Quantum many-body systems understanding them with and using them as new machine learning tools

Christian Gogolin

Vector Institute Toronto
2018-11-22

Outline

0 Foundations of quantum statistical mechanics

1 Machine learning quantum systems

2 Software for quantum machine learning

Outline

0 ~~Foundations of quantum statistical mechanics~~

1 Machine learning quantum systems

2 Software for quantum machine learning

Machine learning quantum systems

I foresee a bright future because:

Machine learning quantum systems

I foresee a bright future because:

- There is BIG data

Machine learning quantum systems

I foresee a bright future because:

- There is BIG data
- Everybody can generate it

Machine learning quantum systems

I foresee a bright future because:

- There is BIG data
- Everybody can generate it
- Classification and control problems are everywhere

Machine learning quantum systems

I foresee a bright future because:

- There is BIG data
- Everybody can generate it
- Classification and control problems are everywhere
- People are used to heuristics

Machine learning quantum systems

I foresee a bright future because:

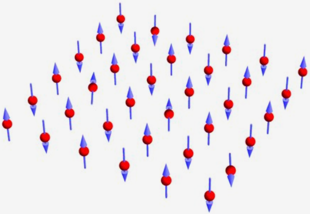
- There is BIG data
- Everybody can generate it
- Classification and control problems are everywhere
- People are used to heuristics
- Applications are not safety critical

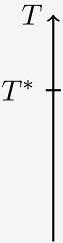
Phase transitions and their characterization

Phase transitions and their characterization

in the 2D ferromagnetic Ising model

$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j \qquad , \quad \sigma_i = \pm 1$$

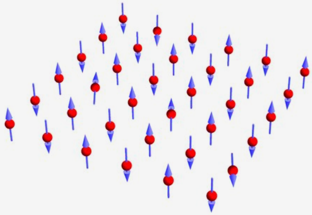


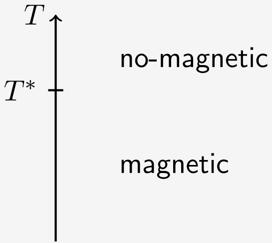


Phase transitions and their characterization

in the 2D ferromagnetic Ising model

$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j \qquad , \quad \sigma_i = \pm 1$$

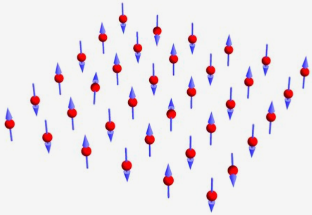




Phase transitions and their characterization

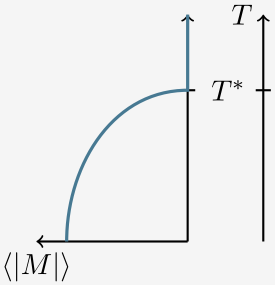
in the 2D ferromagnetic Ising model

$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j \quad , \quad \sigma_i = \pm 1$$



$$M = \sum_i \sigma_i$$

magnetization



no-magnetic

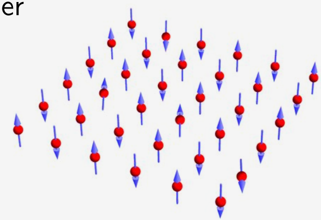
magnetic

Phase transitions and their characterization

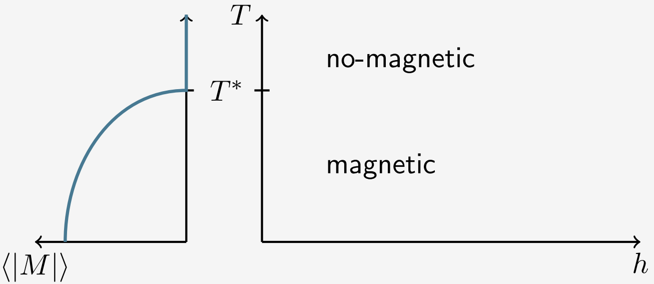
in the 2D ferromagnetic Ising model with disorder

