Data Science

Lecture 2-2: Data Science Fundamentals (Modeling)

UNIVERSITY
OF AMSTERDAM

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Date: Feb 2023

This lecture recaps classification and regression techniques for modeling data.

For this lecture, let us now use the following text classification task as an example: identifying whether a text message is spam or ham (non-spam).

```
✦✦✦✦✦✦✦✦✦✦✦✦ PRIVATE!
Your 2020 Account won $1,000,000
lottery! ✦✦✦✦✦✦✦✦✦ To claim
call 08719180248 ✦✦✦✦✦✦✦
```

Hi Yen-Chia, may we have our meeting on 5/15 by just email update to buy some time? if not, zero worries if you need to talk.

Mail
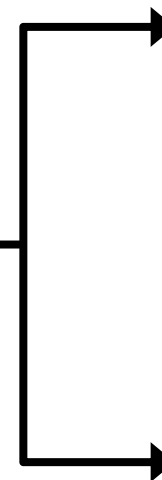
Spam

Ham (Non-spam)

To classify spam messages, we need examples: a dataset with observations (messages) and labels (spam or non-spam).

◆◆◆◆◆◆◆◆◆◆◆◆ PRIVATE! Your 2020 Account won $1,000,000 lottery! ◆◆◆◆◆◆◆◆ To claim call 08719180248 ✧✧✧✧✧✧✧✧

Spam

Hi Yen-Chia, may we have our meeting on 5/15 by just email update to buy some time? if not, zero worries if you need to talk.

Ham

Would you be willing to meet with me on 3/26 Thursday when I was in TU Delft after (or before) giving the guest lecture (10:35am-11:50am)?

Ham

Observations

Labels

We can extract features (information) using human knowledge, which can help distinguish spam and ham messages.

◆◆◆◆◆◆◆◆◆◆◆◆ PRIVATE! Your 2020 Account won $1,000,000 lottery! ◆◆◆◆◆◆◆◆ To claim call 08719180248 ✧✧✧✧✧✧✧

Number of special characters = 34
Number of digits = 22

Spam

Hi Yen-Chia, may we have our meeting on 5/15 by just email update to buy some time? if not, zero worries if you need to talk.

Number of special characters = 5
Number of digits = 3

Ham

5

Using features X (which contains x_1 and x_2), we can represent each message as one data point on an n-dimensional space ($n = 2$ in this case).
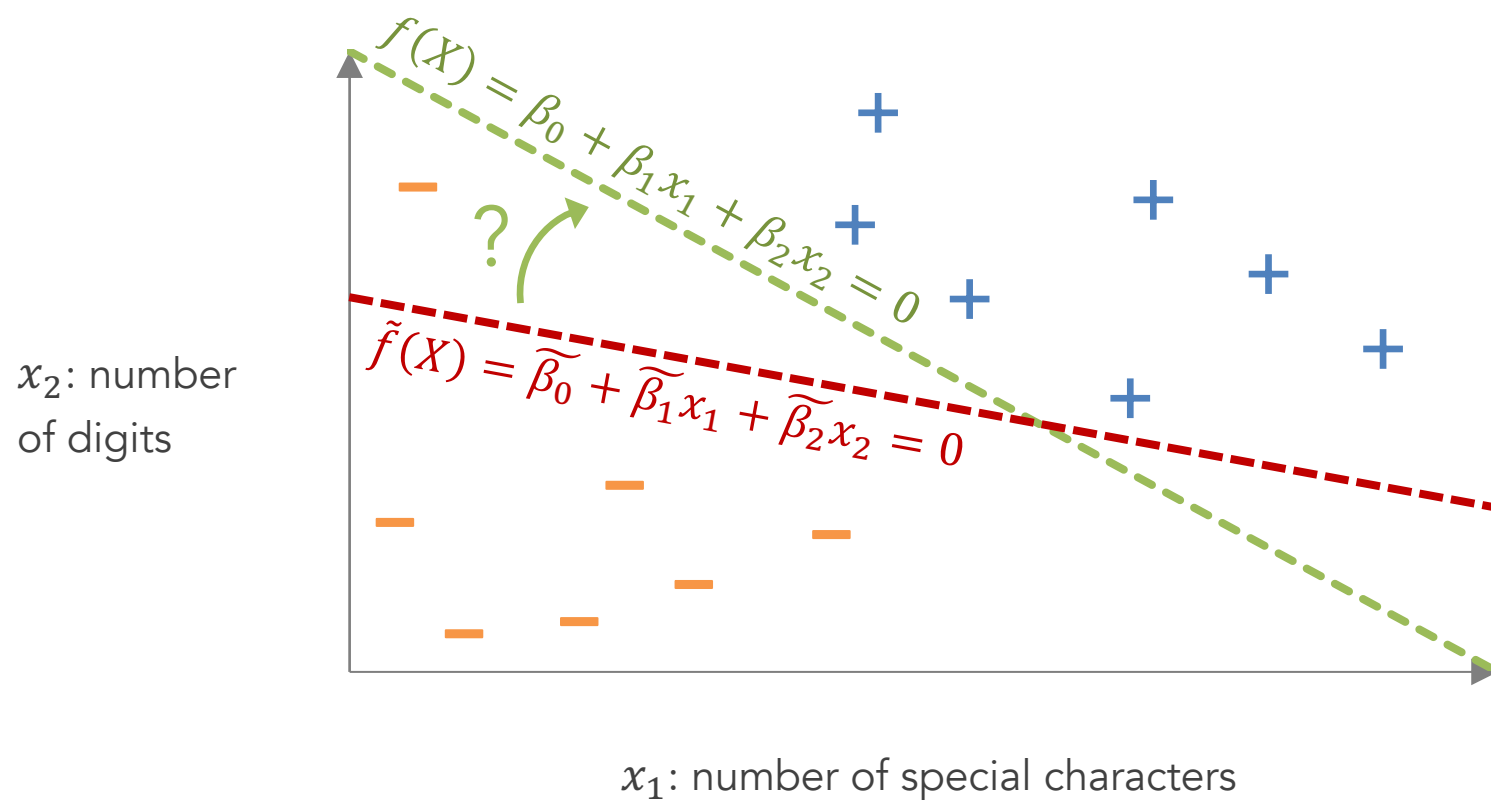

x_2: number of digits

x_1: number of special characters

Spam

Ham

Hi Yen-Chia, may we have our meeting on 5/15 by just email update to buy some time? if not, zero worries if you need to talk.

PRIVATE! Your 2020 Account won $1,000,000 lottery! To claim call 08719180248
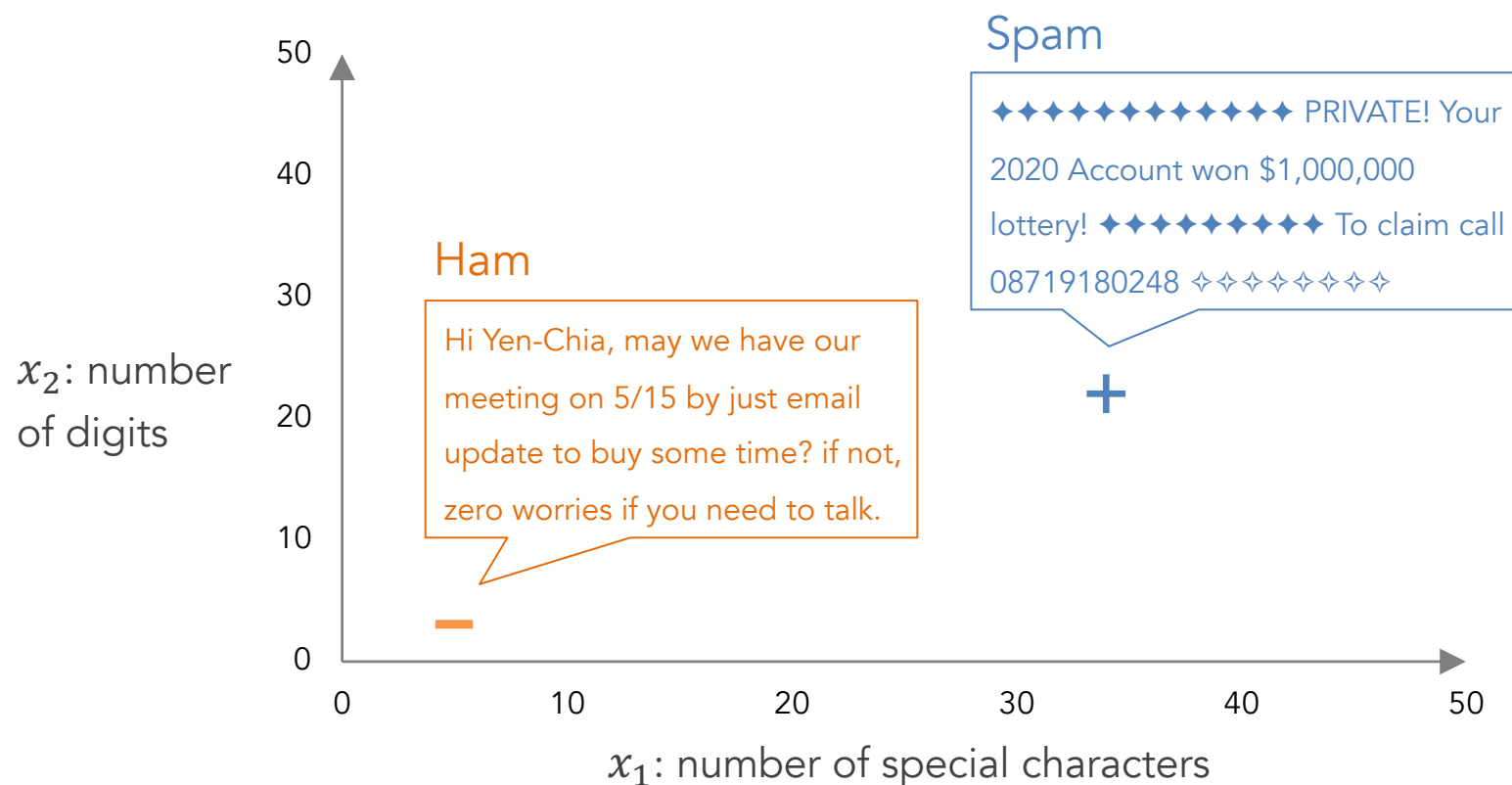
We can think of the model as a function f that can separate the observations into groups (i.e., class labels y) according to their features X.

