

Draft Handout 7: Kernel methods

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Aim. To introduce the ideas of learning machines by introducing data into high-dimensional feature spaces for accuracy gains; introduce the kernel trick, and kernel functions.

Reading list & references:

- (1) Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
 - Ch. 16.2 Support Vector Machine
- (2) Bishop, C. M. (2006). Pattern recognition and machine learning (Vol. 4, No. 4, p. 738). New York: Springer.
 - Ch. 6.1, 6.2 Kernel methods

1. INTRO AND MOTIVATION

Note 1. Consider the Soft SVM with predictive rule $h(x) = \text{sign}(\eta(x))$ with separator $\eta(x) = w_1x_1 + w_2x_2 + b = \langle w, x \rangle + b$ and $x \in \mathbb{R}^2$. It can address learning problems where the data can (up to some degree of violation) be separated by a line (Figure 1.1a). In more challenging cases where the geometry is strongly non-linear this can totally fail (Figure 1.1b).

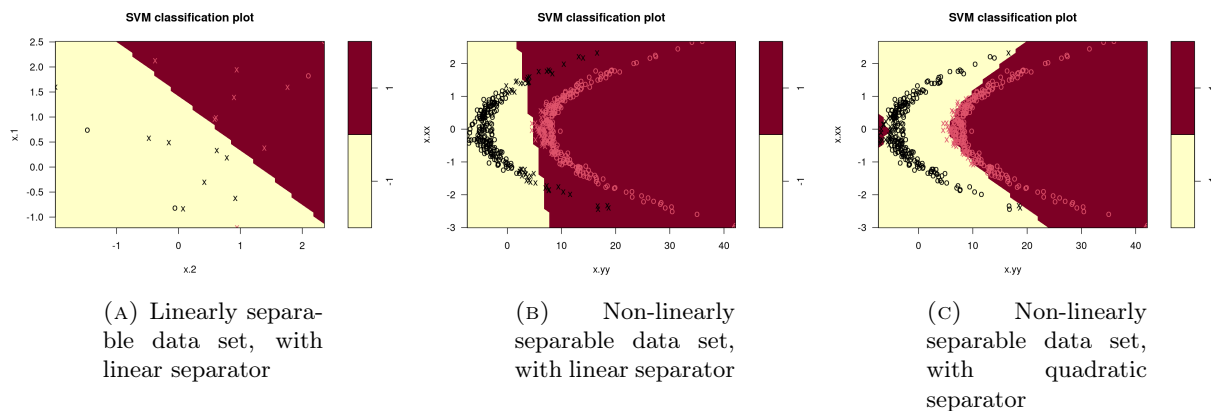


FIGURE 1.1. Soft SVM from Computer practical 4

Note 2. The accuracy of predictive rule can be improved if I take into account the curvature by adding a quadratic term in the 2nd dimension as $\eta'(x) = w'_1x_1 + w'_2x_2 + w'_2x_3 + b = \langle w', \psi(x) \rangle + b$ where $\psi(x) = (x_1, x_2, x_2^2)$ and learning the w' . It works, (Figure 1.1c).

Note 3. Consequently, in order to improve the expressiveness of a hypothesis class $\mathcal{H} = \{x \mapsto f(\langle w, x \rangle)\}$ (for some function f) with purpose to learn a more accurate predictive rule, it is reasonable to consider an embedding $\psi(x)$, which can possibly be a vector of bases functions such as polynomials, splines, etc..., and work on the learning problem with $\mathcal{H} = \{x \mapsto f(\langle w, \psi(x) \rangle)\}$.

Note 4. The above may drastically increase the dimensionality of the problem hence the computational cost and required number of example to train. This challenge is addressed by the Kernel trick.

Note 5. In general, kernel trick allows the design of powerful and cheap extensions of many well known algorithms.

2. IMPROVING EXPRESSIVE POWER

Note 6. To make the class of hypotheses more expressive with purpose to improve accuracy, we can first map the original instance space $x \in \mathcal{X}$ into another space \mathcal{F} (possibly of a higher dimension) via an embedding ψ and then learn a hypothesis in that space.

