Features: Representing your data

COMS21202, Part III

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Introduction

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

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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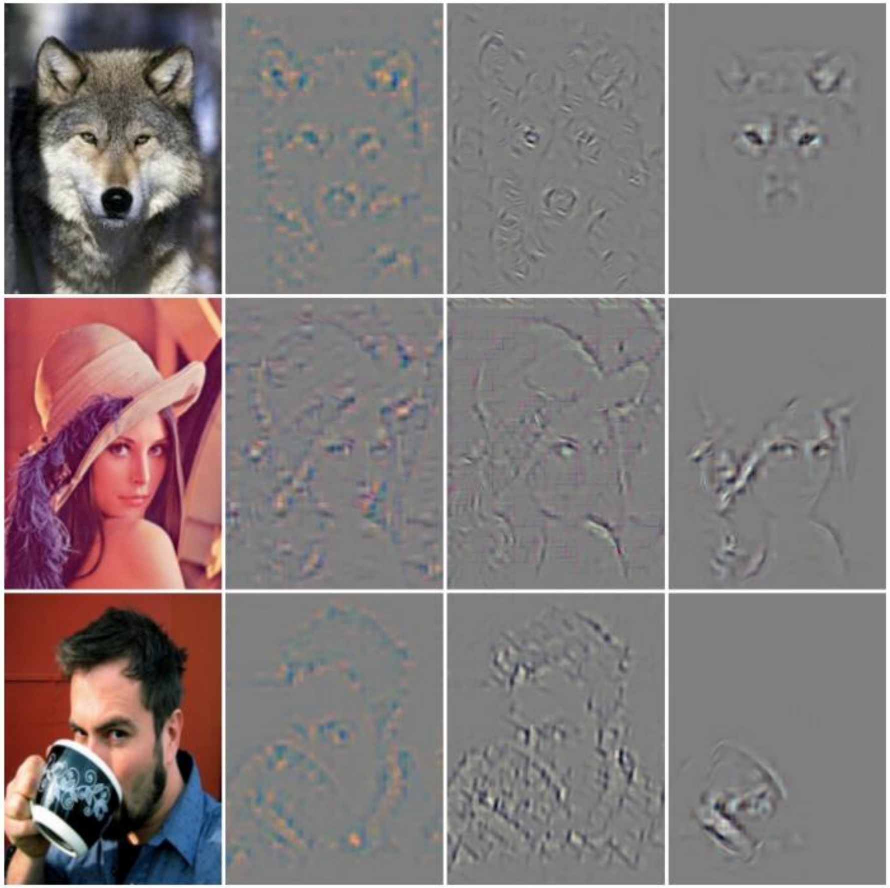
How does machine see the world?

- 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?


Deconvnet output for Alexnet Max pooling layers 1, 2 and 3

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

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**.

An Appetizer

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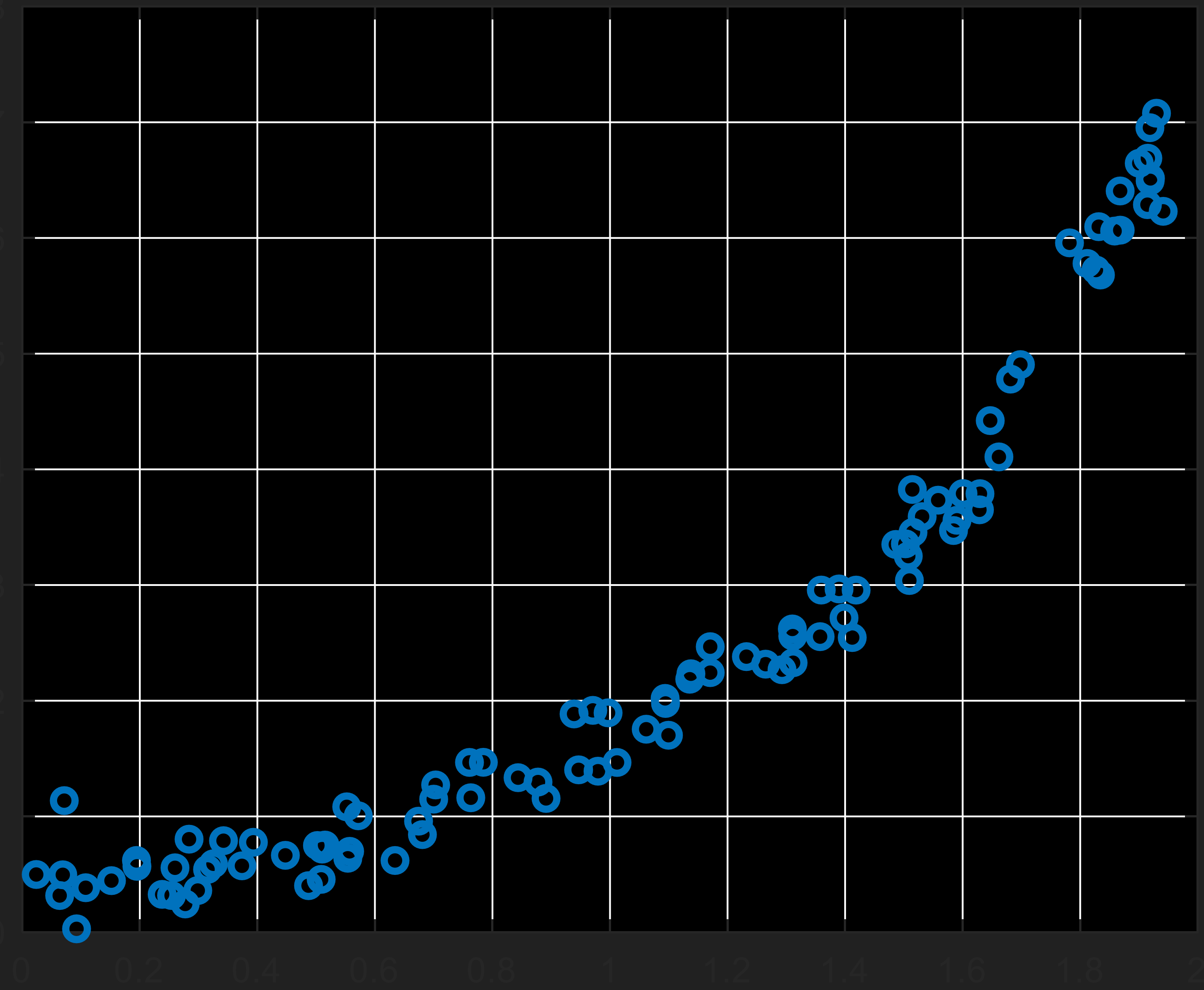
Least Squares (LS) + Feature Transform f

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

LS Regression on Nonlinear Dataset



See Lab 3, Q7 for a similar example

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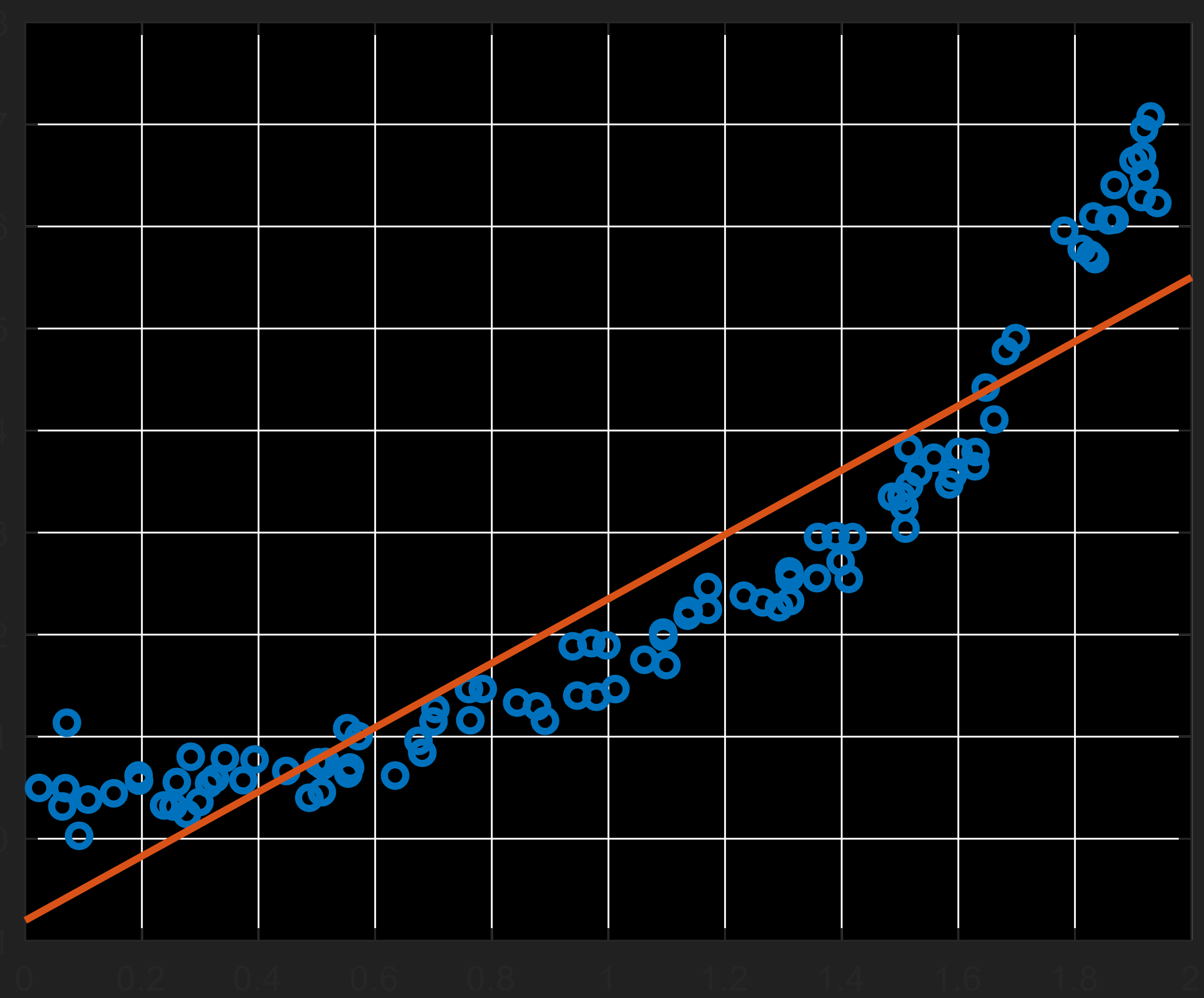
LS Regression on Nonlinear Dataset



