Density estimation via quantum adiabatic computing

Based on arXiv:2303.11346

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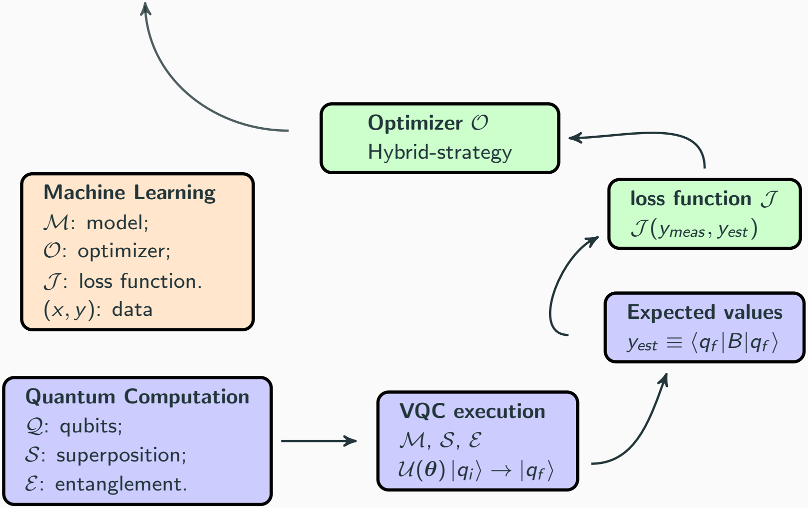
A screenshot of Quantum Machine Learning (QML)



Introduction

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In this work

We focus on to find a **density estimation** strategy.

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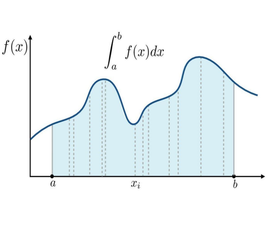

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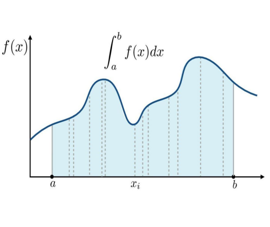

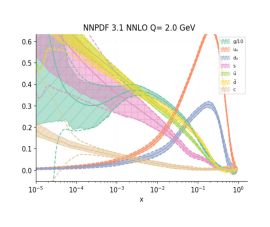

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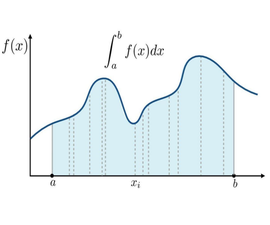
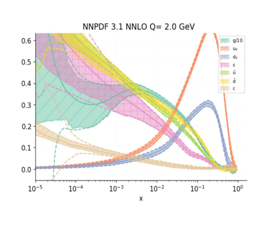
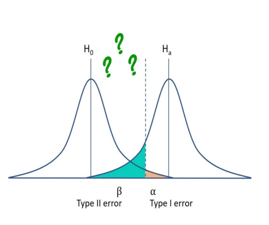
  - **Anomaly detection**: if a PDF is known and punctually evaluable we can use this for hypotesis testing.







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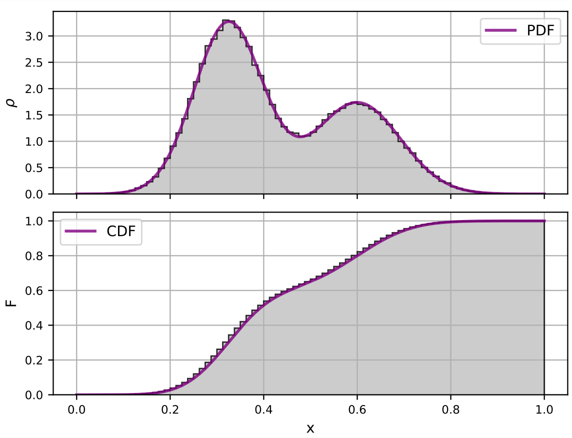
```
import qibo

# in some boxes like this
# we will show how to implement the QAML strategy
```

Code here: qiboteam/adiabatic-fit

METHOD: CDF fit with a VQC

Simple case: 1d data in $\mathcal{D} = [0, 1]$.

➜ Each $x \in \Omega$ can be labeled with its empirical CDF[2] value $F(x)$, which is related to the PDF value via $\rho(x) = \frac{dF(x)}{dx}$.



