QTML 2024, 25.11.2024

Mach. Learn.: Sci. Technol. **5** 025003

On the expressivity of embedding quantum kernels

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1. Quantum Machine Learning (QML)

Quantum model

+

Classical data

+

Classical training algorithm

2. Expressivity

Today: is there more to quantum kernels?

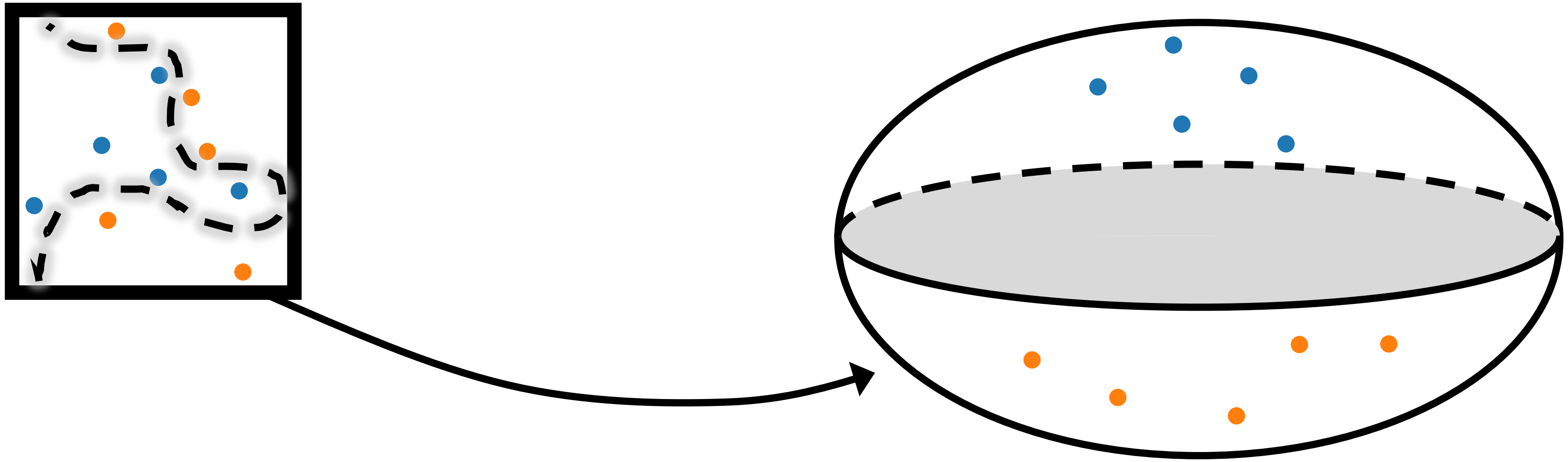
- Quantum kernels beyond the canonical approach?
- What is ultimately possible with quantum kernel methods?

Not today:

- How can I solve cool QML problems?
- How do kernel methods work?

3. Kernel methods

Linear optimization on a feature space:

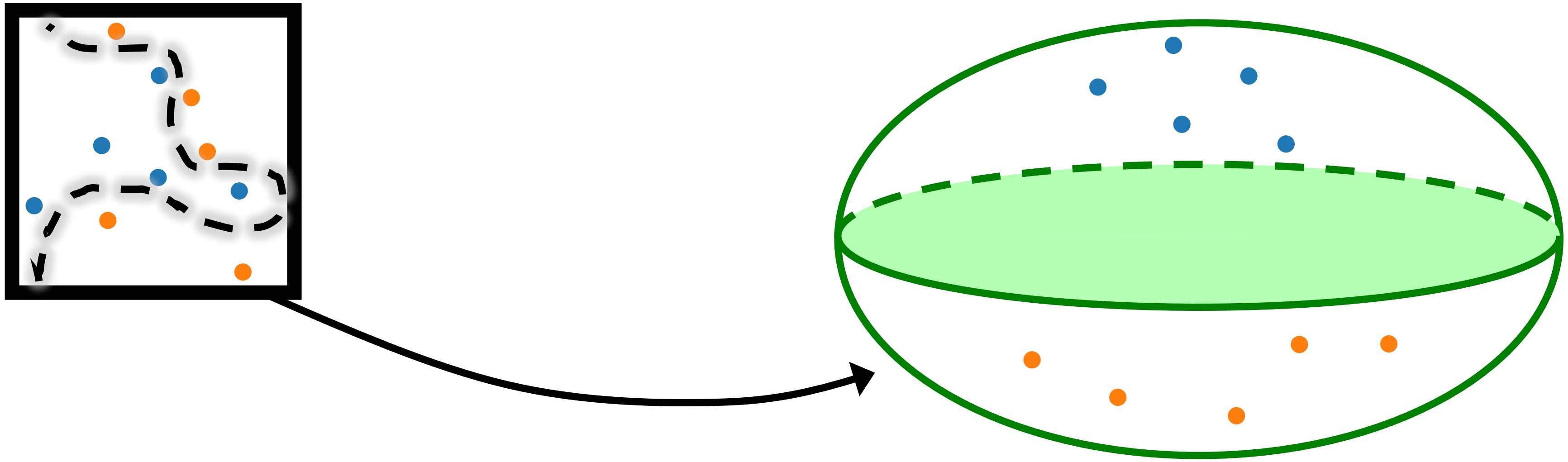


"A kernel is an inner product of feature vectors"

Hubregtsen et al, *PRA* **106** (2022)
Schuld, *2101.11020* (2021)

4. Embedding Quantum Kernels (EQKs)

Linear optimization on quantum feature space:

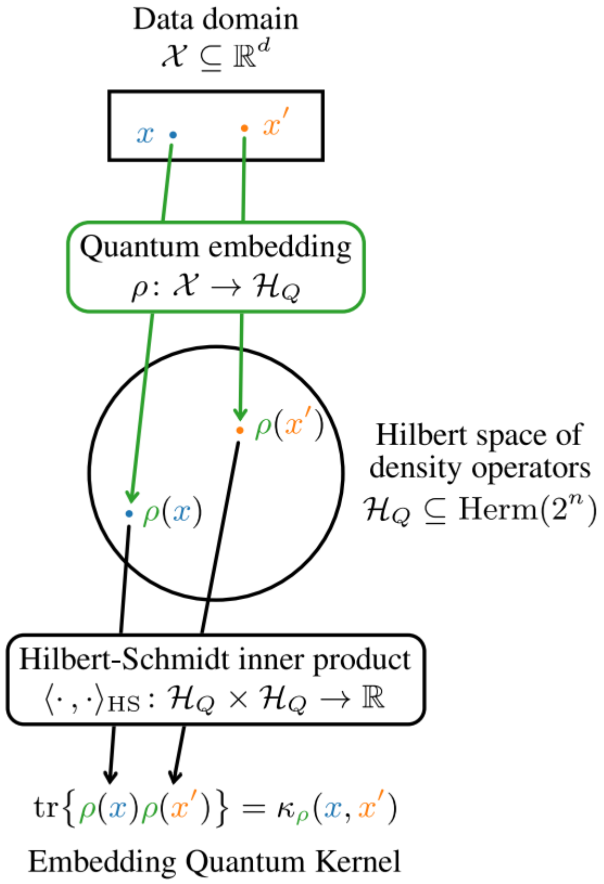


"An Embedding Quantum Kernel is an inner product of quantum feature vectors"

Jerbi et al., *Nat. Comm.* 14 (2023)
GF, Eisert, Dunjko, *MLST.* 5 (2024)

5. Quantum feature maps

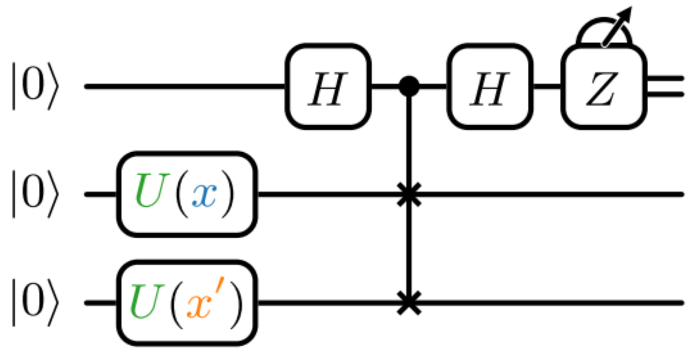
The mathy picture:

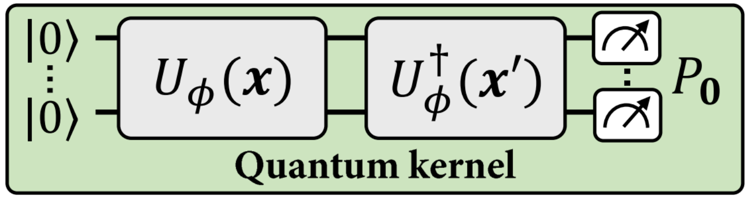


The quantum computer:

$$\rho(x) = U(x)|0\rangle\langle 0|U^\dagger(x)$$

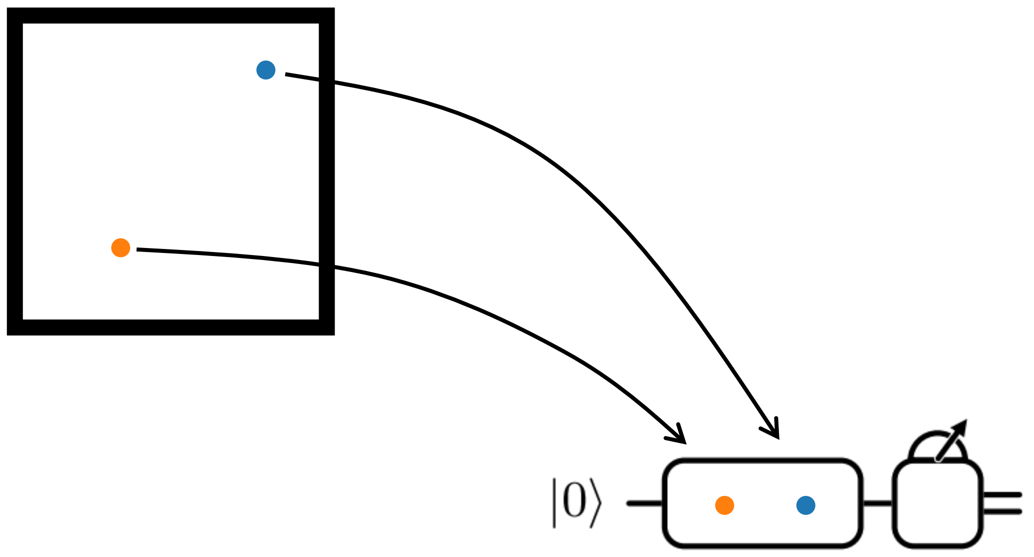
$$\mathrm{tr}\{\rho(x)\rho(x')\}$$





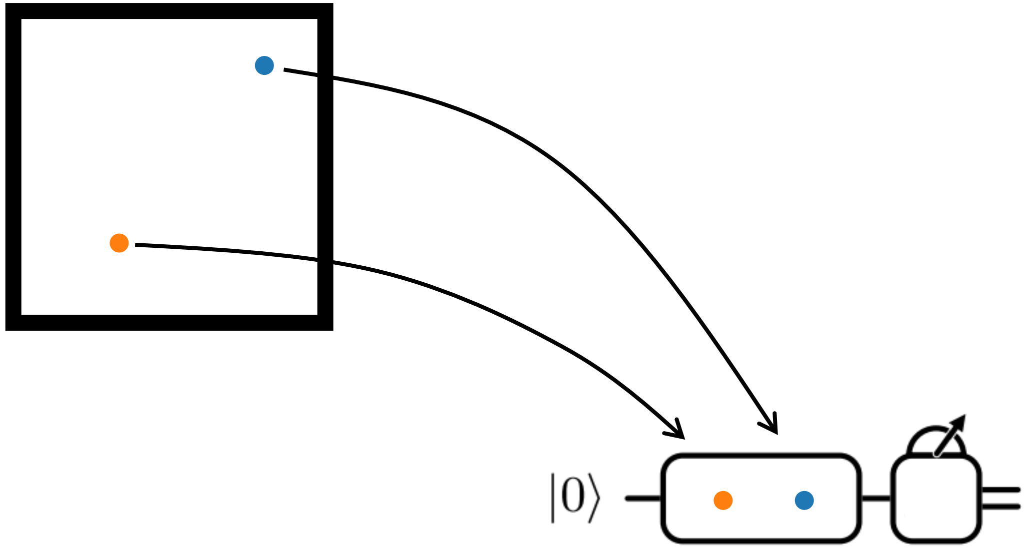