$$f(x) = x$$

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

Square error: 57

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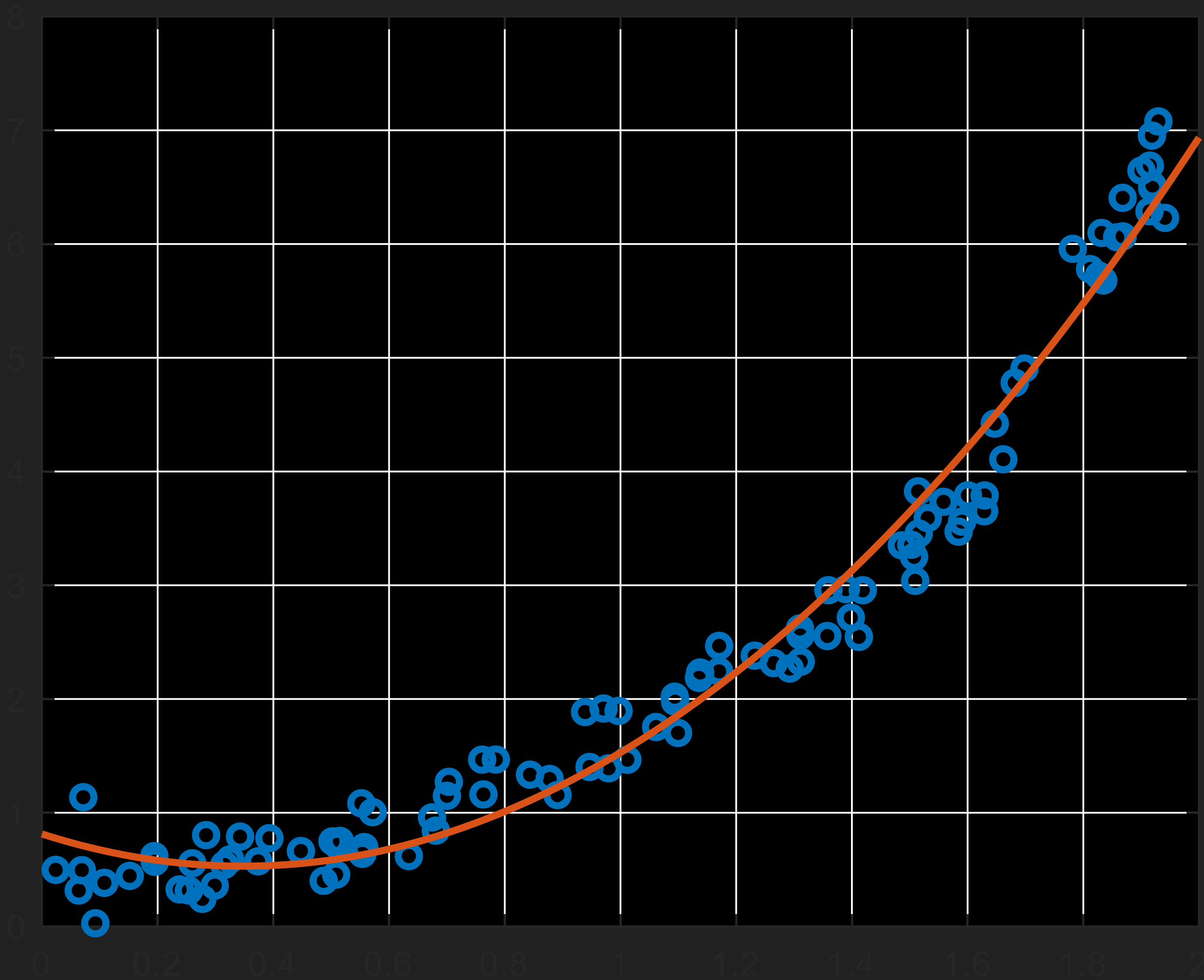
LS Regression on Nonlinear Dataset



$f(x) = x^2$

Square error: 10

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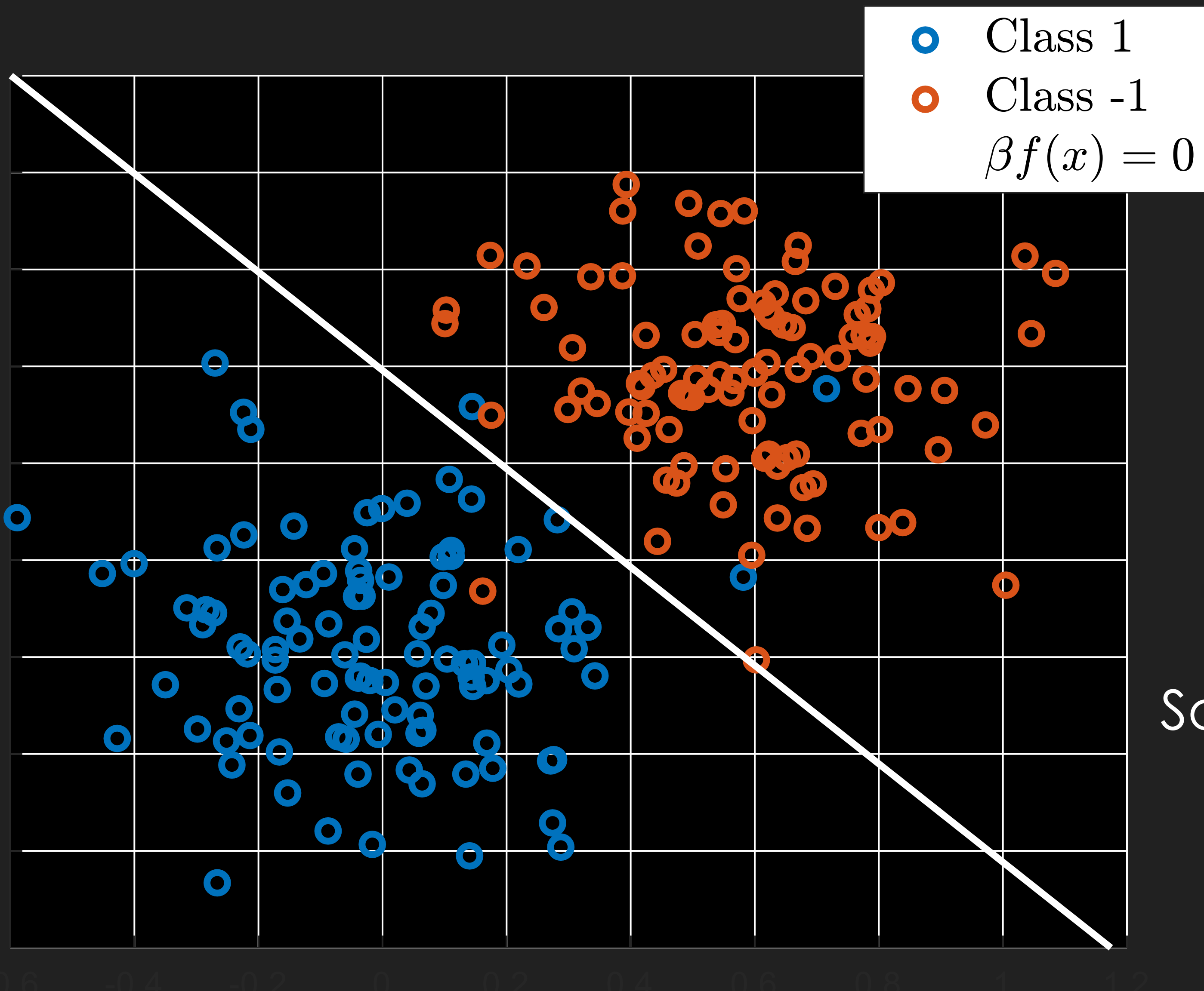
LS Classification + Feature Transform

- 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 $y_i = 1/-1$, $\boldsymbol{x}_i$ 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?

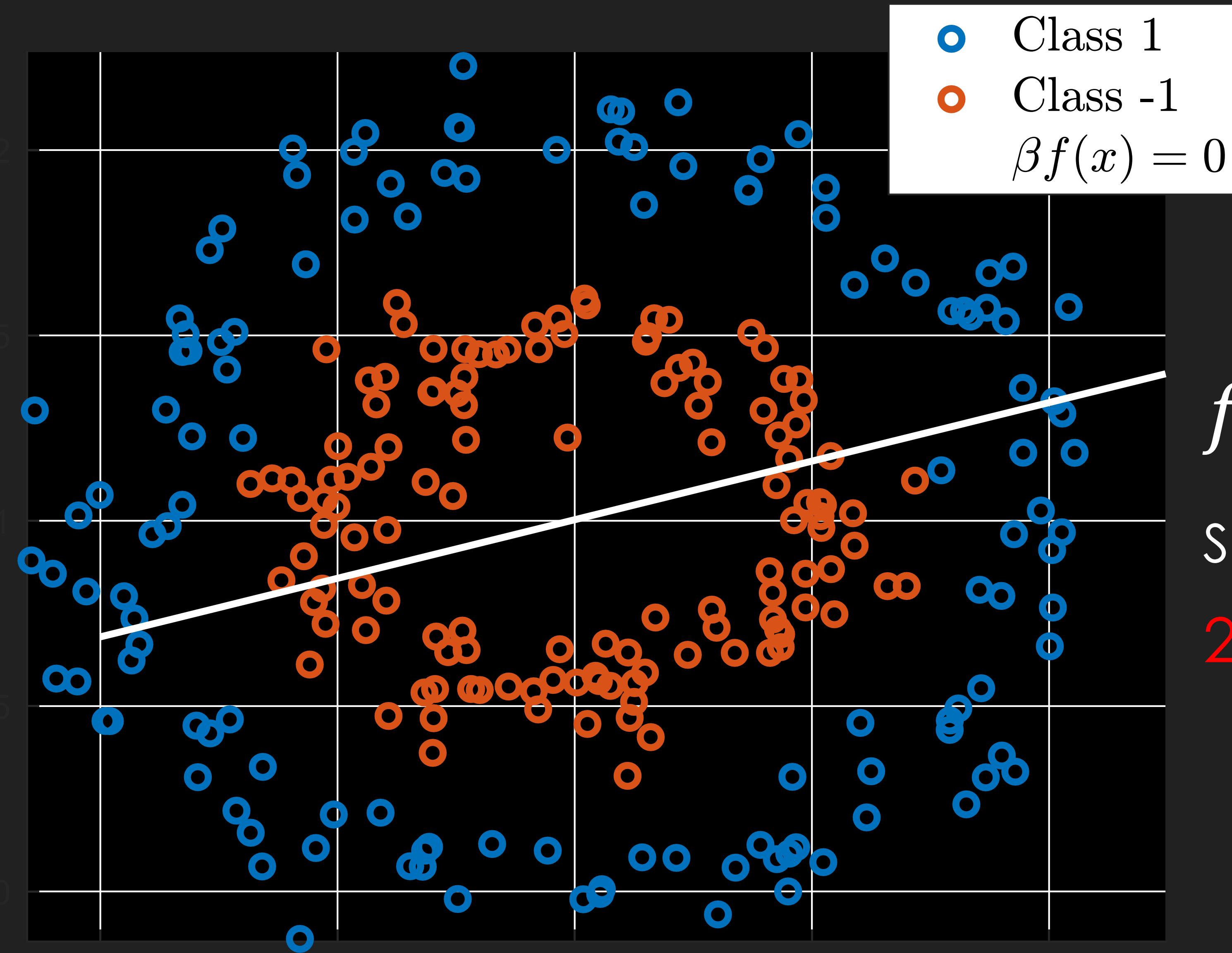
LS Classification



$$f(x) = x$$

Square error: 39.0

LS Classification on Nonlinear Dataset



$$f(x) = x$$

Square error:

252

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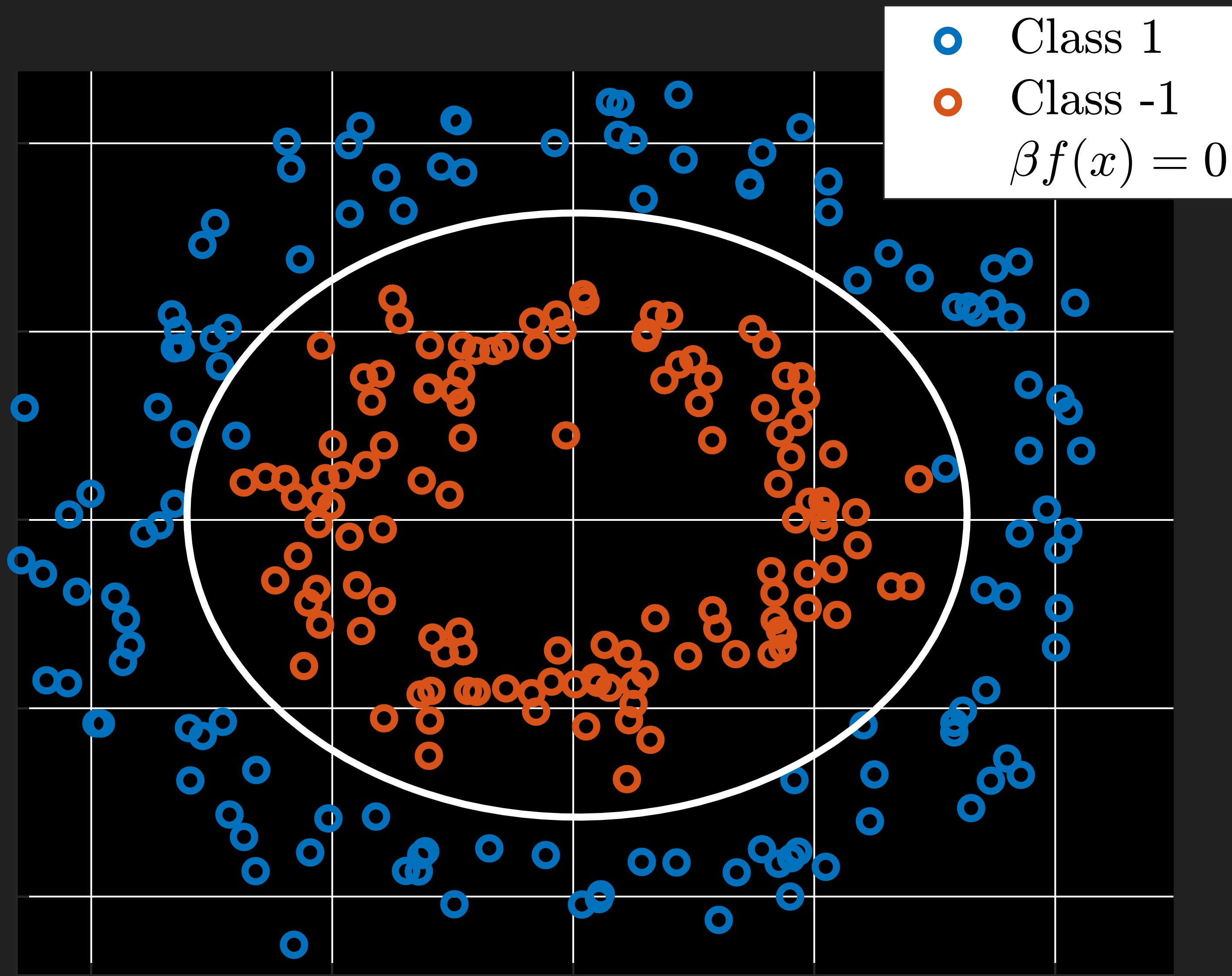
LS Classification on Nonlinear Dataset



$f(x) = \boldsymbol{x}^2$

Square error:

40

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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.

