Quantum-inspired tensor-network machine learning: finding optimal hyperparameters, libraries, and hardware

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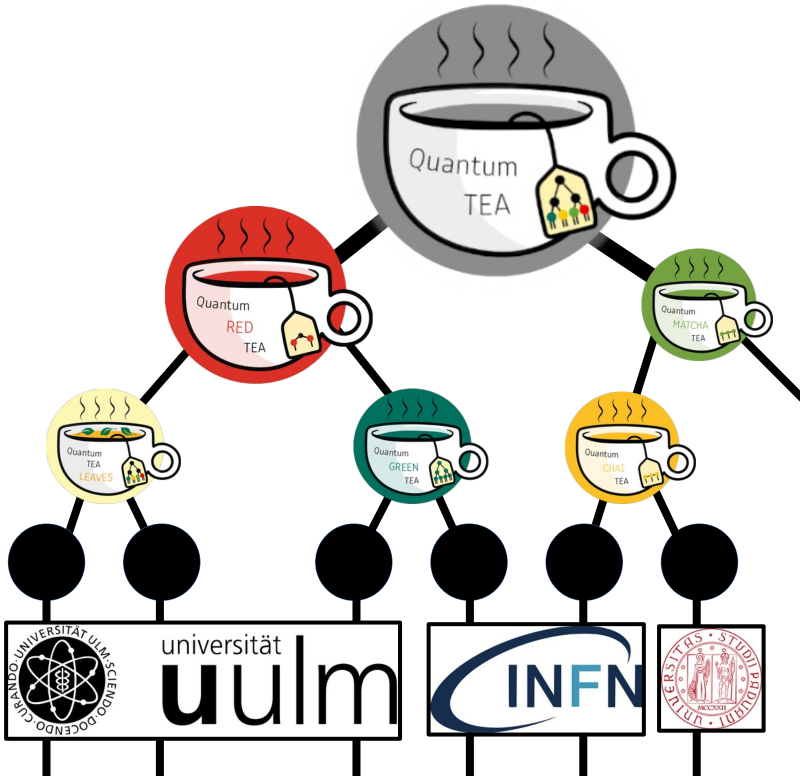
AI @ INFN

Logo by N. Reinic



Outline today's "Tensor network machine learning"

Supervised machine learning

Unsupervised / Generative

Neural Networks & Deep learning

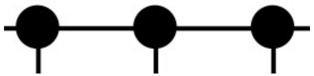
Quantum-inspired methods

Quantum Machine Learning (QML)

What are “quantum-inspired” methods?

Method or idea for quantum technology used on a classical problem without a QPU

Method: tensor network (TN) algorithms



- Quantum wave function represented by TN
- Compress entanglement (quantum correlations)

Problem: supervised learning

- Model represented by TN
- Compress information

What are “quantum-inspired” methods?

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Method: tensor network (TN) algorithms

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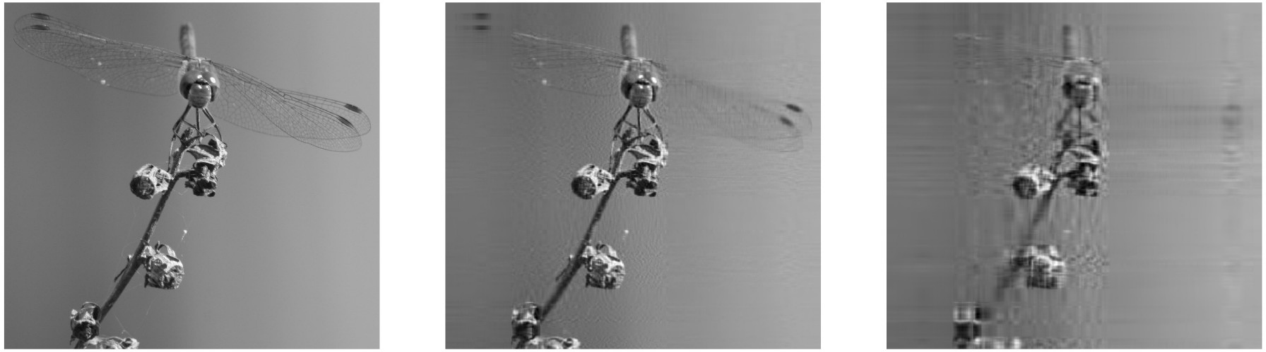
Compression example
Singular Value Decomposition

Singular values kept:
1549 versus 50 versus 15
(1549: no compression)



Quantum TEA: where do we come from?

