Genetic algorithm for Quantum Support Vector Machines

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2.1 Support vector machine

The Support Vector Machine (SVM) is a binary classification alghoritm, whose goal is to build the maximum margin separator between the two classes, that is the separator that maximizes the distance of the closest point from each class. The standard SVM alghoritm is a linear alghoritm, so in particular it will try and build the separating margin as a hyperplane in a d-dimensional space (so a $(d-1)$-dimensional plane), where d is the number of features. The points that touch the margin, or that are on the wrong side of it, are called support vectors. The distance between the decision boundary and the support vectors is called margin. The alghoritm will find the biggest possible margin.

2.1.1 Linear SVM

Let's start assuming that the classes are linearly separable. We are provided with a dataset with N d-dimensional istances $\{\mathbf{x}_i\}_{i=0,\cdots,N-1}$. The two classes will be labelled with

$$y \in \{-1, 1\}.$$

The margin will be the the set of points

$$\{\mathbf{x} \in \mathbb{R}^d : w_0 + \mathbf{w}^T \cdot \mathbf{x} = 0\}, \tag{1}$$

for appropriate parameters $w_0 \in \mathbb{R}$ and $\mathbf{w} \in \mathbb{R}^d$, which define the hyperplane and must be found by the alghoritm. Now we have to find

$$\max_{w_0, \mathbf{w}}(m),$$

with the constraint

$$\frac{1}{||\mathbf{w}||} y_i(w_0 + \mathbf{w}^T \cdot \mathbf{x_i}) \geq m, \, \forall i = 0, \cdots, N-1, \tag{2}$$

that can be rewritten as

$$y_i(w_0 + \mathbf{w}^T \cdot \mathbf{x_i}) \geq m||\mathbf{w}||, \, \forall i = 0, \cdots, N-1. \tag{3}$$

The constraint prevents data points from falling into the margin. Rescaling $\mathbf{w}$ up to a multiplicative factor does not change the hyperplane it defines, so for convenience we can choose its norm such that

$$||\mathbf{w}|| = \frac{1}{m}. \tag{4}$$

Therefore the problem becomes minimizing

$$\frac{1}{2}||\mathbf{w}||,$$

with the constraint

$$y_i(w_0 + \mathbf{w}^T \cdot \mathbf{x_i}) \geq 1, \, \forall i = 0, \cdots, N-1. \tag{5}$$

In the theory of convex optimization one can solve for the Lagrangian dual of this problem. We can introduce the dual variables α_i such that

$$\mathbf{w} = \sum_{i=0}^{N-1} \alpha_i y_i \mathbf{x}_i. \tag{6}$$

One would obtain that the dual problem consists in maximizing, with respect to to the weight vector $\alpha \in \mathbb{R}^N$, the expression

$$f(\alpha_0, \cdots, \alpha_{N-1}) = \sum_{i=0}^{N-1} \alpha_i - \frac{1}{2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i, \mathbf{x}_j), \tag{7}$$

with the constraint

$$\alpha_i \geq 0, \, \forall i = 0, \cdots, N-1, \tag{8}$$

$$\sum_{i=0}^{N-1} \alpha_i y_i = 0. \tag{9}$$

In eq. (7) we indicated as $(\mathbf{x}_i, \mathbf{x}_j)$ the standard dot product of $\mathbb{R}^d$, explicitly

$$(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \cdot \mathbf{x}_j = \sum_{k=0}^{d-1} (\mathbf{x}_i)_k (\mathbf{x}_j)_k.$$

Eq. (7) defines a quadratic programming optimization problem, therefore the global maximum of f can be efficiently found in the context of convex analysis. The parameter w_0 can be found by imposing that, for a support vector

$$y_i(\mathbf{w}^T\mathbf{x}_i + w_0) = 1,$$

that is

$$w_0 = \mathbf{w}^T\mathbf{x}_i - y_i. \tag{10}$$

Once the optimal α_i have been found, given a new istance $\tilde{\mathbf{x}}$, according to eq. (6) and eq. (1), we can predict its class calculating

$$\text{sign}\left[\sum_{i=0}^{N-1} \alpha_i y_i(\tilde{\mathbf{x}}, \mathbf{x}_i) + w_0\right]. \tag{11}$$