$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j + \sum_{i=1}^{N} h_i\sigma_i, \qquad \sigma_i = \pm 1$$

$$M = \sum_i \sigma_i \qquad\qquad h_i \in [-h, h]$$



magnetization phase diagram

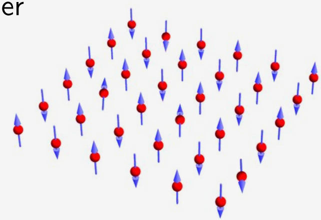


Phase transitions and their characterization

in the 2D ferromagnetic Ising model with disorder

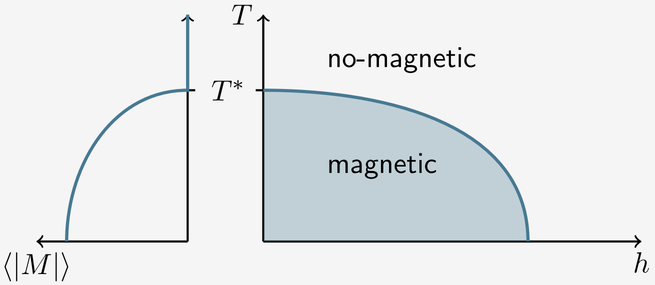
$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j + \sum_{i=1}^{N} h_i \sigma_i, \quad \sigma_i = \pm 1$$

$$M = \sum_i \sigma_i \qquad h_i \in [-h, h]$$



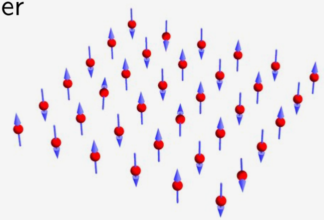
magnetization

phase diagram



Phase transitions and their characterization

in the 2D ferromagnetic Ising model with disorder

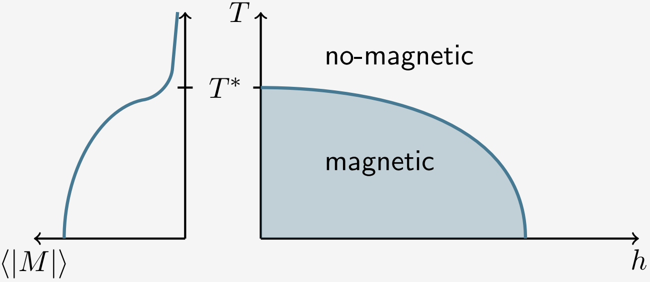


$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j + \sum_{i=1}^{N} h_i\sigma_i, \quad \sigma_i = \pm 1$$

$$M = \sum_i \sigma_i \qquad\qquad h_i \in [-h, h]$$

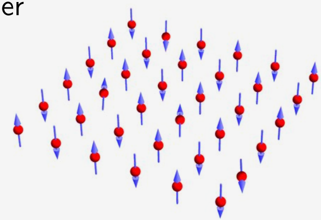
magnetization

phase diagram



Phase transitions and their characterization

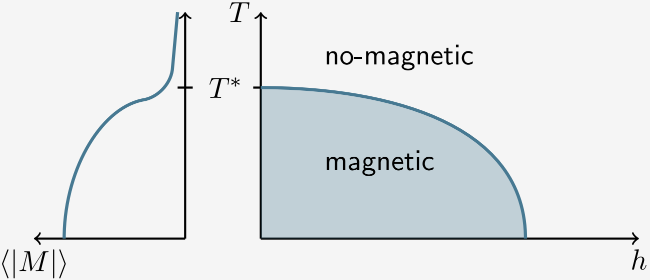
in the 2D ferromagnetic Ising model with disorder



$$H(\vec{\sigma}) = -\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j + \sum_{i=1}^{N} h_i\sigma_i, \qquad \sigma_i = \pm 1$$

$$M = \sum_i \sigma_i \qquad\qquad h_i \in [-h, h]$$

magnetization phase diagram



Can do machine learning necessary, but not really necessary…

Many-body localization

Many-body localization

in the Heisenberg chain

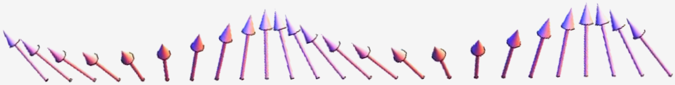
$$H = -\sum_{i=1}^{N}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \sigma_i^z\,\sigma_{i+1}^z) \in \mathbb{C}^{2^N}$$