6. Quantum functions

Prepare and measure:

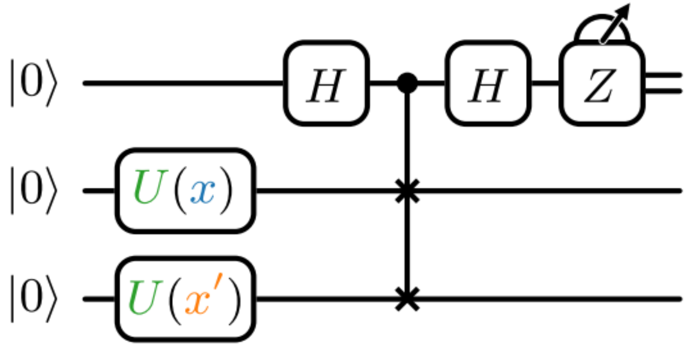


6. Quantum functions

Prepare and measure:

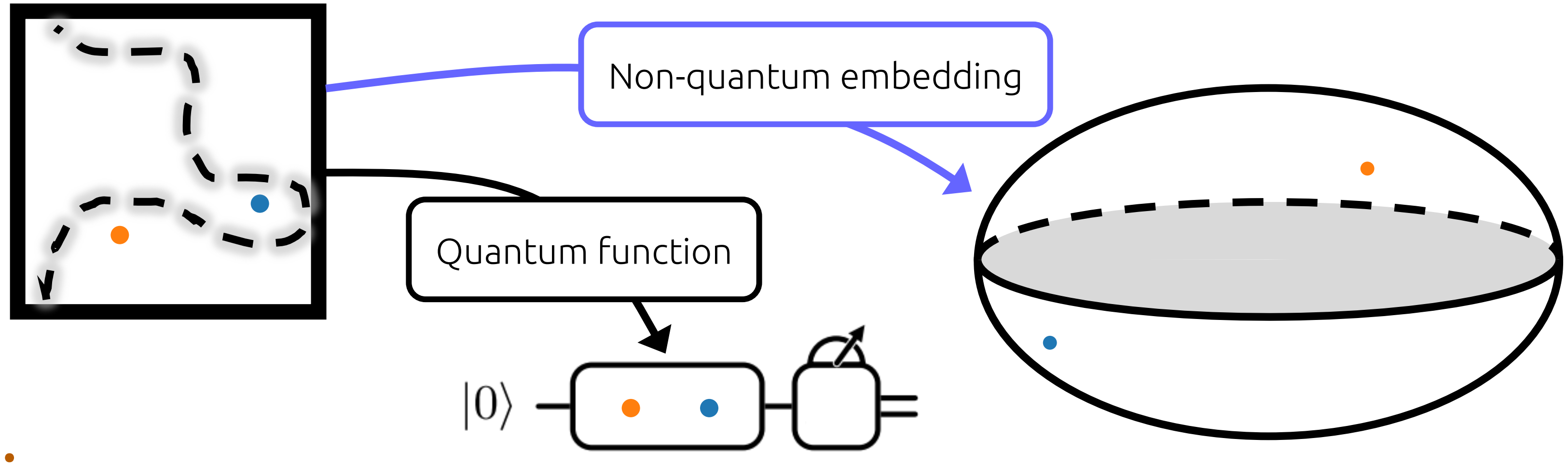


For instance: Embedding Quantum Kernel



7. non-Embedding Quantum Kernels?