[2] **Cumulative Density Function:** after sorting the data, $F(x)$ is calculated by counting how many elements are smaller then the target one.

Variational Quantum Circuits (VQC) as regression model

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where $\mathcal{C}(x;\boldsymbol{\theta})$, $\mathcal{O}$ and ψ_i are the respectively the VQC, a target observable and the initial state on which we apply $\mathcal{C}$.

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- We know how to derivate circuits, *e.g.* using the Parameter Shift Rule (PSR)[3], thanks to which we can calculate:

$$\partial_\mu \hat{F} = r\big[\hat{F}(\mu^+) - \hat{F}(\mu^-)\big]. \tag{3}$$

[3] arXiv:1811.11184

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- In case of rotational gates[4] $\exp\left\{-i\mu\hat{\sigma}\right\}$ we have $r = 0.5$, $\mu^\pm = \mu \pm s$ and $s = \pi/2$.

[3] arXiv:1811.11184

[4] arXiv:1803.00745

PSR

- We can upload x into a rotation angle and calculate $\partial_x \hat{F}$.

```python
from qibo import models, gates, hamiltonians, derivative

# here you define a parametric circuit c as explained during the tutorials
# in which you upload x into the p-th rotation angle, as theta = x*PAR
# then you define an observable
h = hamiltonians.Z(nqubits=1)

# derivative with respect to x of < h >
derivative = derivative.parameter_shift(
    circuit = c,                       # parametric circuit
    hamiltonian = h,                   # target observable
    parameter_index = p,               # parameter index
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In a nutshell

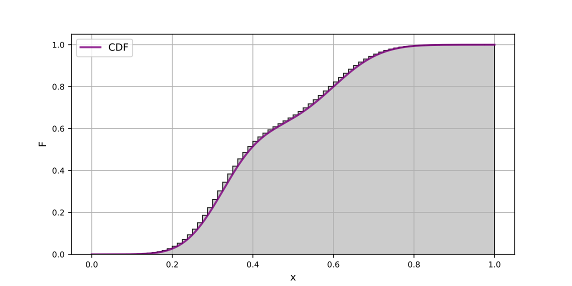
We estimate the CDF using a VQC and we derivate it with the PSR for calculating the PDF.

Two problems

➜ We tried to fit CDFs using a VQC as QML model, but we had two problems:

- by encoding x into the rotation angles, our results often did not retain a **strictly increasing monotony**.
- we need to fix $\hat{F}(0) = 0$ and $\hat{F}(1) = 1$, so we need to manipulate $\hat{F}$ in order to follow these constraints.

➜ These conditions are needed if we deal with CDFs.



METHOD: Quantum Adiabatic ML

Adiabatic Evolution (AE) as QML model

➔ Let's use an Adiabatic Evolution (AE) as model:

$$H_{ad} = H_0\big[1 - s(\tau;\boldsymbol{\theta})\big] + s(\tau;\boldsymbol{\theta})H_1, \tag{4}$$

➔ following a scheduling s, depending on the evolution time $\tau \in [0,1]$ and on some variational parameters $\boldsymbol{\theta}$.

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```python
# with qibo we can implement an Adiabatic Evolution via trotter formula
from qibo import models, hamiltonians, callbacks

# problem's parameters
nqubits = 1
h0 = hamiltonians.X(nqubits)
h1 = hamiltonians.Z(nqubits)
target_observable = h1

# we track the energy of h1 on the evolved ground state
energies = callbacks.Energy(target_observable)
evolution = models.AdiabaticEvolution(
    h0=h0, h1=h1, s = lambda t : t, dt=0.1, callbacks = [energies])

# calculate the evolved final state at time t=final_time
evolved_state = evolution(final_time = final_time)
```

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- we can fix $\hat{F}(0) = 0$ and $\hat{F}(1) = 1$ by chosing H_0 and H_1 such that their ground-state energies are zero and one.

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Optimizing the AE

The task becomes to optimize the scheduling parameters in order to let the AE pass through the training points.

