

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

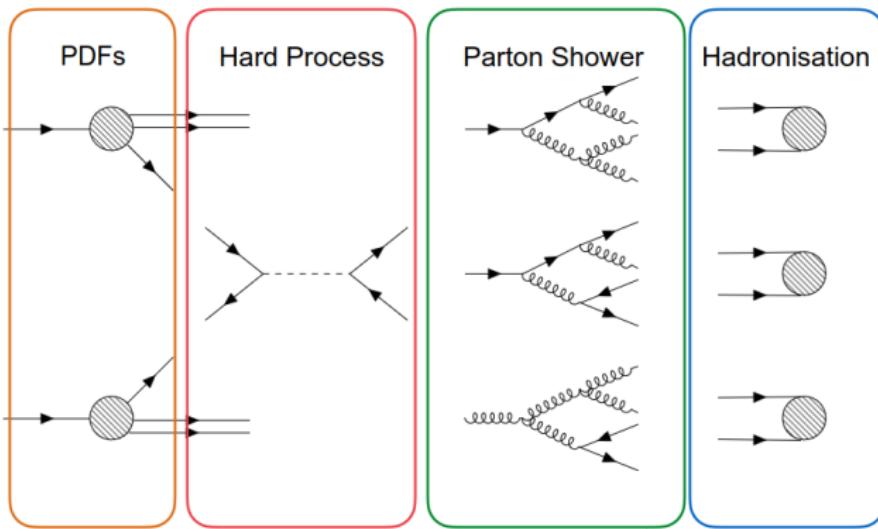
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Introductory concepts

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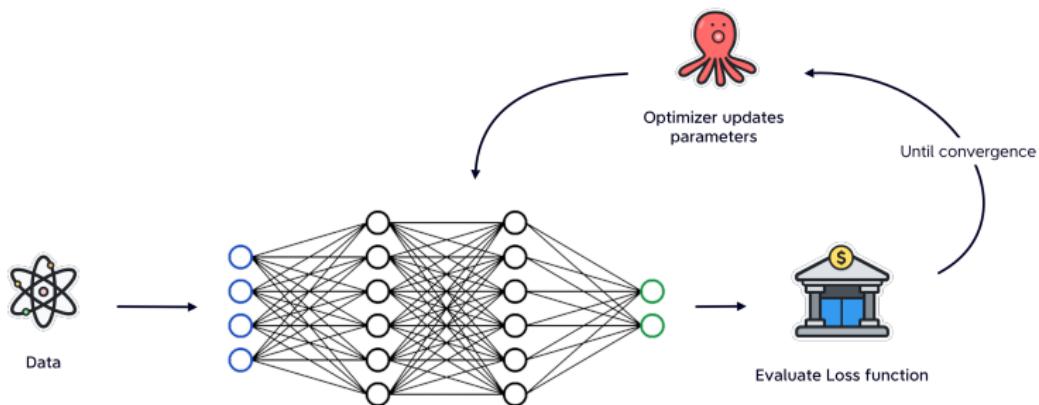
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Parametric Quantum Circuits

