Plan

Cool stuff

- Expectation-Maximization algorithm
  - Gaussian mixture models for clustering
- Kernels
  - Linear regression
  - Support vector machines
- Duality
  - Support vector machines

10-315
Introduction to ML

Nonparametric Regression and Kernels

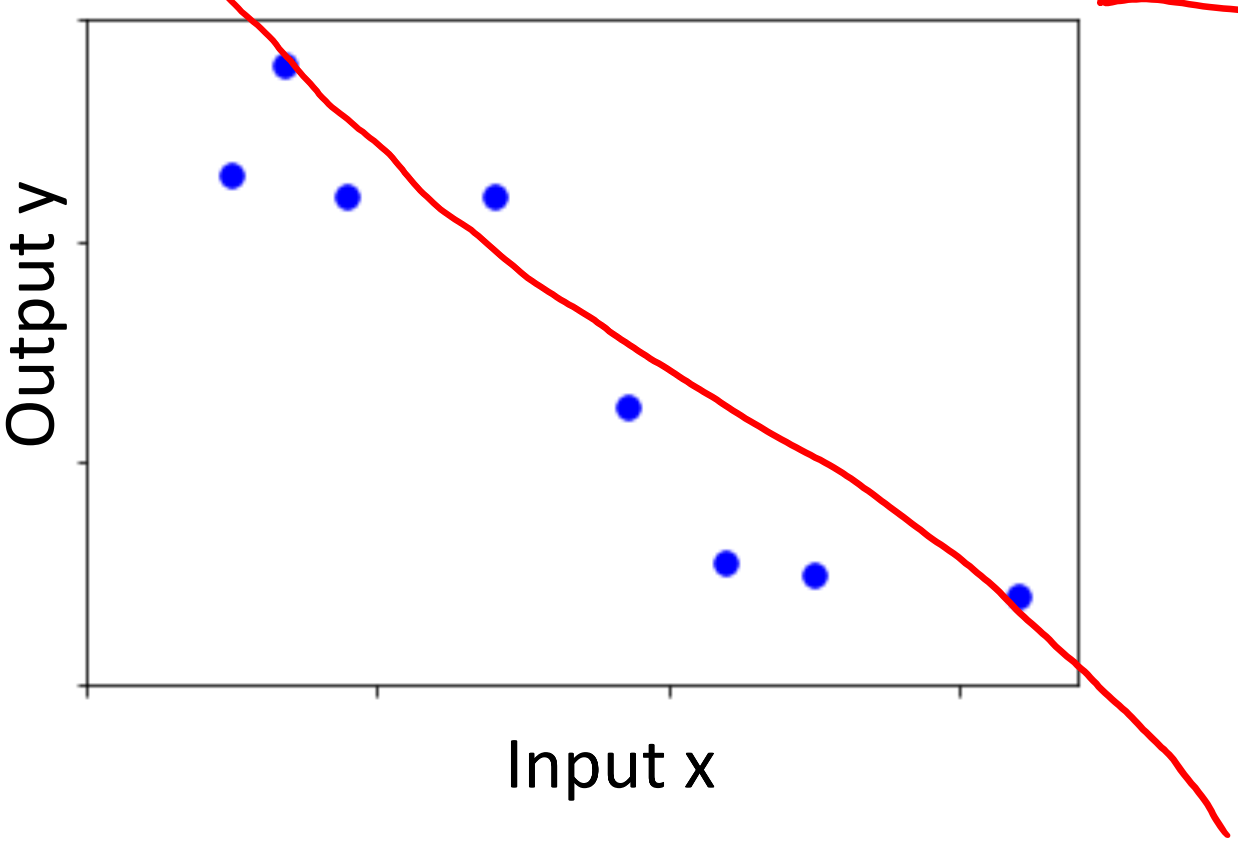
Instructor: Pat Virtue

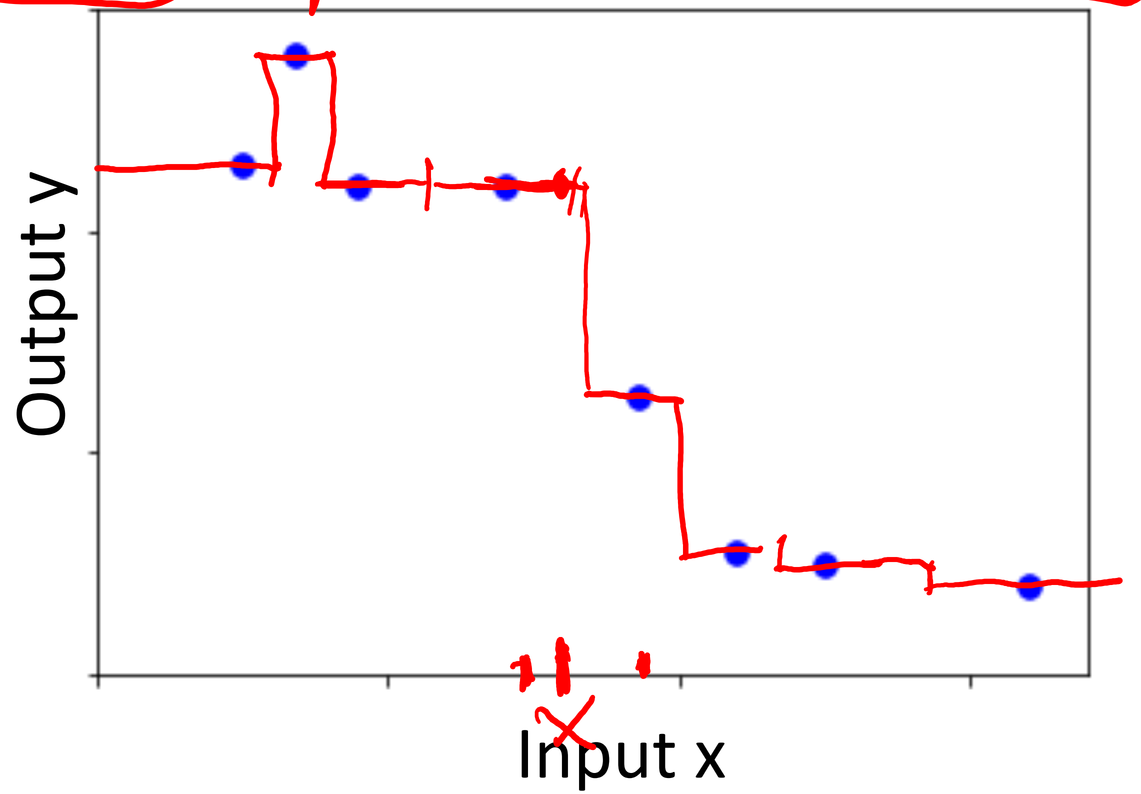
Parametric vs Nonparametric Regression

$\hat{y} = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$

$D \rightarrow \boxed{\text{train}} \rightarrow$ model parameters

$x \rightarrow \boxed{\text{pred (model)}} \rightarrow \hat{y}$





Parametric vs Nonparametric

Two different definitions

Statistics

A nonparametric model does not follow a specific distribution (thus doesn’t have parameters that define that distribution)

Machine learning

The number of parameters in a nonparametric model scales with the number of training data points

Parametric vs Nonparametric

Which models are nonparametric?

Statistics does not follow a specific distribution		Machine learning number of parameters scales with training
No	Linear regression	No
No	Logistic regression	No
Yes	Neural nets	No
No	Naïve Bayes	No
No	Discriminant analysis	No
Yes	K-nearest neighbor	Yes
Yes	Decision trees	

Poll 1

Are decision trees parametric or non-parametric?

A. Param

B.

