Kernel Ridge Regression and the Kernel Trick

Machine Learning Course - CS-433

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Equivalent formulation for Ridge regression

$$\min_{w} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \frac{\lambda}{2} \|w\|^2$$

The solution is given by

$$w_* = \underbrace{\left(\mathbf{X}^\top \mathbf{X} + \lambda I_d\right)}_{\mathbf{X}^\top \in \mathbb{R}^{d \times n} \;\; \to \;\; d \times d}{}^{-1} \mathbf{X}^\top \mathbf{y}$$

But it can be alternatively written as

$$w_* = \mathbf{X}^\top \underbrace{\left(\mathbf{X}\mathbf{X}^\top + \lambda I_n\right)}_{\mathbf{X} \in \mathbb{R}^{n \times d} \;\; \to \;\; n \times n}{}^{-1} \mathbf{y}$$

Proof: let $P \in \mathbb{R}^{m\times n}$ and $Q \in \mathbb{R}^{n\times m}$

$$P(QP + I_n) = PQP + P = (PQ + I_m)P$$

Assume that $QP + I_n$ and $PQ + I_m$ are invertible

$$(PQ + I_m)^{-1}P = P(QP + I_n)^{-1}$$

We get the result with $P = \mathbf{X}^\top$ and $Q = \frac{1}{\lambda}\mathbf{X}$

$$w_* = \Big(\underbrace{\mathbf{X}^\top\mathbf{X} + \lambda I_d}\Big)^{-1}\mathbf{X}^\top\mathbf{y}$$

$$\mathbf{X}^\top \in \mathbb{R}^{d\times n} \quad \rightarrow \quad d \times d$$

But can be alternatively written as

$$w_* = \mathbf{X}^\top\Big(\underbrace{\mathbf{X}\mathbf{X}^\top + \lambda I_n}\Big)^{-1}\mathbf{y}$$

$$\mathbf{X} \in \mathbb{R}^{n\times d} \quad \rightarrow \quad n \times n$$

Usefulness of the alternative form

$$w_* = \underbrace{\mathbf{X}^\top}_{d\times n} \big(\underbrace{\mathbf{X}\mathbf{X}^\top + \lambda I_n}_{n\times n}\big)^{-1} \mathbf{y}$$

1. Computational complexity:
   - For the original formulation $(\mathbf{X}^\top\mathbf{X} + \lambda I_d)^{-1}\mathbf{X}^\top\mathbf{y},\ O(d^3 + nd^2)$
   - For the new formulation $\mathbf{X}^\top(\mathbf{X}\mathbf{X}^\top + \lambda I_n)^{-1}\mathbf{y},\ O(n^3 + dn^2)$

   ➡ Depending on d, n one can be more efficient than the other

2. Structural difference:

$$w_* = \mathbf{X}^\top \alpha_* \ \text{ where } \ \alpha_* = (\mathbf{X}\mathbf{X}^\top + \lambda I_n)^{-1}\mathbf{y}$$

   ➡ $w_* \in \text{span}\{x_1, \cdots, x_n\}$

These two points are the crucial ingredients of the **kernel trick**

Representer Theorem

Claim: For any loss function ℓ, if $w_* = \arg\min_w \sum_{i=1}^{n} \ell(x_i^\top w, y_i) + \frac{\lambda}{2}\|w\|^2$

then there exists $\alpha_* \in \mathbb{R}^n$ such that

$$w_* = \mathbf{X}^\top \alpha_*$$

Meaning: There exists an optimal solution that lies in span$\{x_1, \cdots, x_n\}$

Consequence: It is far more general than LS and we will be able to use the kernel tricks for various problems such as: Kernel SVM, Kernel LS, Kernel Principal Component Analysis

Wahba, G. *Spline models for observational data*. SIAM. 1990
Schölkopf, B., Herbrich, R., & Smola, A. J. *A generalized representer theorem.* COLT*. 2001*

Proof of the representer theorem

We can always rewrite w_* as $w_* = \sum_{i=1}^{n} \alpha_i x_i + u$ where $u^\top x_i = 0$ for all i

Let's denote by $w = w_* - u$

- $\|w_*\|^2 = \|w\|^2 + \|u\|^2$, thus $\|w\|^2 \leq \|w_*\|^2$
- For all i, $w^\top x_i = (w_* - u)^\top x_i = w_*^\top x_i$, thus $\ell(x_i^\top w, y_i) = \ell(x_i^\top w_*, y_i)$