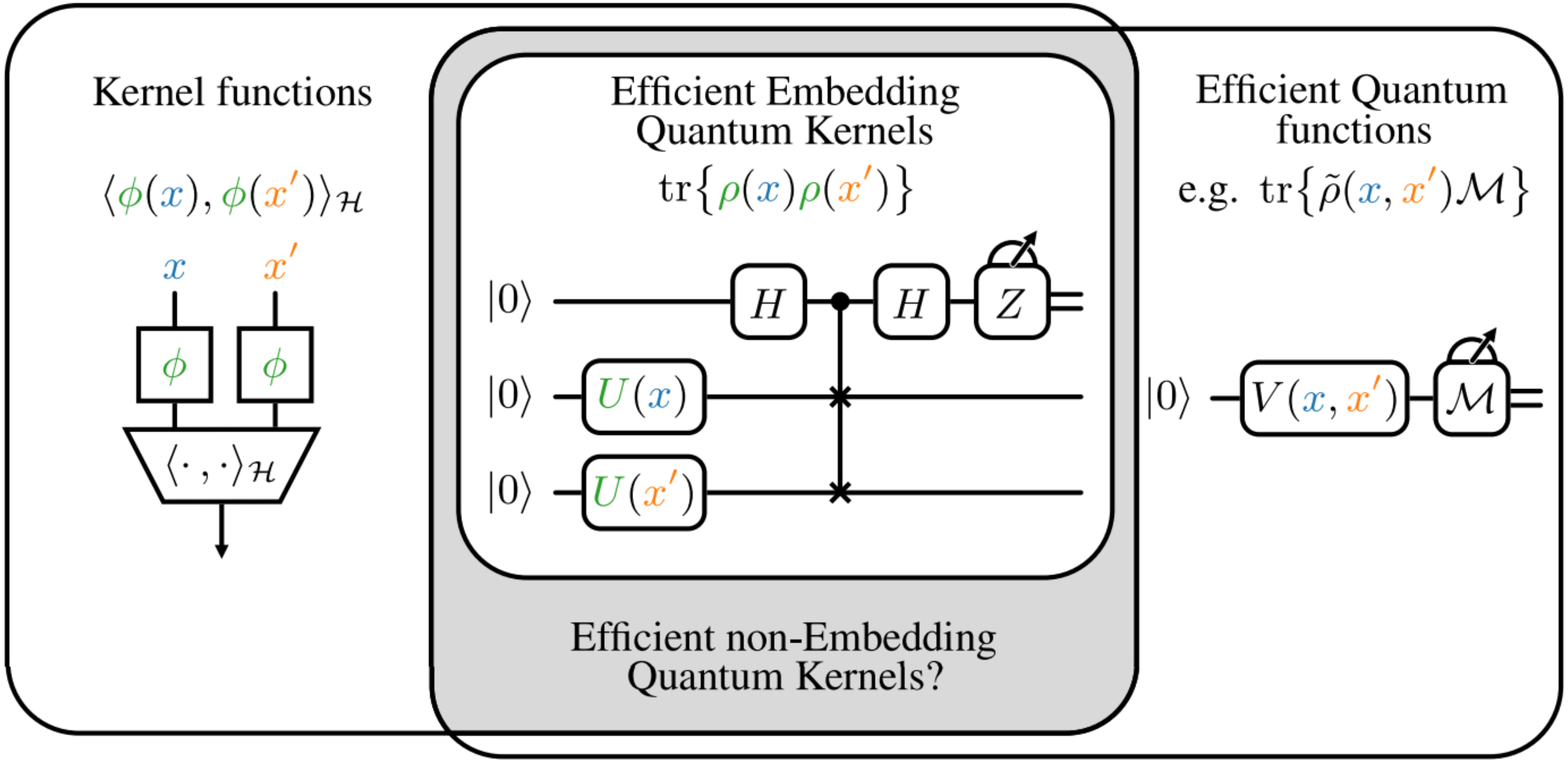
Question: what would a non-EQK look like?



