

Features: Representing your data

COMS21202, Part III

- Song Liu (song.liu@bristol.ac.uk), Lecturer in Data Science and A.I.

Introduction

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Machine Learning Pipeline

Part I

Data Acquisition

sampling/quantization



We are here, Part III

Feature Engineering

representing your data



Part I, II

Training algorithms

classification/regres
sion/clustering...



Prediction/Inference

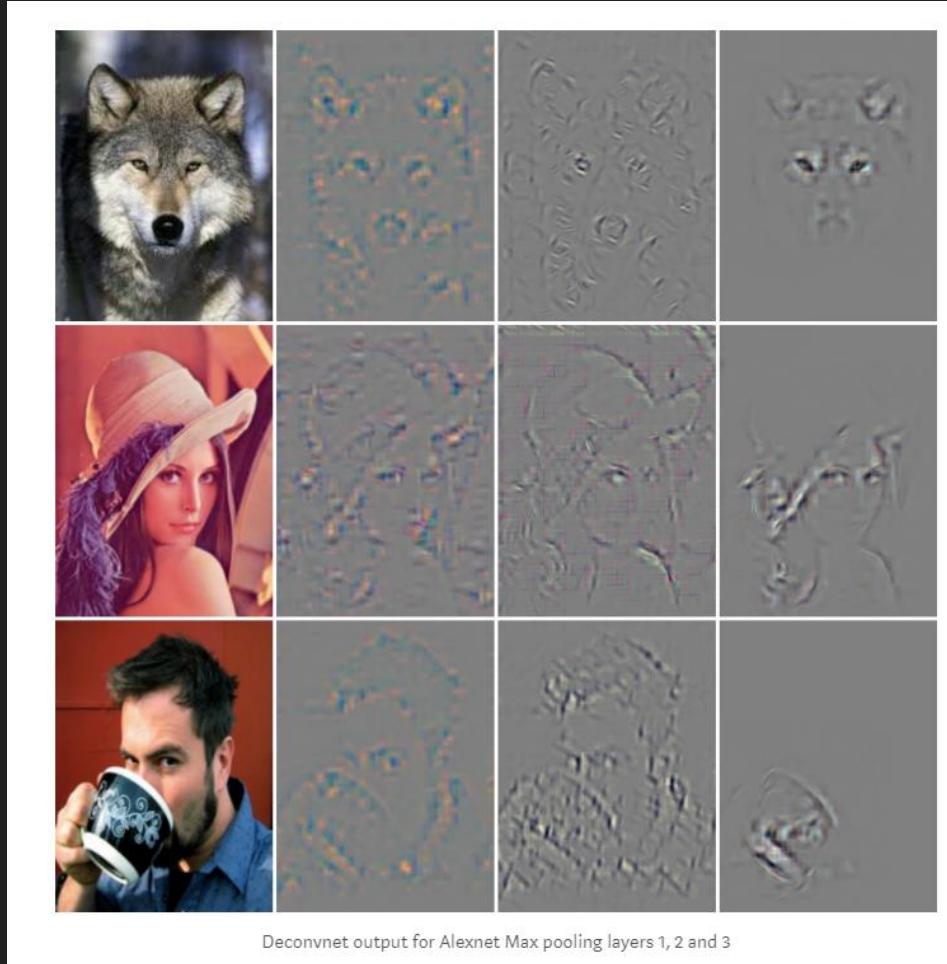
Making decisions,
cats or dogs?

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How does machine see the world?

- Machine does not see the world in the same way we do.
- It does not need to.
- It only needs the representation of info to perform its task.

How does machine learning algorithm see the world?



○ Visualization of layers in Alexnet.
○ Zeiler and Fergus, ECCV 2014

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Turning Data into Features

- Modern machine learning **rarely** uses **raw data** input to perform learning tasks.
- Raw input is usually transformed into a more powerful representation: **features**.
- This procedure of representing data using features is usually referred as **feature engineering** in literatures.

Feature Engineering

- Task: finding a feature **transform function** $f(x)$, which takes a **d -dimensional raw input x** and outputs a **m -dimensional feature vector.**
- Feature function f is the medium through which your learning algorithm interacts with your data.
- Let us put feature engineering in the context of **Least squares**.

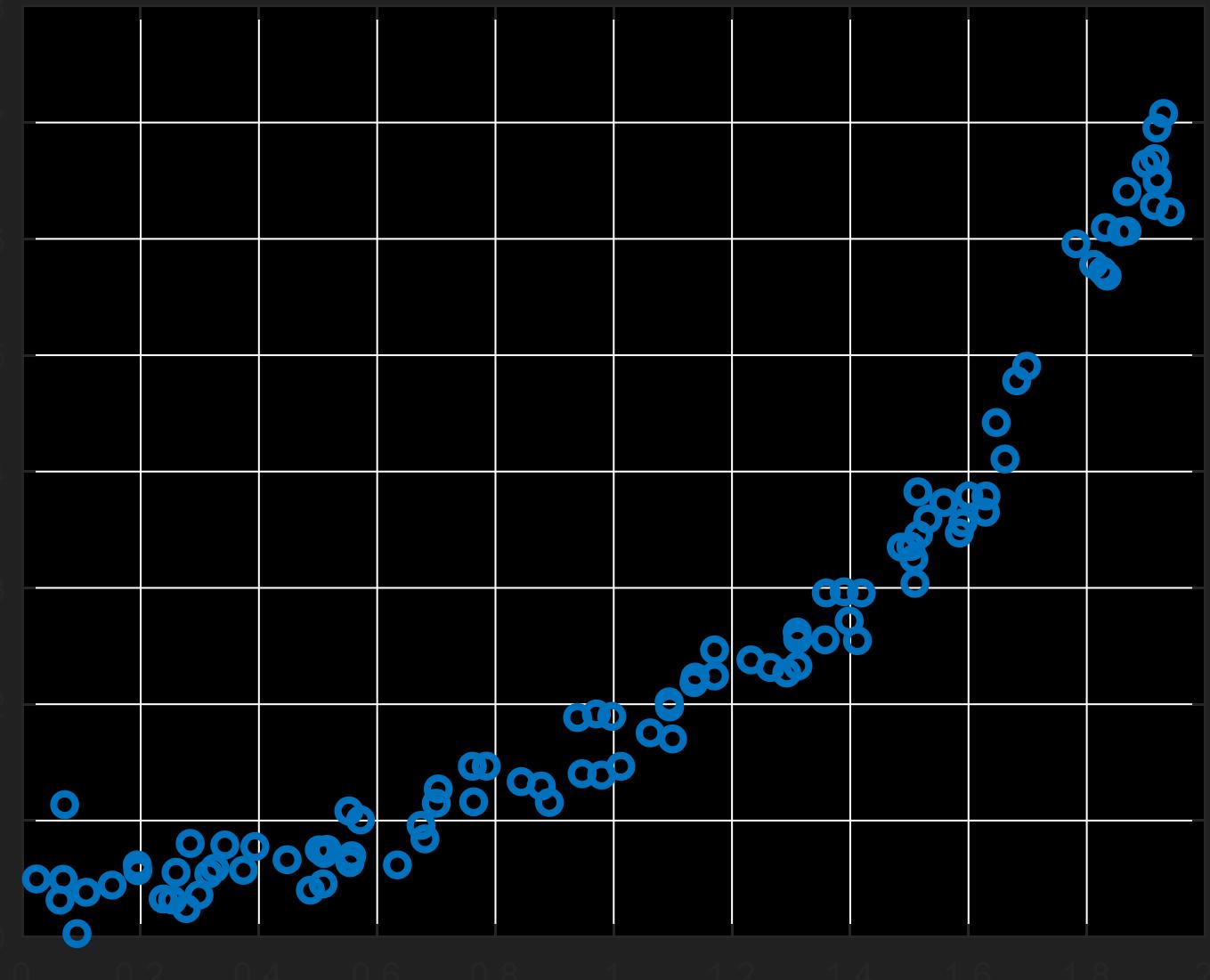
A Teaser

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Least Squares (LS) + Feature Transform f

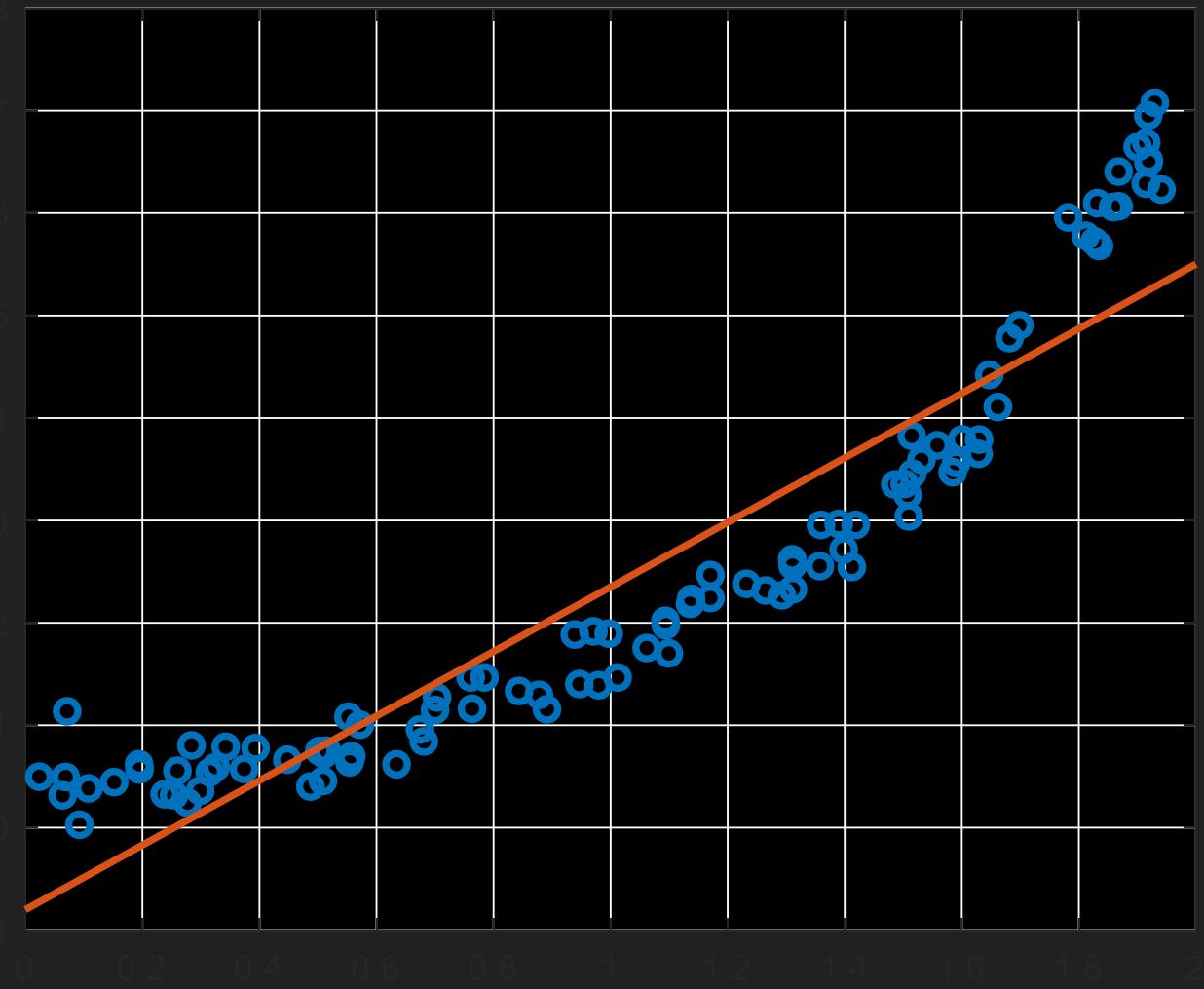
- Recall, given $D = \{(y_i, x_i)\}_i, y_i \in R,$
- LS solves the following minimization:
 - $\hat{\beta} := \arg \min_{\beta} \sum_{i=1}^n (y_i - \beta x_i)^2 \quad (1)$
- Replace x with $f(x)$, a feature transform
 - $\hat{\beta} := \arg \min_{\beta} \sum_{i=1}^n (y_i - \beta f(x_i))^2 \quad (2)$
- (1) and (2) are identical if $f(x) = x.$

