Quantum Machine Learning

Quantum Support Vector Machines

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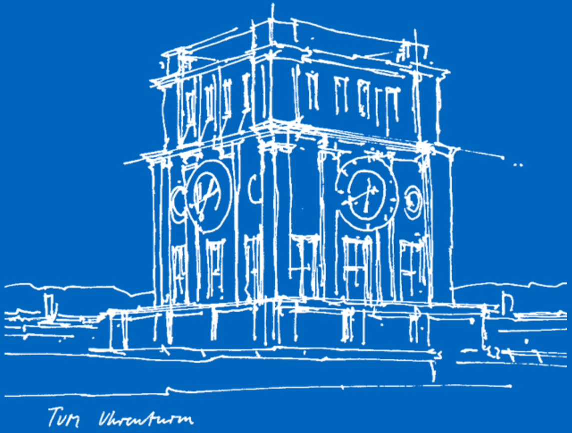

Outline

Introduction to Quantum Machine Learning
Machine Learning

- Training machines to learn from the algorithms implemented to handle the data [1].
- Classical machine learning helps to classify images, recognize patterns and speech, handle big data, ...[1].
- Today, more and more data is being generated.
  $\rightarrow$ Classical algorithms become less efficient [1].

Introduction to Quantum Machine Learning
Machine Learning

- Training machines to learn from the algorithms implemented to handle the data [1].
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- Today, more and more data is being generated.
  $\rightarrow$ Classical algorithms become less efficient [1].

$\Longrightarrow$ **Need to find alternative methods**

- Quantum Machine Learning (QML) is the intersection between quantum computing and machine learning.
- **Motivation**:
  - QML is expected to speed up the performance of ML programs through the use of quantum mechanical properties, i.e. entanglement, superposition.
  - Quantum speed-up in supervised machine learning has recently been shown by researchers of *IBM Quantum* and *University of California, Berkley* [2].
- **How does QML work in general?**
  - QML integrates quantum algorithms within machine learning programs.
    $\Longrightarrow$ Data can be classified, sorted and analyzed using quantum algorithms on a quantum computer.

Outline

Linear Classification
Intro

- Linear Classification, i.e. Perceptron, SVM, seeks to find an optimal separating hyperplane between two classes of data in a dataset such that, with high probability, all training examples of one class are found only on one side of the hyperplane [3].

Linear Classification
Intro

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Setup:

- Input vector $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$ $x_i \in \mathbb{R}^D$
- Labels: $\mathbf{y} = \{\mathbf{y}_1, \mathbf{y}_2, ..., \mathbf{y}_N\}$ $y_i \in \mathcal{C}$
- Classes: $C = \{1, ..., C\}$

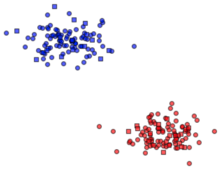

Figure 1 Linearly Separable Data.

Linear Classification
Intro

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Find:

- $f(\cdot) : \mathbb{R}^D \rightarrow \mathcal{C}$
- In the case of a linear decision function:
  $y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$
- Famous perceptron algorithm [4]
  $y_i(\mathbf{w}^T\phi(x_i) + b > 0$

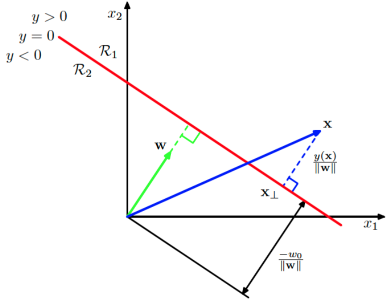

Figure 1 Illustration of Hyperplane Decision Function [4].

Linear Classification

Limitations of LDA

1. No uncertainty measure
2. Hard to optimize
3. Poor generalization
4. Cannot handle noisy data

Linear Classification

Limitations of LDA

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Extension: Introduce variables that allow to maximize the margin of the hyperplane between the classes.

Support Vectors
Hard Margin - Introduction

- Add two hyperplanes to the decision function that are parallel to the decision function.
- Extend the additional hyperplanes until the first datapoint of a data cluster is reached.
- The distance between the two support hyperplanes is called the margin.

$$\mathcal{M} = \frac{2s}{||w||}$$

- A datapoint that is on the hyperplane is called a Support Vector.

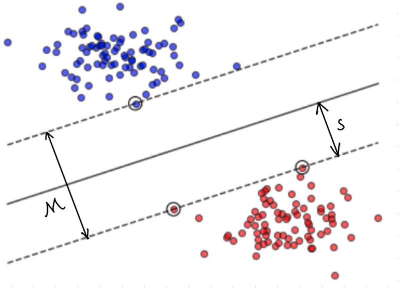

Figure 2 Illustration of Margin and Support Vectors.

Support Vectors

Hard Margin - Optimization Constraints

This setup leads to the following constraints, ($s = 1$):

$$w^T x + b \geq +1 \text{ if } y = 1 \quad (1)$$

$$w^T x + b \geq -1 \text{ if } y = -1 \quad (2)$$

$\Longrightarrow$ Maximize the margin $\mathcal{M}$ (for mathematical convenience, minimize $\mathcal{M} = \frac{1}{2}||w||^2$) given the above constraints [4].

$$\begin{aligned} &\min f_0(\theta) \\ &s.t. \;\; f_i(\theta) \geq 0 \text{ for } i = 1, ..., N \end{aligned} \quad (3)$$

Support Vectors

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$\implies$ Maximize the margin $\mathcal{M}$ (for mathematical convenience, minimize $\mathcal{M} = \frac{1}{2}||w||^2$) given the above constraints [4].

$$\begin{aligned} &\min \frac{1}{2}||w||^2 \\ &s.t.\ y_i(w^T x_i + b - 1) \geq 0 \text{ for } i = 1, ..., N \end{aligned} \tag{3}$$