Quantum Tensor network **E**mulator **A**pplications

Can I just have tensor networks for quantum information?

How to emulate a digital quantum circuits?

+

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How to emulate a digital quantum circuits?

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How to solve the Schrödinger equation?

+

Can we do tensor network machine learning? … soon as well public.

+

Quantum TEA: where do we come from?

Quantum **T**ensor network **E**mulator **A**pplications

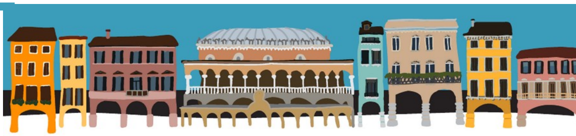
Can I just have tensor networks for quantum information?

How to emulate a digital quantum circuits? +

How to solve the Schrödinger equation? +

And another for performance

Can we do tensor network machine learning? … soon as well public. +



The one-pixel example

Data set: Training & **test**	Feature map	Guess TN	Optimization	Inference
Value: 220 Label: 0	$\begin{pmatrix}\cos(220/255)\\ \sin(220/255)\end{pmatrix}$			
Value: 18 Label: 1	$\begin{pmatrix}0.9975\\ 0.0705\end{pmatrix}$			
Value: 34 Label: 1	$\begin{pmatrix}0.9911\\ 0.1329\end{pmatrix}$			

The one-pixel example

Data set: Training & test

Value: 220
Label: 0

Value: 18
Label: 1

Value: 34
Label: 1

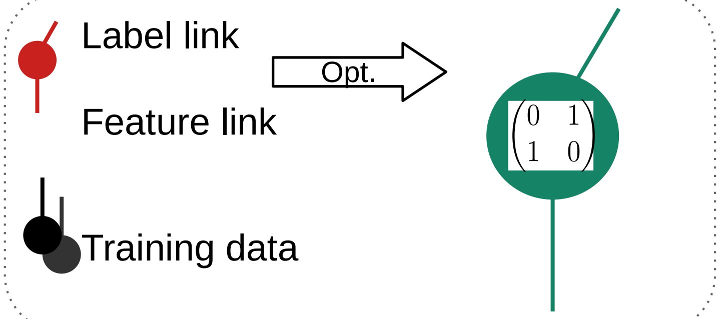
Feature map

$\begin{pmatrix} \cos(220/255) \\ \sin(220/255) \end{pmatrix}$

$\begin{pmatrix} 0.9975 \\ 0.0705 \end{pmatrix}$

$\begin{pmatrix} 0.9911 \\ 0.1329 \end{pmatrix}$

Guess TN / **Optimization**



$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Inference

$\begin{pmatrix} 0.99 \\ 0.07 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\text{argmax} \begin{pmatrix} 0.07 \\ 0.99 \end{pmatrix} = 1$

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Label link

Feature link

Training data

Opt.

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\begin{pmatrix} 0.99 \\ 0.07 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\operatorname{argmax} \begin{pmatrix} 0.07 \\ 0.99 \end{pmatrix} = 1$

$= \begin{pmatrix} 0.13 \\ 0.99 \end{pmatrix}$

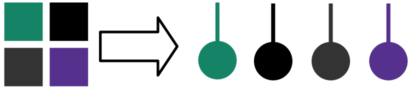
argmax 1

Full-scale algorithm

Based on / original work: E. Miles Stoudenmire and David J. Schwab, Supervised Learning With Quantum-Inspired Tensor Networks, arXiv:1605.05775v2 (2017)

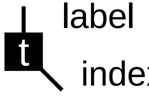
Feature map: list of vectors

One sample: (2x2 pixels)

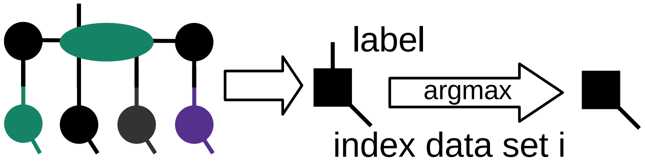


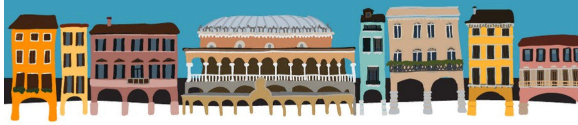
Outer product of vectors (many-body state without quantum correlations)