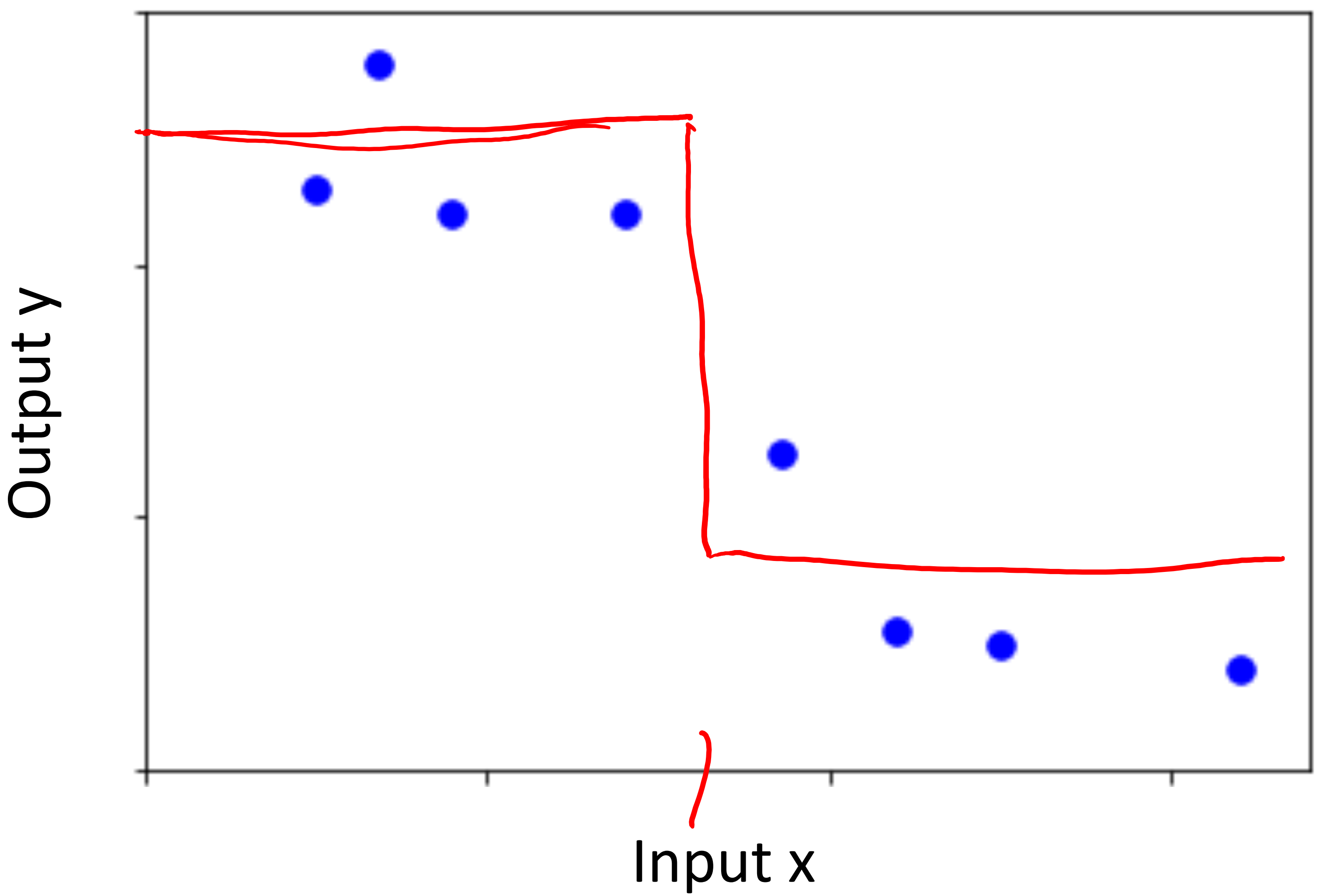
C. Non-Param

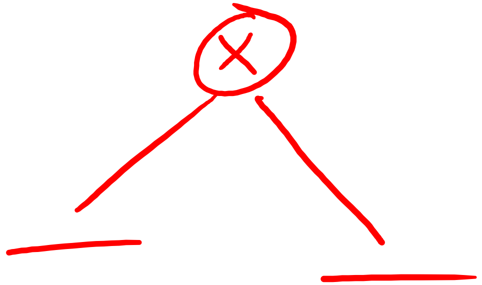
Use ML def

#params scales w/ data

Nonparametric Regression

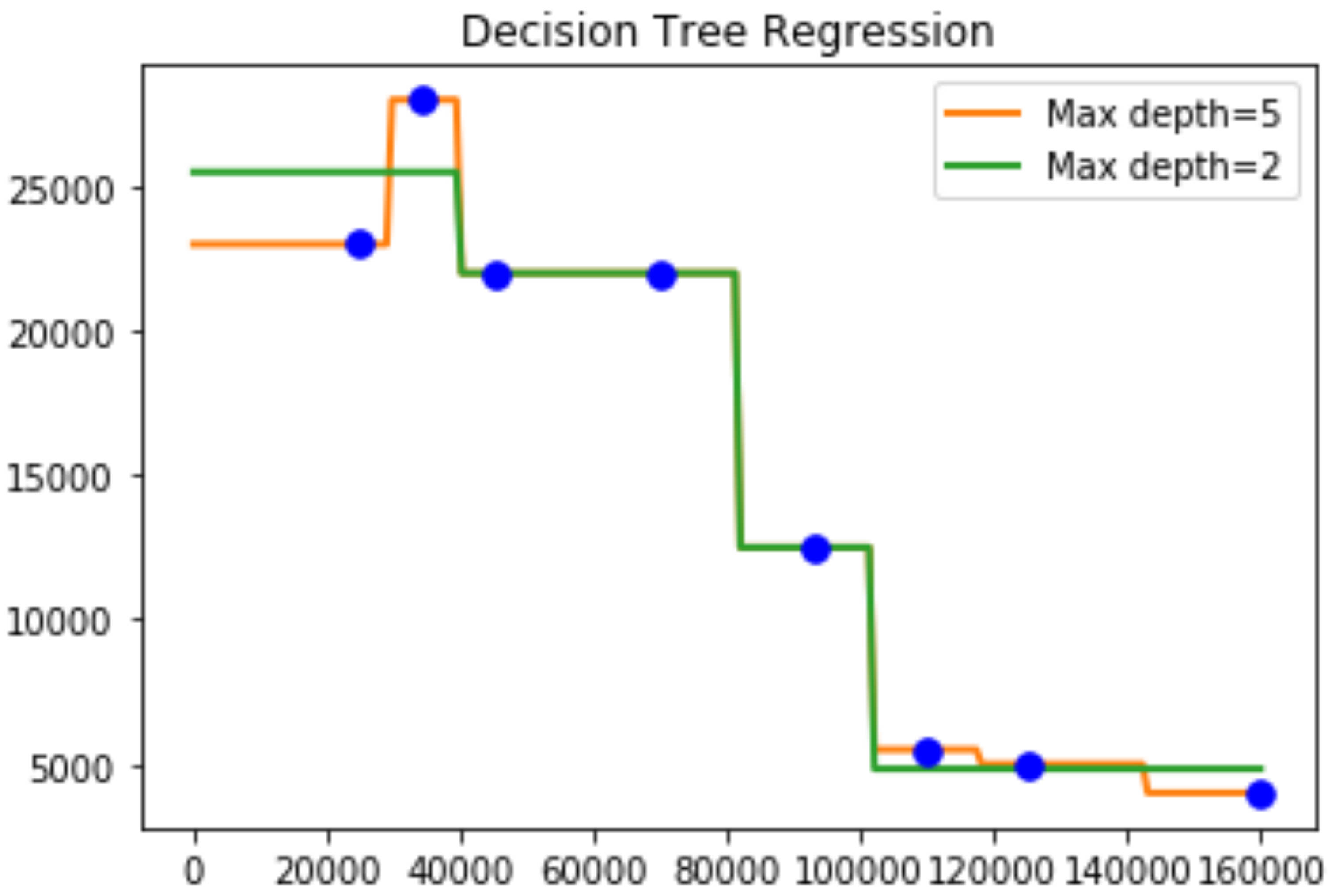
Decision Trees





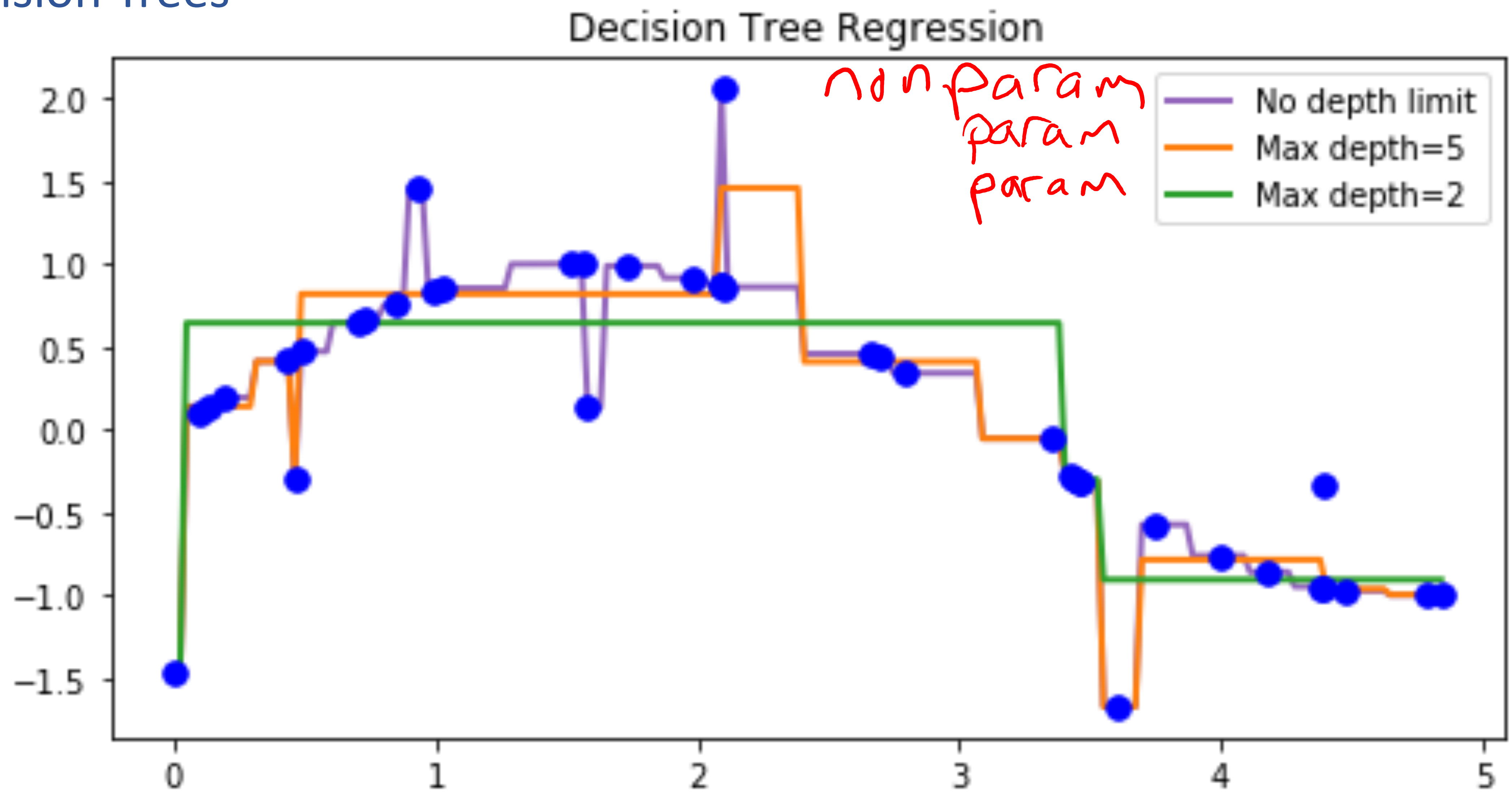
Nonparametric Regression

Decision Trees



Nonparametric Regression

Decision Trees



Poll 1

Are decision trees parametric or non-parametric?

A.

B.

C.

Poll 1

Are decision trees parametric or non-parametric?

It depends :)

- If no limits on depth or reuse of attributes, then non-parametric
  - Model complexity will grow with data
- If pruned/limited to fix size
  - Parametric
- If attributes only used once
  - Parametric; model complexity is limited by number of features