LS Regression on Nonlinear Dataset



See Lab 3, Q7
for a similar
example

LS Regression on Nonlinear Dataset



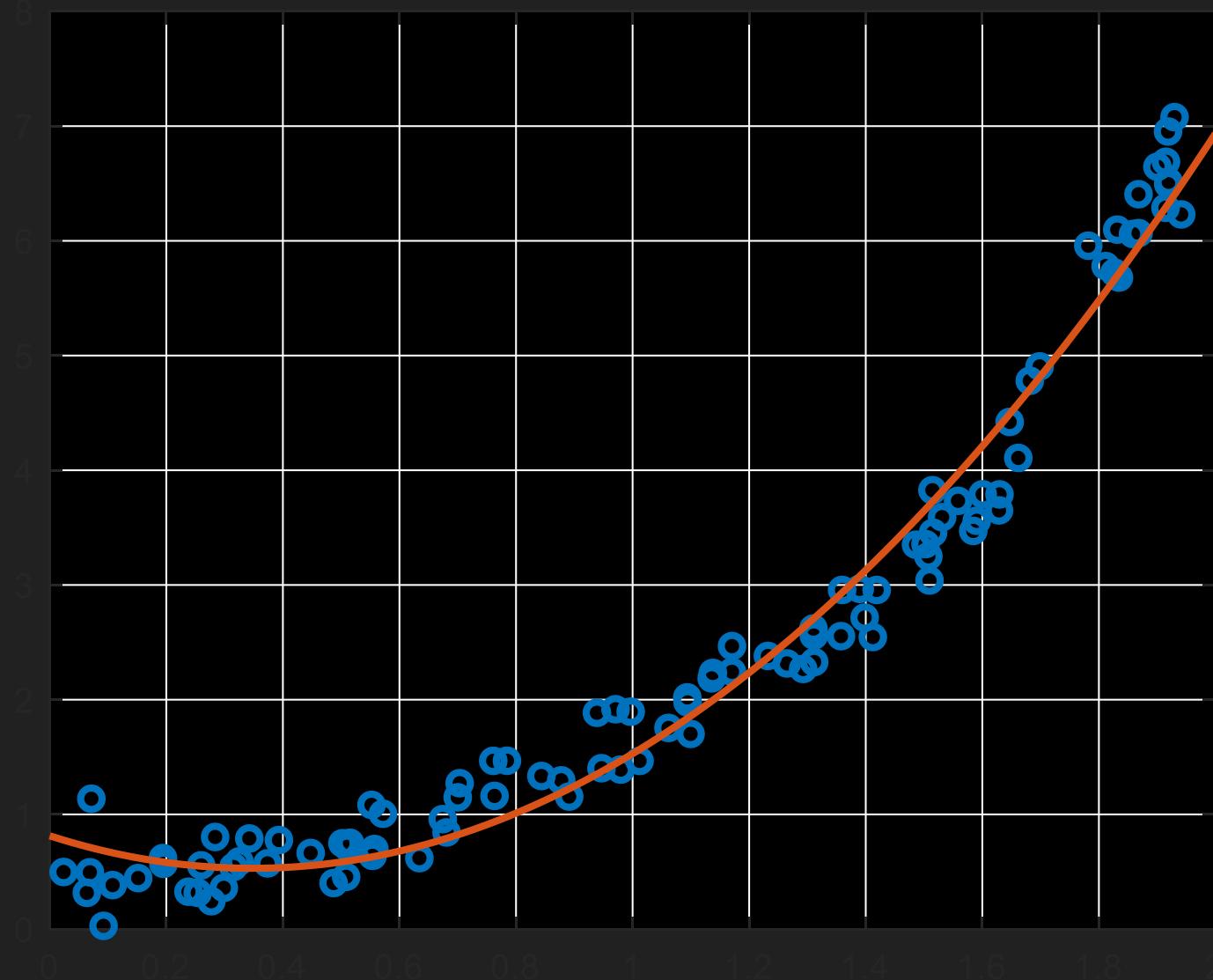
$$f(x) = x$$

Square error:

$$\sum_{i=1}^n (y_i - \hat{\beta} f(x_i))^2,$$

Square error: 57

LS Regression on Nonlinear Dataset



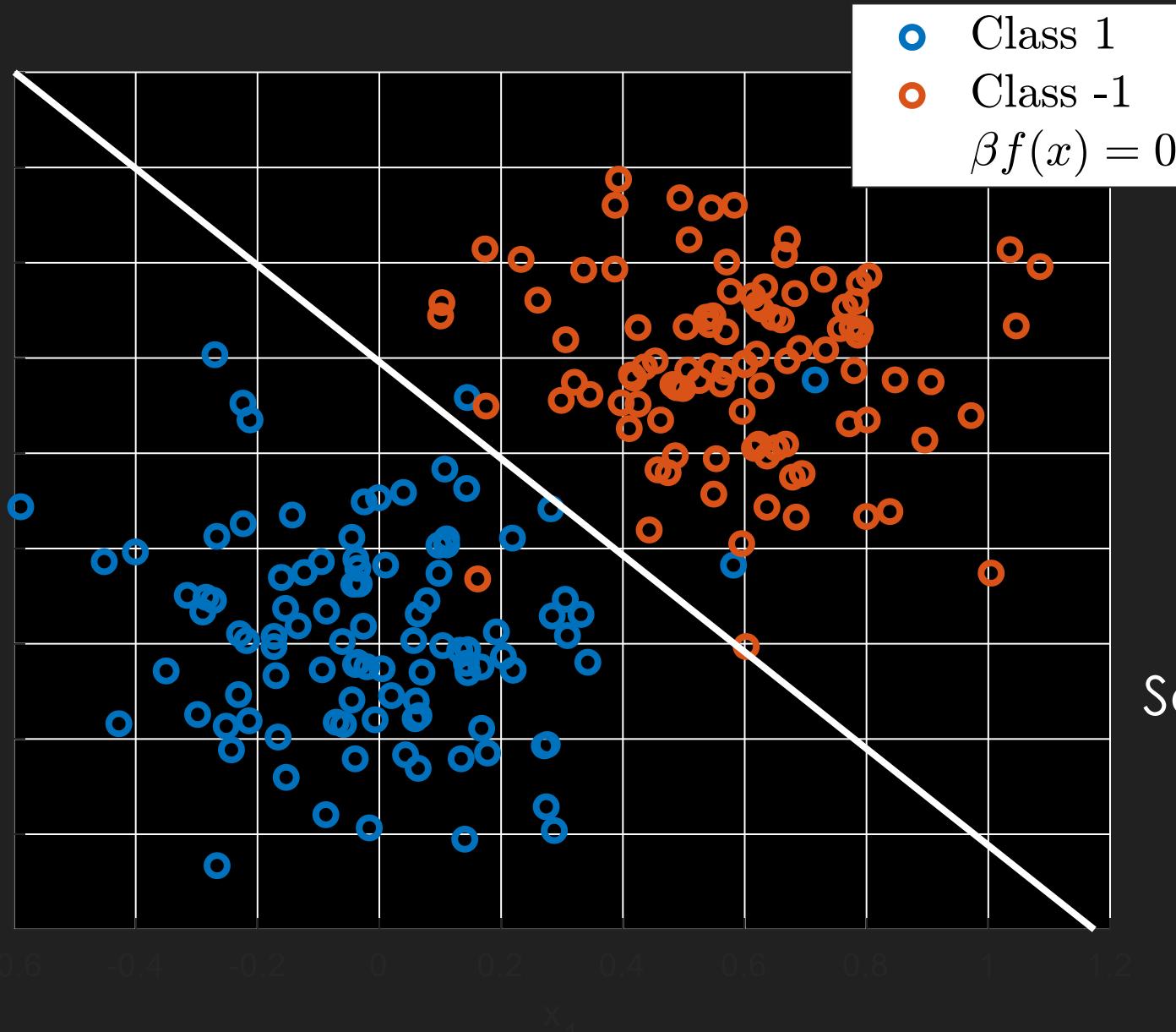
$$f(x) = x^2$$

Square error: 10

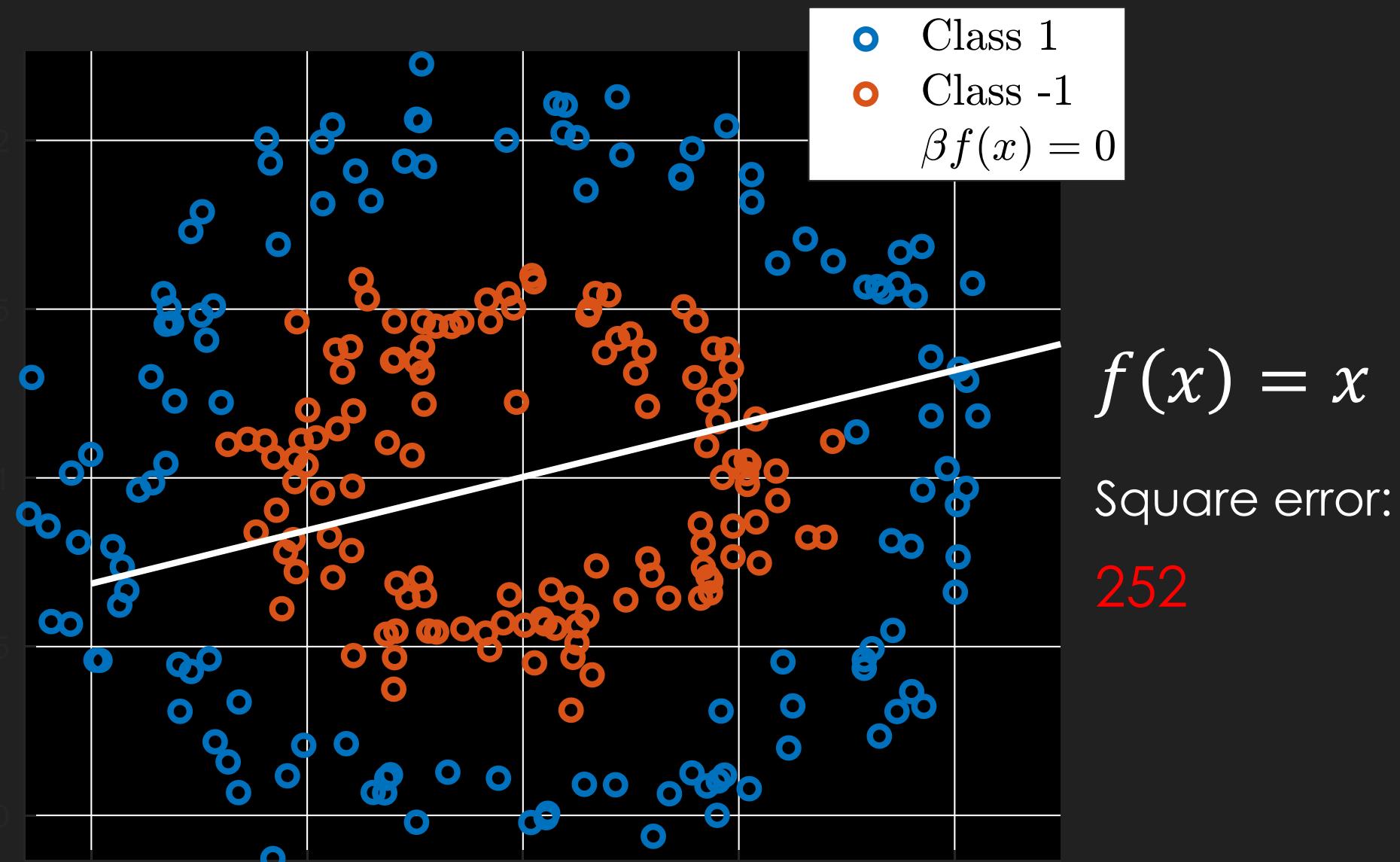
LS Classification + Feature Transform

- Classification dataset: $D = \{(y_i, x_i)\}_{i=1}^n, y \in \{-1, 1\}$.
- Now y only takes two discrete values -1 or 1 as **class labels**.
 - If $y_i = 1/-1$, x_i belongs to pos/neg class.
- Solving LS on D using feature transform f :
 - $\hat{\beta} = \arg \min_{\beta} \sum_{i=1}^n (y_i - \beta f(x_i))^2$
- $\hat{\beta}f(x) = 0$ indicates the **classification boundary**.
 - Why?
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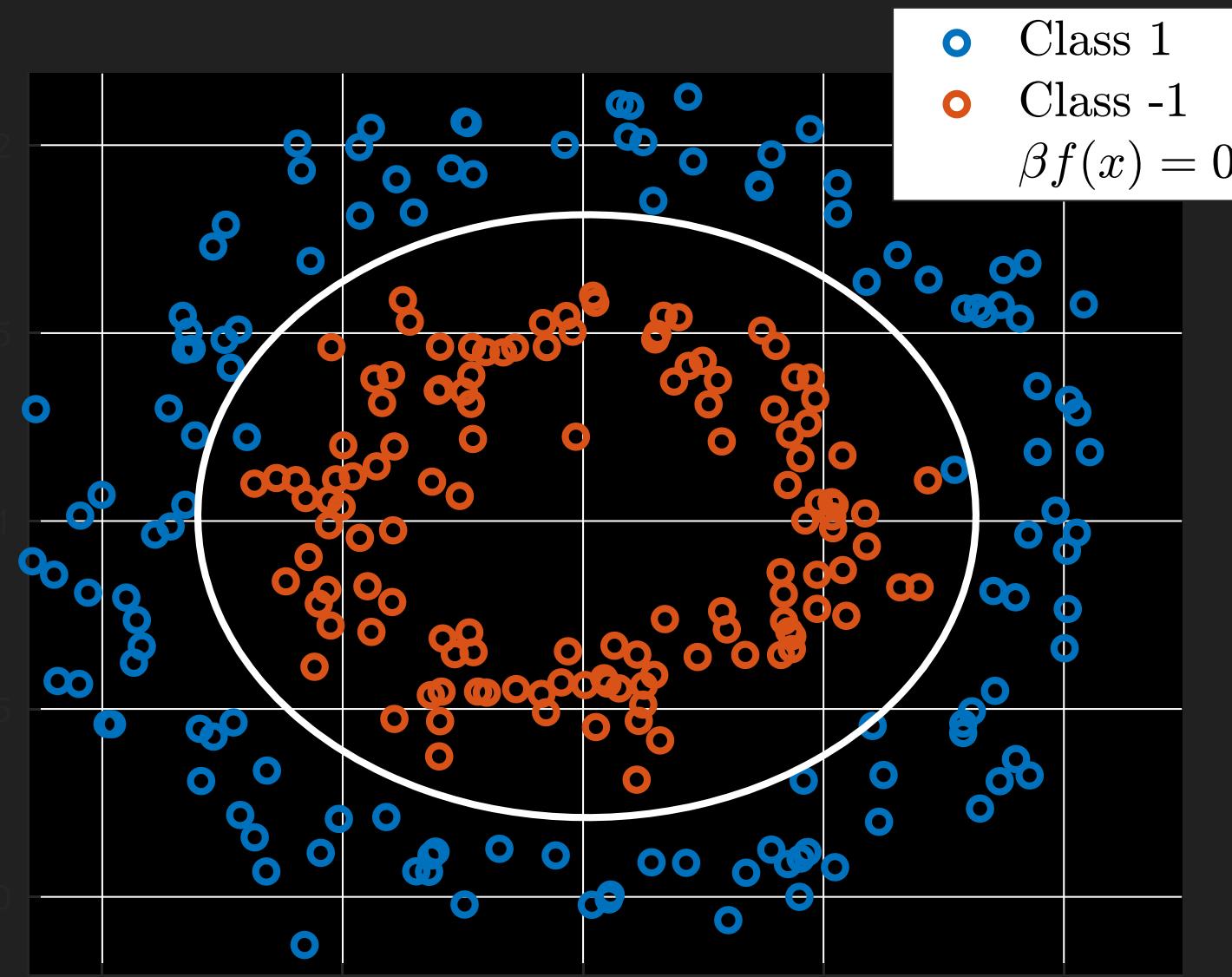
LS Classification



LS Classification on Nonlinear Dataset



LS Classification on Nonlinear Dataset



$$f(x) = x^2$$

Square error:

40



How to construct f in a more principled way?

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Two schools of thoughts:

- Choosing f manually (Week 20,22)
 - **Pros:**
 - Efficient, require little computational effort.
 - Works well if you have domain knowledge.
 - **Cons:** Less flexible, requires tuning on different datasets.
- Choosing f automatically (Week 21)
 - **Pros:** Adaptive, automatically done on different datasets
 - **Cons:**
 - Extra computational burden.
 - Hard to integrate your domain knowledge.
- **Real-world problem solving involves a bit of both!!**

A Note on Math

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Math required in this part

○ Multivariate Linear Algebra

- COMS10003,
- Mathematical Methods for Computer Scientists

○ Probability and Statistics

- COMS10011
- Probability and Statistics

○ Refer to these units for detailed math explanation.

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Formal Notations

○ x, y, z , scalars, $\mathbf{x}, \mathbf{y}, \mathbf{z}$, vectors.

○ $\mathbf{x} \in R^d$, vector in d dimensional real-space.

○ $x^{(i)}$, the i -th dimension of \mathbf{x} .

○ \mathbf{x}_i , the i -th data point in our dataset.

○ $f(\mathbf{x}) \in R^m$, function takes input vector \mathbf{x} and maps it into m dimensional real space.

○ $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \in R^{b \times d}$, **matrices**, with b rows and d columns.

○ “=” is equality, “:=” is definition.

Polynomial Transform

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A Generic Model

- We introduce a generic model.
- $\hat{y} := \langle \beta, f(x) \rangle = \sum_i \beta_i f^{(i)}(x)$.
- Inner product between β and f .
- \hat{y} is linear w.r.t. parameter β .
- Special case:
- when $f(x), \beta \in R, \hat{y} = \beta f(x)$.

Polynomial Transform

- Let $f(x)$ be polynomial functions:
- When $x \in R$, $f(x) := [x^0, x^1, x^2, \dots, x^b]$.
 - b is called the degree of f .
 - $f(x) = [0, x, x^2]$ is called a degree 2 polynomial trans. on x .

Polynomial Transform

- When $x \in R^d$,
- $f(x) := [\mathbf{h}(x^{(1)}), \mathbf{h}(x^{(2)}), \dots, \mathbf{h}(x^{(d)})]$.
- $\mathbf{h}(x) := [x^0, x^1, x^2, \dots, x^b] \in R^b$.
- $f(x) \in R^{d(b+1)}$, which means $\beta \in R^{d(b+1)}$.
- PC: Write down $f^{(i)}(x)$ given i .

Polynomial Transform on Data Matrix

• $X \in R^{n \times d}$ is data matrix with n observations and d dimensions.

• $f(X) := \begin{bmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \dots \\ f(\mathbf{x}_n) \end{bmatrix} \in R^{n \times db}.$

Pairwise Polynomial Transform

○ So far, the polynomial transform is applied on each dimension:

○ i.e., $f(\mathbf{x}) = [\mathbf{h}(x^{(1)}), \mathbf{h}(x^{(2)}), \dots, \mathbf{h}(x^{(d)})]$.

○ It does **not** consider the dependencies between features.

○ Can be solved by appending cross terms i.e., $f(x) := [\mathbf{h}(x^{(1)}), \dots, \mathbf{h}(x^{(d)}), \forall_{u < v} x^{(u)} x^{(v)}]$

LS Solution

$$\textcircled{O} \hat{\beta} = \arg \min \sum_{i=1}^n (y_i - \langle \beta, f(x_i) \rangle)^2$$

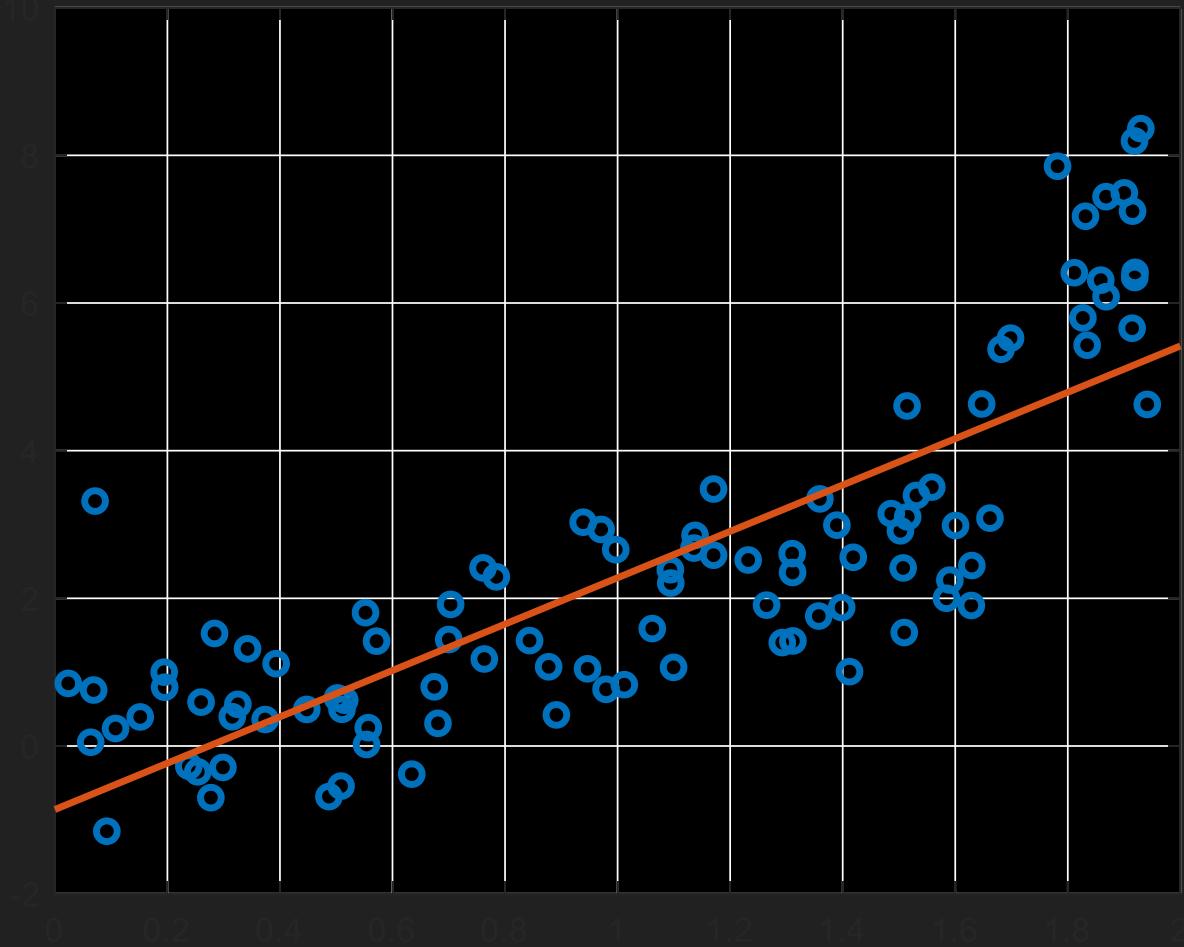
$$\textcircled{O} \hat{\beta} = (f(X)^\top f(X))^{-1} f(X)^\top y$$

