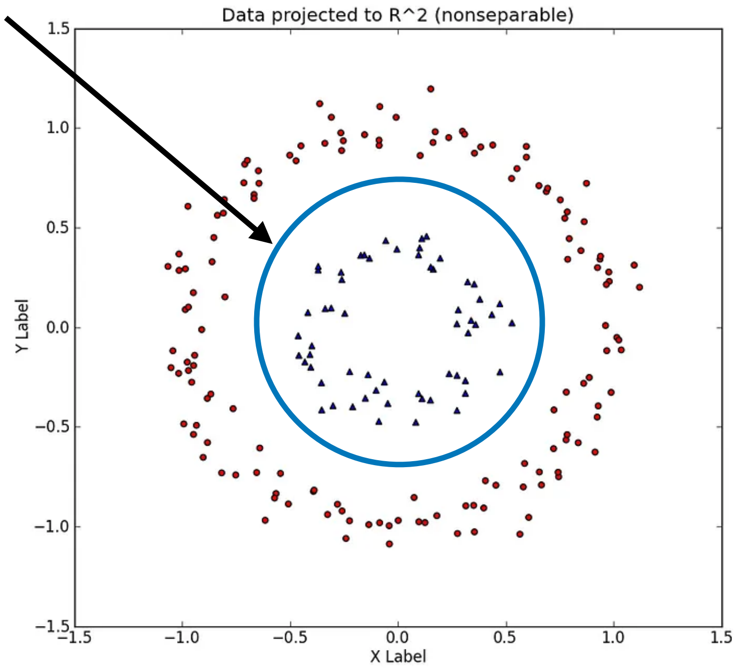
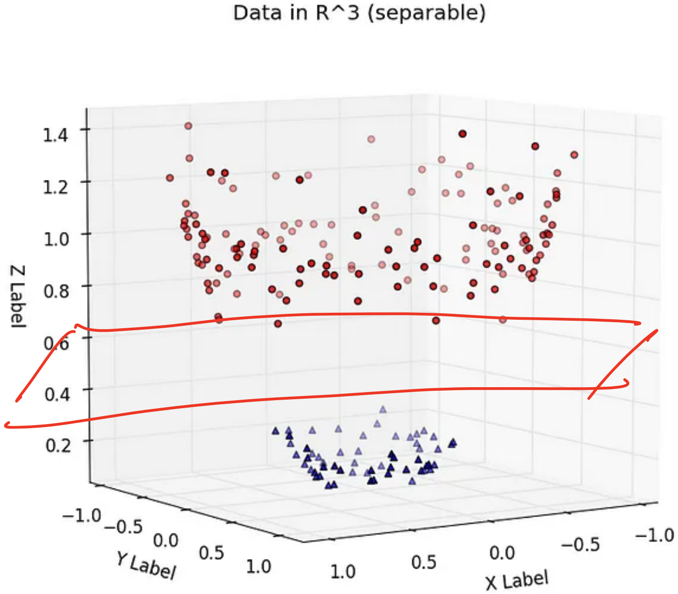
Kernel

Objective today

Use kernels to design nonlinear regression & classification models

Goal: Non-linear decision boundary





Outline

1. Kernel

2. Kernel trick and Kernel regression

3. Kernel SVM

Common Kernels

Linear kernel: $k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z}$

$\underline{\phi(x)} = x$

Common Kernels

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Polynomial kernel: $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + 1)^p$

$$\phi(x) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_d \\ x_1^2 \\ \vdots \\ x_d^2 \\ x_i x_j \\ x_1^3 \\ \vdots \\ x_1^p \end{bmatrix}$$

$$\phi(x)^\top \phi(z) = (x^\top z + 1)^p$$

Common Kernels

Linear kernel: $k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z}$

$\phi(x) \in R^\infty$

Polynomial kernel: $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + 1)^p$

Gaussian kernel (aka RBF):

$$k(\mathbf{x}, \mathbf{z}) = \exp\left(-\|\mathbf{x} - \mathbf{z}\|_2^2 / \sigma^2\right)$$

$x = z \quad 1$

$\|x - z\|_2^2 \to +\infty$

$\exp(-+\infty) \to 0$

Well-defined Kernels

Given any symmetric function $k(\mathbf{x}, \mathbf{z})$, can it be used as a kernel?