$$f(X)$$

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 = 0$$

x_2: number of digits

Spam $f(X) > 0$

Ham $f(X) < 0$

x_1: number of special characters
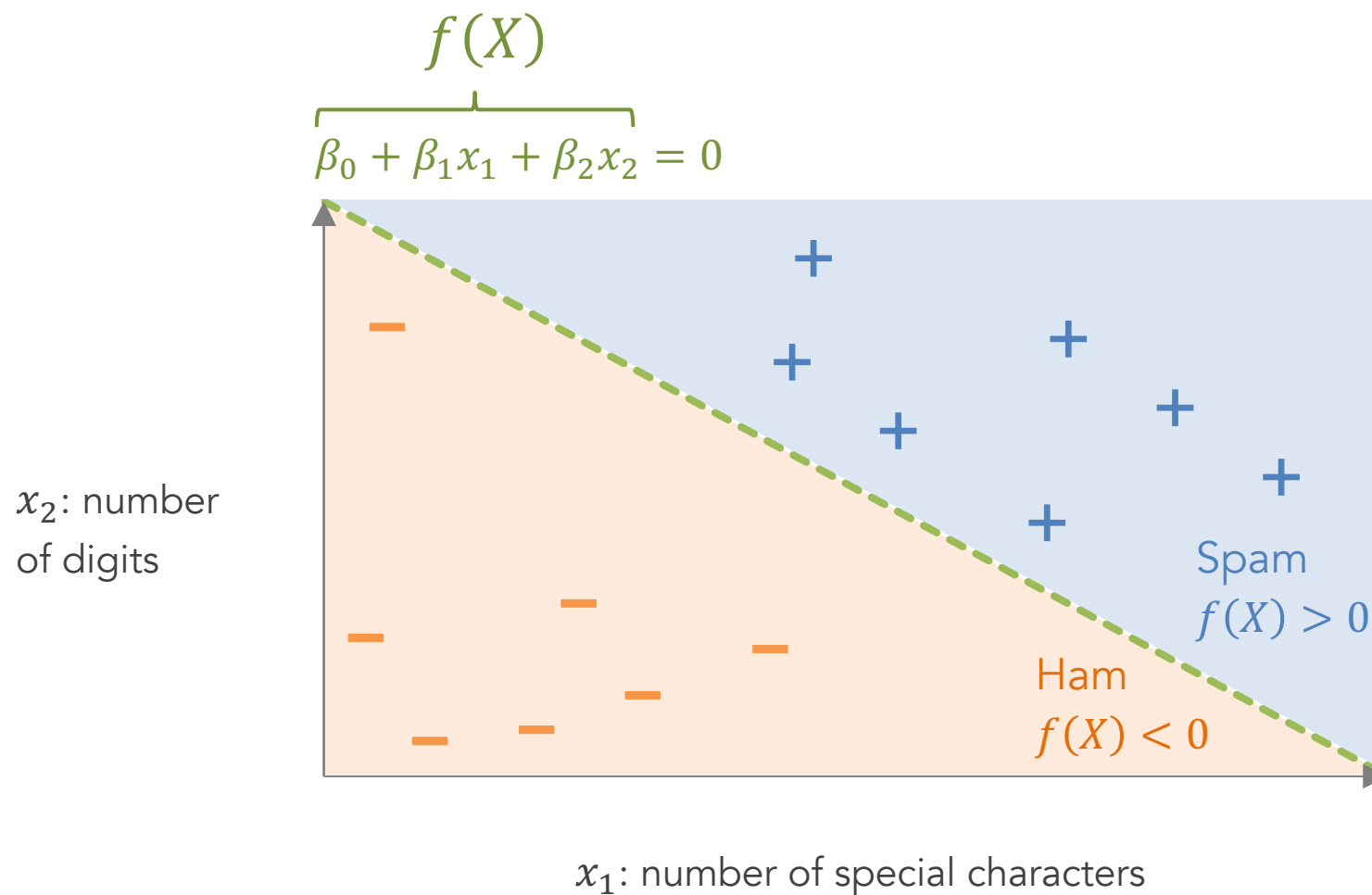
Classification   To find a good function f, we start from some f and train it until satisfied. We need something to tell us which direction and magnitude to update.
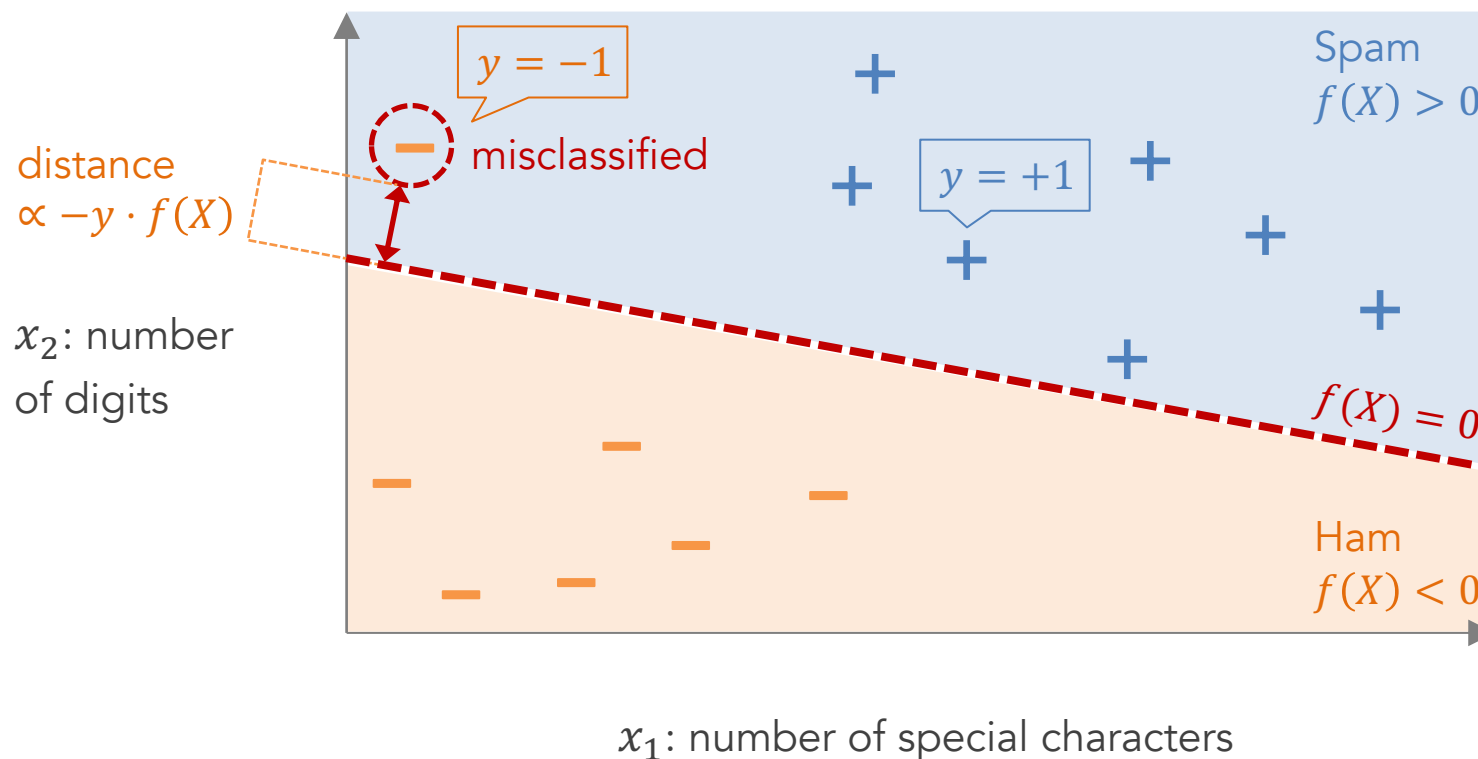
$f(X) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 = 0$

$\tilde{f}(X) = \widetilde{\beta_0} + \widetilde{\beta_1} x_1 + \widetilde{\beta_2} x_2 = 0$

x_2: number of digits

?

