On the Determination of Uncertainties in Parton Densitites

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Summary

1. Uncertainty Quantification Methods Explained

2. Description of Toy Model

3. Neural Network Comparison
Uncertainty Quantification Methods Explained
Bayesian Methods

Bayes’ Theorem:

\[ p(a|m) = \frac{1}{\mathcal{Z}} p(m|a) p(a), \text{ with evidence: } \mathcal{Z} = \int da \ p(m|a) p(a) \]

and likelihood: \[ p(m|a) = \mathcal{N} \exp \left[ -\frac{1}{2} \chi^2(a, m) \right] . \]
Expectation value and variance of any observable $\mathcal{O}$ can be written as:

$$E_{\text{Bayes}}\{\mathcal{O}(a)\} = \frac{1}{n} \sum_{k=1}^{n} \mathcal{O}(a_k),$$

$$V_{\text{Bayes}}\{\mathcal{O}(a)\} = \frac{1}{n} \sum_{k=1}^{n} \left[ \mathcal{O}(a_k) - E_{\text{Bayes}}\{\mathcal{O}(a)\} \right]^2.$$

Metropolis-Hastings and Hamiltonian Monte Carlo (HMC) are examples of MCMC algorithms that obtain samples $a_k$. Nested Sampling is an alternative Bayesian technique that primarily aims to evaluate the evidence $\mathcal{Z}$, also produces samples as a byproduct.
Approximations to Bayesian Posterior: Hessian

Change of variables \( p(a|m) \to p(t|m) \): \( a(t) = a_0 + \sum_{k=1}^{n_{\text{par}}} t_k \frac{e_k}{\sqrt{w_k}}, \)

\[
E_{\text{Hess}} \{ \mathcal{O}(a) \} = \int d^n t \, p(t|m) \, \mathcal{O}(a(t)) \approx \mathcal{O}(a_0).
\]

\[
V_{\text{Hess}} \{ \mathcal{O}(a) \} \approx \sum_k T_k^2 \left( \frac{\partial \mathcal{O}(a(t))}{\partial t_k} \bigg|_{a_0} \right)^2 , \text{ where: } T_k^2 = \int dt_k \, p_k(t_k|m) \, t_k^2.
\]

\( T_k^2 \) is set between 5–10, inflating uncertainties to 68% coverage in global PDF fits according to ad hoc "tolerance criterion". This is motivated by statistical inconsistencies in data.
Data resampling uses frequentist logic to approximate Bayesian posterior with distribution in maximum likelihood estimators:

\[ E_{\text{freq}} \{ \mathcal{O}(a) \} = \frac{1}{n_{\text{rep}}} \sum_{n_{\text{rep}}} \mathcal{O}(a_{\text{rep}}), \]

\[ V_{\text{freq}} \{ \mathcal{O}(a) \} = \frac{1}{n_{\text{rep}}} \sum_{n_{\text{rep}}} \left[ \mathcal{O}(a_{\text{rep}}) - E_{\text{freq}} \{ \mathcal{O}(a) \} \right]^2. \]
Description of Toy Model
Description of Toy Model

Toy 4D Quark model

\[ q_i(x) = x^{\alpha_i}(1 - x)^{\beta_i}, \]
\[ i = 1, 2. \]

\[ \sigma_j = \sum_{i=1,2} c_{ji} q_i, \]
\[ c_{11} = 4c_{12} = 4c_{21} = c_{22}. \]
Equivalency of Parametric Methods

\[
\sigma(x) = \sigma_1 \quad \text{or} \quad \sigma_2 \\
\sigma_{\text{dat}}^1 \quad \text{or} \quad \sigma_{\text{dat}}^2
\]

\[
f(x) = q_1 \quad \text{or} \quad q_2 \\
\text{DR} \quad \text{or} \quad \text{HMC} \quad \text{or} \quad \text{NS} \quad \text{or} \quad \text{Hessian}
\]

\[
\text{ratio to } \sigma_1 \\
\text{ratio to } q_1
\]

\[
\text{ratio to } \sigma_2 \\
\text{ratio to } q_2
\]
Neural Network Comparison
Overfitting with NNs

\[ \sigma(x) \]

- **NN prediction**
- **data**

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Overfitting with NNs

![Loss function over epochs](image)

- Training loss function
- Validation loss function

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Overfitting with NNs

\[
\sigma(x) = \begin{cases} 
\sigma_1 & \text{NN with CV} \\
\sigma_{1}^{\text{dat}} & \text{NN no CV}
\end{cases}
\]
Uncertainty Dependence on Partition Fraction

Neural Network Comparison

Uncertainty Determination in PDFs
Uncertainty Dependence on Partition Fraction

The graph shows the uncertainty ratio to \( f = 0.5 \) for different values of \( f \) ranging from 0.1 to 0.9. The x-axis represents the number of points, and the y-axis represents the uncertainty ratio. The graph illustrates how the uncertainty changes as the number of points increases for each value of \( f \).
Comparison of Neural Nets to Parametric Methods

\[ \sigma(x) \]

\[ \sigma_1 \]

\[ \sigma_{1\text{dat}} \]

- DR
- NN
- NN with preprocess

Ratio to \( \sigma_1 \) with \( x \) values from 0.0 to 1.0.
Closure Test of Neural Nets

![Graph showing percentage of true law within uncertainty for different models.](image)

- **DR + CV**
  - $f = 0.6$

- **NN**
  - $f = 0.2$

- **NN**
  - $f = 0.6$

- **NN + preprocess**
  - $f = 0.6$