Density estimation via adiabatic quantum computing

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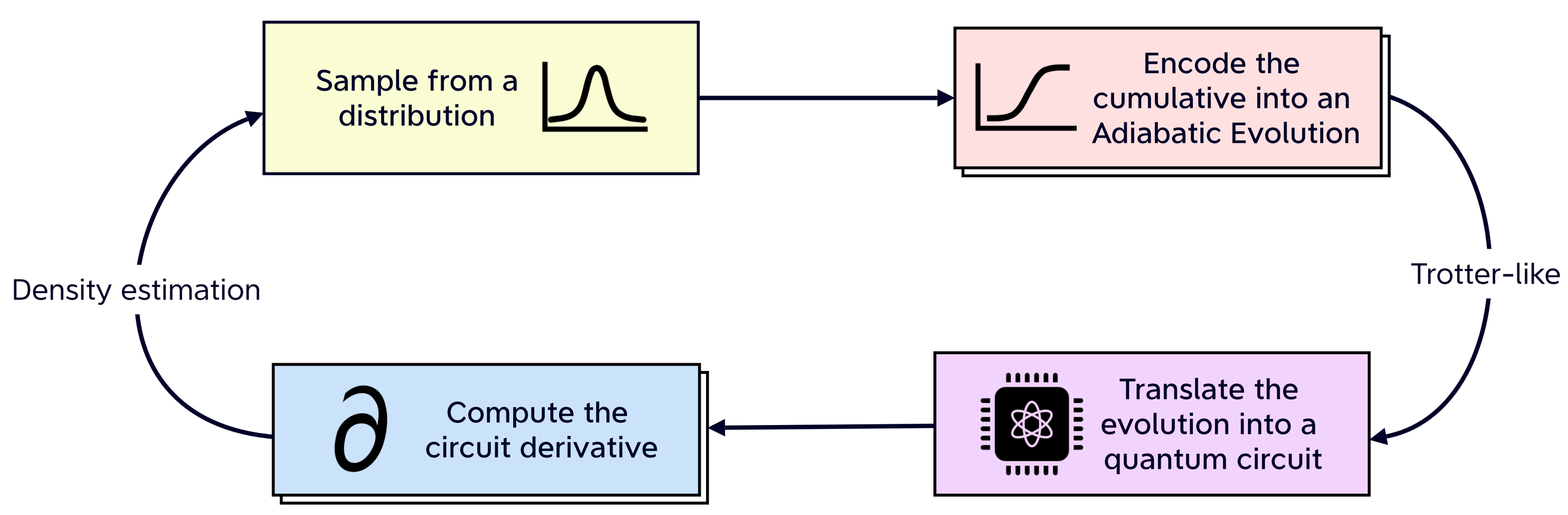
Aim of the project

We propose a novel strategy to perform density estimation: given a variable x sampled from an unknown distribution $\rho(\boldsymbol{x})$, we aim to estimate the puntual probability density value $\hat{\rho}(\boldsymbol{x})$.

To know the value of the probability of a given data x is important in many situations, for example while calculating integrals via Monte Carlo Integration, where ρ is used to correctly weight the sample points in the integral approximation.