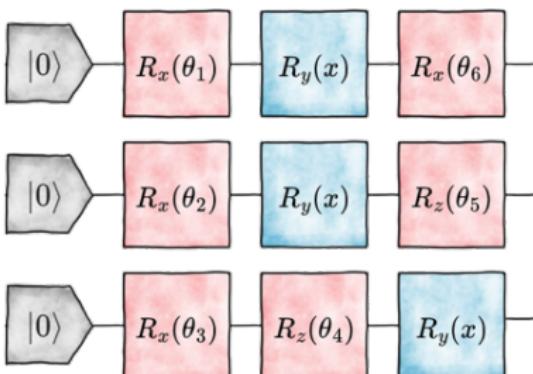
Parametric Quantum Circuits

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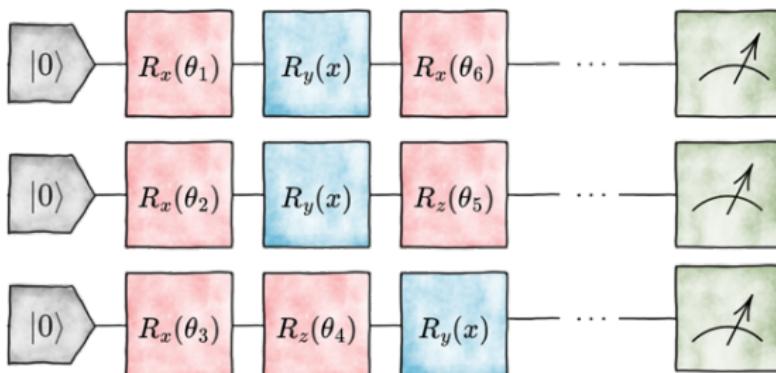
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Rotational gates $R_j(\theta) = e^{-i\theta\hat{\sigma}_j}$ are used to build parametric circuits $\mathcal{C}(\theta)$;
- 👁️ information is accessed calculating expected values $E[\hat{O}]$ of target observables \hat{O} on the state obtained executing \mathcal{C} .



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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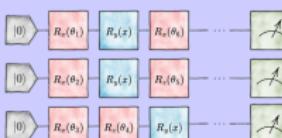
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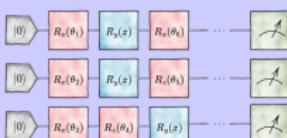
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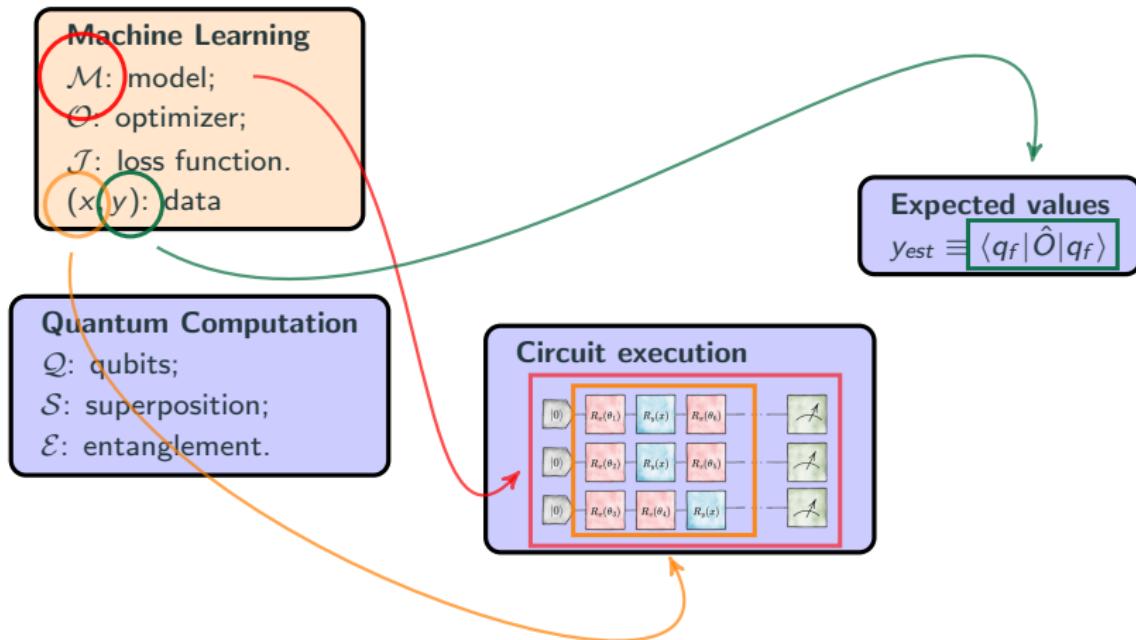
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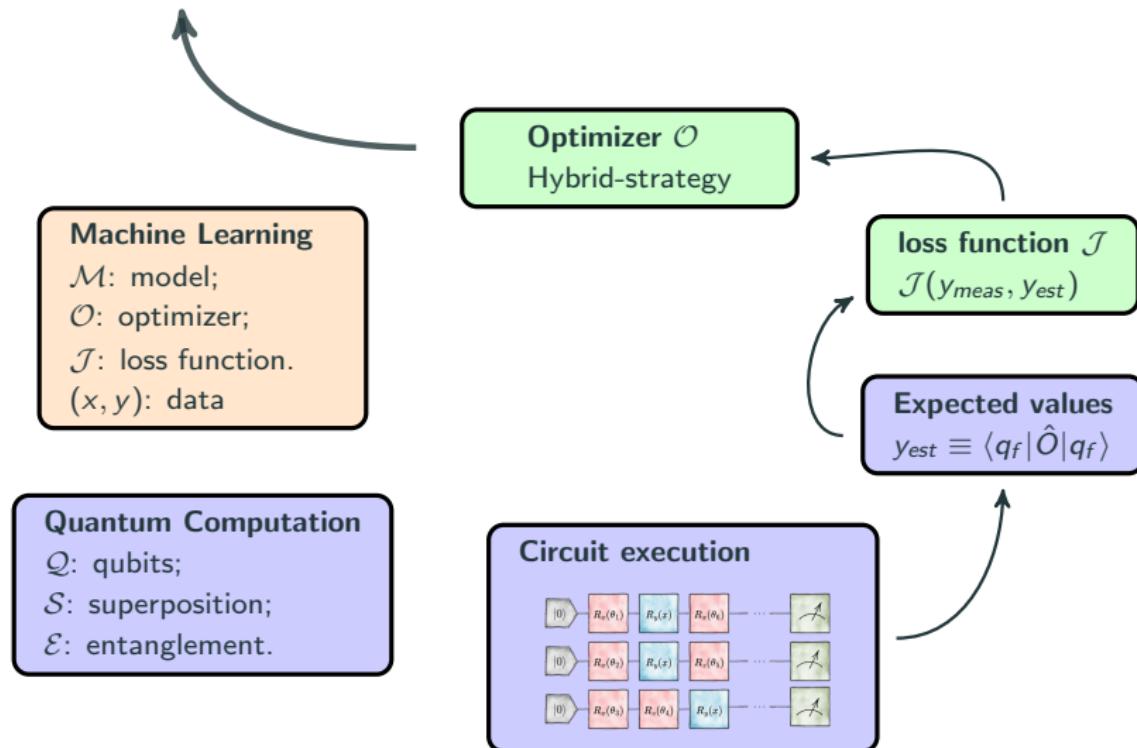
Expected values