Formal Notations

- x, y, z, scalars, $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$, vectors.
- $\boldsymbol{x} \in R^d$, vector in d dimensional real-space.
- $x^{(i)}$, the i-th dimension of $\boldsymbol{x}$.
- $\boldsymbol{x}_i$, the i-th data point in our dataset.
- $\boldsymbol{f}(\boldsymbol{x}) \in R^m$, function takes input vector $\boldsymbol{x}$ and maps it into m dimensional real space.
- $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z} \in R^{b \times d}$, **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.
- $\hat{y} := < \boldsymbol{\beta}, \boldsymbol{f}(\boldsymbol{x}) > = \sum_i \beta^{(i)} f^{(i)}(\boldsymbol{x})$.
  - Inner product between $\boldsymbol{\beta}$ and $\boldsymbol{f}$.
  - $\hat{y}$ is linear w.r.t. parameter $\boldsymbol{\beta}$.
- Special case:
  - when $f(x), \beta \in R, \hat{y} = \beta f(x)$.

Polynomial Transform

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

Polynomial Transform

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

Polynomial Transform on Data Matrix

- $\boldsymbol{X} \in R^{n\times d}$ is data matrix with n observations and d dimensions.
- $f(\boldsymbol{X}) := \begin{bmatrix} f(\boldsymbol{x}_1) \\ f(\boldsymbol{x}_2) \\ \dots \\ f(\boldsymbol{x}_n) \end{bmatrix} \in R^{n\times d(b+1)}$.
- We expanded our data matrix.
  - from d to $d(b+1)$

Pairwise Polynomial Transform

- So far, the polynomial transform is applied on each dimension:
  - i.e., $\boldsymbol{f}(\boldsymbol{x}) = \left[\boldsymbol{h}\left(x^{(1)}\right), \boldsymbol{h}\left(x^{(2)}\right), \dots, \boldsymbol{h}\left(x^{(d)}\right)\right].$
- It does **not** consider the dependencies between features.
  - Can be solved by appending cross terms i.e., $\boldsymbol{f}(\boldsymbol{x}) := \left[\boldsymbol{h}\left(x^{(1)}\right), \dots, \boldsymbol{h}\left(x^{(d)}\right), \forall_{u<v} x^{(u)} x^{(v)}\ \right]$

LS Solution

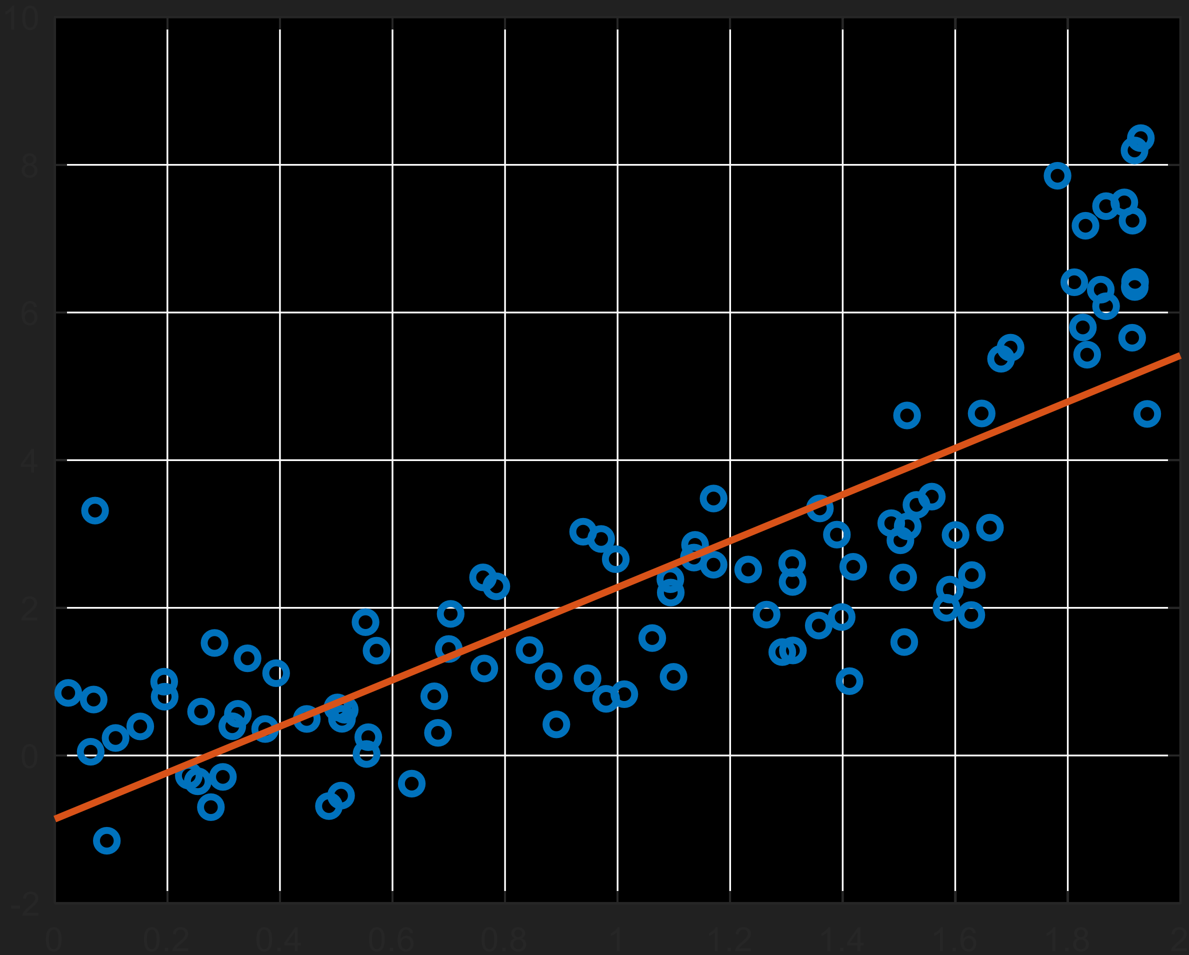
- $\hat{\boldsymbol{\beta}} = \arg\min \sum_{i=1}^{n} (y_i - < \boldsymbol{\beta}, \boldsymbol{f}(\boldsymbol{x}_i) >)^2$
- $\hat{\boldsymbol{\beta}} = \left(\boldsymbol{f}(\boldsymbol{X})^\top \boldsymbol{f}(\boldsymbol{X})\right)^{-1} \boldsymbol{f}(\boldsymbol{X})^\top \boldsymbol{y}$

Questions

- At least, how many observations are needed to compute $\hat{\boldsymbol{\beta}}$ with $\boldsymbol{f} \in R^{d(b+1)}$ 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

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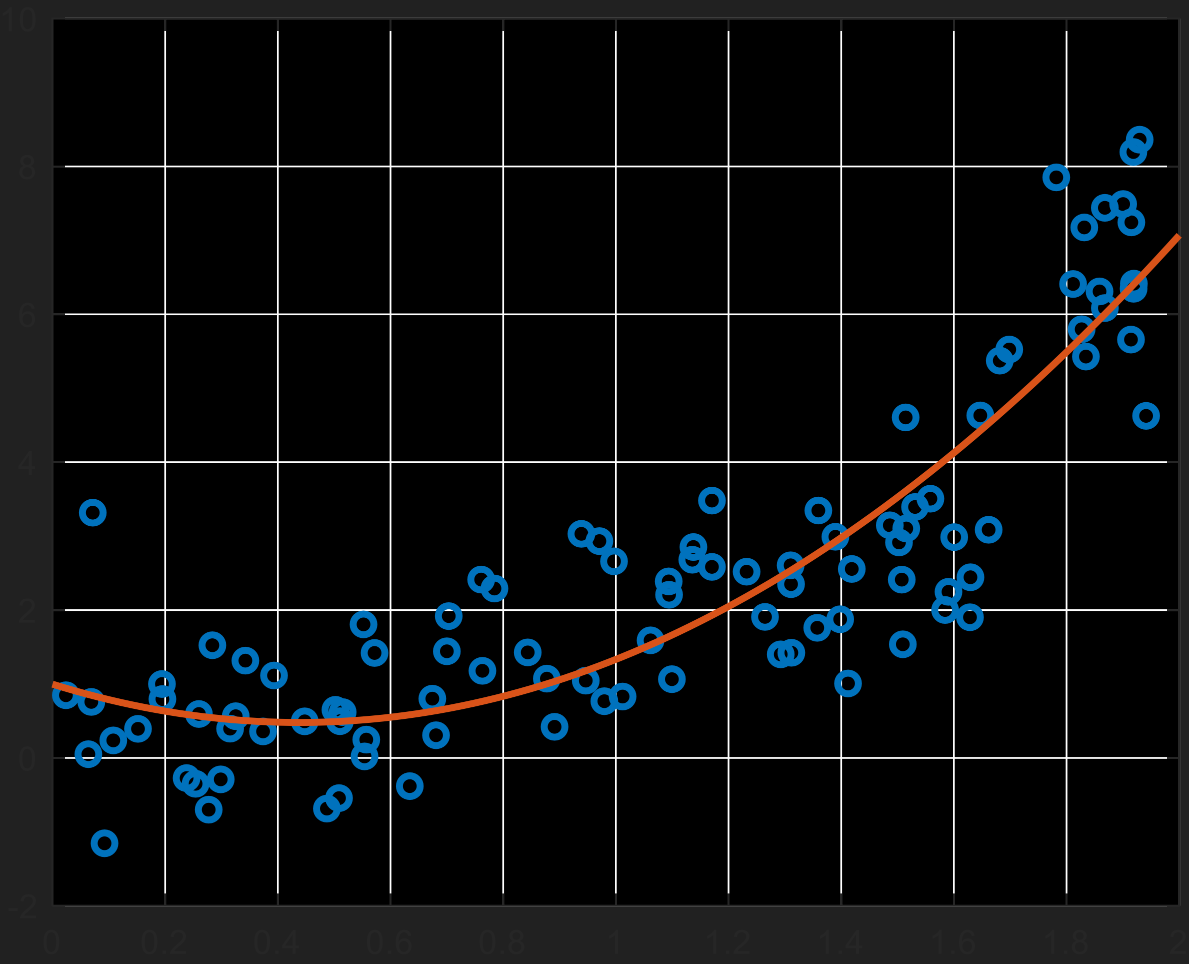
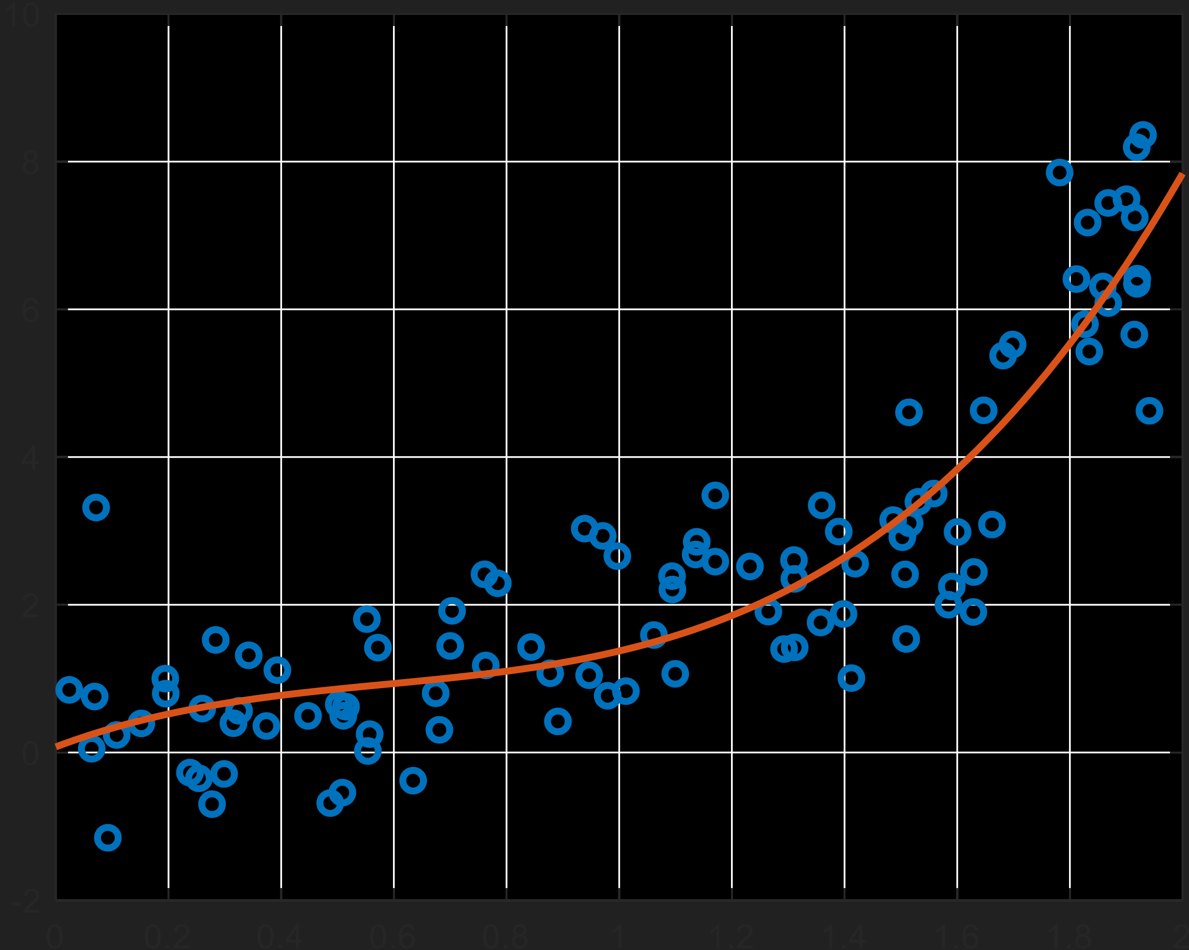
Example: $y = \exp(1.5x - 1) + \epsilon$, $\epsilon \sim N(0,1)$