x_1: number of special characters

8

First, we need an error metric (i.e., loss function). For example, we can use the sum of distances between the misclassified points and line f.
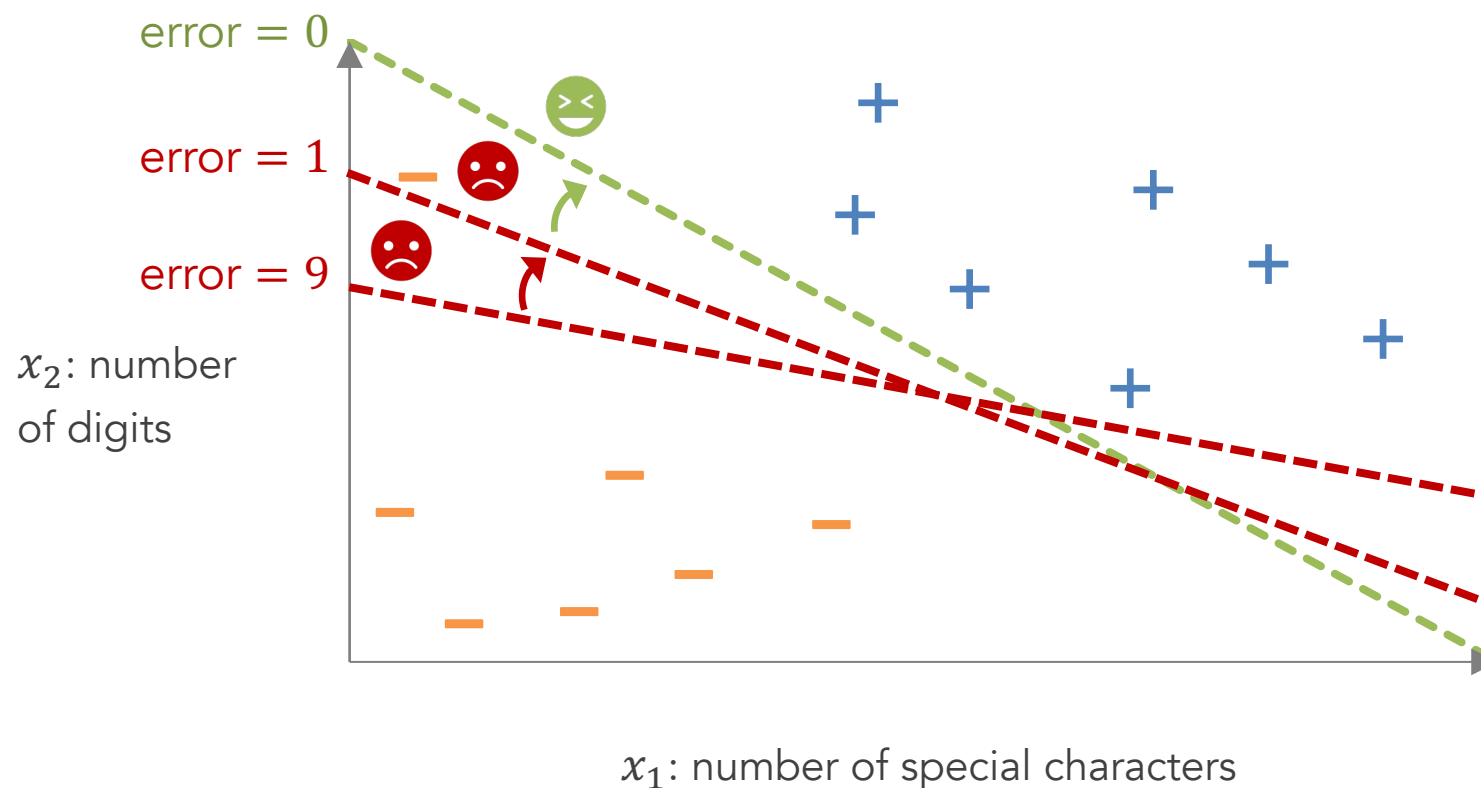
$$\text{error} = \sum -y \cdot f(X) \quad \text{for each misclassified point } X$$

Distance from point to plane: https://mathinsight.org/distance_point_plane

We can use gradient descent (an optimization algorithm) to minimize the error to train the model f iteratively. This example is the Perceptron algorithm.

$$\text{minimize error} = \sum -y \cdot f(X) \quad \text{for each misclassified point } X$$

error $= 0$

error $= 1$

error $= 9$

x_2: number of digits

x_1: number of special characters

More about the Perceptron Algorithm -- http://www.cs.cmu.edu/~mgormley/courses/10601bd-f18/slides/lecture6-perc.pdf

Depending on the needs, we can train different models (using different loss functions) with various shapes of decision boundaries.

x_2: number of digits

x_1: number of special characters
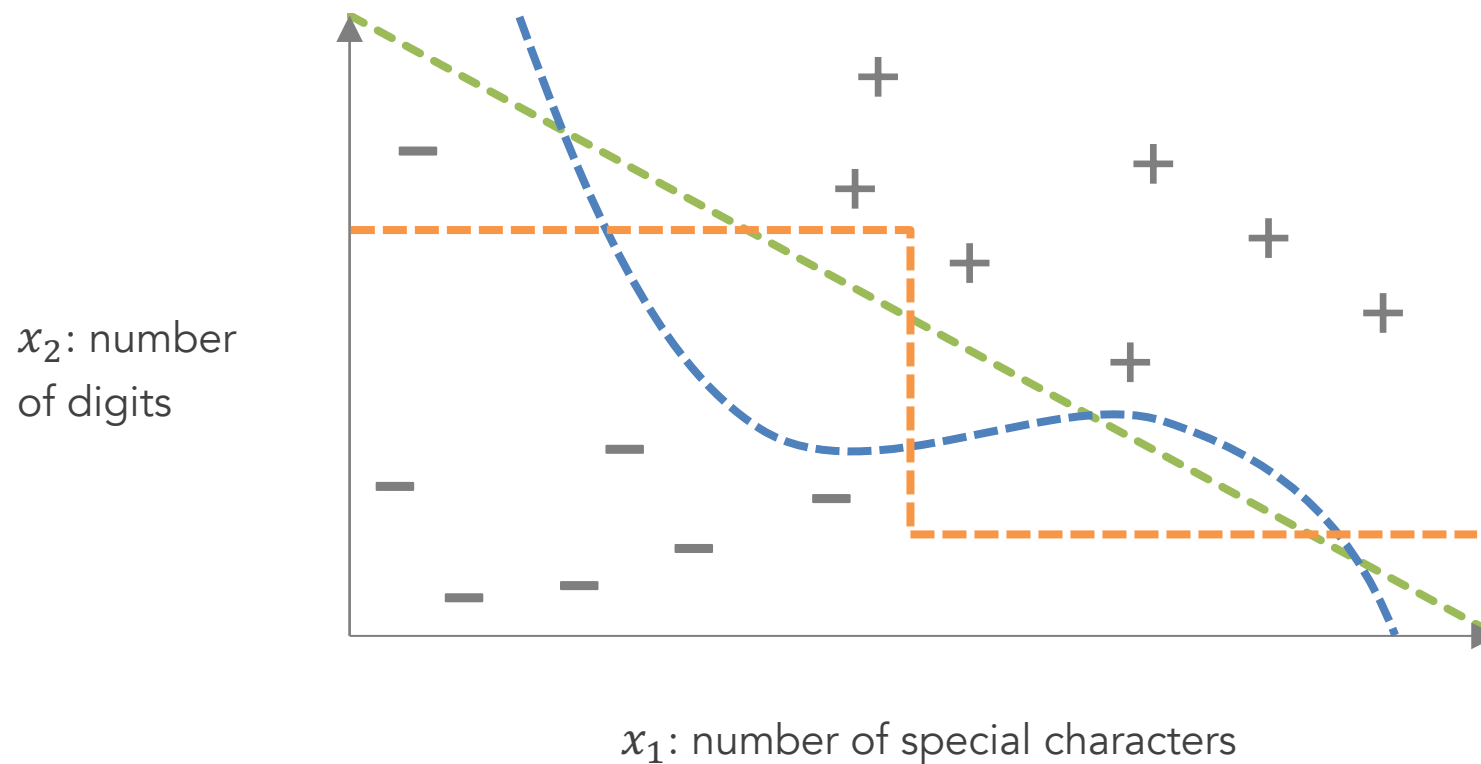
Depending on the needs, we can train different models (using