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

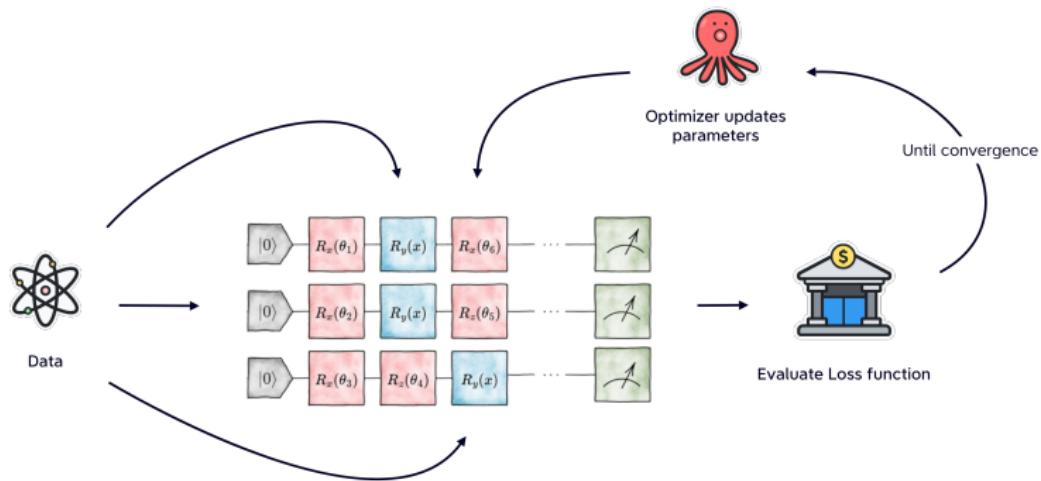
Quantum Machine Learning - encoding the problem



Quantum Machine Learning!

