Multi-dimensional integration with quantum circuits

Based on arXiv:2308.05657

Juan Manuel Cruz-Martinez, Matteo Robbiati, Stefano Carrazza

19 October 2023

Aim and motivation

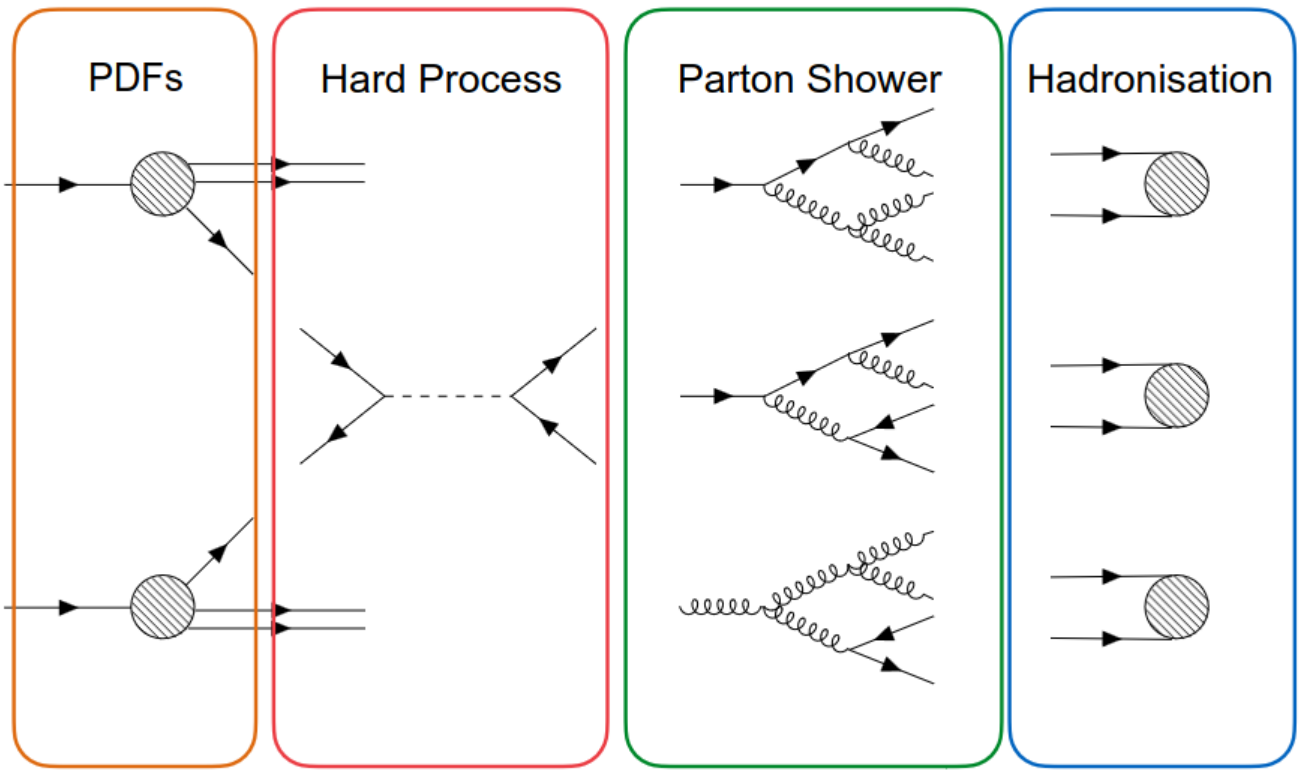
- Calculate multi-dimensional integrals like:

$$I(\boldsymbol{\alpha}) = \int_{\boldsymbol{x}_a}^{\boldsymbol{x}_b} g(\boldsymbol{\alpha}; \boldsymbol{x}) \mathrm{d}^n \boldsymbol{x}. \tag{1}$$

Aim and motivation

- Calculate multi-dimensional integrals like:

$$I(\alpha) = \int_{x_a}^{x_b} g(\alpha; \boldsymbol{x}) \mathrm{d}^n \boldsymbol{x}. \tag{1}$$



Introductory concepts

Machine Learning

Machine Learning helps in solving statistical problems, such as data generation, classification, regression, forecasting, etc.

Machine Learning

Machine Learning helps in solving statistical problems, such as data generation, classification, regression, forecasting, etc.

- we aim to know some hidden law between two variables: $\boldsymbol{y} = f(\boldsymbol{x})$;

Machine Learning

Machine Learning helps in solving statistical problems, such as data generation, classification, regression, forecasting, etc.

- we aim to know some hidden law between two variables: $\boldsymbol{y} = f(\boldsymbol{x})$;
- we define a parameteric model with returns $\boldsymbol{y}_{\text{est}} = f_{\text{est}}(\boldsymbol{x}; \boldsymbol{\theta})$;

Machine Learning

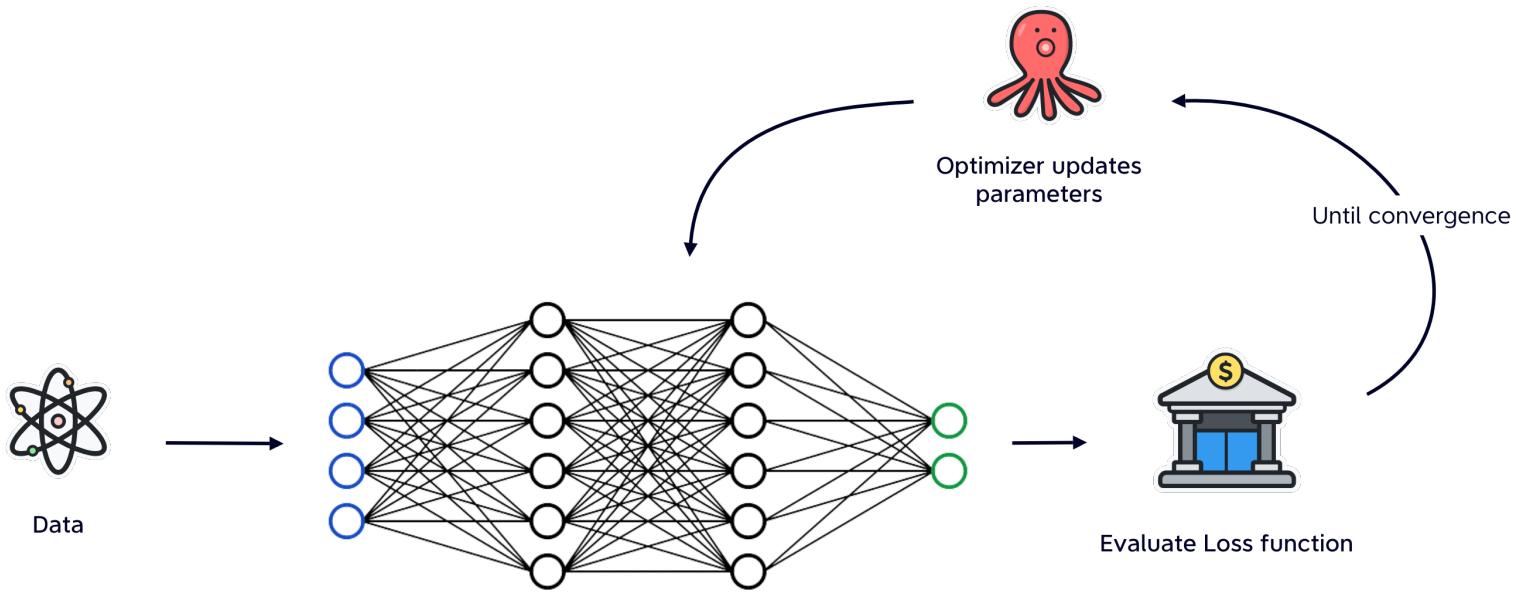
Machine Learning helps in solving statistical problems, such as data generation, classification, regression, forecasting, etc.

