Analytical derivates of neural networks: making a fit faster

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3DSPIN MAPPING THE PROTON IN 3D

Defining the problem

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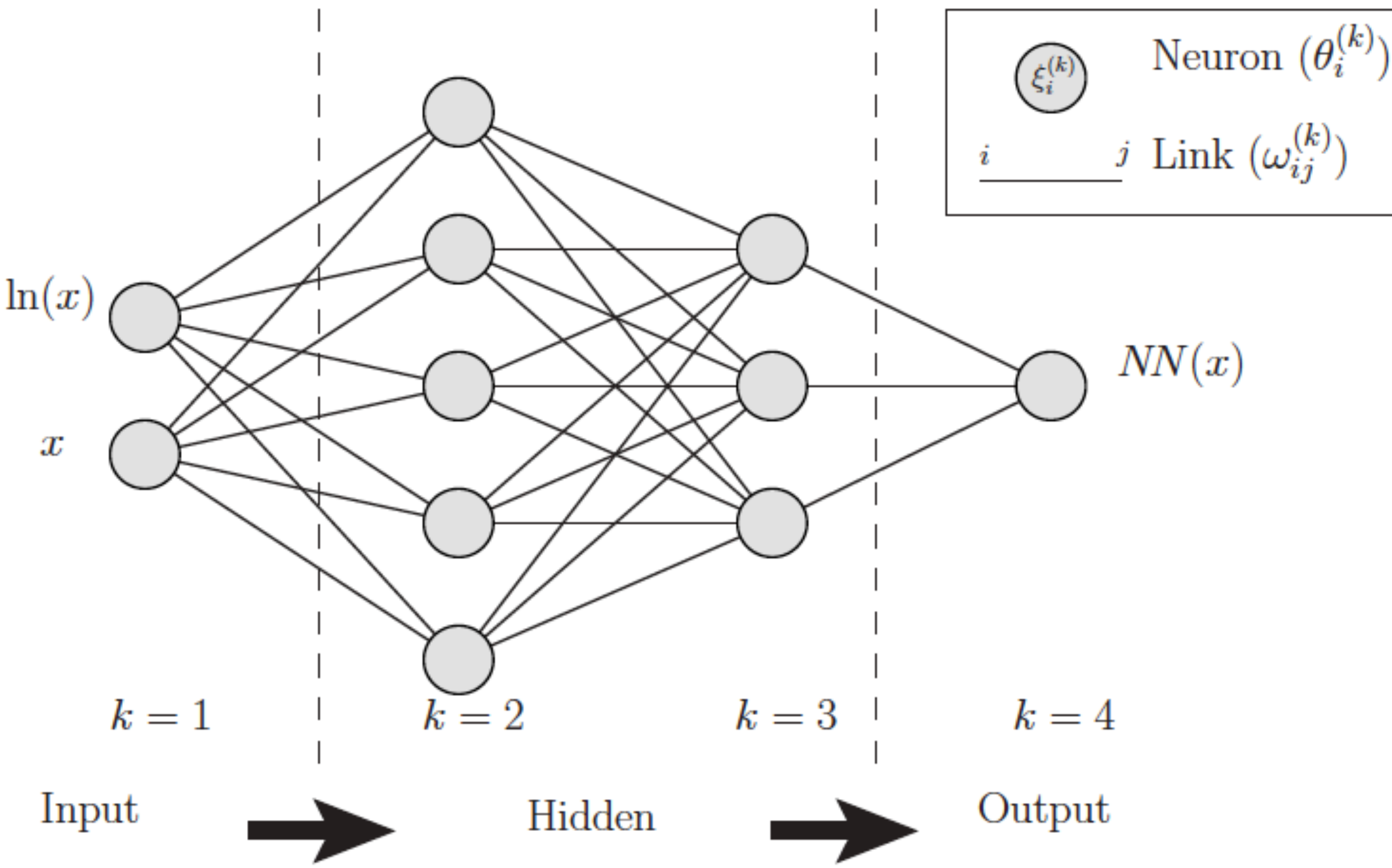
- Therefore the theoretical prediction is a **functional** of the initial-scale distributions and so is the χ^2:

$$\hat{F} \equiv \hat{F}[\{N_i\}] \quad \text{and} \quad \chi^2 \equiv \chi^2[\{N_i\}]$$