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Questions

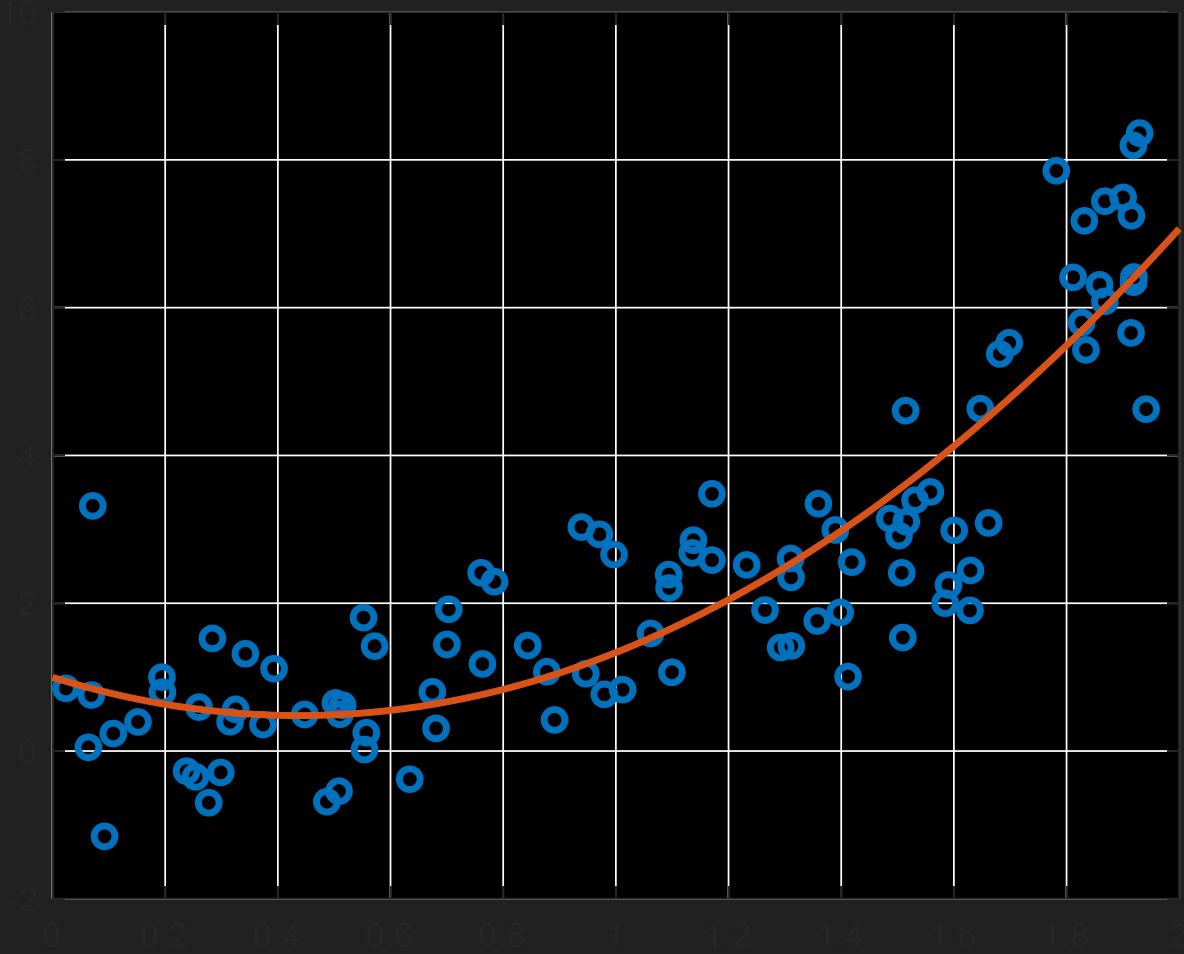
- At least, how many observations are needed to compute $\hat{\beta}$ with $f \in R^{db}$ using the formula above?
- <https://pollev.com/songliu644>
- PC: what is the computational complexity?

Example: $y = \exp(1.5x - 1) + \epsilon$,
 $\epsilon \sim N(0,1)$



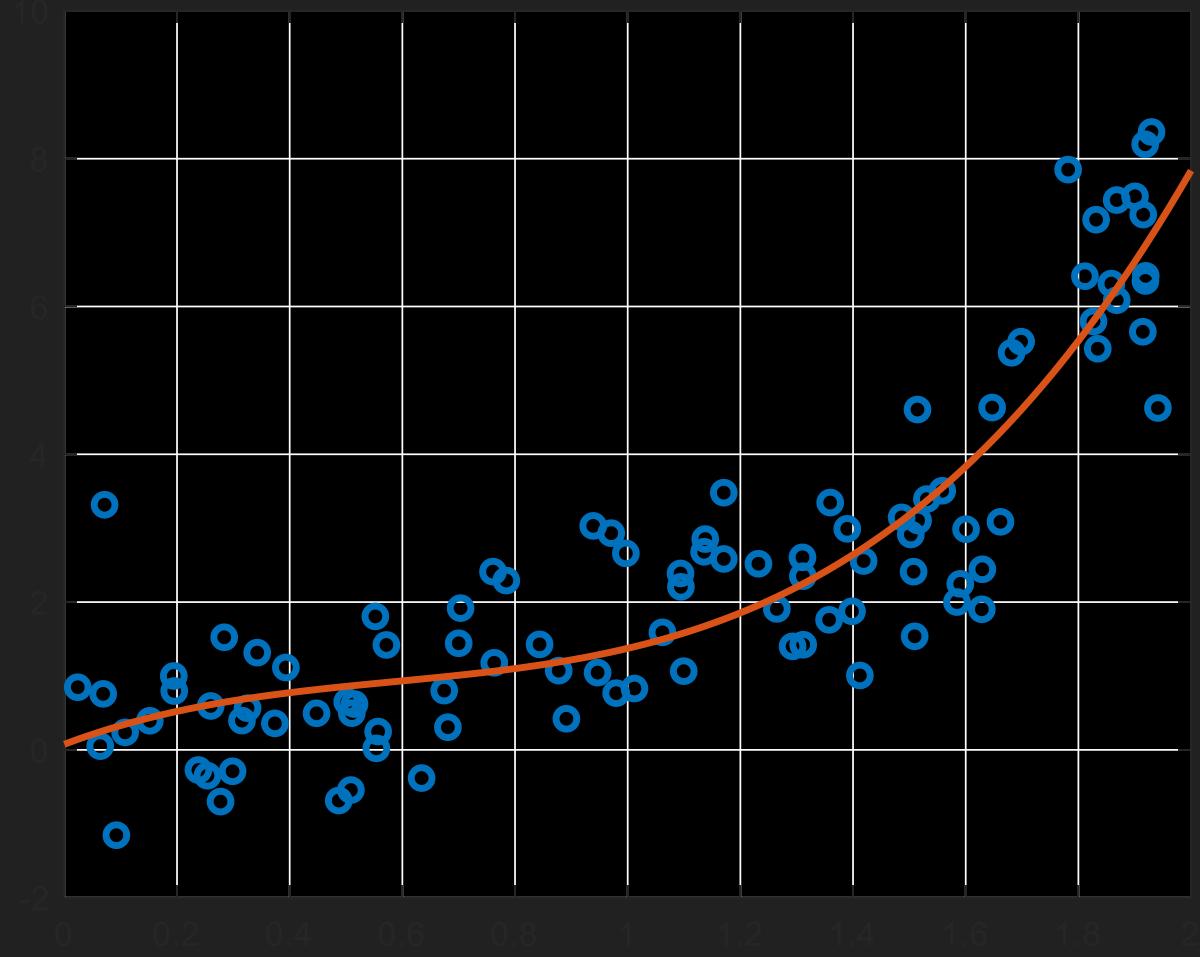
- Polynomial transform with $b = 1$.
- Square error: 171.0

Example: $y = \exp(1.5x - 1) + \epsilon$,
 $\epsilon \sim N(0,1)$



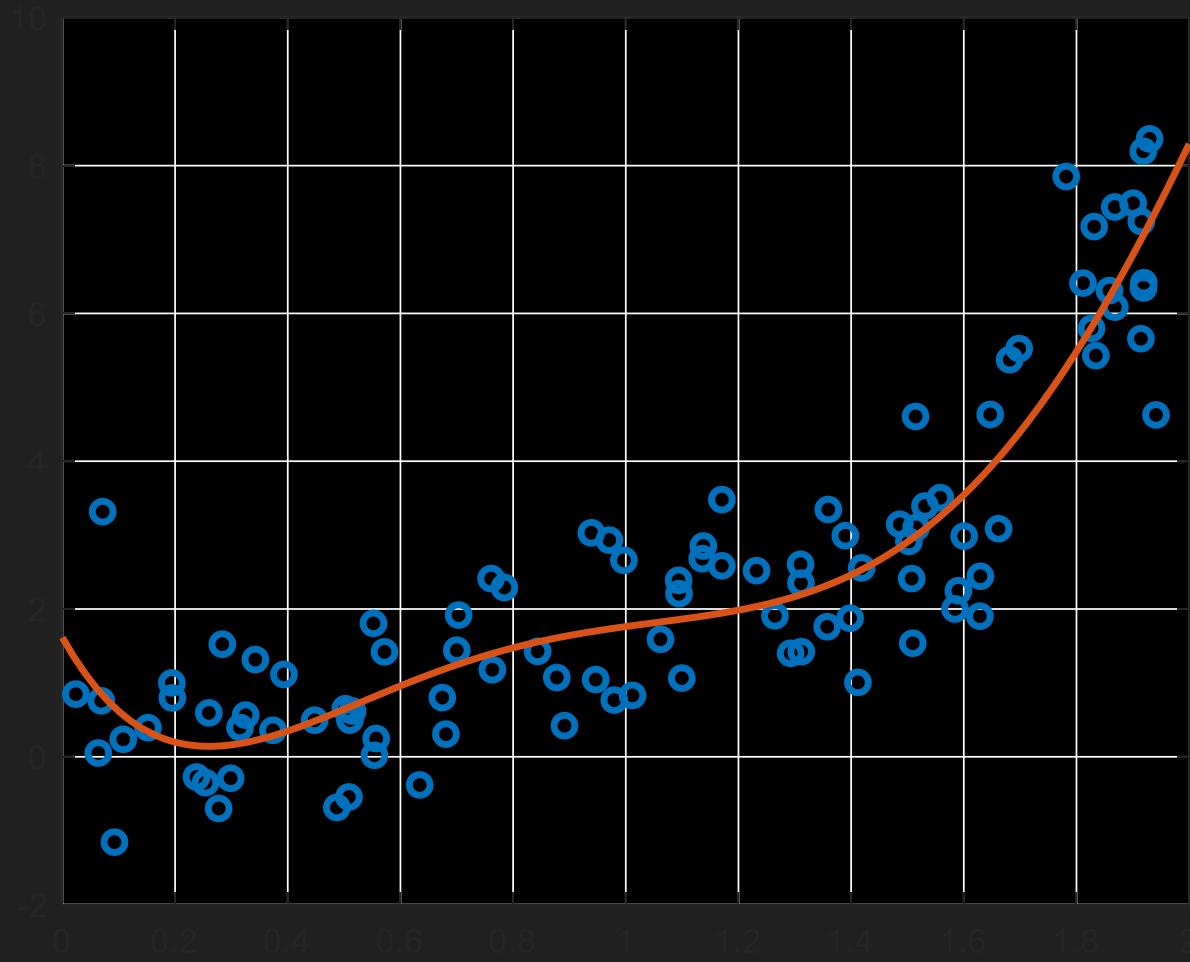
- Polynomial transform with $b = 2$.
- Square error: 108.97

Example: $y = \exp(1.5x - 1) + \epsilon$,
 $\epsilon \sim N(0,1)$



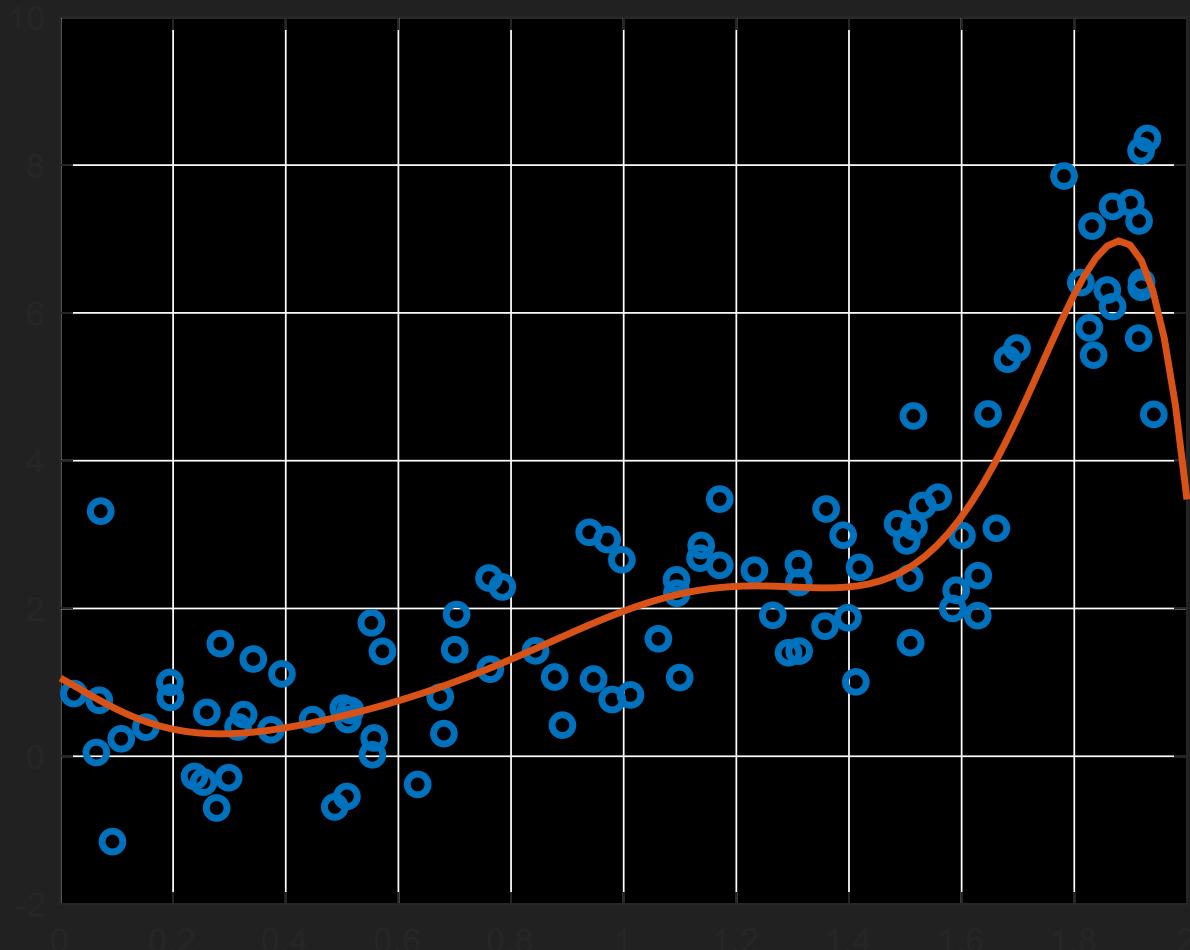
- Polynomial transform with $b = 3$.
- Square error: 99.618