True labels for a data set:



Inference





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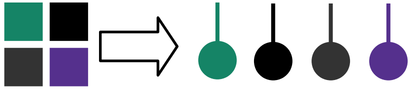

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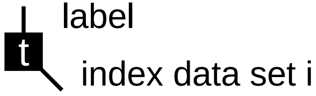
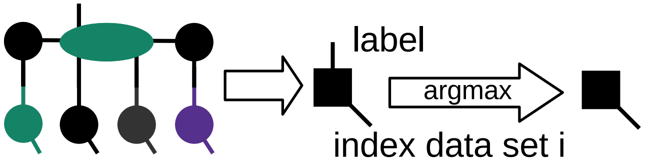
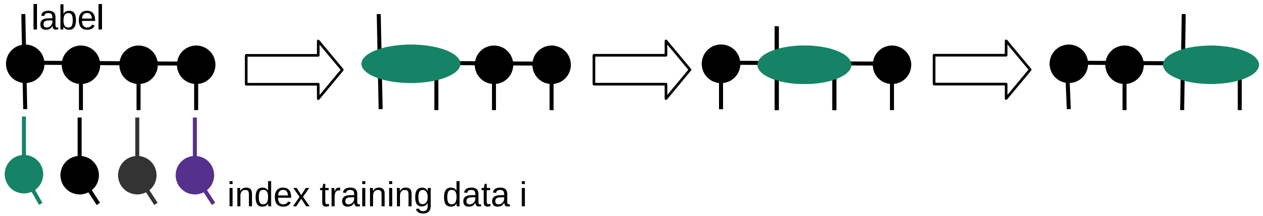


Inference



Optimization step: (no, no backpropagation & gradient descent)

→ One sweep optimizes each nearest-neighbor tensor-pair once



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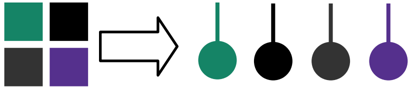

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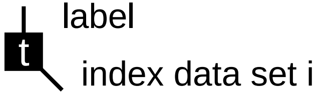
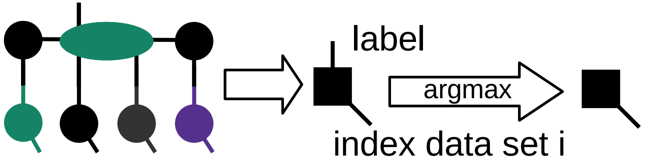


Inference



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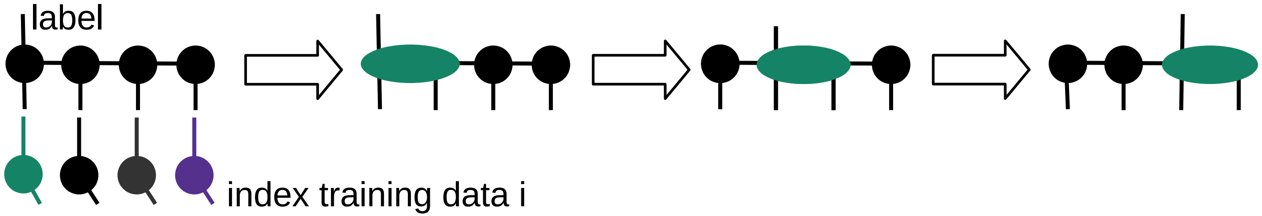
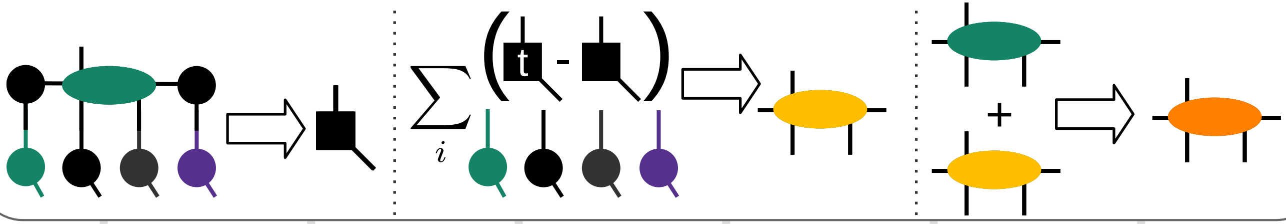


