A new generation of PDFs with deep learning models

Operator implementation in TensorFlow

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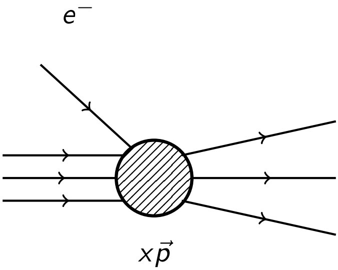
Outline

1. Introduction. General structure of a process.
2. Structure of n3fit. Motivation for operator implementation.
3. Operator implementation in TensorFlow.
4. Results & Conclusions.

General structure of a process

Deep Inelastic Scattering



Convolute the partonic $\hat{\sigma}_{ij}$ with the PDF $\longrightarrow$ Observable σ.

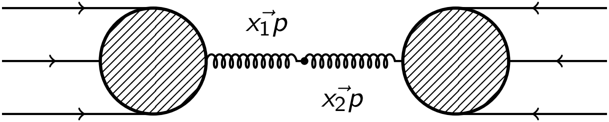
$$\sigma^{DIS} = \int_0^{\infty} dx\ f_\alpha(x) * \hat{\sigma}_{ij}(\mu_F, \mu_R(\alpha_s)) \ . \tag{1}$$

In our language $\longrightarrow$ vector of observables from a grid of x_i:

$$y_N^{DIS} = \sum_{i,\alpha} f_\alpha(x_i) FK_{Ni\alpha} \ . \tag{2}$$

General structure of a process

Hadronic (Example: Drell-Yan)



Convolute the partonic $\hat{\sigma}_{ij}$ with the PDF $\longrightarrow$ Observable σ.

$$\sigma^{DY} = \int_0^\infty dx_1 \, dx_2 \, f_\alpha(x_1) * f_\beta(x_2) * \hat{\sigma}_{ij}(\mu_F, \mu_R(\alpha_s)) \, . \tag{3}$$

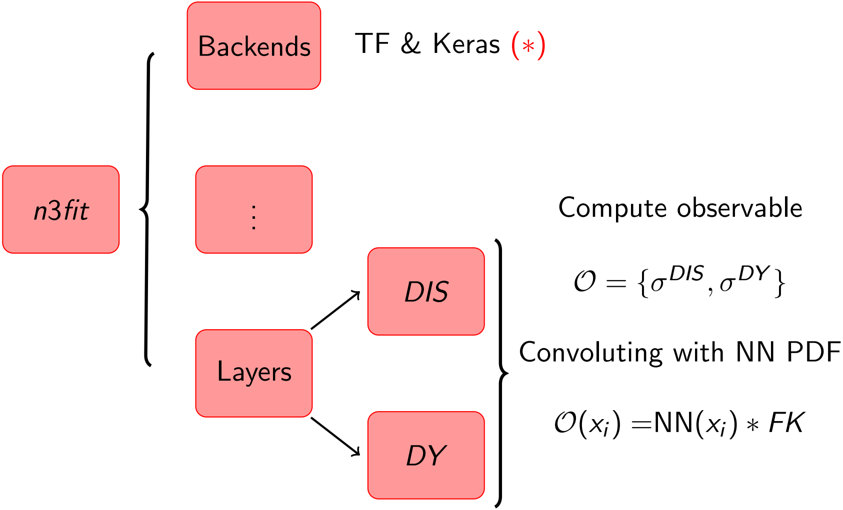
In our language $\longrightarrow$ vector of observables from a grid of x_i:

$$y_N^{DY} = \sum_{i,j,\alpha,\beta} f_\alpha(x_i) f_\beta(x_j) FK_{Nij\alpha\beta} \, . \tag{4}$$

Note: We will use DY to refer hadronic events

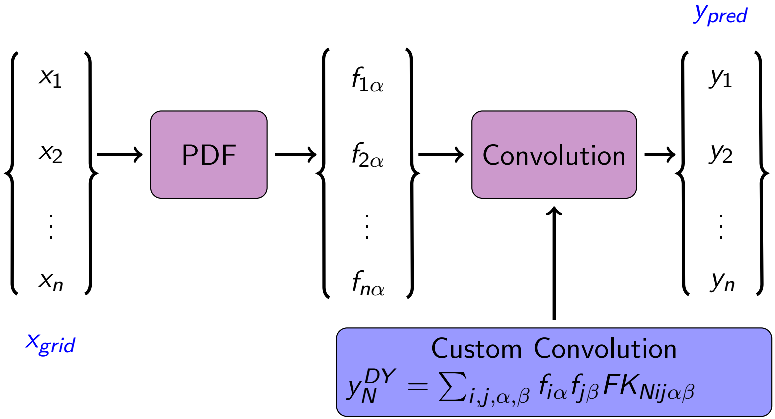
General structure of the model

General structure of n3fit



Operator implementation

i) General structure of observable layers



1. Build model to compute y_{pred} from x_{grid}
2. Compute χ^2 loss by comparing with data
   $\chi^2 = \sum_{i=1}^{N} y_i^{pred} - y_i^{data}$
3. Compute gradient $\nabla\chi^2$ and update values of PDF $\longrightarrow$ Fit

Operator implementation

ii) TF computation of the gradient

1. Computing gradient of the χ^2 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.

$$\frac{\partial\chi^2}{\partial x_i} = \frac{\partial\chi^2}{\partial\mathbf{Op}}\frac{\partial\mathbf{Op}}{\partial f_{\mu\nu}}\cdots\frac{\partial f_{\mu\nu}}{\partial x_i} \tag{5}$$

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.