`METHOD`: Optimizing the AE

Optimizing the AE - ansatz and optimizer

- We use a **CMA-ES**[5] genetic algorithm and the following loss function:

$$J_{\mathrm{MSE}} = \frac{1}{N_{\mathrm{train}}} \sum_{k=1}^{N_{\mathrm{train}}} \left[F(x_k) - E_k(\theta) \right]^2. \qquad (5)$$

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- Thus we evolve the system using a **polynomial scheduling** function[6]:

$$s(t;\theta) = \frac{1}{\eta} \sum_{i=1}^{p} \theta_i x^i, \qquad \text{with} \qquad \eta = \sum_{i=1}^{p} \theta_i, \tag{6}$$

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In each optimization step

We execute the evolution collecting $\{E_k\}$, thanks to which we evaluate J_{MSE}. Then, we update $\boldsymbol{\theta}$ according to the chosen technique.

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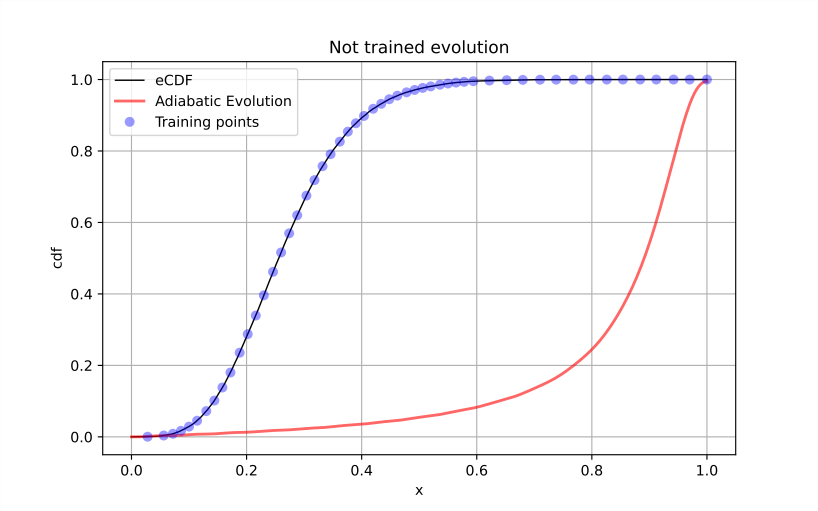
- The optimization step is performed using qibo:

```python
import qibo

# before we define a loss_evaluation function as J_MSE
def loss_evaluation(parameters): {...}

# then we use the cma optimizer provided by qibo
def optimize(force_positive=False, method="cma"):
    """Use qibo to optimize the parameters of the schedule function"""

    options = {
        "ftarget": target,            # Target loss function
        "maxiter": max_iterations,    # Maximum number of iterations
        "maxfeval": max_evals,        # Maximum number of function evaluations
    }

    # forcing the parameters to be positive; unused in this case.
    if force_positive:
        options["bounds"] = [0, 1e5]

    result = qibo.optimizers.optimize(loss_evaluation, parameters, method=method,
      options=options)
    return result
```

A toy example with `nqubits=1` - starting point

- `nparams=20`, `dt=0.1`, `final_time=50` , `target_loss=None`



A toy example - until $J_{\mathrm{MSE}} = 10^{-1}$

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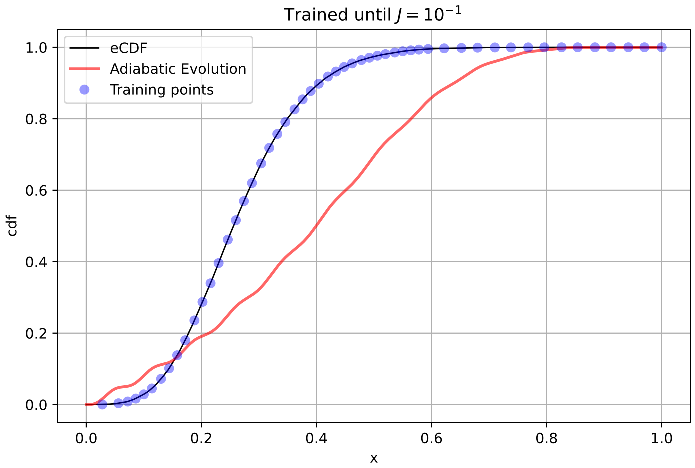
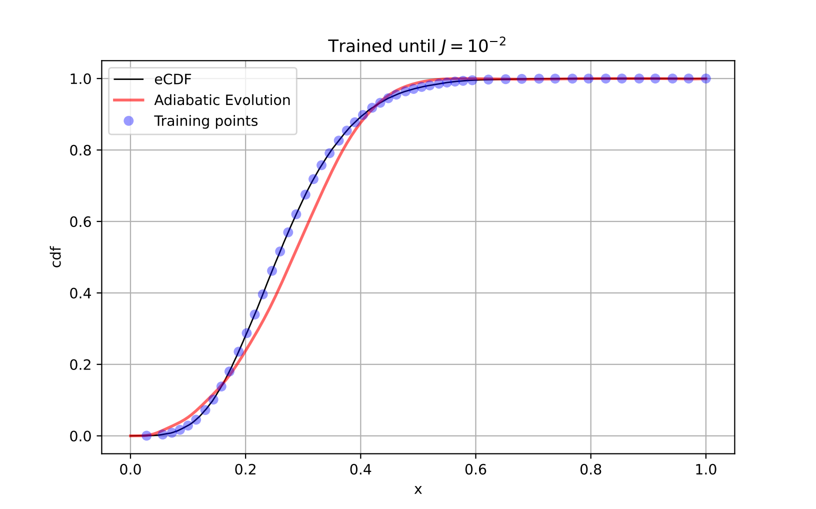