Support Vectors

Hard Margin - Quadratic Programming

This formulated optimization problem is a *quadratic programming* problem, which, in Python, can be solved with the CVXOPT library.

$$\min_{x} \frac{1}{2}\mathbf{x}^T\mathbf{P}\mathbf{x} + \mathbf{q}^T\mathbf{x}$$
$$s.t.\ \mathbf{G}\mathbf{x} \leq \mathbf{h}, \mathbf{A}\mathbf{x} = \mathbf{b}$$

$\mathbf{q} \rightarrow N \times 1$ vector

$\mathbf{P} \rightarrow N \times N$ symmetric matrix

$\mathbf{G} \rightarrow N \times N$ diagonal matrix

$\mathbf{h} \rightarrow N \times 1$ vector

$\mathbf{A} \rightarrow M \times M$ matrix

$\mathbf{b} \rightarrow M \times 1$ vector

Support Vectors

Hard Margin - Lagrangian

In order to solve the optimization problem, eq. (3), we introduce the Lagrangian,

$$\mathcal{L}(\theta, \alpha) = f_0(\theta) - \alpha_i f_i(\theta) \tag{4}$$

and the Duality perspective.
The principle of Duality in optimization theory states that there are two perspectives of approaching an optimization problem [5]. The two approaches:

- **Primal**
- **Dual**

Support Vectors
Hard Margin - Lagrangian

In order to solve the optimization problem, eq. (3), we introduce the Lagrangian and the Duality perspective.

Primal Problem: Solves the lower bound of the constrained optimization $(f_0(\theta^*) = p^*)$

$$\mathcal{L}(w, b, \alpha) = \frac{1}{2} w^T w - \sum_{i=1}^{N} \alpha_i (y_i (w^T x_i + b) - 1) \tag{5}$$

$$g(\alpha) = \min_{w,b} \mathcal{L}(w, b, \alpha) \tag{6}$$

$$\nabla_w \mathcal{L}(w, b, \alpha) = w - \sum_{i=1}^{N} \alpha_i y_i x_i \overset{!}{=} 0 \tag{7}$$

$$\nabla_b \mathcal{L}(w, b, \alpha) = - \sum_{i=1}^{N} \alpha_i y_i \overset{!}{=} 0 \tag{8}$$

Support Vectors

Hard Margin - Lagrangian

Dual Problem: The best lowest bound to the solution of the Primal problem ($g(\alpha^*) = d^*$)
$\rightarrow$ Substitute eq. (7) and eq. (8) back into the Langrangian, $\mathcal{L}(w^*, b^*, \alpha)$.

$$g(\alpha) = \mathcal{L}(w^*, b^*, \alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j \tag{9}$$

From here, set up a new constraint optimization problem:

$$\begin{aligned} &\max_{\alpha} \; g(\alpha) \\ s.t. \; &\sum_{i=1}^{N} \alpha_i y_i = 0, \;\; \alpha_i \geq 0 \text{ for } i = 1, ..., N \end{aligned} \tag{10}$$

Support Vectors

Hard Margin - Implementation

- With the constraint optimization problem, eq. (10), we can formulate a quadratic *programming problem* that can be implemented in Python with the CVXOPT library.

$$\max_{\alpha} \boldsymbol{\alpha} \mathbf{1}_N - \frac{1}{2}\alpha^T \mathbf{Q} \alpha \quad \| \text{ where } \mathbf{Q} = \mathbf{y}\mathbf{y}^T \circ \mathbf{x}^T \mathbf{x}$$
$$s.t. \sum_{i=1}^{N} \alpha_i y_i = 0, \;\; \alpha_i \geq 0 \text{ for } i = 1, ..., N \tag{11}$$

Support Vectors
Hard Margin - Implementation

- With the constraint optimization problem, eq. (10), we can formulate a quadratic *programming problem* that can be implemented in Python with the CVXOPT library.

$$\min_{\alpha} \frac{1}{2}\alpha^T \mathbf{P}\alpha - \mathbf{1}_N^T \boldsymbol{\alpha}$$
$$s.t.\ y^T\alpha = 0,\ -\alpha_i \leq 0 \text{ for } i = 1, ..., N \tag{11}$$

$$\mathbf{q} := -\mathbf{1_N} \in \mathbb{R}^{Nx1}$$
$$\mathbf{P} := \mathbf{Q} \in \mathbb{R}^{NxN}$$
$$\mathbf{G} := -\mathbf{diag}(\mathbf{1_N}) \in \mathbb{R}^{NxN}$$
$$\mathbf{h} := \mathbf{0_N} \in \mathbb{R}^{Nx1}$$
$$\mathbf{A} := \mathbf{y} \in \mathbb{R}^{Nx1}$$
$$\mathbf{b} := 0 \in \mathbb{R}$$

Support Vectors

Hard Margin - Support Vectors

Duality: We use the duality gap between the Primal and Dual solution, $p^* - d^*$, to find the Support Vector (strong duality = $p^* - d^* = 0$):
$\rightarrow$ Strong duality holds if,

$$\alpha_i(y_i(w^T x_i + b) - 1) = 0$$

implying that given $\alpha_i > 0$, if

$$y_i(w^T x_i + b) = 1$$

$\implies$ **Support Vector**

Support Vectors
Hard Margin - Classification

Parameters:

$$w^* = \sum_{i=1}^{N} \alpha_i y_i x_i = (\boldsymbol{\alpha} \cdot \mathbf{y})^T \mathbf{X} \tag{12}$$

$$b = y_i - w^T x_i \tag{13}$$

Classification:

$$\mathbf{y}_{pred} = \text{sign}((w^*)^T \mathbf{x} + b) \tag{14}$$

Support Vectors
Hard Margin - Implementation

Link to the implementation on GITHUB:

- linear-classifier

Support Vectors
Hard Margin - Example Plot

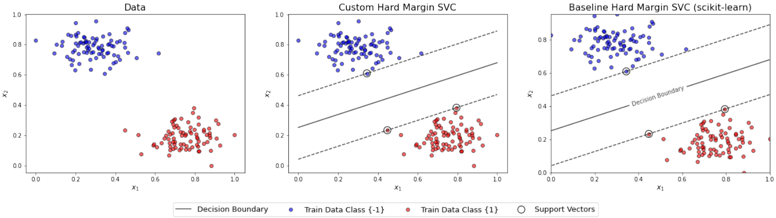


Figure 3 Custom Hard Margin SVC versus scikit-learn linear SVC.

