Kernel

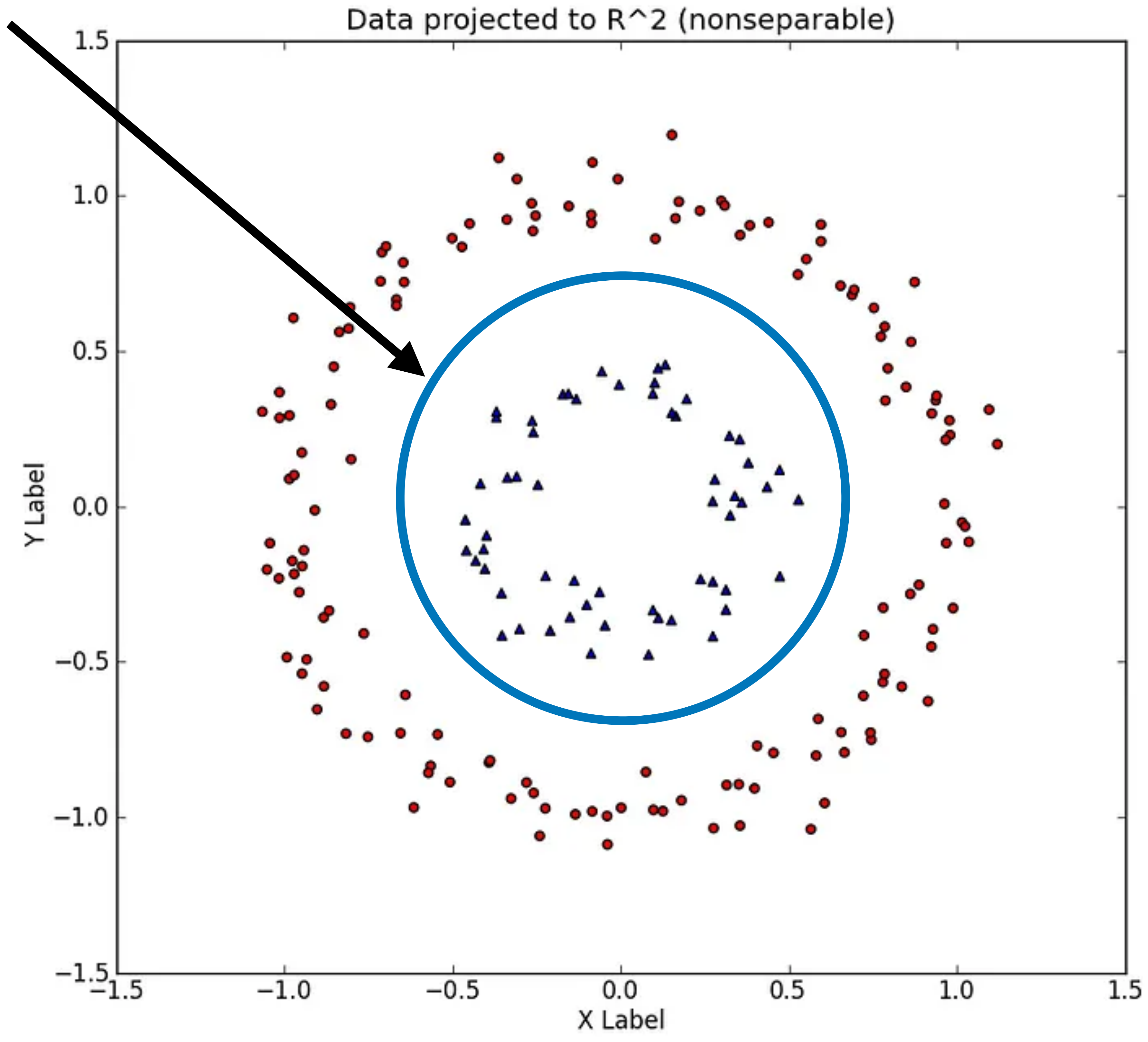
Announcements

HW5 and P5 are released (due in one week)