Therefore

$$\sum_{i=1}^{n} \ell(x_i^\top w, y_i) + \frac{\lambda}{2}\|w\|^2 \leq \sum_{i=1}^{n} \ell(x_i^\top w_*, y_i) + \frac{\lambda}{2}\|w_*\|^2$$

And w is an optimal solution for this problem. Since the objective is strongly convex, there is unicity of the solution and $w_* = w$

Kernelized ridge regression

Classical formulation in w:

$$w_* = \arg\min_w \frac{1}{2}\|\mathbf{y} - \mathbf{X}w\|^2 + \frac{\lambda}{2}\|w\|^2$$

Alternative formulation in α:

$$\alpha_* = \arg\min_\alpha \frac{1}{2}\alpha^\top(\mathbf{X}\mathbf{X}^\top + \lambda I_n)\alpha - \alpha^\top \mathbf{y}$$

Claim: These two formulations are equivalent

Proof: Set the gradient to 0, to obtain $\alpha_* = (\mathbf{X}\mathbf{X}^\top + \lambda I_n)^{-1}\mathbf{y}$, and $w_* = \mathbf{X}^\top \alpha_*$

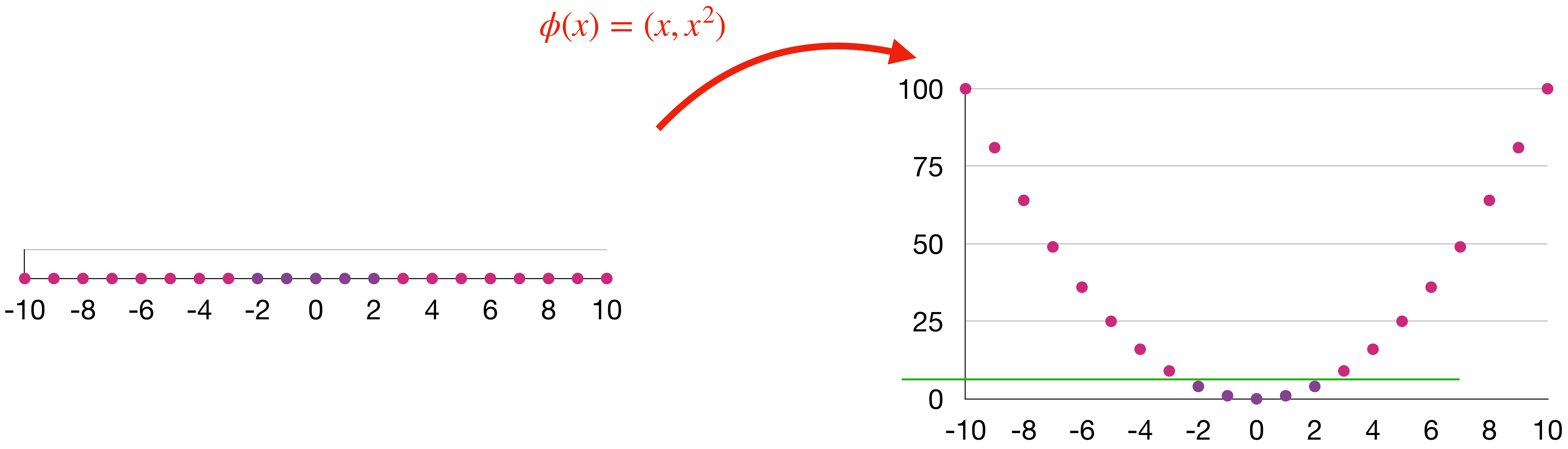
Interest:

- Computational complexity - depending on d, n
- The dual formulation only uses $\mathbf{X}$ through the kernel matrix $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$

Kernel matrix

$$\mathbf{K} = \mathbf{X}\mathbf{X}^\top = \begin{pmatrix} x_1^\top x_1 & x_1^\top x_2 & \cdots & x_1^\top x_n \\ x_2^\top x_1 & x_2^\top x_2 & \cdots & x_2^\top x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^\top x_1 & x_n^\top x_2 & \cdots & x_n^\top x_n \end{pmatrix} = (x_i^\top x_j)_{i,j} \in \mathbb{R}^{n\times n}$$