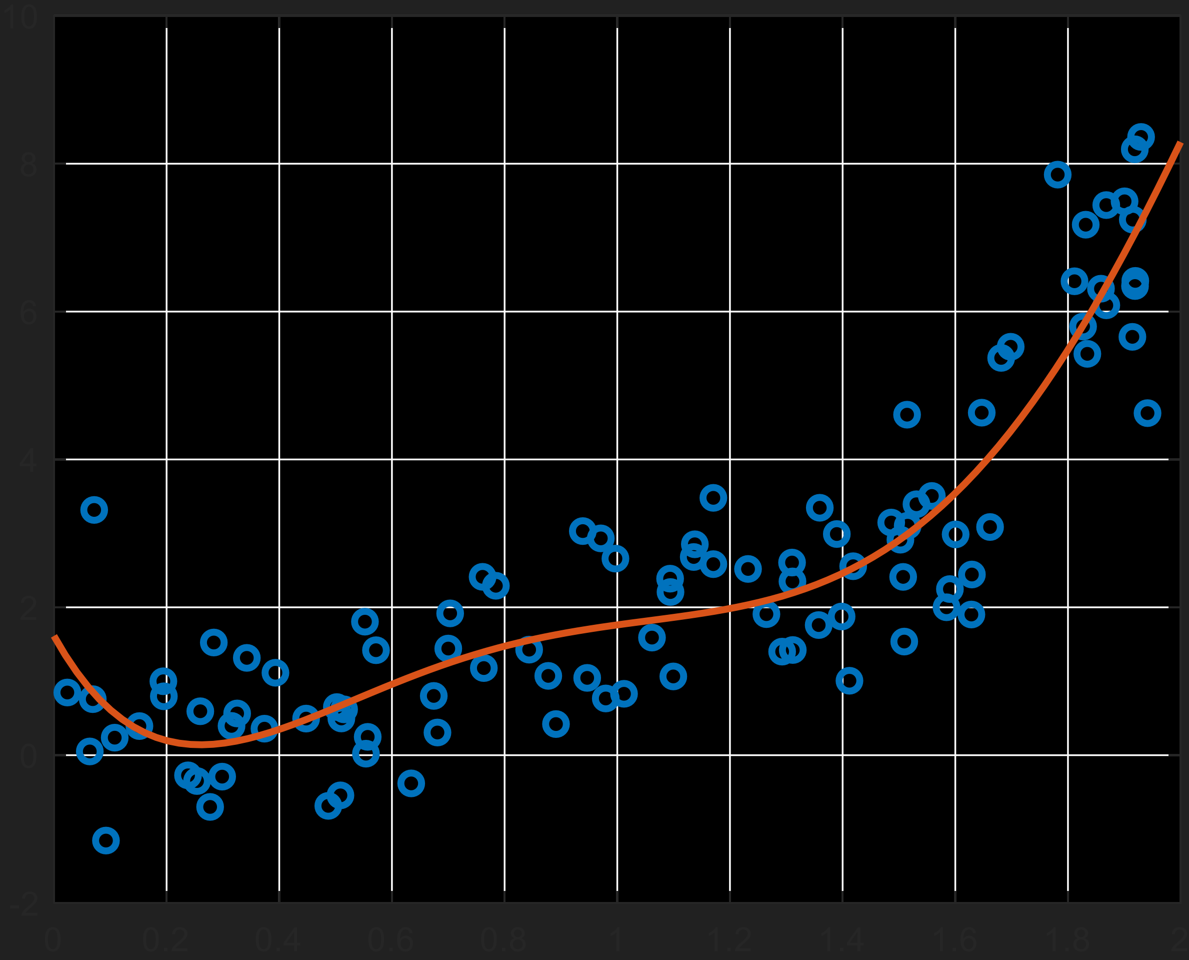
- Polynomial transform with $b = 2$.
- Square error:108.97

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



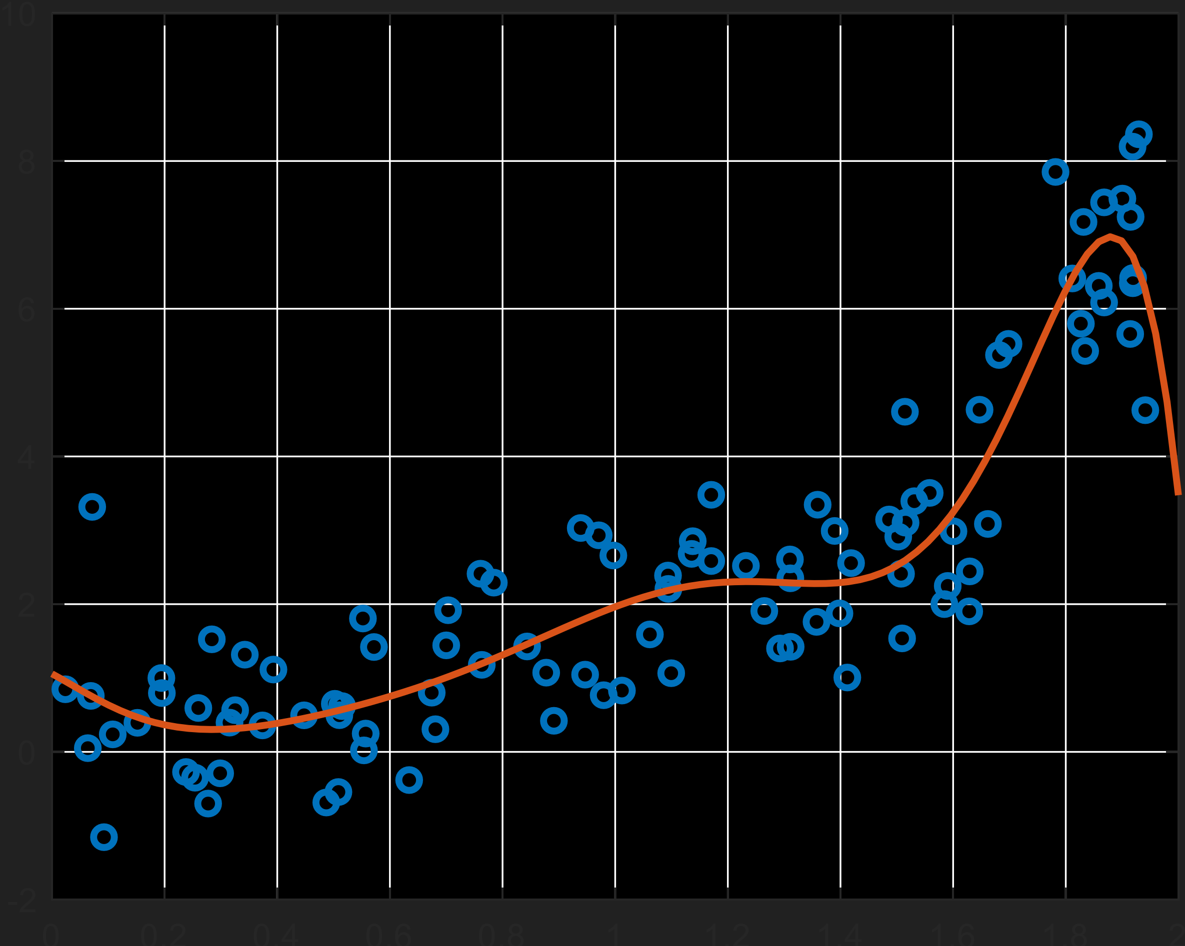
- Polynomial transform with $b = 3$.
- Square error:99.618

