Determining probability density functions with adiabatic quantum computing

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Abstract

We present a method for estimating Probability Density Functions (PDFs) of one dimensional samples using adiabatic quantum computing. We use an adiabatic evolution to encode the cumulative distribution (CDF), exploiting the natural monotonicity of the evolution and choosing the boundary Hamiltonians to perfectly fit the target problem. We then translate the evolution into a continuous-in-time circuit using a Trotter-like procedure. Finally, we derivate the circuit using the Parameter Shift Rule (PSR) in order to get the PDF.

Goal

Estimating the PDF value $\rho(x)$ for each element of a sample of data $\Omega = \{x_j\}_{j=1}^{N_{\rm data}}$. We define the following Quantum Adiabatic Machine Learning (QAML) strategy:

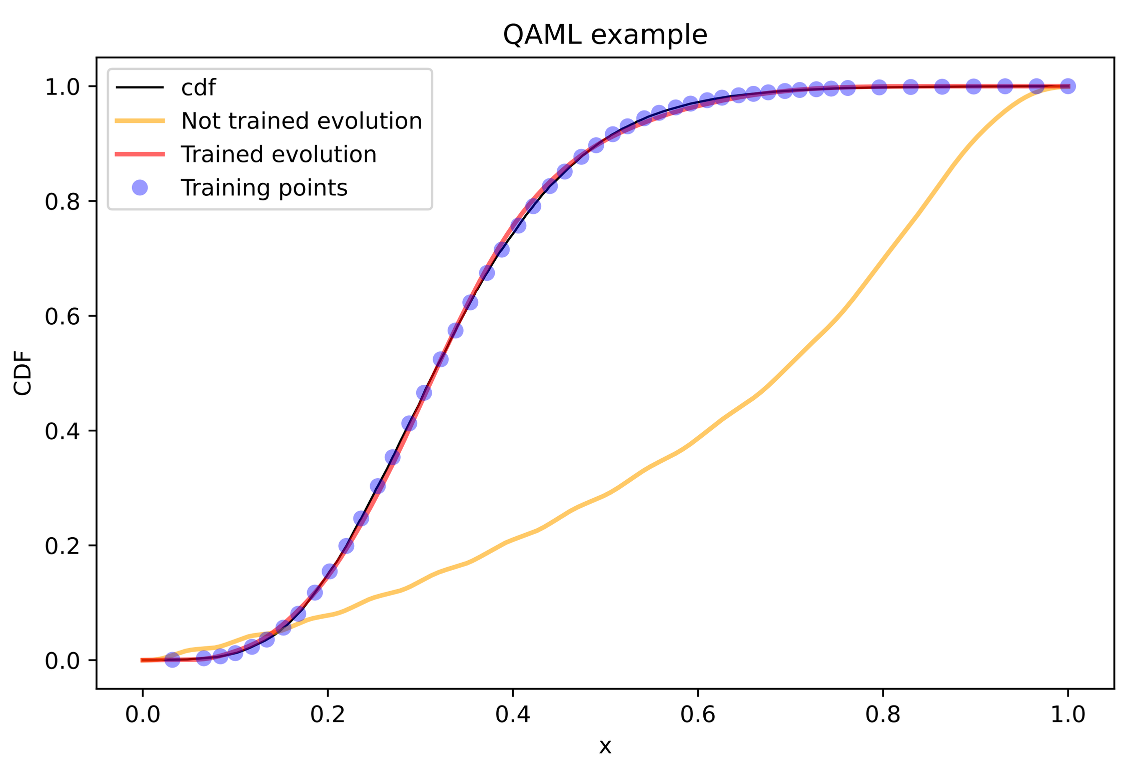
- encoding the CDF values $F(x)$ into an adiabatic evolution;
- translating the adiabatic Hamiltonian into a circuit $\mathcal{C}$ callable at any time τ;
- Derivating the circuit using the parameter shift rule [3] obtaining the PDF.

Encoding a CDF into an adiabatic evolution

We use `qibo` [2] to simulate an adiabatic evolution on time τ:

$$H_{\rm ad}(\tau, \boldsymbol{\theta}) = \big[1 - s(\tau, \boldsymbol{\theta})\big] H_0 + s(\tau, \boldsymbol{\theta}) H_1. \tag{1}$$

We map $\{x, F(x)\}$ into $\{\tau, E(\tau)\}$, where $E(\tau)$ energy of a non-interacting Pauli Z over the evolved ground state of $H_{\rm ad}$ at τ.