→ Calculate the local gradient for the two-site tensor



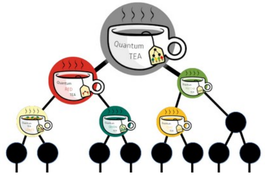
Hyper-parameters, libraries, and hardware

What do we want to bechmark / tune?

Ansätze

MPS

TTN



Parameters in ansatz:

- Bond dimension (compression)
- Precision: double, single, half
- Update 1- or 2-tensors together
- Mapping 2d image
- Label link or “pure overlap”

Libraries & hardware

- CPU versus GPU
- numpy/cupy versus torch

Machine:
leonardo booster partition with A100 GPU

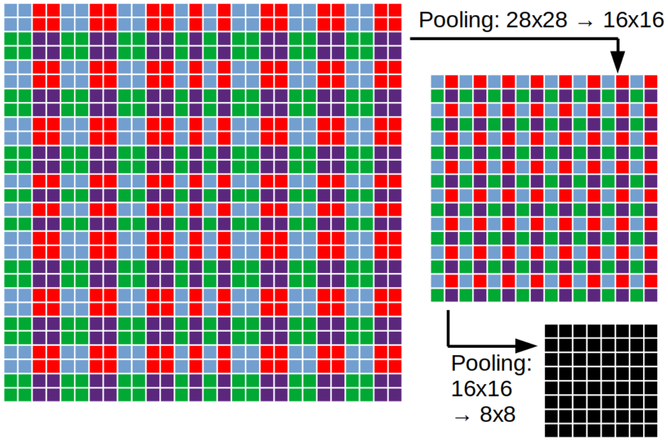
Reference point: MNIST

Training: 2,000
Training batch: 1000
Test: 2,000
Averaged: no (1 run)
MNIST: 70,000

Training precision: 96.2%
Test precision: 92.3% *
Walltime: 1372 seconds

$\chi = 32$

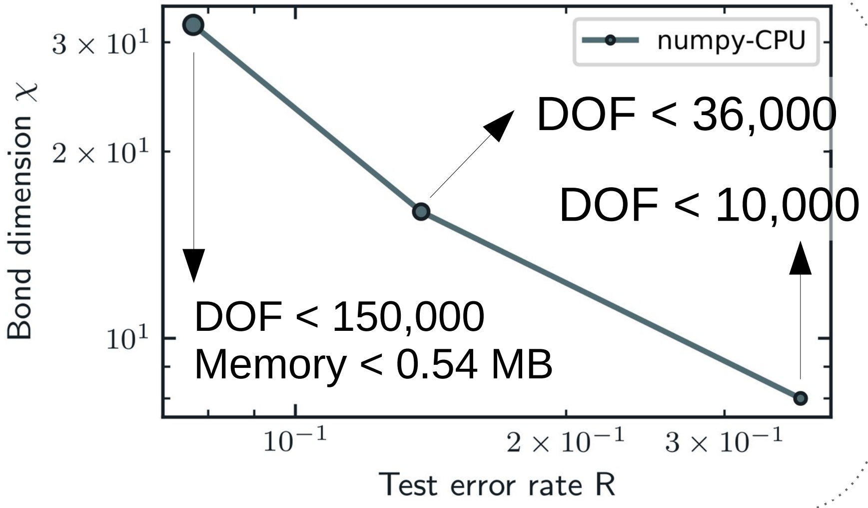
* and one can do better, see Stoudenmire & Schwab, arXiv:1605.05775v2 with > 99%