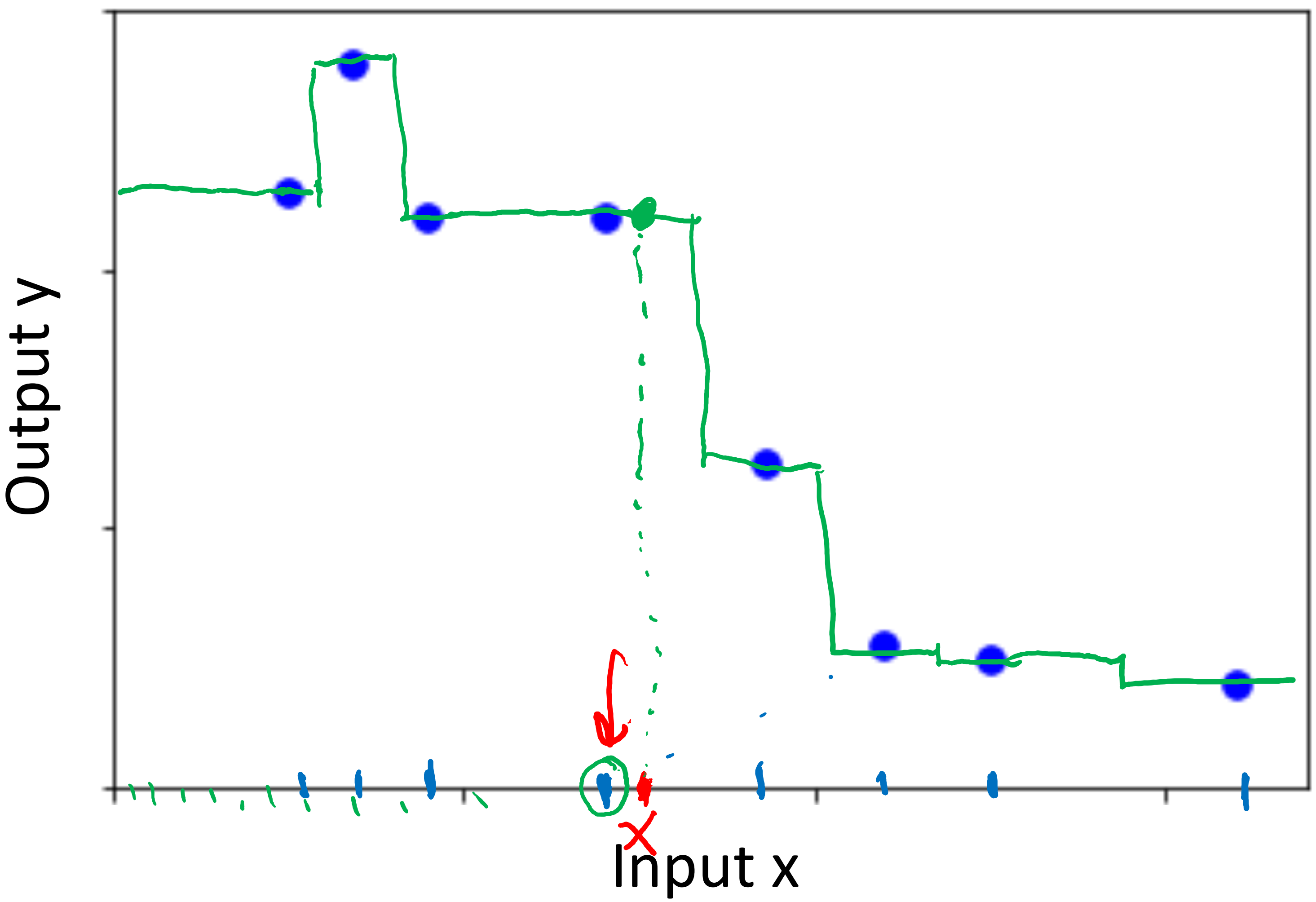
Trade-offs

- Non-parametric methods have very powerful representation capabilities
- But
  - Easily overfit
  - Can take up memory proportional to training size too

Nonparametric Regression

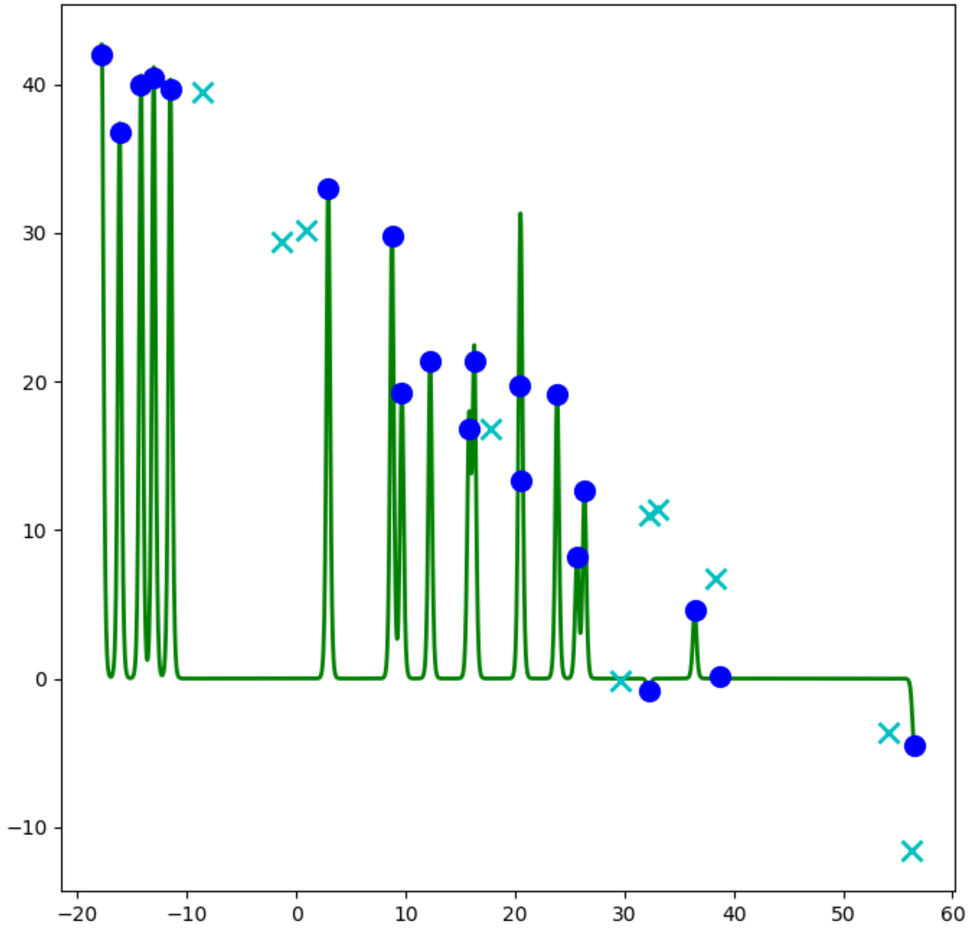
$\hat{y} = h(x)$

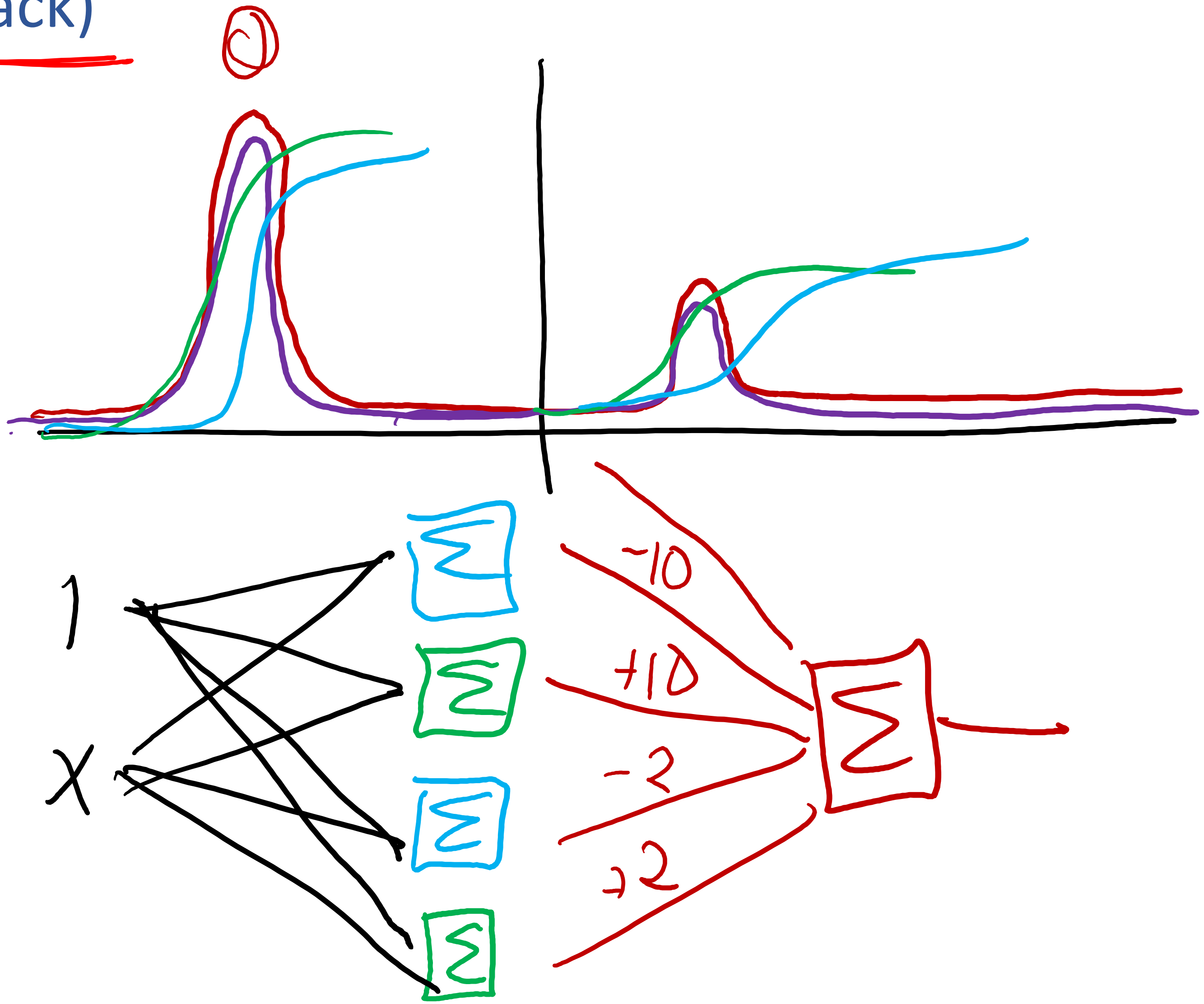
Nearest Neighbor



Nonparametric Regression

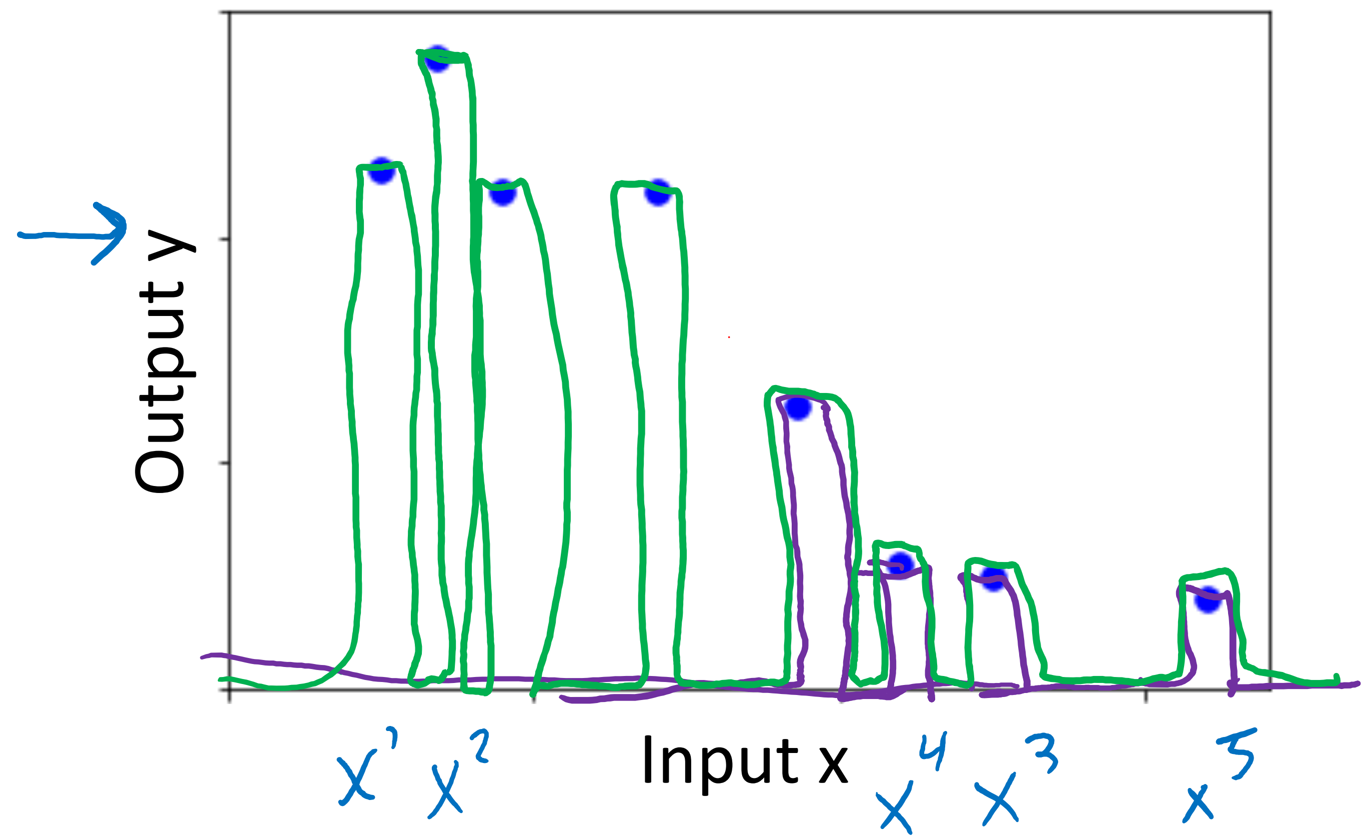
Neural Networks (nonparametric hack)