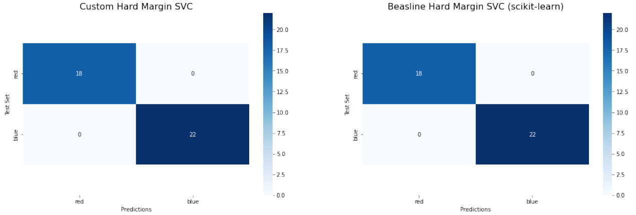


Figure 4 Confusion Matrices for custom hard margin SVC and SCIKIT baseline gard margin SVC.

Support Vectors
Soft Margin

- Hard Margin classification assumes that the data is linearly separable, i.e. does not overlap.
- Unrealistic in real world problems.
- **Extend** the previous Support Vector method to allow misclassification .

Support Vectors
Soft Margin

- Hard Margin classification assumes that the data is linearly separable, i.e. does not overlap.
- Unrealistic in real world problems
- **Extend** the previous Support Vector method to allow misclassification.

- Introduce *slack variables*, $\xi_i \geq 0$, which measure the violation of the margin (in units of $||w||$).

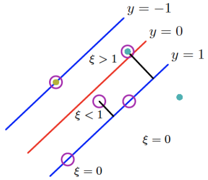


Figure 5 Depiction of Slack Variables ξ [4].

Support Vectors
Soft Margin

$$
\begin{aligned}
&\min f_0(\theta) \\
&s.t.\ \ f_i(\theta) \geq 0 \text{ for } i = 1, ..., N
\end{aligned} \tag{15}
$$

Support Vectors
Soft Margin

$$
\begin{aligned}
&\min \ \frac{1}{2}||w||_2^2 + C\sum_{i=1}^{N}\xi_i \\
&s.t. \ y_i(w^T x_i + b - 1) \geq 1 - \xi_i \ \forall_i
\end{aligned} \tag{15}
$$

Support Vectors
Soft Margin

$$\min \ \frac{1}{2}||w||_2^2 + C\sum_{i=1}^{N}\xi_i$$
$$s.t. \ y_i(w^T x_i + b - 1) \geq 1 - \xi_i \ \forall_i \tag{15}$$

Repeat the procedure:

1. Calculate the Primal
2. Calculate the Dual
3. Use Duality to determine support vectors and to calculate the decision function to perform the classification.

Support Vectors
Soft Margin - Primal

$$\mathcal{L}(w,b,\xi,\alpha,\mu) = \frac{1}{2}||w||_2^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}(\alpha_i(y_i(w^T x_i + b) - 1 + \xi_i) - \sum_{i=1}^{N}\mu_i\xi_i \quad (16)$$

$$g(\alpha) = \min_{w,b,\xi}\mathcal{L}(w,b,\xi,\alpha,\mu) \quad (17)$$

- KKT conditions:

$$\alpha_i \geq 0 \quad (18) \qquad \mu_i \geq 0 \quad (21)$$

$$y_i(w^T x_i + b) - 1 + \xi_i \geq 0 \quad (19) \qquad \xi_i \geq 0 \quad (22)$$

$$\alpha_i(y_i(w^T x_i + b) - 1 + \xi_i) = 0 \quad (20) \qquad \mu_i\xi_i = 0 \quad (23)$$

- Determine w^*, b^* and ξ^*

Support Vectors
Soft Margin - Dual

$$g(\alpha) = \mathcal{L}(w^*, b^*, \xi^*, \alpha) = \sum_{i=0}^{N} \alpha_i - \frac{1}{2} \sum_{i=0}^{N} \sum_{j=0}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j \tag{24}$$

$$\max \;\; g(\alpha) \tag{25}$$

$$s.t. \;\; 0 \leq \alpha_i \leq C \tag{26}$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0 \quad \text{for } i = 1, .., N \tag{27}$$

- Similarly, as with eq. (11), we reformulate eq. (24) as a *quadratic programming problem*.

Support Vectors
Soft Margin - Quadratic Programming

$$\min_{\alpha} \frac{1}{2}\alpha^T \mathbf{P}\alpha - \mathbf{1}_N^T \boldsymbol{\alpha} \tag{28}$$

$$s.t.\ y^T\alpha = 0 \tag{29}$$

$$-\alpha_i \leq 0 \text{ for } i = 1, ..., N \tag{30}$$

$$\alpha_i \leq C \text{ for } i = 1, ..., N \tag{31}$$

$$\mathbf{q} := -\mathbf{1_N} \in \mathbb{R}^{Nx1}$$

$$\mathbf{P} := \mathbf{Q} \in \mathbb{R}^{NxN}$$

$$\mathbf{G} := -\begin{pmatrix} -\mathbf{diag}(\mathbf{1_N}) \\ \mathbf{diag}(\mathbf{1_N}) \end{pmatrix} \in \mathbb{R}^{2NxN}$$

$$\mathbf{h} := \begin{pmatrix} \mathbf{0_N} & C \cdot \mathbf{1_N} \end{pmatrix} \in \mathbb{R}^{2N\times 1}$$

$$\mathbf{A} := \mathbf{y} \in \mathbb{R}^{Nx1}$$

$$\mathbf{b} := 0 \in \mathbb{R}$$

Support Vectors
Soft Margin Implementation

Link to the implementation on GITHUB:

- linear-classifier

Support Vectors
Soft Margin - Example Plot

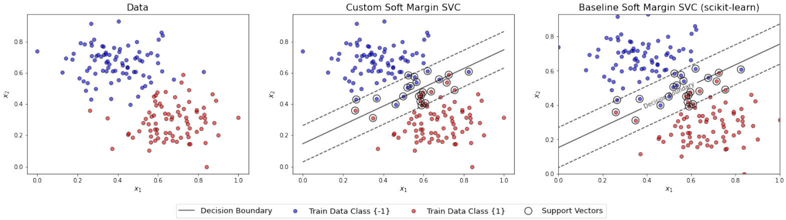


Figure 6 Classification result of the custom soft margin SVC and SCIKIT baseline soft SVC.

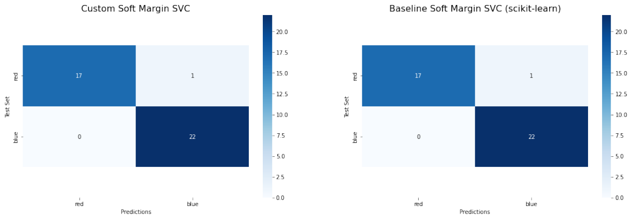


Figure 7 Confusion Matrices for custom soft margin SVC and SCIKIT baseline soft margin SVC.

Kernel Methods

Soft Margin - Example Plot

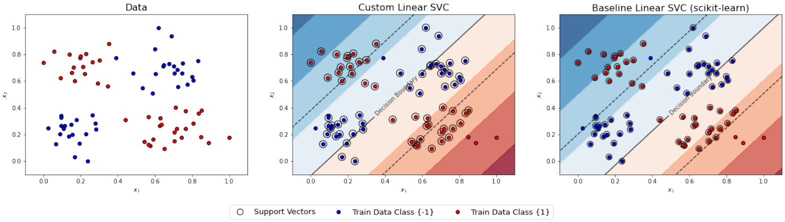


Figure 8 Displays the classification result of the custom soft margin SVC and SCIKIT baseline soft SVC.

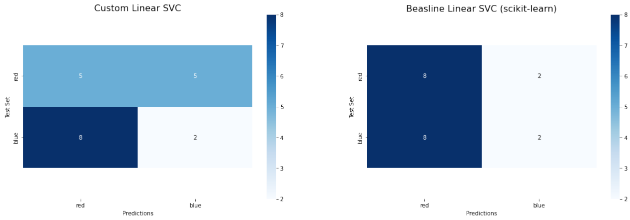


Figure 9 Confusion Matrices for custom soft margin SVC and SCIKIT baseline soft margin SVC.

Kernel Methods

- So far, we still considered the data to be linearly separable in a feature space $\mathbf{X}$.
- In **extending** the Support Vector Machines for higher-dimensional data or non-linear data, we can further generalize the previous approaches by mapping d-dimensional data vectors into an n-dimensional feature space:

$$\phi : \mathbf{X} \rightarrow \mathcal{R}^n$$

- Further, we make use of the *Kernel Trick*:

$$-\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{N}\alpha_i\alpha_j y_i y_j \phi(x_i)^T\phi(x_j)$$

$$-\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{N}\alpha_i\alpha_j y_i y_j k(x_i, x_j), \quad \text{where } k(x_i, x_j) = \phi(x_i)^T\phi(x_j)$$

$\rightarrow$ Increase computational speed for higher dimensional finite data.

Kernel Methods

- So far, we still considered the data to be linearly separable in a feature space $\mathbf{X}$.
- In **extending** the Support Vector Machines for higher-dimensional data or non-linear data, we can further generalize the previous approaches by mapping d-dimensional data vectors into an n-dimensional feature space:

$$\phi : \mathbf{X} \rightarrow \mathcal{R}^n$$

- Further, we make use of the *Kernel Trick*. Therefore, eq. (24) can be written as,

$$g(\alpha) = \sum_{i=0}^{N} \alpha_i - \frac{1}{2} \sum_{i=0}^{N} \sum_{j=0}^{N} \alpha_i \alpha_j y_i y_j k(x_i, x_j) \tag{32}$$

- Kernel can be seen as a measure of similarity.

Kernel Methods

Linear:

$$k(x_1, x_2) = x_1^T x_2$$

Polynominal:

$$k(x_1, x_2) = (c + x_1^T x_2)^d$$

Radial Basis Function:

$$k(x_1, x_2) = \exp(-\gamma ||x_1 - x_2||^2)$$

Sigmoid:

$$k(x_1, x_2) = \tanh(\gamma x_1^T x_2 + c)$$

Classification: If the kernel is not linear, the classification function, eq. (14), must be adopted,

$$y_{pred} = \sum_{i \in SV} \alpha_i y_i k(x, x_i) \tag{33}$$

Kernel Methods
Implementation

Link to the implementation on GITHUB:

- [nonlinear- classifier]

Kernel Methods
Kernel Method - Example Plot

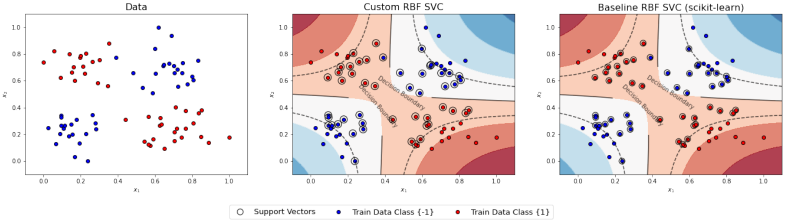


Figure 10 Displays the classification result of the custom RBF SVC and SCIKIT baseline RBF SVC.