Summary 7. Consider a hypothesis class $\mathcal{H} = \{x \mapsto \langle w, x \rangle : w \in \mathbb{R}^n\}$ where the predictive rule $h \in \mathcal{H}$ defined over \mathcal{X} is to be trained against data set $\mathcal{S} = \{z_i = (x_i, y_i)\}_{i=1}^m$. The basic paradigm involves:

- (1) Choose a mapping $\psi : \mathcal{X} \rightarrow \mathcal{F}$ with $\psi(x) := (\psi_1(x), \dots, \psi_d(x))$ for some feature space \mathcal{F} .
- (2) Create the image sequence $\tilde{\mathcal{S}} = \{z_i^\psi = (\psi(x_i), y_i)\}_{i=1}^m$ from the original training set \mathcal{S} .
- (3) Train a linear predictor h against $\tilde{\mathcal{S}}$.
- (4) Predict the label or the output of a new point x^{new} by $h^\psi(x^{\text{new}}) := h \circ \psi(x^{\text{new}}) = h(\psi(x^{\text{new}}))$

Note 8. The introduction of mapping $\psi : \mathcal{X} \rightarrow \mathcal{F}$ induces

- (1) probability distribution G^ψ over domain $\mathcal{X} \times \mathcal{F}$ with $G^\psi(A) = G(\psi^{-1}(A))$ for every set $A \subseteq \mathcal{X} \times \mathcal{F}$.
- (2) predictive rule $h^\psi(\cdot) := h \circ \psi(\cdot)$, where $h \circ \psi(\cdot) = h(\psi(\cdot))$
- (3) risk function $R_{G^\psi}(h) := R_G(h \circ \psi)$, as

$$R_G(h \circ \psi) = \int \ell(h \circ \psi, z = (x, y)) dG(z) = \int \ell(h, z^\psi) dG^\psi(x, y) = R_{G^\psi}(h)$$

Definition 9. A Hilbert space is a vector space, with an inner product, which is also complete¹.

Lemma 10. If \mathcal{X} is a linear subspace of a Hilbert space, then every $x \in \mathcal{X}$ can be written as $x = u + v$ where $u \in \mathcal{X}$ and $\langle u, v \rangle = 0$ for all $v \in \mathcal{X}$.

Note 11. Feature space \mathcal{F} is a Hilbert space preferably due to Lemma 10 that enables the Kernel trick via the representation Theorem 20. Eg, a Euclidean space such as \mathbb{R}^d for some d . That includes infinite dimensional spaces.

Note 12. As feature mapping ψ any function that maps the original instances \mathcal{X} into some Hilbert space \mathcal{F} can be used.

¹Going deeper to completeness is out of the scope.

Note 13. The success of the learning paradigm in Summary 7 depends on choosing a good embedding ψ for the particular learning task. Eg, in SVM, ψ will make the image of the data distribution (close to being) linearly separable in the feature space \mathcal{F} , thus making the resulting learning algorithm a good learner for a given task. This requires prior knowledge of the problem (In Section 4, we see popular recipes for that).

Note 14. Using a $\psi(x) := (\psi_1(x), \dots, \psi_d(x))$ that is high dimensional (d is too large) may improve accuracy (expressiveness) of the learner (e.g. recall in polynomial regression increasing the polynomial degree). However this increases the computational effort/cost required to perform calculations to minimize the associated risk function in the high dimensional space, as well as we need more data. This is addressed via the Kernel trick.

3. THE KERNEL TRICK

Definition 15. Kernel function K is defined as $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ with $K(x, x') = \langle \psi(x), \psi(x') \rangle$ given an embedding $\psi(x)$ of some domain space \mathcal{X} into some Hilbert space \mathcal{F} . Kernel functions describe inner products in the feature space \mathcal{F} .

Note 16. Kernel function K can be considered as specifying similarity between instances via the embedding $\psi(\cdot)$ as mapping the domain set \mathcal{X} into a space where these similarities are realized as inner products.

Problem 17. (Learning problem) Consider a prediction rule $h : \mathcal{X} \rightarrow \mathcal{Y}$ with $h(x) = \langle w, \psi(x) \rangle$ which is trained against a training sample $\{z_i = (x_i, y_i)\}_{i=1}^m$ with the following general optimization problem

$$(3.1) \quad \underset{w}{\text{minimize}} \left(f(\langle w, \psi(x_1) \rangle, \dots, \langle w, \psi(x_m) \rangle) + R(\|w\|) \right),$$

where $f : \mathbb{R}^m \rightarrow \mathbb{R}$ is an arbitrary function and $R : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a monotonically non-decreasing function.

Example 18. In Soft SVM (Proposition 24, Handout 6), it is $f(a_1, \dots, a_m) = \frac{1}{m} \sum_{i=1}^m \max\{0, 1 - y_i a_i\}$ and $R(a) = \lambda a^2$.

Note 19. The following result states a duality in the learning problem 17 that facilitates the implementation of the extension to a possibly high dimensional feature space (hence improving the expressiveness/accuracy) by using kernel functions (hence reducing dimensionality, computational cost, and required data size).

Theorem 20. (Representation theorem) Assume mapping $\psi : \mathcal{X} \rightarrow \mathcal{F}$ where \mathcal{F} is a Hilbert space. There exists a vector $\alpha \in \mathbb{R}^m$ such that $w = \sum_{i=1}^m \alpha_i \psi(x_i)$ is the optimal solution of (3.1) in Problem 17.