Defining the problem

- A feed-forward neural network (NN) is parameterised in terms of **links** and **biases**, *e.g.*:



$$\xi_i^{(j)} = \sigma\left(\sum_k^{\text{(j-1)th layer}} \xi_k^{(j-1)} \omega_{ki}^{(j)} - \theta_i^{(j)}\right)$$

Activation function associated to each neuron

- Effectively, a NN is nothing but a **parametric function**:

$$\begin{aligned} N_i \equiv N_i(x; \{\omega_{ij}^{(\ell)}, \theta_i^{(\ell)}\}) &= \sigma_L\left(\sum_{j^{(1)}=1}^{N_{L-1}} \omega_{ij^{(1)}}^{(L)} y_{j^{(1)}}^{(L-1)} + \theta_i^{(L)}\right) \\ &= \sigma_L\left(\sum_{j^{(1)}=1}^{N_{L-1}} \omega_{ij^{(1)}}^{(L)} \sigma_{L-1}\left(\sum_{j^{(2)}=1}^{N_{L-2}} \omega_{j^{(1)}j^{(2)}}^{(L)} y_{j^{(2)}}^{(L-2)} + \theta_{j^{(1)}}^{(L-1)}\right) + \theta_i^{(L)}\right) \\ &= \ldots \end{aligned}$$

Defining the problem

- In order to minimise the χ^2 **optimally**, we want to be able to compute the following derivatives:

$$\frac{\partial \chi^2}{\partial \omega_{ij}^{(\ell)}} = 2\left(\frac{\mathbf{C}\otimes\mathbf{N} - F}{\sigma^2}\right)\mathbf{C}\otimes\frac{\partial \mathbf{N}}{\partial \omega_{ij}^{(\ell)}}$$

$$\frac{\partial \chi^2}{\partial \theta_{i}^{(\ell)}} = 2\left(\frac{\mathbf{C}\otimes\mathbf{N} - F}{\sigma^2}\right)\mathbf{C}\otimes\frac{\partial \mathbf{N}}{\partial \theta_{i}^{(\ell)}}$$

- This boils down to computing the **derivative of the NN** w.r.t. to its free parameters.
- We can surely do it **numerically** (incremental ratio).
- Can we also do it **analytically** for a generic architecture?
  - better **numerical stability**,
  - **faster**.

Deriving a Neural Network

- Yes, we can derive a feed-forward NN by using the **chain rule**:

$$\frac{\partial N_k}{\partial \theta_i^{(\ell)}} = \Sigma_{ki}^{(\ell)} z_i^{(\ell)} \qquad \text{and} \qquad \frac{\partial N_k}{\partial \omega_{ij}^{(\ell)}} = \Sigma_{ki}^{(\ell)} z_i^{(\ell)} y_j^{(\ell-1)}$$

with:

$$x_i^{(\ell)} = \sum_{j=1}^{N_{\ell-1}} \omega_{ij}^{(\ell)} y_j^{(\ell-1)} + \theta_i^{(\ell)} \,,$$

$$\boldsymbol{\Sigma}^{(\ell)} = \prod_{\alpha=L}^{\ell+1} \mathbf{S}^{(\alpha)}$$

$$y_i^{(\ell)} = \sigma_\ell\left(x_i^{(\ell)}\right) \,,$$

$$z_i^{(\ell)} \omega_{ij}^{(\ell)} = S_{ij}^{(\ell)} \left(= \frac{\partial y_i^{(\ell)}}{\partial y_j^{(\ell-1)}} \right)$$

$$z_i^{(\ell)} = \sigma'_\ell\left(x_i^{(\ell)}\right) \,,$$

Tests against numerical derivatives show that it works beautifully!

