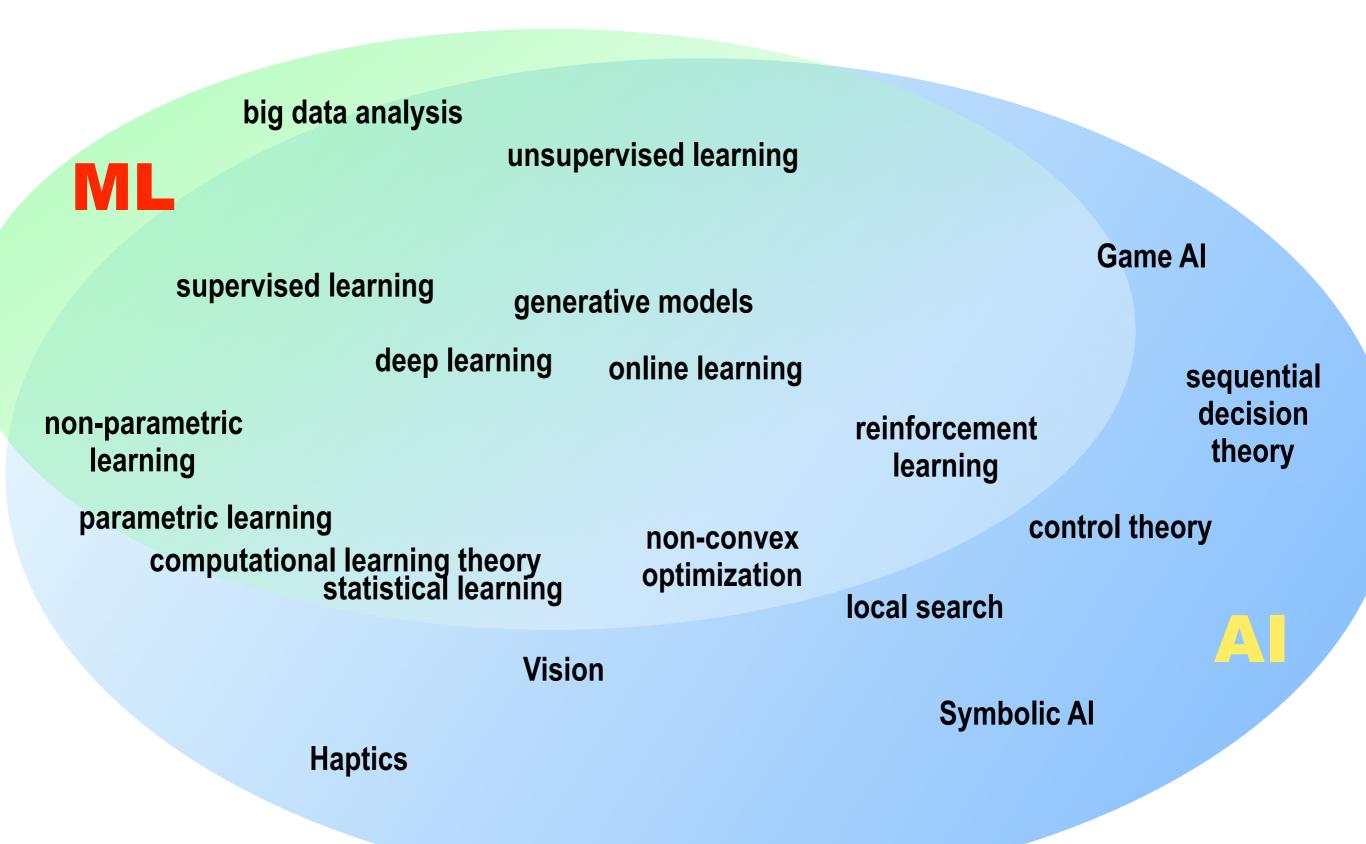
Quantum-enhanced Machine Learning (with near-term devices)

Contents & Literature

- 1) Background 1: machine learning (ML)
 - what is ML, and basic ML models
- 2) QC meets ML (big picture) [for more info: arXiv:1709.02779]
- 3) ML and parametrized circuits [for more info: arXiv:1906.07682]
- 4) QeML with quantum feature spaces [based on: arXiv:1804.11326]
 - Support vector machines
 - Explicit and implicit quantum-embedded SVMs

Machine learning and Al

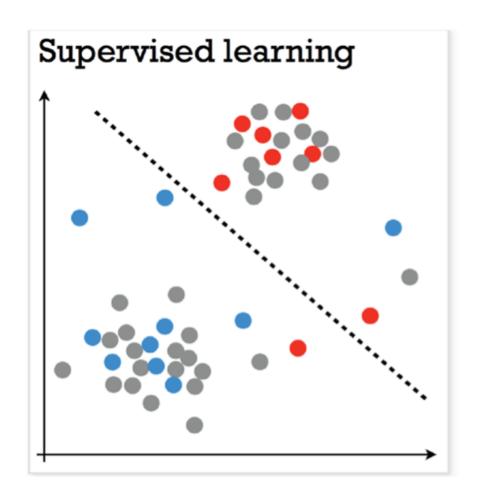


Three main (cannonical) modes of ML:

- Supervised learning
- Unsupervised learning
- Reinforcement learning

• forest of in-between models; semi-supervised, active, transductive, on-line...

Supervised learning: the *what* (is the objective)









7

Supervised learning: the *what* (is the objective)

Basic concepts and math

Data (feature vectors) & Labels:

$$\mathbf{x} \in S \subseteq \mathbb{R}^n$$
; $y \in Labels$

Label function:

$$f: S \rightarrow Labels$$

Dataset, "training examples"

$$D = \{ (\mathbf{x}_i, y_i) | \mathbf{x}_i \in S; y_i = f(\mathbf{x}) \}$$

-need to correctly label unlabeled data

Given D, output a good guess for f.

- -classification (categorical or discrete label) v.s. regression (contiuous label)
- -classification, prediction, regression....

Supervised learning: the *what* (is the objective)

Basic concepts and math

More generally (probabilistic)

BTW: Distributions generalize functions

Data (feature vectors) & Labels:

$$\mathbf{x} \in S \subseteq \mathbb{R}^n$$
; $y \in Labels$

Label function:

$$P(\mathbf{x}, \mathbf{y})$$

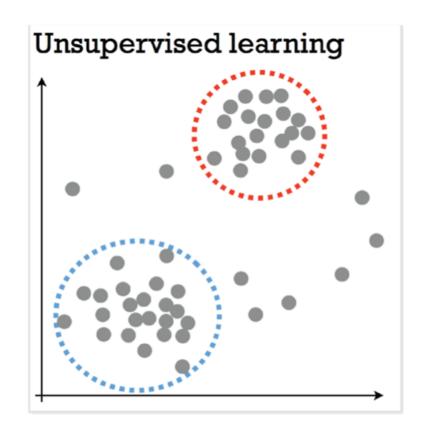
Dataset, "training examples"

$$D \sim P^{\times |D|}$$

Given D, output a good guess for $P(y | \mathbf{x})$

Learning about data-label relationships in a bivariate distribution from samples

Unsupervised learning: the what (is the objective)





?