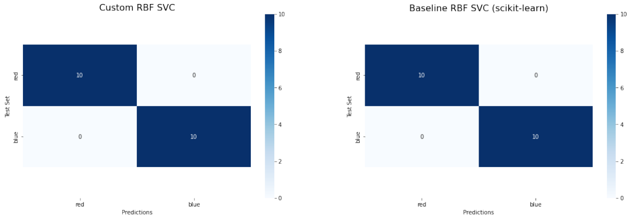


Figure 11 Confusion Matrices for custom RBF SVC and SCIKIT baseline RBF SVC.

Limitations to SVM

- Feature space becomes large $\implies$ Kernel functions become computationally expensive.
- No probabilistic interpretation of the classification.
- Not suitable for large datasets.

Outline

Quantum Kernel Estimation
Introduction

- Idea: Use the quantum advantage to speed up the computation of support vector classifiers (potential use of the exponentially large quantum state space).
- Two methods:
  1. *Quantum Variational Classifier*
  2. *Quantum Kernel Estimation*

Quantum Kernel Estimation
Introduction

- Idea: Use the quantum advantage to speed up the computation of support vector classifiers (potential use of the exponentially large quantum state space).
- Two methods:
  1. *Quantum Variational Classifier*
  2. *Quantum Kernel Estimation*
- In order to make use of the quantum advantage, the classical data needs to be transformed into the quantum state space.
  - Requires a data map (encoding function).
  - Requires a *quantum feature map* as a parameterized circuit.
- From the quantum state space, we can estimate a kernel matrix that can be used with a classical Support Vector Classifier.

Quantum Kernel Estimation

Quantum Feature Map

- Transforms low dimensional real space onto high dimensional quantum state space [6].

$$\Phi : \mathbf{x} \in \Omega \rightarrow |\Phi(x)\rangle \langle\Phi(x)| \, [7] \tag{34}$$

- This is facilitated by a unitary operator $\mathcal{U}_{\Phi(x)}$ on a initial state $|0\rangle^n$ with $n =$ number of qubits [8],

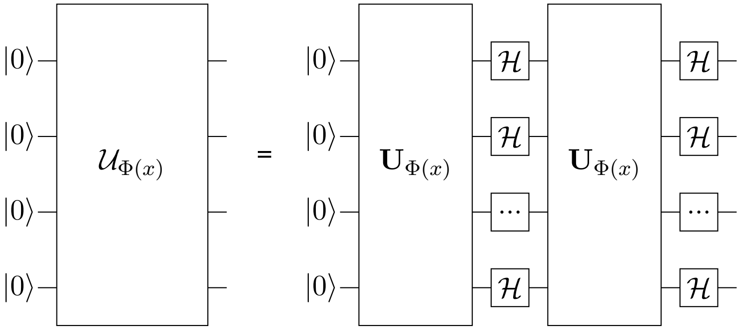
$$\Phi(x) = \mathcal{U}_{\Phi(x)} |0\rangle^{\otimes n} \tag{35}$$

$$\mathcal{U}_{\Phi(x)} = \prod_d \mathbf{U}_{\Phi(x)} \mathcal{H}^{\otimes n} \tag{36}$$

- Dimensions of the feature space have to align with the number of qubits.
- Feature maps have a high influence on the classification accuracy, as they are the basis for the kernel estimation $\implies$ Careful analysis of the feature space is necessary [6].

Quantum Kernel Estimation

Quantum Feature Map - Quantum Circuit



Quantum Kernel Estimation
Pauli Feature Map

- The Pauli-Feature Map is a customizable example of a *quantum feature map* where the $\mathbf{U}_{\Phi(x)}$ from eq. (36) is a diagonal gate in the Pauli basis,

$$\mathbf{U}_{\Phi(x)} = \exp\left\{ i \sum_{S \subseteq [n]} \phi_S(x) \prod_{k \in S} P_i \right\} \tag{37}$$

  with
  - $P_i \in$ {I, Pauli-X, Pauli-Y, Pauli-Z}
  - $S \in \{ \binom{n}{k}$ combinations, $k = 1, ..., n\}$
  - $\phi_S \rightarrow$ data mapping function (encoding function)
- Gives rise the *Z-Feature Map* and the *ZZ-Feature Map*.

Quantum Kernel Estimation
Data Mapping functions

- Standard function used in QISKIT,

$$\phi_S : x \to \begin{cases} x_i & \text{if } S = \{i\} \\ (x_i - \pi)(x_j - \pi) & \text{if } S = \{i, j\} \end{cases}$$

- Further examples [6]:

$$\phi_S : x \to \begin{cases} x_i & \text{if } S = \{i\} \\ \exp\left(\frac{|x_i - x_j|^2}{8/\ln(\pi)}\right) & \text{if } S = \{i, j\} \end{cases} \tag{38}$$

$$\phi_S : x \to \begin{cases} x_i & \text{if } S = \{i\} \\ \frac{\pi}{3\cos x_i \cos x_j} & \text{if } S = \{i, j\} \end{cases} \tag{39}$$