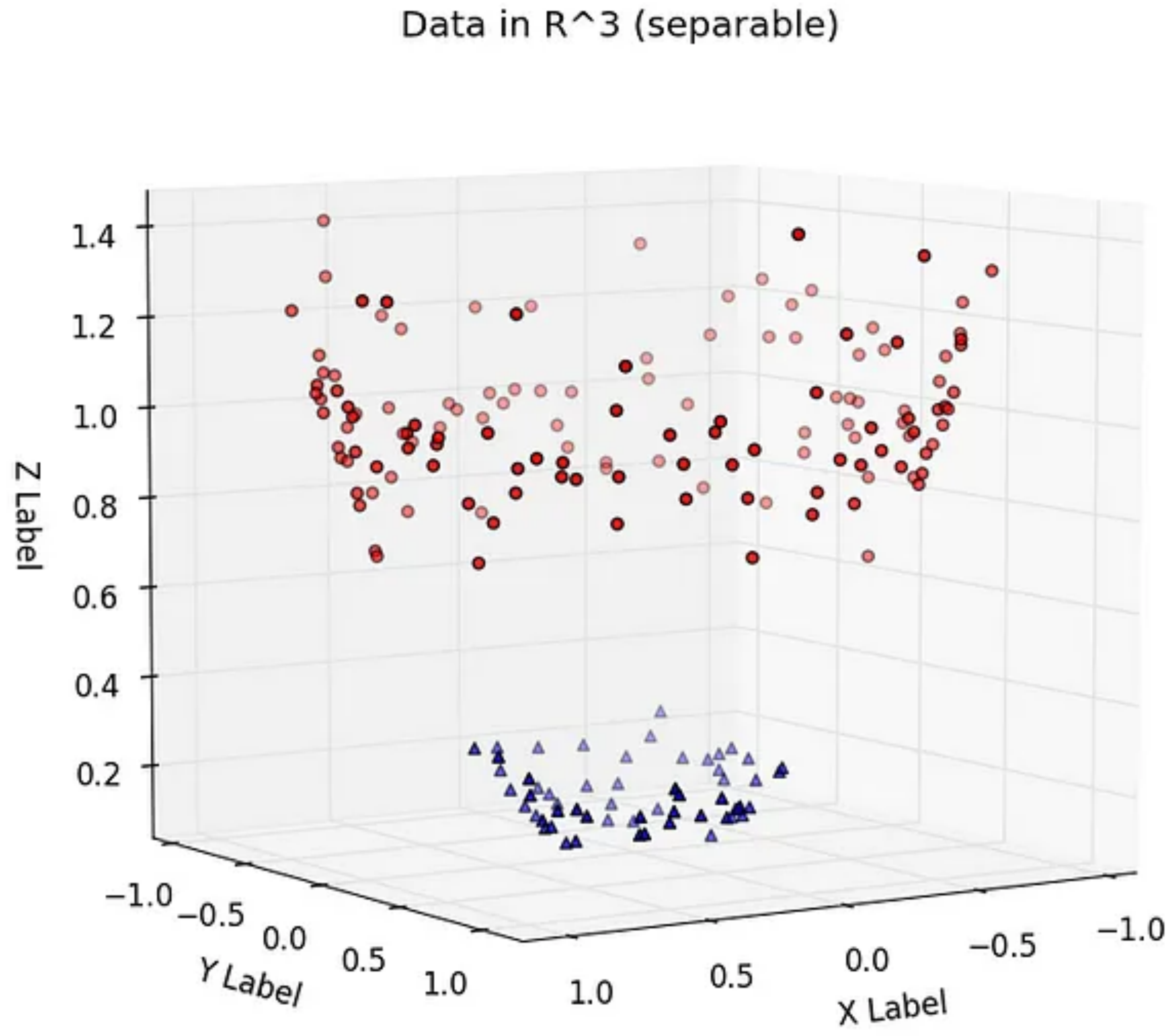
Objective today (and next Tuesday)

