Good Quantum Kernels and Where to Find Them

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Why?

» Supervised quantum machine learning models are kernel methods [arXiv:2101.11020]

» So, one could use a quantum algorithm to:

compute a kernel $\longrightarrow$ feed it to a classical SVM algorithm

» We focus on the feature map, as it encodes the classical data into the quantum circuit

» This opens the possibility to explore unique features, such as entanglement and superposition, which couldn't be achieved via classical methods

» The feature map layer, however, may be constructed with a quite large freedom — and this is the point underlying this project!

How?

We've built a framework to study these quantum-generated kernels

- It comprises of generic tools for exploring, testing and assessing the performance of quantum kernels, given by different configurations for the feature map

- Dimensionality reduction can be performed via DPPs and/or PCA

- Several quantum feature maps can be tested via grid/random search & their performance may be assessed by some numerical metrics

- Moreover, we provide visualization routines for the Gram matrix, for the state vectors of the quantum encoding of single datapoints, for the decision boundaries, etc...

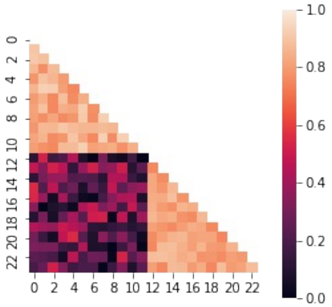
How?

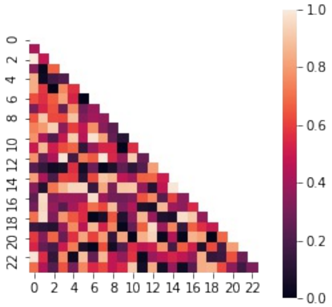
» Some evaluation metrics come from the usual ones in classification problems

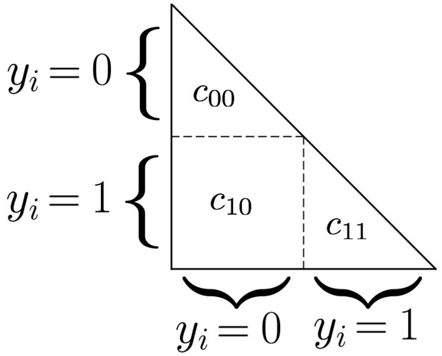
» But that are one, in particular, that needs only the Gram matrix (i.e. the kernel)

$$\Delta_\mu \equiv \frac{1}{2}(\mu_{c_{00}} + \mu_{c_{11}}) - \mu_{c_{10}} \qquad\qquad \Delta_\mu \in [-1, 1]$$

This is the density_diff metric, where μ is the mean of the matrix entries.

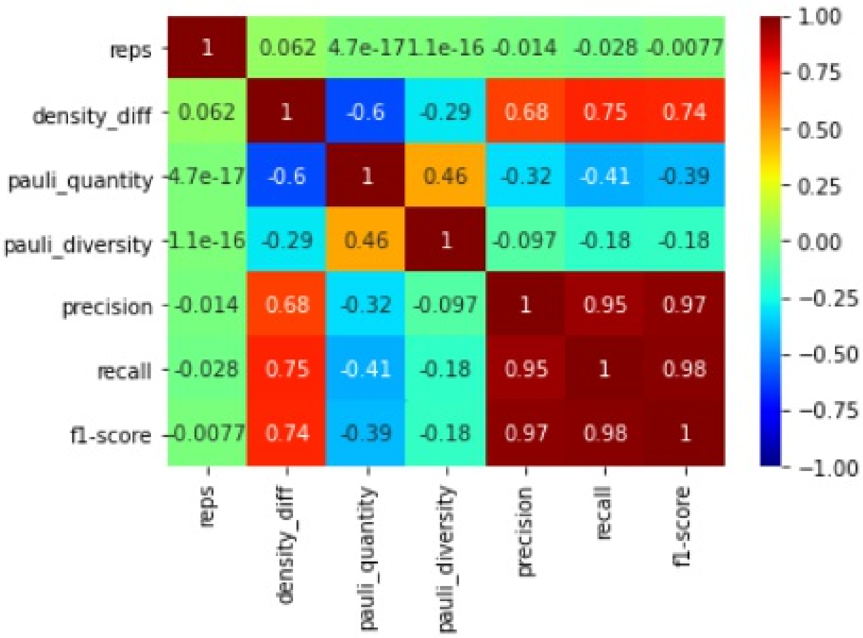






Results – Pt.I

» Correlation matrix between features and metrics



Results – Pt.II

» Decision boundary for the best quantum kernel we've found