Example: $y = \exp(1.5x - 1) + \epsilon$,
 $\epsilon \sim N(0,1)$



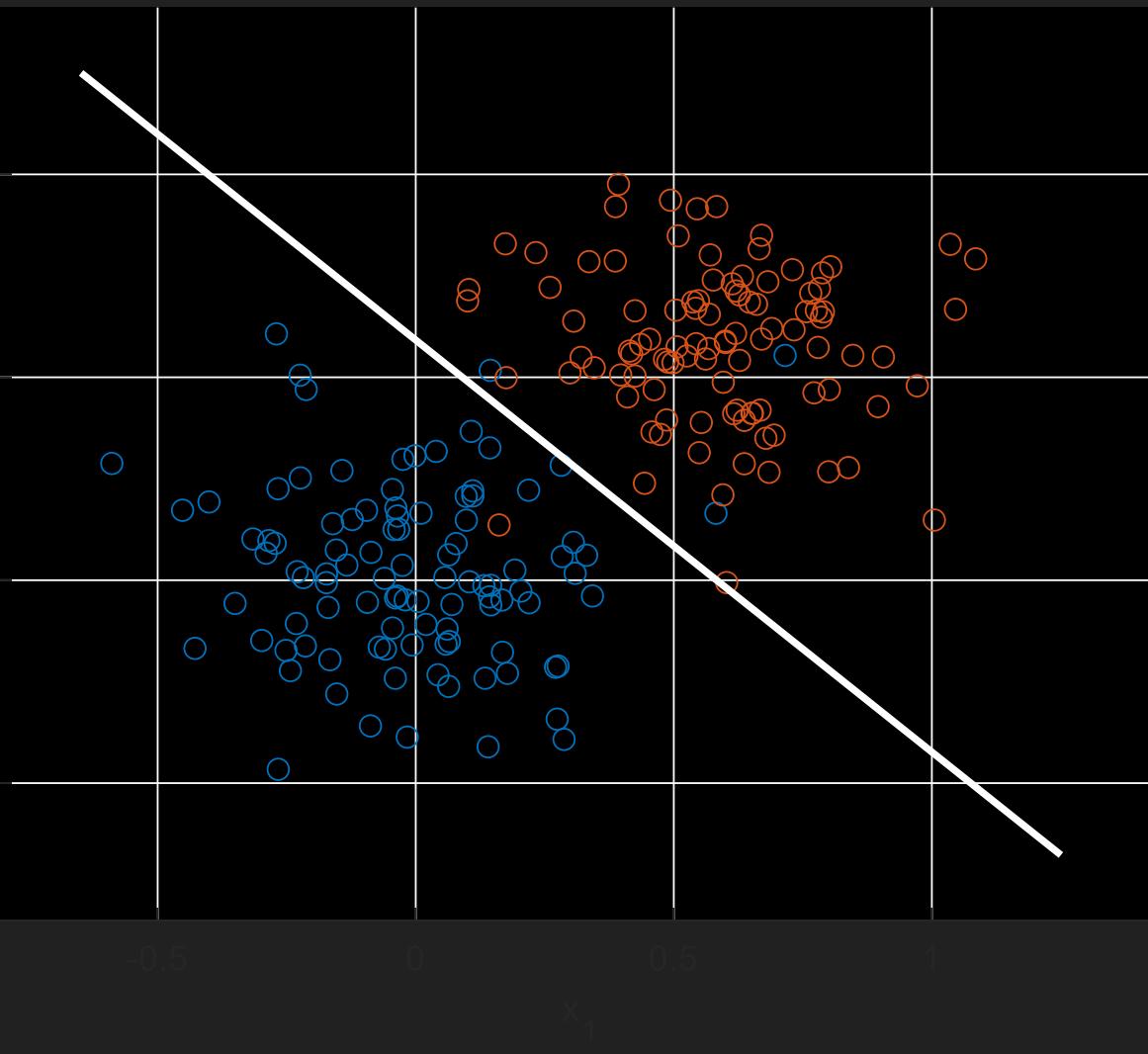
- Polynomial transform with $b = 5$.
- Square error: 89.378

Example: $y = \exp(1.5x - 1) + \epsilon$,
 $\epsilon \sim N(0,1)$



- Polynomial transform with $b = 8$.
- Square error: 78.87

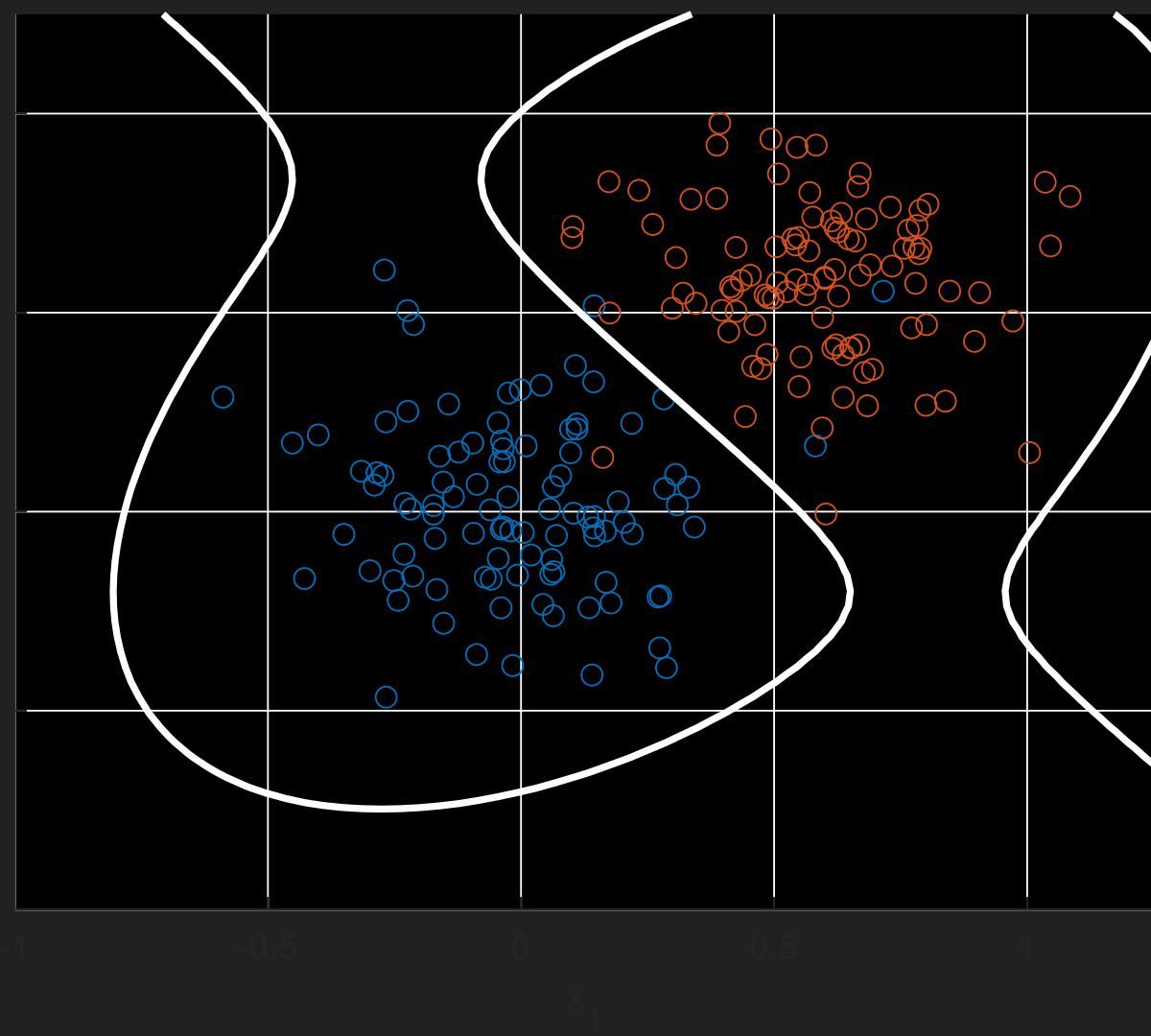
Example: Binary Classification



○ Polynomial transform with $b = 1$.

○ Square Error:
39.0547

Example: Binary Classification



○ Polynomial
transform
with $b = 3$.

○ Square
Error:
32.0632

Observations:

- Pay attention on
- how square error keeps **dropping** when **increasing** degree b .
- how \hat{y} becomes more **flexible** when **increasing** b .
- We will revisit this point in the next lecturer.

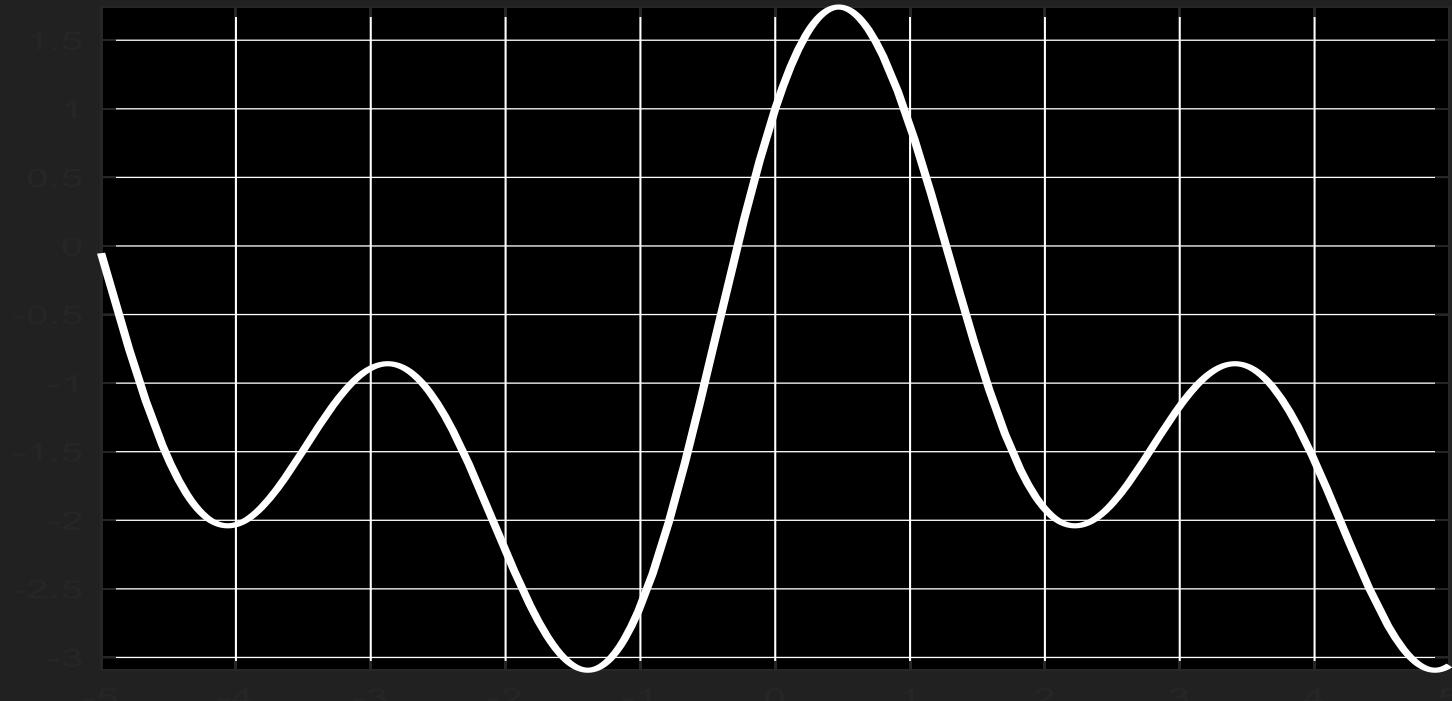
Why it works?