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

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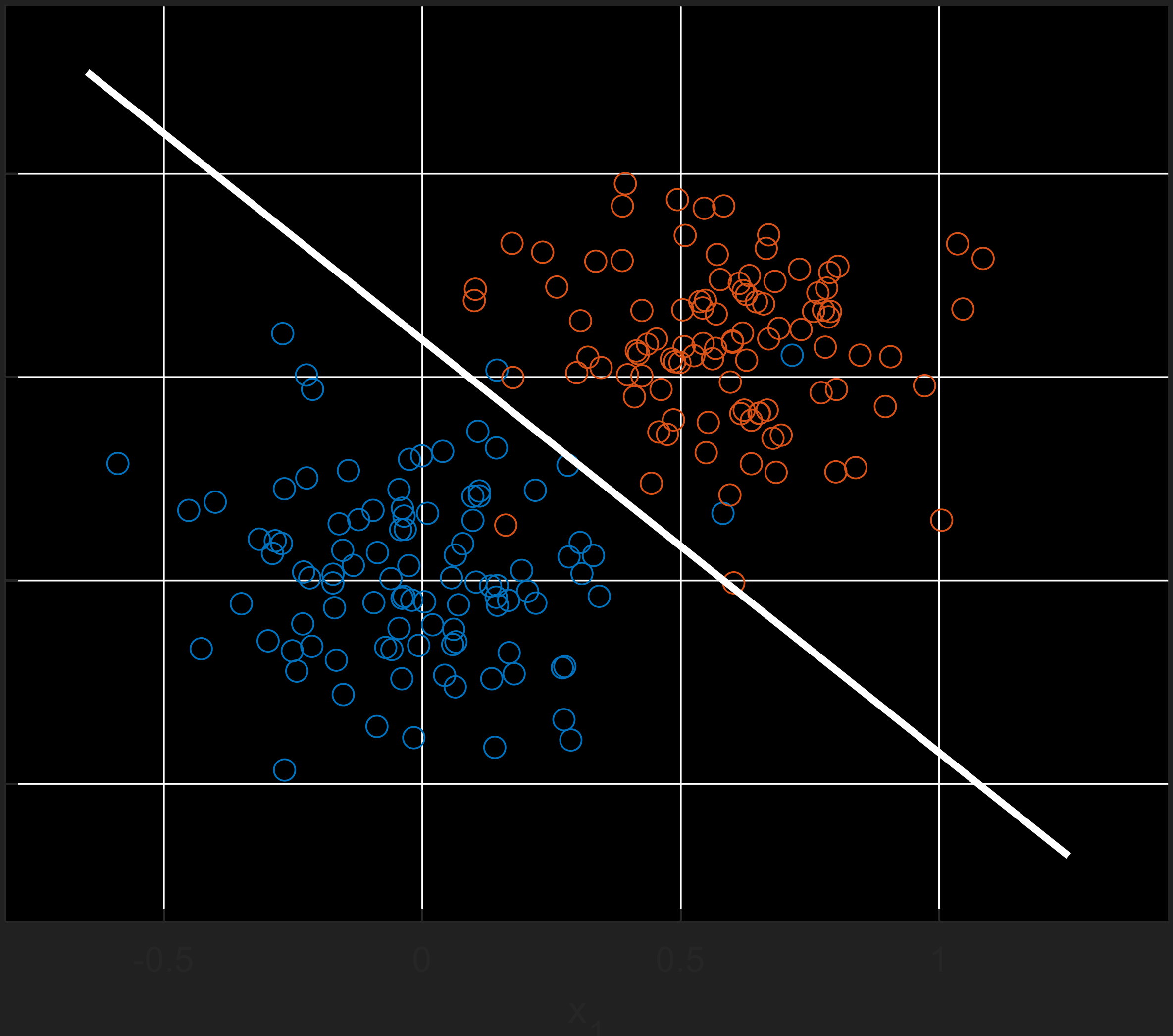
Example: Binary Classification



- Polynomial transform with $b = 1$.
- Square Error: 39.0547

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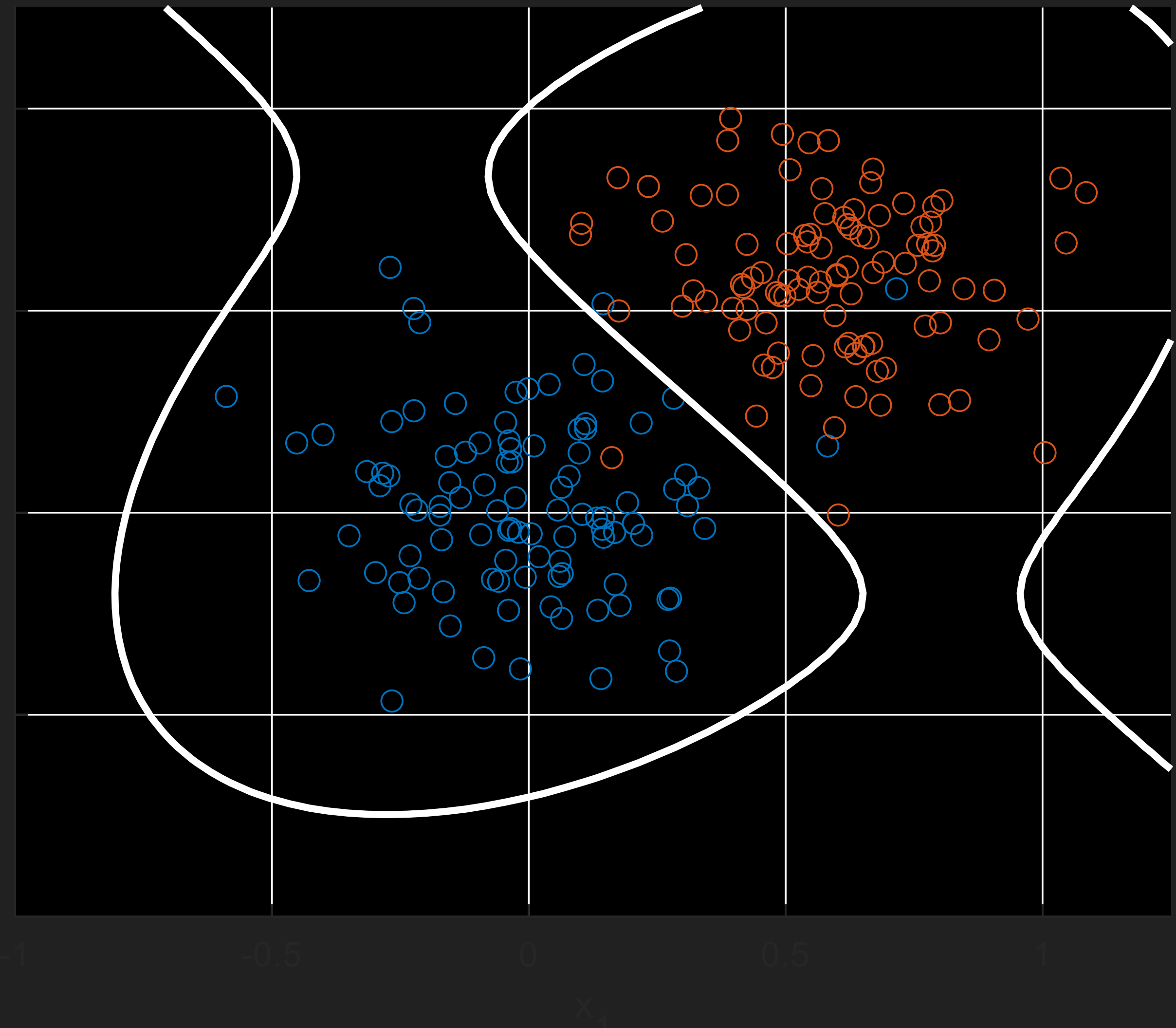
Example: Binary Classification



- 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 lecture.

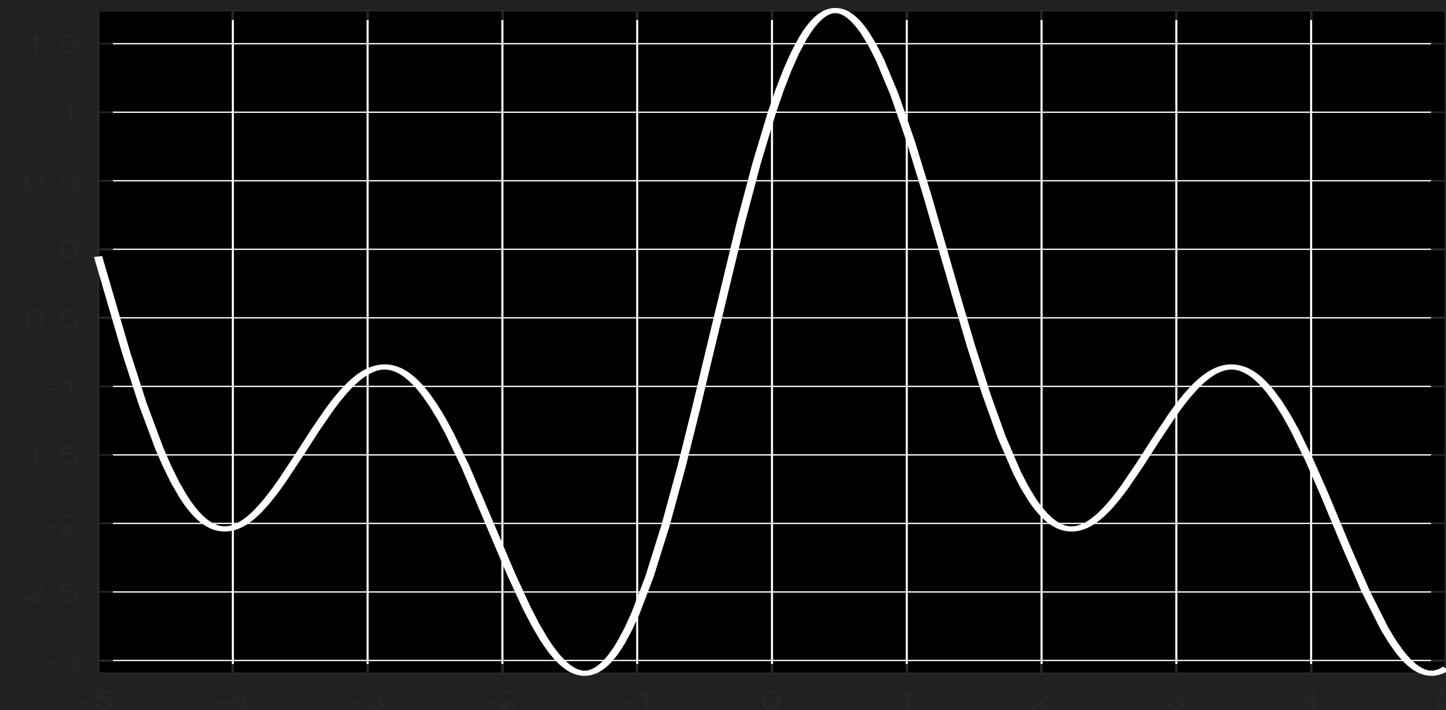
Why it works?

- 1-dimensional intuition: Taylor Series.
- Taylor Series of $g(x)$ at 0:
  - $g(x) = g(0)(x-0)^0 + g'(0)(x-0)^1 + \\ + \frac{g''(0)}{2!}(x-0)^2 + \frac{g'''(0)}{3!}(x-0)^3 + \cdots$
- 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



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

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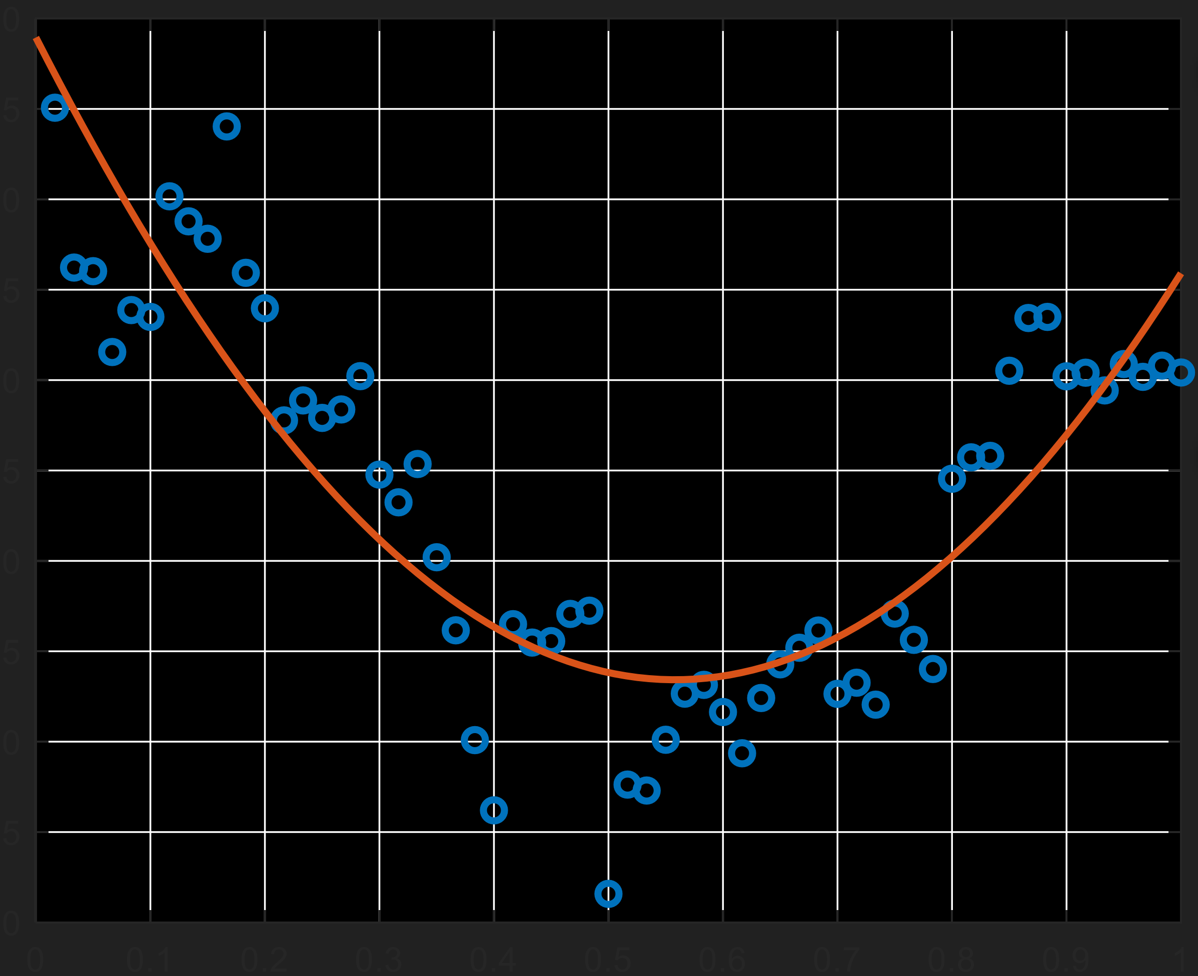
Trigonometric Transform