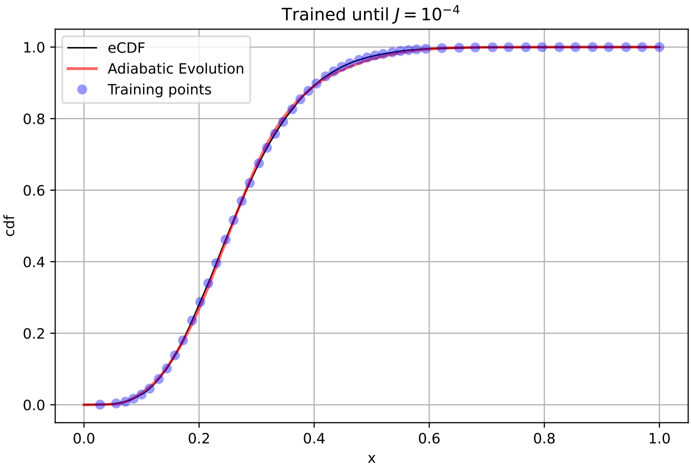
A toy example - until $J_{\mathrm{MSE}} = 10^{-2}$

- `nparams=20`, `dt=0.1`, `final_time=50` , `target_loss=1e-2`



A toy example - ending at $J_{\mathrm{MSE}} = 10^{-4}$

- `nparams=20`, `dt=0.1`, `final_time=50` , `target_loss=1e-4`



`DERIVATION`: from $\{H_j\}$ to a circuit

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- Each of these can be associated with an **instantaneous** time evolution operator U_j, which at $\tau_j = j\,\mathrm{d}t$ should be applied on to the state obtained in τ_{j-1}.
- The time-evolved state τ_n is obtained as follows:

$$|\psi(\tau_n)\rangle = \prod_{j=0}^{n} U(\tau_j)\,|\psi(\tau_0)\rangle\,, \tag{7}$$

where the initial state is the ground state of H_0 by construction.

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$$\mathcal{C}(\tau) = \Lambda_{t0} P_t \exp\left\{ - it \int_0^t \hat{D}(t) \mathrm{d}t \right\} P_0^{-1}, \tag{8}$$

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4. Now we have a circuit $\mathcal{C}$ after which evaluate $\hat{Z}$.

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in which the relationships between the angles and the elements of $\mathcal{C}$ are:

$$\begin{cases} \phi = \pi/2 - \arg(c_{01}) - \arg(c_{00}) \\ \theta = -2 \arccos(|c_{00}|) \\ \psi = \arg(c_{01}) - \pi/2 - \arg(c_{00}). \end{cases} \tag{10}$$

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$$\begin{cases} \phi = \pi/2 - \arg(c_{01}) - \arg(c_{00}) \\ \theta = -2\arccos(|c_{00}|) \\ \psi = \arg(c_{01}) - \pi/2 - \arg(c_{00}). \end{cases} \tag{10}$$

- Now we can derivate with respect to the rotation angles!

`DERIVATION`: derivating $\mathcal{C}_R$ via PSR

Derivating $\mathcal{C}_R$ to get the PDF

- I we call θ one of the three angles, we get $\partial_\tau \hat{F}$ by calculating:

$$\partial_\tau \hat{F}(\tau; \boldsymbol{\theta}) = \sum_{i=1}^{3} \frac{\partial \hat{F}}{\partial \theta_i} \frac{\partial \theta_i}{\partial s} \frac{\partial s}{\partial \tau}, \tag{11}$$

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Summary

- We fit the eCDF via QAML;
- we translate $\{H_j\}$ into $\mathcal{C}_R$;
- we derivate the result via chain rule.