Use kernels to design nonlinear ML models (regression & classification)

Goal: Non-linear decision boundary



Our approach



Outline

1. A new perspective on ridge linear regression

2. Feature mapping and Kernel

3. Kernel trick and demo of kernel regression

Linear regression revisited

Dataset $\mathscr{D} = \{\mathbf{x}_i, y_i\}, \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$

Ridge Linear regression solves the following problem:

$$\arg\min_{w} \sum_{i=1}^{n} (w^\top \mathbf{x}_i - y_i)^2 + \lambda \|w\|_2^2$$

Closed-form solution exists, i.e.,

$$\hat{w} = (XX^\top + \lambda I)^{-1} XY$$

Linear regression revisited

Claim: $\hat{w} = (XX^\top + \lambda I)^{-1} XY \in \text{Span}(X)$

An intuitive proof: GD (or SGD)

$$w_0 = \mathbf{0}, w^{t+1} = w^t - \eta \left[\sum_{i=1}^{n} (\mathbf{x}_i^\top w^t - y_i)\mathbf{x}_i + \lambda w^t \right]$$

A new perspective of linear regression

Since we know optimal solution lives in span(X), we can re-parameterize

$$w = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i = X\alpha, \ \ \alpha_i \in \mathbb{R}, \forall i$$

$$\arg\min_{w} \sum_{i=1}^{n} \left\| X^\top w - Y \right\|_2^2 + \lambda \|w\|_2^2 \quad \Rightarrow \quad \arg\min_{\alpha} \left\| X^\top X\alpha - Y \right\|_2^2 + \|X\alpha\|_2^2$$

Original formulation

New formulation w/ α as our variables

A new perspective of linear regression

$$\arg\min_{\alpha} \left\| X^\top X\alpha - Y \right\|_2^2 + \lambda \|X\alpha\|_2^2$$

Solution:

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

$$X^\top X \in \mathbb{R}^{n\times n},\ (X^\top X)_{i,j} = \mathbf{x}_i^\top \mathbf{x}_j = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

A new perspective of linear regression

When we make prediction on a test example $\mathbf{x} \in \mathbb{R}^d$, we have:

$$\hat{w}^\top \mathbf{x} = (\sum_{i=1}^{n} \alpha_i \mathbf{x}_i)^\top \mathbf{x} = \sum_{i=1}^{n} \alpha_i \cdot \langle \mathbf{x}_i, \mathbf{x} \rangle$$

Notice a theme here:

Linear regression can be done by just using inner product of features

$\langle \mathbf{x}, \mathbf{z} \rangle, \mathbf{x} \in \mathbb{R}^d, \mathbf{z} \in \mathbb{R}^d$