- we aim to know some hidden law between two variables: $\boldsymbol{y} = f(\boldsymbol{x})$;
- we define a parameteric model with returns $\boldsymbol{y}_{\mathrm{est}} = f_{\mathrm{est}}(\boldsymbol{x}; \boldsymbol{\theta})$;
- we define an optimizer, which task is to compute $\mathrm{argmin}_{\boldsymbol{\theta}} \left[J(\boldsymbol{y}_{\mathrm{meas}}, \boldsymbol{y}_{\mathrm{est}}) \right]$.

Machine Learning

Machine Learning helps in solving statistical problems, such as data generation, classification, regression, forecasting, etc.

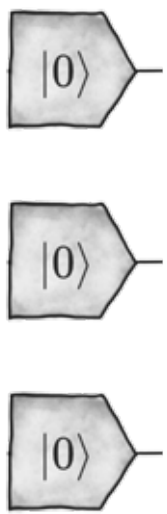
- we aim to know some hidden law between two variables: $\boldsymbol{y} = f(\boldsymbol{x})$;
- we define a parameteric model with returns $\boldsymbol{y}_{\text{est}} = f_{\text{est}}(\boldsymbol{x}; \boldsymbol{\theta})$;
- we define an optimizer, which task is to compute $\text{argmin}_{\boldsymbol{\theta}} \left[J(\boldsymbol{y}_{\text{meas}}, \boldsymbol{y}_{\text{est}}) \right]$.



Parametric Quantum Circuits

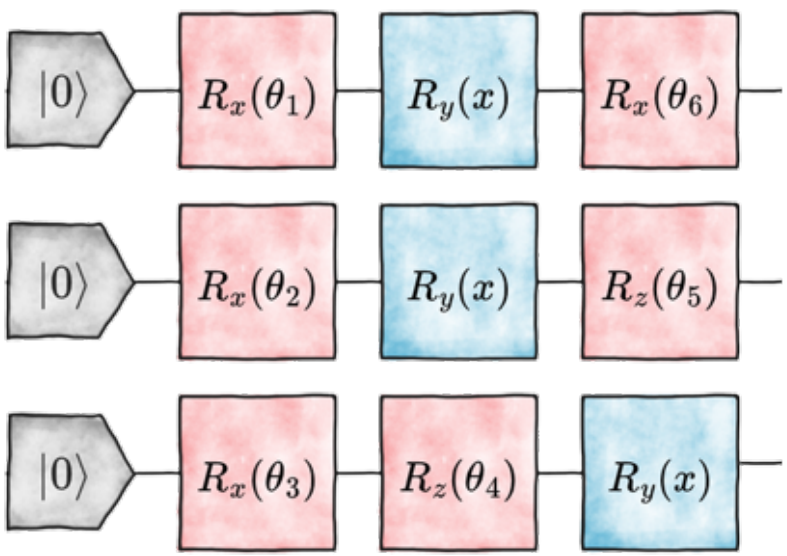
Parametric Quantum Circuits

- Classical bits are replaced by **qubits**: $|q\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$;



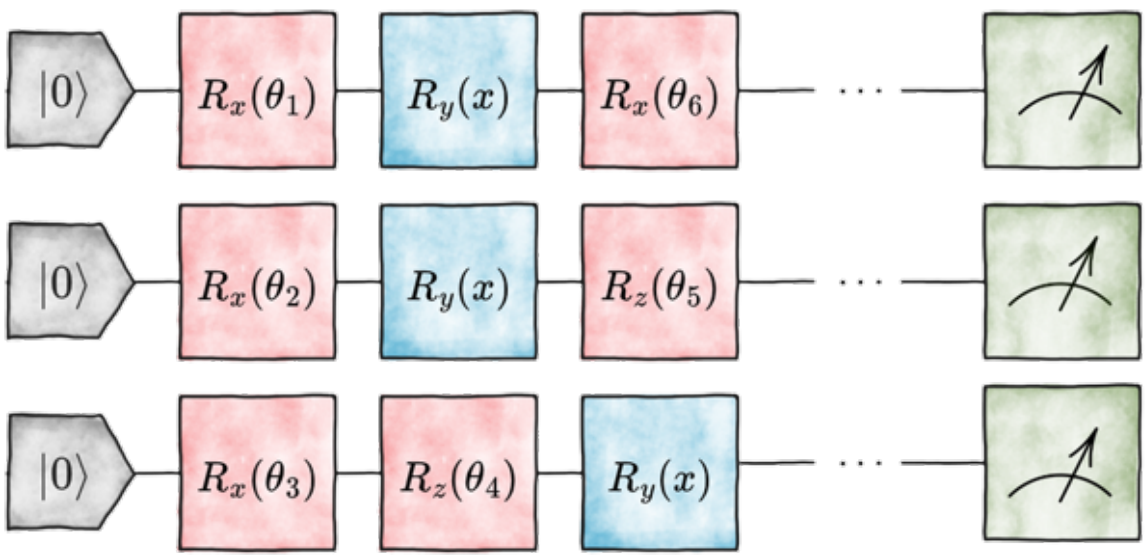
Parametric Quantum Circuits

- Classical bits are replaced by **qubits**: $|q\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$;
- we modify the qubits state by applying unitaries, which we call **gates**. Rotational gates $R_j(\theta) = e^{-i\theta\hat{\sigma}_j}$ are used to build parametric circuits $\mathcal{C}(\boldsymbol{\theta})$;



Parametric Quantum Circuits

- Classical bits are replaced by **qubits**: $|q\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$;
- we modify the qubits state by applying unitaries, which we call **gates**. Rotational gates $R_j(\theta) = e^{-i\theta\hat{\sigma}_j}$ are used to build parametric circuits $\mathcal{C}(\boldsymbol{\theta})$;
- information is accessed calculating expected values $\mathrm{E}[\hat{O}]$ of target observables $\hat{O}$ on the state obtained executing $\mathcal{C}$.



Quantum Machine Learning - doing ML using QC

Machine Learning

$\mathcal{M}$: model;

$\mathcal{O}$: optimizer;

$\mathcal{J}$: loss function.

(x, y): data

Quantum Computation

$\mathcal{Q}$: qubits;

$\mathcal{S}$: superposition;

$\mathcal{E}$: entanglement.

Quantum Machine Learning - operating on qubits

Machine Learning

$\mathcal{M}$: model;

$\mathcal{O}$: optimizer;

$\mathcal{J}$: loss function.

(x, y): data

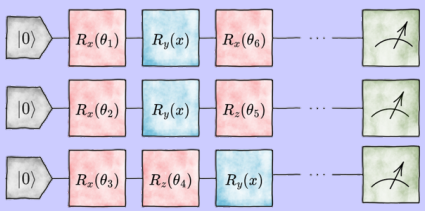
Quantum Computation

$\mathcal{Q}$: qubits;

$\mathcal{S}$: superposition;

$\mathcal{E}$: entanglement.