Answer:

1. The feature map is a “non-quantum embedding”.
2. The kernel function is still a quantum function.

8. Our question



9. Our contribution

Hypothesis:

Embedding Quantum Kernels (EQKs) are very expressive.

Test:

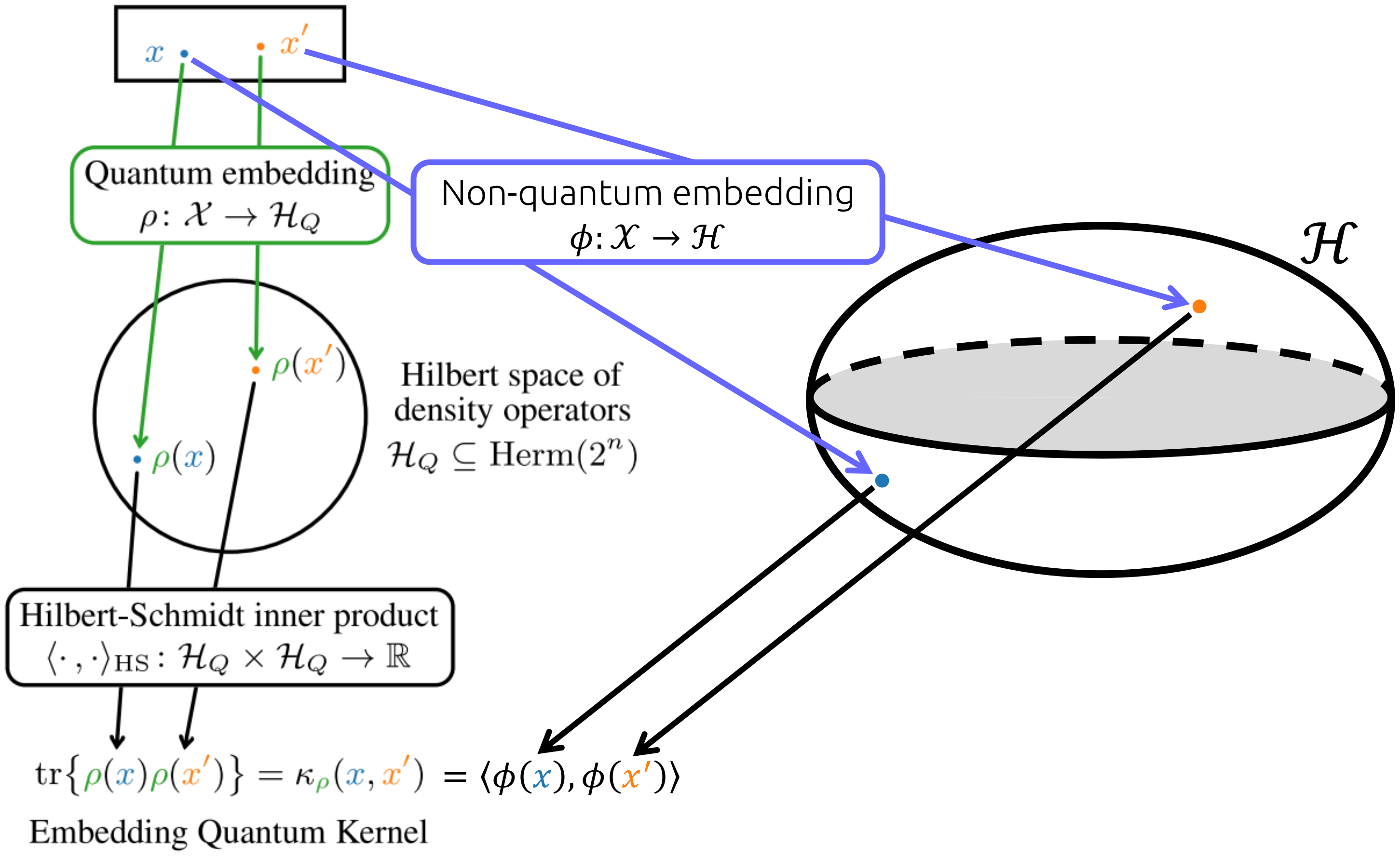
"Take a kernel, can it be expressed as an EQK?"