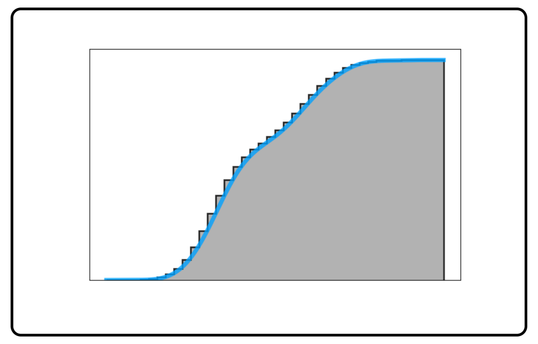


How we optimize the evolution

1. perform the evolution with initial guess $\boldsymbol{\theta}_0$ in the scheduling;
2. estimating a loss function $J_{\rm mse}\big[F, E(\boldsymbol{\theta})\big]$;
3. updating $\boldsymbol{\theta}$ using a chosen optimizer until convergence.

Building a derivable circuit

After encoding the CDF into the evolution, we translate $H_{\rm ad}$ into a circuit derivable via PSR:



Sequence of $\{H_j\}$

$$\hat{F}(x) \to |\psi(\tau)\rangle = \overleftarrow{\prod_j} U_j |\psi_0\rangle$$

$d\tau \to 0$ limit

$$|\psi(\tau)\rangle = \mathcal{C}(\tau)\,|\psi_0\rangle$$

From $\mathcal{C}$ to $\mathcal{C}_R$

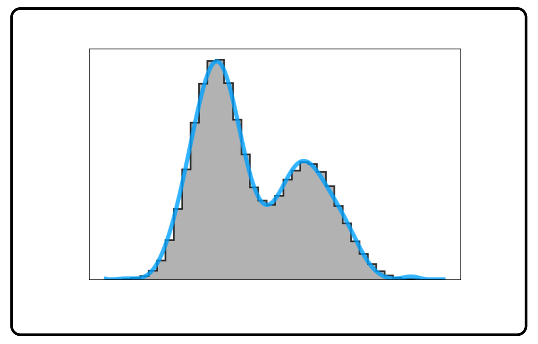
$$|\psi(\tau)\rangle = R_z(\theta_1) R_x(\theta_2) R_z(\theta_3)\,|\psi_0\rangle$$

with $\theta_i \equiv \theta\big(s(\tau)\big)$.

Derivative of $\mathcal{C}_R$

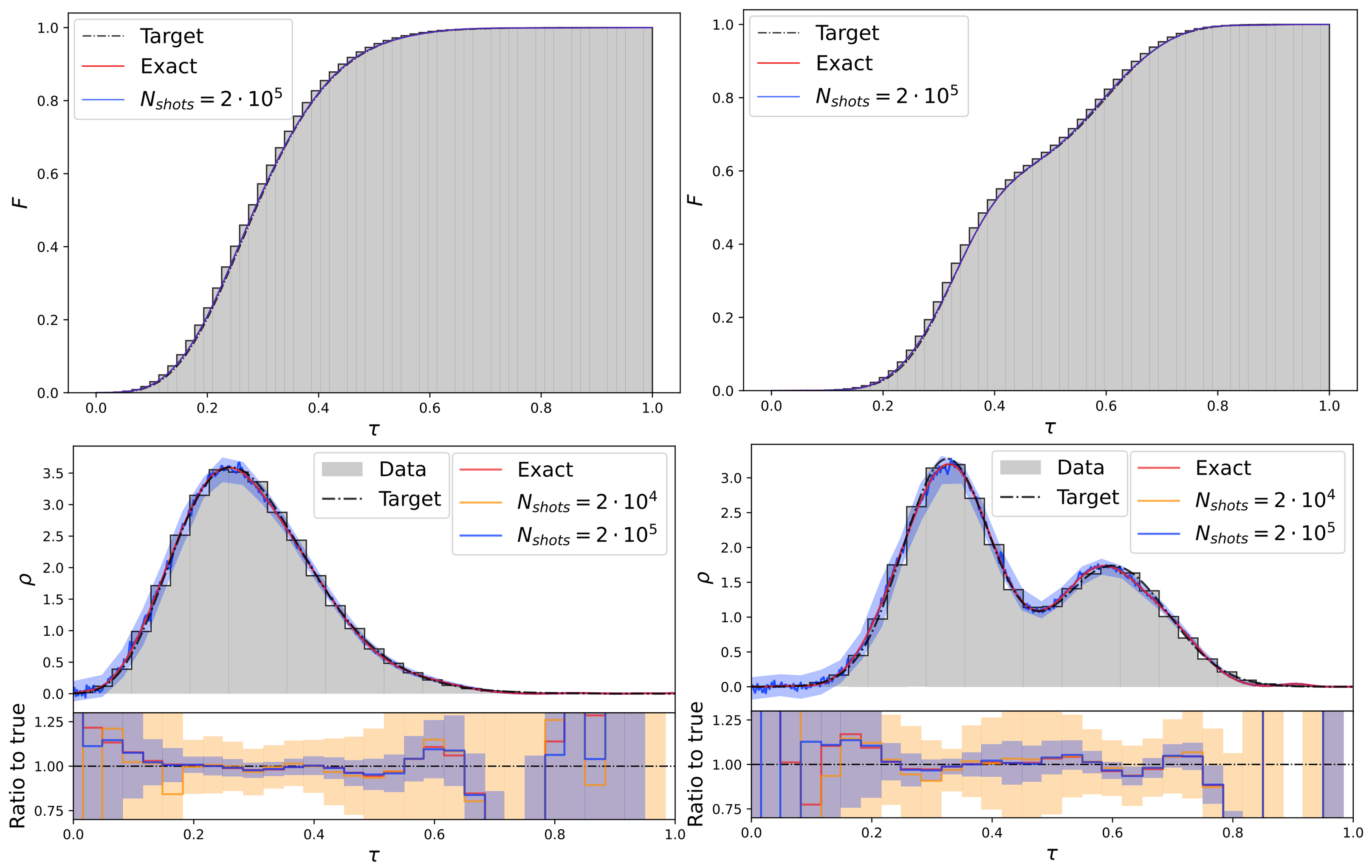
$$\rho(x) = \partial_\tau \hat{F} = \sum_{i=1}^{3} \frac{\partial \hat{F}}{\partial \theta_i} \frac{\partial \theta_i}{\partial \tau}$$