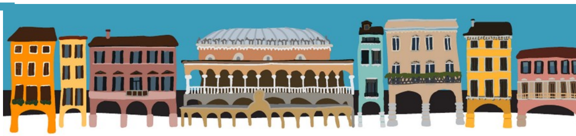


Bond dimension χ

- compression rate quantum correlations as quantum-inspired explanation

- Degrees of freedom (DOF) or memory-need or expressability

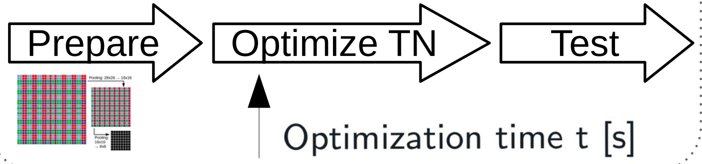


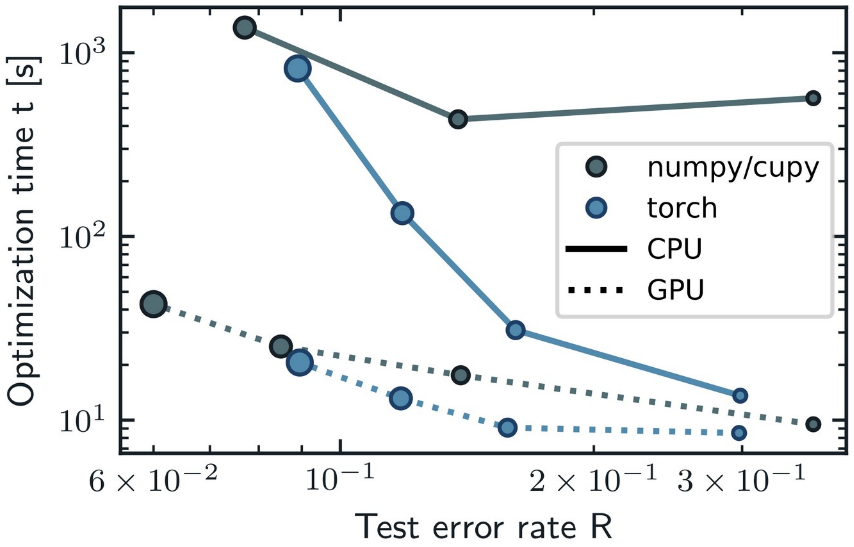


Numpy versus torch, CPU versus GPU

Torch: despite machine learning, no backpropagation used here

Time to run simulation

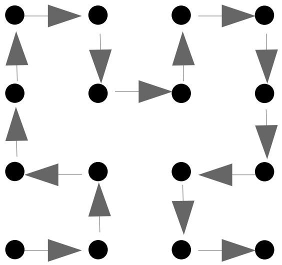




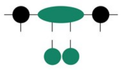
Continue with torch, GPU, and $\chi = 64$

2d image … how to get to a 1d system?

Hilbert curve



Test accuracy
91.05%



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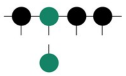
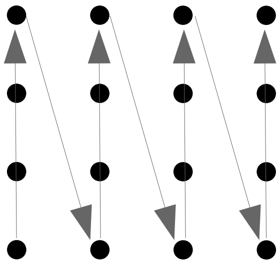
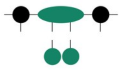