What we just described is the so called hard margin SVM, because we did not allow points to fall inside the margin. One could relax this assumption, modifing the constraint in eq. (5) into

$$y_i(w_0 + \mathbf{w}^T \cdot \mathbf{x_i}) \geq 1 - \xi_i, \; \forall i = 0, \cdots, N-1, \tag{12}$$

where we introduced the slack variables ξ_i. We limit the softness of the margin by setting a positive constant C such that

$$\begin{aligned} \xi &\geq 0, \\ \sum_{i=0}^{N-1} \xi_i &\leq C. \end{aligned} \tag{13}$$

This is called soft margin SVM.

scikit-learn provides a straightforward implementation of the SVM algorithm, which we can use to observe the algorithm in action through an example. We use a mock dataset with 2 features, so we can easily print the data, the decision boundary and the margin.

```
from sklearn.svm import SVC
from sklearn.datasets import make_blobs
```

```
X,y = make_blobs(n_samples=100) #create mock dataset
svm = SVC(kernel='linear', C=1) #create svm
svm.fit(X, y) #fit the svm
```

The result of the fit is shown in Figure (1). We can observe how the alghoritm built the largest possible margin.

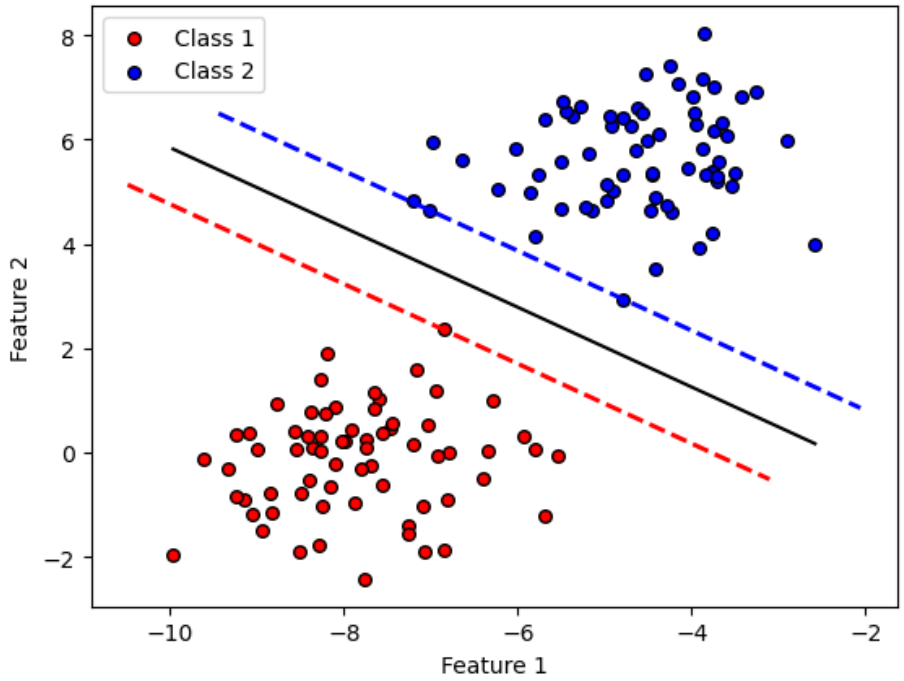


Figure 1: SVM decision boundary and margin border, fitted on a 2 feature mock dataset of 200 istances.