- Trigonometric Transform are used to approximate function over time domain.
  - $f(x) \coloneqq [1, \sin(x), \cos(x), \sin(2x),$
  $\cos(2x) \ldots \sin(bx), \cos(bx)]$
  - $f(x) \in R^{2b+1}$

Example: Apple Stock Price, Feb 2019



- Trigonometric transform with $b = 1$.
- Squared error: 1.5681e+03

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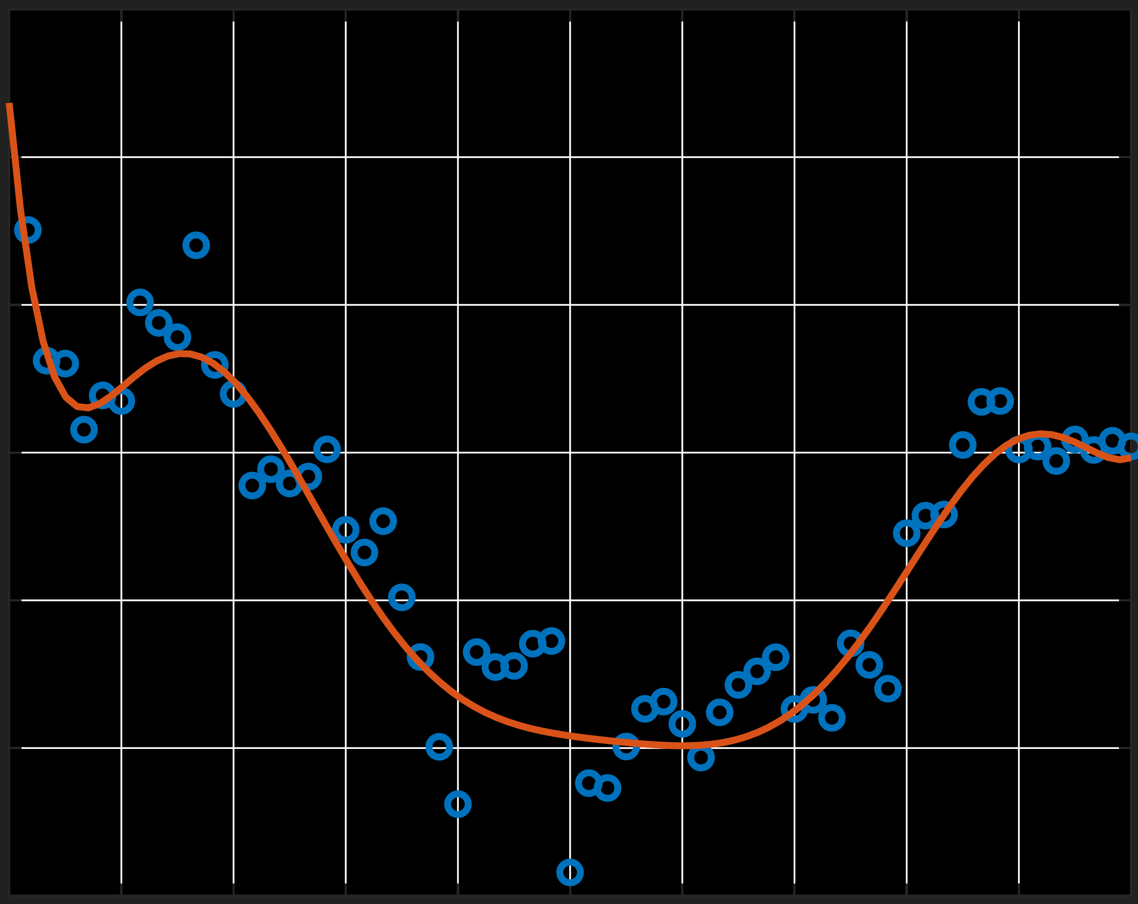
Example: Apple Stock Price, Feb 2019



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

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Linear Expansion of Basis Functions

- Polynomial and Trigonometric transforms based on the idea a function can be approximated by:
  - $y \approx \hat{y} = \sum_{i=1}^{m} \beta^{(i)} f^{(i)}(x)$
  - called a linear basis expansion of y
  - $f^{(i)}$ are called **basis function**
    - Polynomial basis, Trigonometric basis…

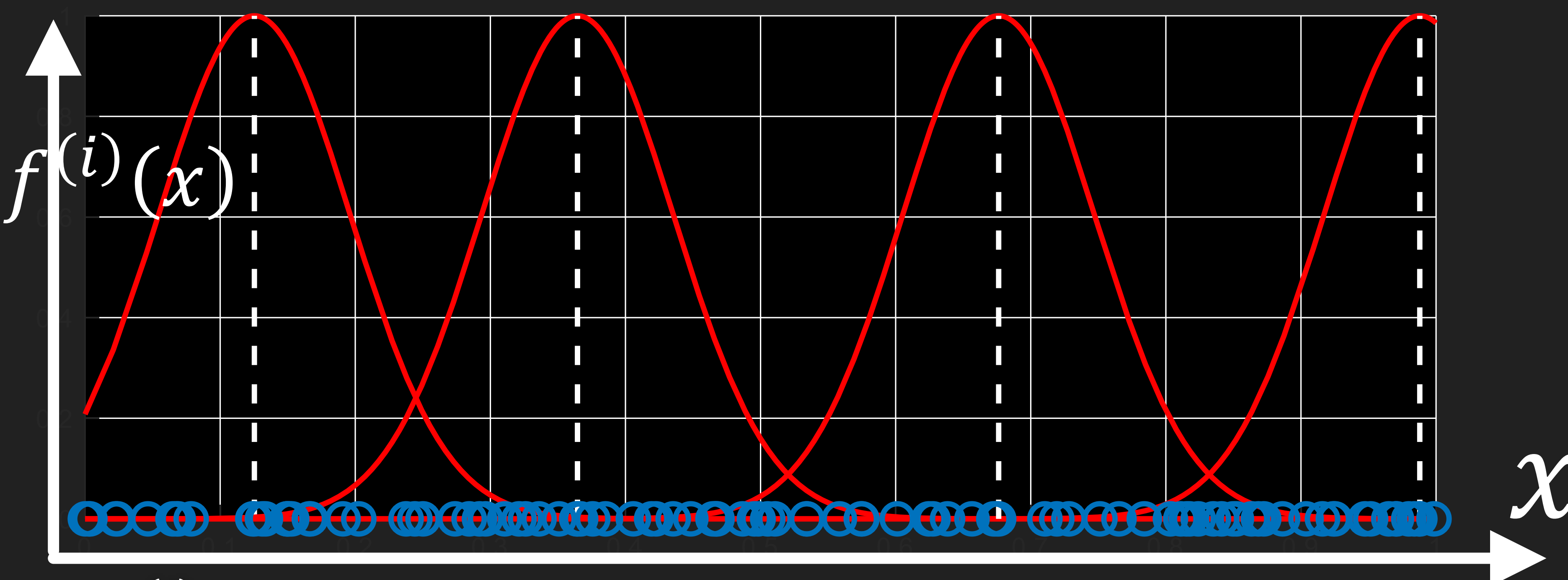
Radial Basis Function (RBF)

- RBF is another widely used basis function for function approximation.
- $f^{(i)}(x) := \exp\left(-\frac{\left\|x - x_i\right\|^2}{\sigma^2}\right)$
  - $\sigma > 0$ is called width
  - σ is determined before fitting
  - A practice is setting σ as the median of all pairwise distances of $\boldsymbol{x}$ in your data.

Radial Basis Function (RBF)

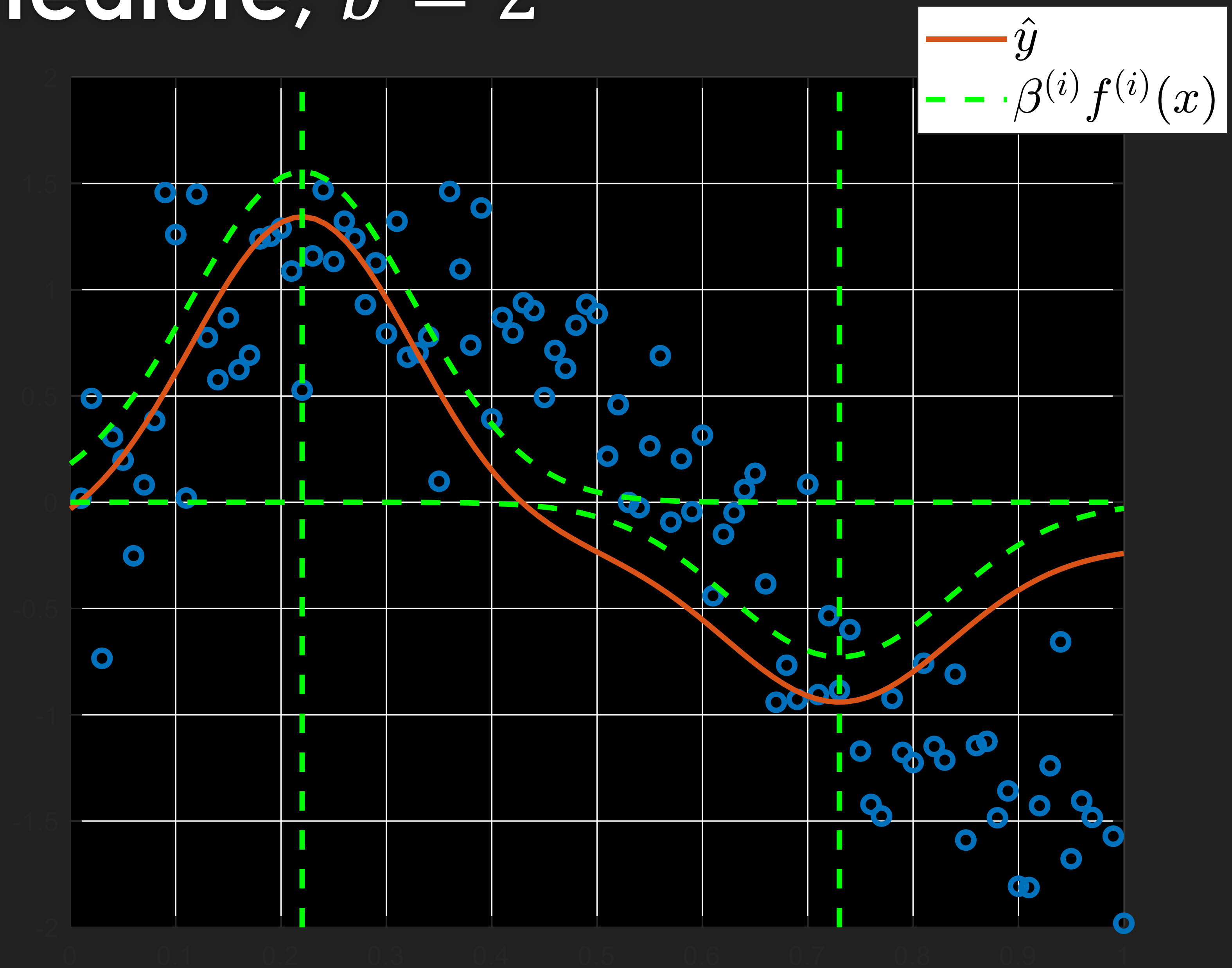
- $\boldsymbol{x}_i$ are called **RBF centroids.**
- $\boldsymbol{x}_i$ can be **randomly chosen** from the $\boldsymbol{x}$ in your dataset
- $\boldsymbol{f}(\boldsymbol{x}) \coloneqq [1, f^{(1)}(x), f^{(2)}(x), \ldots, f^{(b)}(x)]$
  - Do not forget 1!