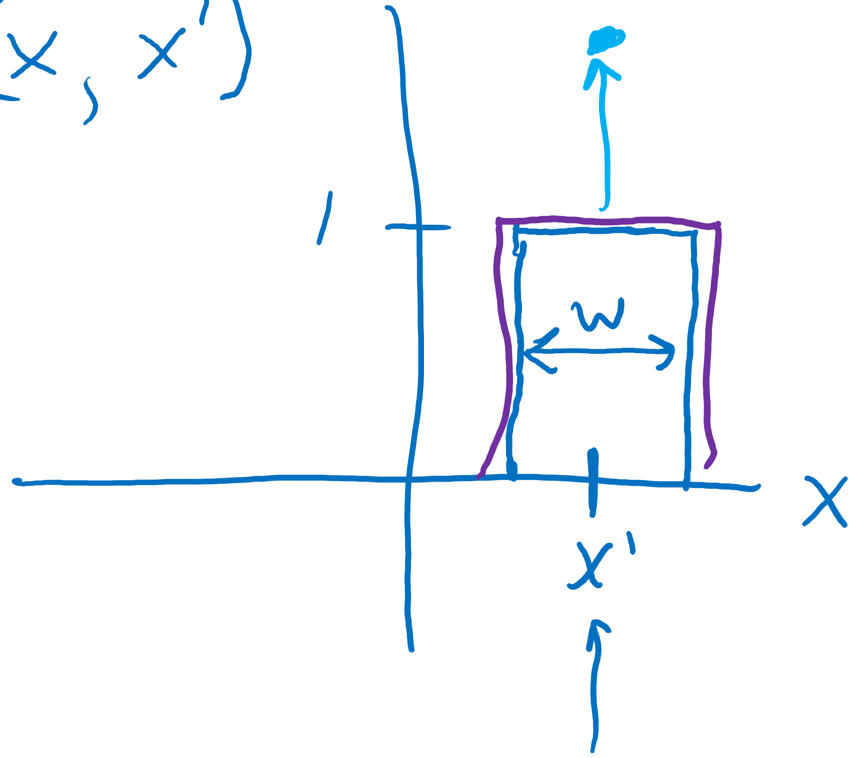


Nonparametric Regression

Kernel Regression



$k(x, x')$



$\hat{y} = h(x)$

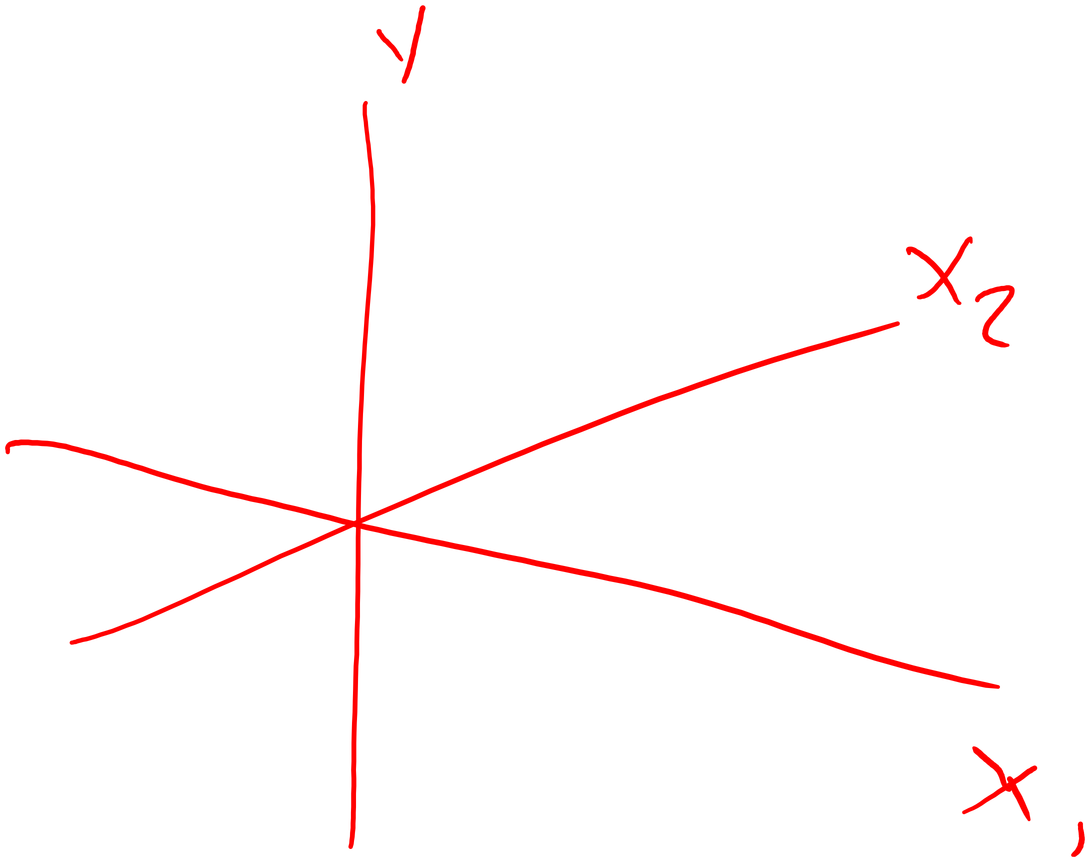
$\hat{y} = \sum_{i=1}^{N} y^{(i)} \boxed{k(x, x^{(i)})}$