2.1.2 Kernel SVM

We now need to address the issue of dealing with a highly non-linearly separable dataset. Let's consider as an example another mock dataset, shown in Figure (2). It is clear that in this case we cannot use the SVM alghoritm in its basic form, not even with a soft margin. We must introduce the idea of kernelization. Let's introduce a function, called feature map, which projects the data in a

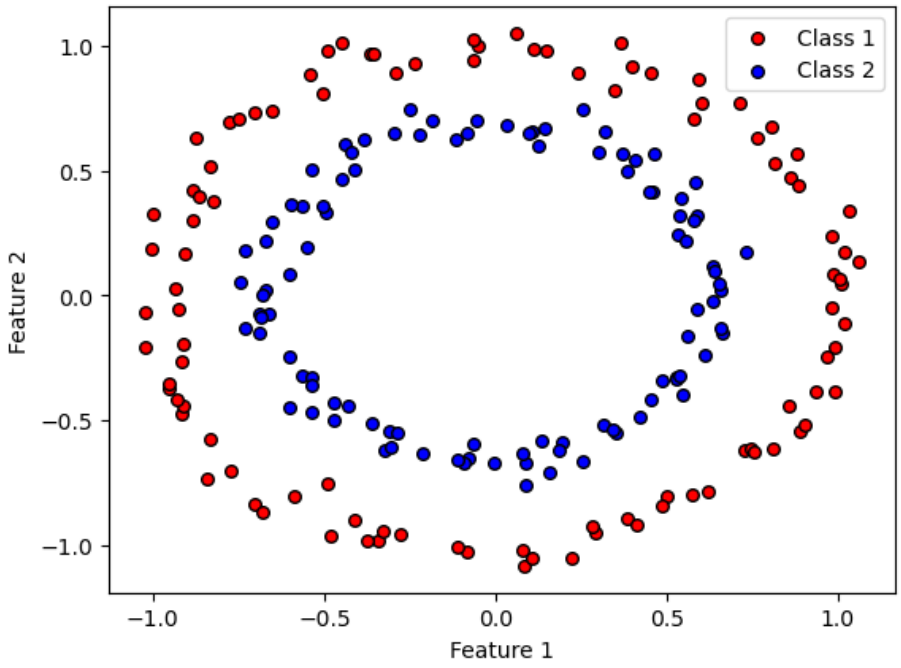


Figure 2: Higly non-linear 2 feature mock dataset with 200 istances.

higher dimensional space. That means a function

$$\phi : \mathbb{R}^d \to \mathbb{R}^D, \tag{14}$$

with $D > d$. The codomain of the feature map is called feature space. If we choose a suitable feature map we can hope to obtain a linearly separable dataset in the feature space. The choice of the feature map is completely arbitrary, as long as it is a bijective function. Therefore, in principle, each time we are given a dataset we must choose an appropriate feature map for this strategy to work. For our example let's consider the feature map

$$\phi : \mathbb{R}^2 \to \mathbb{R}^3,$$
$$\begin{pmatrix} x_0 \\ x_1 \end{pmatrix} \mapsto \begin{pmatrix} x_0^2 \\ x_1^2 \\ \sqrt{2}x_0x_1 \end{pmatrix}. \tag{15}$$

The data of Figure (2) after the application of the feature map ϕ are represented in Figure (3). The dataset is now linearly separable in the feature space, so the