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Many-body localization

in the Heisenberg chain

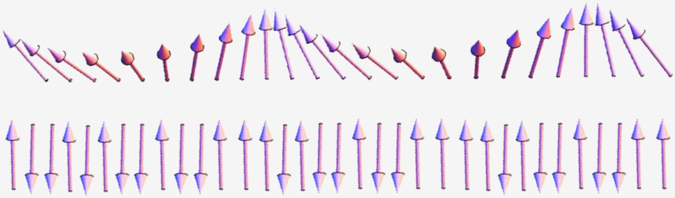
$$H = -\sum_{i=1}^{N} (\sigma_i^x \, \sigma_{i+1}^x + \sigma_i^y \, \sigma_{i+1}^y + \sigma_i^z \, \sigma_{i+1}^z)$$



Many-body localization

in the Heisenberg chain with disorder

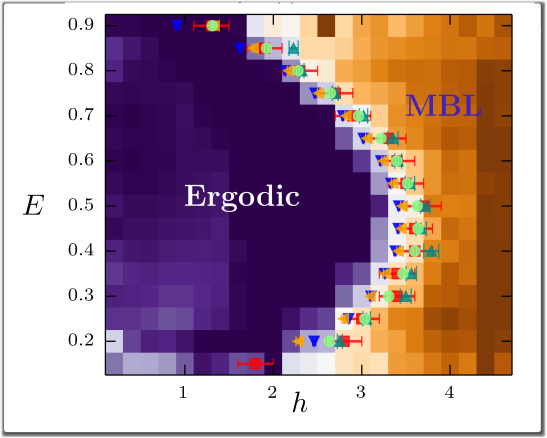
$$H = -\sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z) + \sum_{i=1}^{N} h_i \sigma_i^z$$



Many-body localization

in the Heisenberg chain with disorder

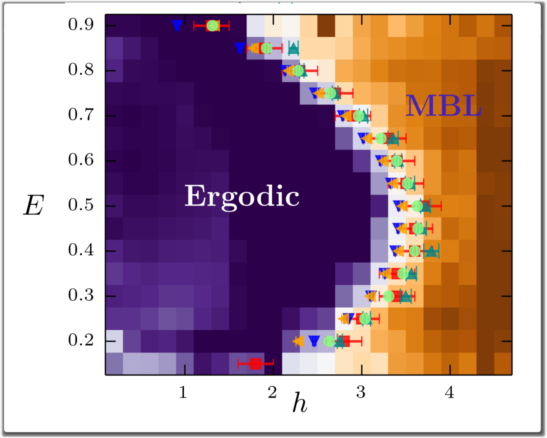
$$H = -\sum_{i=1}^{N}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \sigma_i^z\,\sigma_{i+1}^z) + \sum_{i=1}^{N} h_i\,\sigma_i^z$$



Many-body localization

in the Heisenberg chain with disorder

$$H = -\sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z) + \sum_{i=1}^{N} h_i \sigma_i^z$$

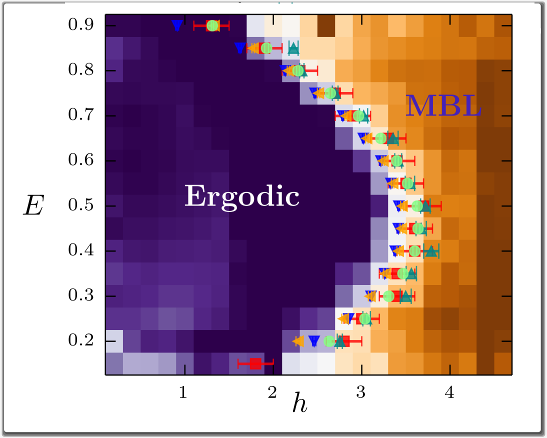


- No local oder parameter

Many-body localization

in the Heisenberg chain with disorder

$$H = -\sum_{i=1}^{N}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \sigma_i^z\,\sigma_{i+1}^z) + \sum_{i=1}^{N} h_i\,\sigma_i^z$$