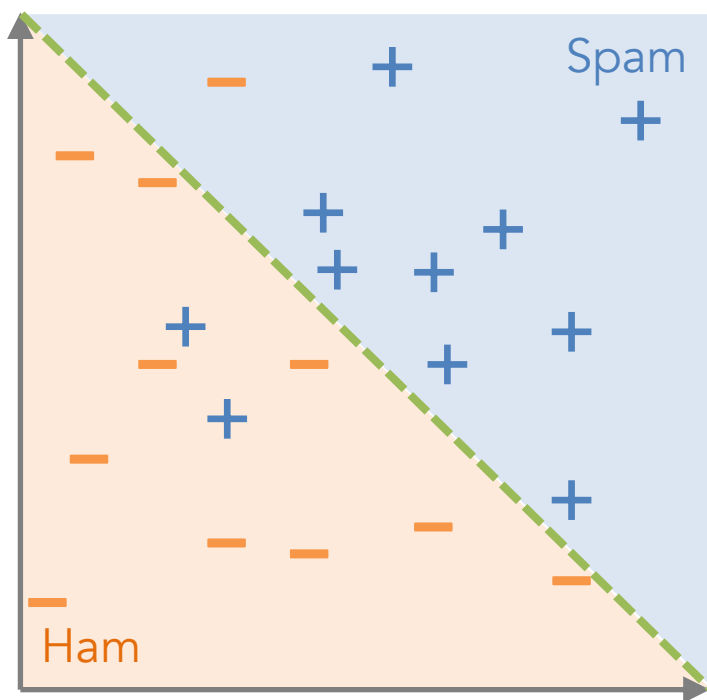different loss functions) with various shapes of decision boundaries.
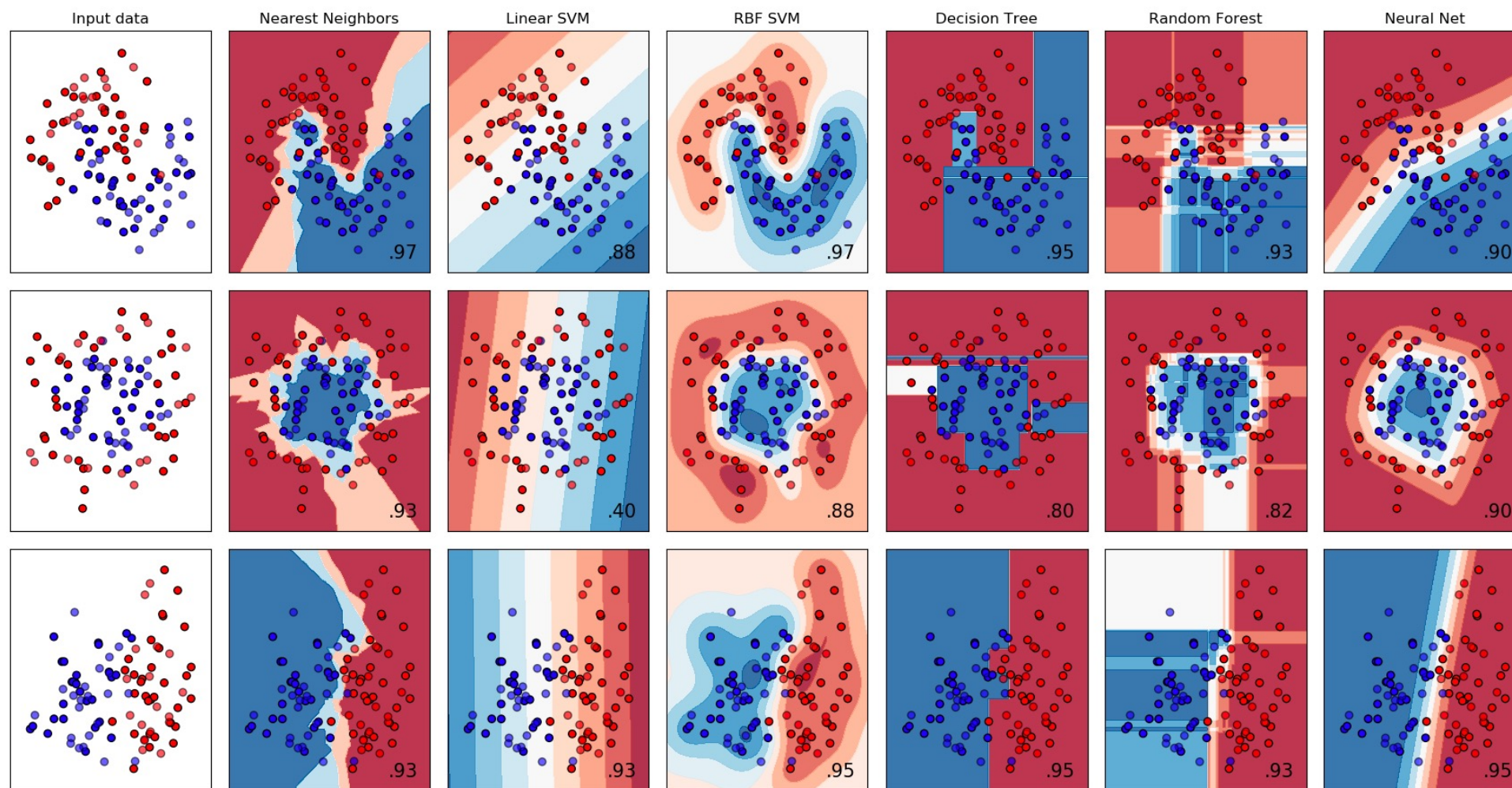
To evaluate our classification model, we need to compute evaluation metrics to measure and quantify model performance, such as the accuracy of all data.
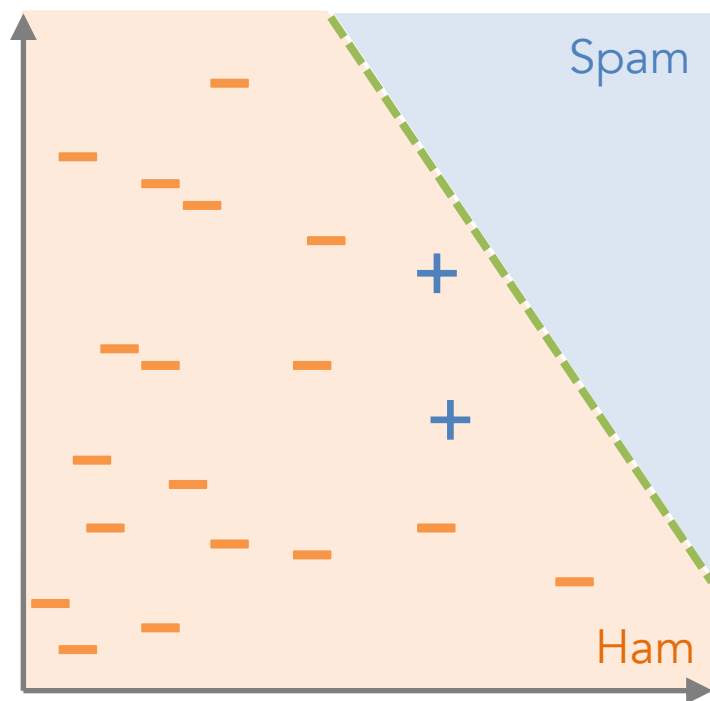

Accuracy for all data

$$= \frac{\text{\# of correctly classified points}}{\text{\# of all points}}$$

$$= \frac{19}{22} = 0.86$$

But what if the dataset is imbalanced (i.e., some classes have significantly fewer data)? In this case, the accuracy of all data is a bad evaluation metric.
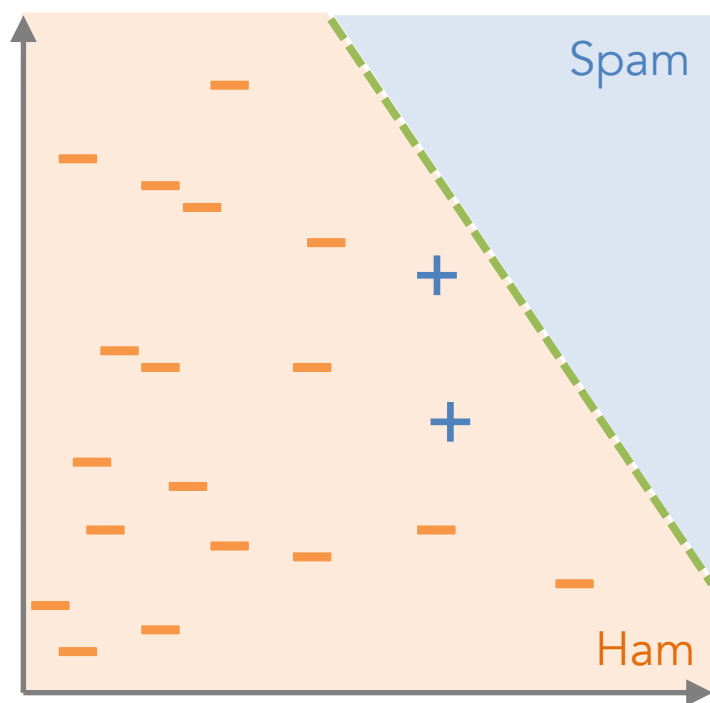

Classify all data as non-spam

Accuracy for all data

$$= \frac{\text{\# of correctly classified points}}{\text{\# of all points}}$$

$$= \frac{18}{20} = 0.9$$

Instead of computing the accuracy for all the data, we can compute accuracy for each class, which allows us to see the performance of different labels.