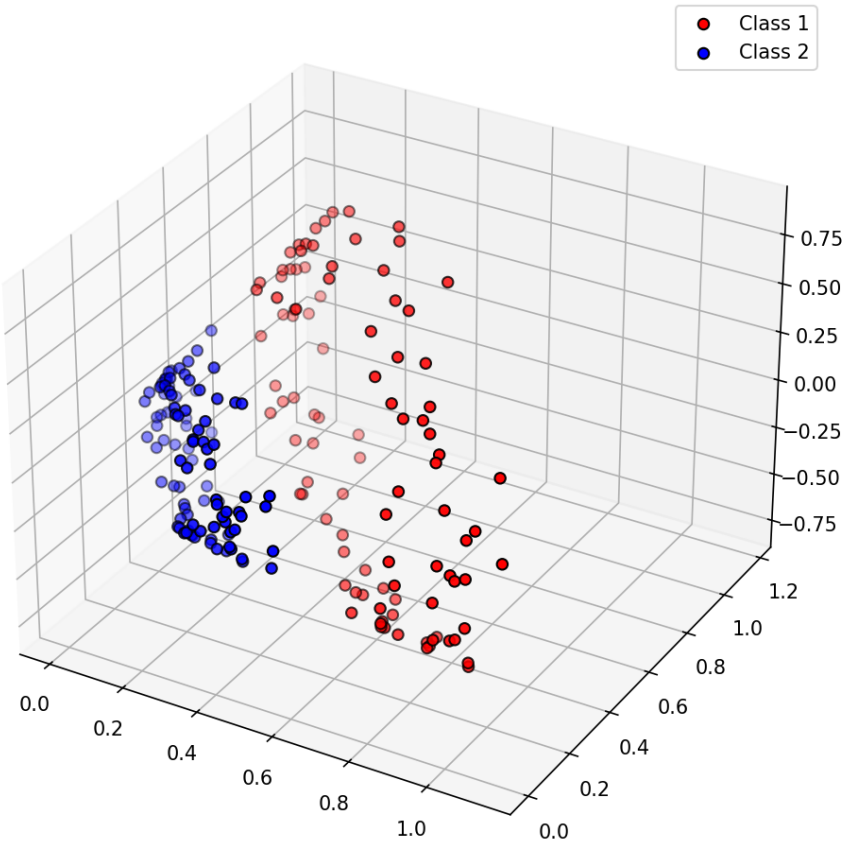


Figure 3: Higly non-linear mock dataset in the feature space after the application of the feature map ϕ. We observe now that the dataset is linearly separable.

strategy worked. We can now apply the SVM alghoritm in this space Consider the two central equations of the algorithm: equation (7), which provides the expression to maximize in order to find the margin, and equation (11), which gives the rule for predicting the class of a new instance. This two equations are now modified into

$$f(\alpha_0, \cdots, \alpha_{N-1}) = \sum_{i=0}^{N-1} \alpha_i - \frac{1}{2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \alpha_i \alpha_j y_i y_j (\phi(\mathbf{x}_i,) \phi(\mathbf{x}_j)), \tag{16}$$

$$\text{sign}\left[\sum_{i=0}^{N-1}\alpha_i y_i(\phi(\tilde{\mathbf{x}}),\phi(\mathbf{x}_i))+w_0\right]. \tag{17}$$

A crucial observation is that in these two expressions only the scalar product of the feature map values appears. Therefore we can conclude that the specific form of the feature map is not important, but rather the scalar product it produces. We can define the kernel K as

$$K:\mathbb{R}^d\times\mathbb{R}^d\to\mathbb{R},$$

$$\mathbf{x},\mathbf{y}\mapsto(\phi(\mathbf{x}),\phi(\mathbf{y})), \tag{18}$$

where $(\phi(\mathbf{x}),\phi(\mathbf{y}))=\phi(\mathbf{x})^T\cdot\phi(\mathbf{y})$ is the standard scalar product of $\mathbb{R}^D$. Eq. (16) and eq. (17) now become

$$f(\alpha_0,\cdots,\alpha_{N-1})=\sum_{i=0}^{N-1}\alpha_i-\frac{1}{2}\sum_{i=0}^{N-1}\sum_{j=0}^{N-1}\alpha_i\alpha_j y_i y_j K(\mathbf{x}_i,\mathbf{x}_j), \tag{19}$$

$$\text{sign}\left[\sum_{i=0}^{N-1}\alpha_i y_i K(\tilde{\mathbf{x}},\mathbf{x}_i)+w_0\right]. \tag{20}$$