Quantum Kernel Estimation

Quantum Feature Map - Example

- Given eq. (37), if $k = 2, P_0 = Z$ and $P_1 = ZZ \implies$ *ZZ-Feature Map*:

$$\mathbf{U}_{\Phi(x)} = \exp\left\{\left(i\sum_{jk}\phi_S(j,k)Z_j \otimes Z_k\right)\left(i\sum_{j}\phi_S(j)Z_j\right)\right\} \tag{40}$$

$$\mathcal{U}_{\Phi(x)} = \left(\exp\left\{\left(i\sum_{jk}\phi_S(j,k)Z_j \otimes Z_k\right)\left(i\sum_{j}\phi_S(j)Z_j\right)\right\}\mathcal{H}^{\otimes n}\right)^d$$

$$\mathcal{U}_{\Phi(x)} = \left(\exp\left(ix_0 Z_0 + ix_1 Z_1 + i(x_0 - \pi)(x_1 - \pi)Z_0 Z_1\right)\mathcal{H}^{\otimes n}\right)^d \tag{41}$$

Quantum Kernel Estimation
Quantum Kernel

- *Quantum feature maps* $\Phi(x)$ naturally give rise to *quantum kernels*:

$$k(x_i, x_j) = \Phi(x_i)^\dagger \Phi(x_j) \tag{42}$$

- As the kernel entries are the fidelities between two feature vectors, we need to establish a way to estimate the fidelities of a quantum state.
- For finite data, this scan be achieved by estimating the transition amplitude [7]:

$$K_{ij} = |\langle \Phi(x_i)^\dagger | \Phi(x_j) \rangle|^2 \tag{43}$$

- Plugging in eq. (35) into eq. (43):

$$K_{ij} = |\langle 0|^{\otimes n} \mathcal{U}^\dagger_{\Phi(x)} \mathcal{U}_{\Phi(x)} |0\rangle^{\otimes n}|^2 \tag{44}$$

Quantum Kernel Estimation
Quantum Kernel

- *Quantum feature maps* $\Phi(x)$ naturally give rise to *quantum kernels*:

$$k(x_i, x_j) = \Phi(x_i)^\dagger \Phi(x_j) \tag{42}$$

- As the kernel entries are the fidelities between two feature vectors, we need to establish a way to estimate the fidelities of a quantum state.
- For finite data, this scan be achieved by estimating the transition amplitude [7]:

$$K_{ij} = |\langle \Phi(x_i)^\dagger | \Phi(x_j) \rangle|^2 \tag{43}$$

- Plugging in eq. (35) into eq. (43):

$$K_{ij} = |\langle 0|^{\otimes n} \mathcal{U}^\dagger_{\Phi(x)} \mathcal{U}_{\Phi(x)} |0\rangle^{\otimes n}|^2 \tag{44}$$

$\Longrightarrow$ *Quantum kernel matrix estimate*

Implementation of Quantum Support Vector Machines

Quantum Kernel Estimation

Implementation of Quantum Support Vector Machines

Quantum Kernel Estimation

1. **Build a parameterized quantum circuit that emulates a *quantum feature map* for each data pair.**
   Example: ZZ-Feature Map for 2-dimensional input
   Recall: eq. (41)

$$\mathcal{U}_{\Phi(x)} = \left(\exp\left(ix_0 Z_0 + ix_1 Z_1 + i(x_0 - \pi)(x_1 - \pi) Z_0 Z_1\right) \mathcal{H}^{\otimes n}\right)^d$$

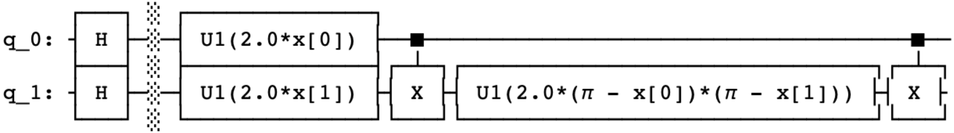


Figure 12 ZZ-Feature Map Circuit.

Implementation of Quantum Support Vector Machines

Quantum Kernel Estimation

1. Build a parameterized quantum circuit that emulates a *quantum feature map* for each data pair.
2. **Construct the *quantum kernel* circuits for each data pair**.
   Recall: eq. (44) and eq. (41)

$$K_{ij} = |\langle 0|^{\otimes n} \mathcal{U}^{\dagger}_{\Phi(x)} \mathcal{U}_{\Phi(x)} |0\rangle^{\otimes n}|^2$$

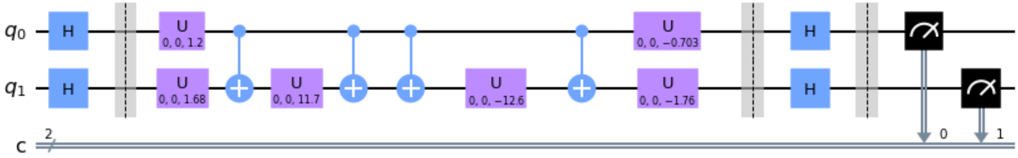


Figure 13 Parameterized Quantum Kernel Circuit.

Implementation of Quantum Support Vector Machines

Quantum Kernel Estimation

1. Build a parameterized quantum circuit that emulates a *quantum feature map* for each data pair.
2. Construct the *quantum kernel* circuits for each data pair.
3. **Measure the number of all zero strings 0^n.**

Implementation of Quantum Support Vector Machines

Quantum Kernel Estimation

1. Build a parameterized quantum circuit that emulates a *quantum feature map* each data pair.
2. Construct the *quantum kernel* circuits for each data pair.
3. Measure the number of all zero strings 0^n.
4. **Calculate the frequency of the zero strings to find the transition probability $\Longrightarrow$ Kernel entry of the the *quantum kernel*.**

Note**: Step 3. and 4. compute the kernel values from the results of the inner products based on the measurements of the quantum circuits created for the *quantum kernel estimate*.

Implementation of Quantum Support Vector Machines
Quantum Kernel Estimation

1. Build a parameterized quantum circuit that emulates a *quantum feature map* each data pair.
2. Construct the *quantum kernel* circuits for each data pair.
3. Measure the number of all zero strings 0^n.
4. Calculate the frequency of the zero strings to find the transition probability $\implies$ Kernel entry of the the *quantum kernel*.