Circuit execution



Quantum Machine Learning - natural randomness

Machine Learning

$\mathcal{M}$: model;

$\mathcal{O}$: optimizer;

$\mathcal{J}$: loss function.

(x, y): data

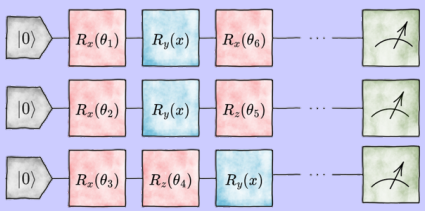
Quantum Computation

$\mathcal{Q}$: qubits;

$\mathcal{S}$: superposition;

$\mathcal{E}$: entanglement.

Circuit execution



Expected values

$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

Quantum Machine Learning - encoding the problem

Machine Learning

$\mathcal{M}$: model;

$\mathcal{O}$: optimizer;

$\mathcal{J}$: loss function.

(x, y): data

Expected values

$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

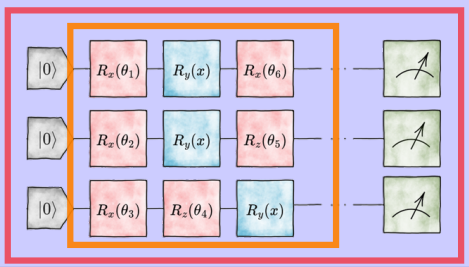
Quantum Computation

$\mathcal{Q}$: qubits;

$\mathcal{S}$: superposition;

$\mathcal{E}$: entanglement.

Circuit execution



Quantum Machine Learning!

Optimizer $\mathcal{O}$
Hybrid-strategy

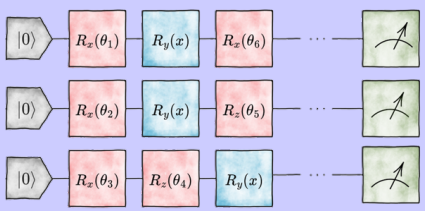
Machine Learning
$\mathcal{M}$: model;
$\mathcal{O}$: optimizer;
$\mathcal{J}$: loss function.
(x, y): data

loss function $\mathcal{J}$
$\mathcal{J}(y_{meas}, y_{est})$

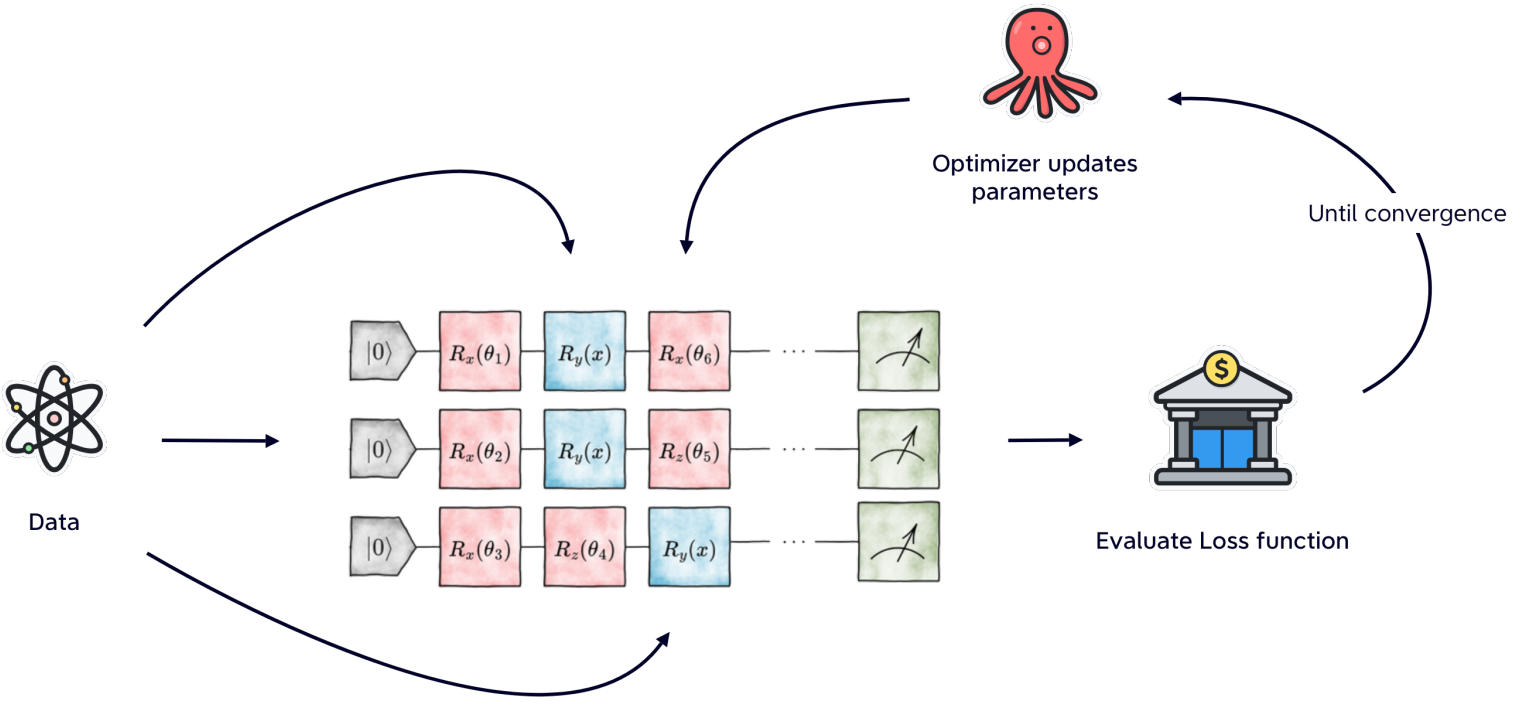
Expected values
$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

Quantum Computation
$\mathcal{Q}$: qubits;
$\mathcal{S}$: superposition;
$\mathcal{E}$: entanglement.