VALIDATION: **test cases**

Test results

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[7] Exact state vector simulation

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- In the following table we collect realistic results in which we used $N_{\text{shots}} = 2 \cdot 10^5$ shots for evaluating $\hat{F}$.

Fit function	N_{sample}	p	J_f	N_{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	$1.45 \cdot 10^{-3}$

Table 1: Summary. $N_{\text{shots}} = 5 \cdot 10^4$.

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- The last three elements in the table refers to a $pp \to t\bar{t}$ production.

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[8] Sampling the frequencies from the simulated state

Test 1: Gamma CDF

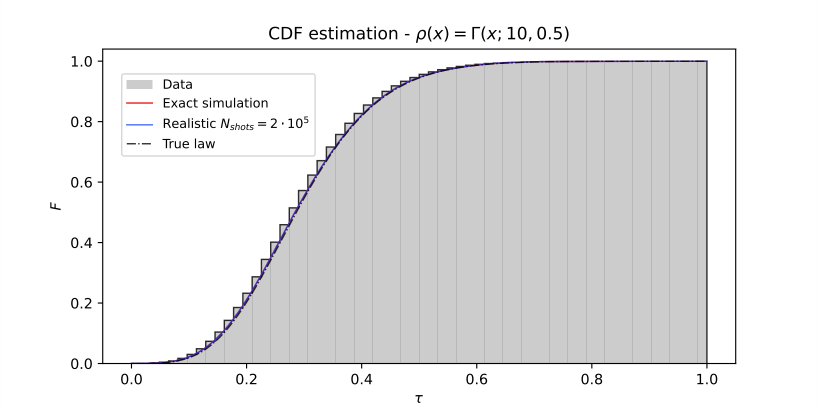


Figure 1: We show the sample (grey hist), ideal (red line) and realistic (blue line) simulation, theoretical CDF of the gamma distribution (dashed black line).

Test 1: Gamma PDF

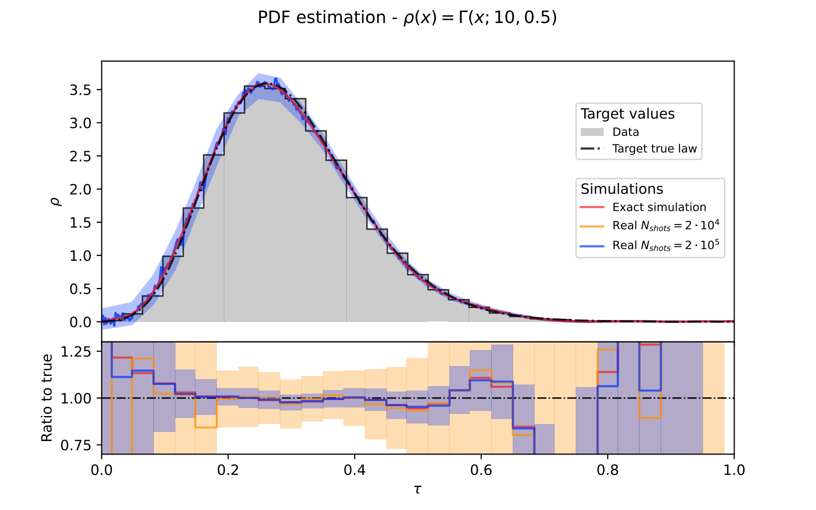


Figure 2: Above: data (grey hist), ideal (red) and realistic (blue) simulation, theoretical PDF law (dashed black line). Below: same quantities but normalized with respect to the true law with the addition of a second realistic simulation (yellow) line.