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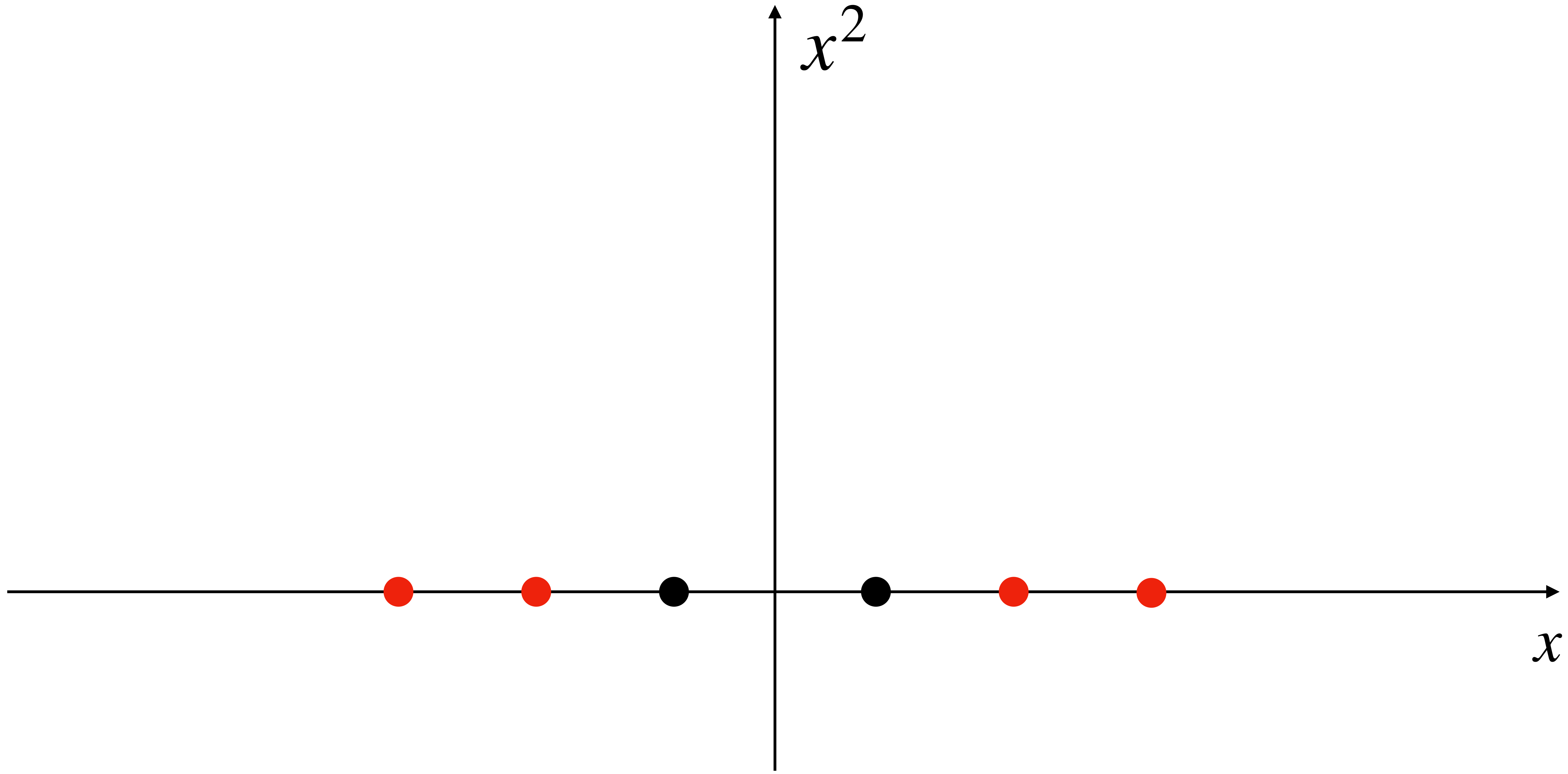
Feature mapping

Define $\phi(\mathbf{x}) \in \mathbb{R}^m$ as a feature mapping (often $m > d$)

Ex 1: $\mathbf{x} \in \mathbb{R}$, $\phi(\mathbf{x}) = [x, x^2]^\top \in \mathbb{R}^2$



Feature mapping

Define $\phi(\mathbf{x}) \in \mathbb{R}^m$ as a feature mapping (often $m > d$)

Ex 2: quadratic
feature mapping ϕ

$$\mathbf{x} = [x_1, x_2]^\top,$$

$$\phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2, x_1 x_2]^\top$$

Feature mapping

Define $\phi(\mathbf{x}) \in \mathbb{R}^m$ as a feature mapping (often $m > d$)

Ex 2: cubic feature mapping ϕ

$$\mathbf{x} = [x_1, x_2]^\top,$$

$$\phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2, x_1 x_2, x_1^3, x_2^3, x_1 x_2^2, x_1^2 x_2]^\top$$

Q: in general, for $\mathbf{x} \in \mathbb{R}^d$, and a p-th order polynomial feature ϕ, what's the dimension of $\phi(\mathbf{x})$?

at least $\binom{d}{p}$

Dim of $\phi(\mathbf{x})$ can be very large!