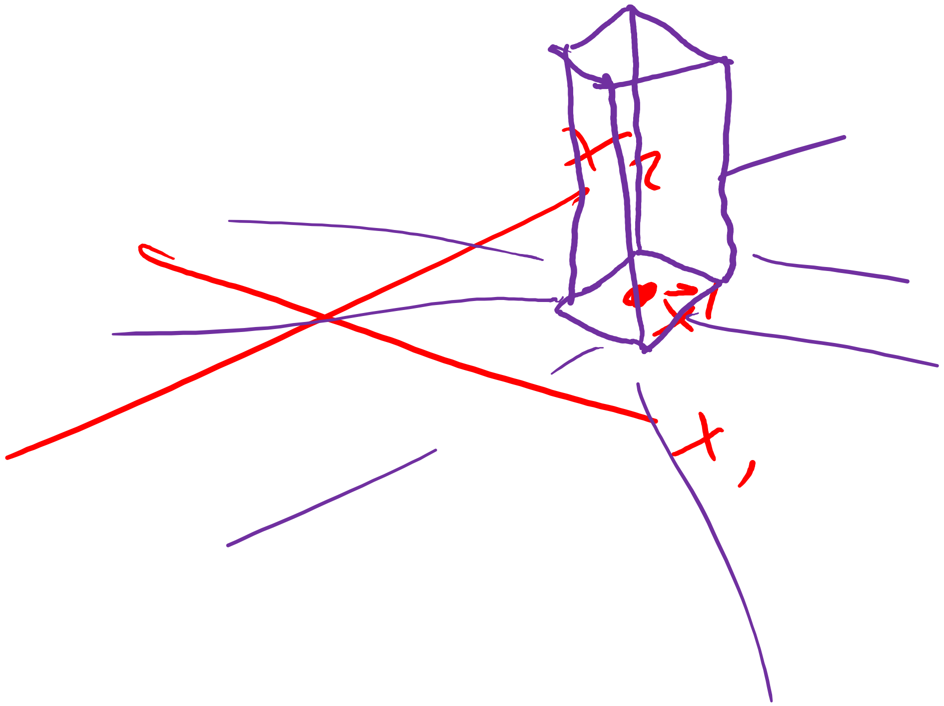
Nonparametric Regression

Kernel Regression

$\vec{x} \in \mathbb{R}^2$

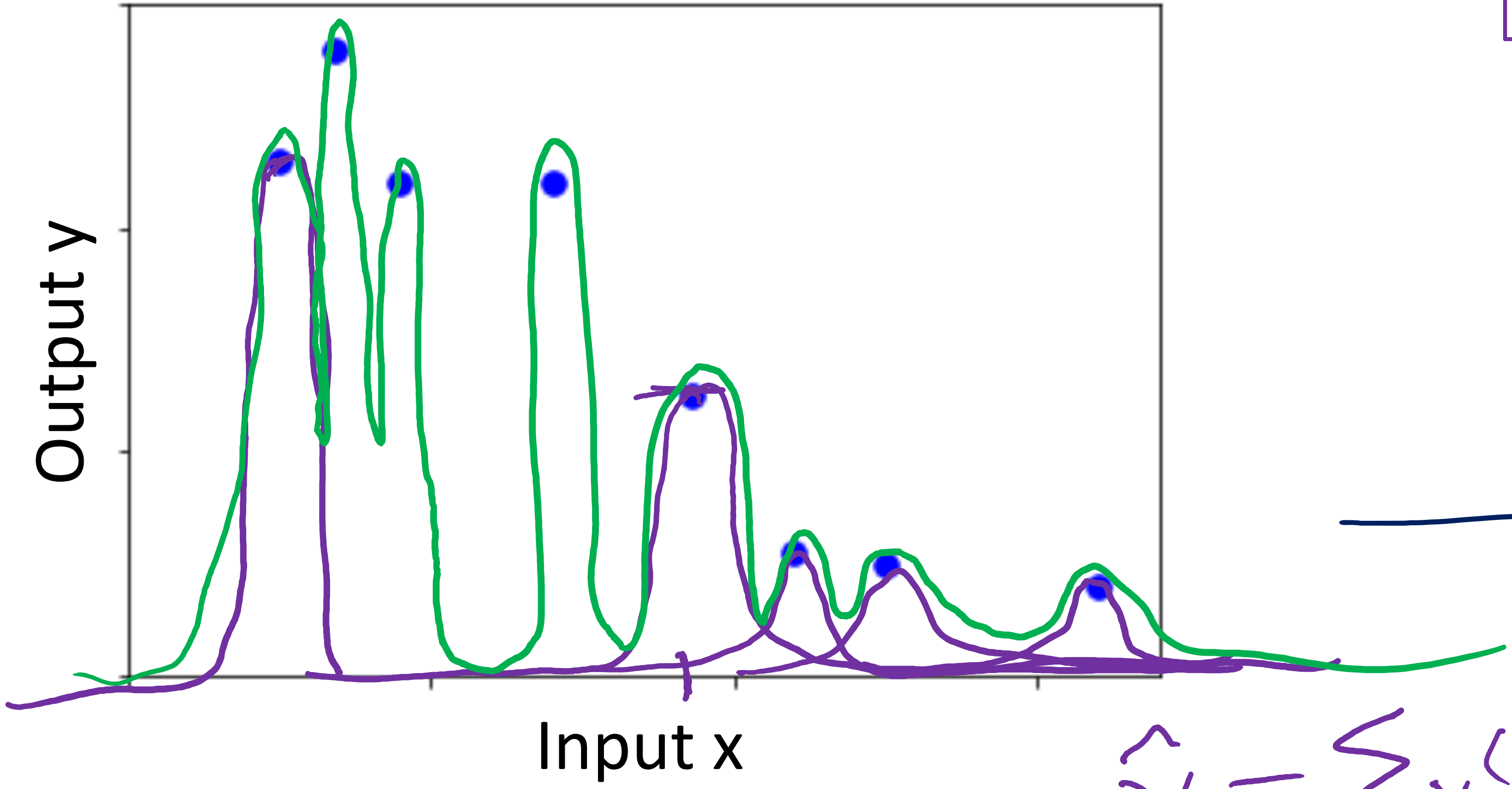
$k(\vec{x}, \vec{x}')$





Nonparametric Regression

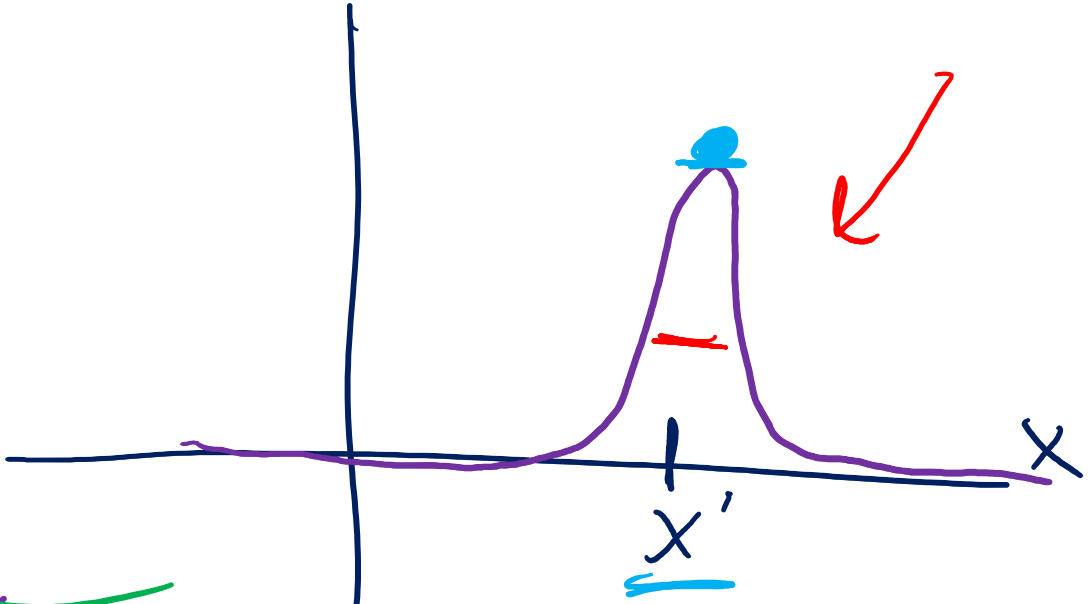
Kernel Regression



RBF Kernel function

$$k(x, x') = e^{\frac{-\|x - x'\|_2^2}{2\sigma^2}}$$

$$= e^{-\gamma \|x - x'\|_2^2}$$



$$\hat{y} = \sum y^{(i)} k(x, x^{(i)})$$

Poll 2

As x and x' get closer the RBF function:

A. Increases

B. Decreases

C. Stays the same

RBF Kernel function

$$k(x, x') = e^{\frac{-\|x-x'\|_2^2}{2\sigma^2}}$$

$$= e^{-\gamma\|x-x'\|_2^2}$$

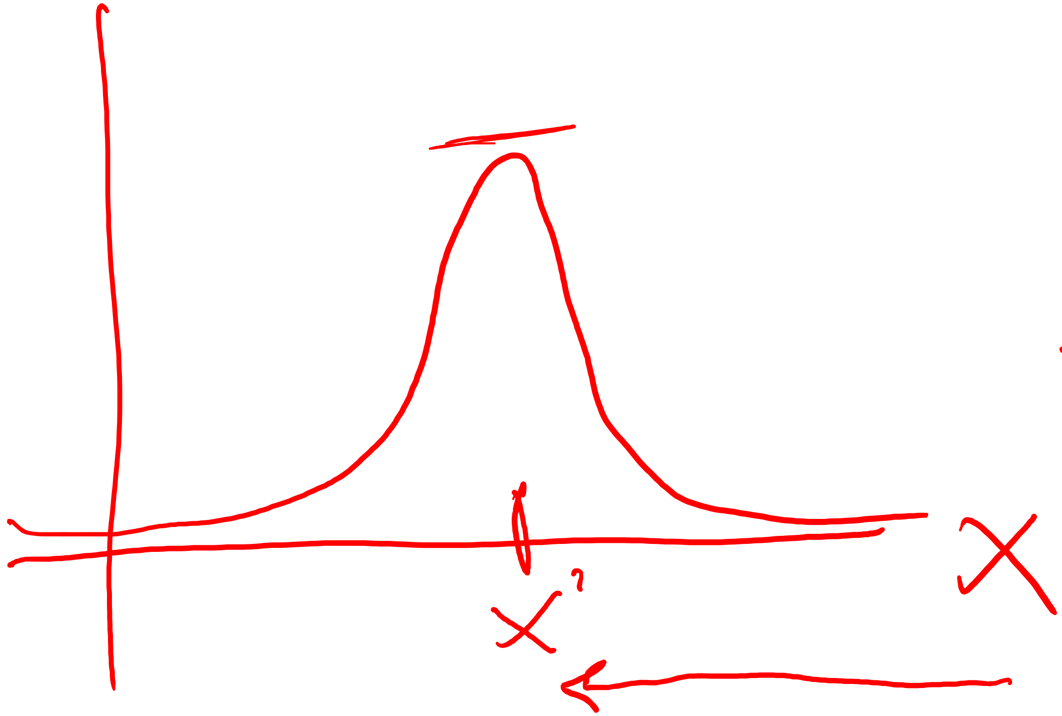
$x - x'$

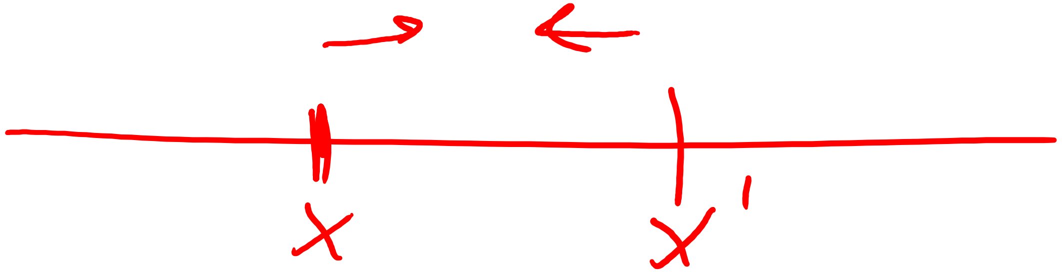
$\downarrow$

0

e^{-0}

$e^{-?}$





Poll 3

As γ increases the RBF function:

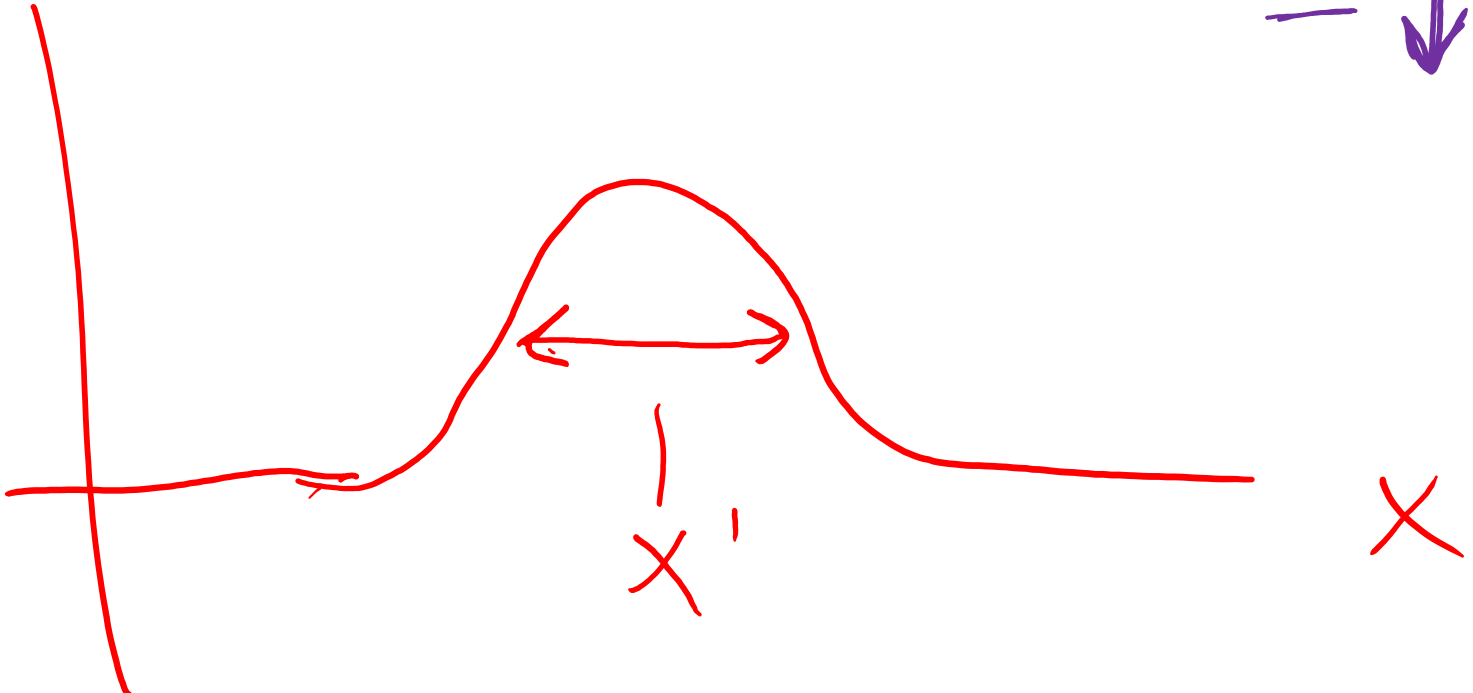
A. Gets wider
B. Gets narrower
C. Stays the same

