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:

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

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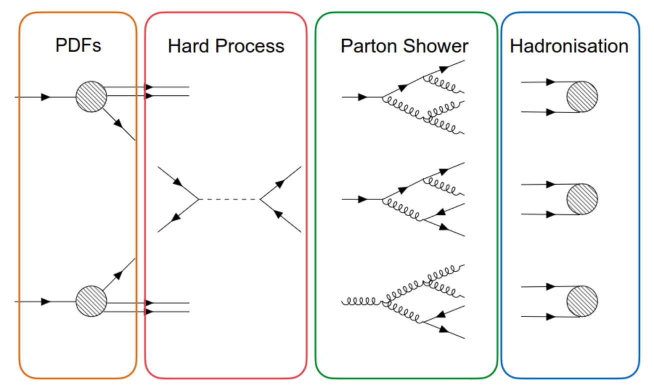

Introductory concepts

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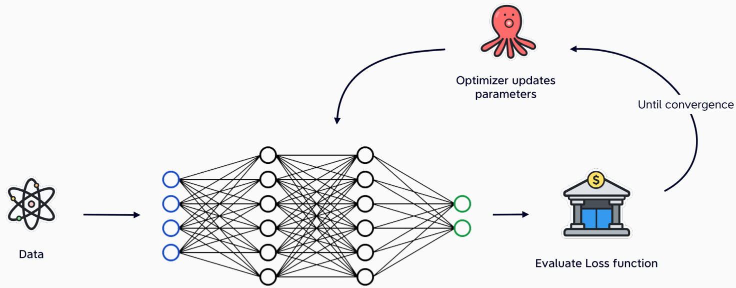
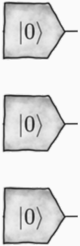


Parametric Quantum Circuits

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



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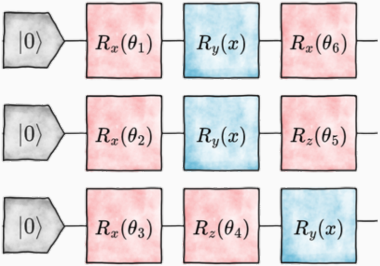

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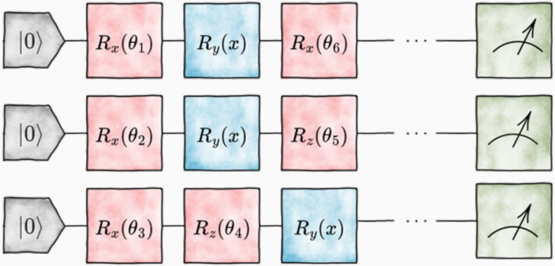
- information is accessed calculating expected values $\mathrm{E}[\hat{O}]$ of target observables $\hat{O}$ on the state obtained executing $\mathcal{C}$.



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

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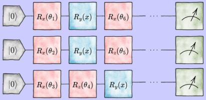

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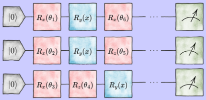

Expected values
$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

Quantum Machine Learning - encoding the problem

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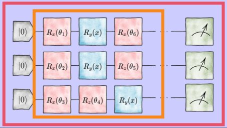

Quantum Machine Learning!

Optimizer $\mathcal{O}$
Hybrid-strategy

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

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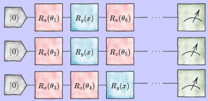
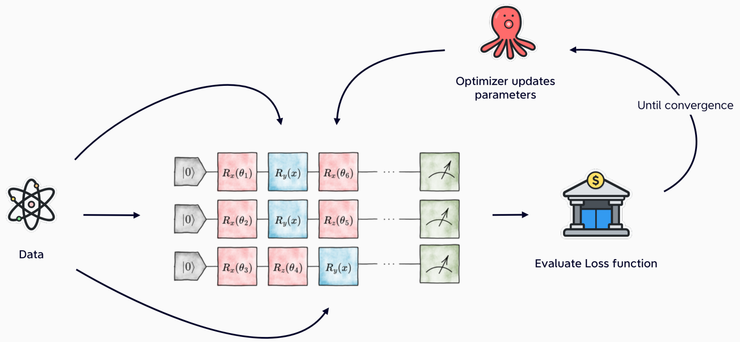
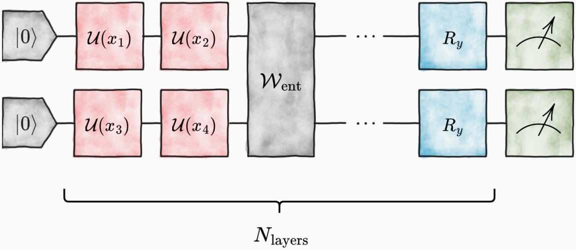