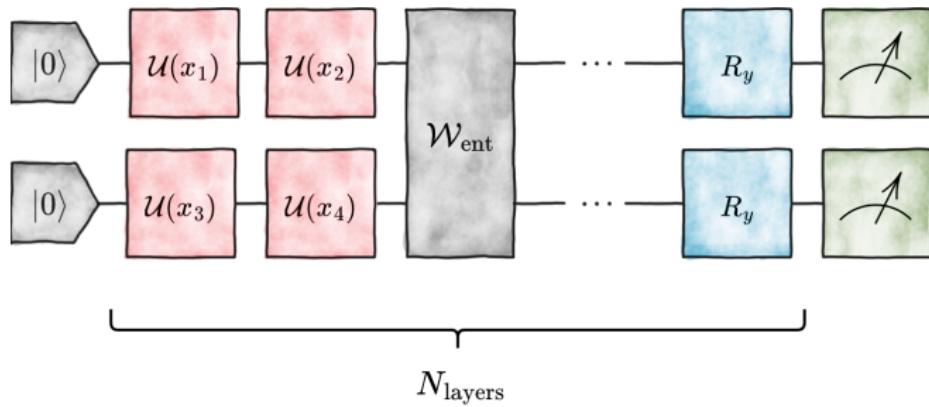


From ML to QML

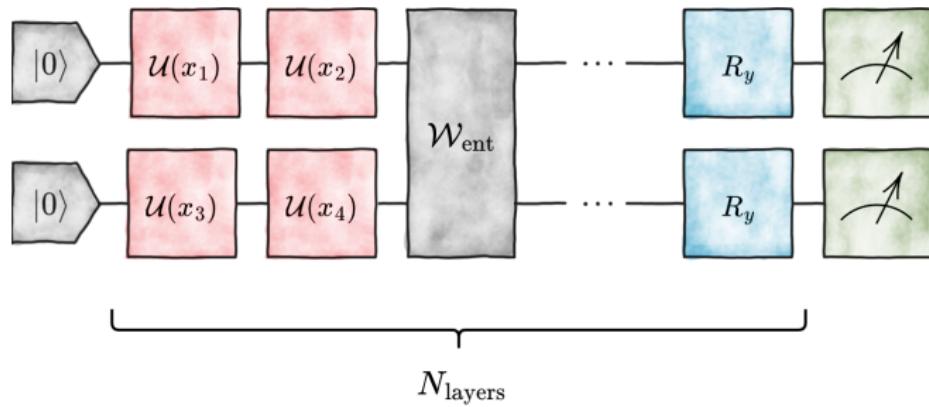


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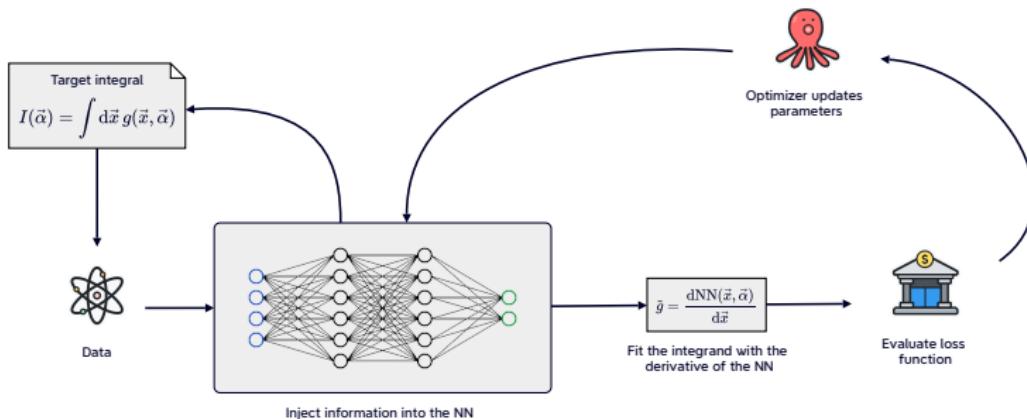


It has been proved this approach is equivalent to approximate a function with an N -term Fourier Series.