We see explicitly that the only quantity that matters is the kernel K. In our specific example the value of the kernel is

$$K(\mathbf{x},\mathbf{y})=\begin{pmatrix}x_0^2 & x_1^2 & \sqrt{2}x_0x_1\end{pmatrix}\cdot\begin{pmatrix}y_0^2\\ y_1^2\\ \sqrt{2}y_0y_1\end{pmatrix}=(\mathbf{x}^T\cdot\mathbf{y})^2. \tag{21}$$

Therefore once we are given a dataset it is sufficient for us to choose an appropriate kernel, and forget about the feature map. Once the kernel has been chosen the SVM can be trained using eq. (19), and we can use it to predict a new class using eq. (20). There are some properties that the kernel must satisfy:

- The kernel must be symmetric, that is

$$\forall\,\mathbf{x},\mathbf{y}\in\mathbb{R}^d,\ K(\mathbf{x},\mathbf{y})=K(\mathbf{y},\mathbf{x}).$$

- The kernel must be positive definite, that is

$$\forall\,\mathbf{x},\mathbf{y}\in\mathbb{R}^d,\ K(\mathbf{x},\mathbf{y})\geq 0.$$

Common choices of kernels are

- Linear kernel:

$$K(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \cdot \mathbf{y}.$$

  This goes back to the standard SVM we used in Figure (1). It is suitable only for linearly separable (or close to, using soft margin) datasets.

- Polynomial kernel:

$$K(\mathbf{x}, \mathbf{y}) = (\gamma \mathbf{x}^T \cdot \mathbf{y} + c)^{\delta}.$$

  For $c = 0$, $\gamma = 1$ and $\delta = 2$ we obtain the kernel of eq. (21).

- Gaussian kernel:

$$K(\mathbf{x}, \mathbf{y}) = \exp(-\gamma ||\mathbf{x} - \mathbf{y}||).$$

  This is also known as Radial Basis Function (RBF) kernel.

- Sigmoid kernel:

$$K(\mathbf{x}, \mathbf{y}) = \tanh(\mathbf{x}^T \cdot \mathbf{y} + c).$$

scikit learn offers an easy way to easily implement all these common kernels. For example the kernel in eq. (21) can be implemented as

```
svm = SVC(kernel='poly', degree=2, gamma=1, coef0=0)
```

One can also create a custom kernel, passing as an argument a callable function to be used to calculate the kernel. Fitting this SVC function to the non-linear dataset of Figure (2) yields the result shown in Figure (4).