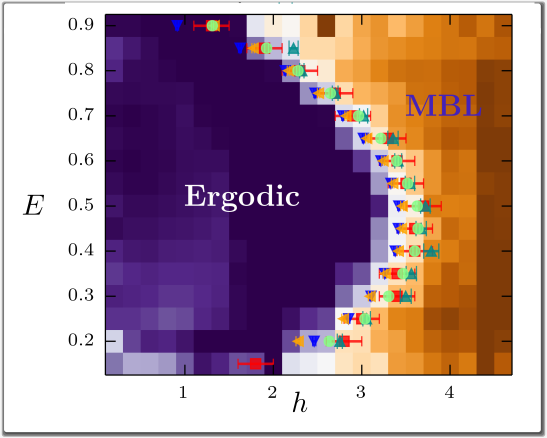


- No local oder parameter
- No universally accepted order parameter

Many-body localization

in the Heisenberg chain with disorder

$$H = -\sum_{i=1}^{N}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \sigma_i^z\,\sigma_{i+1}^z) + \sum_{i=1}^{N} h_i\,\sigma_i^z$$

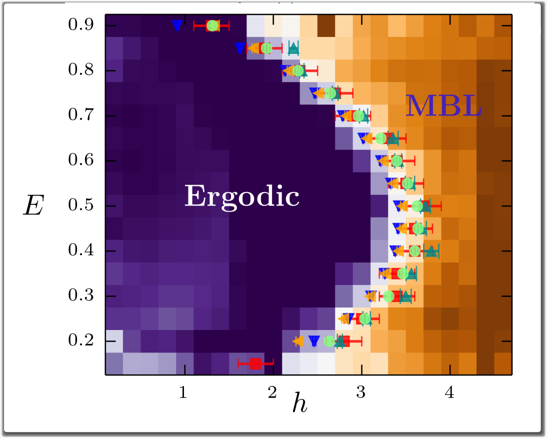


- No local oder parameter
- No universally accepted order parameter
- Do not agree within error bars

Many-body localization

in the Heisenberg chain with disorder

$$H = -\sum_{i=1}^{N}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \sigma_i^z\,\sigma_{i+1}^z) + \sum_{i=1}^{N} h_i\,\sigma_i^z$$

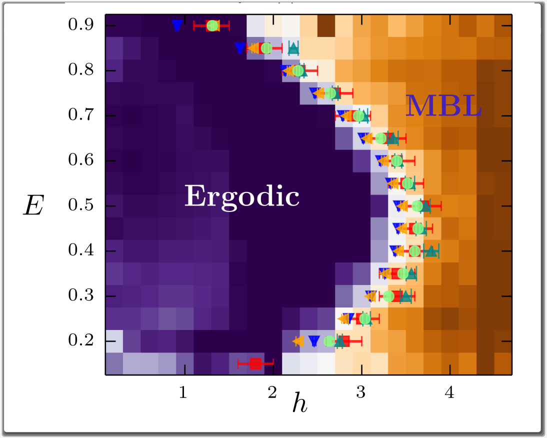


- No local oder parameter
- No universally accepted order parameter
- Do not agree within error bars
- strong finite size effects

Many-body localization

in the Heisenberg chain with disorder

$$H = -\sum_{i=1}^{N} (\sigma_i^x \, \sigma_{i+1}^x + \sigma_i^y \, \sigma_{i+1}^y + \sigma_i^z \, \sigma_{i+1}^z) + \sum_{i=1}^{N} h_i \, \sigma_i^z$$