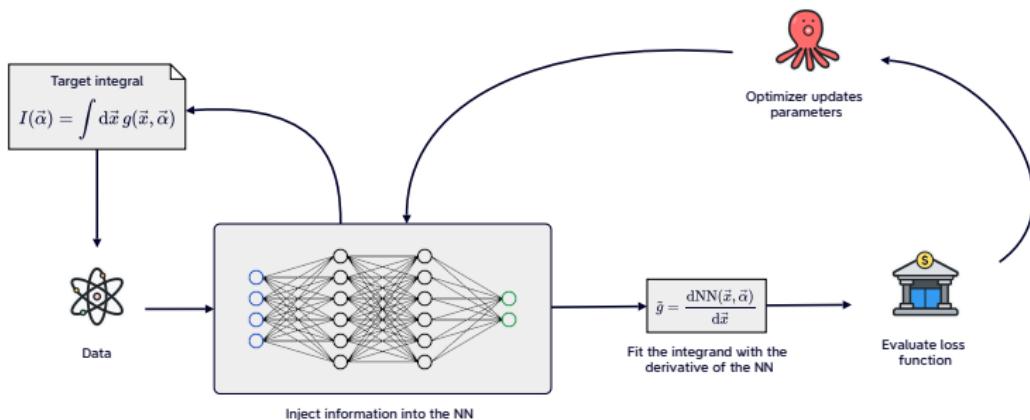
Two inspirations

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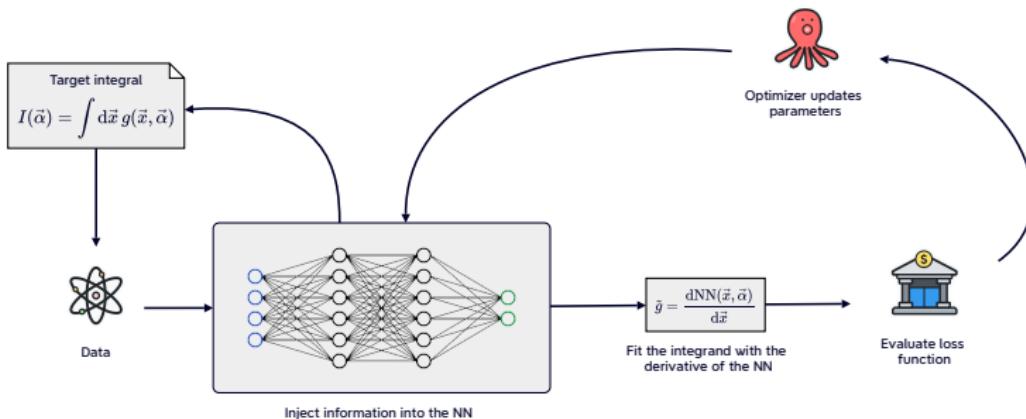


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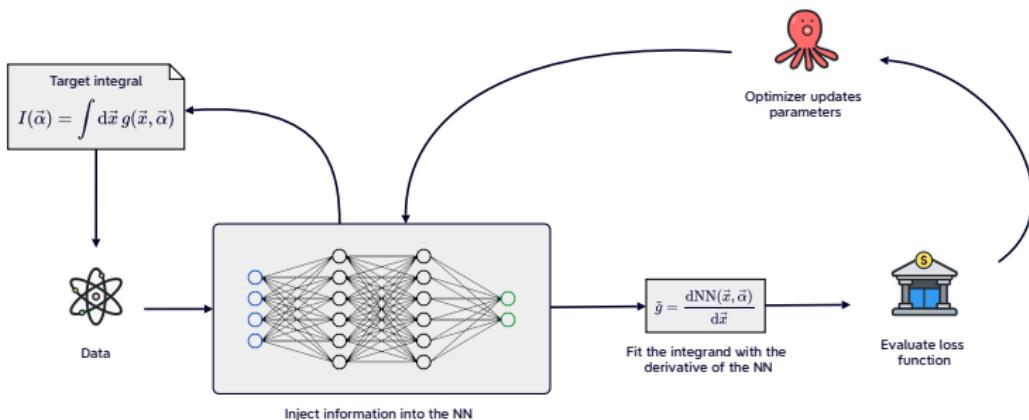
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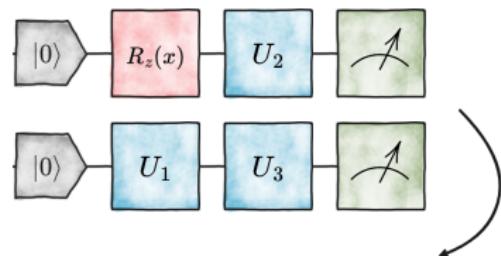


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- once trained, the NN can be called with any combination of data and parameters. Monte Carlo Integration (MCI), instead, has to be recomputed every time;