data: $\mathbf{x} \in S \subseteq \mathbb{R}^n$

"world": $P(\mathbf{x})$

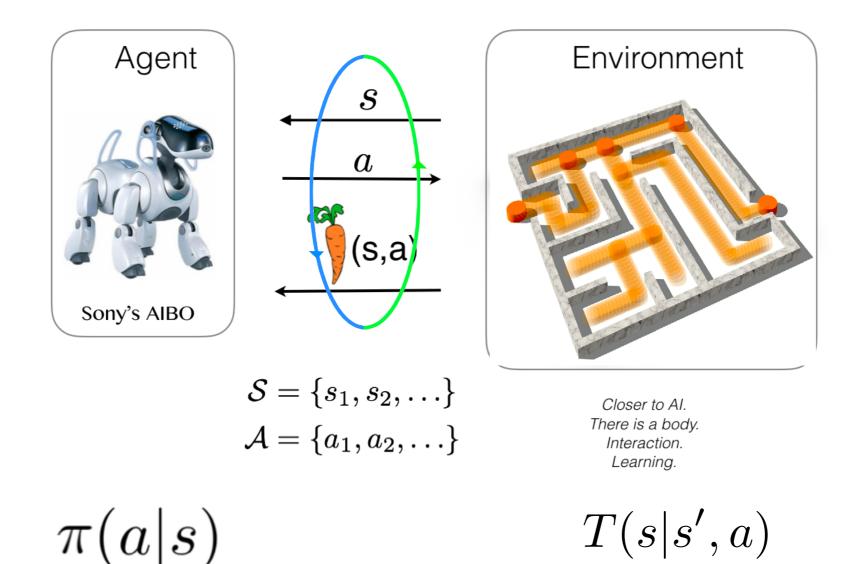
training: $D \sim P^{\times |D|}$

-discriminative (clustering), "labeling w/o examples"

-generative (make more cats): approximate sampling from P given D

Learning about (all) <u>features</u> in a distribution <u>from samples</u>

Reinforcement learning: the what (is the objective)



Learning correct behaviour (policies) by trial-and-error (incl. data generation online). E.g. AlphaGo.

Supervised learning: the *how* (is it achieved)

Recall: need to "guess" $f: S \subseteq \mathbb{R}^n \to Labels$ from $D = \{(\mathbf{x}_i, y_i = f(\mathbf{x}_i))\}$

- Hypothesis family: $\{f^{\theta} | f^{\theta} : S \subseteq \mathbb{R}^n \to Labels, \theta\}$ (c.f. "model/model family")
- Learning = training \approx fitting: $argmin_{\theta} \ Error_on_D(f^{\theta}) + R(f^{\theta})$ R = regularization

- "Loss", "empirical risk", e.g. $\sum_{(\mathbf{x},y)\in D} |f^{\theta}(\mathbf{x}) y|^2$
- Generalization performance: (no overfitting, Occam's razor)

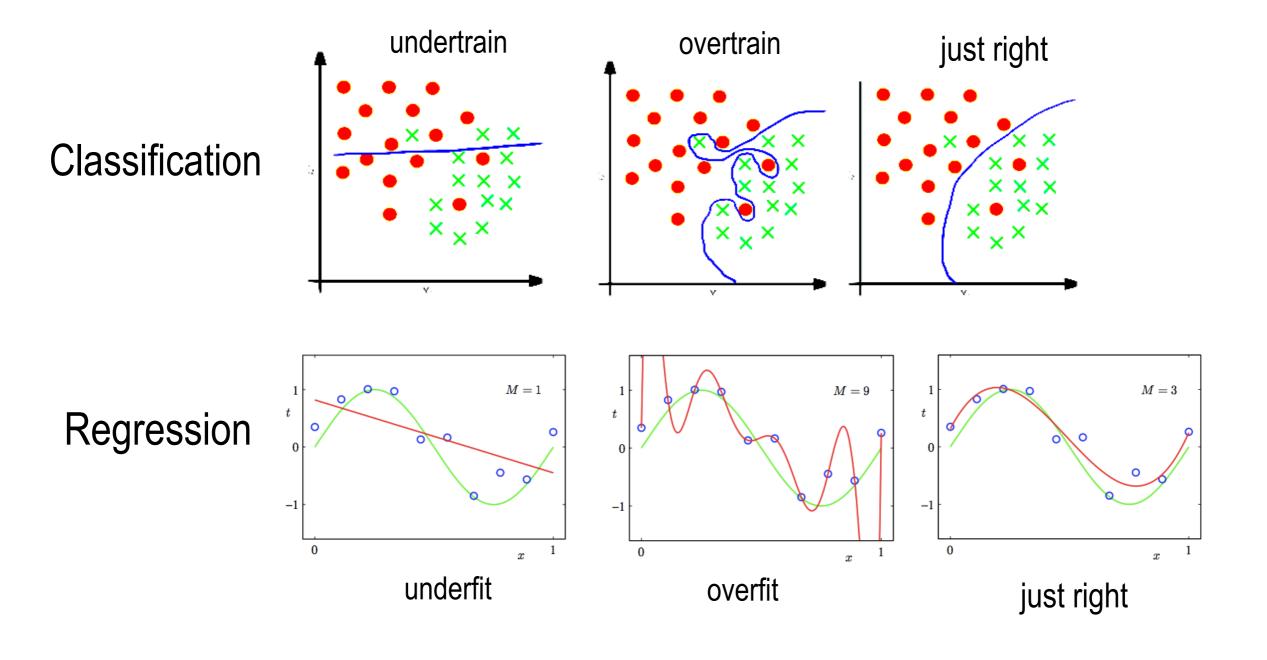
Supervised learning: the *how* (is it achieved)

Recall: need to "guess" $f: S \subseteq \mathbb{R}^n \to Labels$ from $D = \{(\mathbf{x}_i, y_i = f(\mathbf{x}_i))\}$

- Hypothesis family: $\{f^{\theta} | f^{\theta} : S \subseteq \mathbb{R}^n \to Labels, \theta\}$ (c.f. "model/model family")
- Learning = training \approx fitting: $argmin_{\theta} \ Error_on_D(f^{\theta}) + R(f^{\theta})$ R = regularization

the same elements will be present for unsupervised learning

- "Loss", "empirical risk", e.g. $\sum_{(\mathbf{x},y)\in D} |f^{\theta}(\mathbf{x}) y|^2$
- Generalization performance: (no overfitting, Occam's razor)