Test 2: gaussian mixture CDF

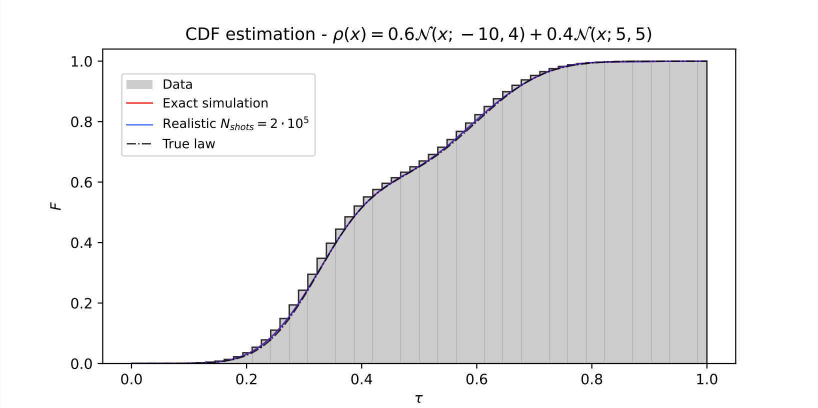


Figure 3: We show the sample (grey hist), ideal (red line) and realistic (blue line) simulation, theoretical CDF of the gamma distribution (dashed black line).

Test 2: gaussian mixture PDF

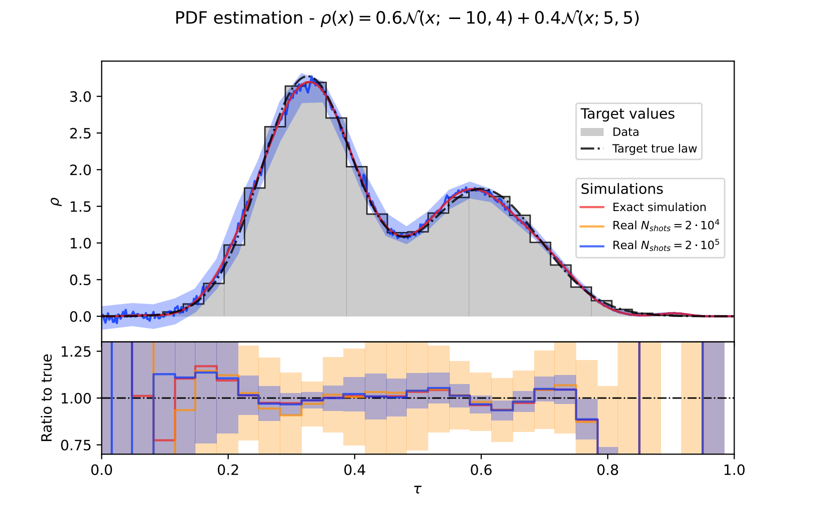
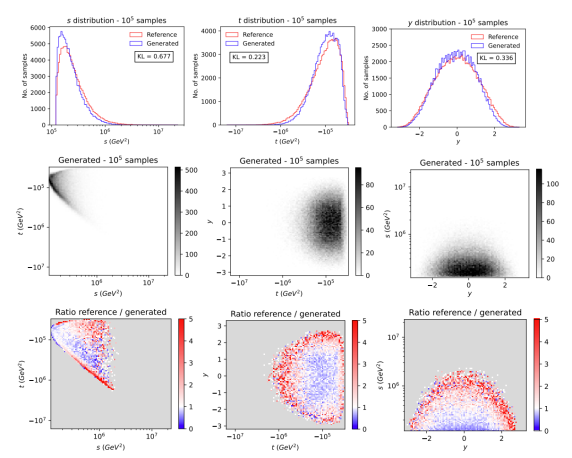


Figure 4: Above: data (grey hist), ideal (red) and realistic (blue) simulation, theoretical PDF law (dashed black line). Below: same quantities but normalized with respect to the true law with the addition of a second realistic simulation (yellow) line.

Test 3: quantum generation of $pp \to t\bar{t}$

- In a previous TH work[9] a sample of 10^5 events for $pp \to t\bar{t}$ at a center of mass $\sqrt{s} = 13$ TeV for LHC configuration was generated[10].



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[9] arXiv:2110.06933

[10] s and t Mandelstam variables, y rapidity.

HEP 1: y CDF

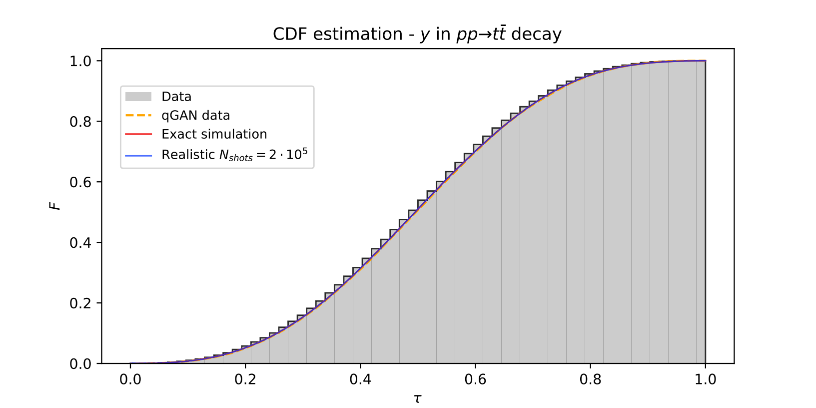

Figure 5: We show the sample (grey hist), ideal (red line) and realistic (blue line) simulation, quantum GAN eCDF (yellow).