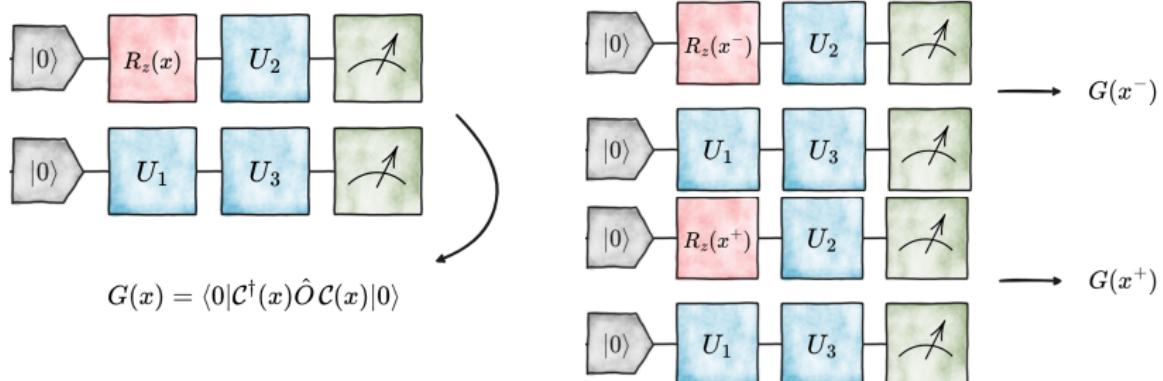
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- once trained, the NN can be called with any combination of data and parameters. Monte Carlo Integration (MCI), instead, has to be recomputed every time;
- in the INN is the integrand to be approximated, instead of the integral (as in MCI), swaps **variance** for approximation error.



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



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:

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

Where $x^\pm = x \pm s$ and, considering rotational gates, we have $s = \pi/2$ and $r = 1/2$.

Combining inspirations: qinntegrate

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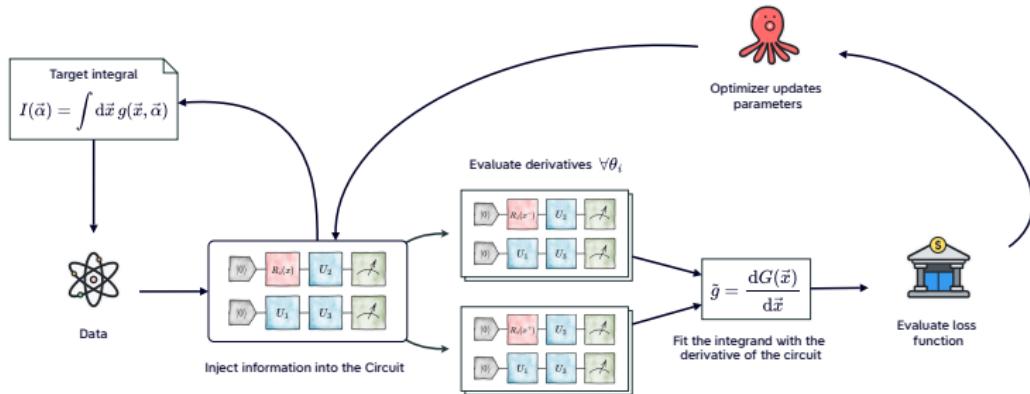
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If independent variables, $\frac{dG(x)}{dx}$ is obtained by summing all PSR contributions.

Validation examples

Toy model: 3-dimensional trigonometric function

We firstly consider a simple multi-dimensional target:

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

And we target a differential distribution $\frac{dI(\alpha, \alpha_0; \mathbf{x})}{dx_i}$ for fixed i but varying α_0 's.

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

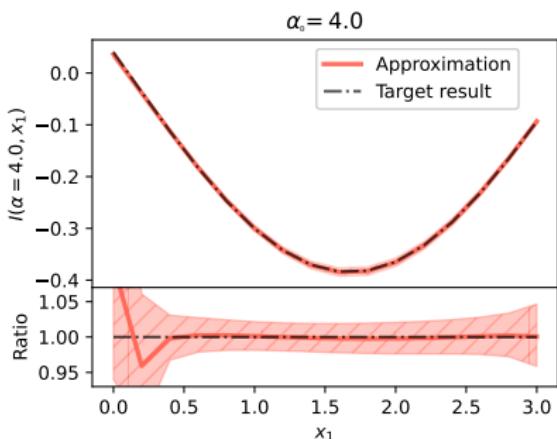
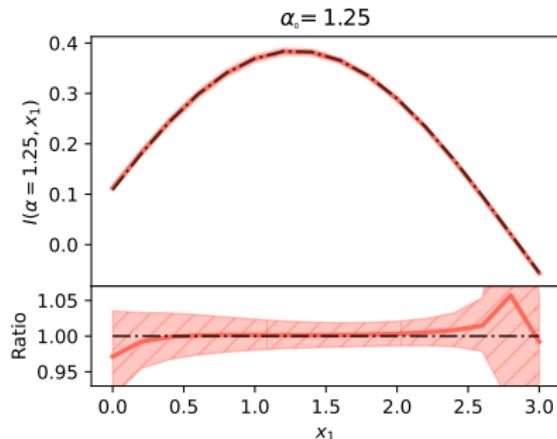
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$$I_u(Q^2) = \int_{10^{-4}}^{0.7} x u(x, Q) dx. \quad (3)$$