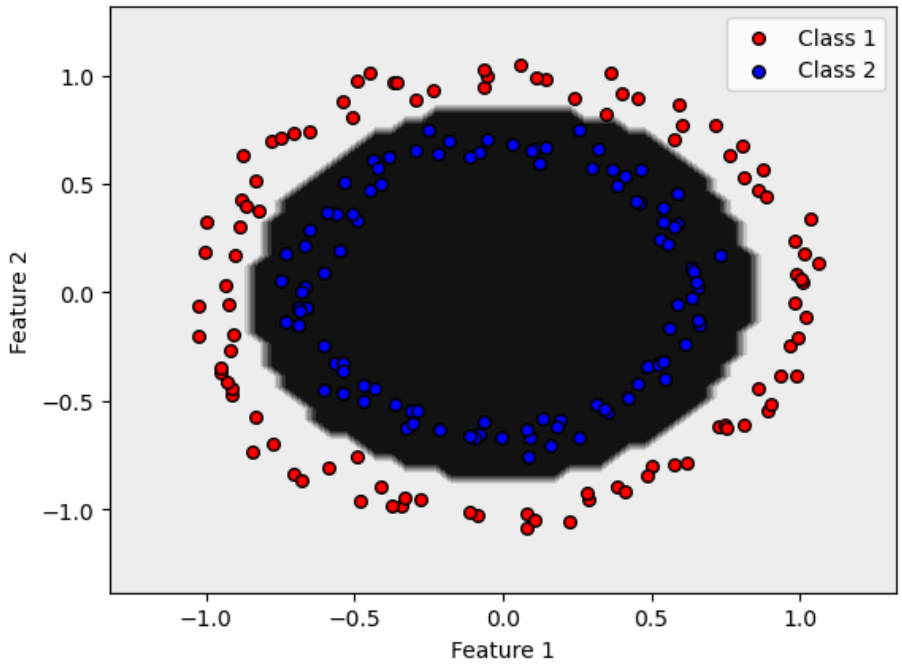


Figure 4: Higly non-linear mock dataset decision boundary, fitted with a SVM using kernel of eq. (21). The white and black areas are the two predicted classes. We observe how, using the kernel, we obtained a non-linear decision boundary.

3 Quantum machine learning

Introduction bla bla

3.1 Quantum Support Vector Machine

3.1.1 Quantum feature map and Quantum Kernels

The SVM alghoritm faces some important limitations when the feature space becomes large, as estimating kernel functions becomes computationally intensive. Quantum computing could enhance the algorithm's performace by providing access to exponentially large Hilbert feature spaces. The idea is to construct a feature map which maps classical data into a quantum state which lives in an exponentially large Hilbert feature space. Therefore in this context a feature

map is a function

$$\phi : \mathbb{R}^d \to \mathcal{H}, \tag{22}$$

$$\mathbf{x} \mapsto \phi(\mathbf{x}) \equiv |\phi(\mathbf{x})\rangle.$$

In the framework of quantum computing $\mathcal{H}$ is a n-qubit Hilbert space, that is a space of the form

$$\mathcal{H} = \bigotimes_{i=0}^{n} \mathcal{H}_{qubit}, \tag{23}$$

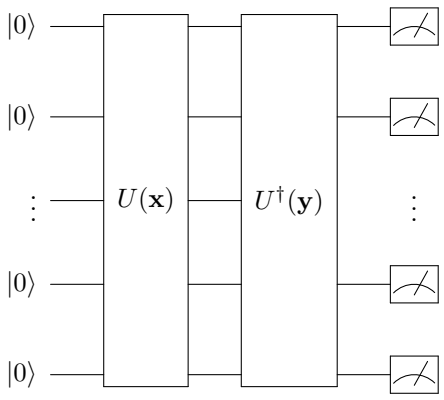
where $\mathcal{H}_{qubit}$ is the Hilbert space of a single qubit. The dimension of $\mathcal{H}$ is 2^n. The feature map will implemented by the means of a parametrised quantum circuit. That means that it exists a unitary operator that depends on d classical parameters $U(\mathbf{x}) = U(x_0, \cdots, x_{d-1})$ such that

$$|\phi(\mathbf{x})\rangle = U(\mathbf{x})|0\rangle^{\otimes n}. \tag{24}$$

This circuit is called quantum encoding circuit, because it encodes classical data into a quantum state. The classical data is passed to the circuit as a parameter. We will later make examples of frequently used encoding circuits. Once we have the feature map the kernel is constructed as

$$K(\mathbf{x}, \mathbf{y}) = |\langle \phi(\mathbf{x}) | \phi(\mathbf{y}) \rangle|^2 . \tag{25}$$

Here $\langle\ ,\ \rangle$ denotes the standard internal scalar product between vectors in $\mathcal{H}$. This definition clearly yields a kernel that satisfies the two kernel properties. How do we calculate the kernel in practice? Suppose we want to calculate the kernel $K(\mathbf{x}, \mathbf{y})$ and consider the following circuit.