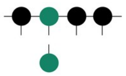
ZigZag map



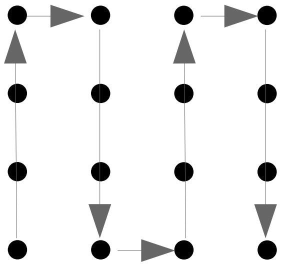
Test accuracy
91.35%



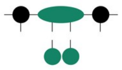
Test accuracy
91.45%



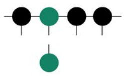
Snake map



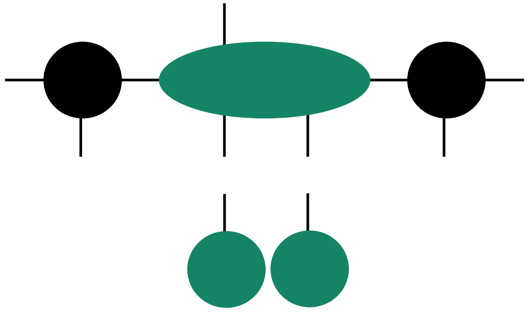
Test accuracy
90.9%

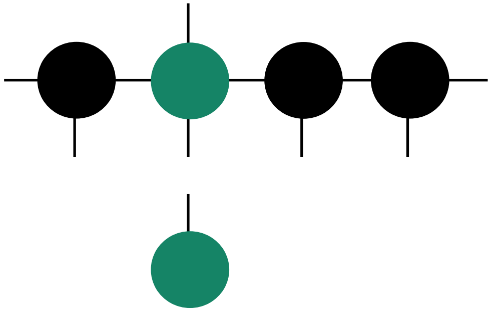


Test accuracy
91.15%



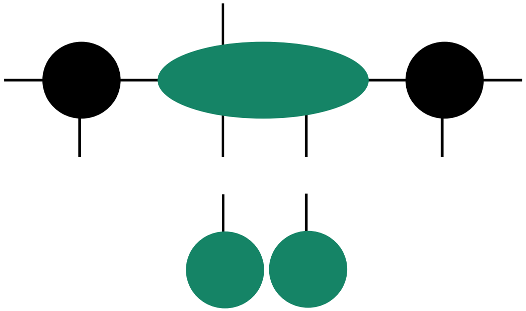
Single-tensor updates





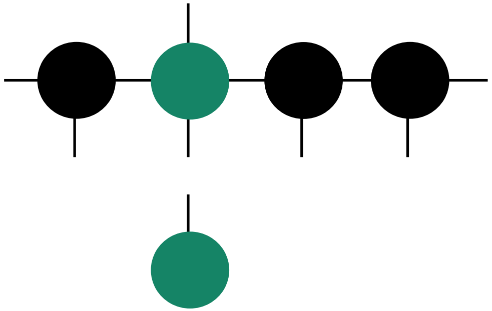
Single-tensor updates

Two-tensor update



$O(\chi^3 \cdot d^3 \cdot l), d = 2, l = 10$

Single-tensor update



$O(\chi^3 \cdot d^2 \cdot l), d = 2, l = 10$

Test accuracy: 91.05%
Time: 20.59s

Test accuracy: 91.05%
Time: 14.43s

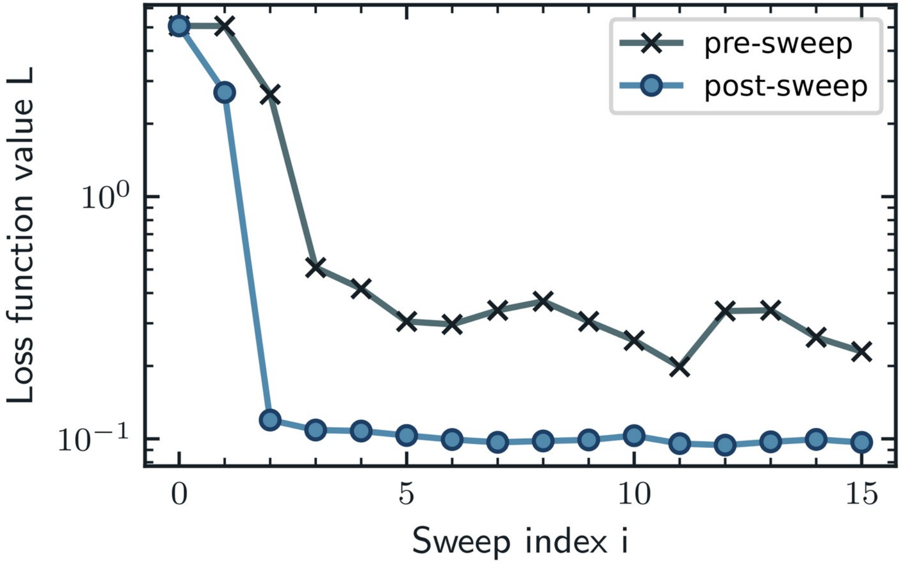
Apply lessons learned to the full data set

Single-tensor update

Training: 60,000
Training batch: 20,000
Test: 10,000
Averaged: no (1 run)
MNIST: 70,000