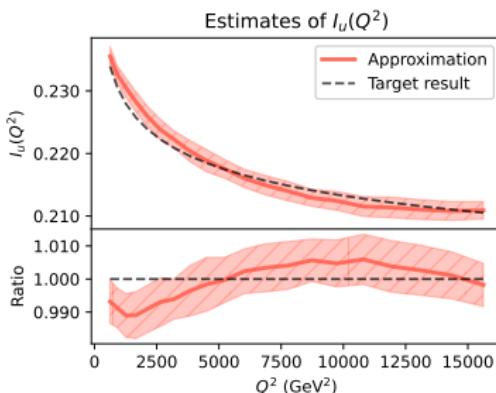
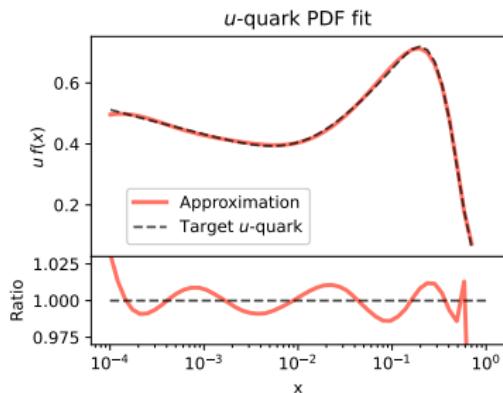
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$N_{x,\text{train}}$	500
Q	1.67
N_{layers}	4
N_{params}	27
$ I - \tilde{I} $	$1.2 \cdot 10^{-5}$
N_{shots}	Exact simulation
Optimizer	L-BFGS

Parameter	Value
$(N_x, N_Q)_{\text{train}}$	(120, 100)
$N_{Q,\text{est}}$	20
N_{runs}	100
N_{layers}	4
N_{params}	36
$ I - \tilde{I} $	$7.4 \cdot 10^{-5}$
N_{shots}	10^6
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Toy model on a superconducting quantum chip

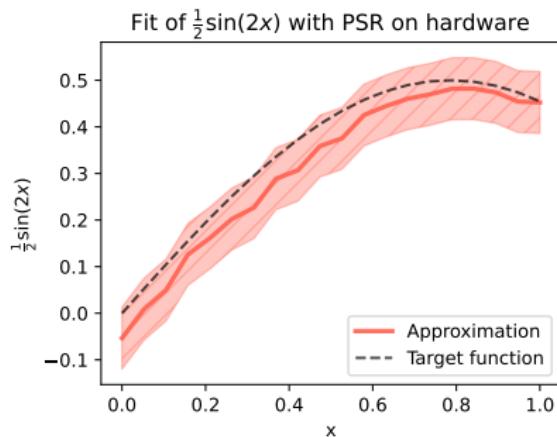
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Parameter	Value
$N_{x,\text{train}}$	50
$N_{x,\text{est}}$	20
N_{runs}	10
N_{layers}	1
N_{params}	6
$ I - \tilde{I} $	$2.8 \cdot 10^{-2}$
N_{shots}	$2 \cdot 10^3$
Optimizer	L-BFGS

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Some final comments

- ❑ the algorithm **successfully approximates** multi-dimensional integrals;
- ❑ once a winning architecture is defined, this can be used to fit the integrand and to perform **any differential distribution** of the integral;
- ❑ we have used **shallow models** as VQCs;
- ❑ computing the derivatives scales **exponentially** with the dimensionality;
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How to do better?

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⌚ Code available [here](#).

📄 Pre-print: arXiv:2308.05657

Thank you for your attention!