(26)

Suppose we run this circuit R times, and we call A the number of times that we measure the bit string $000\cdots0$. We state that

$$\lim_{R\to+\infty}\frac{A}{R}=K(\mathbf{x},\mathbf{y}). \tag{27}$$

The proof is straightforward. The LHS of eq. (27) is the probability of measuring $000\cdots0$, which according to quantum mechanics can be calculated as

$$|^{\otimes n}\langle 0|U(\mathbf{x})U^{\dagger}(\mathbf{y})|0\rangle^{\otimes n}|^2=|^{\otimes n}\langle 0|U^{\dagger}(\mathbf{y})U(\mathbf{x})|0\rangle^{\otimes n}|^2=$$

$$=|\langle\phi(\mathbf{y})|\phi(\mathbf{x})\rangle|^2=K(\mathbf{x},\mathbf{y}).$$

□

Therefore, to evaluate the kernel, it suffices to construct the quantum circuit (26) and measure the frequency with which the string $000\cdots00$ occurs. We have to perform this operation for each pair of instances, and construct the matrix

$$K_{ij}=K(\mathbf{x}_i,\mathbf{x}_j). \tag{28}$$

This kernel matrix is then plugged into eq. (19) to train a classical SVM.

3.1.2 Quantum encoding circuits

Let's now discuss some possible choices of quantum encoding circuits:

- Basis encoding: this can be applied if the istances live in a finite dimensional space, whose dimension 2^n, where n is the number of qubits. If the dimensione is smaller that 2^n we can still apply this encoding by using padding. The istances can be mapped into bit strings of lenght n and the feature map corresponds to

$$\phi:\{0,1\}^n\to\mathcal{H}, \tag{29}$$

$$x=(x_0\cdots x_{n-1})\mapsto|x_0\rangle\otimes\cdots\otimes|x_{n-1}\rangle\equiv|x_0\cdots x_{n-1}\rangle=|x\rangle.$$

Here $|x\rangle$ is a state of the so called computational basis. For example the bit string 01001 is mapped to the quantum state

$$|0\rangle \otimes |1\rangle \otimes |0\rangle \otimes |0\rangle \otimes |1\rangle = |01001\rangle.$$

The kernel that originates from this feature map is

$$K(x, y) = |\langle x|y\rangle|^2 = |\delta_{x,y}|^2 = \delta_{x,y} \tag{30}$$

since vectors in the computational basis are orthogonal.

- Amplitude encoding: this can be applied with istances that are normalized vector, that is vectors of the form

$$\mathbf{x} = (x_0, \cdots, x_{d-1})^T \in \mathbb{R}^d, \tag{31}$$

such that

$$\sum_{i=0}^{d-1} x_i^2 = 1.$$

In this case the encoding consists in sending

$$\mathbf{x} = (x_0, \cdots, x_{d-1})^T \mapsto |\phi(\mathbf{x})\rangle = \sum_{i=0}^{d-1} x_i |i\rangle, \tag{32}$$

where $|i\rangle$ is the i-th vector of the computational basis. The fact that $\mathbf{x}$ is normalized ensures that the feature vector is normalized as well, and therefore represents a physical state. The kernel generated by this feature map is

$$K(x, y) = \left| \sum_{i,j} x_i y_j \langle i|j\rangle \right|^2 = \left| \sum_{i,j} x_i y_j \delta_{i,j} \right|^2 = (\mathbf{x}^T \cdot \mathbf{y})^2. \tag{33}$$

We went back to a polynomial kernel.

- By creating more copies of the feature vector of amplitude encoding we can create higher order polynomial kernels.

- Product encoding: in this case each feature of the input is encoded in the amplitudes of one separate qubit. For example we can send

$$\mathbf{x} = (x_0, \cdots, x_{d-1})^T \mapsto \begin{pmatrix} \cos x_0 \\ \sin x_0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} \cos x_{d-1} \\ \sin x_{d-1} \end{pmatrix}, \tag{34}$$