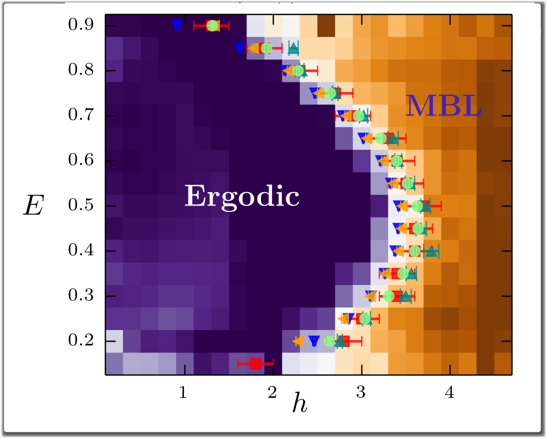


- No local oder parameter
- No universally accepted order parameter
- Do not agree within error bars
- strong finite size effects
- 10.000 disorder averages

Many-body localization

in the Heisenberg chain with disorder

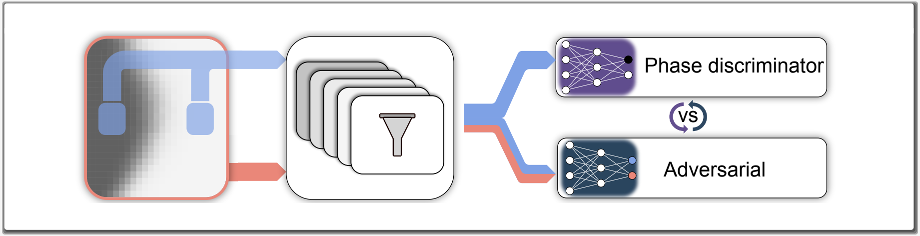
$$H = -\sum_{i=1}^{N} (\sigma_i^x \, \sigma_{i+1}^x + \sigma_i^y \, \sigma_{i+1}^y + \sigma_i^z \, \sigma_{i+1}^z) + \sum_{i=1}^{N} h_i \, \sigma_i^z$$



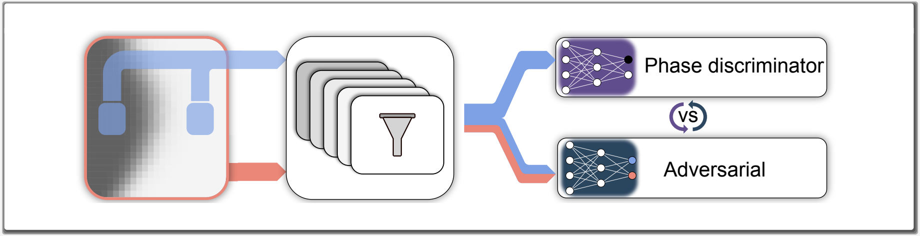
- No local oder parameter
- No universally accepted order parameter
- Do not agree within error bars
- strong finite size effects
- 10.000 disorder averages

Machine learning to the rescue?