Exploiting analytic derivatives

- Use **APFEL/APFELgrid** as it give access to the initial-scale PDFs:

$$F(Q) = \underbrace{C(Q) \otimes \Gamma(Q, \mu_0)}_{\text{FK table}} \otimes f(\mu_0)$$

- Use **ceres-solver** to assess the impact of different derivation strategies:
  - **analytic** derivatives,
  - **numerical** derivatives (incremental ratio: forward/backward/central),
  - **automatic** derivatives:

Dual Numbers & Jets

Dual numbers are an extension of the real numbers analogous to complex numbers: whereas complex numbers augment the reals by introducing an imaginary unit ι such that $\iota^2 = -1$, dual numbers introduce an *infinitesimal* unit ϵ such that $\epsilon^2 = 0$. A dual number $a + v\epsilon$ has two components, the *real* component a and the *infinitesimal* component v.

http://ceres-solver.org/automatic_derivatives.html#chapter-automatic-derivatives

Dual numbers and Jets

For example, consider the function

$$f(x) = x^2,$$

Then,

$$\begin{aligned} f(10+\epsilon) &= (10+\epsilon)^2 \\ &= 100 + 20\epsilon + \epsilon^2 \\ &= 100 + 20\epsilon \end{aligned}$$

Observe that the coefficient of ϵ is $Df(10) = 20$. Indeed this generalizes to functions which are not

A Jet is a n-dimensional dual number, where we augment the real numbers with n infinitesimal units $\epsilon_i,\ i = 1, \ldots, n$ with the property that $\forall i, j\ : \epsilon_i \epsilon_j = 0$. Then a Jet consists of a *real* part a and a n-dimensional *infinitesimal* part $\mathbf{v}$, i.e.,

$$x = a + \sum_j v_j \epsilon_j$$

The summation notation gets tedious, so we will also just write

$$x = a + \mathbf{v}.$$

where the ϵ_i's are implict. Then, using the same Taylor series expansion used above, we can see that:

$$f(a + \mathbf{v}) = f(a) + Df(a)\mathbf{v}.$$

Automatic derivation

- Automatic derivatives are available **through ceres** if one **templates** the function to be derived in such a way to **evaluate** it, not just on real numbers, but also **on dual numbers/jets**:

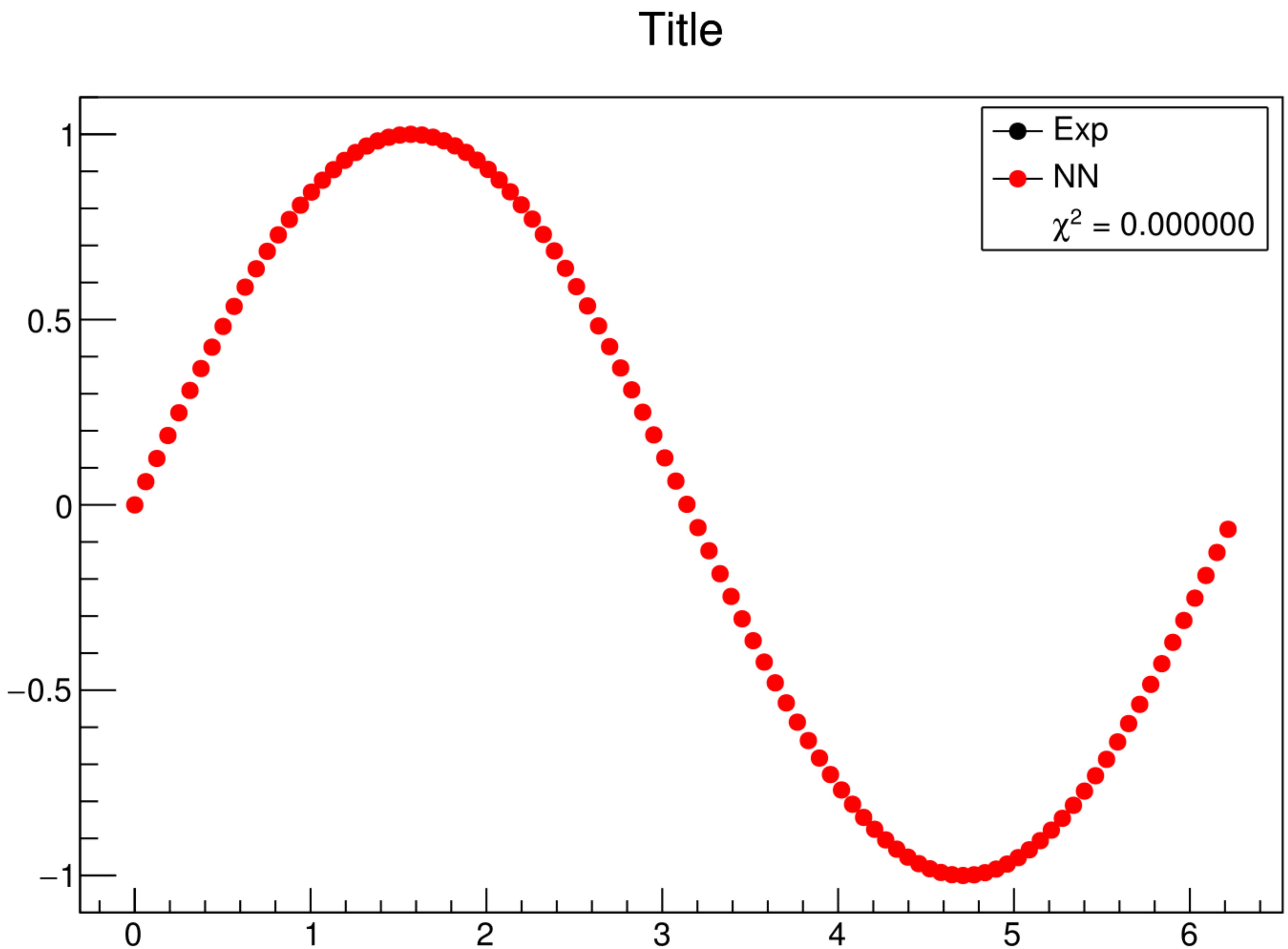
```
template<class T>
class FeedForwardNN
{
 public:

  // Constructors
  FeedForwardNN(std::vector<int> const &Arch,
                int const &RandomSeed = 0,
                std::function<T(T const &)> const &ActFun = Sigmoid<T>,
                std::function<T(T const &)> const &dActFun = dSigmoid<T>,
                bool const &LinearOutput = true);
```

- During the fit ceres takes care of computing the derivatives w.r.t. the free parameters by **evaluating the (jet-valued) function on a jet**.

