Learning with quantum kernels: early applications to material damage prediction

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Quantum machine learning

Some informal definitions

Quantum-enhanced machine learning

Quantum computation to speed-up classical machine learning operations.

Example: SVM with quantum linear systems solver algorithm

Machine learning in quantum feature spaces

Information is *encoded* into quantum states and classical algorithms find the optimal model

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Note: not all quantum machine learning is done on quantum computers. QML can also mean to use classical machine learning for quantum mechanics.

Quantum machine learning in the near term

Quantum-enhanced ML gives provable speed-up, but requires **fault-tolerant hardware**. However . . .

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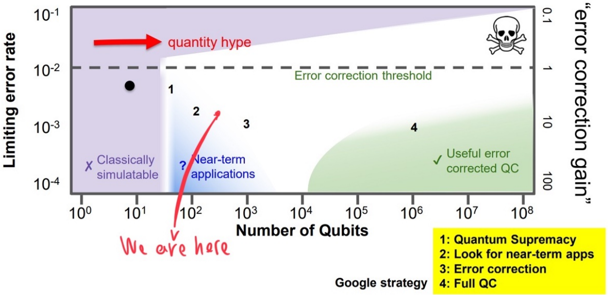

Source: https://www.hpcwire.com/2018/04/26/google-frames-quantum-race-as-two-dimensional/

Quantum-enhanced ML is not viable in the near term.

ML in quantum feature spaces

Can we learn data patterns that are *hard to learn classically*?

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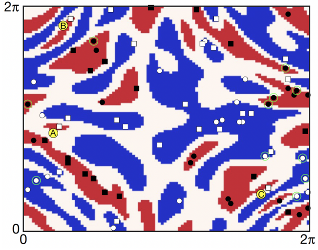
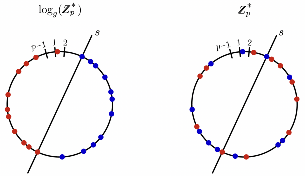


Source: Havlicek *et al.*, 2019, Nature Physics

Data generated from a 'quantum model' such to be hard to access classically.



Source: Liu *et al.*, 2020, arXiv:2010.02174

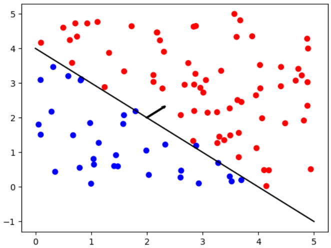
Data labelled by discrete loagarithm over a group generated by a large prime number.
Classically hard to compute, but efficient with Shor's quantum algorithm.

ML in quantum feature spaces

Are there *real world* datasets that are classically hard to classify, but 'understandable' for quantum computers?

Maximum margin classifier

Assume that the data is linearly separable (perhaps with some noise)



Model:

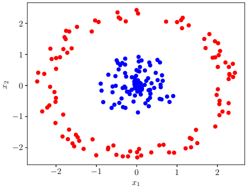
$$y = \operatorname{sgn}\left(\langle \mathbf{w}, \mathbf{x} \rangle + b\right)$$

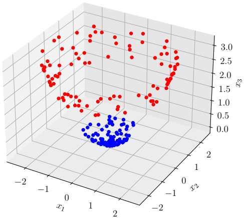
Support vector machine, primal form (*maximum geometric-margin classifier*)

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{s.t.} \quad & y^{(i)}\left(\mathbf{w}^\top \mathbf{x}^{(i)} + b\right) \geq 1, \quad i = 1, \dots, m \end{aligned}$$

Maximum margin classifier

What if the data is *not* linearly separable? We can introduce a feature map $\phi(x)$





$$\xrightarrow[\phi(x)=\left\{x_1, x_2, 0.5\left(x_1^2+x_2^2\right)\right\}]{\qquad\qquad\qquad}$$

Model: $y = \operatorname{sgn}\left(\langle \mathbf{w}, \phi(\mathbf{x})\rangle + b\right)$

Kernels

Representer theorem

The vector that expresses the optimal separating hyperplane in feature space is a linear combination of feature vectors.

$$\mathbf{w} = \sum_{i=1}^{N' \leq N} \alpha_i \phi\left(\mathbf{x}_i\right)$$

Kernels

Representer theorem

The vector that expresses the optimal separating hyperplane in feature space is a linear combination of feature vectors.

$$\mathbf{w} = \sum_{i=1}^{N' \leq N} \alpha_i \phi\left(\mathbf{x}_i\right)$$

So we can rewrite our model as

$$y = \operatorname{sgn}\left(\sum_{i=1}^{N' \leq N} \alpha_i \langle \phi\left(\mathbf{x}_i\right), \phi\left(\mathbf{x}\right) \rangle + b\right),$$

which is *linear in the feature space*.