Classify all data as non-spam
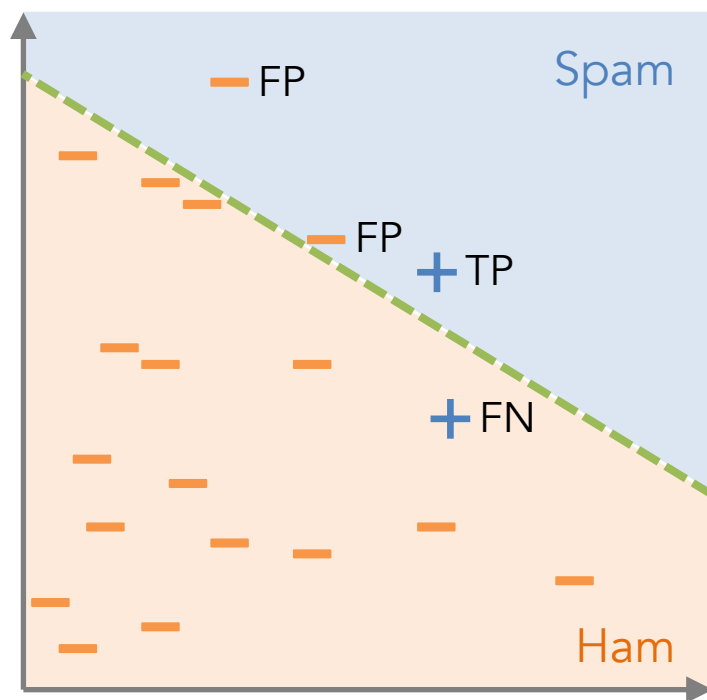
$$\text{Accuracy for spam} = \frac{0}{2} = 0$$

(true positive rate, recall, sensitivity)

$$\text{Accuracy for ham} = \frac{18}{18} = 1$$

(true negative rate, specificity)

If we care more about the positive class (e.g., spam), we can use precision and recall, with its best value at 1 and the worst value at 0.

Spam

FP

FP

+ TP

+ FN

Ham

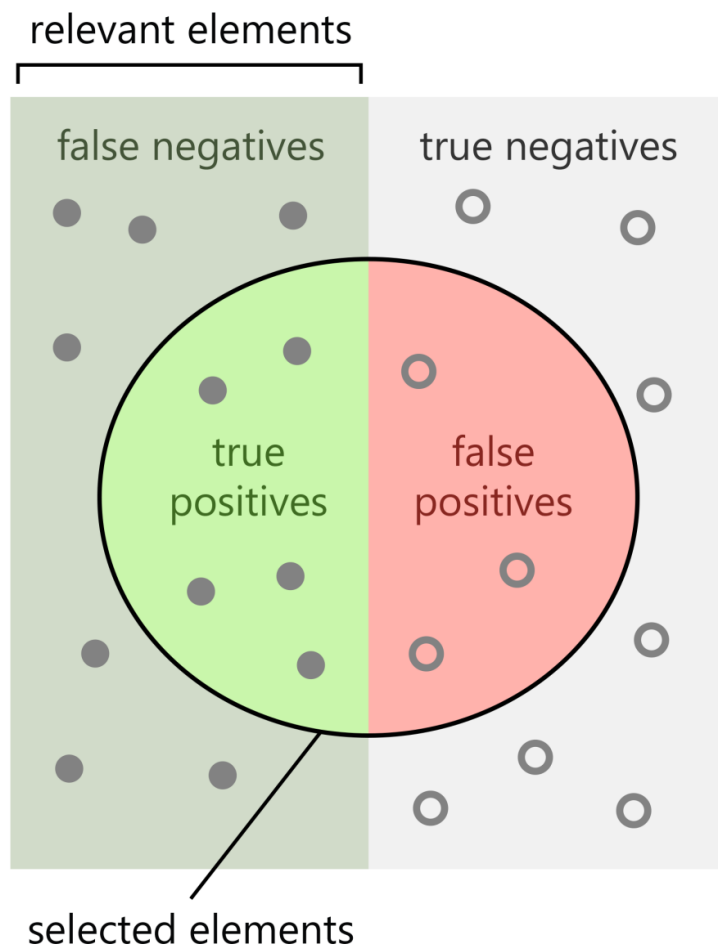TP = 1 (True Positive)

FP = 2 (False Positive)

FN = 1 (False Negative)

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} = 0.33$$

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} = 0.5$$

He and Garcia. 2009. Learning from imbalanced data. IEEE TKDE.

Precision and recall can be aggregated into F-score as a general model performance, with its best value at 1 and worst value at 0.

relevant elements

false negatives | true negatives

true positives | false positives

selected elements

How many selected items are relevant?

How many relevant items are selected?

$$\text{Precision} = \frac{}{}$$

$$\text{Recall} = \frac{}{}$$

$$\text{F–score} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

Retrieved from https://en.wikipedia.org/wiki/Precision_and_recall

We can train different types of models. But how do we know which one is better? Can we just pick an evaluation metric to determine which model is good?
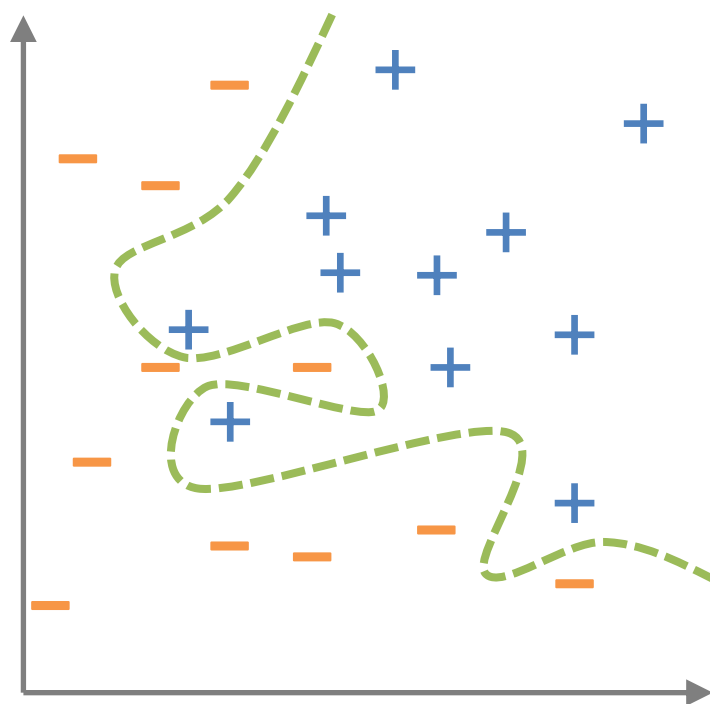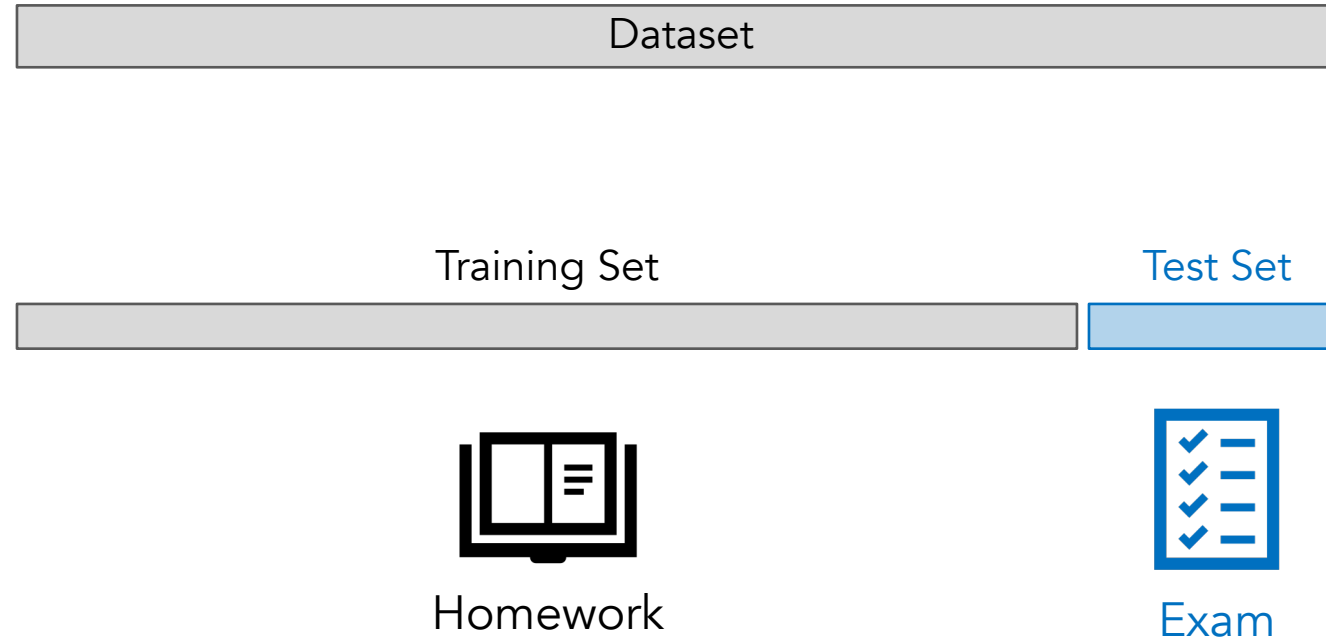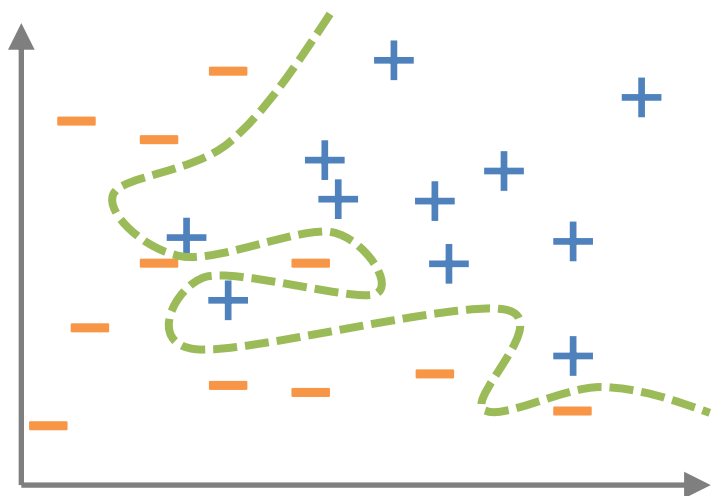