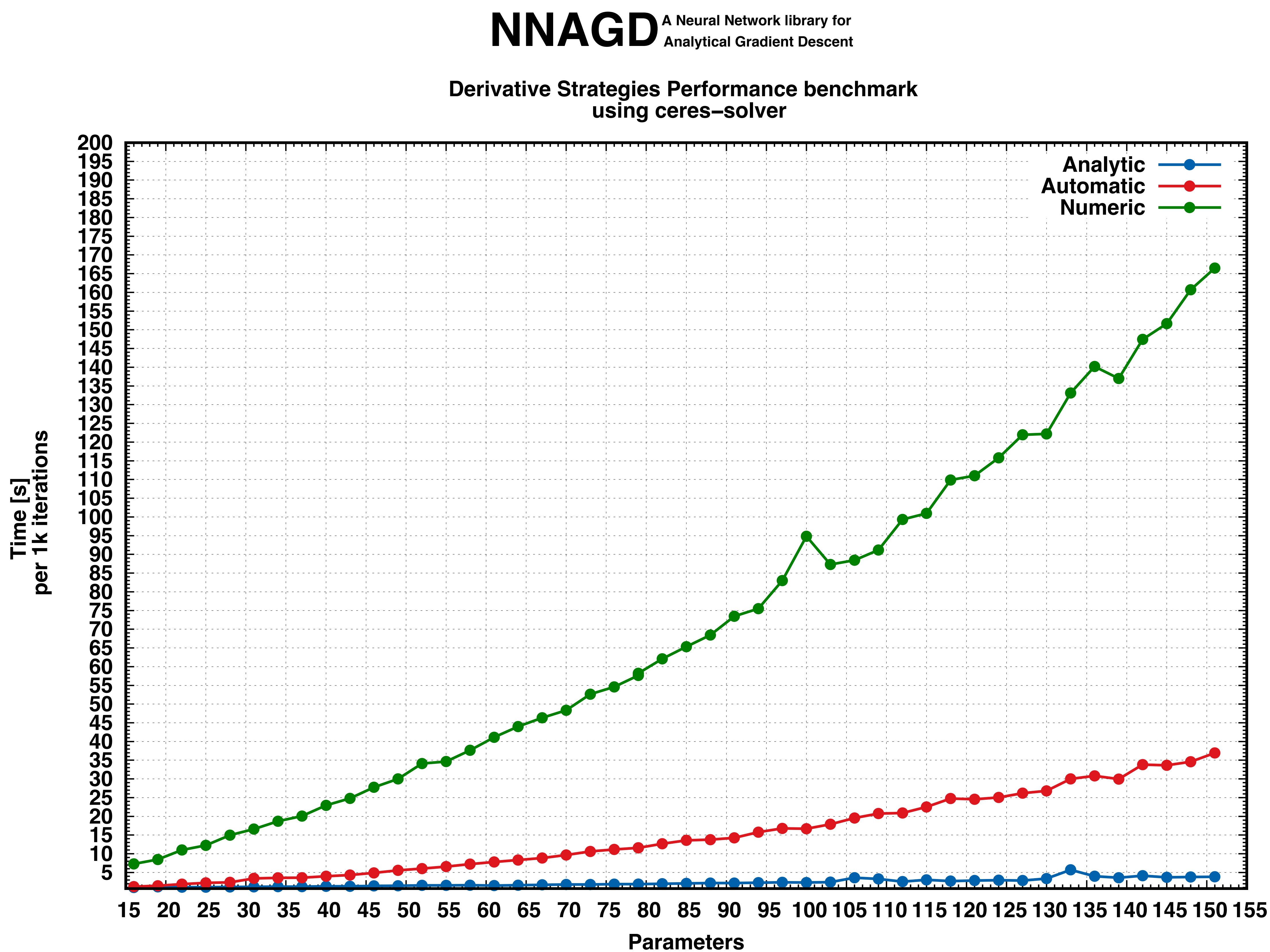
Performance

- Fit 100 points of a **sine function** using a NN with one single hidden layer with an increasing number of nodes:



- Let the code run for **1k iterations** ($\chi^2 \simeq 10^{-9}$ - 10^{-12}).