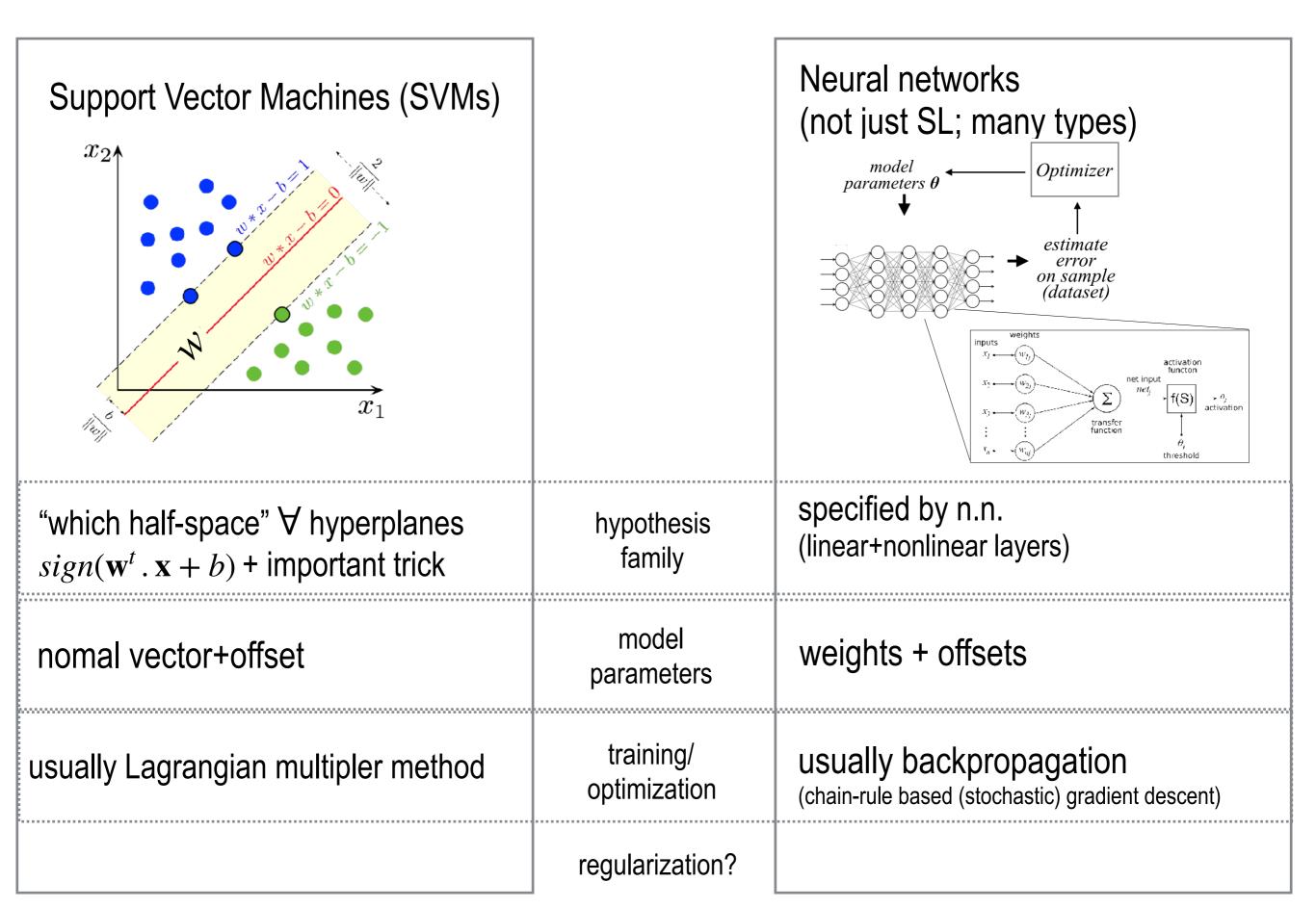


Supervised learning: the *how* (is it achieved); examples

- support vector machines (SVM)
- neural networks

- k-nearest neighbours [classification]
- decision trees [classification]
- naïve Bayes
- (linear) regression [regression]
- Gaussian process regression

Supervised learning: the how (is it achieved); examples



When discussing QML, keep an eye on

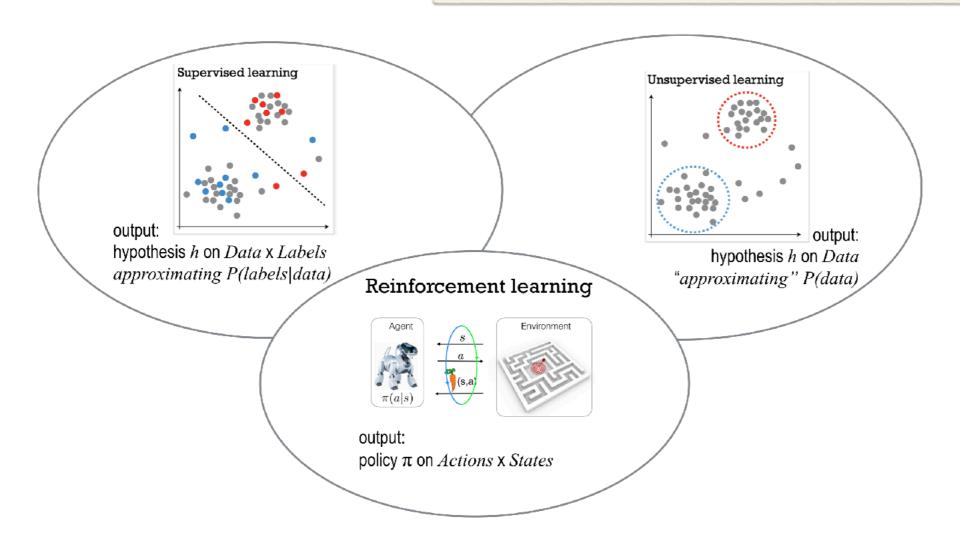
- the What (what is the objective/goal)
- the **How** (how is it done: algorithm; does is achieve the goal)
- the Why
 (why do it on a QC; what is the expected advantage/other motivation)

actually, same questions apply to much of *classical* ML approaches the why is tricky tho; makes a good model model is though

Big picture take home:

the learning/training is optimization:

$$\operatorname{argmin}_{\theta} \operatorname{Err_training_set}(\theta) + \operatorname{Reg}(\theta)$$



but machine learning is more; which model; how it generalizes; good choices...

A connection... variational methods in physics.. incl VQE are very similar

Var. Q chem	ML	
"Ansatz"	"model"/hypothesis family	
loss: energy	loss: training set error+regul.	
explicit, error free ground truth	implicit ground truth, errors	
optimization	learning/training	

no regularization	statistical,	regularization
or generalization	parameteric learning	generalization

-ground truth...

Cat v.s. no-cat example



QC meets ML: big picture ideas

-QC and the optimization bottleneck

training *is optimization* and can be hard (NP-hard) → quantum optimization

-QC and the high dimension bottleneck

much of ML is linear algebra; quantum computing is good at that, under conditions

-QC and the hard model bottleneck

topic of the next two lectures

Supervised Machine learning with Parameterized Quantum Circuits

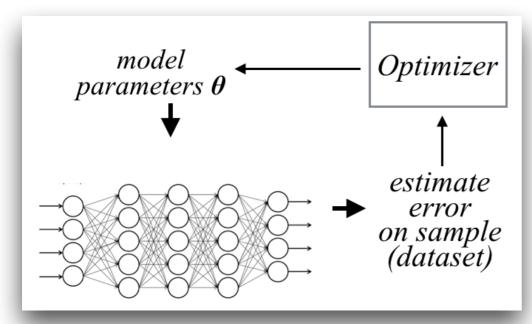
What: supervised learning for classification

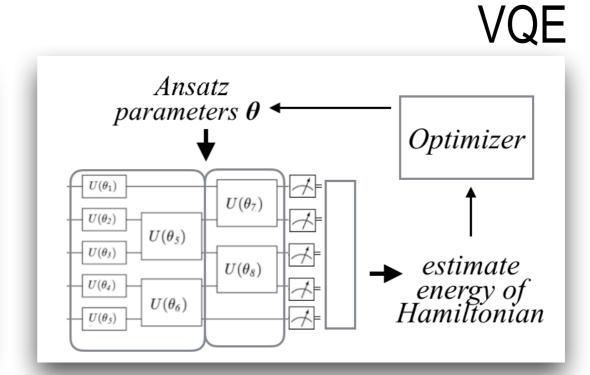
Using quantum computing... but not for optimization needs