Accuracy:
94.55%

Loss history



Bonus: binary label optimizations

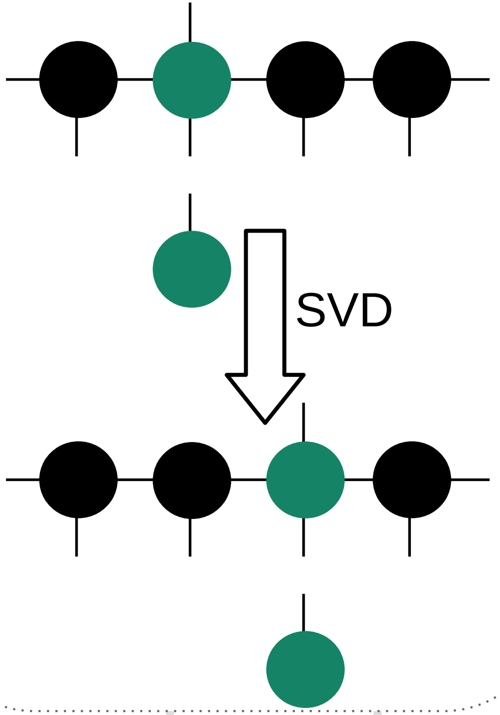
Label-link & argmax

(a, b)

↓ argmax(..)

0 if a > b else 1

Move label link



One-dimensional label link & rounding

(a)

↓ round(..)

0 if a < 0.5 else 1

SVD no longer needed
(no Krylov space needed)

Full and native support for half precision data type

Bonus: binary label runtimes

	float64	float32	float16
One-dimensional label link & rounding … with SVD	Accuracy: 99.75% T = 7.6s	Accuracy: 99.75% T = 6.9s	Accuracy: 99.7% T = 7.8s
One-dimensional label link & rounding … without SVD	Accuracy: 99.55% T = 4.4s	Accuracy: 99.55% T = 4.2s	Accuracy: 99.4% T = 4.3s

Memory-friendly

Conclusion and outlook

Quantum-inspired machine learning for supervised ML tasks

Hyper-parameters from quantum many-body physics

Option for GPU support + option to switch to torch

Also integrate jax and tensorflow as in DJ et al., arXiv 2409.03818

Explore high-energy data and follow path of FPGA triggers

See L. Borella, Alberto Coppi, et al. arxiv:2409.16075

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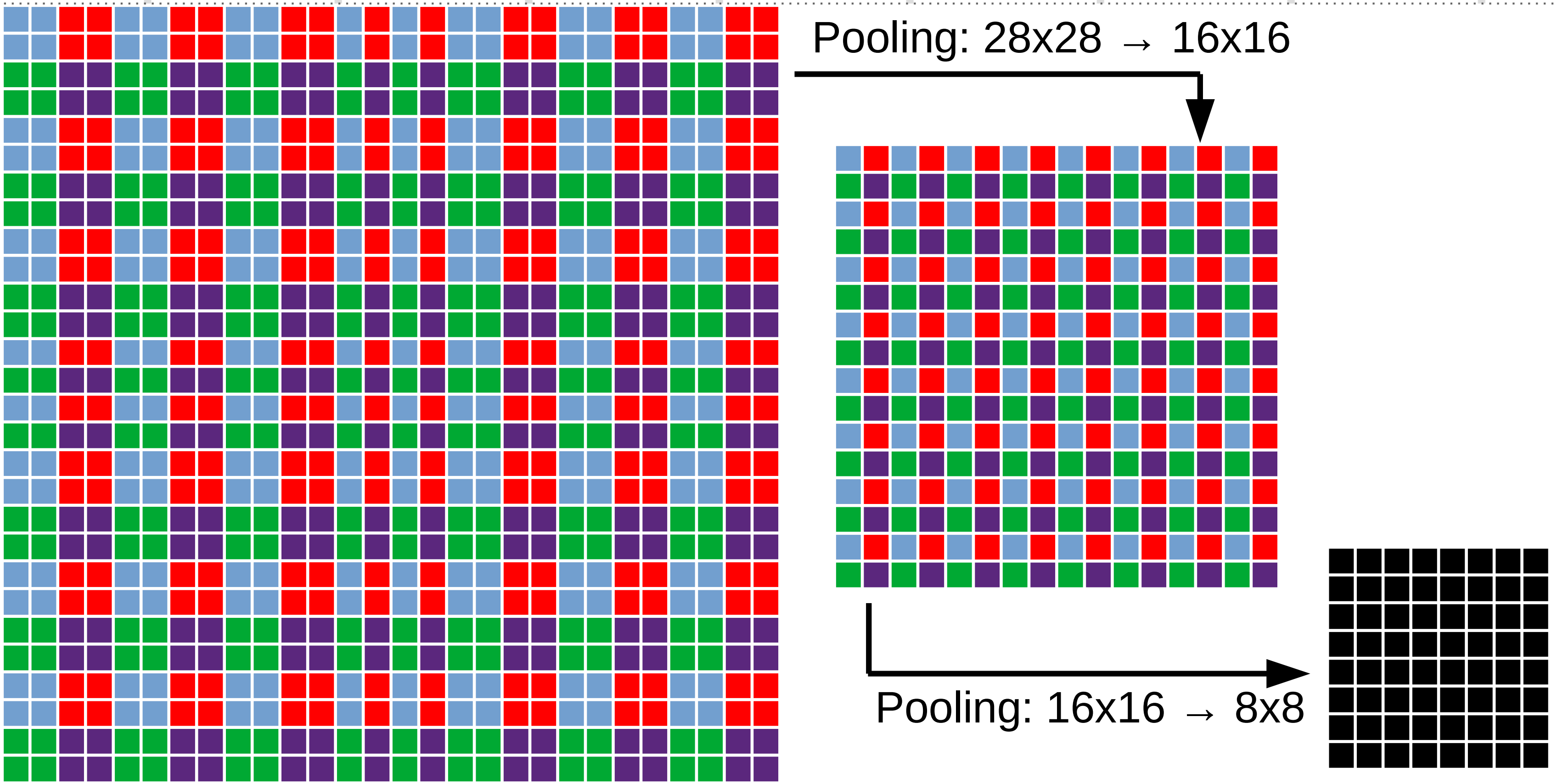
Backup slides