$K(x, z) = K(z, x)$

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$$\exists \phi, \text{s.t.,}\ k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z}), \forall \mathbf{x}, \mathbf{z}$$

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$K_{ij} = k(x_i, x_j)$

$\mathbb{R}^{m \times m}$

$$\cancel{\exists \phi, \text{ s.t.}}, \forall \mathbf{x}_1, \ldots, \mathbf{x}_m, \text{ the kernel matrix } K = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_2) & \ldots & k(\mathbf{x_1}, \mathbf{x_m}) \\ k(\mathbf{x}_2, \mathbf{x}_1) & \ldots & k(\mathbf{x_2}, \mathbf{x_m}) \\ \ldots & \ldots & \ldots \\ k(\mathbf{x}_m, \mathbf{x}_1) & \ldots & k(\mathbf{x_m}, \mathbf{x_m}) \end{bmatrix} \text{ is PSD}$$

Construction of well-defined kernels

Kernels built by recursively applying the following one or more rules are well-defined kernels

Given well-defined k_1, k_2

$k_1 = x^T z$

1. $k(\mathbf{x}, \mathbf{z}) = ck_1(\mathbf{x}, \mathbf{z}), c > 0$

$k_1(x, z) = \phi_1^T(x)\, \phi_1(z)$

$c \cdot k_1(x, z) = \Big(\underbrace{\sqrt{c}\, \phi_1(x)}_{\phi'}\Big)^T \Big(\sqrt{c}\, \phi_1(z)\Big)$

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4. $k(\mathbf{x}, \mathbf{z}) = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{z})f(\mathbf{z})$

$f(x) \in \mathbb{R}$

$\big(\underbrace{f(x)\phi_1(x)}_{\phi'(x)}\big)^T \big(f(z)\phi_1(z)\big)$

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In class exercise:

Given $k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z}$ being well defined,

Prove Gaussian kernel

$\exp\left(-\|\mathbf{x} - \mathbf{z}\|_2^2/\sigma^2\right)$ is well defined

Construction of well-defined kernels $\exp(-x^\top z)$

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Hint:

Rule 1

$\exp(-\mathbf{x}^\top\mathbf{x}/\sigma^2) \cdot \exp(2\mathbf{x}^\top\mathbf{z}/\sigma^2) \cdot \exp(-\mathbf{z}^\top\mathbf{z}/\sigma^2)$

$f(x)$ ✓ Rule 5 $f(z)$

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Solution: recall linear regression can be done by just using inner product of two features!

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A recipe:

1. Write the learning algorithm in terms of $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$

2. Define a kernel $k(\mathbf{x}, \mathbf{z})$ (e.g., Gaussian kernel, poly kernel)

3. Replace all $\langle \mathbf{x}, \mathbf{z} \rangle$ operation in the Alg by $k(\mathbf{x}, \mathbf{z})$

$O(d)$

$\exp\left(-\frac{\|x-z\|_2^2}{\sigma^2}\right)$

Kernel ridge regression

1. Recall linear regression can be done via just using inner product:

$$\alpha = \left(X^\top X + \lambda I\right)^{-1} Y \in \mathbb{R}^n$$

$$\|X^\top w - y\|_2^2 + \lambda \|w\|_2^2$$

$$\Leftrightarrow \|X^\top X \alpha - y\|_2^2 + \lambda \|X\alpha\|_2^2$$

$$w = \sum_{i=1}^{n} \alpha_i x_i = X\alpha$$

$$X = \begin{bmatrix} | & & | \\ x_1 & \cdots & x_n \\ | & & | \end{bmatrix} \in \mathbb{R}^{d\times n}$$

$$X^\top X = \begin{array}{c|c} & j \\ \hline i & \begin{bmatrix} & \vdots & \\ \cdots & x_i^\top x_j & \cdots \\ & \vdots & \end{bmatrix} \end{array} \in \mathbb{R}^{n\times n}$$

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3. Replace $X^\top X$ by a kernel matrix K

$$X^\top X = \begin{array}{cc} & j \\ i & \left[\; x_i^\top x_j \;\right] \end{array}$$

$$\underset{\mathbb{R}^{n\times n}}{K} = \begin{array}{cc} & j \\ i & \left[\; k(x_i, x_j) \;\right] \end{array}$$

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$$K \in \mathbb{R}^{n\times n}, \;\; K_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$$

$$\alpha = (K + \lambda I)^{-1} Y$$

Kernel ridge regression

In test time, recall linear regression makes prediction at $\mathbf{x}$:

$$\hat{y} = \sum_{i=1}^{n} \alpha_i \langle \mathbf{x}_i, \mathbf{x} \rangle$$

$$w = \sum_{i=1}^{n} \alpha_i x_i$$

$$w^T x$$

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$$\hat{y} = \sum_{i=1}^{n} \alpha_i \cdot k(\mathbf{x}_i, \mathbf{x})$$

Demo

Training data is generated as follows: $x \sim \text{uniform}[0,10]$,
$y = \sin(x\pi/2) + \epsilon, \epsilon \sim \mathcal{N}(0,0.1)$