- 1-dimensional intuition: Taylor Series.
- Taylor Series of $g(x)$ at 0:
 - $$g(x) = g(0)(x - 0)^0 + g'(0)(x - 0)^1 + \frac{g''(0)}{2!}(x - 0)^2 + \frac{g'''(0)}{3!}(x - 0)^3 + \dots$$
 - You can approximate a **smooth** function using polynomial terms (at some cost).

Fourier Series

- What are **other ways** of decomposing a function?
- Suppose we have a periodic signal $g(x)$ over the time domain.
 - e.g. a sound wave or a stock price
 - $$g(x) = a_0 + \sum_{i=1}^{\infty} [a_i \sin(ix) + b_i \cos(ix)]$$
 - This decomposition is called Fourier Series.

Fourier Series



O $g(x) = \sin(x) + \cos(x) + \sin(2x) + \cos(2x)$

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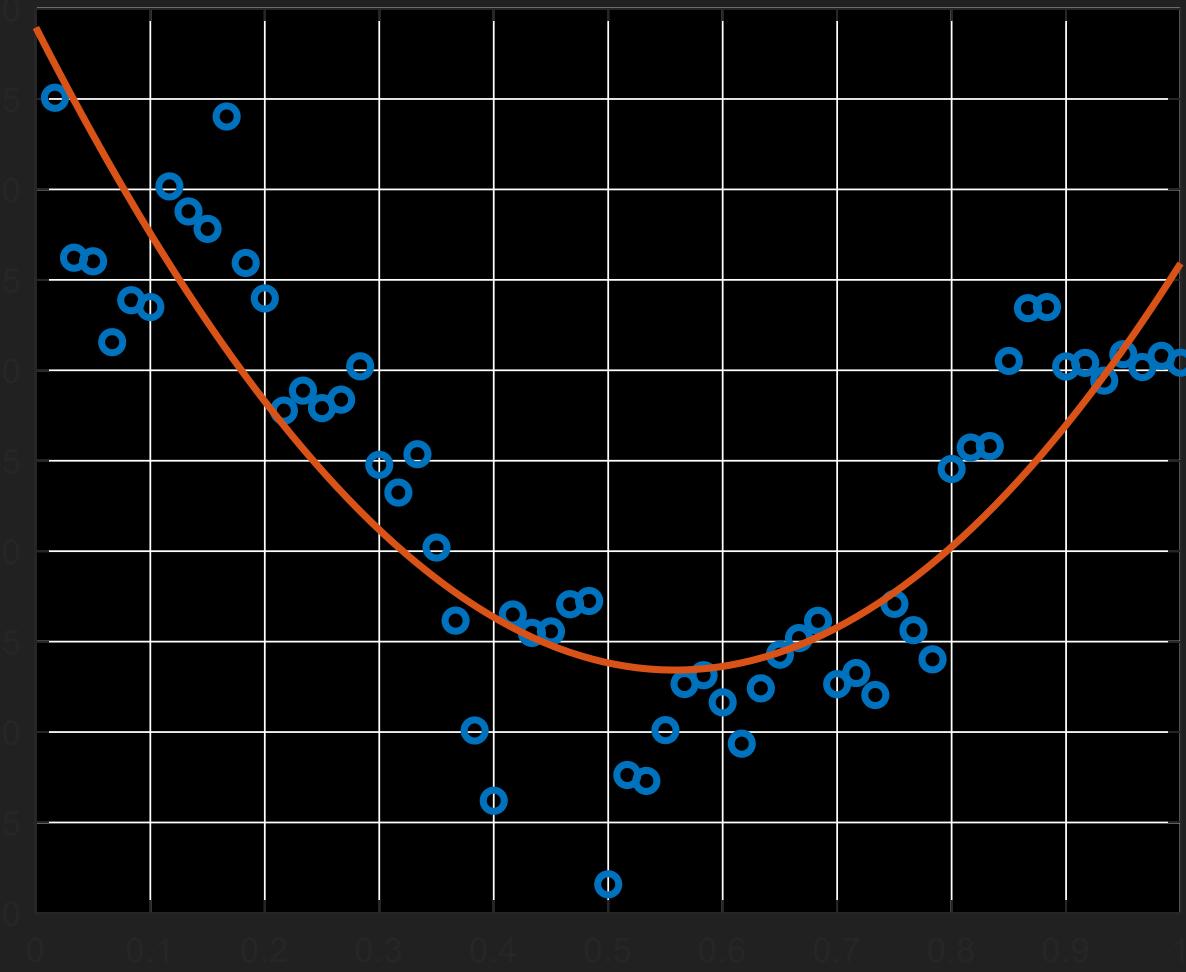
Trigonometric Transform

○ Trigonometric Transform are used to approximate function over **time domain**.

○ $f(x) := [1, \sin(x), \cos(x), \sin(2x), \cos(2x) \dots \sin(bx), \cos(bx)]$

○ $f(x) \in R^{2b+1}$

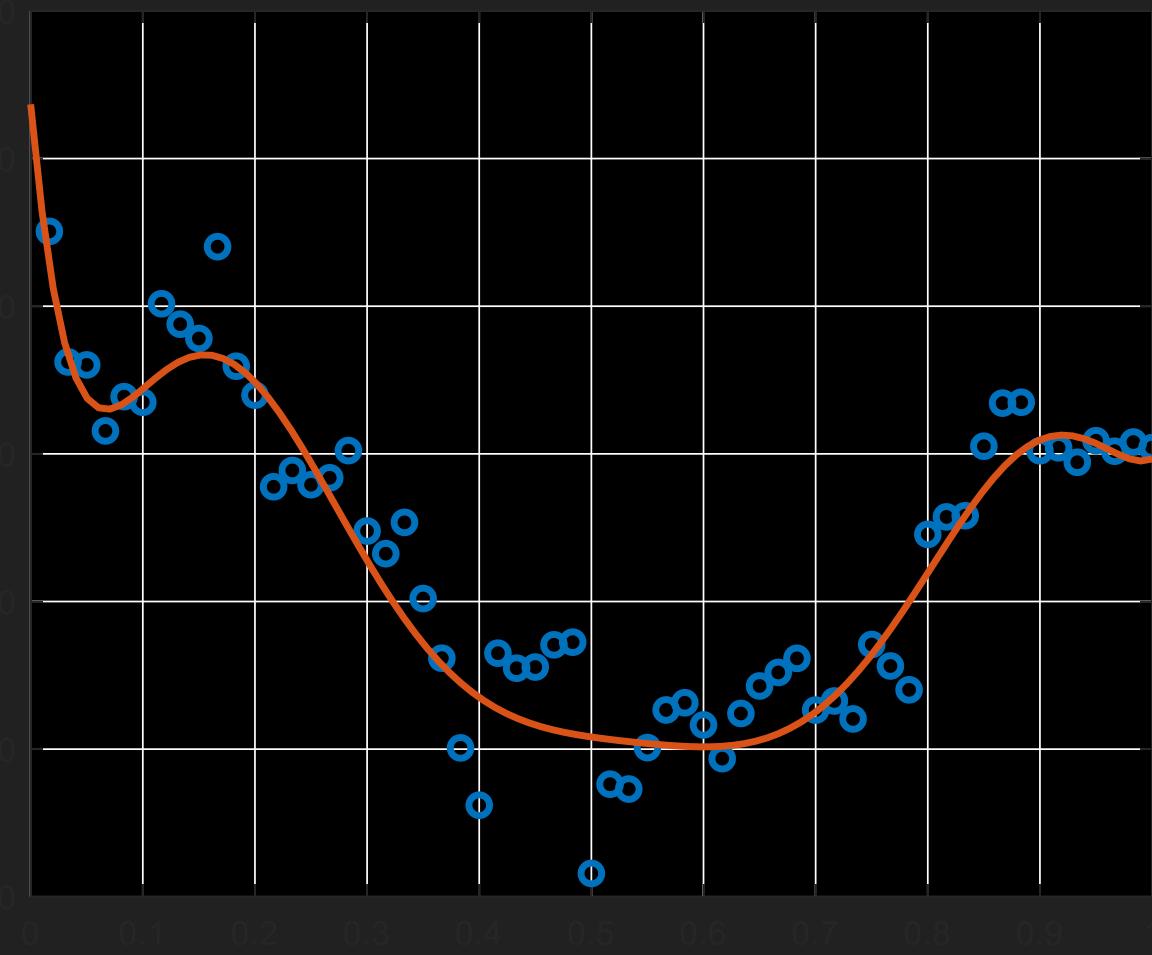
Example: Apple Stock Price, Feb 2019



○ Trigonometric transform with $b = 1$.

○ Squared error:
 1.5681×10^3

Example: Apple Stock Price, Feb 2019



- Trigonometric transform with $b = 4$.
- Squared error: 699.9117

Linear Expansion of Basis Functions

○ Polynomial and Trigonometric transforms based on the idea a function can be approximated by:

$$y \approx \sum_{i=1}^m \beta_i f^{(i)}(x)$$

○ called a linear basis expansion of y

○ $f^{(i)}$ are called **basis function**

○ Polynomial basis, Trigonometric basis...

Radial Basis Function (RBF)

○ RBF is another widely used basis function for function approximation.

○ $f^{(i)}(x) := \exp\left(-\frac{\|x-x_i\|^2}{\sigma^2}\right)$

○ σ is called kernel width

○ σ is determined **before** fitting

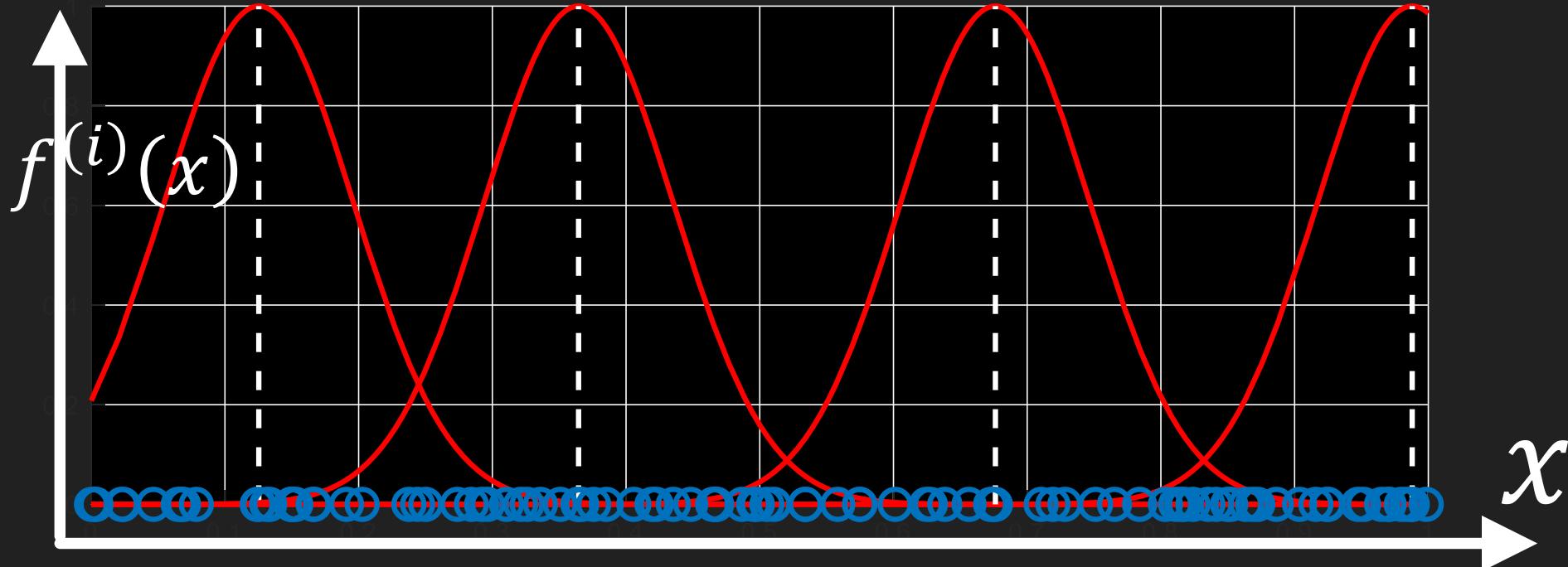
○ x_i are called **RBF centroids**.