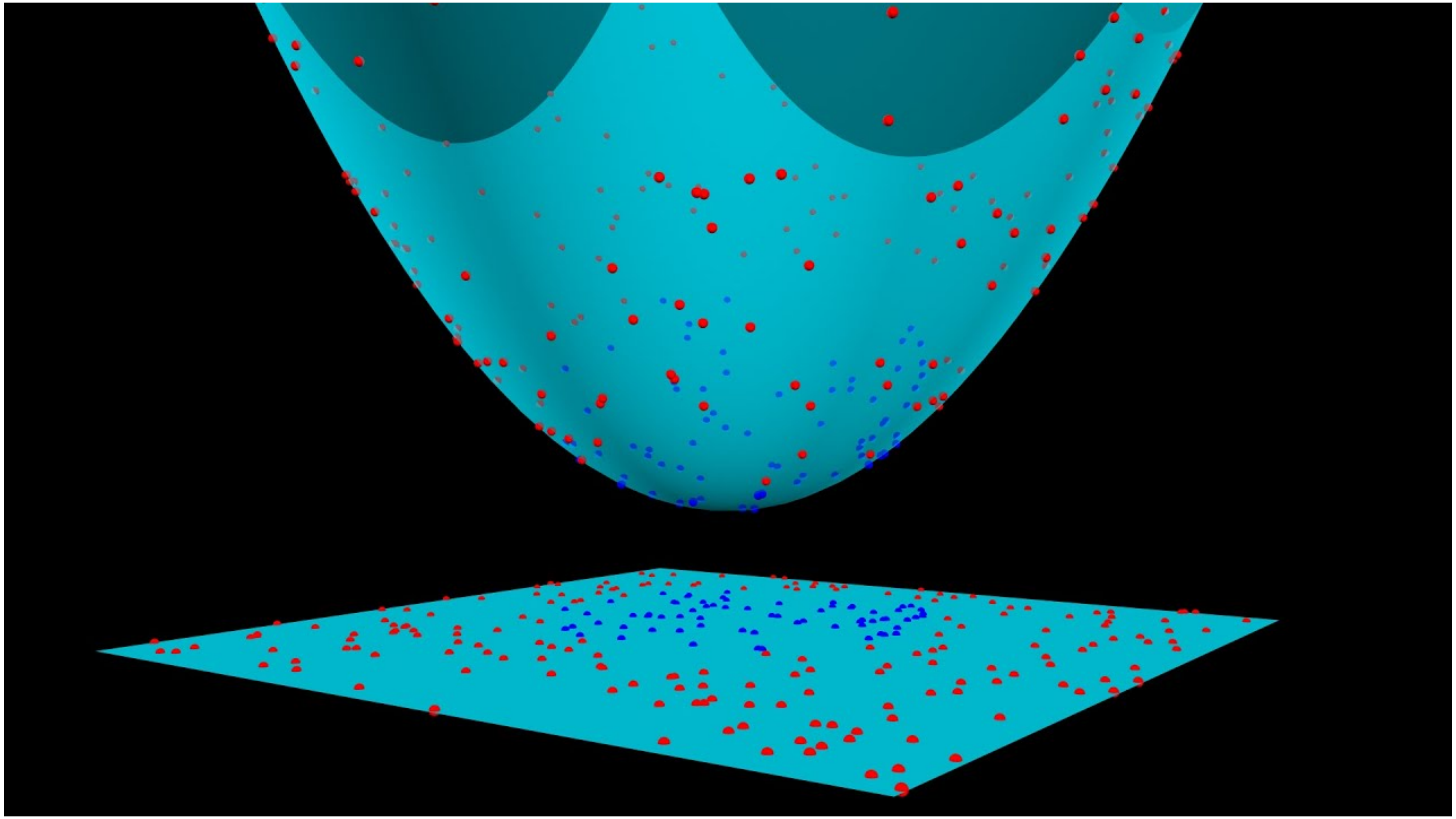
Embedding into feature spaces



Not separable by a half space

Separable by a half space

Usefulness of feature spaces



Kernel matrix with feature spaces

When a feature map $\phi : \mathbb{R}^d \to \mathbb{R}^{\tilde{d}}$ is used,

$$(x_i)_{i=1}^n \hookrightarrow \big(\phi(x_i)\big)_{i=1}^n$$

The associated kernel matrix is

$$\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\top = \begin{pmatrix} \phi(x_1)^\top\phi(x_1) & \phi(x_1)^\top\phi(x_2) & \cdots & \phi(x_1)^\top\phi(x_n) \\ \phi(x_2)^\top\phi(x_1) & \phi(x_2)^\top\phi(x_2) & \cdots & \phi(x_2)^\top\phi(x_n) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(x_n)^\top\phi(x_1) & \phi(x_n)^\top\phi(x_2) & \cdots & \phi(x_n)^\top\phi(x_n) \end{pmatrix} \in \mathbb{R}^{n\times n}$$