HEP 1: y PDF

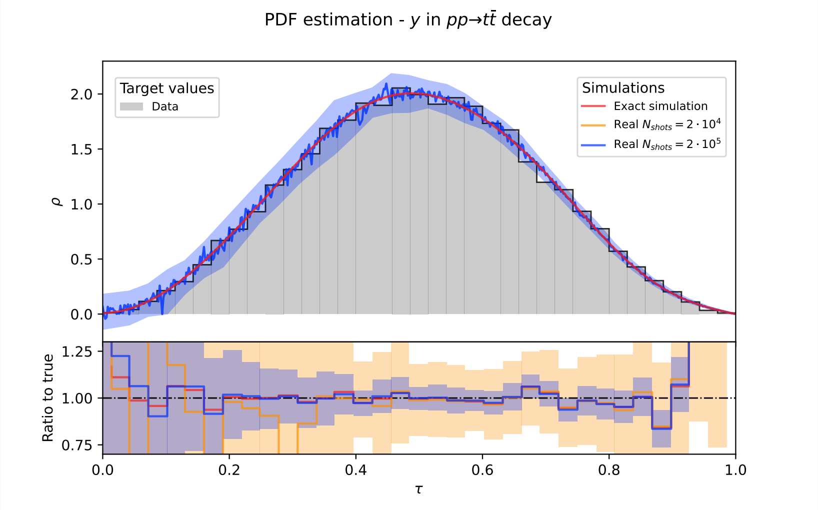

Figure 6: Above: data (grey hist), ideal (red) and realistic (blue) simulation. Below: same quantities but normalized with respect to the true law with the addition of a second realistic simulation (yellow) line.

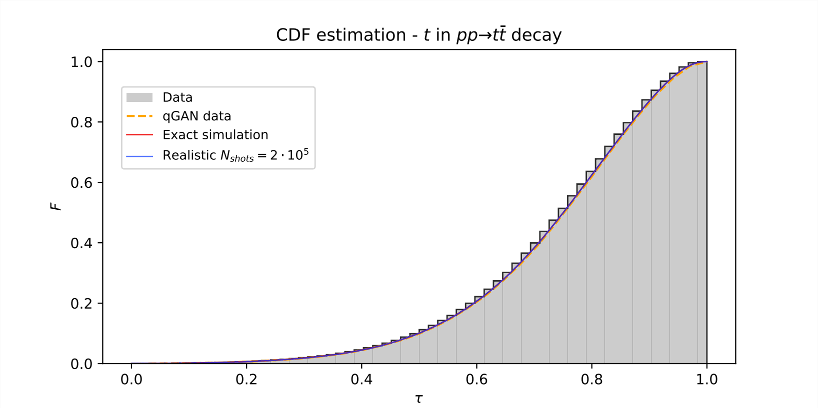

Figure 7: We show the sample (grey hist), ideal (red line) and realistic (blue line) simulation, quantum GAN eCDF (yellow).