From ML to QML

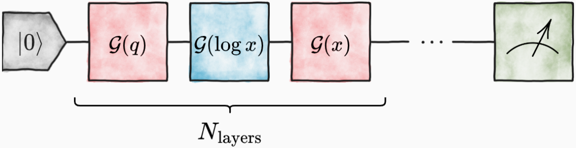


Our QML reuploading model

In case of multi-dimensional target:



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



Two inspirations

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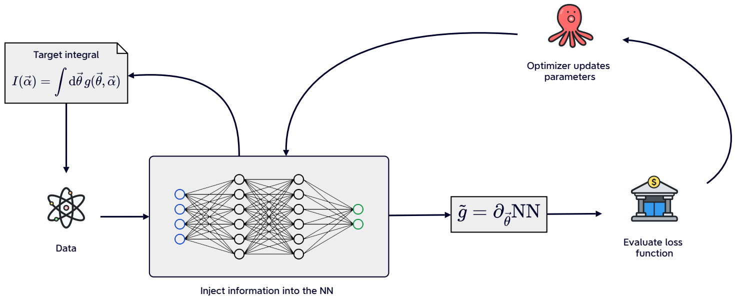

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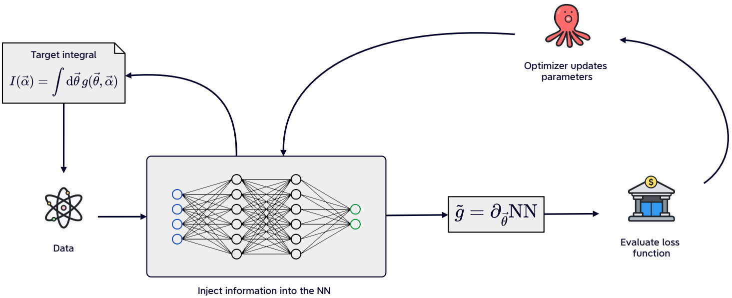

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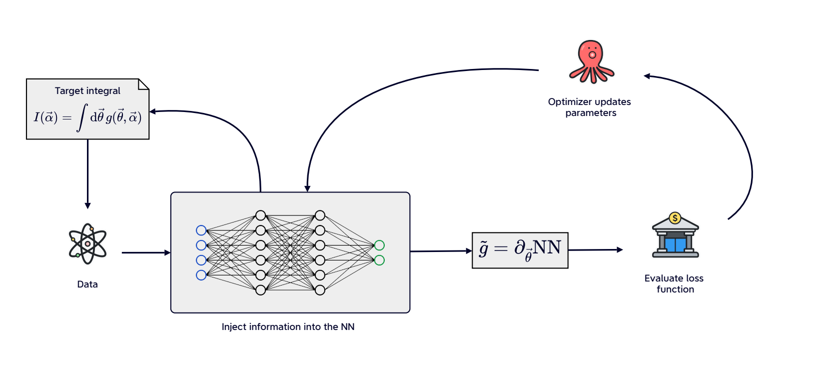

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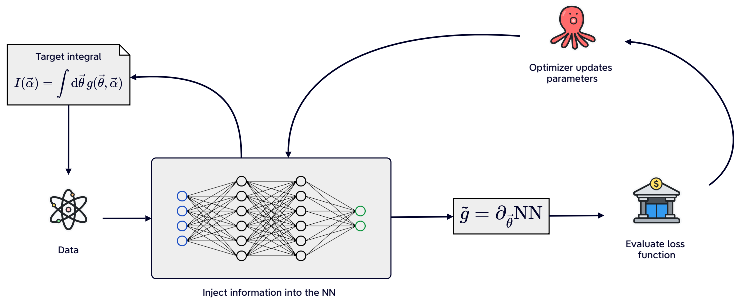
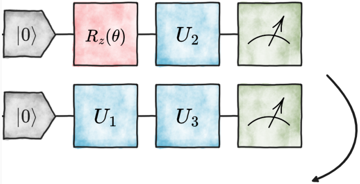
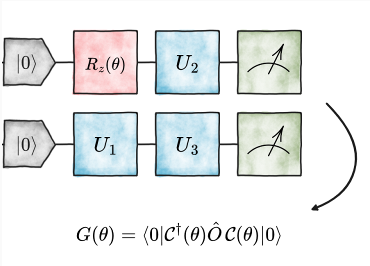


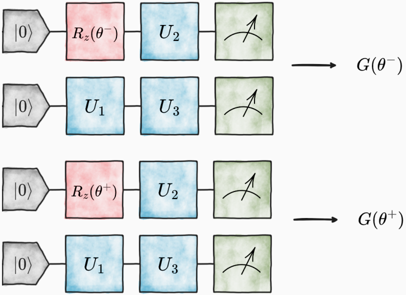
This is interesting for at least two reasons:

- having an **analytical** estimator of the integral prevents us to re-compute the whole integral for every parameter combination;
- in the INN is the integrand to be approximated, instead of the integral (as in MCI), and this leads to a **smaller variance**.