Schematic pipeline of the algorithm

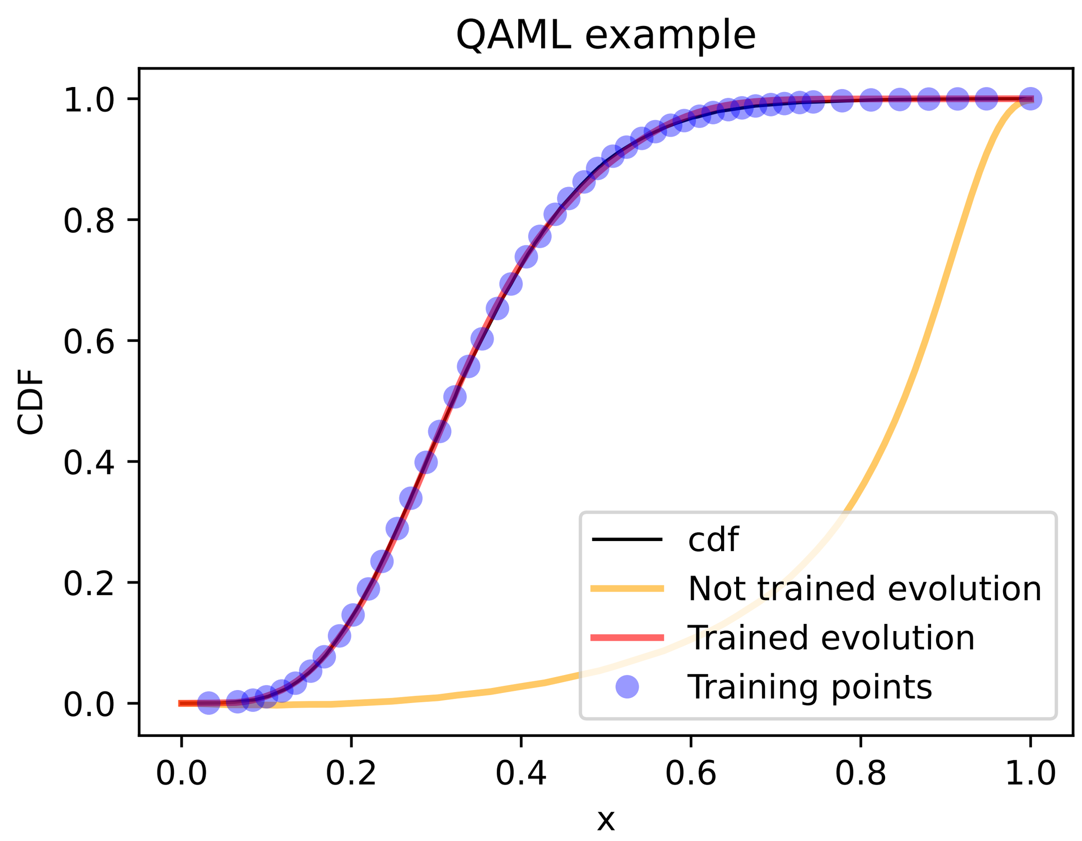


Encoding a CDF into an adiabatic evolution

We use `qibo` [1] 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.