Performance



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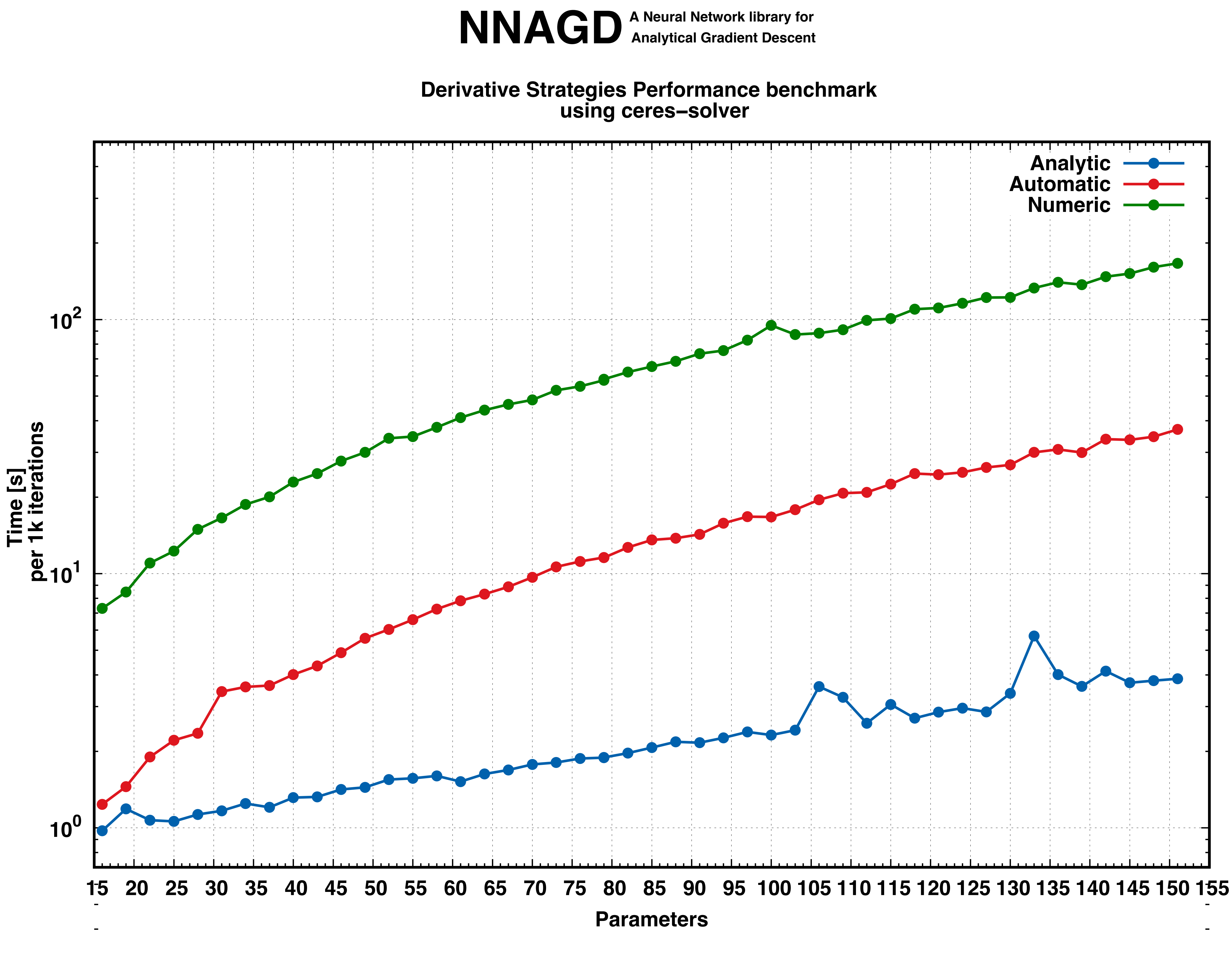
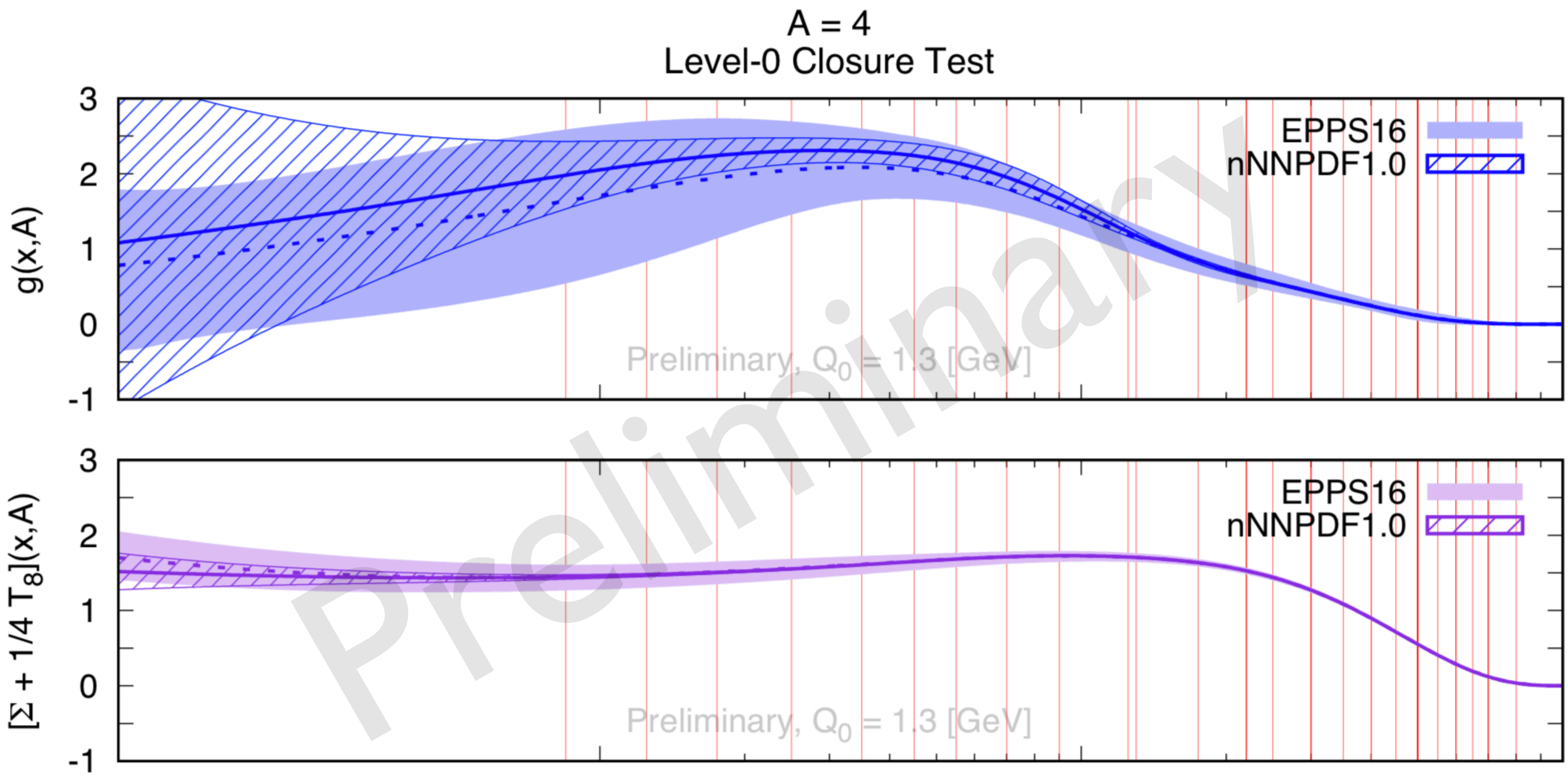


Preliminary closure tests

- Use **analytic derivatives** of a feed-forward NN to extract nuclear PDFs from **DIS pseudo-data** (closure test) using **APFELgrid** and **ceres**:



Summary

- Feed-forward NNs can be **derived analytically** by using the chain rule,
- this allows one to compute the gradient of the χ^2 analytically:
  - provided that one uses an **APFELgrid-like computation**.
- The analytic knowledge of the gradient of the χ^2 makes a fit much faster.
- We have used **ceres** to assess the performance of analytic, numeric, and automatic differentiation.
- Analytic derivatives seem to perform substantially better.