RBF Kernel function

$$k(x, x') = e^{\frac{-\|x-x'\|_2^2}{2\sigma^2}}$$

$$= e^{-\gamma\|x-x'\|_2^2}$$

$$\gamma = \frac{1}{2\sigma^2}$$



Poll 4

As γ increases the max height of the RBF:

A. Increases

B. Decreases

C. Stays the same

RBF Kernel function

$$k(x, x') = e^{\frac{-\|x - x'\|_2^2}{2\sigma^2}}$$

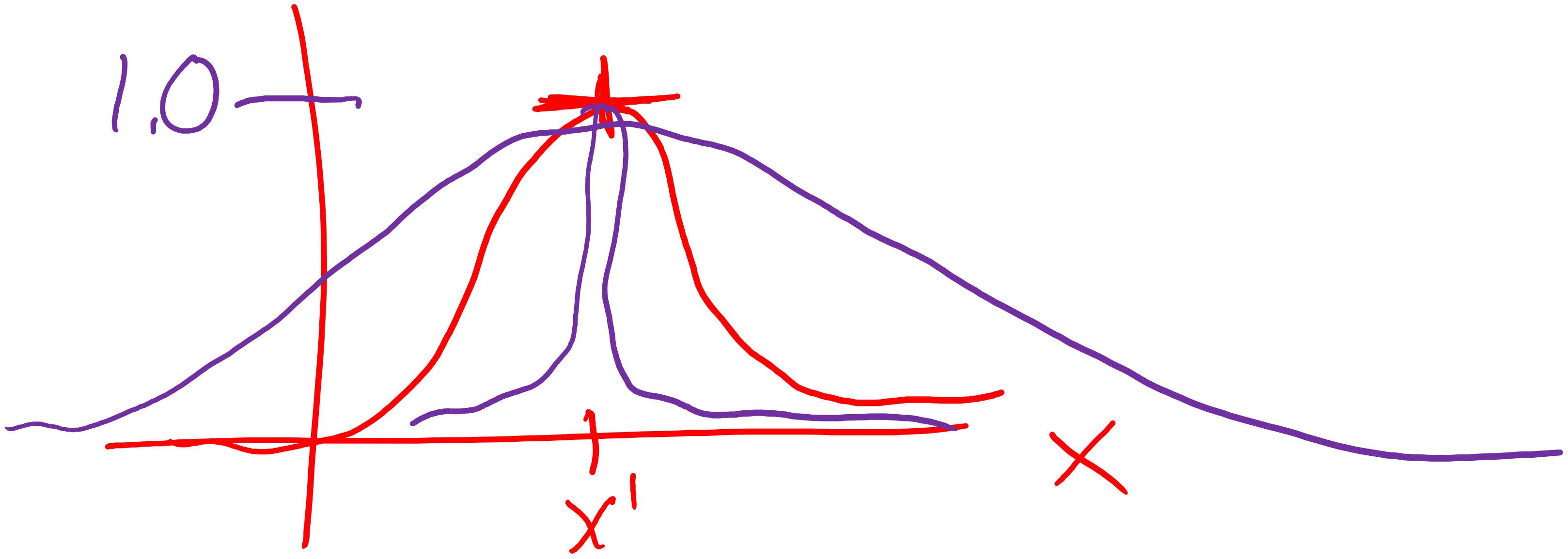
$$= e^{-\gamma\|x - x'\|_2^2}$$

$$\gamma = \frac{1}{2\sigma^2}$$

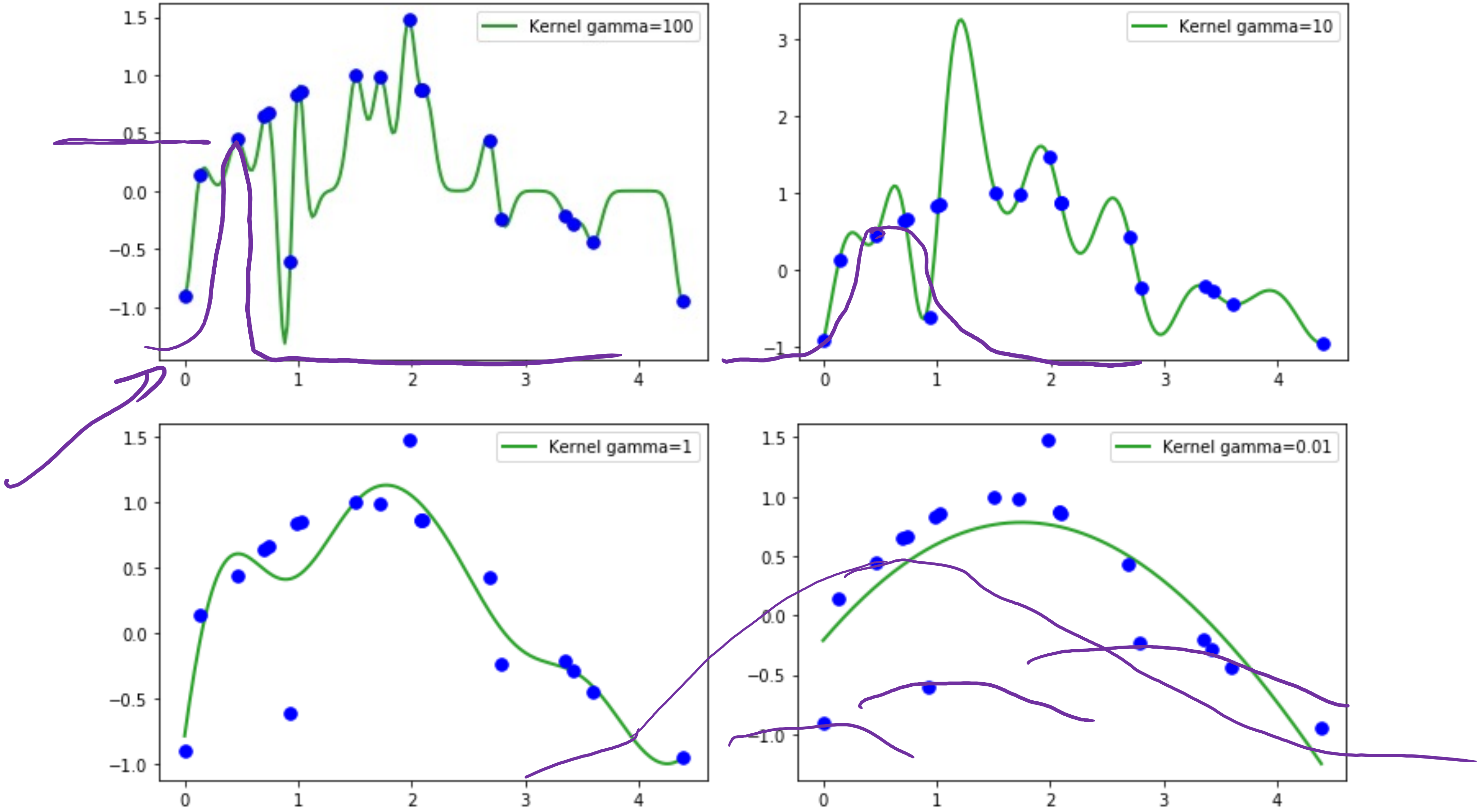
$$x = x'$$

$$e^{-\gamma\|0\|_2^2}$$

$$e^{-\gamma 0}$$



Kernel Regression



Kernel Regression

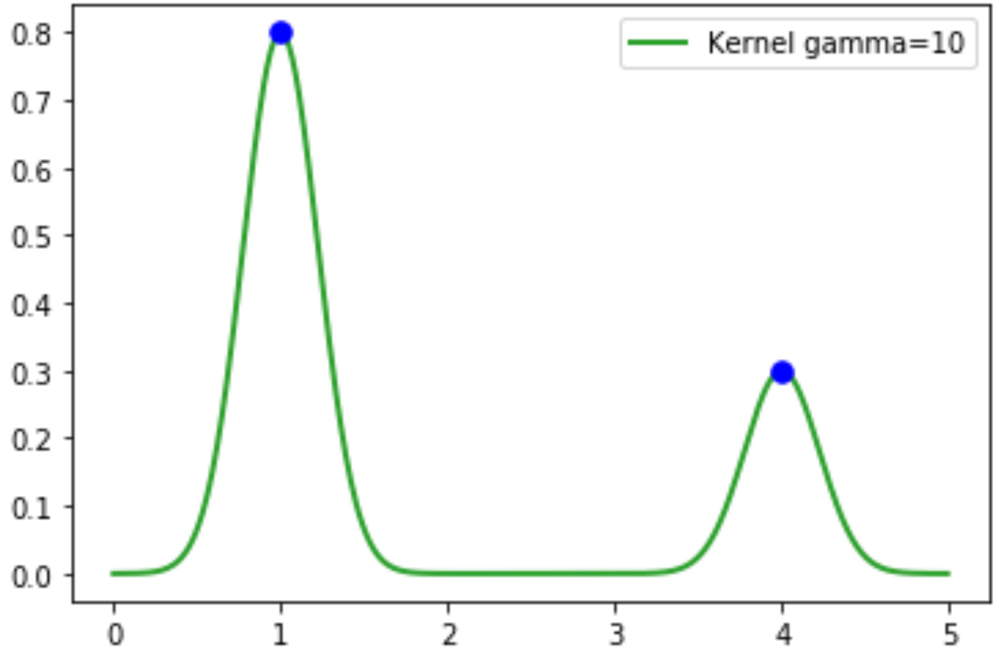
RBF kernel and corresponding hypothesis function

Distance kernel (Gaussian / Radial Basis Function)

- Close to point should be that point
- Far should be zero
- Mini Gaussian window

$$k(x, x') = e^{\frac{-\|x-x'\|_2^2}{2\sigma^2}} = e^{-\gamma\|x-x'\|_2^2}$$

- We control the variance γ

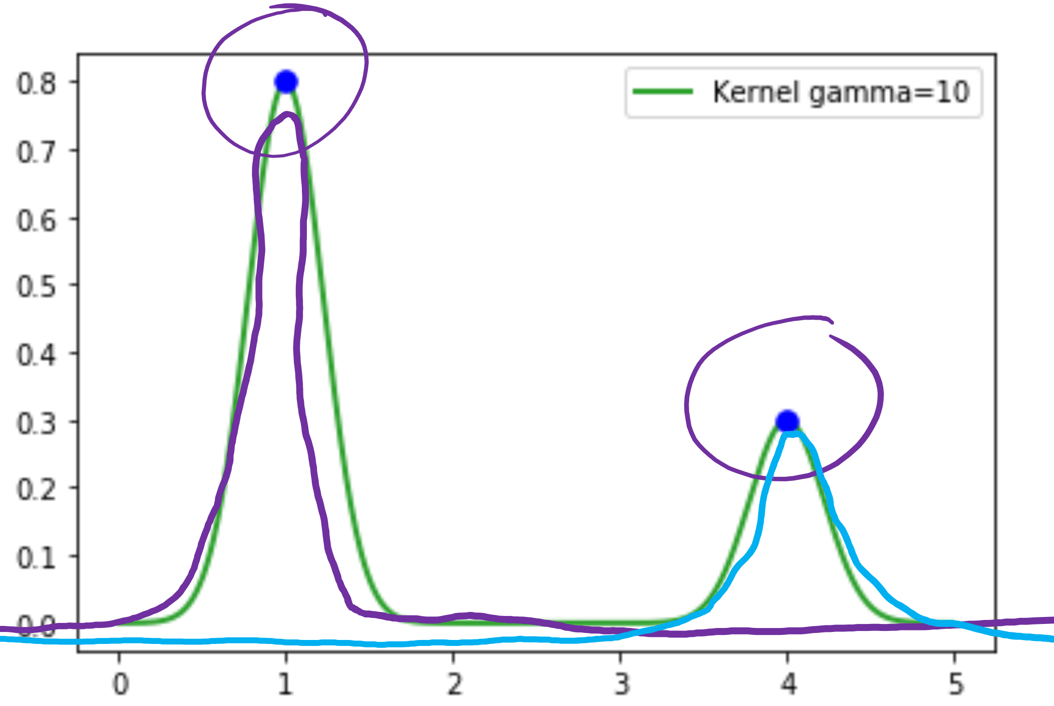


Kernel Regression

RBF kernel and corresponding hypothesis function

Prediction?