where $\frac{\partial \hat{F}}{\partial \theta_i}$ with PSR



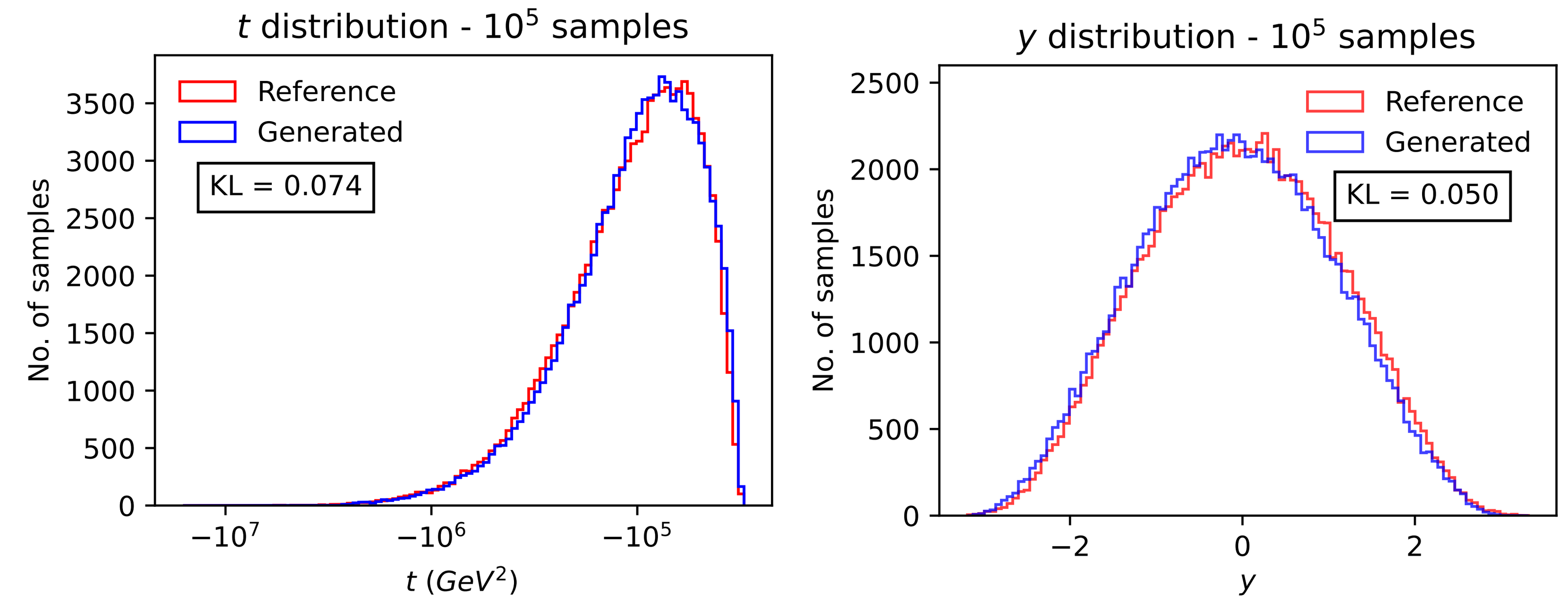
Validation cases

We firstly test the QAML procedure on a Gamma distribution and on a Gaussian mixture.

