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:

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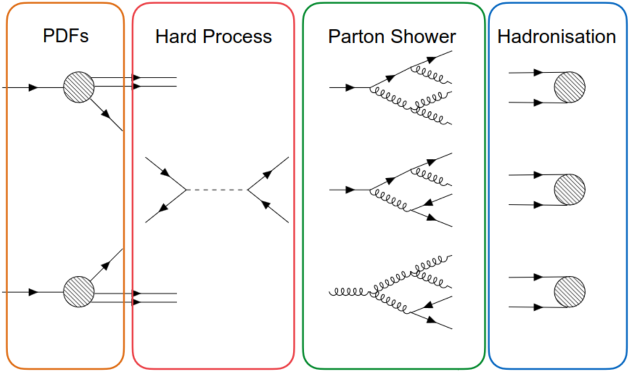

Introductory concepts

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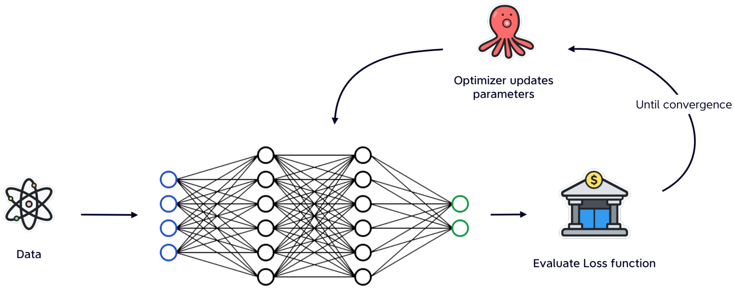

Parametric Quantum Circuits

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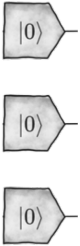

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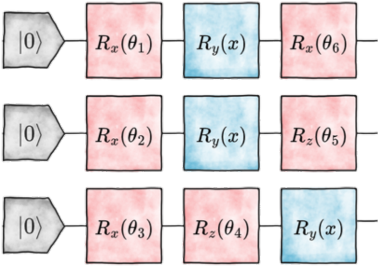

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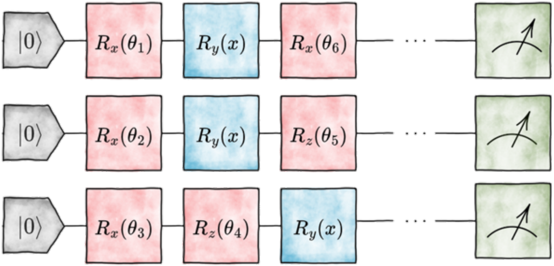
- information is accessed calculating expected values $\mathrm{E}[\hat{O}]$ of target observables $\hat{O}$ on the state obtained executing $\mathcal{C}$.



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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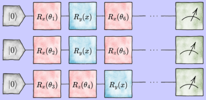

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$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

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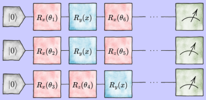

Quantum Machine Learning - encoding the problem

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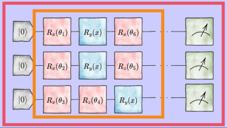

Quantum Machine Learning!

Optimizer $\mathcal{O}$
Hybrid-strategy

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

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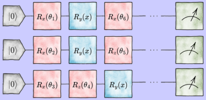
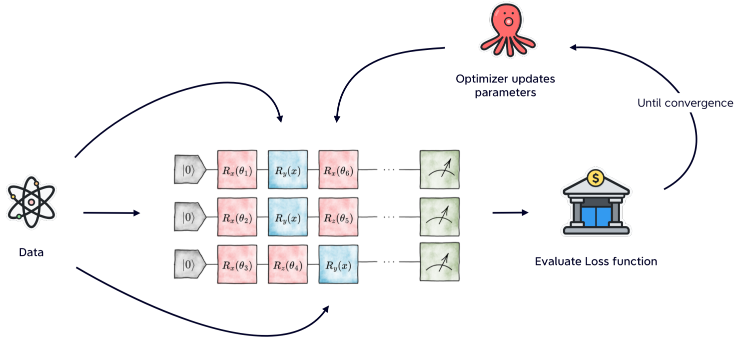


From ML to QML



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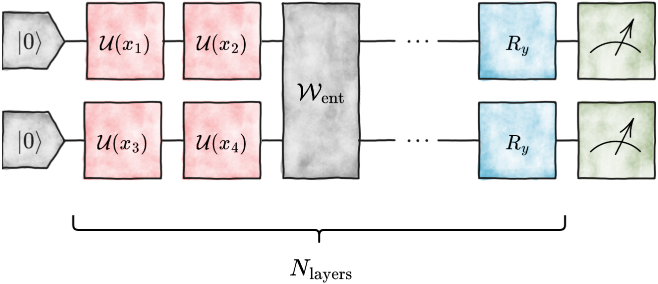