- Weighted sum of these little windows
  - $\hat{y} = h(x) = \boxed{\sum_i \alpha_i k(x, x^{(i)})}$
  - What should α_i be?
    - $\boxed{\alpha_i = y_i,}$ $\alpha = y$?
    - Need to account for points that are close together



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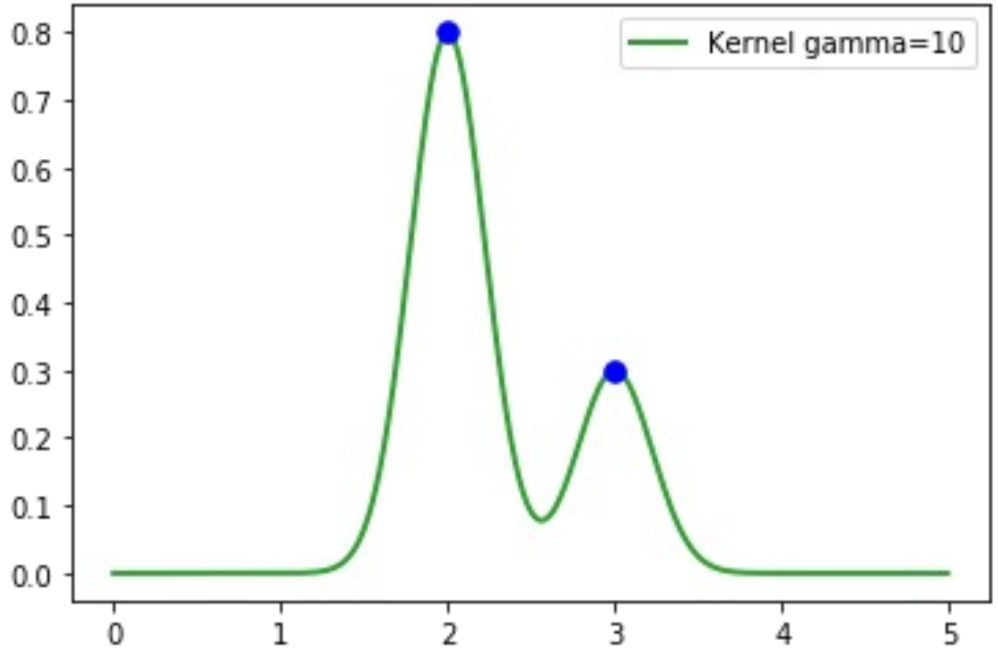

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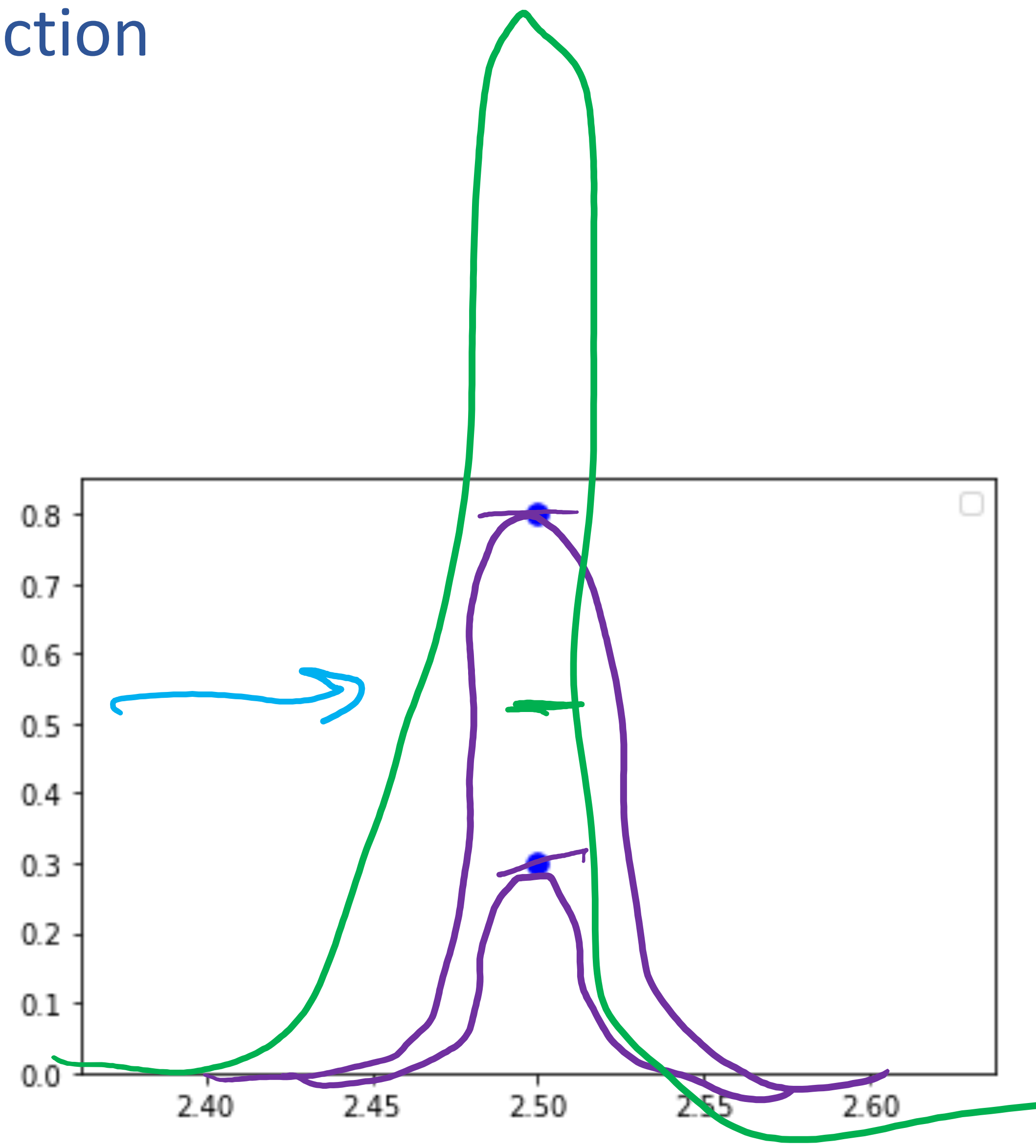

Kernel Regression

RBF kernel and corresponding hypothesis function

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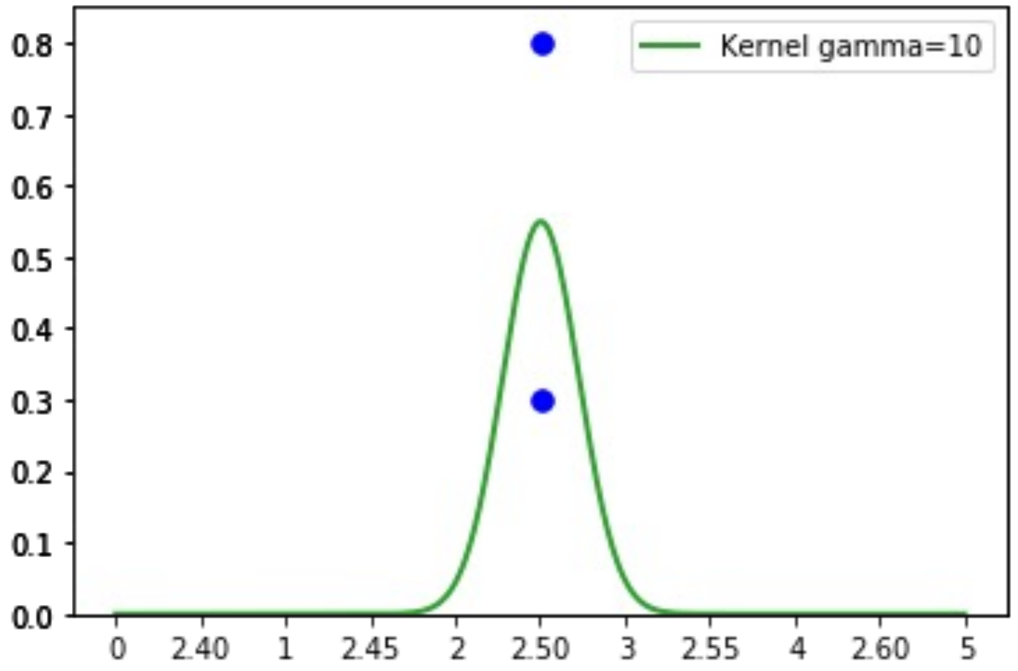


Kernel Regression

RBF kernel and corresponding hypothesis function

$$\alpha^{(i)} = \frac{y^{(i)}}{\text{density of } x^{(i)}}$$

all

Prediction?

