Quantum Circuit Learning and SVM

Faris Sbahi

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Quantum Circuit Learning

Introduction

- Approximate any analytical function (with sufficient number of qubits)
- Hybrid classical-quantum algorithm
- Parameterize quantum gates by some θ, optimize θ iteratively using gradient descent or the like
- Low-depth quantum circuit. Goal: realizable near-term

Quantum Circuit Learning

Algorithm

- Inputs: training data $\{\vec{x}_i\}$ with outputs $\{f(\vec{x}_i)\}$
- Outputs: $\{y_i\}$ which closely approximates $\{f(\vec{x}_i)\}$.
- In particular, minimizes some loss function (locally) e.g. quadratic loss for least-squares $\sum_i |y_i - f(\vec{x}_i)|^2$

Quantum Circuit Learning

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1. Encode data into quantum state. $|\psi_{in}(\vec{x_i})\rangle = U(\vec{x_i})\,|0\rangle$ for some unitary U
2. Apply θ-parameterized unitary. $|\psi_{out}(\vec{x_i})\rangle = U(\theta)\,|\psi_{in}(\vec{x_i})\rangle$
3. Measure expectation of some tensor products of Paulis i.e. some set of operators $\{B_j\} \subseteq \{I, X, Y, Z\}^{\otimes N}$. Output $y_i \equiv g(\{\langle B_j(\vec{x_i})\rangle\})$ using some function g.
4. Minimize loss L by tuning θ iteratively
5. Evaluate L on validation set $\{\vec{v_i}\}$ disjoint from $\{\vec{x_i}\}$

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Why QCL?

- Closed form exists for least-squares (orthogonal projection of vector of y_i's onto the column space of the data matrix)
- Hence, we can use HHL. But requires high depth.
- With QCL, we can solve iteratively and use a short-depth circuit

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Example

- Consider 1-d input $\{x_i\}$
- Let $\{P_k\} = \{I, X, Y, Z\}^{\otimes N}$
- Expand $\rho_{in}(x) = |\psi_{in}(x)\rangle \langle\psi_{in}(x)| = \sum_k a_k P_k$
- Similarly, $\rho_{out}(x) = U(\theta)\rho_{in}(x)U(\theta)^\dagger = \sum_k b_k P_k$
- $b_m = \sum_k U_{(m,k)} a_k$ since this is a unitary change of basis
- Therefore, expectation measurement is a linear combination of input coefficients
- Constraint: row vector $U_{(m,k)}$ has unit norm for fixed m

Quantum Circuit Learning

Example

- Recall that for a single qubit, $\rho = \frac{1}{2}[I + \vec{a} \cdot \sigma]$, $|a| \leq 1$
- Rotate $a = (0, 0, 1)$ about Y axis by some $\theta = \sin^{-1}(x_{in})$ for each of N qubits and call this ρ_{in}
- $\rho_{in} = \frac{1}{2^N} \otimes_{i=1}^{N} [I + xX_i + \sqrt{1 - x^2} Z_i]$
- Hence, unitary transformation can give arbitrary N^{th} order polynomial
- Generalize to d dimensional input

Quantum Circuit Learning

Compute Gradient

- Assume chain of unitary transformations $U_{l:1}(\theta)$
- $\langle B(\theta)\rangle = \mathrm{tr}\big(BU_{l:1}(\theta)\rho_{in}U_{l:1}(\theta)^{\dagger}\big)$
- Assume $U_j(\theta) = \exp(-i\theta P_j/2)$ for pauli product P_j
- $\frac{\partial\langle B\rangle}{\partial\theta_j} = -\frac{i}{2}\,\mathrm{tr}\Big(BU_{l:1}[B, U_{j-1:1}\rho_{in}U^{\dagger}_{j-1:1}]U^{\dagger}_{l:j}\Big)$
- Use identity for commutator of arbitrary ρ with a Pauli product
- Gives gradient in terms of additional $U(\pm\pi/2)$ transformations

$$\frac{\partial\langle B\rangle}{\partial\theta_j} = \frac{1}{2}\mathrm{Tr}\left[BU_{l:j+1}U_j\left(\frac{\pi}{2}\right)\rho_j U_j^{\dagger}\left(\frac{\pi}{2}\right)U^{\dagger}_{l:j+1}\right] - \frac{1}{2}\mathrm{Tr}\left[BU_{l:j+1}U_j\left(-\frac{\pi}{2}\right)\rho_j U_j^{\dagger}\left(-\frac{\pi}{2}\right)U^{\dagger}_{l:j+1}\right]$$