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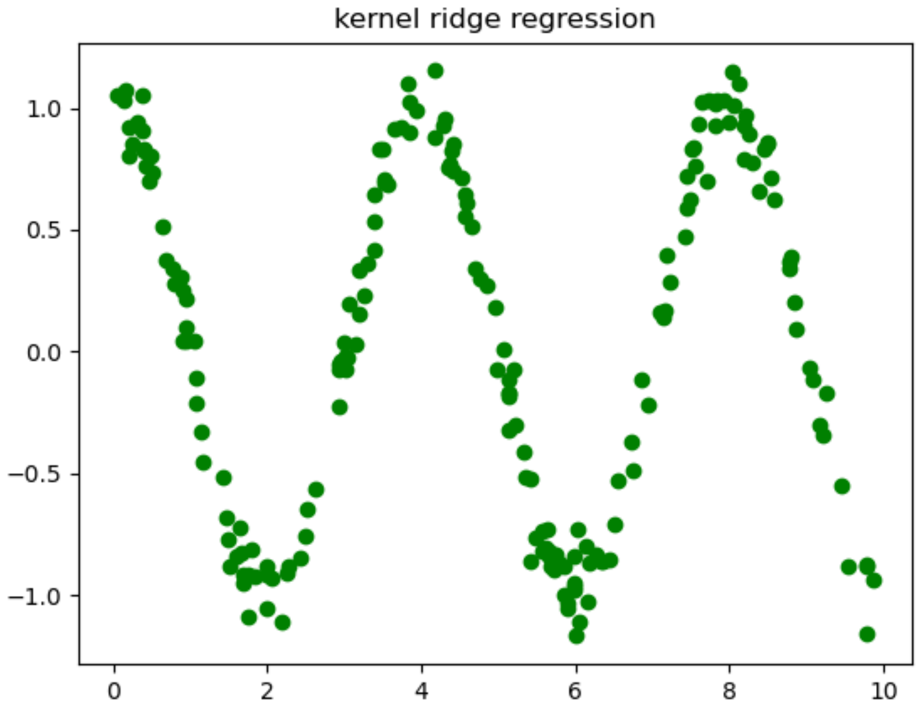

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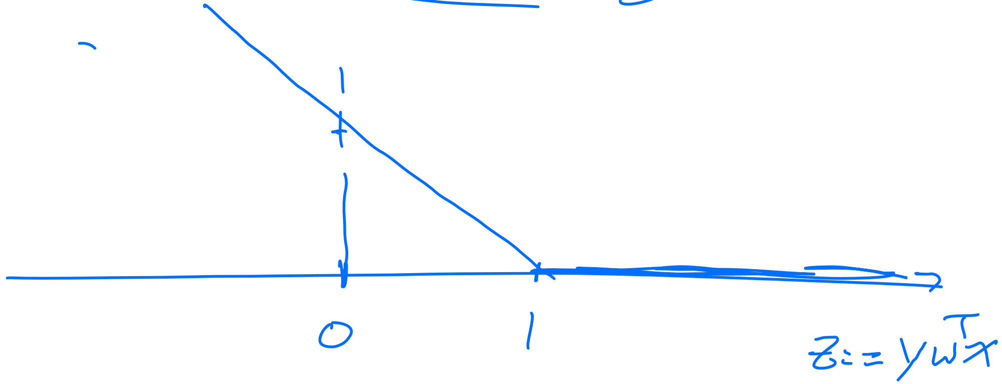
Recall the soft-margin SVM formulation

$$\min_{w} \|w\|_2^2/2 + C \sum_{i=1}^{n} \max\left\{0, 1 - y_i(w^\top \mathbf{x}_i)\right\}$$

hinge loss



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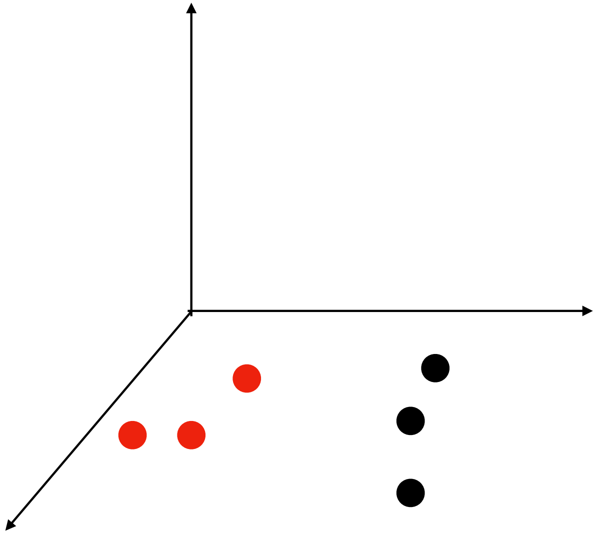
Intuitive proof:



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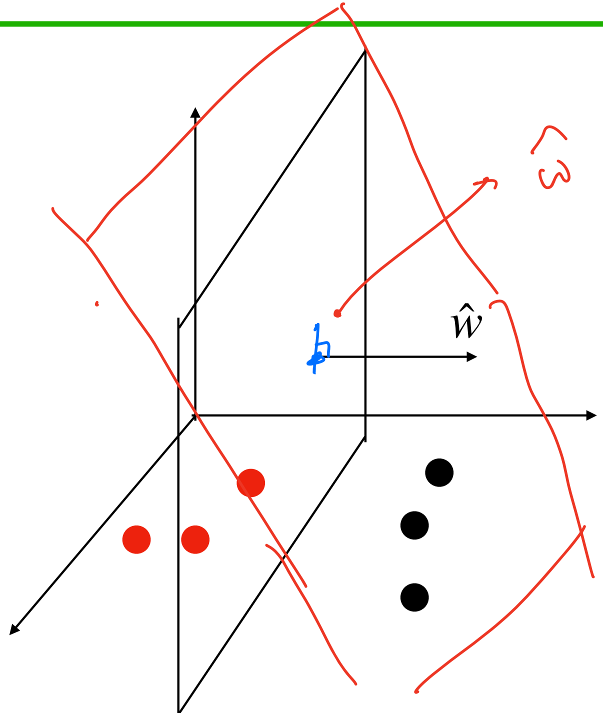

A new formulation of soft-margin SVM formulation

$$\text{Re-parameterize } w = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i = X\alpha$$

learn $\alpha \in \mathbb{R}^n$

Replace w by $X\alpha$ in soft-margin SVM objective

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w w

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$\ell(\alpha)$

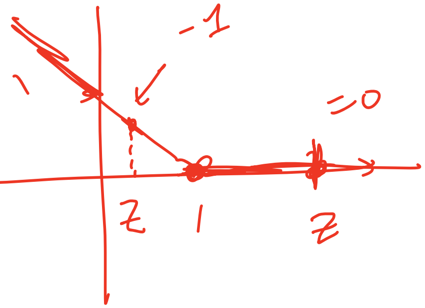
$\nabla_\alpha \ell(\alpha)$

Alg: gradient descent to optimize $\alpha \in \mathbb{R}^n$

$X^\top X\alpha$

$X^\top X = [\ \cdots\ ]$ $\quad x_i^\top x_j$

$C \cdot \sum_{i=1}^{n} -1(\underbrace{y_i x_i^\top X\alpha}_{z_i} \le 1)(y_i X^\top x_i)$



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$$\nabla_\alpha \ell(\alpha) = \cancel{2}X^\top X\alpha + C\sum_{i=1}^{n} \mathbf{1}\left\{y_i(x_i^\top X\alpha) \le 1\right\}(-y_i X^\top x_i)$$

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$X^\top x_i$

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$$= \begin{bmatrix} - & x_1^\top & - \\ & \vdots & \\ - & x_n^\top & - \end{bmatrix} x_i = \begin{bmatrix} x_1^\top x_i \\ \vdots \\ x_n^\top x_i \end{bmatrix}$$

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Q: Can we apply kernel trick??

Kernelized GD for SVM

$$\min_{\alpha} \|X\alpha\|_2^2 + C\sum_{i=1}^{n} \max\left\{0, 1 - y_i(\mathbf{x}_i^\top X\alpha)\right\}$$

While not converged:

$$g = X^\top X\alpha + C\sum_{i=1}^{n} \mathbf{1}\left\{y_i(x_i^\top X\alpha) \leq 1\right\}(-y_i X^\top x_i)$$

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Replace $X^\top \mathbf{x}_i$ by $\mathbf{k}_i = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_\mathbf{i}) \\ k(\mathbf{x}_2, \mathbf{x}_\mathbf{i}) \\ \dots \\ k(\mathbf{x}_n, \mathbf{x}_\mathbf{i}) \end{bmatrix} \in \mathbb{R}^n$

$k(x_j, x_i)$

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Replace

$$g = K\alpha + C\sum_{i=1}^{n} \mathbf{1}\{y_i(\mathbf{k}_i^\top \alpha) \le 1\}(-y_i \mathbf{k}_i)$$

Summary for kernel SVM so far

1. Ideally, want to do the SVM in the lifted high-dim feature space, i.e.,

$$\min_{\alpha} \|w\|_2^2 + C\sum_{i=1}^{n} \max\left\{0, 1 - y_i(w^\top \phi(x_i))\right\}$$

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2. Via the re-parameterization step, we see GD can be implemented ***via just using*** $\langle \mathbf{x}, \mathbf{z} \rangle$

3. We apply kernel trick, i.e., replace all $\langle \mathbf{x}, \mathbf{z} \rangle$ by $k(\mathbf{x}, \mathbf{z})$

Take-home message today

Kernel trick allows us to do regression / classification in $\phi(\mathbf{x})$ space (possibly infinite dim) **without ever explicitly computing $\phi(\mathbf{x})$!**