Radial Basis Function (RBF)



- $f^{(i)}(x)$ are visualized in red at random 4 centroids among 100 uniformly drawn x.
- At each "bump",
  - If $\beta^{(i)} > 0$, basis at $x^{(i)}$ gives $\hat{y}$ a "lift".
  - If $\beta^{(i)} < 0$, basis at $x^{(i)}$ gives $\hat{y}$ a "push".

RBF feature, $b = 2$



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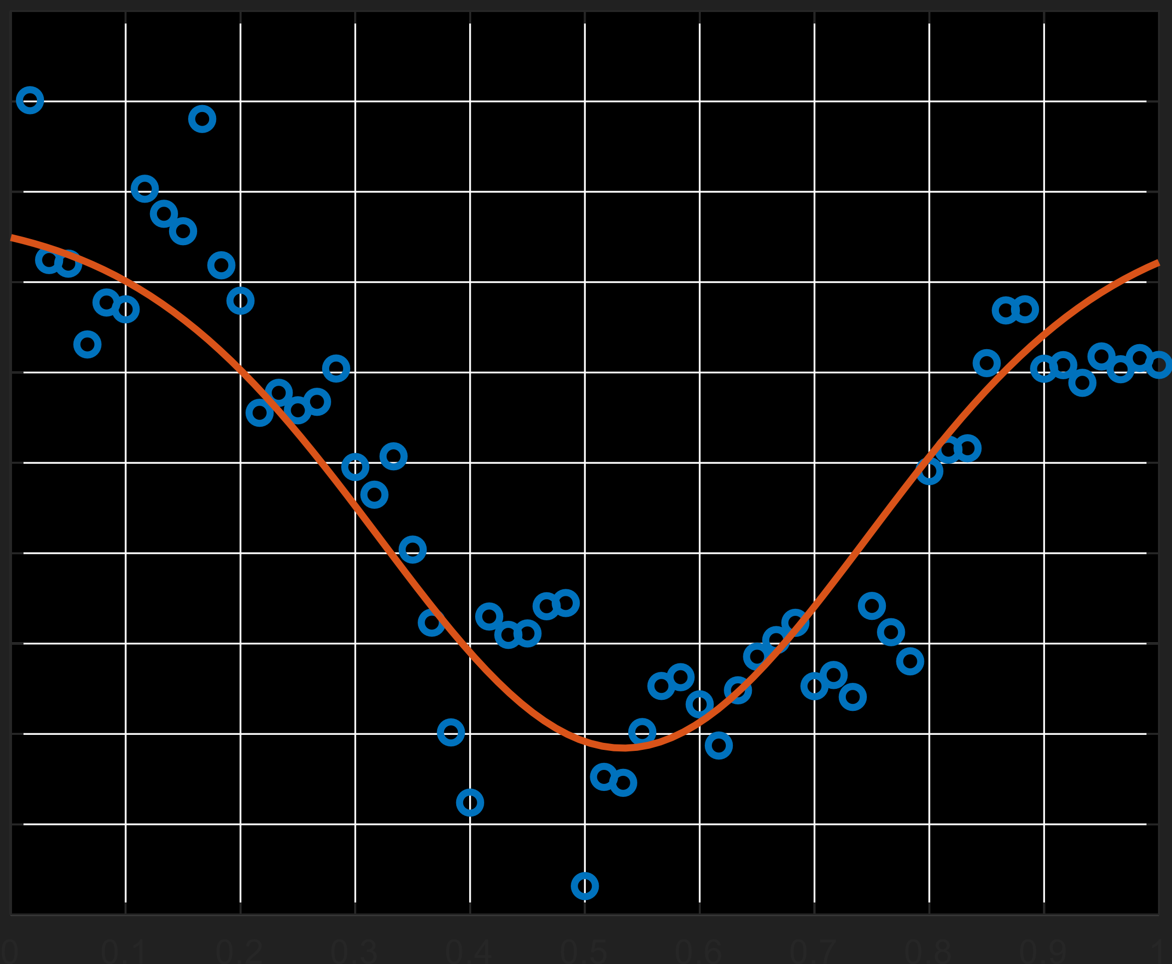
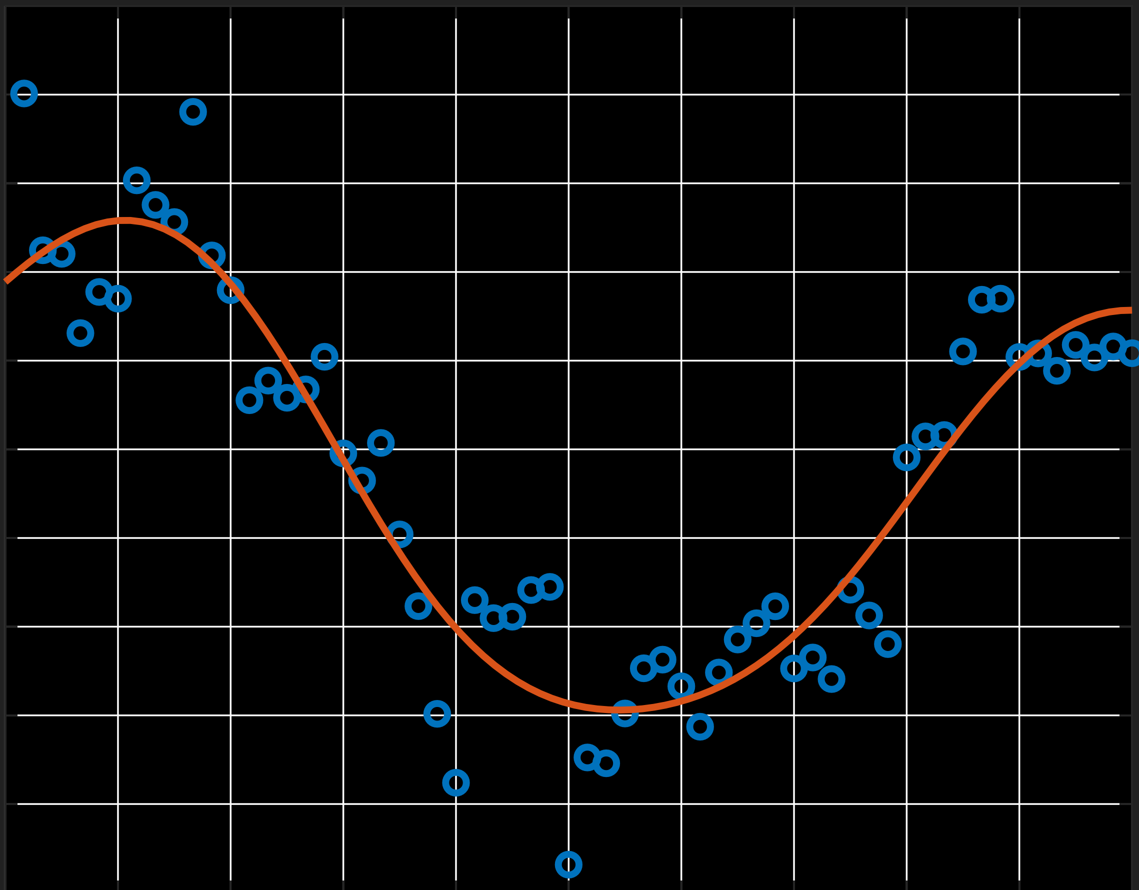
Example: Apple Stock Price, Feb 2019



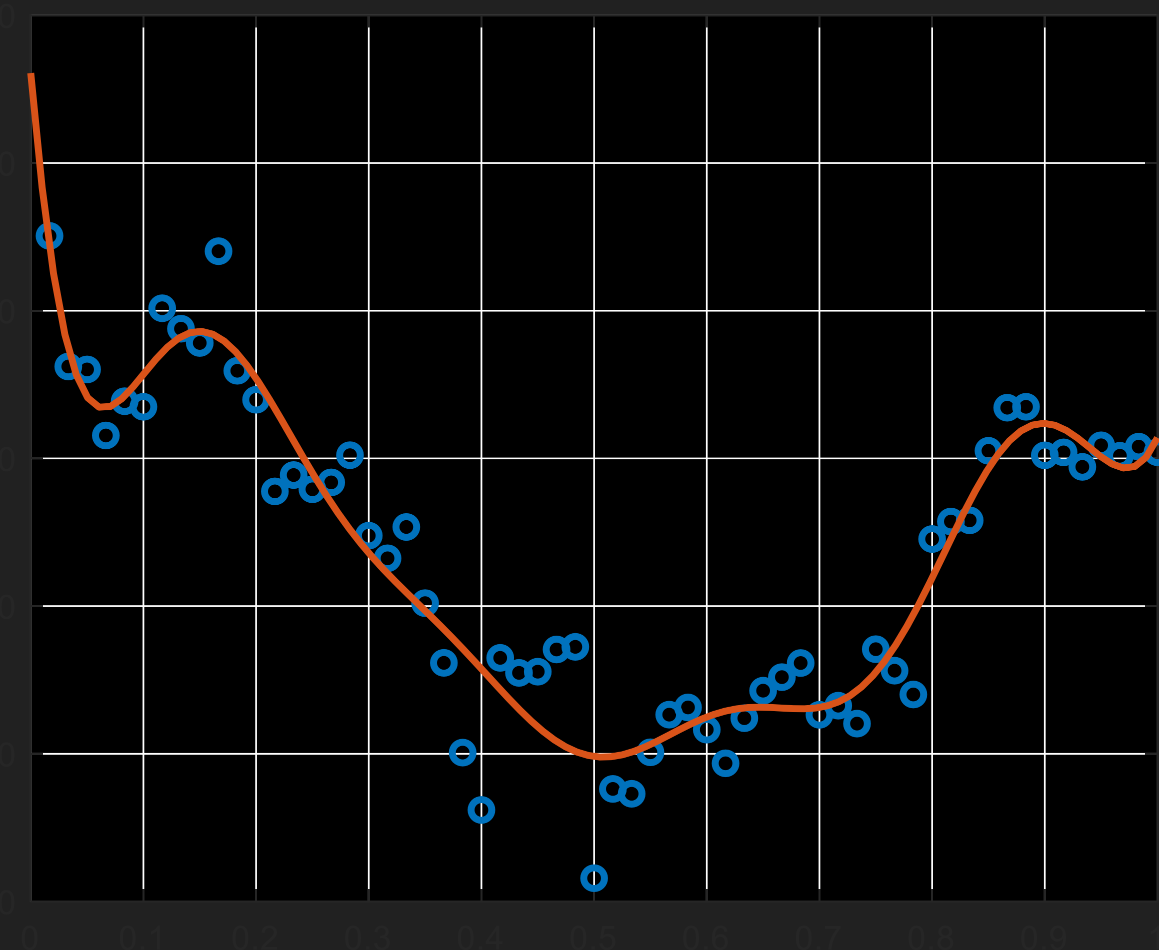
- RBF
  - σ =0.2121
  - $b = 1.$
- Squared error: 1.1908e+03