The quantity $k\left(\mathbf{x}, \mathbf{x}'\right) = \langle \phi\left(\mathbf{x}\right), \phi\left(\mathbf{x}'\right) \rangle$ is called the *kernel* induced by the feature map ϕ.

Kernel trick

If we find an efficient explicit formula for the kernel, we don't need to compute the feature map directly and we can *implicitly* compute distances and classify in the feature space.

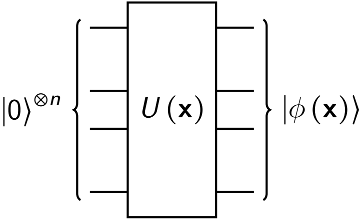
Example: quadratic kernel

$$
\begin{aligned}
\mathbf{x} &= \left(x_1,\, x_2\right)^{\top} \\
\phi\left(\mathbf{x}\right) &= \left(x_1^2,\, \sqrt{2}x_1x_2,\, x_2^2\right)^{\top} \\
k\left(\mathbf{x}, \mathbf{x}'\right) &= \left\langle \phi\left(\mathbf{x}\right),\, \phi\left(\mathbf{x}'\right)\right\rangle \\
&= \left(x_1x_1' + x_2x_2'\right)^2 \\
&= \left\langle \mathbf{x},\, \mathbf{x}'\right\rangle^2
\end{aligned}
$$

i.e. the kernel can be computed in the original space of data.

Quantum kernels

In terms of quantum states, we can encode $\mathbf{x}$ into a unitary operator $U(\mathbf{x})$. This creates $|\phi(\mathbf{x})\rangle = U(\mathbf{x})|0\rangle$



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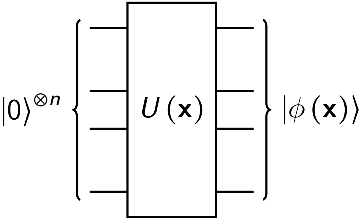
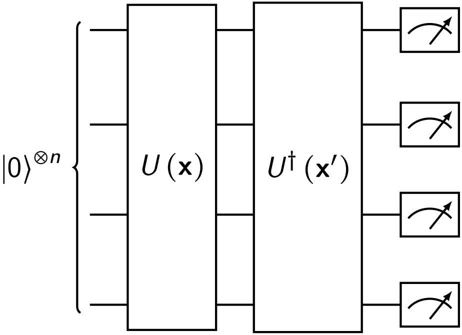
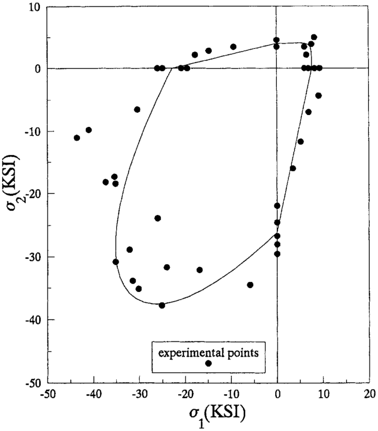


Defining $\rho(\mathbf{x}) = |\mathbf{x}\rangle\langle\mathbf{x}'|$, the *quantum kernel* $k(\mathbf{x},\mathbf{x}') = \mathrm{Tr}\{\rho(\mathbf{x})\rho(\mathbf{x}')\}$ implicitly accesses the 4^n-dimensional complex space



Material damage prediction

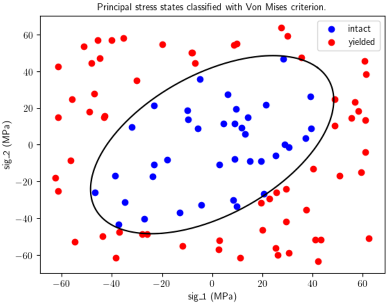
- Failure criteria are models of material failure. They generally come from semi-empirical relations (data + physics)
- They are effectively *classification problems*, where the decision boundary is the *failure envelope*



Source: Echaabi *et al.*, 1996, Polymer Composites

Von Mises criterion

A `hello, world!` example in material damage prediction



$$\sigma_1^2 + \sigma_2^2 - \sigma_1 \sigma_2 - \sigma_y^2 = 0$$

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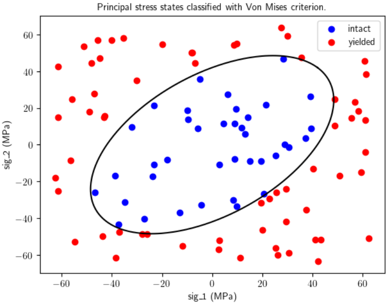