Why? TBD

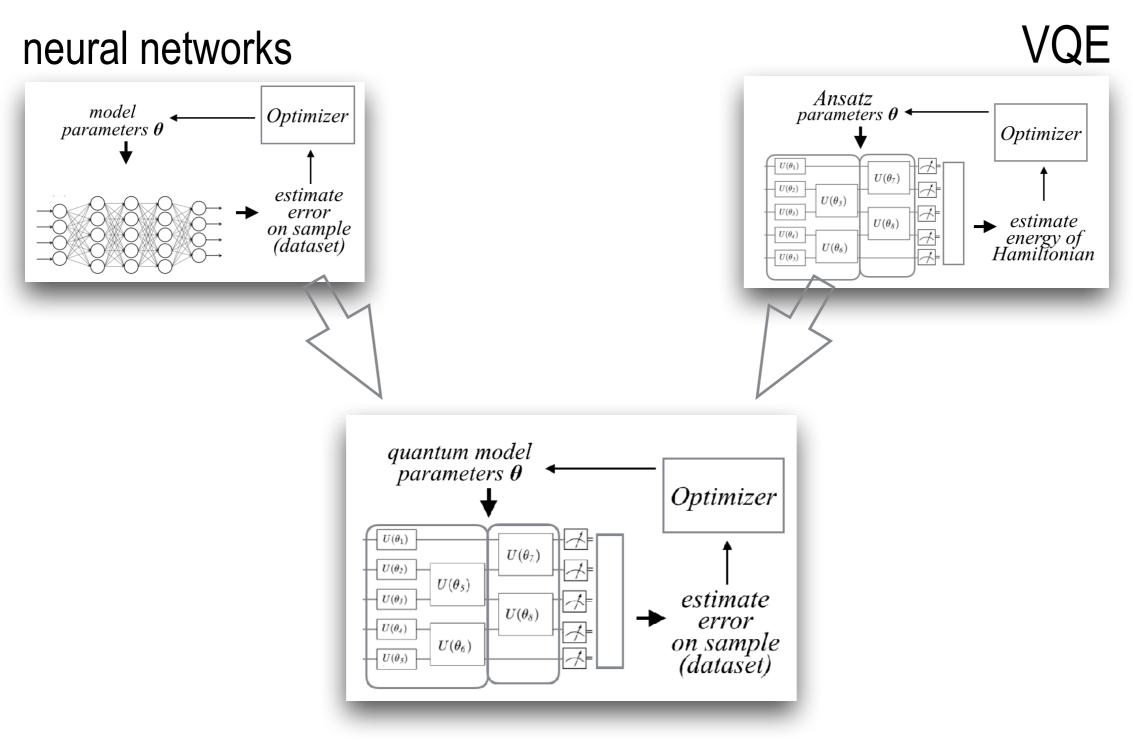
Supervised Machine learning with Parameterized Quantum Circuits

neural networks





Machine learning with Parameterized Quantum Circuits



PQC-based ML

- 1) can we train it?
- 2) does it work?
- 3) does it do anything interesting? why do this?

Same Q's for VQE, but there 3) is clear. Here it is not.

Motivations: cannot do it classically? Curiosity driven?

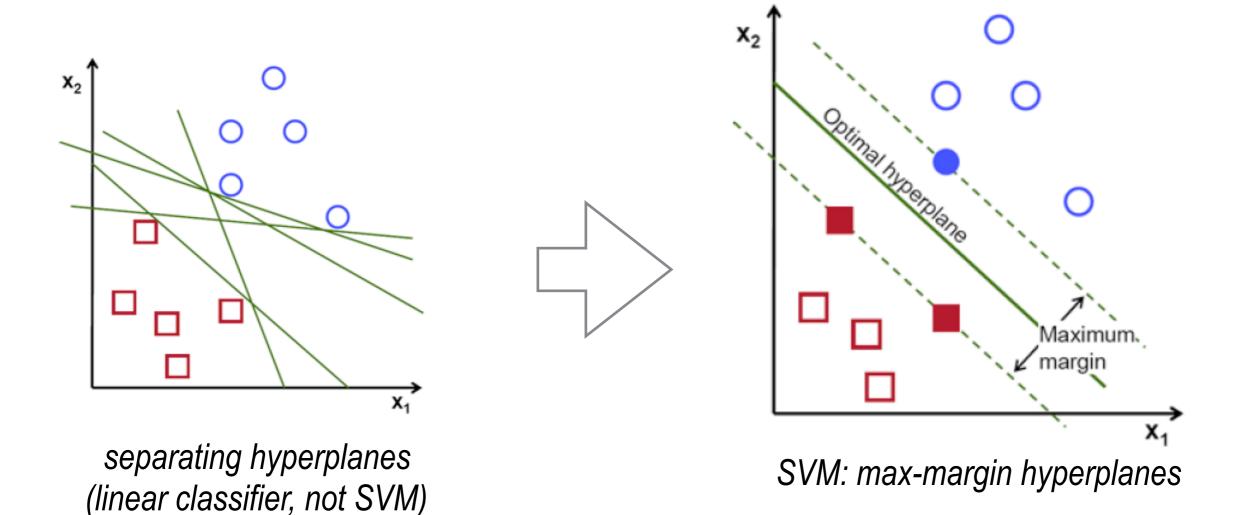
We don't really understand the model...

Next:

- 1) a way to understand some of it.
- 2) reasons to do it

Background 2: SVMs in detail

$$D = \{(x_i, y_i)\}_i \ x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$$



for now, assume linearly separable data

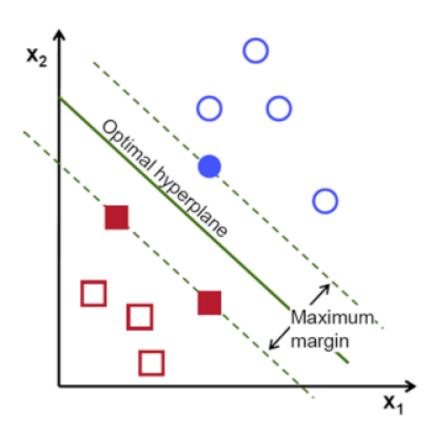
$$D = \{(x_i, y_i)\}_i \ x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$$

A number of equivalent formulations...

$$\underset{\mathbf{w},b}{\operatorname{arg\,max}} \min_{i \in \{1,...,N\}} \frac{y_i(\mathbf{w}^\mathsf{T} \mathbf{x}_i + b)}{\|\mathbf{w}\|}$$

 $y_i(\mathbf{w}^{\mathsf{T}}\mathbf{x}_i + b)$ - "functional margin"

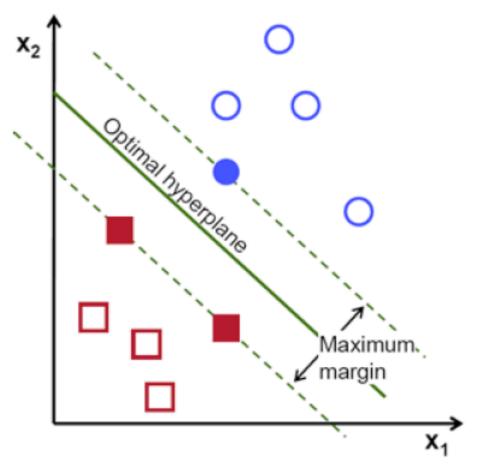
$$\frac{y_i(\mathbf{w}^\mathsf{T}\mathbf{x}_i + b)}{\|\mathbf{w}\|}$$
 - "geometric margin"



$$D = \{(x_i, y_i)\}_i \ x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$$

After some work: quadratic problem

$$\label{eq:argmin} \begin{split} & \underset{\mathbf{w},b}{\text{arg min}} \ \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{such that } y_i(\mathbf{w}^\intercal \mathbf{x}_i + b) \geq 1, \quad i = 1, \dots, N. \end{split}$$



SVM: max-margin hyperplanes

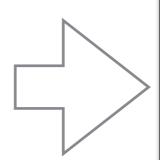
"Support vectors": points closest and equidistant to hyperplane

Hyperplane fully defined in terms of *support vectors*

Lagrangian approach

Primal problem:

$$\label{eq:such that point} \begin{split} & \underset{\mathbf{w},b}{\text{arg min}} \ \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{such that } y_i(\mathbf{w}^\intercal \mathbf{x}_i + b) \geq 1, \quad i = 1, \dots, N. \end{split}$$



Dual problem:

$$\arg\max_{\alpha} \ \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i)^\mathsf{T} \mathbf{x}_j,$$
 such that $\alpha_i \geq 0$, for $i = 0, \dots, N$,
$$\operatorname{and} \ \sum_{i=1}^{N} \alpha_i y_i = 0.$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i^* y_i \mathbf{x}_i.$$