Circuit execution

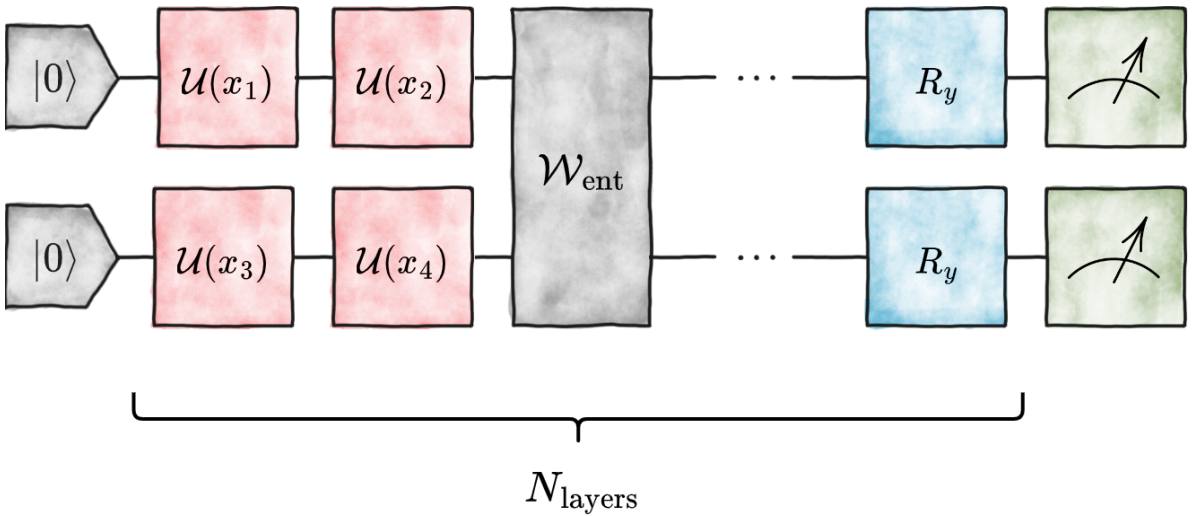


From ML to QML

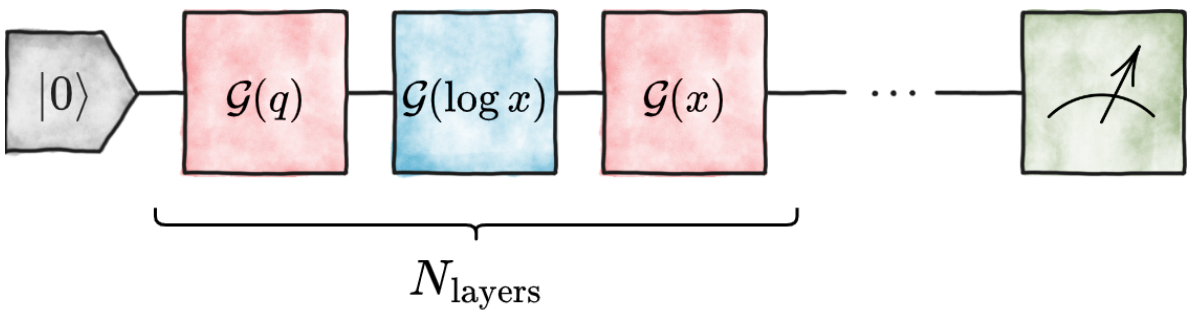


Our QML reuploading model

In case of multi-dimensional target:



In case of 1-dimensional target (used for a Parton Distribution Function fit):



Two inspirations

Classical inspiration - The INN algorithm

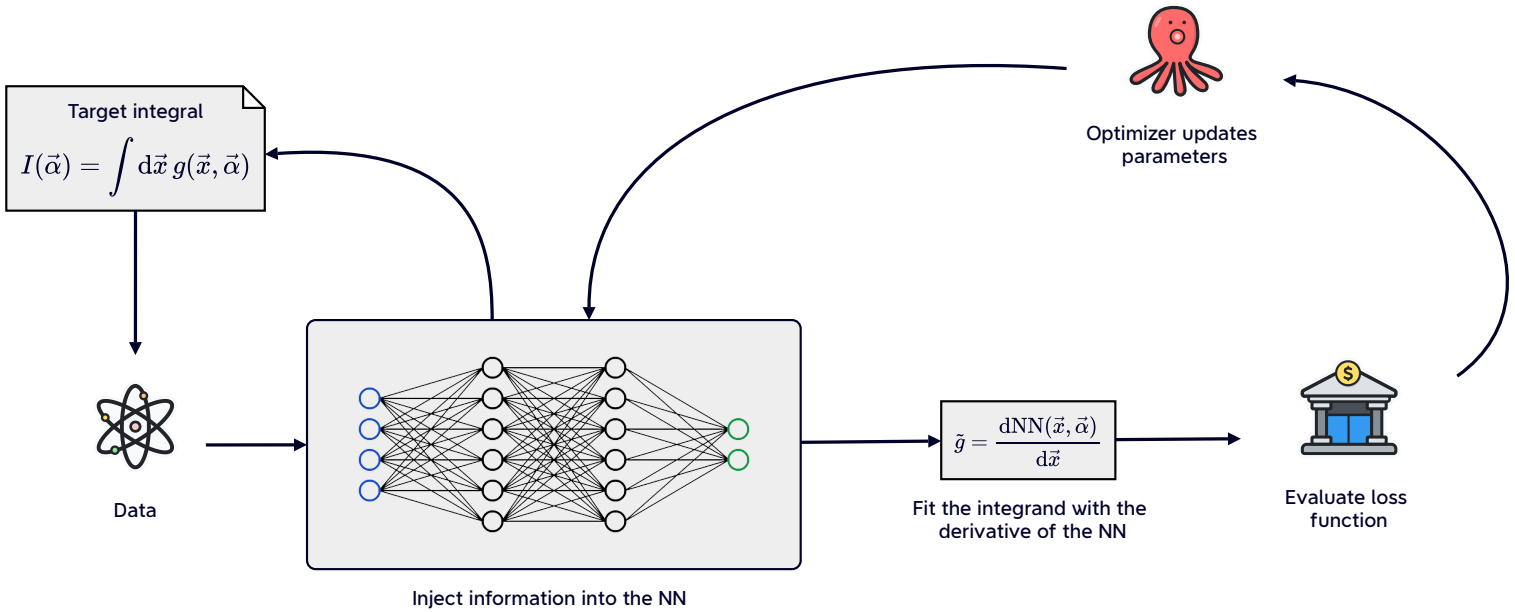
arXiv:2211.02834

In 2022, D. Maitre and R. Santos-Mateus presented a method to estimate multi-variable integrals using Neural Networks:

Classical inspiration - The INN algorithm

arXiv:2211.02834

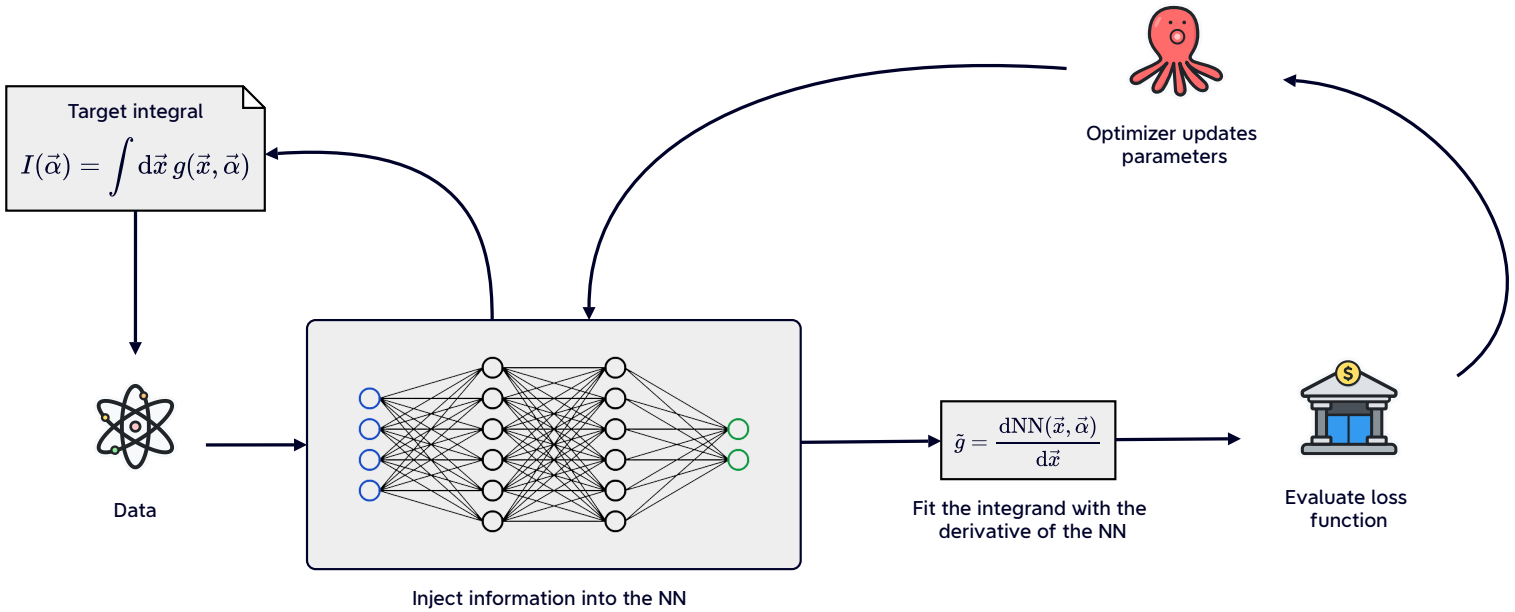
In 2022, D. Maitre and R. Santos-Mateus presented a method to estimate multi-variable integrals using Neural Networks:



Classical inspiration - The INN algorithm

arXiv:2211.02834

In 2022, D. Maitre and R. Santos-Mateus presented a method to estimate multi-variable integrals using Neural Networks:

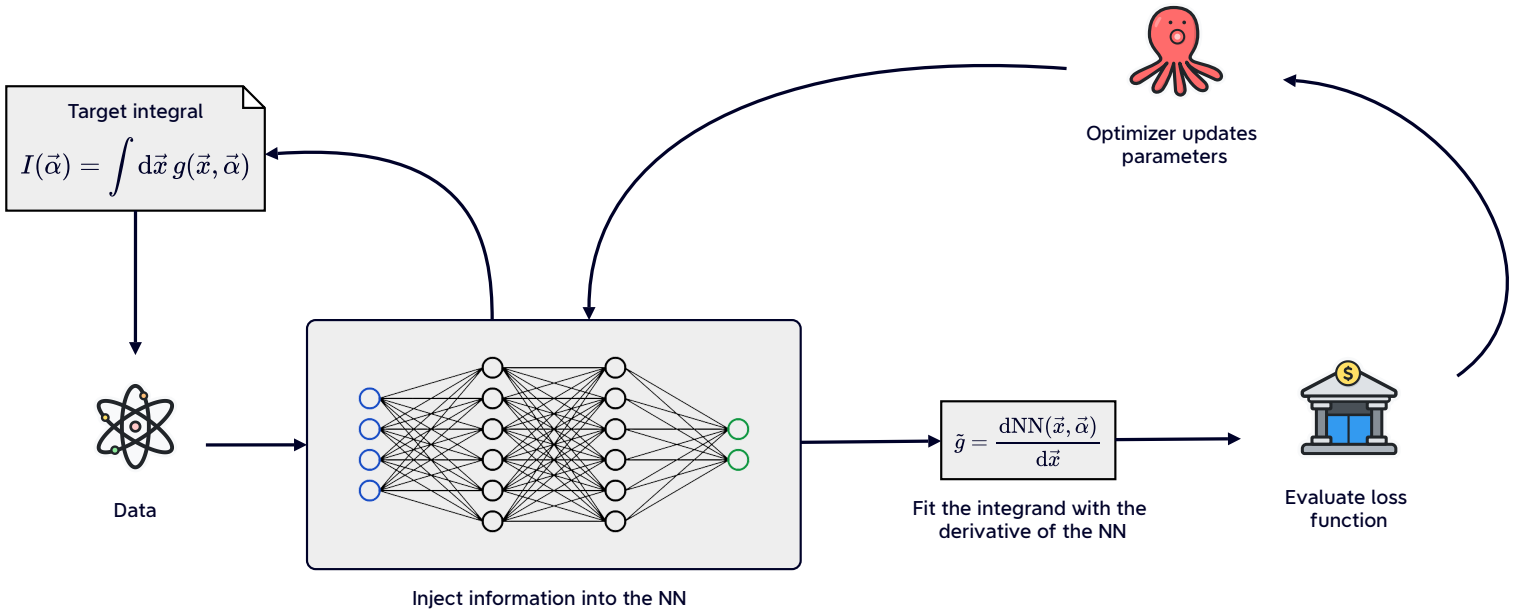


- both NN and dNN are analytical models;

Classical inspiration - The INN algorithm

arXiv:2211.02834

In 2022, D. Maitre and R. Santos-Mateus presented a method to estimate multi-variable integrals using Neural Networks:

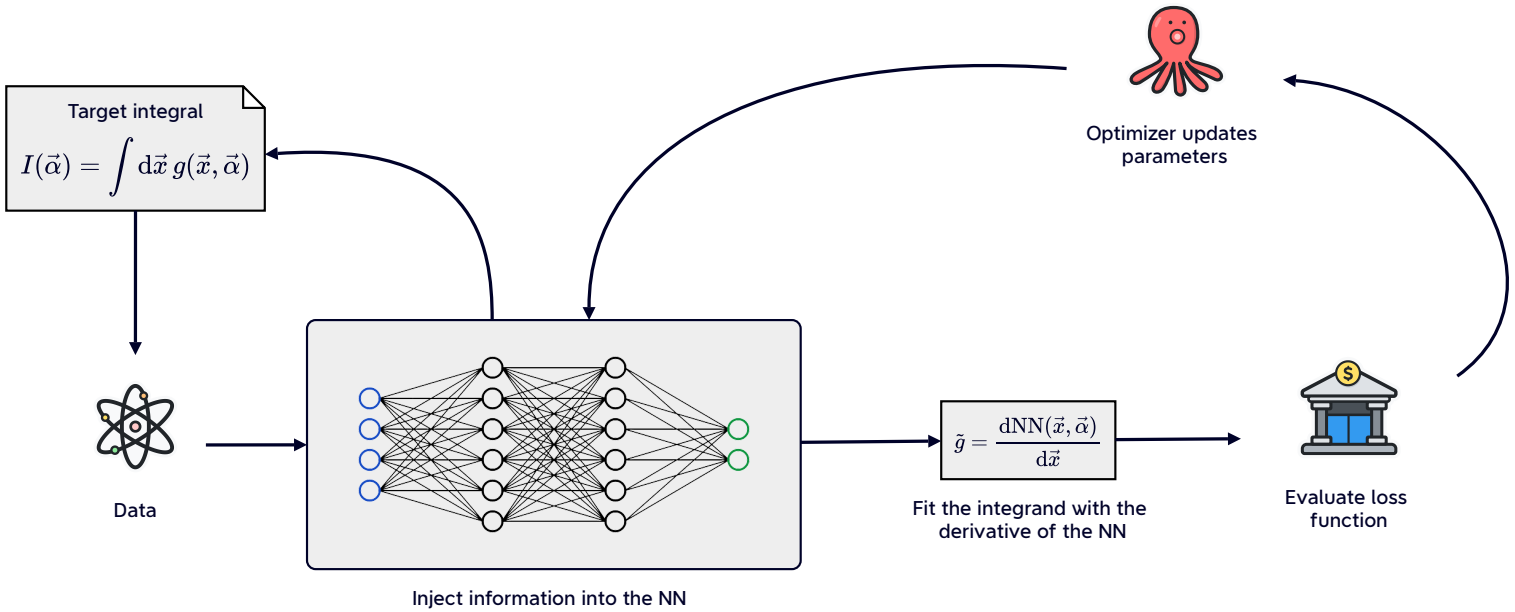


- both NN and dNN are analytical models;
- once trained, the NN can be called with any combination of data and parameters (MCI, instead, has to be recomputed every time);

