2 + \alpha_S, \beta_S + 1)} \quad i = g, u_v \text{ and } d_v$$

Parameters

Dimensions

25

Normalization coefficients: N_g, N_{u_v}, N_{d_v} and N_s

20 free shape parameters

The data -Toy

Dimensions

| | | |
|-------|--|-------|
| 101 n | | 171 n |
| 101 p | | 171 p |

Cross sections:

$$\sigma_p(x, Q^2) = 4u(x, Q^2) + d(x, Q^2),$$

$$\sigma_n(x, Q^2) = 4d(x, Q^2) + u(x, Q^2).$$

Here σ_p and σ_n mimic what in reality could be the F_p2 And F_n2 structure functions, respectively.

Parameters:

where the Q^2 -dependent shape parameters $p = \{N_{u,d}, \alpha_{u,d}, \beta_{u,d}, \gamma_{u,d}, \delta_{u,d}\}$ are given by

Dimensions

10

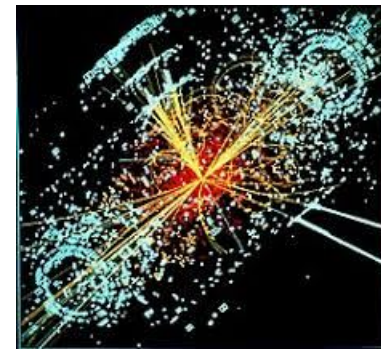
$$p(Q^2) = p^{(0)} + p^{(1)}s(Q^2), \quad s(Q^2) = \log \left(\frac{\log(Q^2/\Lambda_{\text{QCD}}^2)}{\log(Q_0^2/\Lambda_{\text{QCD}}^2)} \right). \quad ($$

Parton Distribution Functions:

$$u(x, Q^2) = N_u(Q^2) x^{\alpha_u(Q^2)} (1-x)^{\beta_u(Q^2)} (1 + \gamma_u(Q^2)\sqrt{x} + \delta_u(Q^2)x),$$

$$d(x, Q^2) = N_d(Q^2) x^{\alpha_d(Q^2)} (1-x)^{\beta_d(Q^2)} (1 + \gamma_d(Q^2)\sqrt{x} + \delta_d(Q^2)x),$$

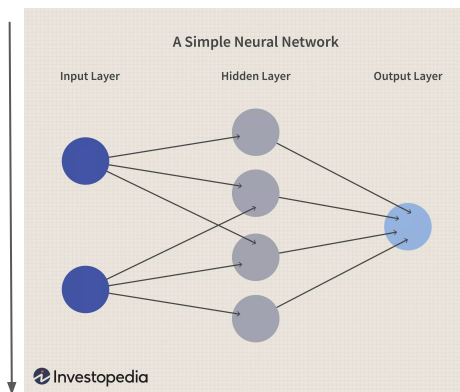
What is ALPhA?



Particle Accelerators



Collision Data



Theory

What do these results mean for our theoretical models describing this process?

How can we represent some of these processes in theoretical functions/terms

Experiment

How can we augment our data (ex fill in missing spots on broken particle track)

How can we design better experiments

Data manipulation

Simulate experimental process and provide researchers with interface