Example:

- ☐ Given a dataset $\mathbf{X} \in \mathbb{R}^{10\times 2}$
- ☐ Build parameterized kernel circuit from parameterized feature map circuits for each data pair $\implies$ 100 circuits.

Implementation of Quantum Support Vector Machines

Quantum Feature Map and Quantum Kernel Estimation

Links to the implementation on GITHUB:

- quantum-feature-map
- quantum-kernel-estimation

Implementation of Quantum Support Vector Machines

Quantum SVC

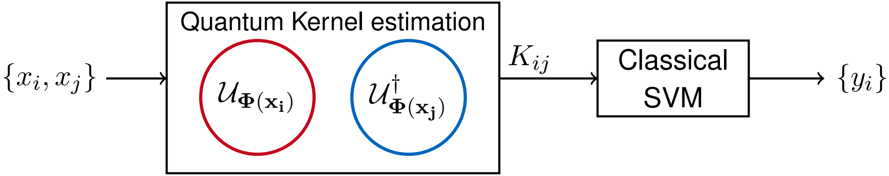
How is the Quantum Kernel embedded into the SVM protocol?

Implementation of Quantum Support Vector Machines

Quantum SVC

How is the Quantum Kernel embedded into the SVM protocol?

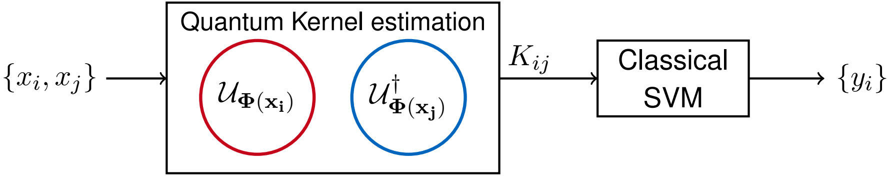
- Instead of using a classical kernel in the constraint optimization problem, eq. (25), just insert the quantum kernel estimate, eq. (44).



Implementation of Quantum Support Vector Machines
Quantum SVC

How is the Quantum Kernel embedded into the SVM protocol?

- Instead of using a classical kernel in the constraint optimization problem, eq. (25), just insert the quantum kernel estimate, eq. (44).



- Now we have a **Quantum Support Vector Machine**.

Outline

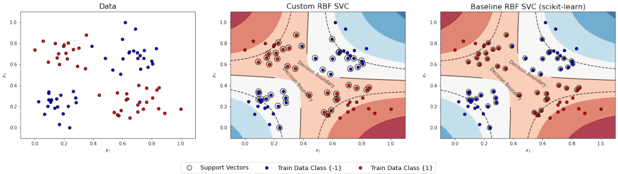
Results
Benchmark SVC

	Linear	Polynomoinal	Sigmoid	RBF C=10	RBF C=100
Linearly Separately Data	0.975	0.975	0.975	0.975	0.975
XOR Data	0.350	0.950	0.400	1.000	1.000
Circles Data	0.400	1.000	0.275	1.000	1.000
Moons Data	0.750	0.750	0.750	0.750	0.850
Adhoc Data	0.300	0.250	0.300	0.500	0.550

(a) Test accuracy Custom SVC.

	Linear	Polynomoinal	Sigmoid	RBF C=10	RBF C=100
Linearly Separately Data	0.975	0.975	0.95	0.975	0.975
XOR Data	0.500	0.950	0.35	1.000	1.000
Circles Data	0.400	0.800	0.30	1.000	1.000
Moons Data	0.750	0.725	0.75	0.725	0.875
Adhoc Data	0.350	0.300	0.40	0.500	0.550

(b) Test accuracy benchmark SVC.



(c) Example plot on XOR data.

Figure 14 Benchmark SVC.

Results
Benchmark Quantum Kernel

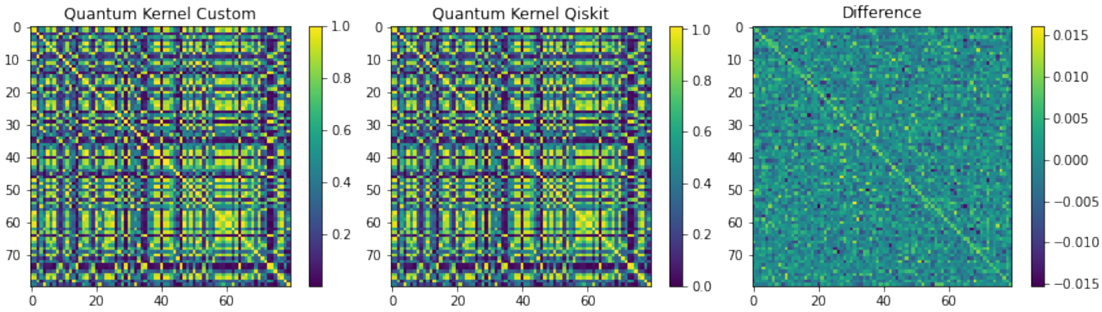


Figure 15 Comparison of Custom Quantum Kernel and QISKIT quantum kernel.

Results

Benchmark Quantum SVC

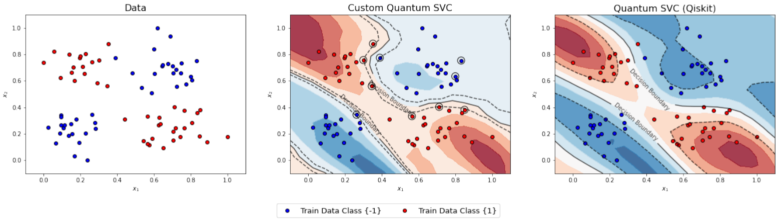


Figure 16 Comparison of Custom Quantum SVC and QISKIT baseline Quantum SVC.