Classical inspiration - The INN algorithm

arXiv:2211.02834

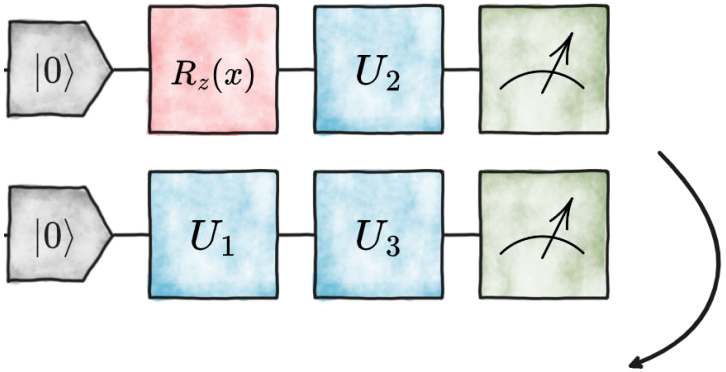
In 2022, D. Maitre and R. Santos-Mateus presented a method to estimate multi-variable integrals using Neural Networks:



- both NN and dNN are analytical models;
- once trained, the NN can be called with any combination of data and parameters (MCI, instead, has to be recomputed every time);
- in the INN is the integrand to be approximated, instead of the integral (as in MCI), and this leads to a **smaller variance**.

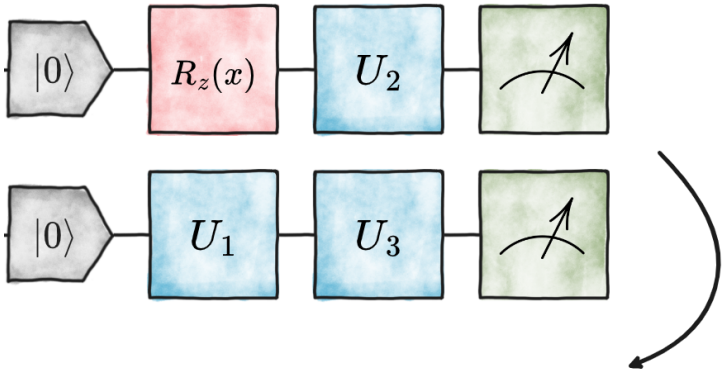
Quantum inspiration - Parameter Shift Rule

arXiv:1811.11184

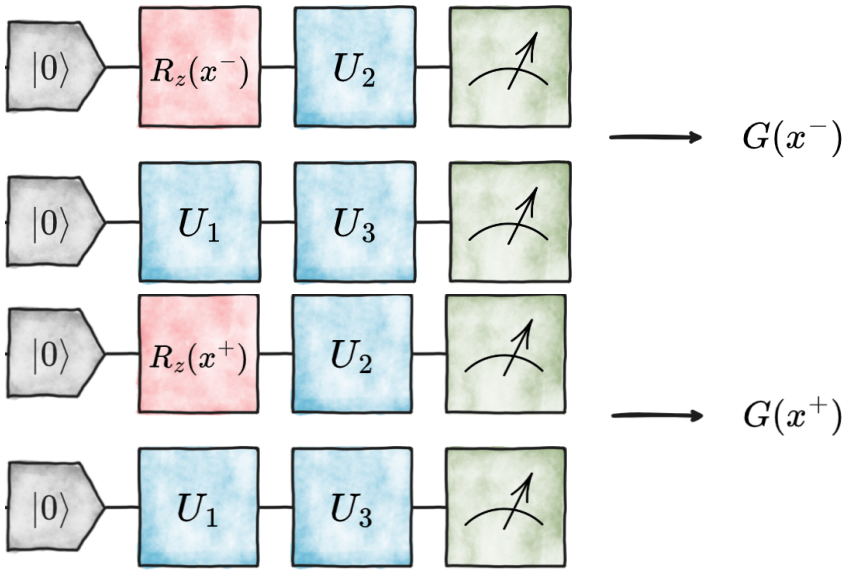


$$G(x) = \langle 0|\mathcal{C}^\dagger(x)\hat{O}\,\mathcal{C}(x)|0\rangle$$

arXiv:1811.11184



$$G(x) = \langle 0|\mathcal{C}^\dagger(x)\hat{O}\,\mathcal{C}(x)|0\rangle$$



Considering the unitary $\mathcal{U}(x) = e^{-ixU}$ affected by one parameter x, if the hermitian generator U has at most two eigenvalues $\pm r$, an exact estimator of $\partial_x G$ is:

$$\partial_x G = r\big[G(x^+) - G(x^-)\big].$$

Combining inspirations: `qinntegrate`

The `qinntegrate` algorithm

At this point, we knew that:

The `qinntegrate` algorithm

At this point, we knew that:

1. **variables** can be **injected** into a quantum circuit as rotational angles;

The `qinntegrate` algorithm

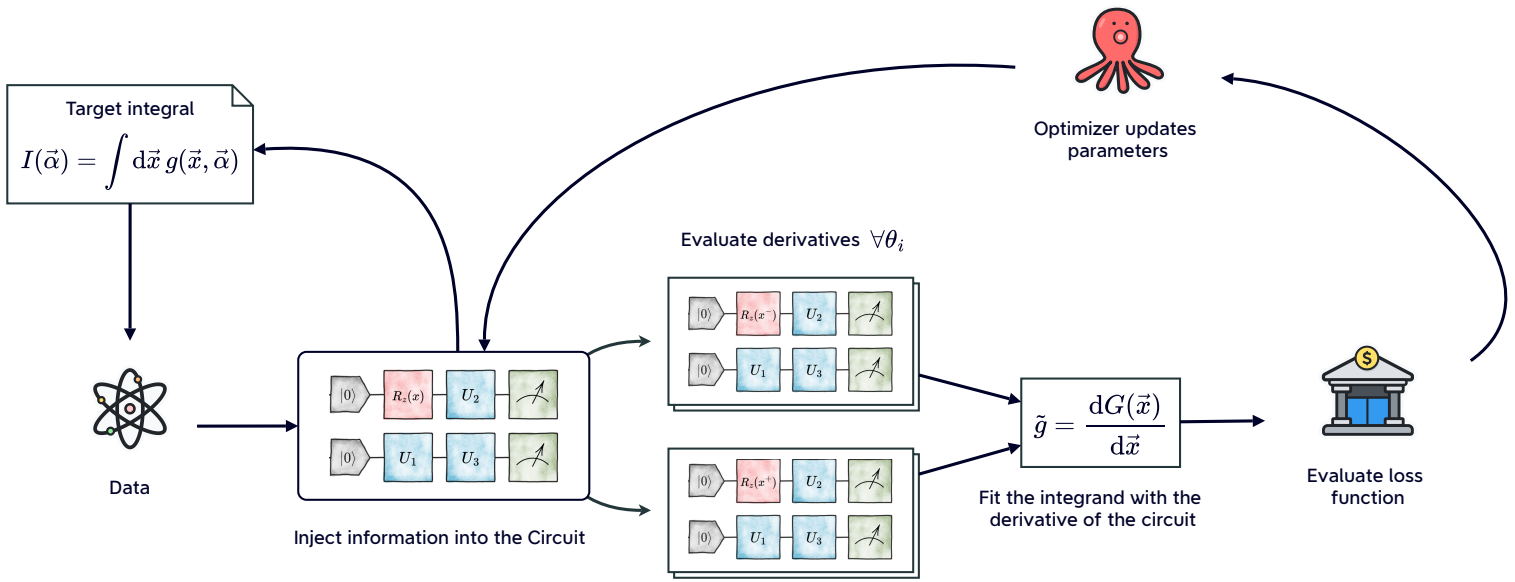
At this point, we knew that:

1. **variables** can be **injected** into a quantum circuit as rotational angles;
2. the same circuit architecture $\mathcal{C}$ can be used to compute **both** the estimator and its derivatives.