Pooling layer



Modularity of the library

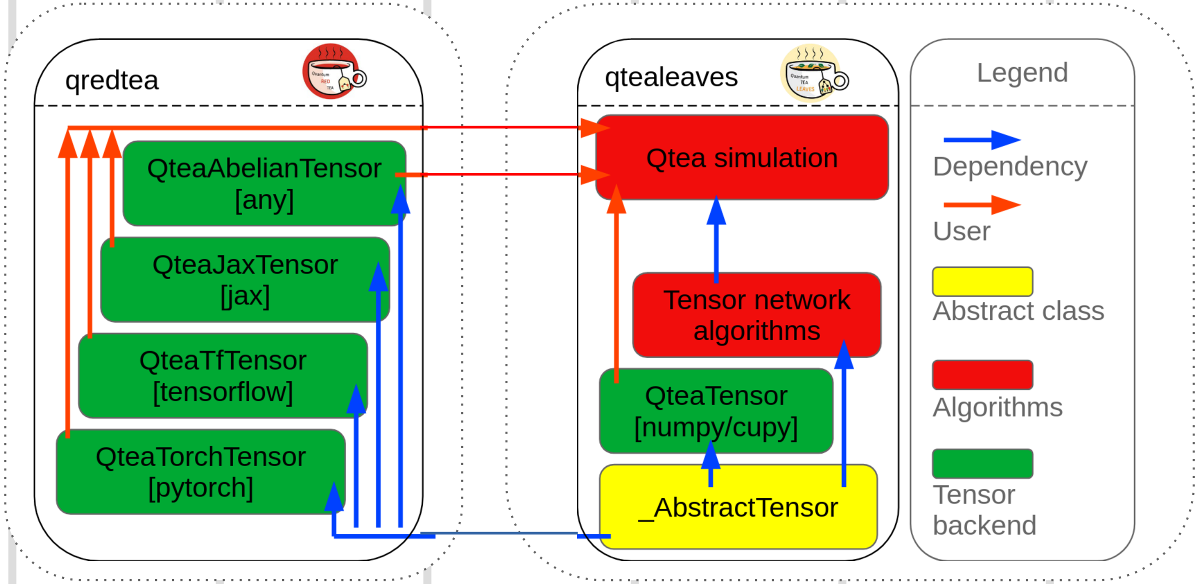
Why do you need another tea flavor?

How to integrate new technology in a library?

Can we use GPUs? … no, because ...

Can we use jax? … no, ...

Major update qtealeaves v1.0.0+



MPS (two-tensor update) versus TTN (single-tensor)