Why bother with dual problem? Representation in terms of datapoints

sparser evaluation

$$(\mathbf{w}^*)^\mathsf{T}\mathbf{x} + b^* = \left(\sum_{i=1}^N \alpha_i y_i(\mathbf{x}_i)^\mathsf{T}\mathbf{x}\right) + b^*.$$

only inner products matter

$$\alpha_i \alpha_j y_i y_j (\mathbf{x}_i)^\mathsf{T} \mathbf{x}_j,$$

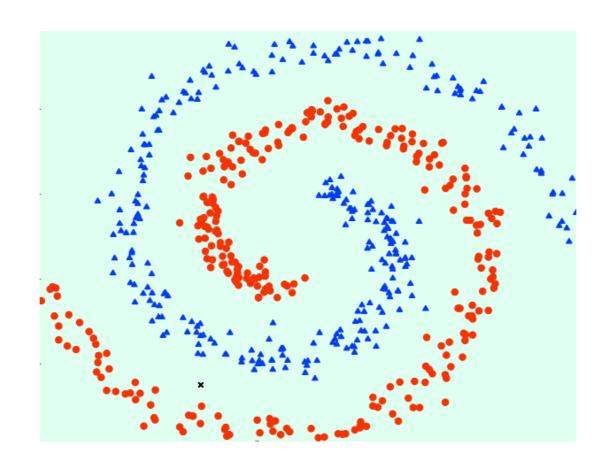
handy for quantum tricks

Comment: the math should not hide the fact we are simply

finding a member of the hypothesis family which is minimizing a loss function

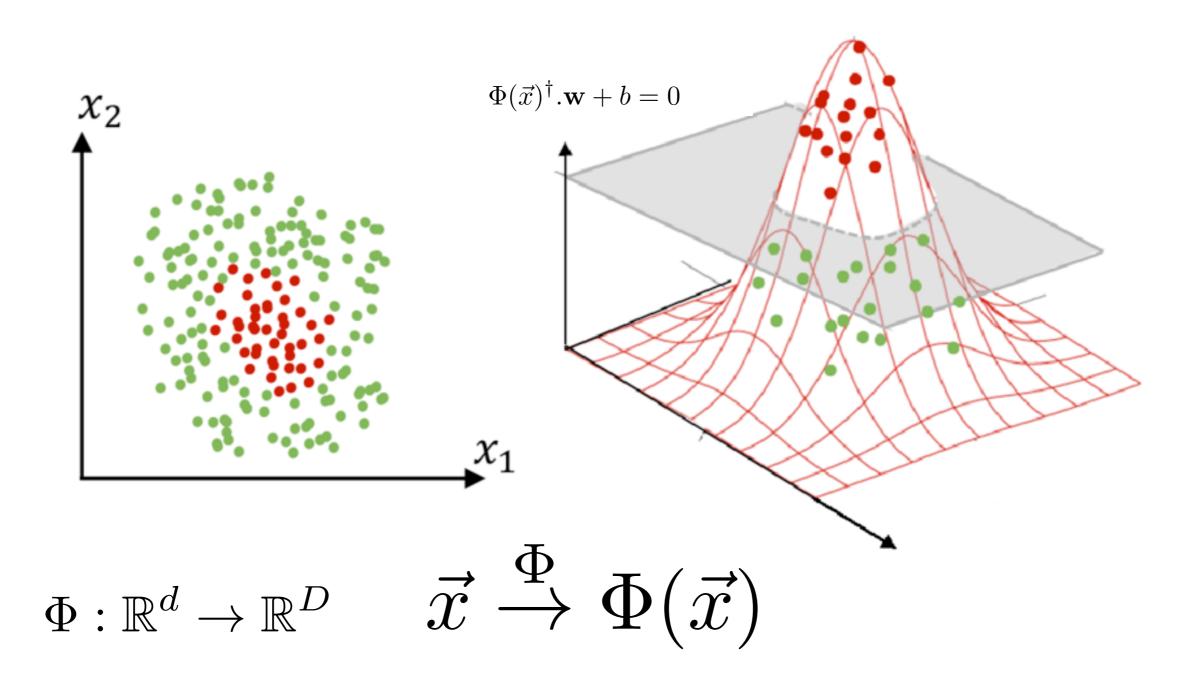
NB: almost true: SVMs is "optimized" to be able to reason about learning performance...

Why should we care about SVMs: what about when data is **not** linearly separable?



Non-separable datasets?

- -slack variables (this lead to QSVM type 1)
- -feature mapping and the kernel trick



c.f.: Cover's theorem...

one can "train" and evaluate SVM classifiers in rich feature spaces without ever mapping data-points into said spaces. They can even be infinite dimensional

Note: in dual... only inner products matter

$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle \ (\phi = \Phi...)$$

$$\underset{\alpha}{\operatorname{arg\,max}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j(\mathbf{x}_i)^{\mathsf{T}} \mathbf{x}_j,$$

$$\underset{\alpha}{\operatorname{arg\,max}} \ \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$$

=
$$\underset{\alpha}{\operatorname{arg\,max}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \ K(\mathbf{x}_i, \mathbf{x}_j)$$

Note: in dual... only inner products matter

$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle \ (\phi = \Phi...)$$

$$\underset{\alpha}{\operatorname{arg\,max}} \ \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j(\mathbf{x}_i)^{\mathsf{T}} \mathbf{x}_j,$$

BTW: this thing is called "the kernel"

Note, we really don't care about the feature map $\,\Phi$ itself...

 $|\mathsf{x}_i),\phi(\mathsf{x}_i)
angle$

Kernels can <u>sometimes</u> be evaluated (much) more efficiently directly:

$$(x_1, x_2, x_3) \mapsto \phi(\mathbf{x}) = (x_1x_1 \quad x_1x_2 \quad x_1x_3 \quad x_2x_1 \quad x_2x_2 \quad x_2x_3 \quad x_3x_1 \quad x_3x_2 \quad x_3x_3)^\mathsf{T}$$

$$\langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle = \sum_{i=1}^{d} \sum_{j=1}^{d} x_i z_i x_j z_j$$
 Runtime for $\phi(\mathbf{x})$: $\mathcal{O}(d^2)$

$$\phi(\mathbf{x}) = \begin{pmatrix} x_1 x_1 & x_1 x_2 & x_1 x_3 & x_2 x_1 & x_2 x_2 & x_2 x_3 & x_3 x_1 & x_3 x_2 & x_3 x_3 \end{pmatrix}^{\mathsf{T}}$$

reverse-engineered:
$$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^{\mathsf{T}} \mathbf{z})^2 = \left(\sum_{i=1}^d x_i z_i\right) \left(\sum_{i=1}^d x_i z_i\right) = \sum_{i=1}^d \sum_{j=1}^d x_i z_i x_j z_j = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle.$$

Directly:

Let
$$\mathbf{x} = (x_1, ..., x_d)^{\mathsf{T}}$$
, $\mathbf{z} = (z_1, ..., z_d)^{\mathsf{T}}$ and

$$K(\mathbf{x},\mathbf{z}) = (\mathbf{x}^{\mathsf{T}}\mathbf{z})^2$$
.

Runtime: $\mathcal{O}(d)$.