Proof. Let w^* be the optimal solution of (3.1). Because w^* is element of Hilbert space, it can be written as $w^* = \sum_{i=1}^m \alpha_i \psi(x_i) + u$ where $\langle u, \psi(x_i) \rangle = 0$ for all $i = 1, \dots, m$. Set $w := w^* - u$.

Because $\|w^*\|^2 = \|w\|^2 + \|u\|^2$ it is $\|w\| \leq \|w^*\|$ implying that

$$R(\|w\|) \leq R(\|w^*\|).$$

Because $\langle w, \psi(x_i) \rangle = \langle w^* - u, \psi(x_i) \rangle = \langle w^*, \psi(x_i) \rangle$ for all $i = 1, \dots, m$, it is

$$f(\langle w, \psi(x_1) \rangle, \dots, \langle w, \psi(x_m) \rangle) = f(\langle w^*, \psi(x_1) \rangle, \dots, \langle w^*, \psi(x_m) \rangle)$$

Then the objective function of (3.1) at w is less than or equal to that of the minimizer w^* which implies that $w = \sum_{i=1}^m \alpha_i \psi(x_i)$ is an optimal solution. \square

Note 21. Let $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a kernel function with $K(x, x') = \langle \psi(x), \psi(x') \rangle$. According to the representation Theorem 20, the Learning problem 17, can be equivalently addressed by re-writing the learning predictive rule as

$$h_\alpha(x) = \sum_{i=1}^m \alpha_i K(x_i, x)$$

and learning $\{\alpha_i\}$ as the solutions of

$$(3.2) \quad \underset{\alpha}{\text{minimize}} \left(f \left(\sum_{i=1}^m \alpha_i K(x_i, x), \dots, \sum_{i=1}^m \alpha_i K(x_m, x) \right) + R \left(\sqrt{\sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j K(x_i, x_j)} \right) \right),$$

This is because

$$\langle w, \psi(x_j) \rangle = \left\langle \sum_{i=1}^m \alpha_i \psi(x_i), \psi(x_j) \right\rangle = \sum_{i=1}^m \alpha_i \langle \psi(x_i), \psi(x_j) \rangle = \sum_{i=1}^m \alpha_i K(x_i, x_j)$$

and

$$\|w\|^2 = \left\langle \sum_{i=1}^m \alpha_i \psi(x_i), \sum_{j=1}^m \alpha_j \psi(x_j) \right\rangle = \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j \langle \psi(x_i), \psi(x_j) \rangle = \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j K(x_i, x_j)$$

Example 22. In Soft SVM (Proposition 24, Handout 6), we can have

$$\underset{\alpha}{\text{minimize}} \left(\lambda \sum_i \sum_j \alpha_i \alpha_j K(x_i, x_j) + \frac{1}{m} \sum_i \max \left(0, 1 - y_i \sum_j \alpha_j K(x_i, x_j) \right) \right)$$

for $h(x) = \text{sign} \left(\sum_j \alpha_j K(x_i, x_j) \right)$. It can be minimised via SGD. As we can just directly specify the kernel function without the need to even think about feature mapping $\psi(\cdot)$ (which is eliminated and replaced by the kernel), we can call it Kernel SVM.

Note 23. In Learning problem 17, direct access to elements $\psi(\cdot)$ in the feature space is not necessary, as equivalently one can calculate or just specify the associated kernel function (that is inner products in the feature space).

Example 24. (Polynomial Kernels) Let $x \in \mathcal{X} \subseteq \mathbb{R}^n$. Assume we want to extend the linear mapping $x \mapsto \langle w, x \rangle$ to the k degree polynomial mapping $x \mapsto h(x)$. The multivariate polynomial can be written as $h(x) = \langle w, \psi(x) \rangle$, where $\psi : \mathbb{R}^n \rightarrow \mathbb{R}^d$ with $\psi(x)$ is a vector of elements $\psi_J(x) = \prod_{i=1}^r x_{J_i}$ for $J \in \{1, \dots, n\}^r$ and $r \leq k$. This learning problem can be equivalently be addressed with the k

degree polynomial kernel

$$K(x, x') = (1 + \langle x, x' \rangle)^k$$

Solution. It is

$$\begin{aligned} K(x, x') &= (1 + \langle x, x' \rangle)^k = \left(\sum_{j=0}^n x_j x'_j \right)^k \quad (\text{by setting } x_0 = x'_0 = 1) \\ &= \sum_{J \in \{1, \dots, n\}^k} \prod_{i=0}^n x_{J_i} x'_{J_i} = \sum_{J \in \{1, \dots, n\}^k} \left(\prod_{i=0}^n x_{J_i} \right) \left(\prod_{i=0}^n x'_{J_i} \right) \\ &= \langle \psi(x), \psi(x') \rangle \end{aligned}$$

where $\psi(x)$ is as defined.