HEP 2: t PDF

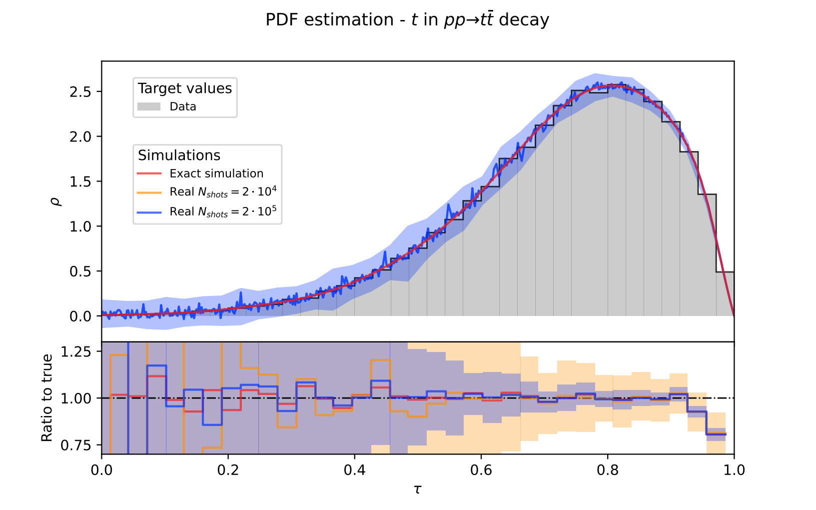

Figure 8: Above: data (grey hist), ideal (red) and realistic (blue) simulation. Below: same quantities but normalized with respect to the true law with the addition of a second realistic simulation (yellow) line.

HEP 3: s CDF

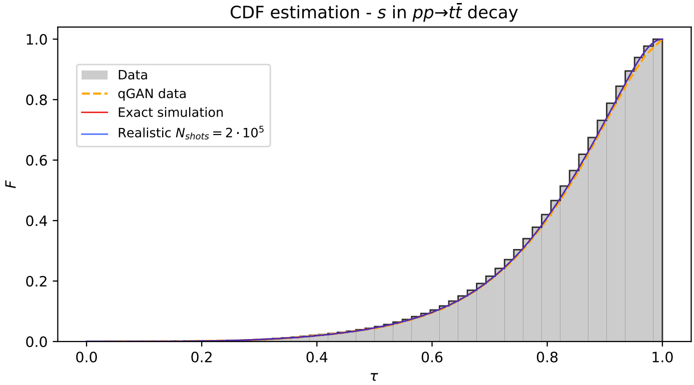

Figure 9: We show the sample (grey hist), ideal (red line) and realistic (blue line) simulation, quantum GAN eCDF (yellow).

HEP 3: s PDF

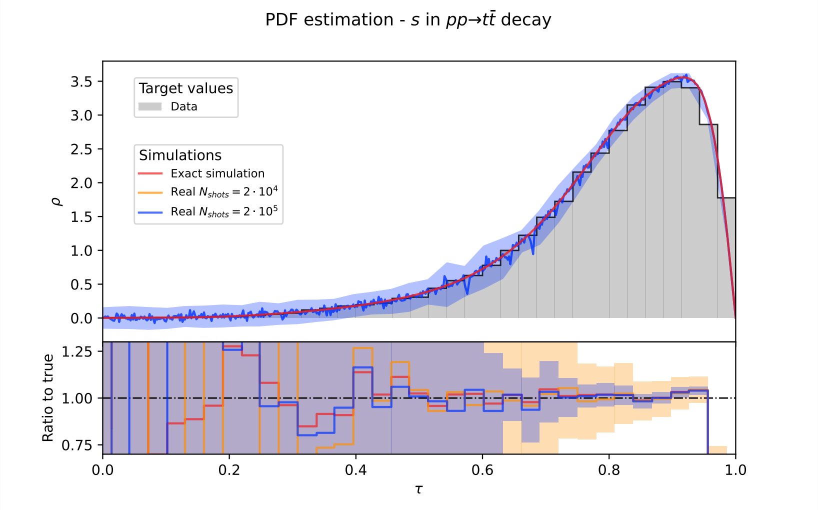

Figure 10: Above: data (grey hist), ideal (red) and realistic (blue) simulation. Below: same quantities but normalized with respect to the true law with the addition of a second realistic simulation (yellow) line.

Outlook and references

Outlook

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  - improve QAML validation: *try more general scheduling functions (e.g. ANNs), benchmarking with other density estimation techniques;*

[11] In case of *iid* random variables this model can be used individually for each dimension.

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  - hardware deployment: *can a NISQ device be used for this? what is the speed-up advantage when running the QAML on annealers?*
  - multi-dimensional[11] PDFs : *how to preserve correlations? how to exploit multi-qubits hamiltonians?*

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  - use the QAML strategy for integrating, *e.g.* deploying of a new NNPDF feature;
  - anomaly detection applications of the QAML algorithm.

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Some references

We leave some references and links thanks to which you can use our codes and read more about the project:

- open-access codes for personal coding or contributing:
  - the qibo package;
  - the qibolab package;
  - the qibocal package;
- our official webpage, with the following documentations:
  - the qibo docs;
  - the qibolab docs;
  - the qibocal docs;

The code is open-source and available here!