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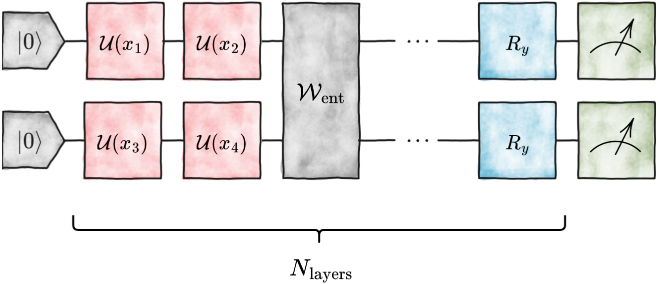

It has been proved this approach is equivalent to approximate a function with an N-term Fourier Series.

Two inspirations

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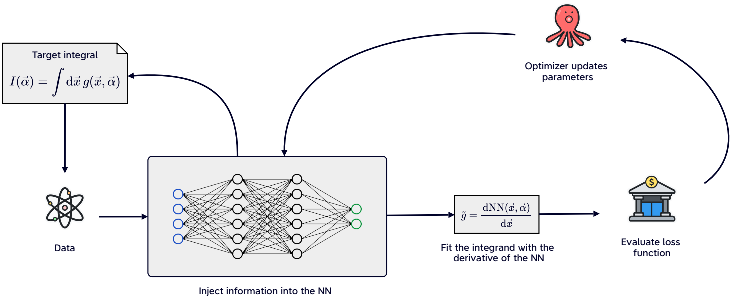

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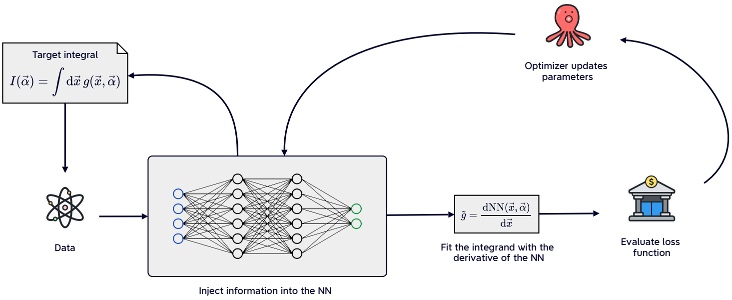

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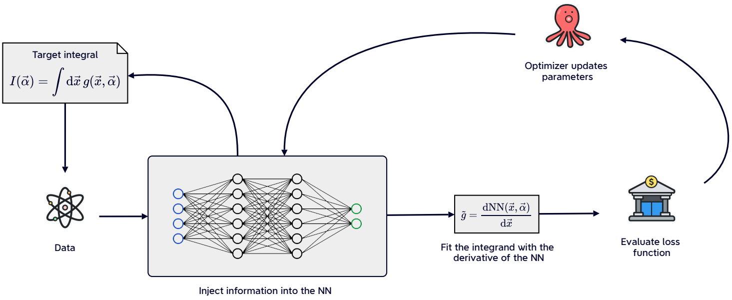

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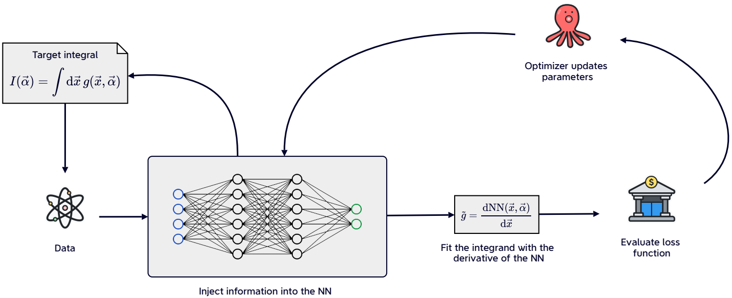

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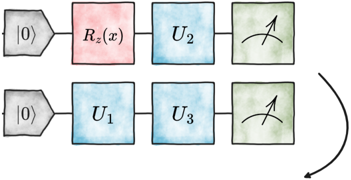
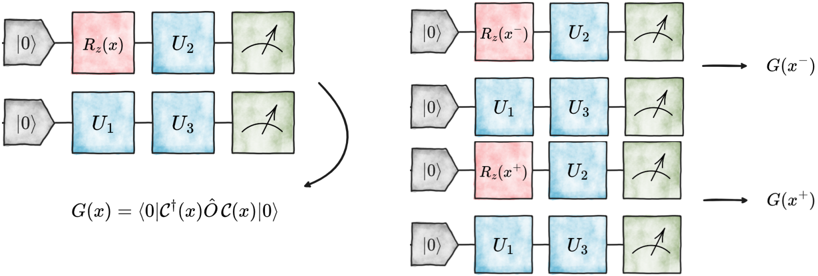
- once trained, the NN can be called with any combination of data and parameters. Monte Carlo Integration (MCI), instead, has to be recomputed every time;
- in the INN is the integrand to be approximated, instead of the integral (as in MCI), swaps **variance** for approximation error.