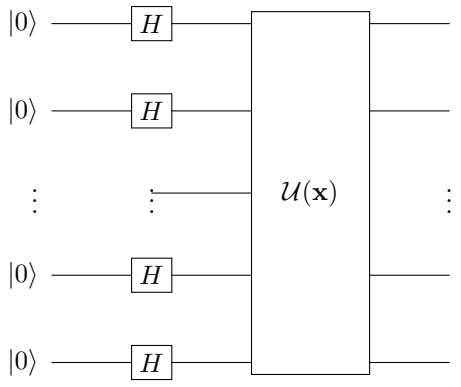
therefore the i-th qubit will be in the state

$$\cos x_i|0\rangle + \sin x_i|1\rangle. \tag{35}$$

This generates the kernel

$$K(x,y) = \prod_{i=0}^{d-1} \cos(x_i - y_i). \tag{36}$$

- ZZ feature map: The previously discussed encoding maps where quantum maps that in the end generated a kernel which is easy to calculate with classical tools, for example a polynomial kernel or a cosine kernel. It is important now to discuss quantum encoding circuits that creates a kernel which is not possible to write as an easy classical kernel, otherwise there is no advantage in using quantum computing for this task if the kernel could have been easily calculated with classical tools. The hope is that by using a purely quantum kernel we obtain better performance that by using a classical kernel. Since general quantum circuits are not expected to be classicaly simulable, there are many choices one can make. One example is generated by the following circuit



where H is the standard Hadamard gate and

$$\mathcal{U}(\mathbf{x}) = \exp\left[i \sum_{S\subseteq[n]} \phi_S(\mathbf{x}) \prod_{i\in S} Z_i \right]. \tag{37}$$

Here $[n] = \{0, \cdots, n-1\}$, Z_i is the third Pauli matrix acting on the i-th qubit and $\phi_S(\mathbf{x})$ are arbitrary coefficients, which are the ones that actually encode the classical data. S runs over all possibile subsets of $[n]$, and can be thought as an index that describes connectivities between different qubits or datapoints. We have 2^n possible choices of the coefficients. It is convenient to choose them in a way such that only the terms with $|S| \leq d$ contribute, in order to obtain a circuit that can be easily implemented on a quantum computer. This is done by asking that

$$\phi_S = 0 \quad \text{if} \quad |S| > d. \tag{38}$$

Let's focus on a simple case where $n = d = 2$. There are two default choices for the coefficients in this case. The first one is to set

$$\phi_{\{i\}}(\mathbf{x}) = x_i, \tag{39}$$

$$\phi_{\{i,j\}}(\mathbf{x}) = 0. \tag{40}$$

The feature maps becomes

$$U(\mathbf{x}) = e^{ix_0 Z_0}\, e^{ix_1 Z_1} H^{\otimes n}. \tag{41}$$

This is called Z feature map. The circuit decomposed in elementary quantum gates is shown in Figure . The other possible choice is

$$\phi_{\{i\}}(\mathbf{x}) = x_i, \tag{42}$$

$$\phi_{\{i,j\}}(\mathbf{x}) = (\pi - x_i)(\pi - x_j). \tag{43}$$

In this case the feature maps becomes

$$U(\mathbf{x}) = e^{i(\pi - x_0)(\pi - x_1) Z_0 Z_1}\, e^{ix_0 Z_0}\, e^{ix_1 Z_1} H^{\otimes n}. \tag{44}$$

This is called ZZ feature map, and it is an encoding circuit thought to be hard to simulate classically. It is shown in Figure . We will see how it behaves later on. Those two are standard choices, but there are many more circuits that can be built starting from the general structure of eq.

(37), especially if we consider a greater number of qubits, and so we allow connectivities of three and more qubits.

- Pauli feature map: Eq. (37) can be generalised to include not only Z gates, but all of the Pauli gates. We can have

$$\mathcal{U}(\mathbf{x}) = \exp\left[i \sum_{S\subseteq[n]} \phi_S(\mathbf{x}) \prod_{i\in S} P_i\right], \tag{45}$$

  where $P \in \{1, X, Y, Z\}$. This allows us to generate not only interaction of the ZZ type, but also for example YY type or ZY type.

- We will now show an example of a feature map which is hard to simulate classically but which yields a classical kernel.