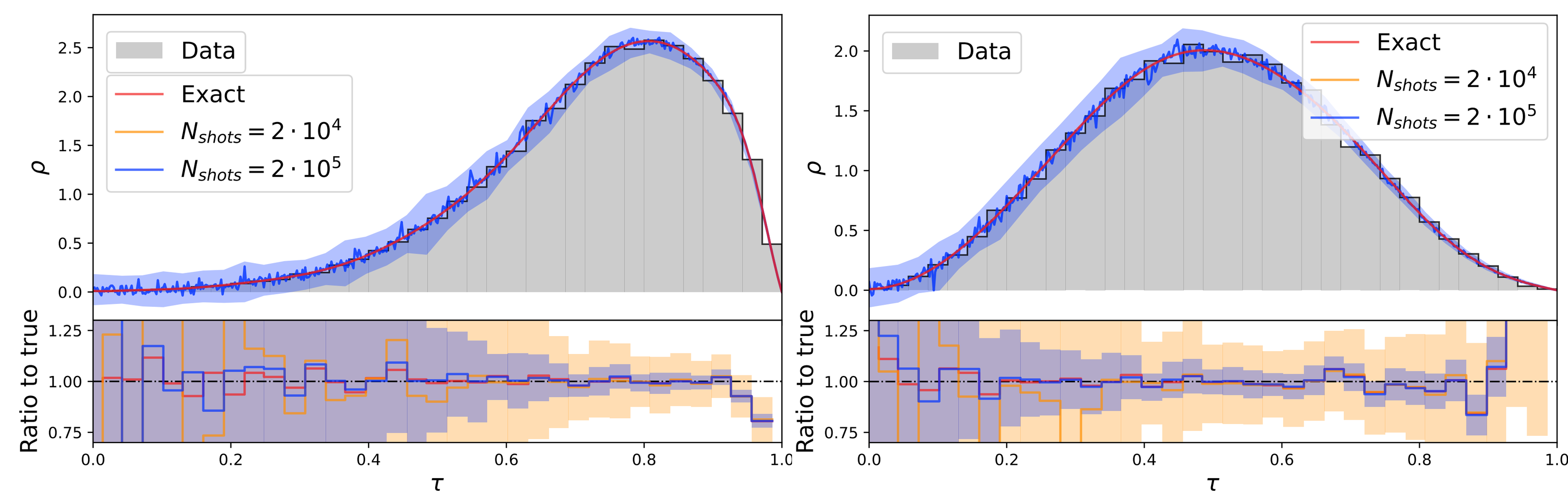


Quantum density estimation after quantum data generation

LHC events of a $pp \to t\bar{t}$ decay generated with a quantum GAN [1].



On which we apply the QAML algorithm:



Results

Simulation with shots noise due to $N_{\rm nshots} = 5 \cdot 10^4$.

Fit function	$N_{\rm sample}$	p	J_f	$N_{\rm ratio}$	χ^2
Gamma	$5 \cdot 10^4$	25	$2.9 \cdot 10^{-6}$	31	$2.2 \cdot 10^{-4}$
Gaussian mix	$2 \cdot 10^5$	30	$2.75 \cdot 10^{-5}$	31	$4.39 \cdot 10^{-3}$
t	$5 \cdot 10^4$	20	$2.1 \cdot 10^{-6}$	34	$3.4 \cdot 10^{-4}$
s	$5 \cdot 10^4$	20	$7.9 \cdot 10^{-6}$	34	$1.20 \cdot 10^{-3}$
y	$5 \cdot 10^4$	8	$3.7 \cdot 10^{-6}$	34	$1.45 \cdot 10^{-3}$

References

[1] Carlos Bravo-Prieto, Julien Baglio, Marco Cè , Anthony Francis, Dorota M. Grabowska, and Stefano Carrazza. Style-based quantum generative adversarial networks for monte carlo events. *Quantum*, 6:777, aug 2022.

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[3] Maria Schuld, Ville Bergholm, Christian Gogolin, Josh Izaac, and Nathan Killoran. Evaluating analytic gradients on quantum hardware. *Physical Review A*, 99(3), mar 2019.