Domain-Adversarial Neural Networks

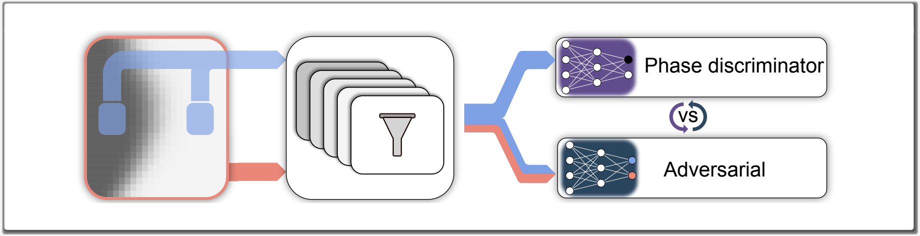


Domain-Adversarial Neural Networks



- No need to know the phase boundary

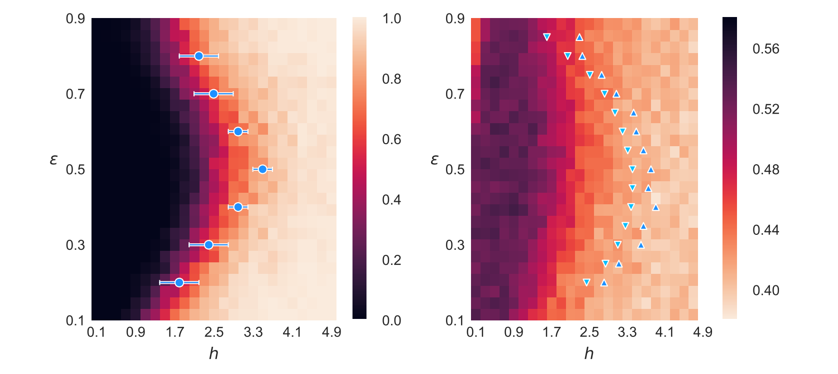
Domain-Adversarial Neural Networks



- No need to know the phase boundary
- No manual feature engineering

Comparison with other "oder parameters"

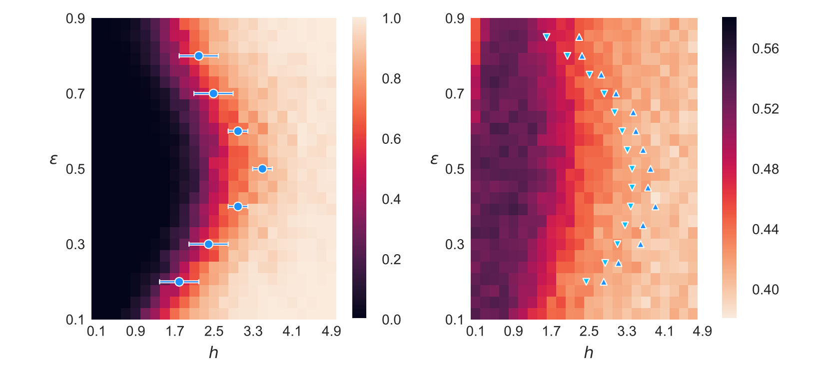
Background: DANN $N = 12$, 50 real. vs AAGR $N = 12$, 50 real.



Datapoints: DANN $N = 18$, 500 real. vs. AAGR $N = 22$, 1.000-10.000 real.

Comparison with other “oder parameters”

Background: DANN $N = 12$, 50 real. vs AAGR $N = 12$, 50 real.



Datapoints: DANN $N = 18$, 500 real. vs. AAGR $N = 22$, 1.000-10.000 real.

- Superior statistical properties
- Vastly less disorder averaging

Outline

Quantum optimization and machine learning

Probably the first relevant application because:

Quantum optimization and machine learning

Probably the first relevant application because:

- Unlocks objective functions and kernel maps that a classical computer cannot calculate

Quantum optimization and machine learning

Probably the first relevant application because:

- Unlocks objective functions and kernel maps that a classical computer cannot calculate
- No error correction/fault tolerance needed

Quantum optimization and machine learning

Probably the first relevant application because:

- Unlocks objective functions and kernel maps that a classical computer cannot calculate
- No error correction/fault tolerance needed
- Some quantum many-body and chemistry problems naturally map to quantum hardware

Quantum optimization and machine learning

Probably the first relevant application because:

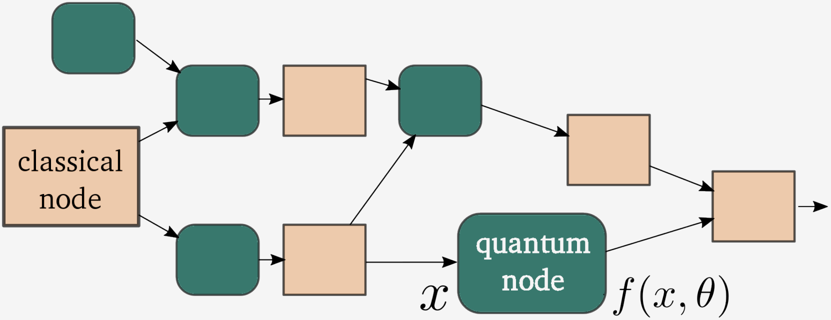
- Unlocks objective functions and kernel maps that a classical computer cannot calculate
- No error correction/fault tolerance needed
- Some quantum many-body and chemistry problems naturally map to quantum hardware
- Hybrid quantum classical computation