<u>Problem</u>: when $d \lll \tilde{d}$ computing $\phi(x)^\top\phi(x')$ costs $O(\tilde{d})$ - too expensive

Kernel trick

Kernel function: $\kappa(x, x')$ such that

$$\kappa(x, x') = \phi(x)^\top \phi(x')$$

Similarity between x_i and x_j

Similarity realized as inner products in the feature space

It is equivalent to

- Directly compute $\kappa(x, x')$
- First augment the features to $\phi(x)$, then compute $\phi(x)^\top \phi(x')$

Interest: enable to compute linear classifier in high-dimensional space without having to do computation in this high-dimensional space.

Examples of kernel (easy)

1. Linear kernel: $\kappa(x, x') = x^\top x'$
   ➡ Feature map is $\phi(x) = x$
2. Quadratic kernel: $\kappa(x, x') = (xx')^2$ for $x, x' \in \mathbb{R}$
   ➡ Feature map is $\phi(x) = x^2$

3. Polynomial kernel

Let $x, x' \in \mathbb{R}^3$

$$\kappa(x, x') = (x_1x_1' + x_2x_2' + x_3x_3')^2$$

<u>Feature map</u>:

$$\phi(x) = [x_1^2, x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3] \in \mathbb{R}^6$$

<u>Proof:</u>

$$\kappa(x, x') = \phi(x)^\top \phi(x')$$

$$\begin{aligned}\kappa(x, x') &= (x_1x_1' + x_2x_2' + x_3x_3')^2 \\ &= (x_1x_1')^2 + (x_2x_2')^2 + (x_3x_3')^2 + 2x_1x_2x_1'x_2' + 2x_1x_2x_3'x_3' + 2x_2x_2x_3'x_3' \\ &= \left(x_1^2, x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3\right)^\top \left(x_1'^2, x_2'^2, x_3'^2, \sqrt{2}x_1'x_2', \sqrt{2}x_1'x_3', \sqrt{2}x_2'x_3'\right)\end{aligned}$$

We obtain ϕ by identification

4. Radial basis function (RBF) kernel

Let $x, x' \in \mathbb{R}^d$

$$\kappa(x, x') = e^{-(x-x')^\top (x-x')}$$

For $x, x' \in \mathbb{R}$

$$\kappa(x, x') = e^{-(x-x')^2}$$

<u>Feature map</u>:

$$\phi(x) = e^{-x^2}\Big(\cdots, \frac{2^{k/2}x^k}{\sqrt{k!}}\cdots\Big)$$

Infinite dimensional vector

<u>Proof:</u> $\kappa(x, x') = e^{-x^2-x'^2+2xx'}$

$$= e^{-x^2}e^{-x'^2}\textstyle\sum_{k=0}^{\infty}\frac{2^k x^k x'^k}{k!}$$ by the Taylor expansion of $\exp$

$$\phi(x) = e^{-x^2}\Big(\cdots, \frac{2^{k/2}x^k}{\sqrt{k!}}\cdots\Big) \implies \phi(x)^\top \phi(x') = \kappa(x, x')$$

<u>Interest</u>: it cannot be represented as an inner product in a finite-dimensional space

Building new kernels from old kernels

Let κ_1, κ_2 be two kernel functions and ϕ_1, ϕ_2 the corresponding feature maps

Claim 1: Positive linear combinations of kernel are kernels

$$\kappa(x, x') = \alpha\kappa_1(x, x') + \beta\kappa_2(x, x') \ \text{ for } \alpha, \beta \geq 0$$