Yay, quadratic speedup

See e.g. Radial basis function kernel

$$K(\mathbf{x},\mathbf{x}') = \exp\!\left(-rac{\|\mathbf{x}-\mathbf{x}'\|^2}{2\sigma^2}
ight)$$

$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle$$

$$\Phi(x) = e^{-x^2/2\sigma^2} \left[1, \sqrt{\frac{1}{1!\sigma^2}} x, \sqrt{\frac{1}{2!\sigma^4}} x^2, \sqrt{\frac{1}{3!\sigma^6}} x^3, \dots \right]^T$$

inf. dim.....

c.f. Mercer's theorem

To keep in mind:

-primal v.s. dual:

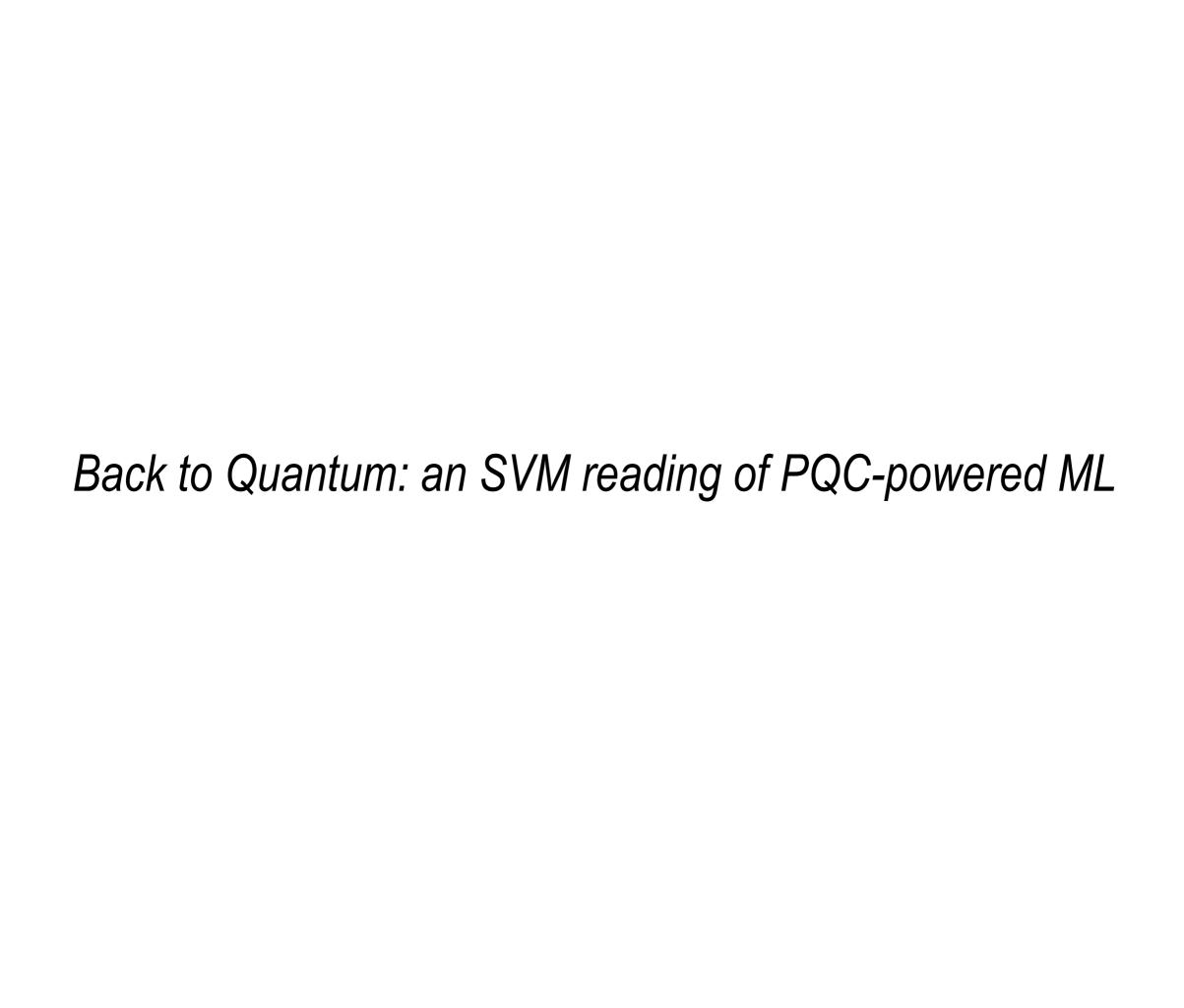
in <u>primal</u>, optimize over normal vector **explicitly**; in <u>dual</u>, it is implicit, and the separating hyperplane is expressed in terms of data points

-feature maps:

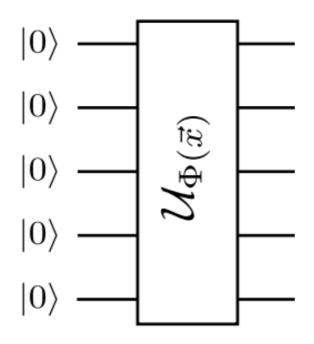
by raising dimension non-linearly, we can achieve linear-separability

-kernel trick:

in dual formulation, only need kernel evaluation on data points for training.



Basic idea: quantum computing offers interesting "natively quantum" feature maps and kernels

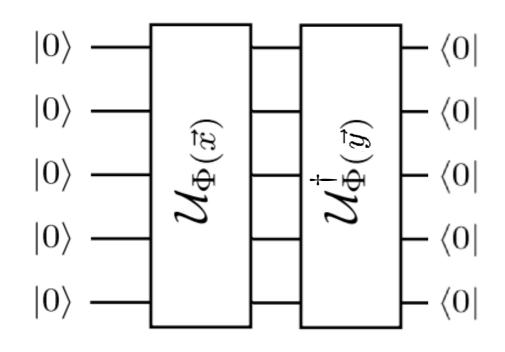


$$\vec{x} \mapsto \mathcal{U}_{\Phi}(\vec{x})|0\rangle = |\Phi(\vec{x})\rangle$$

Data is encoded in the circuit parameters (not input state). More general.

Basic idea: quantum computing offers interesting "natively quantum" feature maps and kernels

One thing we can do with this... is evaluate inner products.



But we can do more

Kernel!

$$|\langle \Phi(\vec{y})|\Phi(\vec{x})\rangle|^2$$

Can be hard to compute.

Do this quantumly (recall QC is good for inner products) also possible: swap tests, hadamard tests

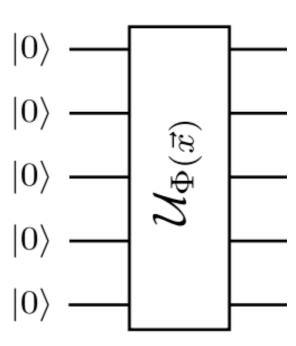
Which feature maps should we construct?

$$U_{\Phi(\vec{x})} = \exp\left(i\sum_{S\subseteq[n]} \phi_S(\vec{x}) \prod_{i\in S} Z_i\right)$$

$$\phi_{\{i\}}(\vec{x}) = x_i \text{ and } \phi_{\{1,2\}}(\vec{x}) = (\pi - x_1)(\pi - x_2)$$

$$e^{i\phi_{\{l,m\}}(\vec{x})Z_lZ_m} = \boxed{\mathbb{Z}_{\phi}}$$

$$\mathcal{U}_{\Phi} = H^{\otimes n} U_{\Phi} H^{\otimes n} U_{\Phi} \cdots H^{\otimes n} U_{\Phi}$$



Which feature maps should we construct...elaborated

- DIMENSION OF FEATURE SPACE = 2 ; # QUBITS = N = INITIAL DIMENSION

• DEFINE "SUBMAPS" ϕ_S S=-individual vector entries; $S \in \{1...N\}$ - Paivs; .-- can be generalized

= correlators (2 or k-local)