Results:

"EQKs are universal for important families of kernel functions".

10. non-EQKs can also be EQKs

Things aren't always what they seem!



11. Theorems

Results: *"EQKs are universal for important families of kernel functions".*

How? Explicit construction

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How? Explicit construction

1. Take kernel

11. Theorems

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How? Explicit construction

1. Take kernel

2. Construct a feature map

11. Theorems

Results: *"EQKs are universal for important families of kernel functions".*

How? Explicit construction

1. Take kernel

2. Construct a feature map

3. Make it a quantum embedding

11. Theorems

Results: *"EQKs are universal for important families of kernel functions".*

How? Explicit construction

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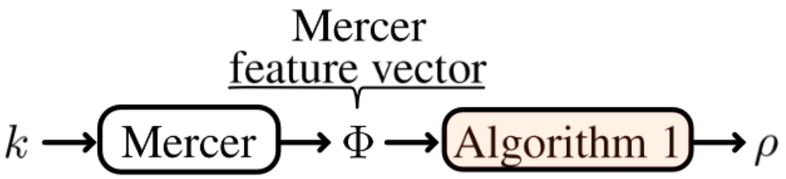

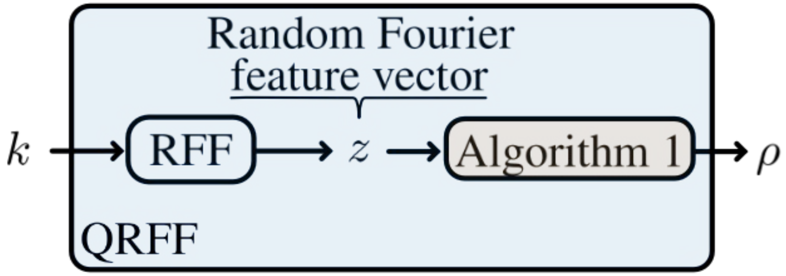

12. Take-home message

1. Although non-EQKs can exist *in principle*, we are not aware of any.

2. If you use EQKs, you're fine... *for now*.

Invitation: Help us search! We give many possible avenues in the paper.

References

“QML smells like kernels”:

Schuld, Killoran, *PRL* 122 4 (2019)
Havlícek *et al.*, *Nature* 567 (2019)

“QML is just kernels”:

Schuld, *arXiv:2101.11020* (2021)

“QML is not just kernels”:

Jerbi *et al.*, *Nat. Comm.* 14 (2023)

Our work: “Are we considering all possible kernels?”:

GF, Eisert, Dunjko, *MLST.* 5 (2024)

Thank you for your attention!

On the expressivity of Embedding Quantum Kernels

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(arXiv:2309.14419)

The kernel trick

Polynomial kernel $(x, x' \in \mathbb{R}^d)$

$$k(x, x') = \langle x, x' \rangle^r$$

<u>Option 1</u>: $2d + r - 2$ ops.

- $\langle x, x' \rangle$: d products and $d - 1$ sums
- $(\ldots)^r$: $r - 1$ products

<u>Option 2</u>: $\gg$ Option 1.

$k(x, x') = \langle \phi_{r,d}(x), \phi_{r,d}(x') \rangle$

$\phi_{r,d}(x)$ all monomials of degree r (combinatorial size, $N_{r,d}$)

$N_{r,d}$ products and $N_{r,d} - 1$ sums

Total $2N_{r,d} - 1$.

Gaussian kernel

$$k(x, x') = \exp(-\|x - x'\|^2)$$

<u>Option 1</u>: $3d - 1$ ops + sth.

- $\|x - x'\|^2$: $3d - 1$ ops.
- $\exp(\ldots)$: dunno…, not much?

<u>Option 2</u>: ∞.

$k(x, x') = \langle \phi_d(x), \phi_d(x') \rangle$

$\phi_d(x)$ all monomials.

There are infinitely many of them.

Construct two ∞-length vectors

Total ∞.