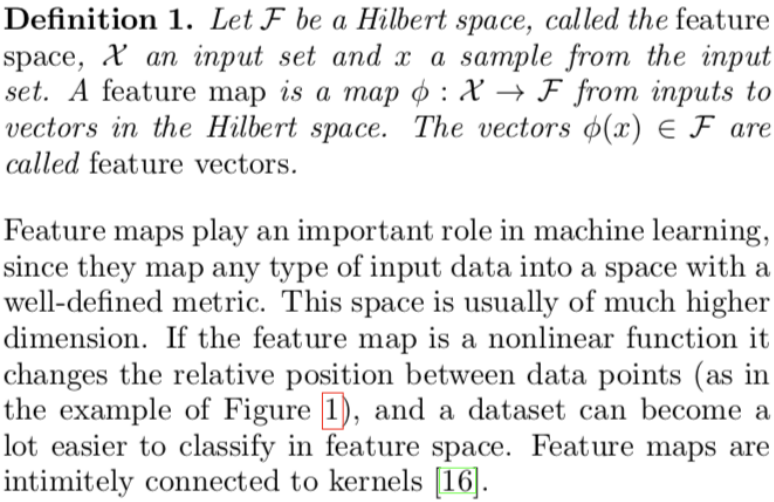
SVM

Kernels

- Linear classifier (e.g. perceptron): perform binary classification by separating labels in feature space with hyperplane.
- Data is not always separable
- Idea: Map data to higher dimensional space where data is separable
- Kernel function does this implicitly by providing a means to compute the inner product in that space

SVM

Kernels

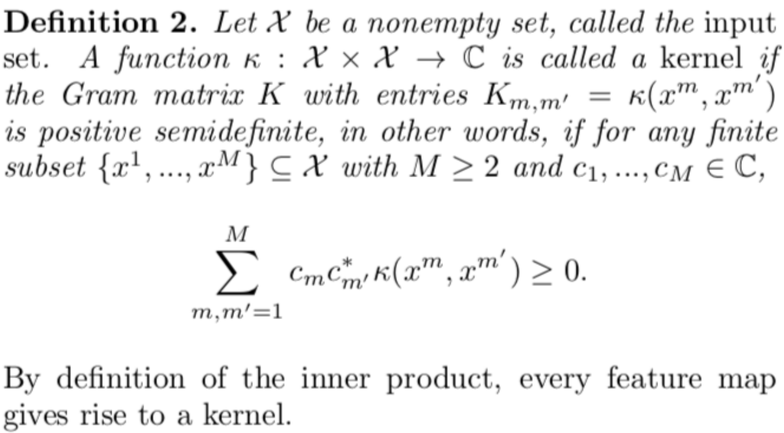


Definition 1. *Let $\mathcal{F}$ be a Hilbert space, called the* feature space, *$\mathcal{X}$ an input set and x a sample from the input set. A* feature map *is a map $\phi : \mathcal{X} \rightarrow \mathcal{F}$ from inputs to vectors in the Hilbert space. The vectors $\phi(x) \in \mathcal{F}$ are called* feature vectors.

Feature maps play an important role in machine learning, since they map any type of input data into a space with a well-defined metric. This space is usually of much higher dimension. If the feature map is a nonlinear function it changes the relative position between data points (as in the example of Figure 1), and a dataset can become a lot easier to classify in feature space. Feature maps are intimitely connected to kernels [16].