Example: Apple Stock Price, Feb 2019



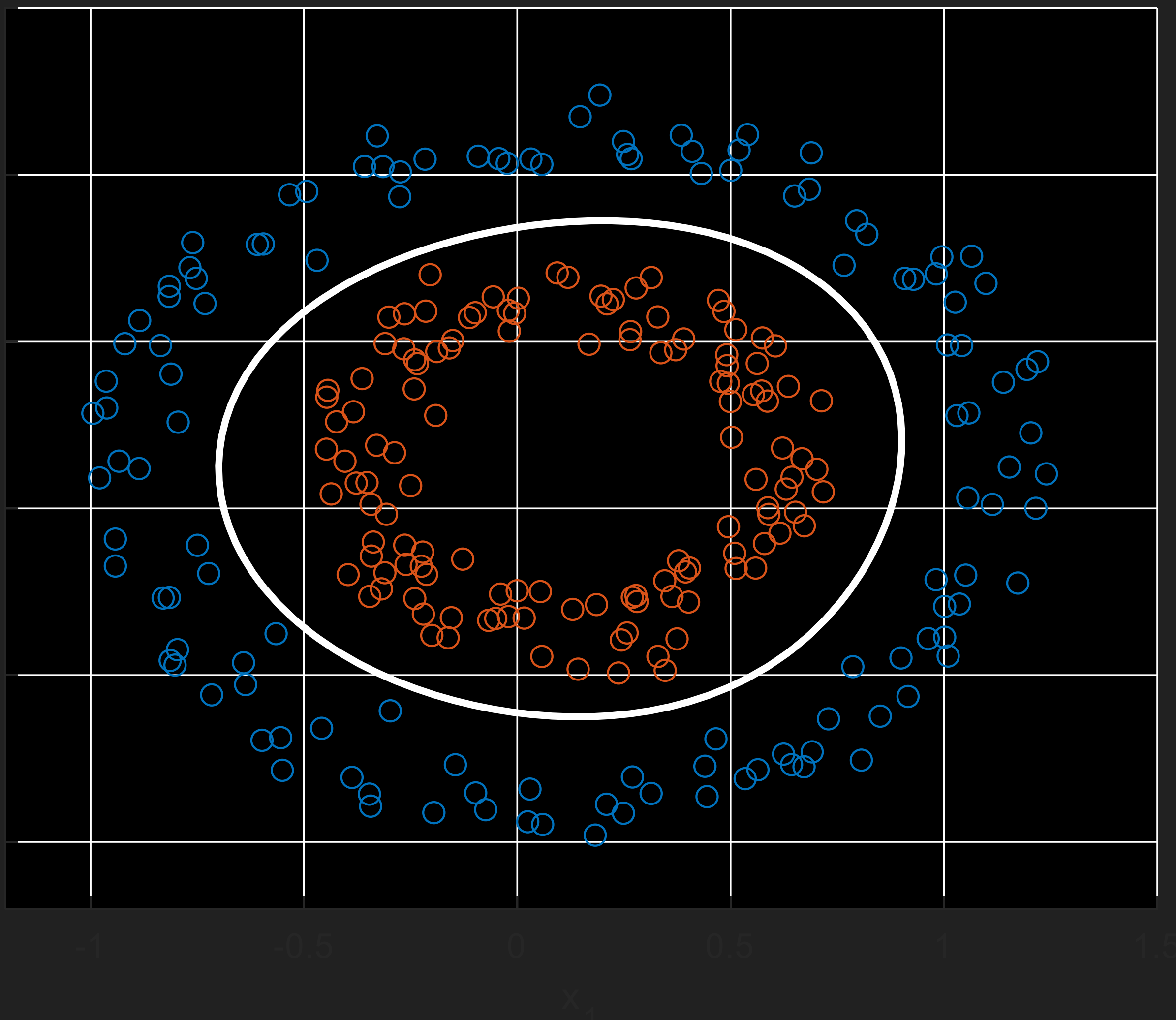
- RBF
  - σ =0.2121
  - b = 5.
- Squared error: 842.7575

Example: Apple Stock Price, Feb 2019



- RBF
  - σ =0.2121
  - $b = 10.$
- Squared error: 593.8104

Example: Double Ring Classification



- RBF
  - σ =0.7041
  - b = 5.
- Squared error: 16.3351

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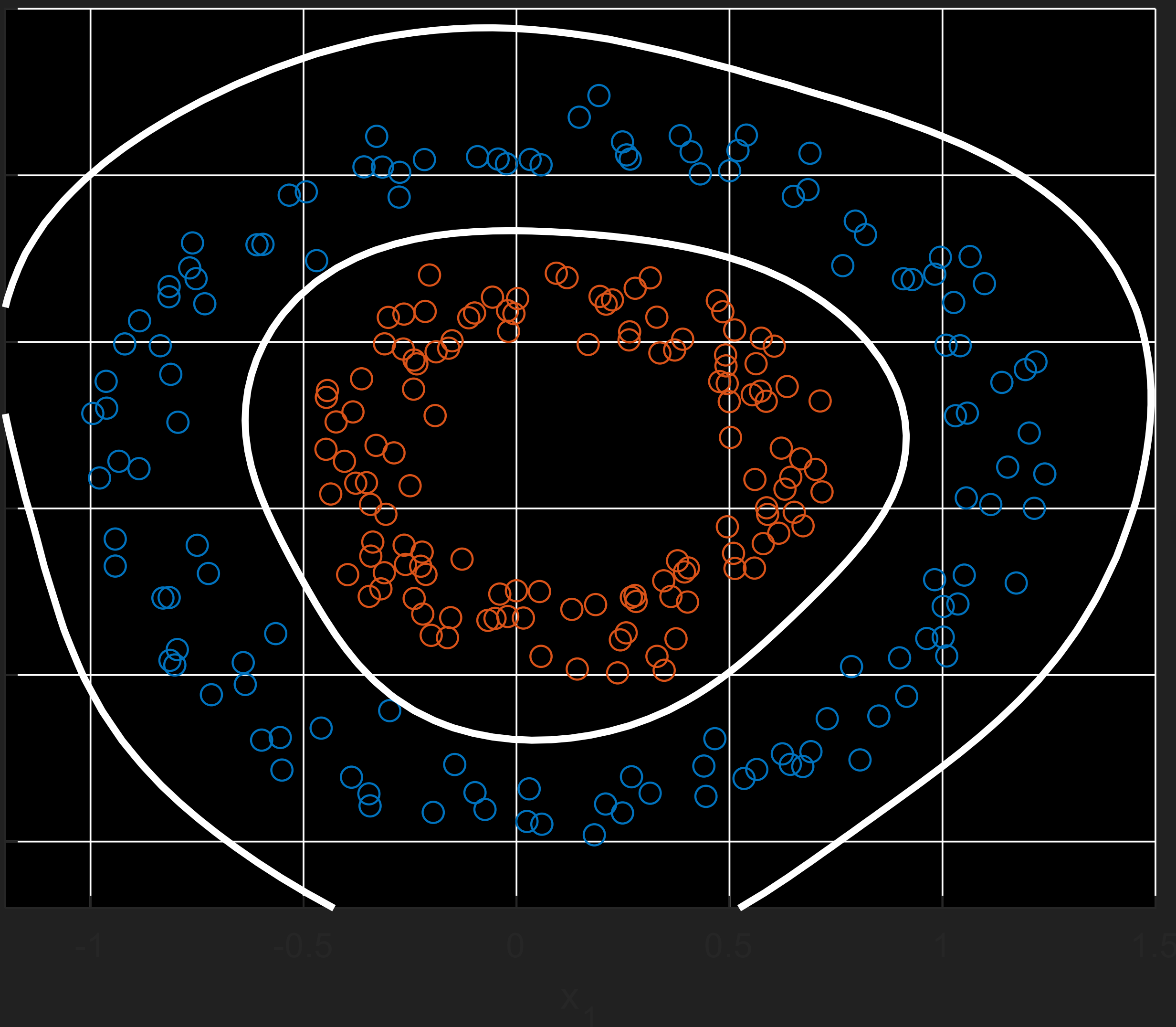
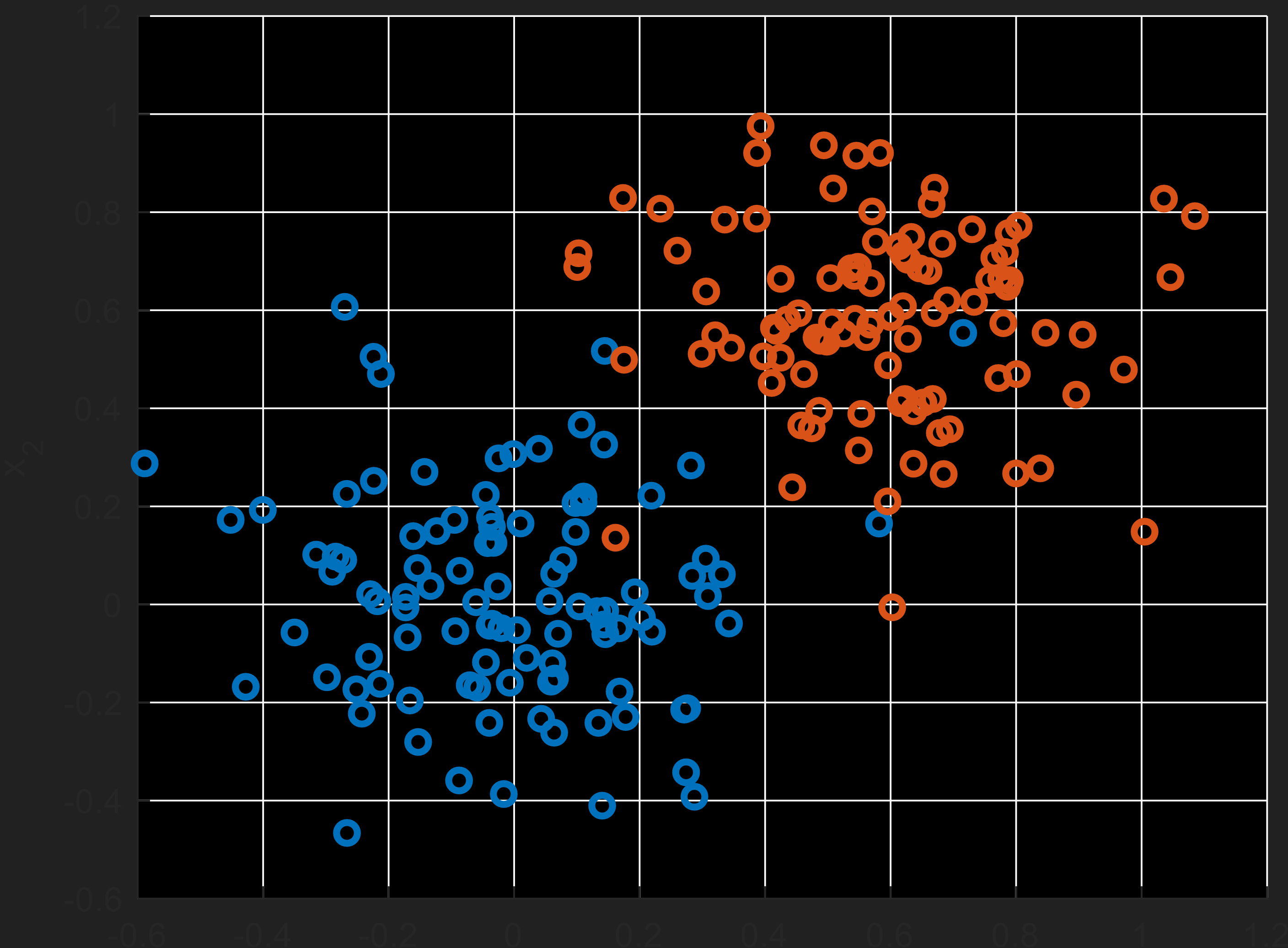
Example: Double Ring Classification



- RBF
  - σ =0.7041
  - $b = 100.$
- Squared error: 9.9890

Selecting Features using Prior Knowledge



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Question

- Seeing your dataset above, what $\boldsymbol{f}$ should you use for classification? Hint: consider computational cost and overfitting
  - Polynomial, $b = 1$
  - Polynomial, $b = 2$
  - Polynomial, $b = 3$
  - RBF, $b = 100$
- **https://bit.ly/2FnjryC**

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 $\boldsymbol{f}$ with a larger b makes $\hat{y}$ more flexible, can we make $b = \infty$?
- Next two lectures, The selection of number of basis $\boldsymbol{b}$ and Kernel methods.

To know more…

- The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Hastie et al., 2009
  - 2.3.1 Linear Models and Least Squares
  - 2.6.3 Function Approximation
  - 2.8.3 Basis Functions