The `qinntegrate` algorithm

At this point, we knew that:

1. **variables** can be **injected** into a quantum circuit as rotational angles;
2. the same circuit architecture $\mathcal{C}$ can be used to compute **both** the estimator and its derivatives.



If indipendent variables, $\frac{\mathrm{d}G(x)}{\mathrm{d}x}$ is obtained by summing all PSR contributes.

Validation examples

Toy model: 3-dimensional trigonometric function

We firstly consider a simple multi-dimensional target:

$$\begin{aligned} I(\boldsymbol{\alpha}; \boldsymbol{x}) &= \int g(\boldsymbol{\alpha}; \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \\ &= \int \cos(\boldsymbol{\alpha} \cdot \boldsymbol{x} + \alpha_0) \, \mathrm{d}\boldsymbol{x}. \end{aligned} \tag{2}$$

And we target a marginalisation $\frac{\mathrm{d}I(\boldsymbol{\alpha};\boldsymbol{x})}{\mathrm{d}x_i}$ for fixed i but varying α's.

Toy model: 3-dimensional trigonometric function

We firstly consider a simple multi-dimensional target:

$$I(\boldsymbol{\alpha}; \boldsymbol{x}) = \int g(\boldsymbol{\alpha}; \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int \cos(\boldsymbol{\alpha} \cdot \boldsymbol{x} + \alpha_0) \, \mathrm{d}\boldsymbol{x}. \tag{2}$$

And we target a marginalisation $\frac{\mathrm{d}I(\boldsymbol{\alpha};\boldsymbol{x})}{\mathrm{d}x_i}$ for fixed i but varying α's.

Parameter	Value
$N_{\boldsymbol{x},\mathrm{train}}$	100
$\boldsymbol{\alpha}$	$\{1, 2, 0.5\}$
N_{α_0}	10
N_{layers}	2
N_{params}	20
$\lvert I - \tilde{I} \rvert$	$4.4 \cdot 10^{-3}$
N_{shots}	Exact simulation
Optimizer	L-BFGS

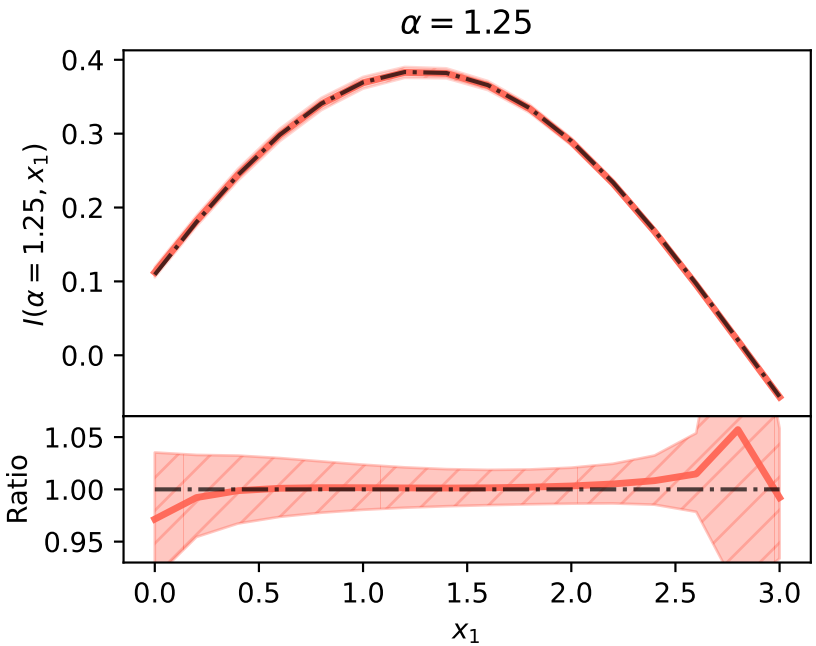
Toy model: 3-dimensional trigonometric function

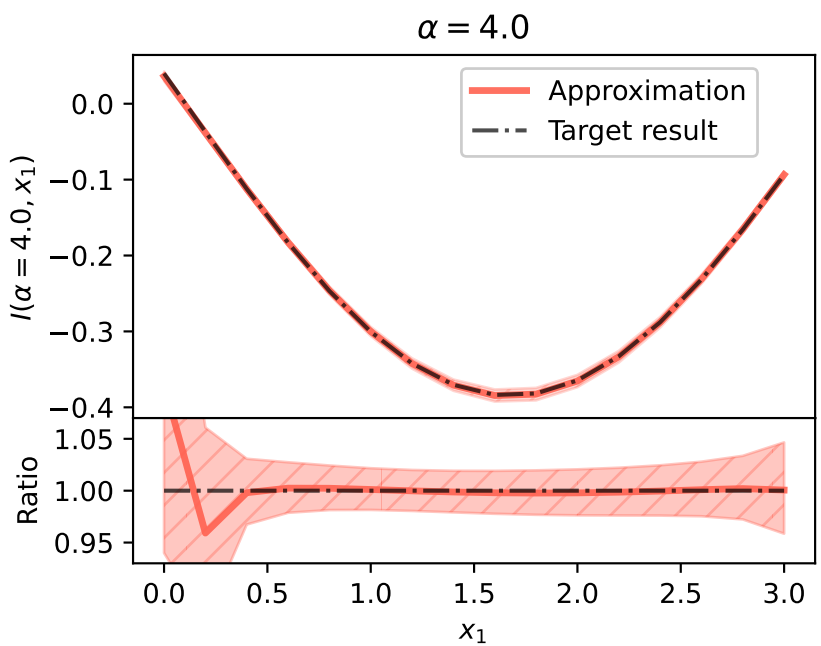
We firstly consider a simple multi-dimensional target:

$$I(\boldsymbol{\alpha}; \boldsymbol{x}) = \int g(\boldsymbol{\alpha}; \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int \cos(\boldsymbol{\alpha} \cdot \boldsymbol{x} + \alpha_0) \, \mathrm{d}\boldsymbol{x}. \tag{2}$$

And we target a marginalisation $\frac{\mathrm{d}I(\boldsymbol{\alpha};\boldsymbol{x})}{\mathrm{d}x_i}$ for fixed i but varying α's.