4. CONSTRUCTION OF KERNELS

Note 25. The kernel formulated as an inner product in a feature space allows us to build interesting extensions of many well-known algorithms by making use of the kernel trick and without the need to have direct access to the feature space.

Note 26. Specifying a kernel function is a way to express prior knowledge without the need to have direct access to the feature space. This is consequence of the Representation theorem 20 that kernel is the inner product of feature mappings ψ which sufficiently replaces them in the learning problem, and the fact that ψ is a way to express and utilize prior knowledge about the problem at hand.

Note 27. The question is whether the specified function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ (by the practitioner) is indeed a kernel function; i.e. if K can be written as inner product $K(x, x') = \langle \psi(x), \psi(x') \rangle$ of feature functions $\psi(x)$. Theorem 30 provides sufficient and necessary conditions to check that.

Definition 28. Gram matrix is called the $m \times m$ matrix G s.t. $[G]_{i,j} = K(x_i, x_j)$.

Definition 29. A symmetric function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is positive semi-definite if its Gram matrix G , $[G]_{i,j} = K(x_i, x_j)$, is a positive semi-definite matrix.

Theorem 30. A symmetric function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ implements an inner product in some Hilbert space if and only if it is positive semi-definite i.e. its Gram matrix G , $[G]_{i,j} = K(x_i, x_j)$, is a positive semi-definite matrix.

Proof. Assume K implements an inner product $K(x, x') = \langle \psi(x), \psi(x') \rangle$ in some Hilbert space; let's consider $\psi : \mathcal{X} \rightarrow \mathbb{R}^d$ for simplicity. Let G be its Gram matrix with $G = \Psi^\top \Psi$ and $\psi(x_i)$ is the i -th column of Ψ . For any $\xi \in \mathbb{R}^d - \{0\}$

$$\begin{aligned} \xi^\top G \xi &= \sum_i \sum_j \xi_i K(x_i, x_j) \xi_j = \sum_i \sum_j \xi_i \langle \psi(x_i), \psi(x_j) \rangle \xi_j = \sum_i \sum_j \langle \xi_i \psi(x_i), \psi(x_j) \xi_j \rangle \\ &= \left\langle \sum_i \xi_i \psi(x_i), \sum_j \psi(x_j) \xi_j \right\rangle = \left\| \sum_i \xi_i \psi(x_i) \right\|_2^2 \geq 0 \end{aligned}$$

Assume the symmetric function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is positive semi-definite. Let $\mathbb{R}^f = \{f : \mathcal{X} \rightarrow \mathbb{R}\}$. For $x \in \mathcal{X}$ let function ψ over \mathbb{R}^f with $\psi(x) = K(\cdot, x)$. This allows to define a vector space consisting of all the linear combinations of elements of the form $K(\cdot, x)$, having an inner product

$$\left\langle \sum_i \alpha_i K(\cdot, x_i), \sum_j \beta_j K(\cdot, x_j) \right\rangle = \sum_i \sum_j \alpha_i \beta_j \underbrace{\langle K(\cdot, x_i), K(\cdot, x_j) \rangle}_{=K(x_i, x_j)}.$$

This satisfies all the properties of inner product, s.t. it is symmetric, linearity, positive definite as $K(x, x) \geq 0$. Then there is some feature vector ψ such that $K(x, x') = \langle \psi(x), \psi(x') \rangle$. \square

Claim 31. In Figure 1.1c, we could see that examples can be distinguished by some ellipse, so it was reasonable to we can define ψ as a vector with elements all the monomials up to order d ; alternatively we could use a degree 2 polynomial kernel.

Example 32. Consider two kernel functions $K_1 : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ and $K_2 : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$. Show that K_3 with $K_3(x, x') = K_1(x, x') + K_2(x, x')$ is a kernel function.

Solution. Let Gram matrix, G_j induced by kernel function K_j . For any $\xi \in \mathbb{R}^d - \{0\}$, it is

$$\xi^\top G_3 \xi = \xi^\top (G_1 + G_2) \xi = \xi^\top G_1 \xi + \xi^\top G_2 \xi \geq 0$$

that completes the proof according to Lemma 30.

5. IMPLEMENTATIONS

Note 33. The concept of a kernel formulated as an inner product in a feature space allows us to build interesting extensions of many well-known algorithms by making use of the kernel trick. One example was the Kernel SVM. We see some popular cases, below.

5.1. **Gaussian process regression.**

5.2. **Kernel PCA (maybe).**