Fit linear functions in the high-dim feature space

The feature mapping $\phi(\mathbf{x}) \in \mathbb{R}^m$ allows us to perform linear regression in the ϕ space

Ex: cubic feature mapping ϕ

$$\mathbf{x} = [x_1, x_2]^\top, \ \phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2, x_1x_2, x_1^3, x_2^3, x_1x_2^2, x_1^2x_2]^\top$$

$w^\top \phi(\mathbf{x})$ now can represent a 3-order polynomials!

To fit a 3-order polynomial in $\mathbf{x}$, we can instead do linear regression in $\phi(\mathbf{x})$

Fit linear functions in the high-dim feature space

Perform linear regression in ϕ space, i.e.,

$$\min_{w} \sum_{i=1}^{n} \left(w^\top \phi(\mathbf{x}_i) - y_i\right)^2 + \lambda \|w\|_2^2$$

Linear in ϕ, but high-order poly in $\mathbf{x}$

What is the potential problem of doing this?

This is where the new perspective of linear regression and kernels come to rescue!

Kernel

Kernel $k(\mathbf{x}, \mathbf{z})$

A valid kernel is a kernel such that $\exists \phi, k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z}), \forall \mathbf{x}, \mathbf{z}$

Ex: quadratic kernel

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + 1)^2$$

$$\phi(\mathbf{x}) = [1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2]^\top$$

Q: what's the computation of $k(\mathbf{x}, \mathbf{z})$?

Q: what's the computation of $\phi(\mathbf{x})^\top \phi(\mathbf{z})$?

Ex: cubic feature mapping ϕ

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + 1)^3$$

Generalizing to p-th order polynomials:

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

Kernel

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

The mapping $\phi(\mathbf{x})$ is infinite-dimensional

Ex: $\mathbf{x} \in \mathbb{R}$, the mapping $\phi(\mathbf{x})$:

$$\phi(\mathbf{x}) = \left[\ldots, \frac{1}{\sqrt{i!}} \exp\left(-\frac{x^2}{2\sigma^2}\right) x^i, \ldots\right]^\top \in \mathbb{R}^\infty$$

Kernel

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

2. Linear function $w^\top \phi(\mathbf{x})$ can model any indefinitely differentiable function f

Why? ϕ contains all polynomials, and f can be written as an infinite Taylor series..

Summary so far

1. Feature mapping $\phi(\mathbf{x})$ lifts $\mathbf{x}$ into high-dimensional space (e.g., high-order polynomials)

2. A kernel $k(\mathbf{x}, \mathbf{z})$ is a symmetric function, such that there exists a ϕ, so that

$$k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z})$$

3. Kernel allows us to compute $\langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$ without ever explicitly computing ϕ

($k(\mathbf{x}, \mathbf{z})$ is easy to compute but $\langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$ is hard to compute)

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Kernel Trick

We wanted to do linear regression in the new features $\phi(\mathbf{x_1}), \ldots, \phi(\mathbf{x_n})$,

BUT, $\phi(\mathbf{x})$ can be very high-dim or even infinite-dim….

Recall linear regression can be done by just using inner product of two features!

The kernel trick

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 by $k(\mathbf{x}, \mathbf{z})$

Kernel ridge regression

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

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

2. Define a kernel, e.g., $k(\mathbf{x}, \mathbf{z}) = \exp(-\|\mathbf{x} - \mathbf{z}\|_2^2/\sigma^2)$

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

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

Kernel ridge regression

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

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

Replace it w/ $k(\mathbf{x}_i, \mathbf{x})$:

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

take-home message

Kernel trick enables to do LR in $\phi(\mathbf{x})$ space (possibly infinite dim) **without ever explicitly computing $\phi(\mathbf{x})$!**