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



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:

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

Combining inspirations: `qinntegrate`

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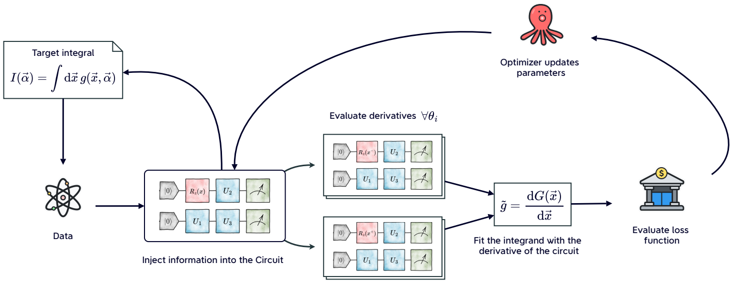

If independent variables, $\frac{\mathrm{d}G(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}}$ is obtained by summing all PSR contributions.

Validation examples

Toy model: 3-dimensional trigonometric function

We firstly consider a simple multi-dimensional target:

$$
\begin{aligned}
I(\boldsymbol{\alpha}, \alpha_0; \boldsymbol{x}) &= \int g(\boldsymbol{\alpha}, \alpha_0; \boldsymbol{x})\, \mathrm{d}\boldsymbol{x} \\
&= \int \cos(\boldsymbol{\alpha} \cdot \boldsymbol{x} + \alpha_0)\, \mathrm{d}\boldsymbol{x}.
\end{aligned} \tag{2}
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And we target a differential distribution $\frac{\mathrm{d}I(\boldsymbol{\alpha}, \alpha_0; \boldsymbol{x})}{\mathrm{d}x_i}$ for fixed i but varying α_0'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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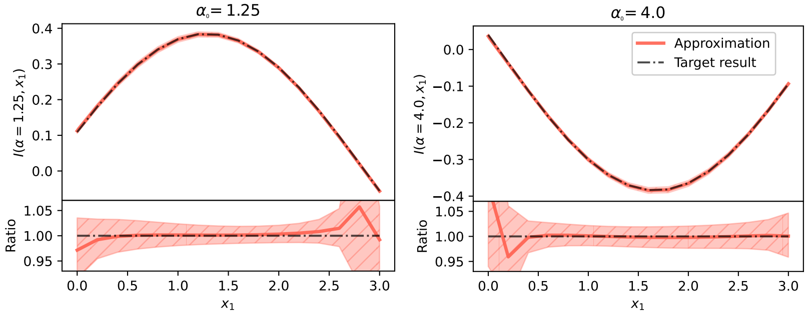

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Parameter	Value
$N_{x,\mathrm{train}}$	500
Q	1.67
N_{layers}	4
N_{params}	27
$\lvert I - \tilde{I}\rvert$	$1.2 \cdot 10^{-5}$
N_{shots}	Exact simulation
Optimizer	L-BFGS

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
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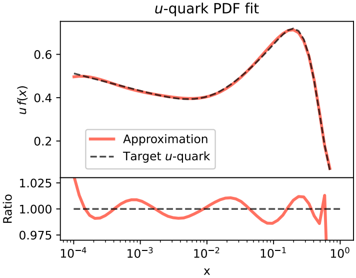

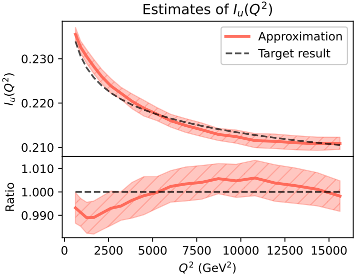

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We finally tackle a dummy target using a real superconducting qubit:

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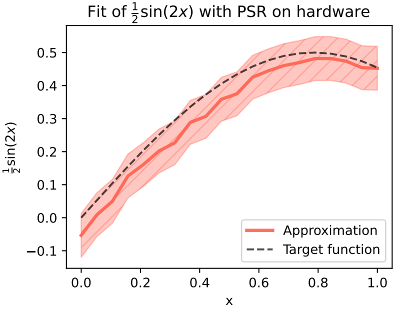

Parameter	Value
$N_{x,\mathrm{train}}$	50
$N_{x,\mathrm{est}}$	20
N_{runs}	10
N_{layers}	1
N_{params}	6
$\lvert I - \tilde{I}\rvert$	$2.8 \cdot 10^{-2}$
N_{shots}	$2 \cdot 10^{3}$
Optimizer	L-BFGS

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- exploit **variables correlation** to reduce the number of required gates.

Thank you for your attention!