Claim 2: Product of kernels are kernels

$$\kappa(x, x') = \kappa_1(x, x')\kappa_2(x, x')$$

Interest: Building blocks to derive new kernels

Proof 1:

$$\kappa(x,x') = \alpha\kappa_1(x,x') + \beta\kappa_2(x,x')$$
$$= \alpha\phi_1(x)\phi(x')_1^\top + \beta\phi_2(x)\phi_2(x')^\top$$
$$= \phi(x)^\top\phi(x')$$

where $\phi(x) = \begin{pmatrix} \sqrt{\alpha}\phi_1(x) \\ \sqrt{\beta}\phi_\beta(x) \end{pmatrix} \in \mathbb{R}^{d_1+d_2}$

kernels from old kernel

s and ϕ_1, ϕ_2 the corresponding feature maps

Claim 1: Positive linear combinations of kernel are kernel

$$\kappa(x,x') = \alpha\kappa_1(x,x') + \beta\kappa_2(x,x')$$

Claim 2: Product of kernels are kernel

$$\kappa(x,x') = \kappa_1(x,x')\kappa_2(x,x')$$

B ... old kernel

Proof 2:

$$\kappa(x, x') = \kappa_1(x, x')\kappa_2(x, x')$$
$$= \phi_1(x)^\top \phi_1(x') \phi_2(x)^\top \phi_2(x')$$

Let $\phi(x) = \begin{pmatrix} (\phi_1(x))_1 \phi_2(x) \\ \vdots \\ (\phi_1(x))_{d_1} \phi_2(x) \end{pmatrix} \in \mathbb{R}^{d_1 \times d_2}$, then

$$\phi(x)^\top \phi(x') = \sum_{i,j} (\phi_1(x))_i (\phi_2(x))_j (\phi_1(x'))_i (\phi_2(x'))_j$$
$$= \sum_i (\phi_1(x))_i (\phi_1(x'))_i \sum_j (\phi_2(x))_j (\phi_2(x'))_j$$
$$= \phi_1(x)^\top \phi_1(x') \phi_2(x)^\top \phi_2(x') = \kappa(x, x')$$

Let ... ding feature maps

Cla ... el

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$$\kappa(x, x') = \kappa_1(x, x')\kappa_2(x, x')$$

Mercer's condition

Question: Given a kernel function κ, how can we ensure that there exists a feature map ϕ such that

$$\kappa(x, x') = \phi(x)^\top \phi(x')$$

Answer: It is true if and only if the following Mercer's conditions are fulfilled:

- The kernel function is symmetric:

$$\forall x, x', \kappa(x, x') = \kappa(x', x)$$

- The kernel matrix is psd for all possible input sets:

$$\forall n \geq 0,\ \forall (x_i)_{i=1}^n, \quad \mathbf{K} = (\kappa(x_i, x_j'))_{i,j=1}^n \succcurlyeq 0$$

Predicting with kernels

Problem: we predict with $y = \phi(x)^\top w_*$ whereas $\phi(x)$ can be expensive to compute

Question: How to do a prediction only using the kernel function, without computing $\phi(x)$?

Answer: $\phi(x)^\top w_* = \phi(x)^\top \phi(\mathbf{X})^\top \alpha_* = \sum_{i=1}^{n} \kappa(x, x_i) \alpha_{*i}$

We can do a prediction only using the kernel function

Important remark:

$$y = \phi(x)^\top w_* = f_{w_*}(x)$$

Linear prediction in the feature space

Non linear prediction in the $\mathcal{X}$ space

Bonus: proof of Mercer theorem

- If κ implements an inner product then it is symmetric and the kernel matrix is psd:
$$v^\top \mathsf{K} v = \sum_{i,j} v_i v_j \phi(x_i)^\top \phi(x_j) = (\sum_i v_i \phi(x_i))^2$$
- Define $\phi(x) = \kappa(\cdot, x)$. Define a vector space of function by taking all linear combinations $\{\sum_i \alpha_i \kappa(\cdot, x_i)\}$. Define an inner product on this vector space by
$$\langle \sum_i \alpha_i \kappa(\cdot, x_i), \sum_j \beta_j \kappa(\cdot, x'_j) \rangle = \sum_{i,j} \alpha_i \beta_j \kappa(x_i, x'_j)$$

This is a valid inner product (symmetric, bilinear and positive definite, with equality only $\phi(x)$ is the zero function)

We have
$$\langle \phi(x), \phi(x') \rangle = \langle \kappa(\cdot, x), \kappa(\cdot, x') \rangle = \kappa(x, x')$$