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'Analytic' feature map and kernel:

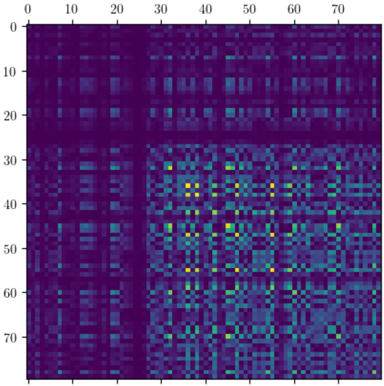
$$\phi(\mathbf{x}) = \left(x_1^2, x_2^2, x_1 x_2\right)^\top$$
$$k\left(\mathbf{x}, \mathbf{x}'\right) = \langle \phi(\mathbf{x}), \phi\left(\mathbf{x}'\right) \rangle$$

Von Mises criterion

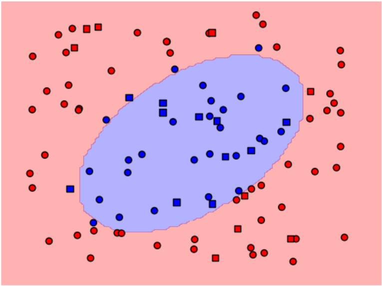
Classification with classical quadratic kernel

$$k(\mathbf{x}, \mathbf{x}') = \left(\gamma \langle \mathbf{x}, \mathbf{x}' \rangle + r\right)^2$$

Kernel matrix



Failure envelope



Von Mises criterion

Using a quantum 'quadratic' kernel

Strictly speaking, if we 'simply' encode **x** as the quantum state $|x\rangle$, it seems that we recover the quadratic kernel.

$$\phi\left(\mathbf{x}\right) = |x\rangle \longrightarrow k\left(\mathbf{x}, \mathbf{x}'\right) = \left|\mathbf{x}^{\dagger}\mathbf{x}'\right|^{2}$$

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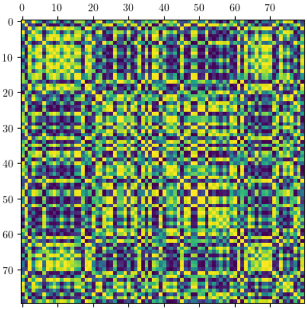
However, the kernel matrix does not show any class separation...



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Reason: normalization in the original feature space confuses the data

$$\phi\left(\mathbf{x}\right) = \left(x_1, x_2\right) / \|\mathbf{x}\|$$

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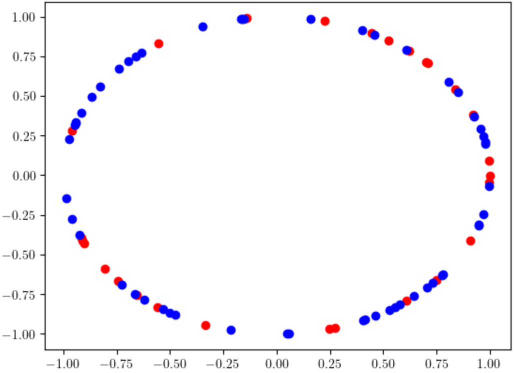
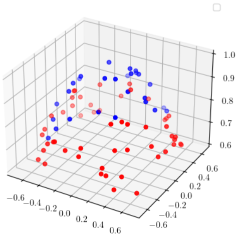


Von Mises criterion

Using the same kernel in a 4-dimensional space of unit vectors

Hack: add a 3rd dimension and normalize on a semi-sphere.

$$\phi(\mathbf{x}) = (x_1, x_2, 1, 0)^\top / \|\mathbf{x}\|$$



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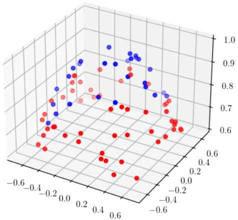
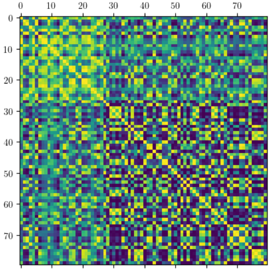
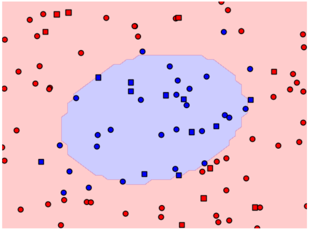






Von Mises criterion

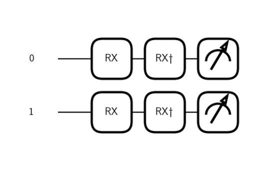
Rotation encoding kernels

Can we do better and avoid feature pre-processing that can confuse the label spaces?