Model A
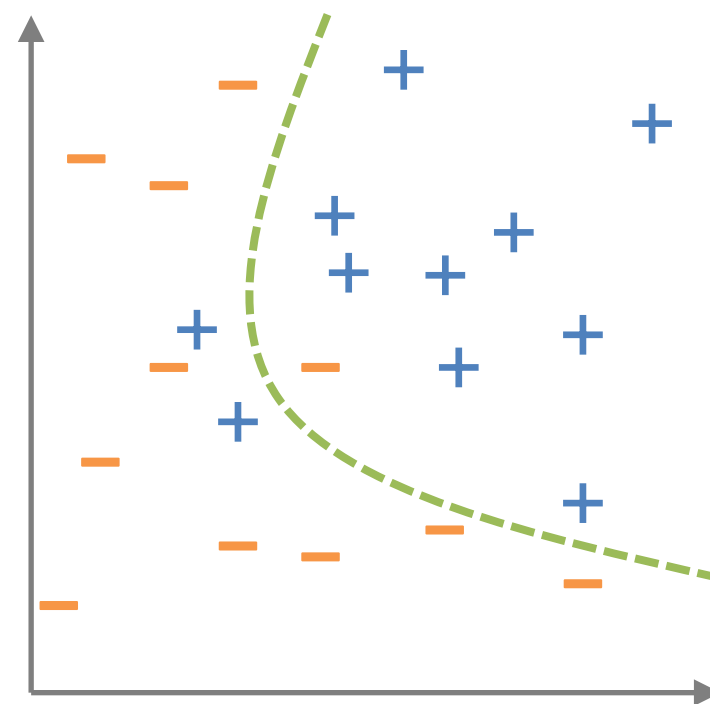
Model B

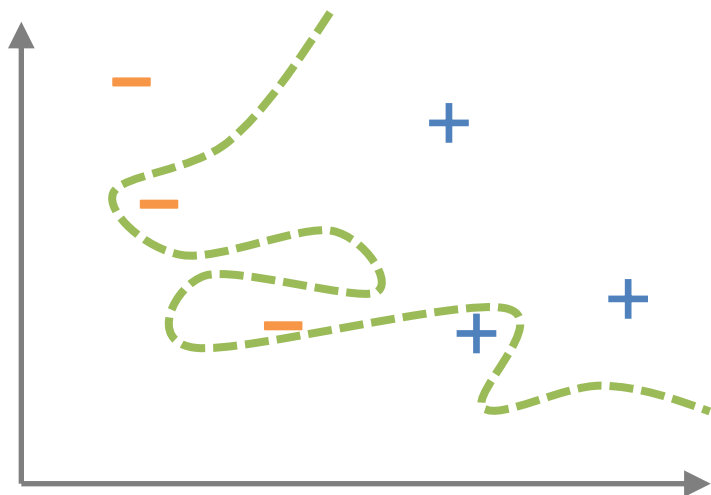To choose models, we need a test set, which contains data that the models have not yet seen before during the training phase.