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





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

$$\partial_\theta G = r\left[G(\theta^+) - G(\theta^-)\right].$$

Combining inspirations: `qinntegrate`

The `qinntegrate` algorithm

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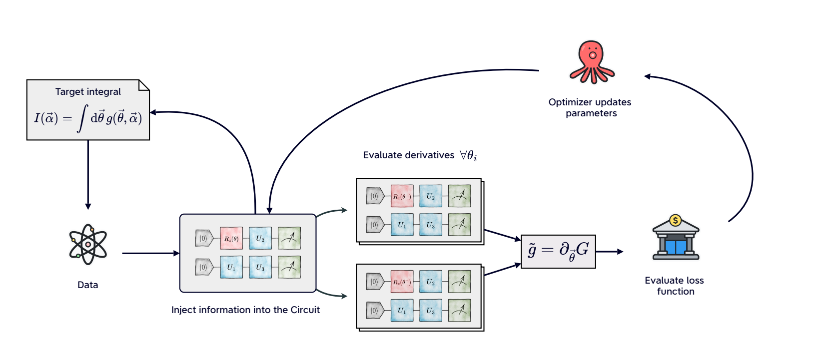

If indipendent variables, $\frac{\mathrm{d}G(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}}$ is obtained by summing all PSR contributes.

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.

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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
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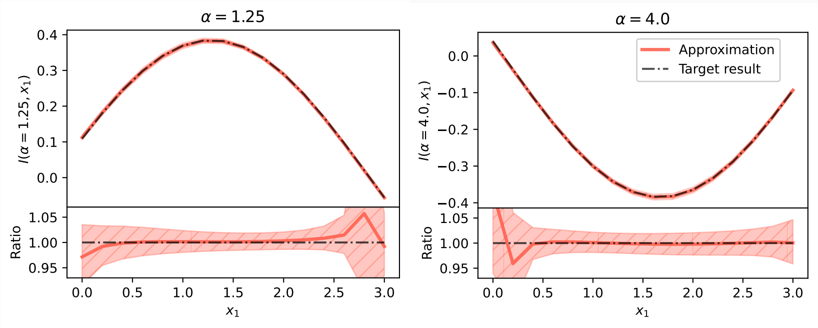

The u-quark PDF

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

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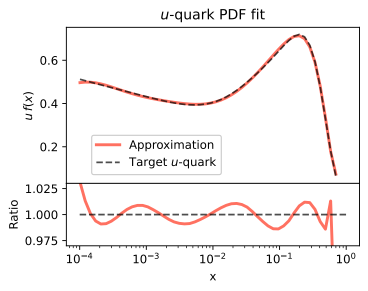
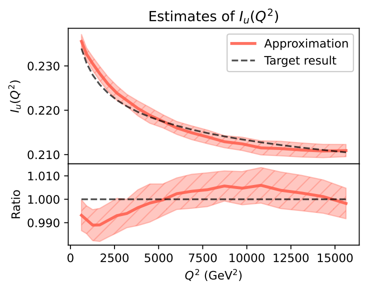
Parameter	Value
$N_{x,\mathrm{train}}$	500
Q	1.67
N_{layers}	4
N_{params}	27
$\lvert I - \tilde{I} \rvert$	$1.2 \cdot 10^{-5}$
N_{shots}	Exact simulation
Optimizer	L-BFGS

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:

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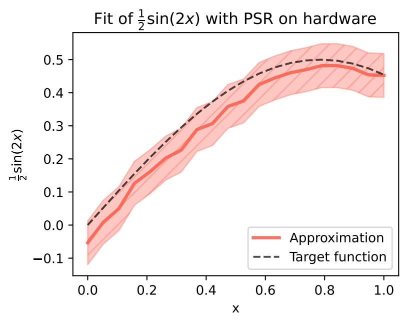

Parameter	Value
$N_{x,\mathrm{train}}$	50
$N_{x,\mathrm{est}}$	20
N_{runs}	10
N_{layers}	1
N_{params}	6
$\lvert I - \tilde{I} \rvert$	$2.8 \cdot 10^{-2}$
N_{shots}	$2 \cdot 10^{3}$
Optimizer	L-BFGS

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.