Rotation encoding

Encode every feature as the rotation angle of a gate.

$$\phi(\mathbf{x}) = R(x_1) \otimes R(x_2) |0\rangle^{\otimes 2}$$



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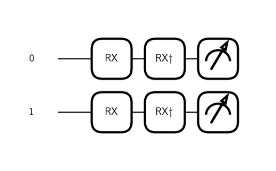

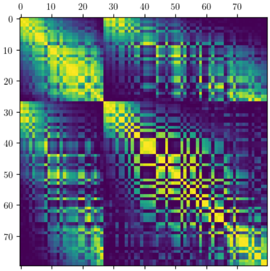

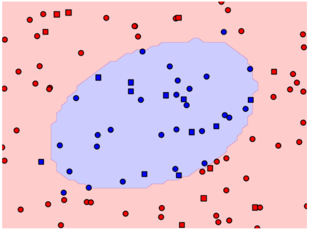

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1. It provides a reality-based example to compare the accuracies of classical and quantum kernels.
2. It highlights the key aspects of data encoding in quantum states
   - normalization
   - data scaling
   - data dimensionality

Where to go from here

- Study more complex datasets, where the 'ground truth' is unknown
  - Experimental data
  - Numerical, high-fidelity data

[1] La Rocca *et al.*, 2022, PRX Quantum

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- Further investigate near-term encodings for damage prediction
  - In particular, quantum kernels generated by Hamiltonian evolution ($e^{iH\mathbf{x}}$) correspond to Fourier series in the data

$$k(\mathbf{x}, \mathbf{x}') = \sum_{\mathbf{n}, \mathbf{n}' \in \Omega} c_{\mathbf{n}, \mathbf{n}'} e^{i\mathbf{n}\mathbf{x}} e^{i\mathbf{n}'\mathbf{x}'}$$

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- Encode problem knowledge in the circuit to have control over the c_{n_i, n_j} coefficients
  - e.g. encoding symmetries [1]

[1] La Rocca *et al.*, 2022, PRX Quantum

Thank you!

Dual formulation of the maximum margin classifier

$$\begin{aligned}
\max_{\alpha} \quad & C(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\
\text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, m \\
& \sum_i \alpha_i y^{(i)} = 0
\end{aligned}$$

Classical kernels

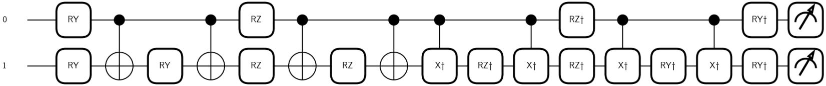
Name	Expression
polynomial	$(\gamma\langle \mathbf{x}, \mathbf{x}' \rangle + c_0)^d$
sigmoid	$\tanh(\gamma\langle \mathbf{x}, \mathbf{x}' \rangle + c_0)$
RBF	$\exp\left(-\gamma\|\mathbf{x} - \mathbf{x}'\|^2\right)$

Table: Some popular kernels

Amplitude encoding circuits

1 qubit

2 qubits



Single rotation kernel encoding for 2 qubits

$$k\left(\mathbf{x}, \mathbf{x}'\right) = \prod_{i=1}^{N} \cos\left(x_i - x_i'\right)$$

With 2 features ($\mathbf{x} = \left(x_1, x_2\right)^\top$),

$$k\left(\mathbf{x}, \mathbf{x}'\right) = \cos\left(x_1 - x_1'\right) \cos\left(x_2 - x_2'\right)$$

Substitute $z_i = \left(x_i - x_i'\right)$ and Mc Laurin expand

$$\begin{aligned} k\left(\mathbf{x}, \mathbf{x}'\right) &\approxeq \left(1 - \frac{1}{2} z_1^2\right)\left(1 - \frac{1}{2} z_2^2\right) \\ &= 1 - \frac{1}{2} z_2^2 - \frac{1}{2} z_1^2 + \frac{1}{4} z_1^2 z_2^2 \\ &= \dots \end{aligned}$$

Re-substituting $\mathbf{x}$, $\mathbf{x}'$, one finds $x_i^2 x_i'^2$ and $x_i x_j x_i' x_j'$ terms as in the classical quadratic kernel, as well as additional 4$^{\text{th}}$ order terms in the features.