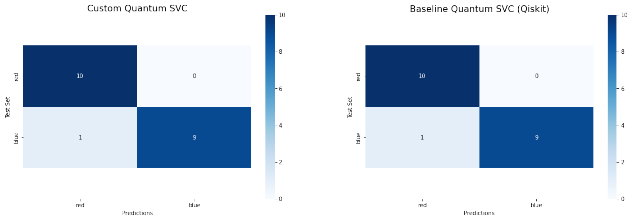


Figure 17 Confusion Matrices for custom Quantum SVC and SCIKIT baseline Quantum SVC.

Results

Comparison of Different Data Maps in QSVC

	Default Data Map	Exp Data Map	Sin Data Map	Cos Data Map
XOR Data	0.9375	1.000	1.0000	1.0000
Cirles Data	1.0000	1.000	1.0000	1.0000
Moons Data	0.6875	0.625	0.8125	0.8125
Adhoc Data	1.0000	0.500	0.7500	0.7500

Figure 18 Test accuracy of different data maps on different data.

Results

Comparison of the Z-Feature Map and the ZZ-Feature Map

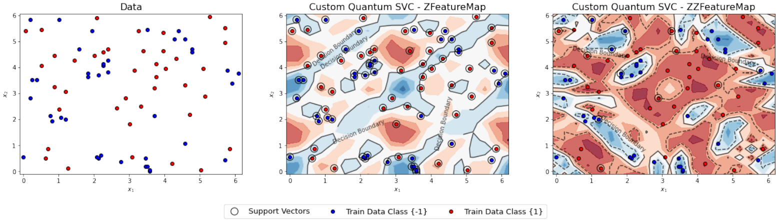


Figure 19 Comparison of the Z-Feature Map and the ZZ-Feature Map on the Adhoc data [7].

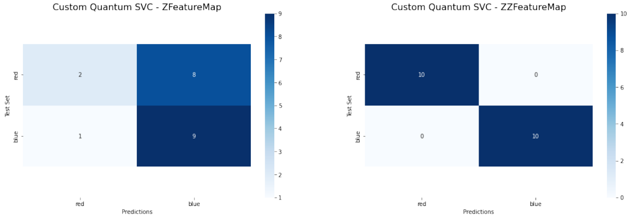


Figure 20 Confusion Matrix of Z-Feature Map and ZZ-Feature Map on the Adhoc data [7].

Results

Comparison of a Quantum Kernel and a RBF Kernel on Adhoc Data

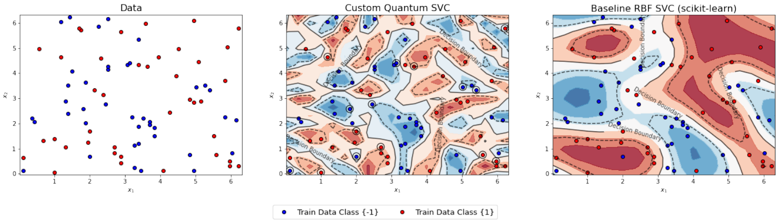


Figure 21 Benchmark on Adhoc data.

	Custom Quantum SVC	Custom RBF SVC
Adhoc Data	1.0	0.7

Figure 22 Test accuracy of custom QSVC and custom rbf SVC.

Results

Comparison of Different Kernels on Different Data

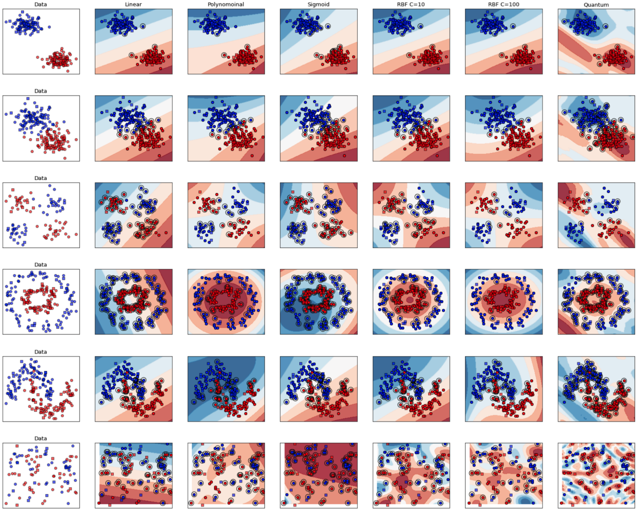


Figure 23 Comparison of different classification models.

Results

Comparison of Different Kernels on Different Data

	Linear	Polynomoinal	Sigmoid	RBF C=10	RBF C=100	Quantum
Linearly Separately Data	0.975	0.975	0.975	0.975	0.975	0.950
XOR Data	0.350	0.950	0.400	1.000	1.000	0.950
Circles Data	0.400	1.000	0.275	1.000	1.000	0.975
Moons Data	0.750	0.750	0.750	0.750	0.850	0.850
Adhoc Data	0.300	0.250	0.300	0.500	0.550	1.000

Figure 24 Comparison of different classification models.

Results
Conclusion

- Implemented a classical Support Vector Machine.
- Implemented a Quantum Kernel Estimation.
- Implemented a Quantum Support Vector Classifier.
- Benchmarked the custom implementations against implementations of established libraries.
- Showed that quantum kernels can perform better on high dimensional data.

- **Potential Improvements**:
  - Improve efficiency of code:
    - Remove unnecessary for-loops
    - Mirror quantum kernel in estimation as $K_{ij} = K_{ji}$
    - Initialize the diagonal elements as 1
  - Implement a general Pauli-Feature Map.
  - Implement a state vector calculation scheme for the quantum kernel estimation.

Outline

References I

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