Dataset

Training Set
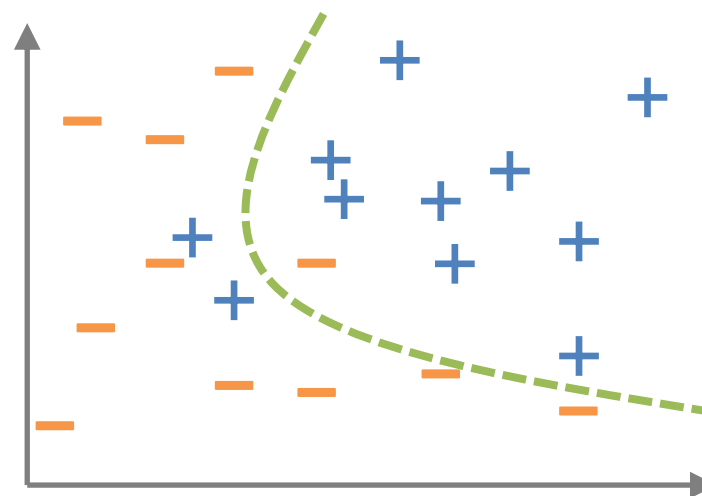
Test Set

Homework

Exam

😣 Model A

Training Accuracy = 1

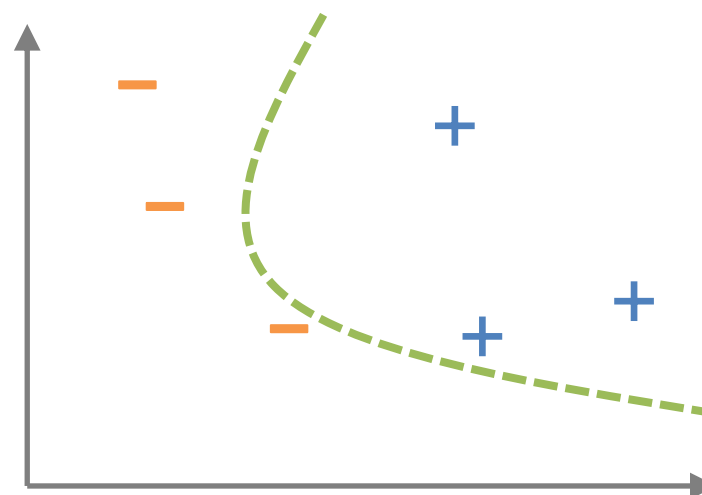Testing Accuracy = 0.5

😆 Model B
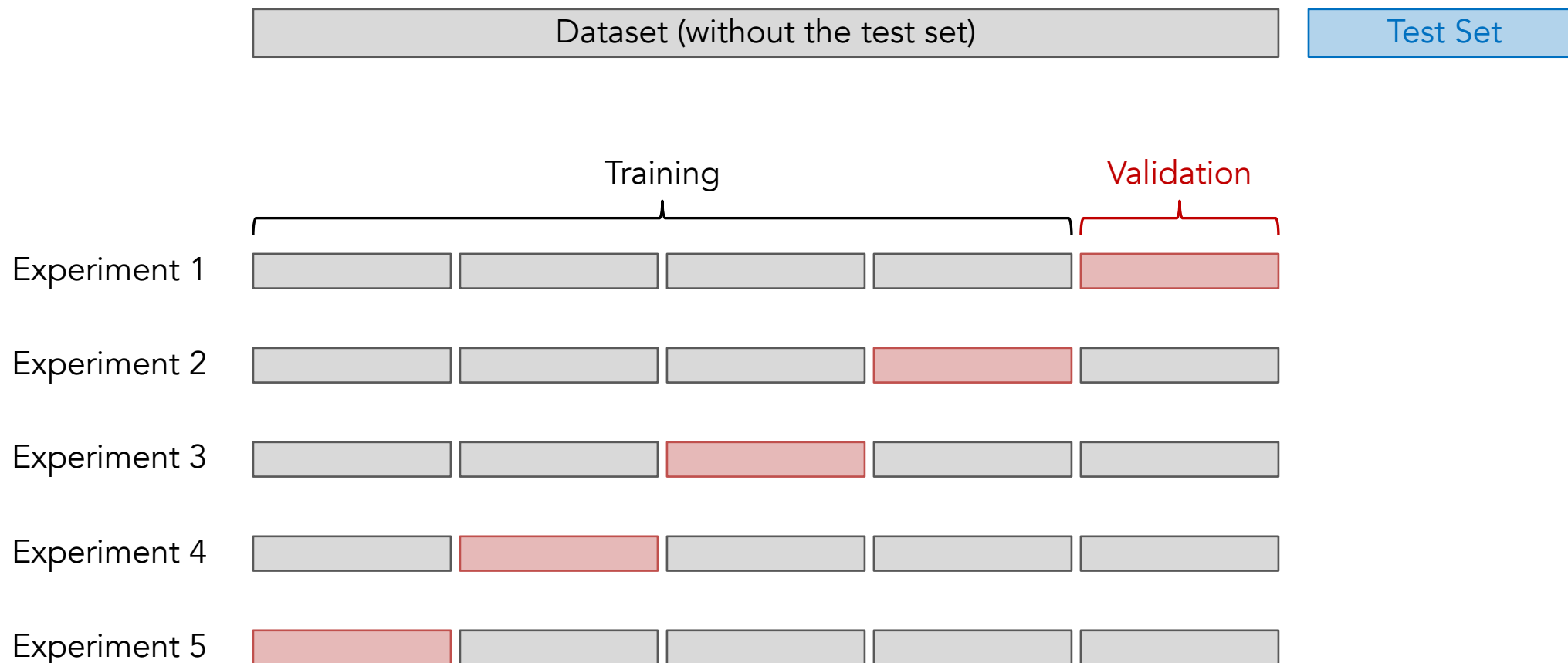

Training Accuracy = 0.86

Testing Accuracy = 1
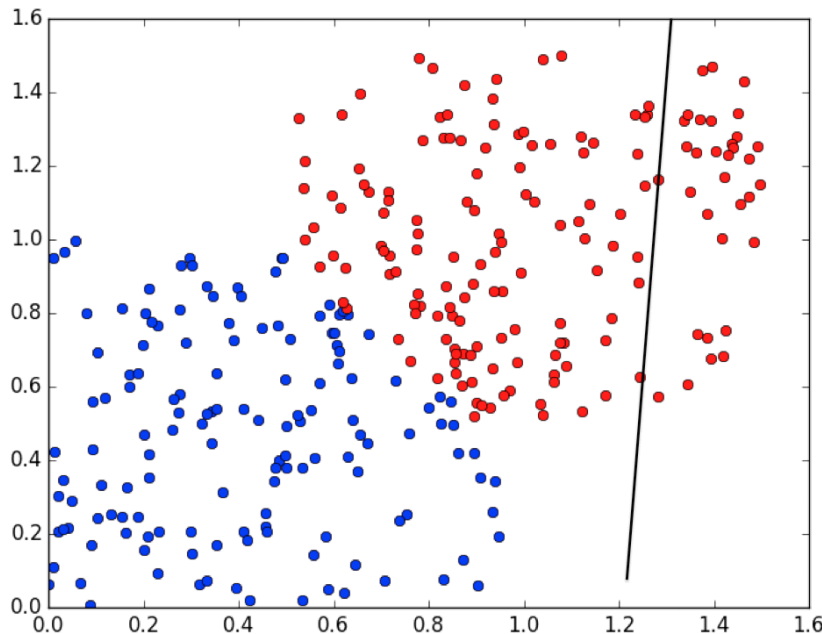
To tune hyper-parameters for a model, we use cross-validation to divide the dataset into folds and use each fold for validation.

Unlike classification (which separates data into categories), regression fits a function that maps features X to a continuous variable y (i.e., the response).

- [Classification] How can we fit a function that separates data points into different groups?
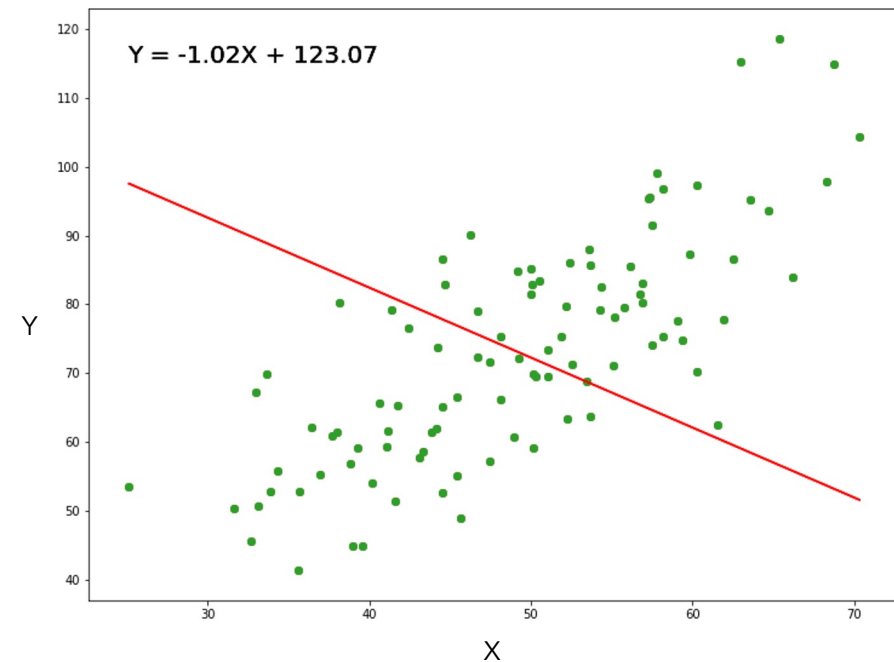
- [Regression] How can we fit a function that maps features (input) to a continuous variable (output)?

Source of Figures -- https://saichandra1199.medium.com/classification-vs-regression-622b83ff8e90

Linear regression fits a linear function that maps X to y using some error metric, which can best describe the linear relationship between variables X and y.
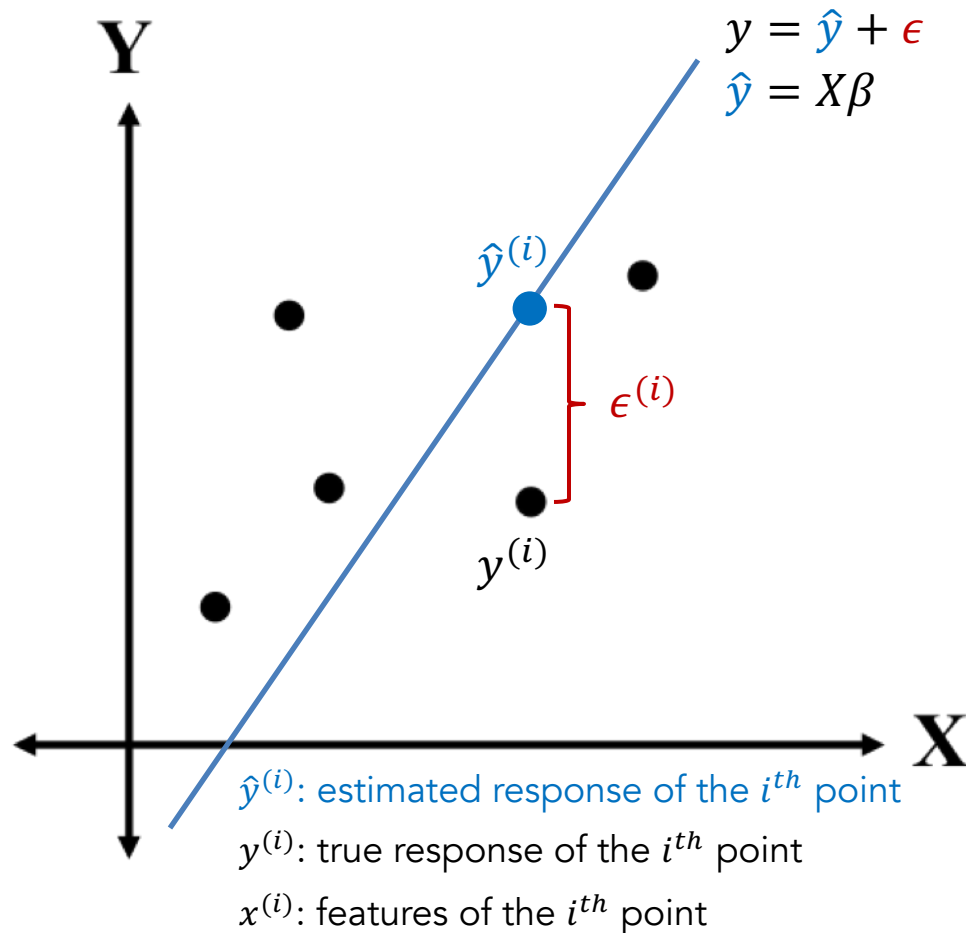

$$y = \hat{y} + \epsilon$$
$$\hat{y} = X\beta$$

$\hat{y}^{(i)}$

$\epsilon^{(i)}$

$y^{(i)}$

$\hat{y}^{(i)}$: estimated response of the ith point
$y^{(i)}$: true response of the ith point
$x^{(i)}$: features of the ith point

y: true response (in vector form)

$\hat{y}$: estimated response (in vector form)

X: predictors/features (in matrix form)

β: coefficient (in vector form)

ϵ: error/noise/residual (in vector form)

$$X = [\mathbf{1} \quad x_1] = \begin{bmatrix} 1 & x_1^{(1)} \\ \vdots & \vdots \\ 1 & x_1^{(n)} \end{bmatrix}$$

β_0: intercept
β_1: slope
x_1: first predictor

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

$$\hat{y} = X\beta = \beta_0 + \beta_1 x_1 = \begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(n)} \end{bmatrix}$$

We use the vector and matrix forms to simplify equations.