φs: Ror R² → "angles"

$$\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
\vdots \\
x_n
\end{bmatrix}
\Rightarrow \phi_s \Rightarrow \theta \Rightarrow \exp\left(i \quad 2_1 \otimes 2_3 \quad \theta\right)$$

$$\begin{matrix}
V_s \quad (\vec{x}) \\
\end{matrix}$$

- $\bigcup \phi(\vec{x}) := \prod \bigcup_{s} (\vec{x})$ All DIAGONAL__
- · FEATURE MAP : U = (HON U(x))

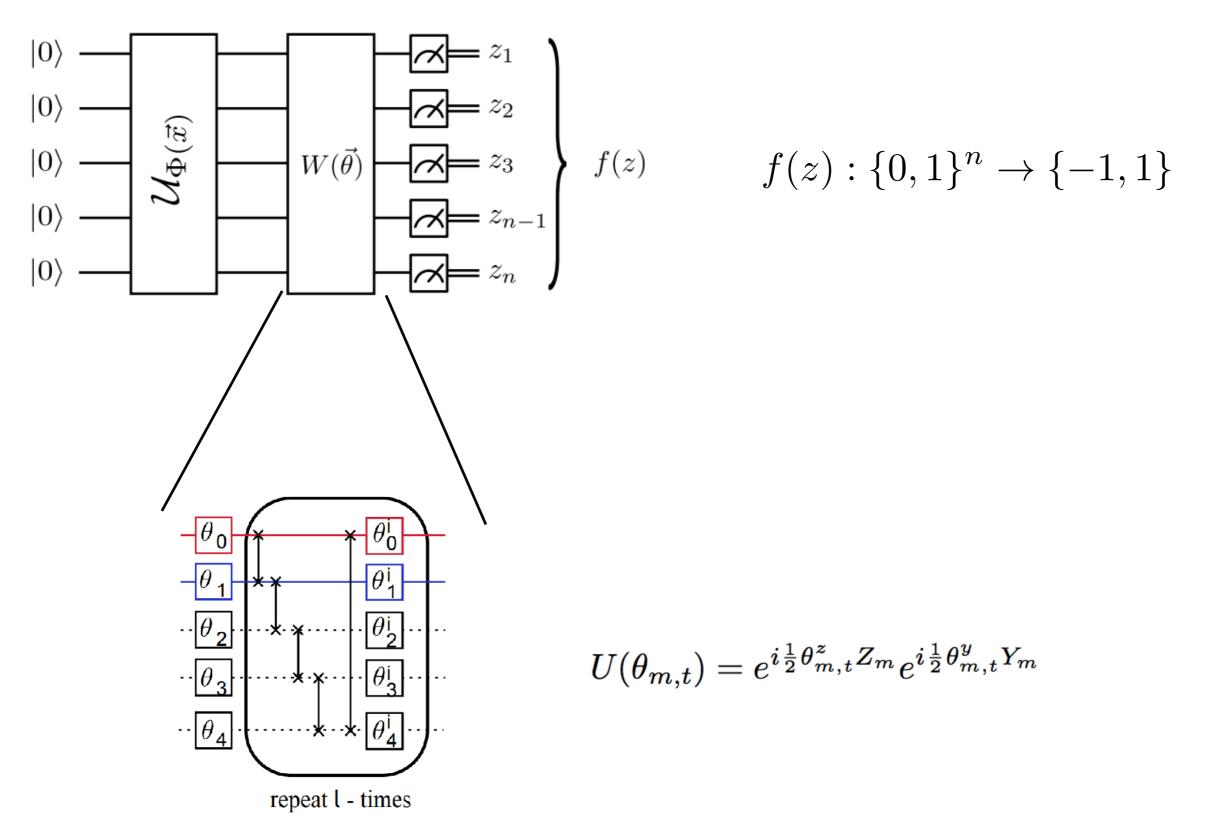
First type of PQC SVM: implicit (dual) model

classifying:
$$out(\mathbf{x}) = sign\left(\sum_{i=1}^{N} y_i \alpha_i^* K(\mathbf{x}_i, \mathbf{x}) + b\right)$$

Quantum parts: needed in both to evaluate the kernels only offline; optimization essentially on classical data.



Fully quantum model: explicit (primal) model



How does it output a label? What is the achieved classfier?

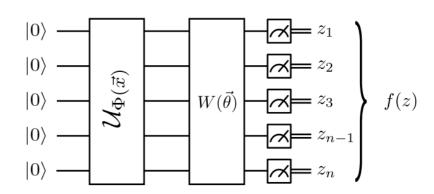
The label (output): (approximately) sign of the expected value f, shifted by b:

$$out(\mathbf{x}, \theta) \approx sign(\mathbb{E}_{z \sim Q.circ}[f(z)] + b)$$

$$out(\mathbf{x}, \theta) \approx \operatorname{sign}(\langle \Phi(\vec{x}) | W^{\dagger}(\vec{\theta}) \mathbf{f} W(\vec{\theta}) | \Phi(\vec{x}) \rangle + b)$$

The algorithm:

- -sample z many times ("shots")
- -average, shift, compute sign.



Comment:

$$out(\mathbf{x},\theta) \approx sign(\mathbb{E}_{z\sim Q.circ}[f(z)] + b)$$

$$out(\mathbf{x},\theta) \approx sign(\langle \Phi(\vec{x}) | W^{\dagger}(\vec{\theta}) \mathbf{f} W(\vec{\theta}) | \Phi(\vec{x}) \rangle + b)$$
 "measure each qubit in comp basis, compare $\{(\vec{z})^{\dagger} = \text{observable}\}$
$$\mathbf{f} := \sum_{\vec{z}} \{(\vec{z}) | \vec{z} \times \vec{z} \}$$

"measure each qubit in comp basis, compute $f(\tilde{z})$ ":= a realization of measurement of $f(\tilde{z})$. Averaging yields the expected value.

How does it learn?

Optimize θ to minimize some loss/error/empirical risk on dataset

Involves evaluation of classifier function many times...

Often: stochastic gradient descent

Q. chemistry optimization and optimization here very similar

But what does it do?

SUM CLASJIFIER: Sign
$$(\vec{n}, \vec{x} + b)$$

HERE: SIGN $(\langle \phi(x) | W^{\dagger}(\theta) | \phi(x) \rangle + b)$

inner product?

 $(\langle \phi(x) | W^{\dagger} | \psi(x) \rangle) = \text{Tr}[\underline{W^{\dagger} | \psi(x) \rangle} | \psi(x) | \psi(x$

$$|out(\vec{x}) = sign(\vec{w}, \vec{\phi}(\vec{x}) + b)$$

the feature space is that of density operators...

Nature. vol. 567, pp. 209-212 (2019) arxiv:1804.11326. p.g. 12.

What does it do?

$$\left[\vec{\mathbf{w}}\left(\mathbf{\theta}\right)\right] = \operatorname{tr}\left[W^{\dagger}(\vec{\theta})\mathbf{f}W(\vec{\theta})P_{\alpha}\right]$$

$$\left[\vec{\Phi}(\vec{\mathbf{x}})\right]_{\mathbf{x}} = \left\langle \Phi(\vec{x}) \left| P_{\alpha} \right| \Phi(\vec{x}) \right\rangle$$

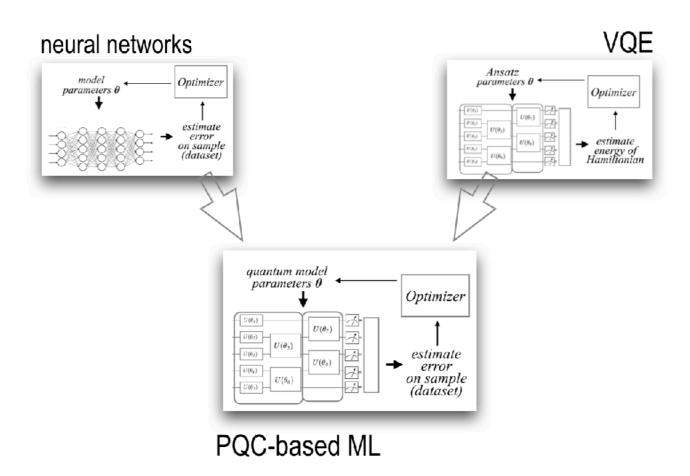
$$out(\vec{\mathbf{x}}) \approx sign(\vec{w} \cdot \vec{\Phi}(\vec{\mathbf{x}}) + b)$$

-limitations on the model come into play here...
-not *all hyperplanes* reachable...