Operator implementation

iii) Manual computation of the gradient

1. From the expression of the output:

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

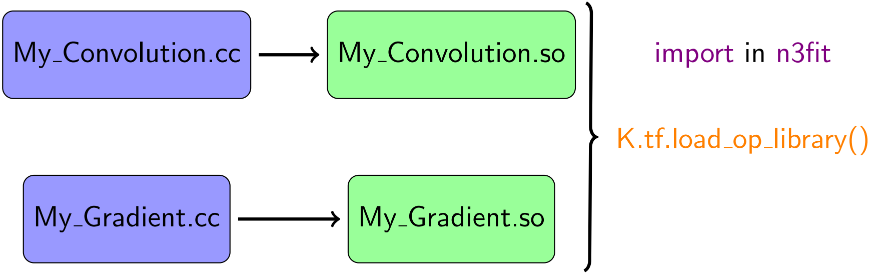
2. Gradient of the output with respect ot the PDFs:

$$\begin{aligned} \frac{\partial y_N}{\partial f_{\mu\nu}} &= \frac{\partial}{\partial f_{\mu\nu}} \sum_{i,j,\alpha,\beta} f_{i\alpha} f_{j\beta} FK_{Nij\alpha\beta} \\ &= \sum_{i,j,\alpha,\beta} (\delta_{\mu i}\delta_{\nu\alpha} f_{\beta j} + \delta_{\mu j}\delta_{\nu\beta} f_{\alpha i}) FK_{Nij\alpha\beta} \qquad (6) \\ &= \sum_{j,\beta} f_{j\beta} FK_{N\mu j\nu\beta} + \sum_{i,\alpha} f_{i\alpha} FK_{Ni\mu\alpha\nu} \end{aligned}$$

Through technical details

i) Generating libraries

1. Build .cc files computing the convolution and the gradient.
2. Compile them to build .so libraries.
   g++ -std=c++11 -shared My_Convolution_.cc -o My_Convolution_.so $TF_FLAGS
3. load the libraries in DIS/DY layers of n3fit with load_op_library() function of TensorFlow.



Through technical details

ii) Writing the convolution in c++

1. Input PDF: $f_{i\alpha}$ and FK table: $FK_{Nij\alpha\beta}$
2. Basis flavors: $basis = \{(1,2),(3,4),...,(3,1)\}$

```
// Define the op's interface. Register the op in the tensorflow system by specify inputs and outputs and required attributes
// Create an op that takes two tensors of float and outputs a the tensor product
REGISTER_OP("MyConvolutionDy")
    .Input("pdf: float")
    .Input("fk_table: float")
    .Attr("basis_flav_1: list(int)")
    .Attr("basis_flav_2: list(int)")
    .Output("y_pred: float")
    // Define the shape of the output tensor
    .SetShapeFn([](::tensorflow::shape_inference::InferenceContext* c) {
        // Give to the output 0 the next shape (the last one of the fk table (input 1))
        c -> set_output(0, c -> MakeShape( { c -> Dim(c -> input(1), 0) } )
        );
        return Status::OK();
    });
```

3. Compute convolution $y_N^{DY} = \sum_{i,j,\alpha,\beta} f_{i\alpha} f_{j\beta} FK_{Nijc} \delta^c_{\alpha\beta}$

```
// Perform the convolution of the PDFs with the FK table
for (int n = 0; n < fk_shape.dim_size(0); n++) {
    y_pred(n) = 0.0;
    for (int i = 0; i < pdf_shape.dim_size(0); i++) {
        for (int k = 0; k < pdf_shape.dim_size(0); k++) {
            for(int c = 0; c < basis_flav_.size(); c++) {
                // PDFs and the FK table are summed only up to the flavour index, given by the flavour basis
                y_pred(n) += pdf(i, basis_flav_1_[c]) * pdf(k, basis_flav_2_[c]) * fk_table(n, c, i, k);
            }
        }
    }
}
```

Through technical details

iii) Writing the observable layer

A DY class written in TF would need at least 3 operations

1. Generate luminosity tensor $\mathcal{L}_{ij\alpha\beta} = f_{i\alpha} * f_{j\beta}$
2. Apply mask to eliminate the non-active flavors
3. Perform the convolution $y_N^{DY} = \sum_{i,j,\alpha,\beta} \mathcal{L}_{ij\alpha\beta} FK_{Nijc} \delta^c_{\alpha\beta}$

```python
class DY_mask(Observable):

    def call(self, pdf):
        # Generate luminosity tensor
        tensor_luminosity = self.tensor_product(pdf, pdf, axes = 0)
        # Permute luminosity tensor for doing the convolution
        permuted_luminosity = self.permute_dimensions(tensor_luminosity, (3,1,2,0))
        # Eliminate the non-active flavours by applying the mask
        masked_luminosity = self.boolean_mask(permuted_luminosity, self.basis, axis = 0)
        # Compute the actual convolution
        result = self.tensor_product(self.fktable, masked_luminosity, axes = 3)
        return result
```

Custom DY class just calls the MyConvolutionDY.cc

```python
class DY(Observable):

    def call(self, pdf):
        # Convolution computed by Custom_Convolution_DY.cc
        my_result = conv_out_module.my_convolution_dy( pdf, self.fktable, basis_flavs_1 = self.basis_flavs_1, basis_flavs_2 = self.basis_flavs_2 )
        return my_result
```

Results

Checking computation

DIS only:

	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

DY-like only:

	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

Checking memory

Global:

	TensorFlow	Custom Convolution	Diff
Virtual	22.3 GB	19.7 GB	2.6 GB
RES	16.7 GB	14.1 GB	2.6 GB

DY-like 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

Conclusions & Next steps

1. Custom convolution takes 3 GB less of memory than TensorFlow.
2. Take full control on the computation of the observables.
3. Load FK tables in GPU: new possibilities.

Thank you!

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