SVM

Kernels



Definition 2. *Let $\mathcal{X}$ be a nonempty set, called the* input set. *A function $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C}$ is called a* kernel *if the Gram matrix K with entries $K_{m,m'} = \kappa(x^m, x^{m'})$ is positive semidefinite, in other words, if for any finite subset $\{x^1, ..., x^M\} \subseteq \mathcal{X}$ with $M \geq 2$ and $c_1, ..., c_M \in \mathbb{C}$,*

$$\sum_{m,m'=1}^{M} c_m c_{m'}^* \kappa(x^m, x^{m'}) \geq 0.$$

By definition of the inner product, every feature map gives rise to a kernel.

SVM

Kernels

Theorem 1. *Let $\phi : \mathcal{X} \to \mathcal{F}$ be a feature map. The inner product of two inputs mapped to feature space defines a kernel via*

$$\kappa(x, x') := \langle \phi(x), \phi(x') \rangle_{\mathcal{F}}, \tag{1}$$

where $\langle \cdot, \cdot \rangle_{\mathcal{F}}$ is the inner product defined on $\mathcal{F}$.

Proof. We must show that the Gram matrix of this kernel is positive definite. For arbitrary $c_m, c_{m'} \in \mathbb{C}$ and any $\{x^1, ..., x^M\} \subseteq \mathcal{X}$ with $M \geq 2$, we find that

$$\begin{aligned} \sum_{m,m'=1}^{M} c_m c_{m'}^* \kappa(x_m, x_{m'}) &= \langle \sum_{m} c_m \phi(x_m), \sum_{m'} c_{m'} \phi(x_{m'}) \rangle \\ &= || \sum_{m} c_m \phi(x_m) ||^2 \geq 0 \end{aligned}$$

□

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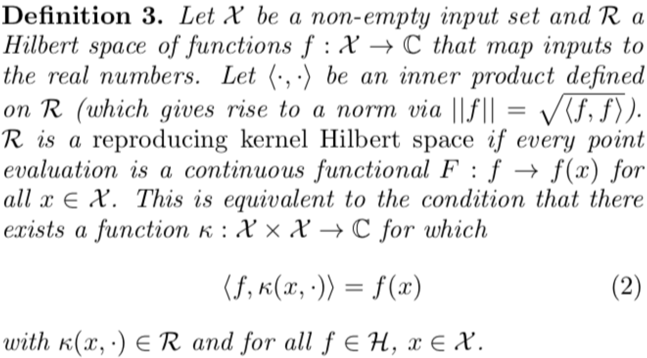
Kernels



Definition 3. *Let $\mathcal{X}$ be a non-empty input set and $\mathcal{R}$ a Hilbert space of functions $f : \mathcal{X} \to \mathbb{C}$ that map inputs to the real numbers. Let $\langle \cdot, \cdot \rangle$ be an inner product defined on $\mathcal{R}$ (which gives rise to a norm via $||f|| = \sqrt{\langle f, f \rangle}$). $\mathcal{R}$ is a* reproducing kernel Hilbert space *if every point evaluation is a continuous functional $F : f \to f(x)$ for all $x \in \mathcal{X}$. This is equivalent to the condition that there exists a function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ for which*

$$\langle f, \kappa(x, \cdot) \rangle = f(x) \tag{2}$$

with $\kappa(x, \cdot) \in \mathcal{R}$ and for all $f \in \mathcal{H}$, $x \in \mathcal{X}$.

- Can construct unique RKHS for any feature map
- Mercer's Theorem: If kernel k is positive, we can expand k (as a uniformly convergent series) in terms of eigenfunctions and eigenvalues of a positive operator that come from k.
- Representer Theorem: Even if were trying to solve an optimization problem in an infinite dimensional space H_k containing linear combinations of kernels centered on arbitrary x_i's, then the solution lies in the span of the n kernels centered on the x_is.