Quantum optimization and machine learning

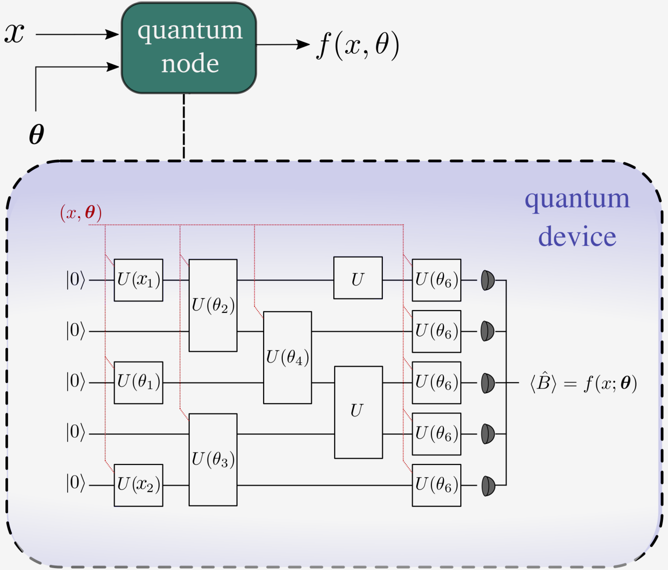
Probably the first relevant application because:

- Unlocks objective functions and kernel maps that a classical computer cannot calculate
- No error correction/fault tolerance needed
- Some quantum many-body and chemistry problems naturally map to quantum hardware
- Hybrid quantum classical computation
- There is now software to do the training/optimization. . .

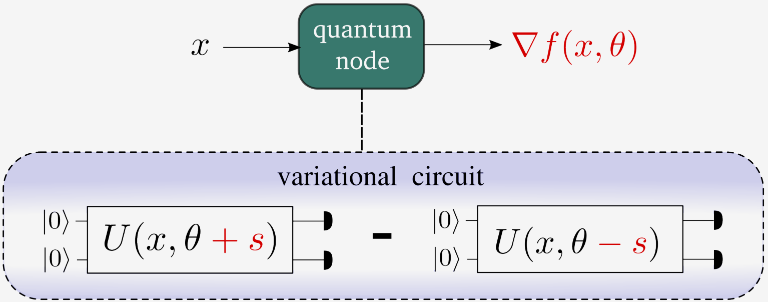
Hybrid quantum classical computation



Variational quantum circuits



Automatic differentiation



Enter PennyLane

PENNYLANE

is a library for quantum optimization and machine learning that:

- Enables optimization via automatic differentiation
- Built for hybrid quantum-classical computation
- Is hardware agnostic and extensible via plugins
- Open-source and extensively documented
- We hope to become the PyTorch of quantum machine learning

PENNYLANE

Let's see this in action!

Summary

- Adversarial domain adaptation for delineating phase transitions

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties
  - Semi un-supervised

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties
  - Semi un-supervised
  - Opens up way to investigate how the network discriminates phases

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties
  - Semi un-supervised
  - Opens up way to investigate how the network discriminates phases
- PennyLane

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties
  - Semi un-supervised
  - Opens up way to investigate how the network discriminates phases
- PennyLane
  - Easy to use PyTorch style automatic differentiation for QML

Summary

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties
  - Semi un-supervised
  - Opens up way to investigate how the network discriminates phases
- PennyLane
  - Easy to use PyTorch style automatic differentiation for QML
  - Hardware agnostic and extensible

Summary

Thank you for your attention!

- Adversarial domain adaptation for delineating phase transitions
  - Objective estimate of the phase boundary
  - Superior statistical properties
  - Semi un-supervised
  - Opens up way to investigate how the network discriminates phases
- PennyLane
  - Easy to use PyTorch style automatic differentiation for QML
  - Hardware agnostic and extensible