○ x_i can be **randomly chosen** from your dataset

Radius Basis Function (RBF)

- $f(\mathbf{x}) := [f^{(1)}(\mathbf{x}), f^{(2)}(\mathbf{x}), \dots, f^{(b)}(\mathbf{x}), \mathbf{1}]$
 - Do not forget 1!
 - A practice is setting σ as the median of all pairwise distances of \mathbf{x} .
 - Compute $\|x_i - x_j\|, \forall i, j$.
 - Sort
 - Find median and set σ to the median.
 - $b < n - 1$. Why?

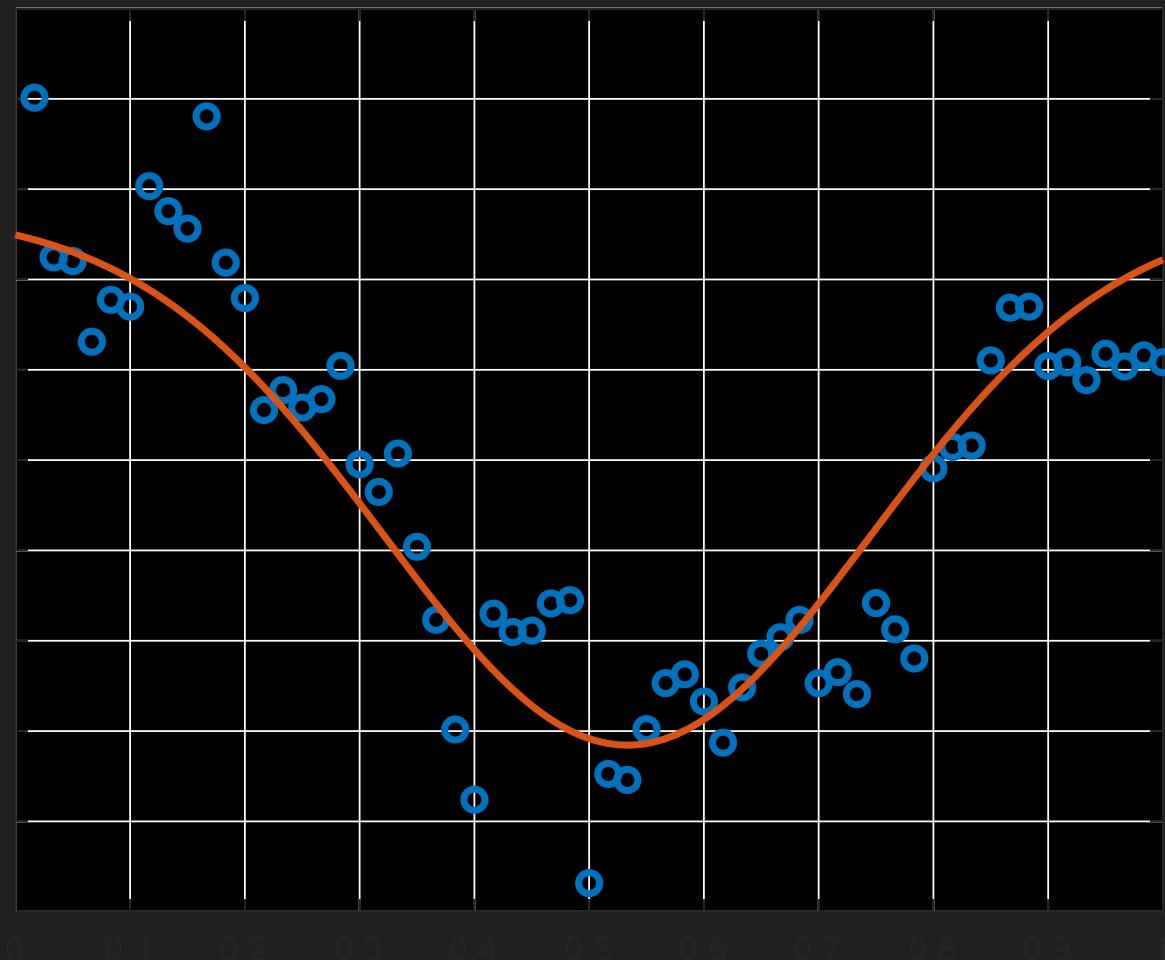
Radius Basis Function (RBF)



○ $f^{(i)}(x)$ are visualized in red at random 4 locations among 100 uniformly drawn x .

○ At each “bump”, basis gives \hat{y} a “lift”.

Example: Apple Stock Price, Feb 2019



ORBF

$\sigma = 0.2121$

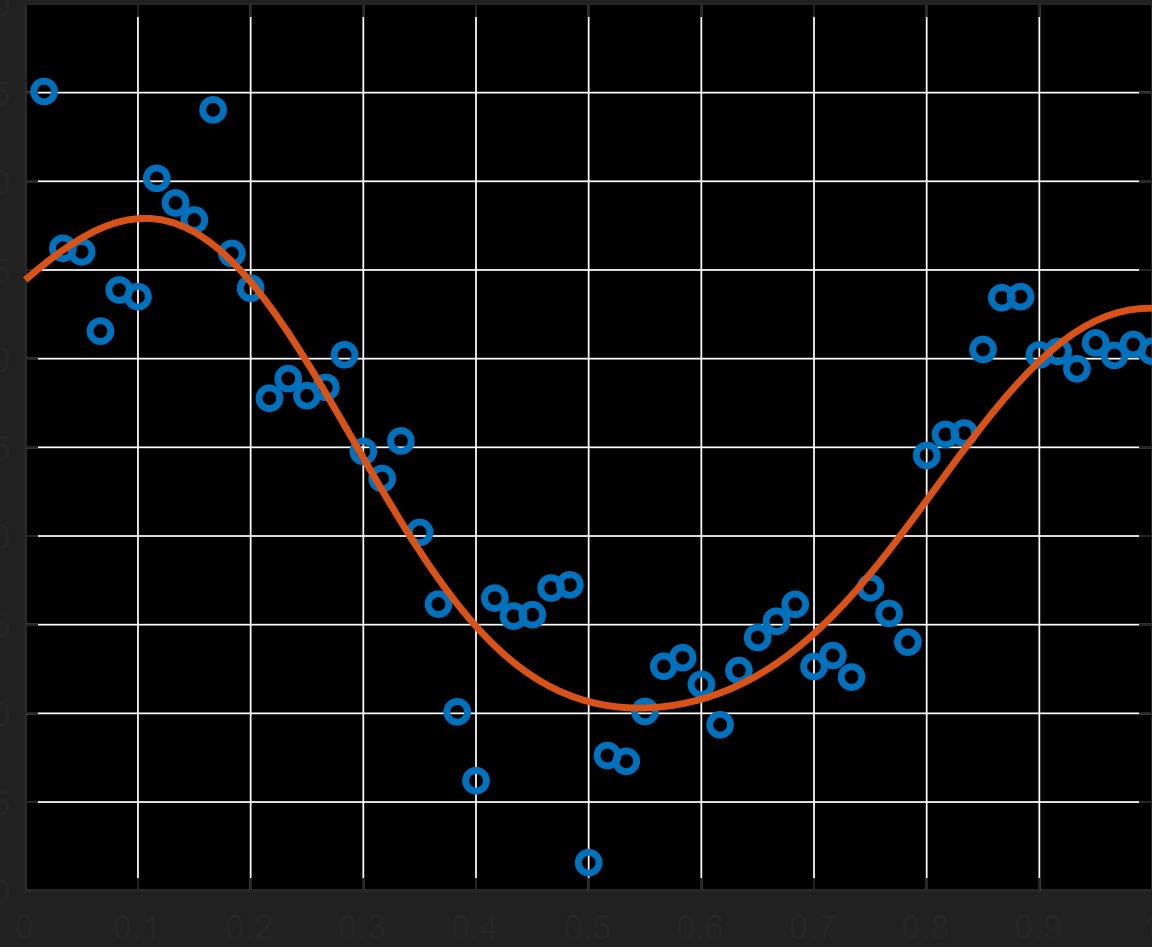
$b = 1.$

Squared

error:

$1.1908e+03$

Example: Apple Stock Price, Feb 2019



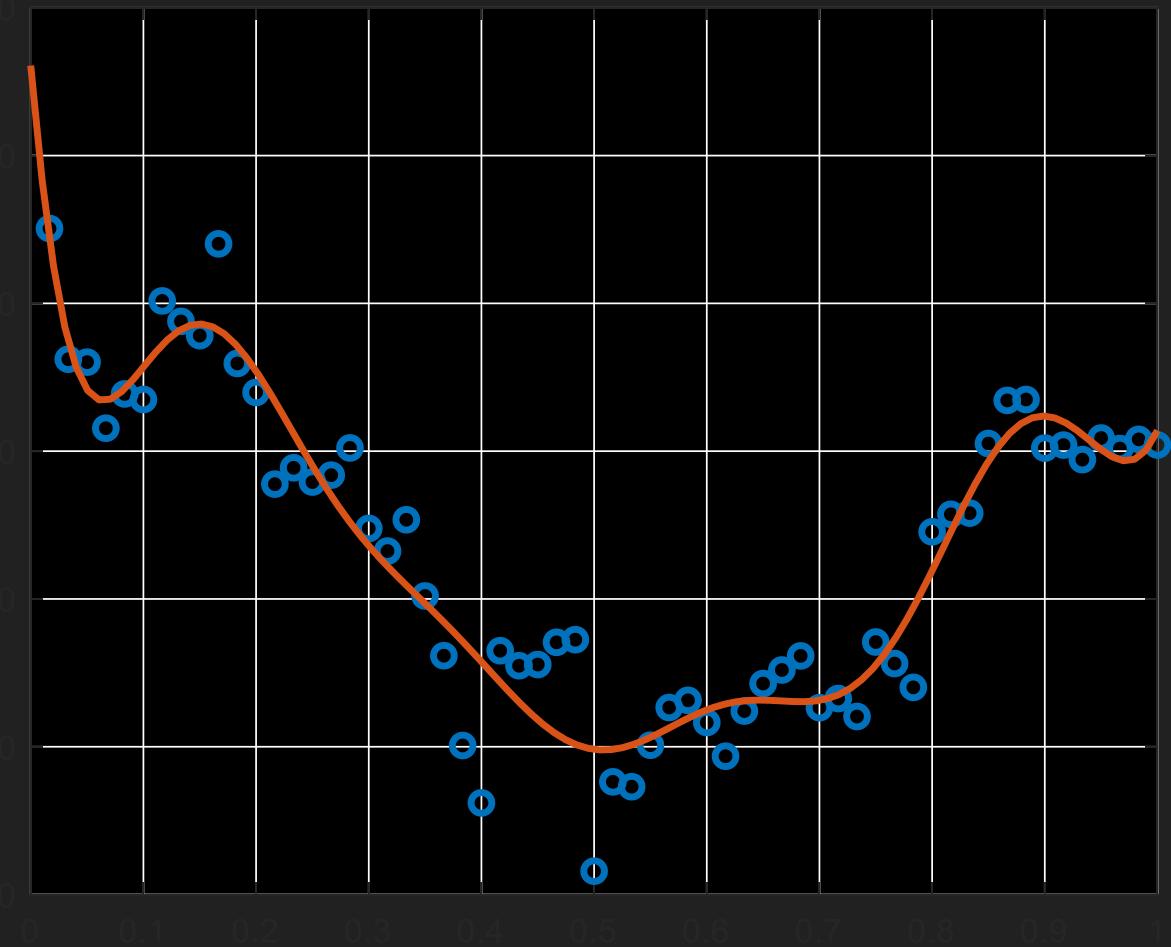
ORBF

$\sigma = 0.2121$

$b = 5.$

Squared
error:
842.7575

Example: Apple Stock Price, Feb 2019



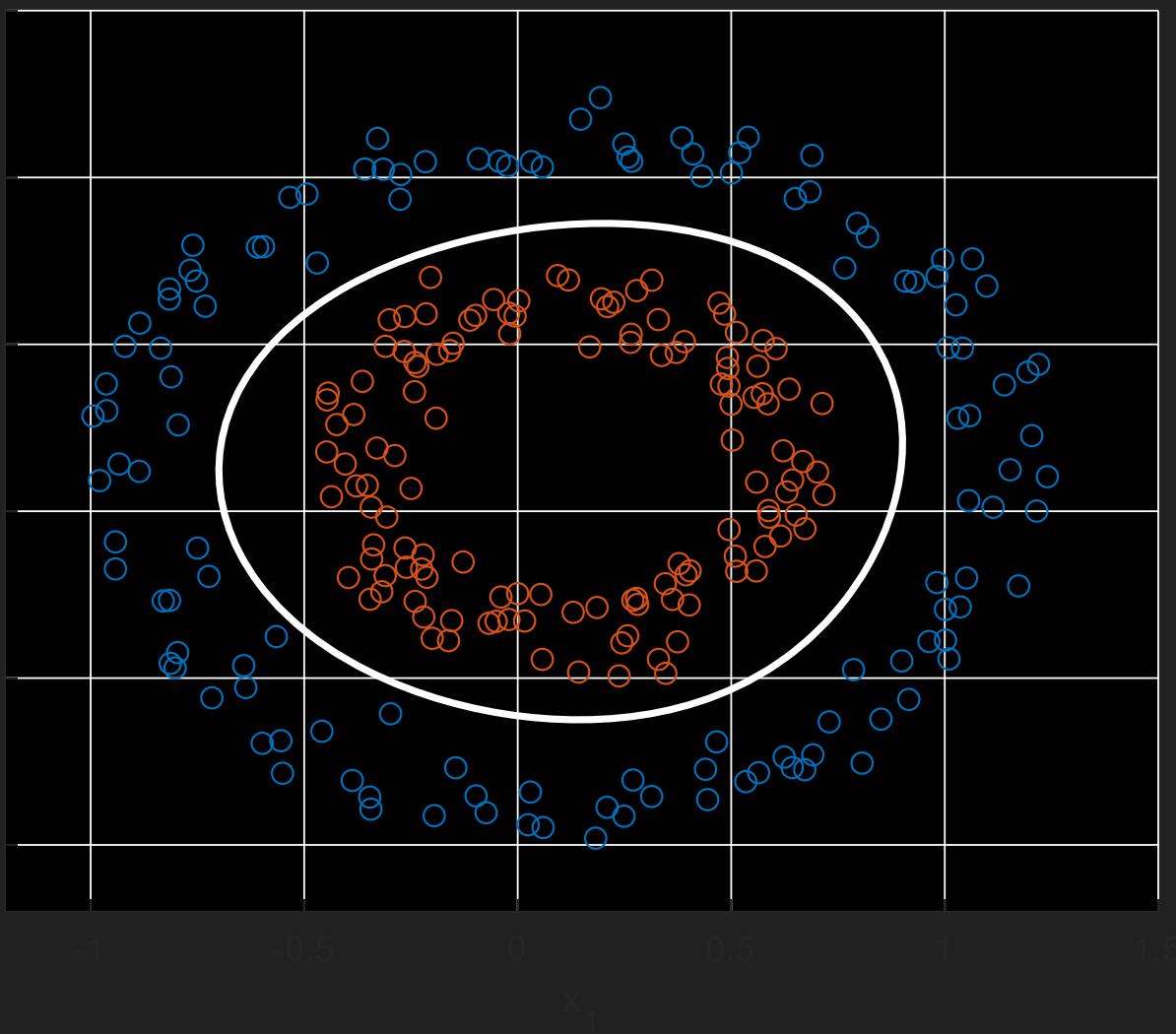
ORBF

$\sigma = 0.2121$

$b = 10.$

Squared
error:
593.8104

Example: Double Ring Classification



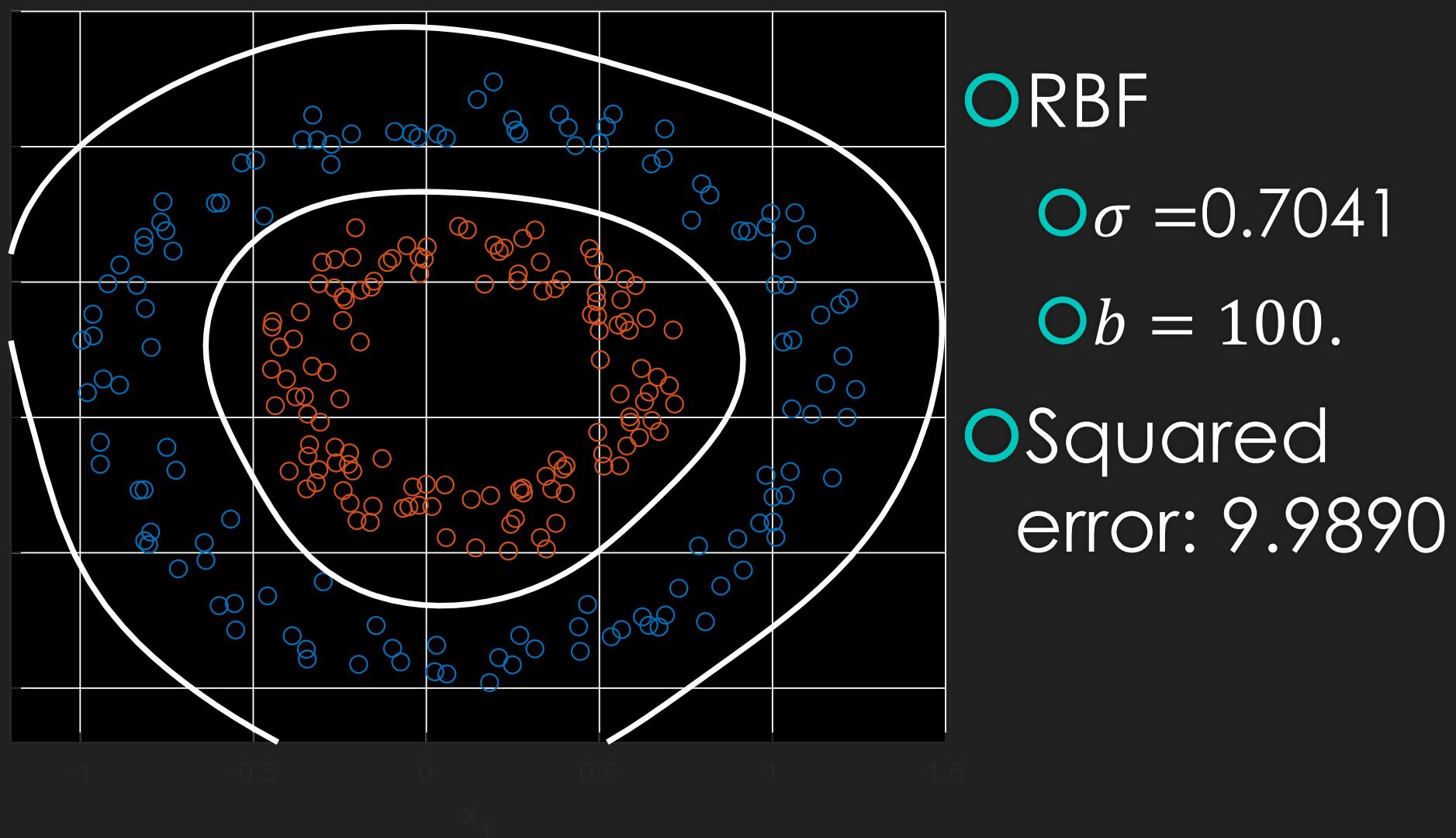
ORBF

$\sigma = 0.7041$

$b = 5.$

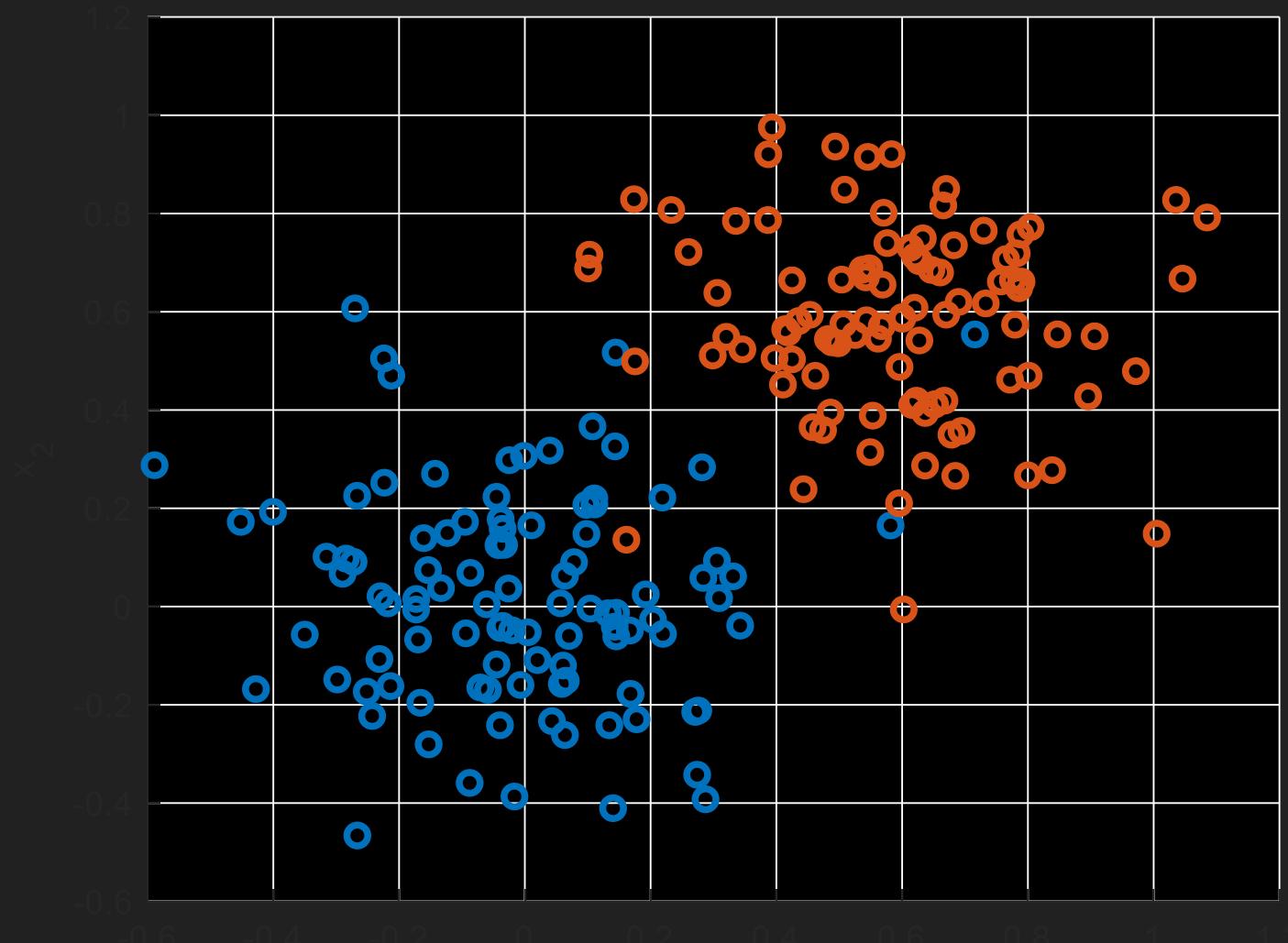
Squared
error:
16.3351

Example: Double Ring Classification



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Selecting Features using Prior Knowledge



Question

- Seeing your dataset above, what f should you use for classification? Hint: consider computational cost and overfitting
 - Polynomial, $b = 1$
 - Polynomial, $b = 2$
 - Polynomial, $b = 3$
 - ORBF, $b = 100$
- <https://pollev.com/songliu644>

Conclusion

- Feature transform can be crucial to regression and classification tasks.
- Three useful feature transform:
 - Polynomial
 - Trigonometric (on time series)
 - RBF
- As b increases, \hat{y} become more flexible, squared error is lowered.

Unanswered Questions

- Increasing b drops squared error.
- How do you select number of basis b ?
- Knowing an f with a larger b makes \hat{y} more flexible, can we make $b = \infty$?
- Next two lectures, The selection of number of basis b and Kernel methods.