- Weighted sum of these little windows
  - $\hat{y} = h(x) = \sum_i \alpha_i k\left(x, x^{(i)}\right)$
  - What should α_i be?
    - Need to account for points that are close together

      $\alpha = (K)^{-1} y$

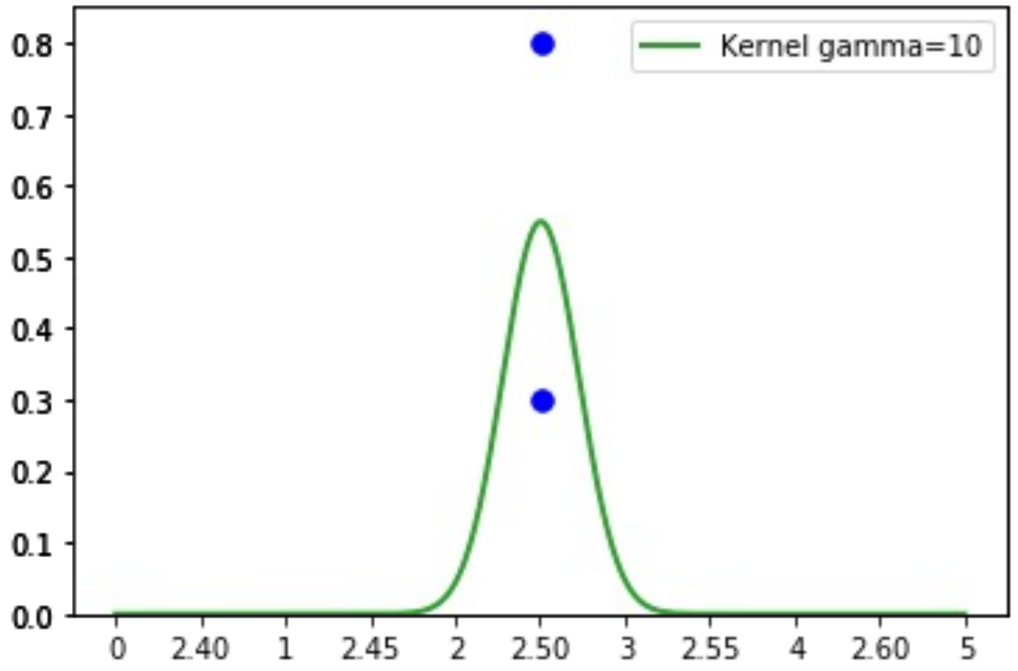
      $\alpha = (K + \lambda I)^{-1} y$

      where $K_{ij} = k\left(x^{(i)}, x^{(j)}\right)$

      and λ is small to help inversion

i

j



Kernelized Linear Regression

Reminder: Polynomial Linear Regression

Polynomial feature function

poly(d)

$$x \xrightarrow{\phi(x)} [1 \; x \; x^2 \; x^3 \; x^4]$$

1   5

$$[x_1, x_2] \xrightarrow{\phi(\vec{x})} [1 \; x_1 \; x_2 \; x_1^2 \; x_2^2 \; x_1 x_2]$$

2   6

$$(X^T X)^{-1} X^T y \rightarrow \hat{\theta}$$

Reminder: Polynomial Linear Regression

Polynomial feature function

Least squares formulation

Least squares solution

Reminder: Polynomial Linear Regression

Polynomial feature function

- $x \to \phi(x) = [1, x, x^2, x^3]^T$
- $X \to \Phi$ $\leftarrow \mathbb{R}^{N \times 4}$

Least squares formulation

- $\min_w \|y - \Phi w\|_2^2$

Least squares solution

- $w = (\Phi^T \Phi)^{-1} \Phi^T y$

Plus L2 regularization

- $\min_w \|y - \Phi w\|_2^2 + \lambda \|w\|_2^2$
- $w = (\Phi^T \Phi + \lambda \mathrm{I})^{-1} \Phi^T y$

Can rewrite as

- $w = \Phi^T (\Phi \Phi^T + \lambda \mathrm{I})^{-1} y$

Kernelized Linear Regression

L2 regularized linear regression (with feature function)

- $\min_{w} \|y - \Phi w\|_2^2 + \lambda \|w\|_2^2$
- $w = (\Phi^T \Phi + \lambda \mathrm{I})^{-1} \Phi^T y$

Can rewrite as

- $w = \Phi^T (\Phi \Phi^T + \lambda \mathrm{I})^{-1} y$

Let $(K + \lambda I)^{-1}$

$\boldsymbol{\alpha} = (\Phi \Phi^T + \lambda \mathrm{I})^{-1} \mathbf{y}$

$\Phi^T \vec{\alpha}$

Prediction

- $\hat{y} = h(x) = \mathrm{w}^{\mathrm{T}} \mathrm{x}$

new

$= x^T w$

$= \phi(x)^T w$

$= \phi(x)^T \Phi^T \vec{\alpha}$

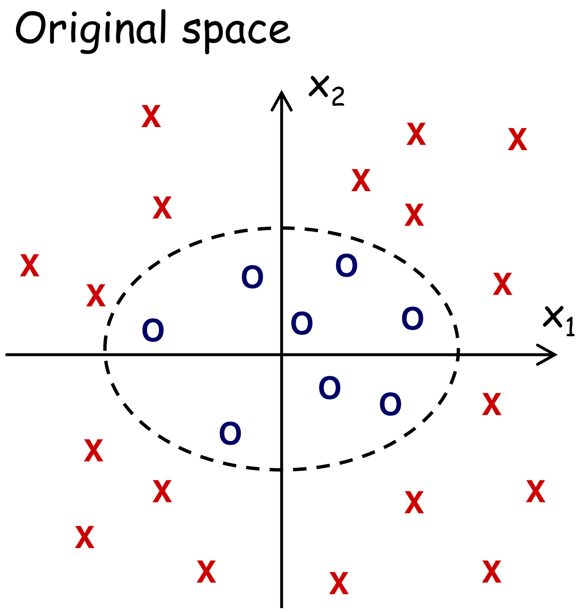
$= \sum_{i=1}^{N} \alpha_i \boxed{\phi(x)^T \phi(x^{(i)})} = \sum_{i=1}^{N} \alpha_i \boxed{k(x, x^{(i)})}$

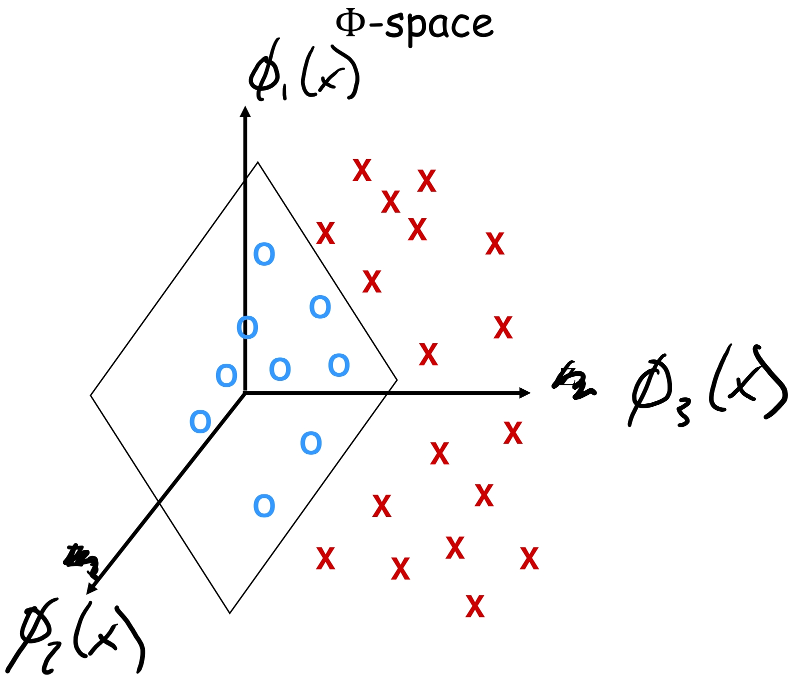
feature dot prod

Kernel

Example: Polynomial Kernel

https://www.youtube.com/watch?v=3liCbRZPrZA





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Kernels: Motivation

Motivation #1: Inefficient Features

- Non-linearly separable data requires **high dimensional** representation
- Might be **prohibitively expensive** to compute or store

Motivation #2: Memory-based Methods

- k-Nearest Neighbors (KNN) for facial recognition allows a **distance metric** between images -- no need to worry about linearity restriction at all

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Kernel Methods

$\cancel{x^T z}$ feature

$\phi(x)^T \phi(z)$

$k(x, z)$

Key idea:

1. Rewrite the algorithm so that we only work with **dot products** $x^T z$ of feature vectors
2. Replace the **dot products** $x^T z$ with a **kernel function** $k(x, z)$

The kernel $k(x,z)$ can be **any** legal definition of a dot product:

$$k(x, z) = \boxed{\phi(x)^T \phi(z)} \text{ for any function } \phi: \mathcal{X} \rightarrow \mathbf{R}^D$$

So we only compute the ϕ dot product **implicitly**

This **"kernel trick"** can be applied to many algorithms:

- classification: perceptron, SVM, …
- regression: ridge regression, …
- clustering: k-means, …

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Kernel Methods

Q: These are just non-linear features, right?

A: Yes, but…

Q: Can't we just compute the feature transformation φ explicitly?

A: That depends...

Q: So, why all the hype about the kernel trick?

A: Because the **explicit features** might either be **prohibitively expensive** to compute or **infinite length** vectors

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Example: Polynomial Kernel

$(x^T z)^d$

$x \in R^2 \quad d=2$ poly

For n=2, d=2, the kernel $\mathrm{K}(\mathrm{x}, \mathrm{z}) = (\mathrm{x} \cdot \mathrm{z})^{\mathrm{d}}$ corresponds to

$$\phi: \mathrm{R}^2 \to \mathrm{R}^3,\ (\mathrm{x}_1, \mathrm{x}_2) \to \Phi(\mathrm{x}) = (\mathrm{x}_1^2, \mathrm{x}_2^2, \sqrt{2}\mathrm{x}_1\mathrm{x}_2)$$

$$\phi(\mathrm{x}) \cdot \phi(z) = \left(\mathrm{x}_1^2, \mathrm{x}_2^2, \sqrt{2}\mathrm{x}_1\mathrm{x}_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1 z_2)$$

$$= (\mathrm{x}_1 z_1 + \mathrm{x}_2 z_2)^2 = (\mathrm{x} \cdot z)^2 = \mathrm{K}(\mathrm{x}, \mathrm{z})$$

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Kernel Examples

Side Note: The feature space might not be unique!

Explicit representation #1:

$$\phi: R^2 \rightarrow R^3,\ (x_1, x_2) \rightarrow \Phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

$$\phi(x) \cdot \phi(z) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)$$

$$= (x_1z_1 + x_2z_2)^2 = (x \cdot z)^2 = K(x, z)$$

Explicit representation #2:

$$\phi: R^2 \rightarrow R^4,\ (x_1, x_2) \rightarrow \Phi(x) = (x_1^2, x_2^2, x_1x_2, x_2x_1)$$

$$\phi(x) \cdot \phi(z) = (x_1^2, x_2^2, x_1x_2, x_2x_1) \cdot (z_1^2, z_2^2, z_1z_2, z_2z_1)$$

$$= (x \cdot z)^2 = K(x, z)$$

These two different feature representations correspond to the same kernel function!

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Kernel Examples

Name	Kernel Function (implicit dot product)	Feature Space (explicit dot product)
Linear	$K(\mathbf{x}, \mathbf{z}) = \mathbf{x}^T \mathbf{z}$	Same as original input space
Polynomial (v1)	$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z})^d$	All polynomials **of** degree d
Polynomial (v2)	$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z} + 1)^d$	All polynomials **up to** degree d
Gaussian (RBF)	$K(\mathbf{x}, \mathbf{z}) = \exp(-\frac{\|\|\mathbf{x} - \mathbf{z}\|\|_2^2}{2\sigma^2})$	Infinite dimensional space
Hyperbolic Tangent (Sigmoid) Kernel	$K(\mathbf{x}, \mathbf{z}) = \tanh(\alpha \mathbf{x}^T \mathbf{z} + c)$	(With SVM, this is equivalent to a 2-layer neural network)

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