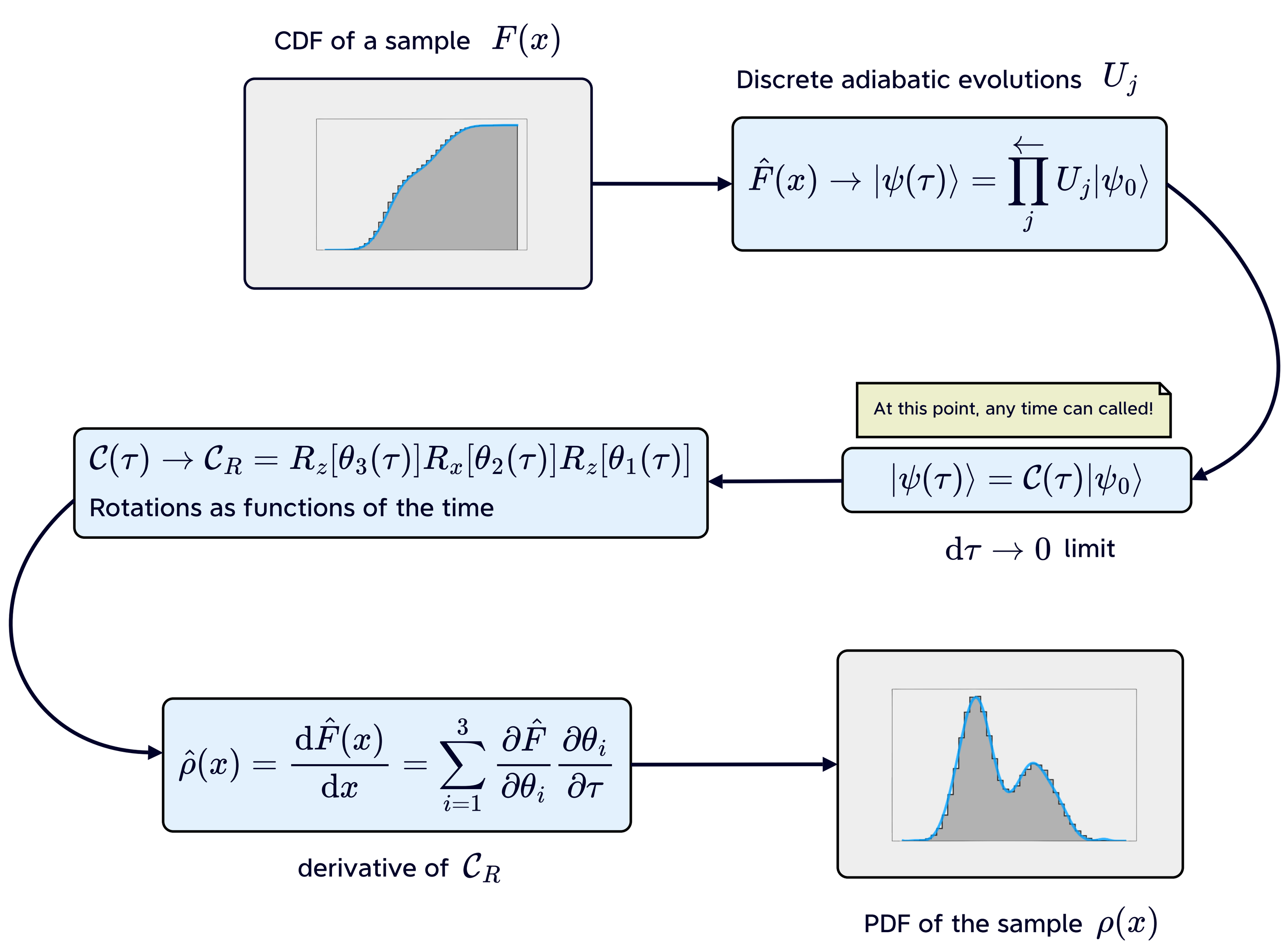


How we optimize the evolution

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

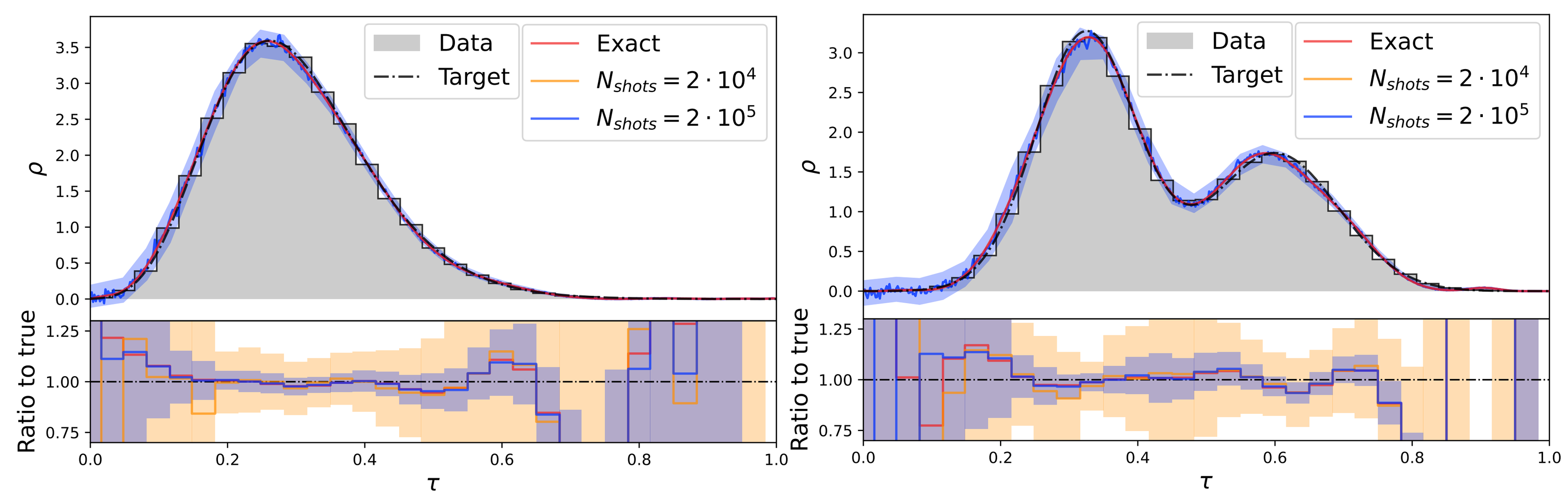
Building a derivable circuit

After encoding the CDF into the evolution, we translate $H_{\rm ad}$ into a circuit derivable via shift rules [2]:



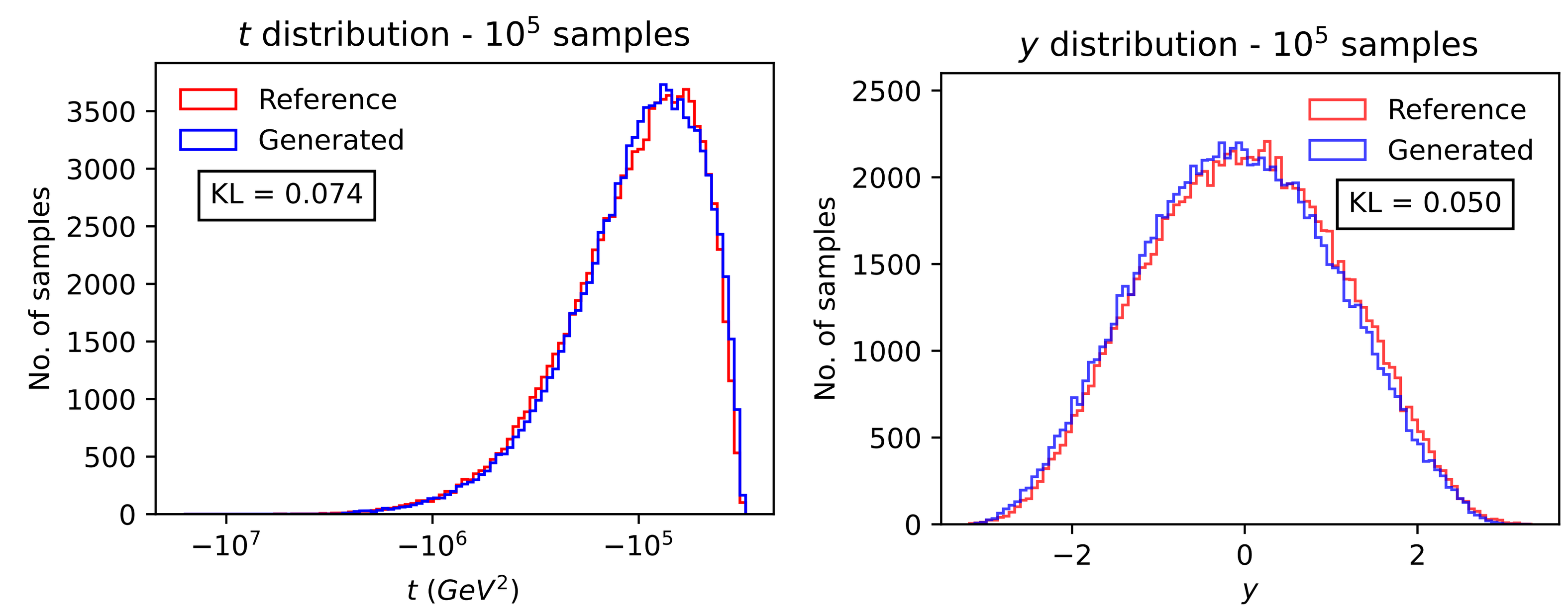
Validation cases

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

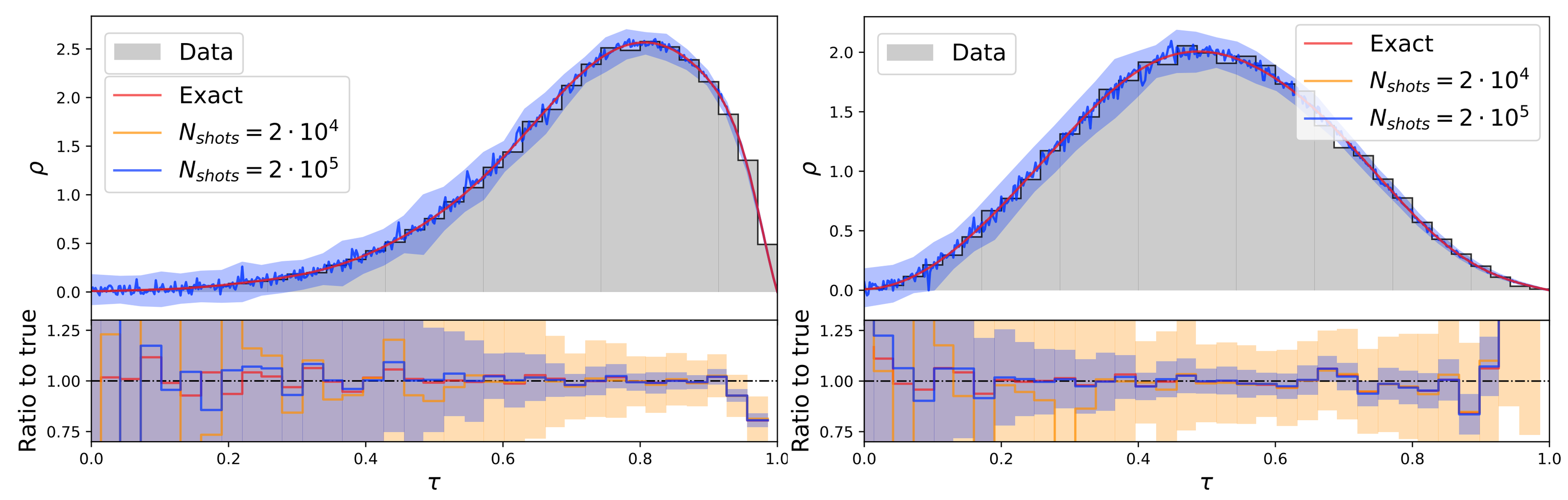


Quantum density estimation of quantum generated data

LHC events of a $pp \to t\bar{t}$ decay generated with a quantum GAN [3].



On which we apply the QAML algorithm:



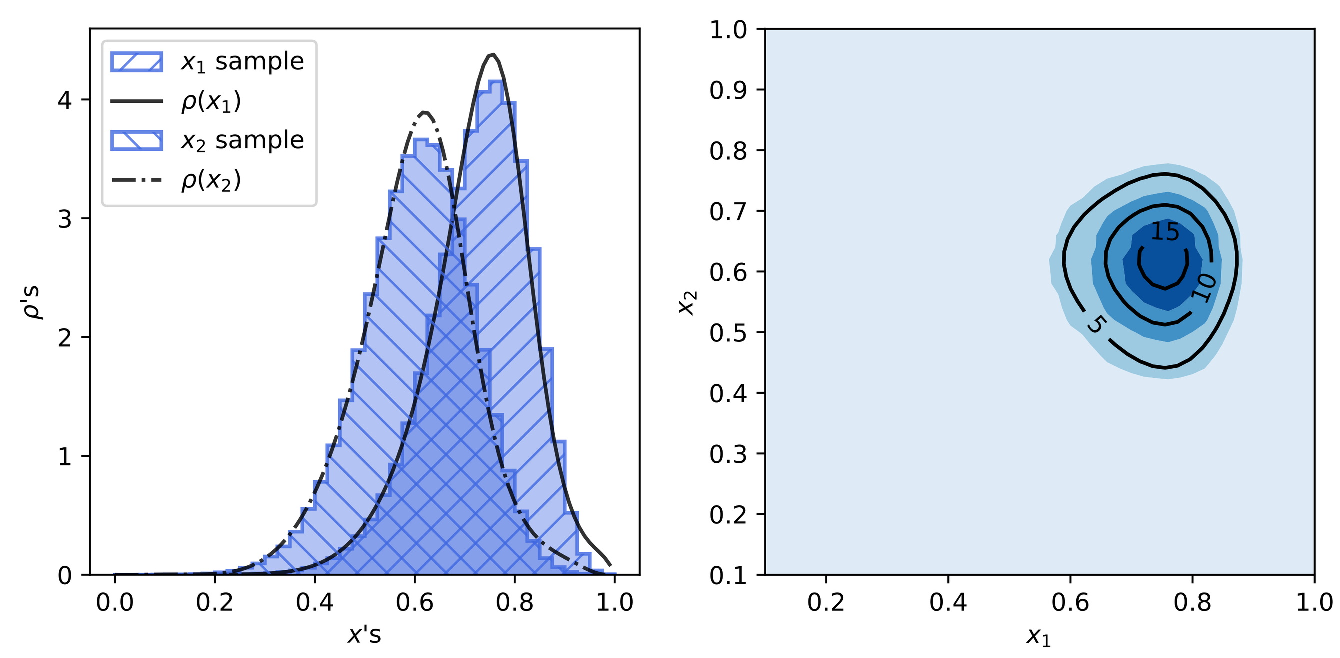
Results

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	$1.45 \cdot 10^{-3}$

Scale up with dimensionality

This same framework can be used to determine a d-dimensional PDFs in case of d *iid* variables. We can do this by composing a d-qubits circuit which encodes the rotations corresponding to d adiabatic evolutions. The global PDF is calculated as product of the marginalised ones. In the following we estimate $\rho_g(x_1, x_2) = \rho_1(x_1)\rho_2(x_2)$.



References

[1] S. Efthymiou, S. Ramos-Calderer, C. Bravo-Prieto, A. Pérez-Salinas, D. García-Martín, A. Garcia-Saez, J. I. Latorre, and S. Carrazza, "Qibo: a framework for quantum simulation with hardware acceleration," *Quantum Science and Technology*, vol. 7, p. 015018, dec 2021.

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