Parameter	Value
$N_{\boldsymbol{x},\mathrm{train}}$	100
$\boldsymbol{\alpha}$	$\{1, 2, 0.5\}$
N_{α_0}	10
N_{layers}	2
N_{params}	20
$\lvert I - \tilde{I} \rvert$	$4.4 \cdot 10^{-3}$
N_{shots}	Exact simulation
Optimizer	L-BFGS





The u-quark PDF

We then consider the u-quark PDF:

$$I_u(Q^2) = \int_{10^{-4}}^{0.7} x\, u(x, Q)\, \mathrm{d}x. \tag{3}$$

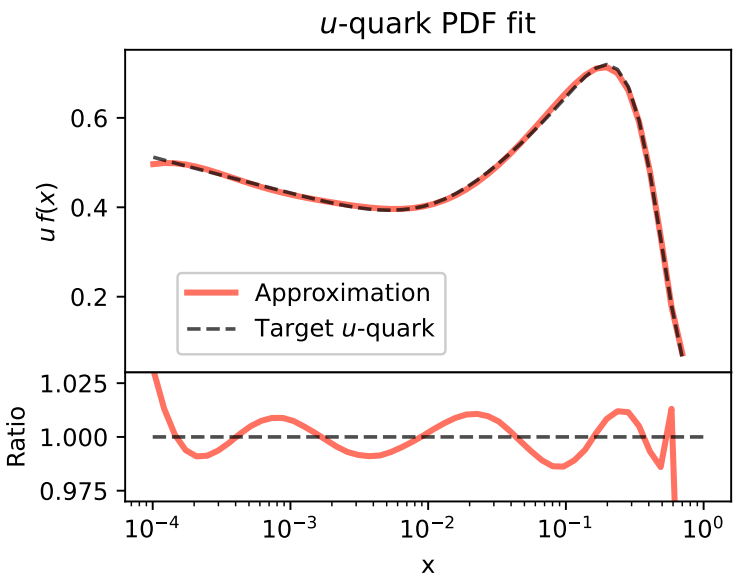
The u-quark PDF

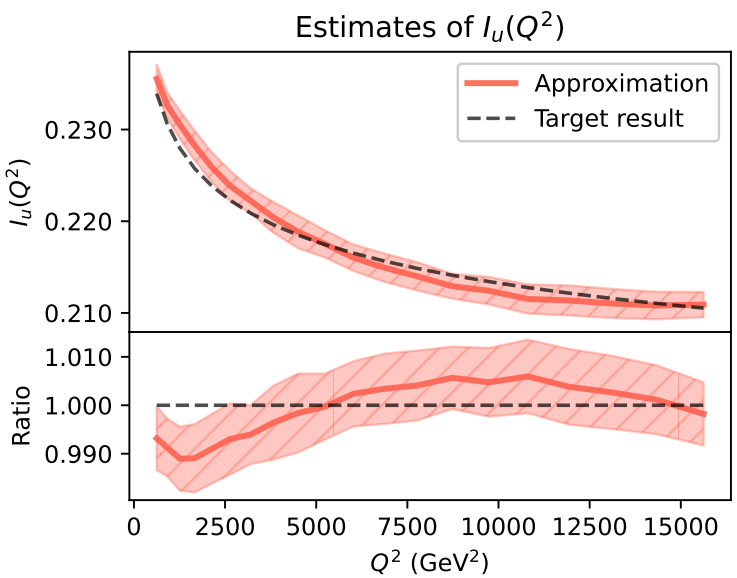
We then consider the u-quark PDF:

$$I_u(Q^2) = \int_{10^{-4}}^{0.7} x\, u(x, Q)\, \mathrm{d}x. \tag{3}$$

Parameter	Value
$N_{x,\mathrm{train}}$	500
Q	1.67
N_{layers}	4
N_{params}	27
$\lvert I - \tilde{I}\rvert$	$1.2 \cdot 10^{-5}$
N_{shots}	Exact simulation
Optimizer	L-BFGS

Parameter	Value
$(N_x, N_Q)_{\mathrm{train}}$	(120, 100)
$N_{Q,\mathrm{est}}$	20
N_{runs}	100
N_{layers}	4
N_{params}	36
$\lvert I - \tilde{I}\rvert$	$7.4 \cdot 10^{-5}$
N_{shots}	10^6
Optimizer	L-BFGS





Toy model on a superconducting quantum chip

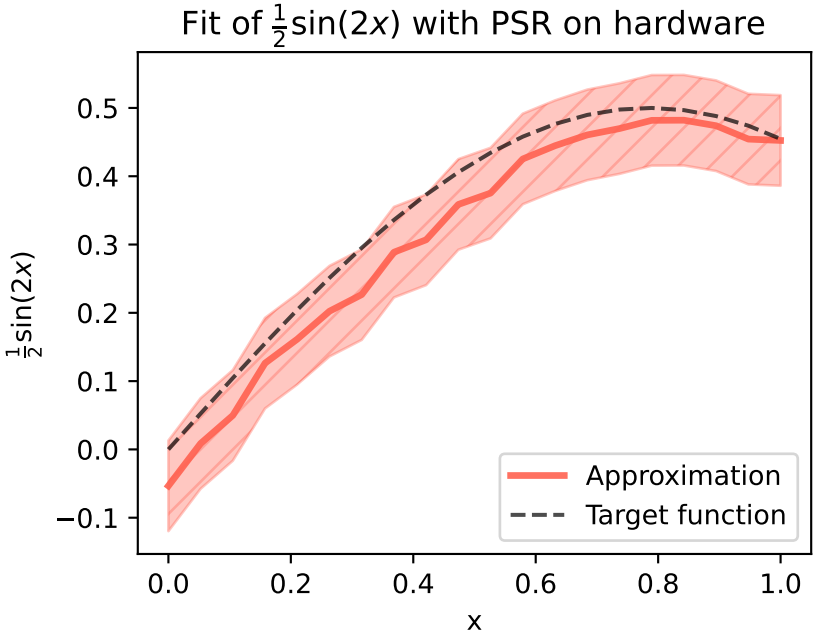
We finally tackle a dummy target using a real superconducting qubit:

$$I = \int_0^1 \frac{1}{2} \cos(2x)\, \mathrm{d}x. \tag{4}$$

Toy model on a superconducting quantum chip

We finally tackle a dummy target using a real superconducting qubit:

$$I = \int_0^1 \frac{1}{2} \cos(2x)\, \mathrm{d}x. \tag{4}$$



Parameter	Value
$N_{x,\mathrm{train}}$	50
$N_{x,\mathrm{est}}$	20
N_{runs}	10
N_{layers}	1
N_{params}	6
$\lvert I - \tilde{I} \rvert$	$2.8 \cdot 10^{-2}$
N_{shots}	$2 \cdot 10^{3}$
Optimizer	L-BFGS

Conclusions

Conclusions and outlook

As final comment we can say that:

- 👍 the proposed model successfully approximates multi-dimensional integrals;
- 👍 once a winning architecture is defined, this can be used to fit the integrand and to perform any "marginalisation" of the integrand;
- 👍 using VQCs, we build particularly shallow models;
- 👎 the current method used to calculate derivatives scales bad with the problem dimensionality;
- 👎 the hardware noise complicates the derivatives calculation.

How to do better?

- try different differentiation strategies (natural gradient, non-demolition measurements, etc);
- define even more shallow models to reduce the number of quantum gates;
- exploit variables correlation to reduce the number of required gates.