-not maximal margin attained!

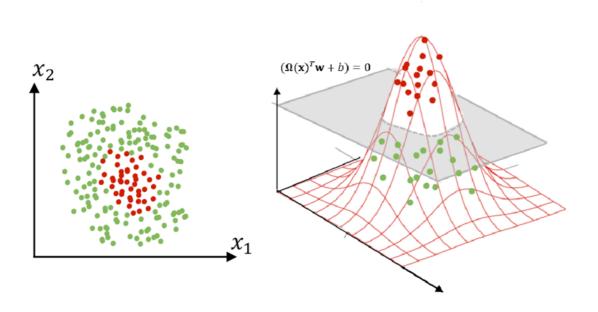
BECAUSE W(B) & ARE RESTRICTED.

Note the explicit model is much like training a NN/VQE

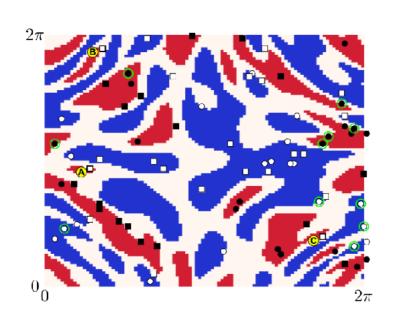


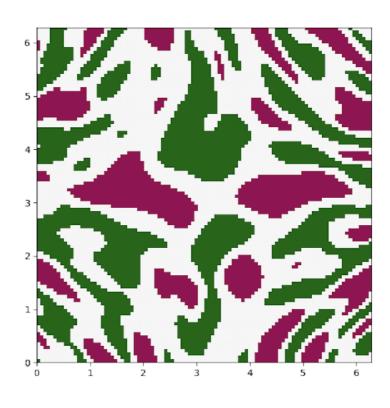
-but with a connection with a well-understood classical model

Illustration of quantum decision boundaries



Two slices of quantum kernels:





-for quantum advantage: useful and classically hard

-for advantage for near-term quantum: useful and doable

-for quantum advantage: useful and classically hard

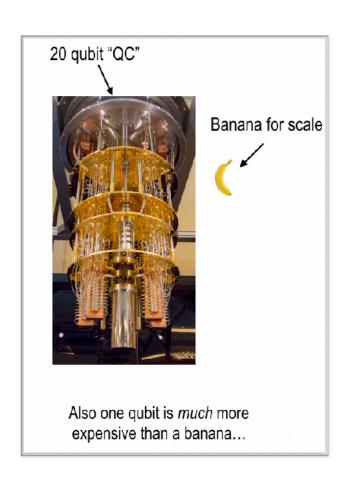
-useful: remains to be seen;

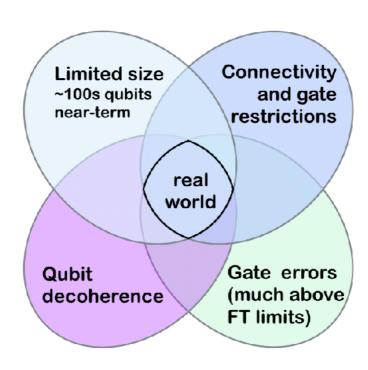
- almost all models useful in some settings;
 here when data has complex correlations.
- Bleeding edge reasearch:
- theory for ML is difficult;
- QCs just becoming large enough for experiments

-for quantum advantage: useful and classically hard

- -classically hard:
 - trivially there exist "BQP-hard" kernels (for deep circuits)
 - for "functional problems" no hard separation results but; very likely hard.
 - more interestingly; likely hard in shallow circuit regime

-for advantage for near-term quantum: useful and doable

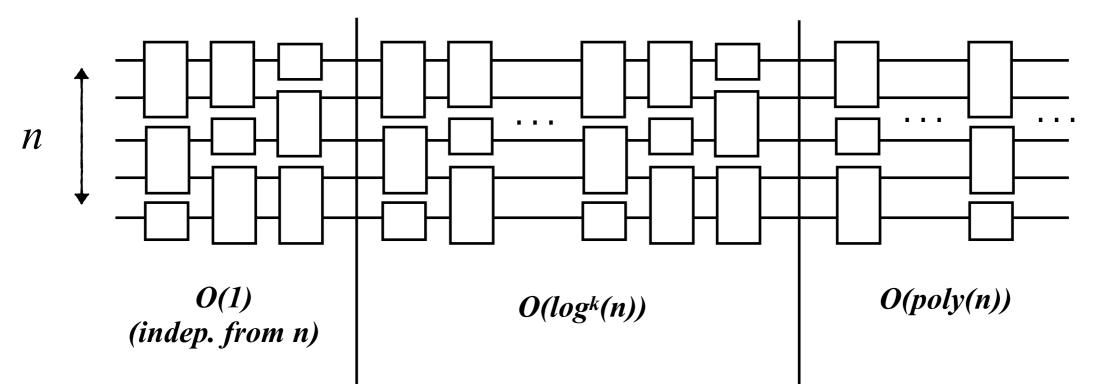




doable: makes sense with: ~100 qubits, limited depth, errors

- 1) ~100 qubits probably yes 2^{100} is interesting
- 2) depth?
- 3) noise?

Recall Quantum depth complexity



- -better than *classical* const depth for relational problems
- -*likely* better for sampling problems, <u>no matter what</u> depth of classical computer
- -NOT better than CC for decision problems

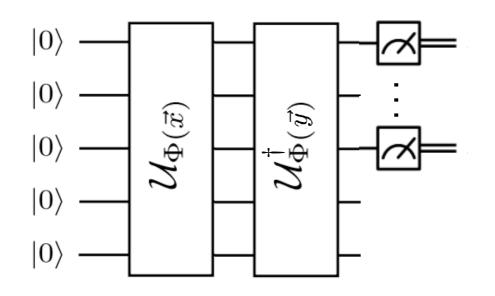
Hard part of Shor's algo.

Ground states

of complex systems in polytime (multi-scale entanglement renormalization ansatz)

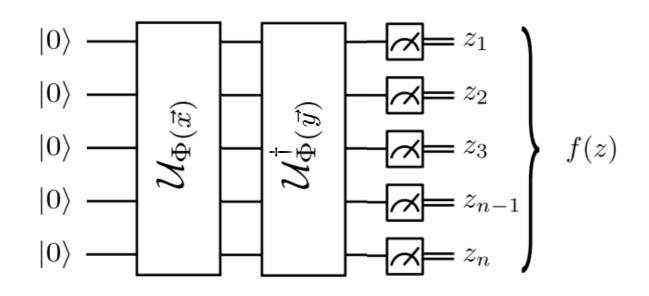
"BQP" = full QC

can we have limited depth and classically hard?



Lm: full exact simulation of output of **log-many qubits** in constant depth, can be done in poly-time

This is the situation in chemistry with log-local Hamiltonians - depth must be at least log.



Not log-many! No known efficient classical algorithm

- 1) ~100 qubits **√**
- 2) depth ✓
- 3) noise?

Reasons for optimism:

- a) ML as signal-from-noise + source shifting
- b) stochastic hypothesis families and noisy data (distinct from mathematical optimization)
- c) brains are noisy:)