SVM

Optimization – Dual Formulation

$$\begin{aligned}\text{maximize } f(c_1 \ldots c_n) &= \sum_{i=1}^{n} c_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i c_i (\varphi(\vec{x}_i) \cdot \varphi(\vec{x}_j)) y_j c_j \\ &= \sum_{i=1}^{n} c_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i c_i k(\vec{x}_i, \vec{x}_j) y_j c_j\end{aligned}$$

$$\text{subject to } \sum_{i=1}^{n} c_i y_i = 0, \text{ and } 0 \leq c_i \leq \frac{1}{2n\lambda} \text{ for all } i.$$

- Use quadratic programming, coordinate descent, gradient descent, SMO...
- Representer's Theorem
- Only ever need to evaluate inner product in RKHS to train and test model

SVM

Explicit Classification

- Encode data, just as with QCL. This time, encode data under feature map transformation directly.
- $U_\phi(x)\,|0\rangle^N = |\Phi(x)\rangle$
- Hence, $K(x,z) = |\,\langle\phi(x)|\phi(z)\rangle\,|^2$
- Map must be hard to compute classically. Simple kernel like RBF allows efficient classical computation in infinite-dimensional Hilbert space. Large quantum Hilbert space is not enough.

SVM

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- Consider feature map $U_\phi(x) = V_{\phi(x)} H^{\otimes n} V_{\phi(x)} H^{\otimes n}$ where $V_{\phi(x)} = exp\Big(i \sum\limits_{S \subseteq [n]} \phi_S(x) \prod_{i \in S} Z_i\Big)$, $|S| \leq 2$
- Conjecture: Classical evaluation of inner products generated from circuits with two basis changes and diagonal gates up to additive error is "hard"

SVM

Havlicek et al

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- Conjecture: Classical evaluation of inner products generated from circuits with two basis changes and diagonal gates up to additive error is "hard"
- $n = d = 2$ qubits
- $\phi_{\{i\}}(\vec{x}) = x_i$ and $\phi_{\{1,2\}} = (\pi - x_1)(\pi - x_2)$ with $\vec{x} \in (0, 2\pi]^2$
- Take some random unitary $V \in SU(4)$ and defined data "gap" $\Delta = 0.3$.
- Then, we define $\langle \Phi(x) | V^\dagger Z_1 Z_2 V | \Phi(x) \rangle \geq \Delta \implies +1$ label and -1 otherwise

SVM

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- Now, apply θ-parameterized layers of l unitaries. $\theta \in \mathbb{R}^{2N(l+1)}$
- For binary classication, $y \in \{+1, -1\}$.
- In our case, $\vec{f} = Z_1 Z_2$ and $0 \leq l \leq 4$
- Measure $M_y = \frac{1}{2}(I + y\vec{f})$ with $\vec{f} = \sum_{z \in \{0,1\}^N} f(z) \left|z\right\rangle \left\langle z\right|$ and $f : \{0, 1\}^n \to \{+1, -1\}$
- Obtain empricial distribution $p_y(x)$ which is expectation of M_y sampled with repeated shots
- Classify by comparing $p_y(+1)$ to $p_{-1}(x)$ (can add bias as well)
- Define loss function to be average number of missclassifications

SVM

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- How is this SVM?
- Decision rule for label:
  $m(x) = sgn(\langle\Phi(x)| W^{\dagger}(\theta)\vec{f}W(\theta) |\Phi(x)\rangle$
- Decompose density operator ρ_{in} and ρ_{out} in *Pauli* product basis $\{P_\alpha\}$.
- Expectation value of binary measurement and decision rule can be expressed in terms of $w_\alpha(\theta) = \mathrm{tr}\left[W^{\dagger}(\theta)\vec{f}W(\theta)P_\alpha\right]$ and $\Phi_\alpha(x) = \langle\Phi(x)| P_\alpha |\Phi(x)\rangle$
- $m(x) = sgn(1/2^N \sum_\alpha w_\alpha(\theta)\Phi_\alpha(x))$. SVM separating hyperplane.
- Decomposition shows we should think of $|\phi(x)\rangle\langle\phi(x)|$ as the feature vectors i.e. feature vectors don't live directly in the Hilbert space $H = (\mathbb{C}^2)^{\otimes N}$. As expected, since global phase would make this problematic.