Matrix

Scalar

Vector

$$X = \begin{bmatrix} \mathbf{1} & x_1 & \cdots & x_p \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_p^{(1)} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_1^{(n)} & \cdots & x_p^{(n)} \end{bmatrix}$$

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

Vector

$$\hat{y} = f(X) = X\beta = \begin{bmatrix} \mathbf{1} & x_1 & \cdots & x_p \end{bmatrix} \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(n)} \end{bmatrix}$$
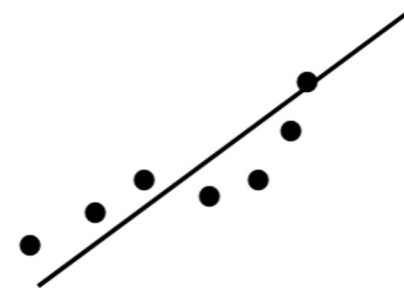
Usually, we assume that the error is IID (independent and identically distributed) and follows a normal distribution with zero mean and some variance σ^2.

$$y = \hat{y} + \epsilon$$
$$\hat{y} = X\beta$$

$$\hat{y}^{(i)}$$

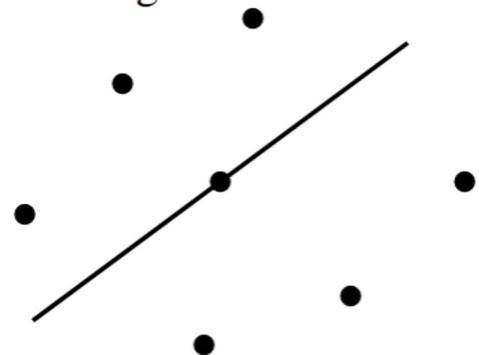$$\epsilon^{(i)} = \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

$$y^{(i)}$$
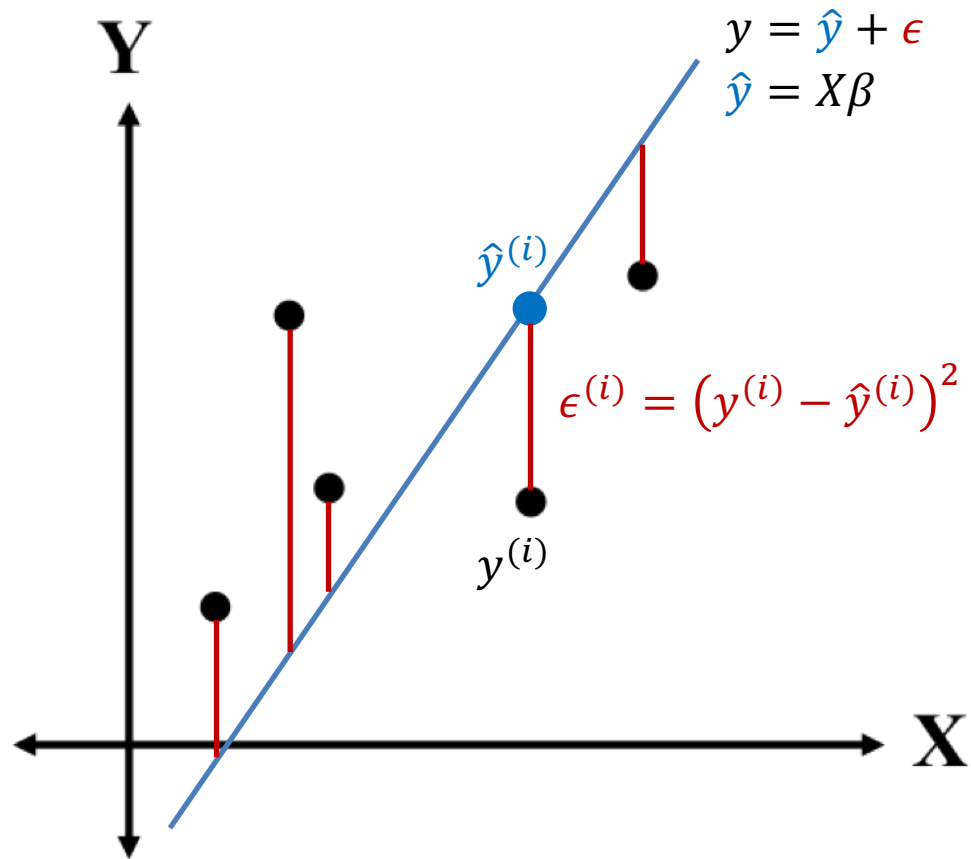
$$\epsilon \sim^{iid} N(0, \sigma^2)$$

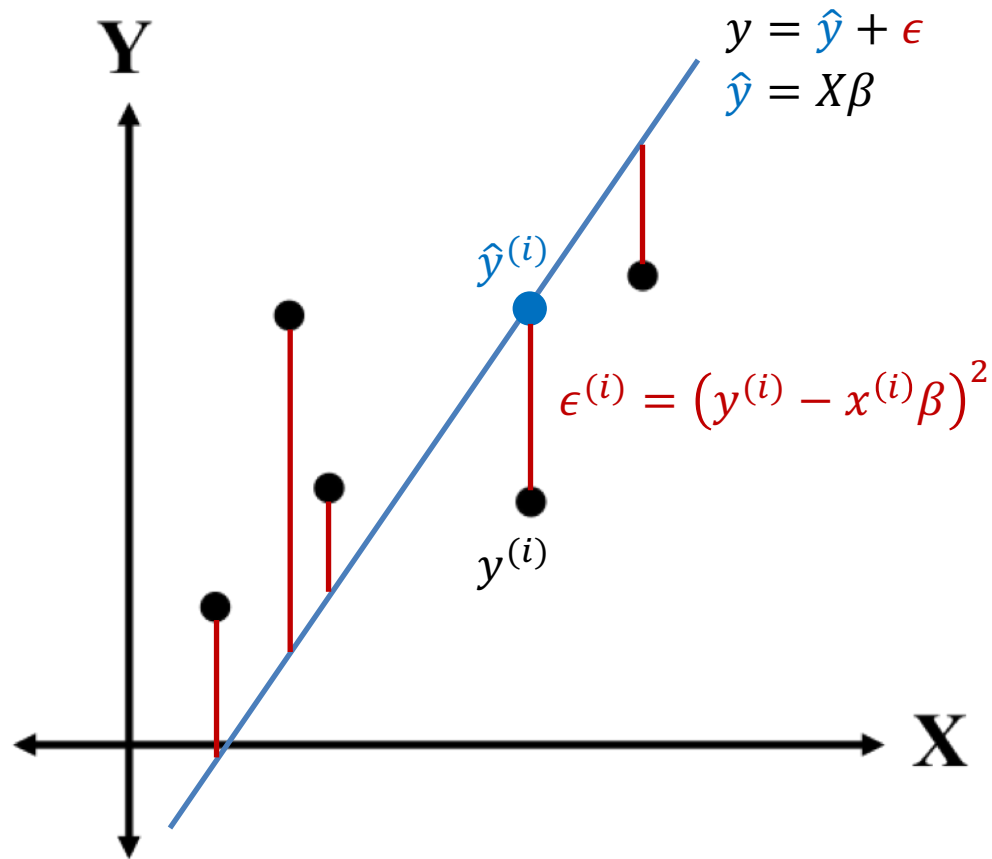$$\epsilon = \|y - \hat{y}\|_2^2 = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

Small σ^2

Large σ^2
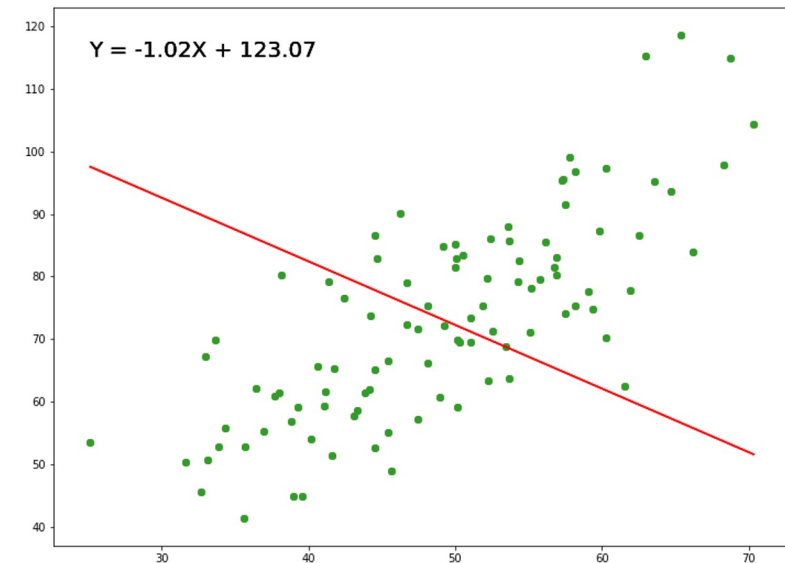
To find the optimal coefficient β, we need to minimize the error (the sum of squared error) using gradient descent or taking the derivative of its matrix form.

$$y = \hat{y} + \epsilon$$
$$\hat{y} = X\beta$$

$\hat{y}^{(i)}$

$$\epsilon^{(i)} = \left(y^{(i)} - x^{(i)}\beta\right)^2$$

$$y^{(i)}$$

$$\min_{\beta} \epsilon = \min_{\beta} \sum_{i=1}^{n} \left(y^{(i)} - x^{(i)}\beta\right)^2$$

$$= \min_{\beta} (y - X\beta)^T (y - X\beta)$$

Y = -1.02X + 123.07

More about linear regression -- https://www.stat.cmu.edu/~cshalizi/mreg/15/lectures/13/lecture-13.pdf

We can generalize linear regression to have multiple predictors (i.e., multiple linear regression) and keep the original mathematical representation.

$$y = \hat{y} + \epsilon$$
$$\hat{y} = X\beta$$
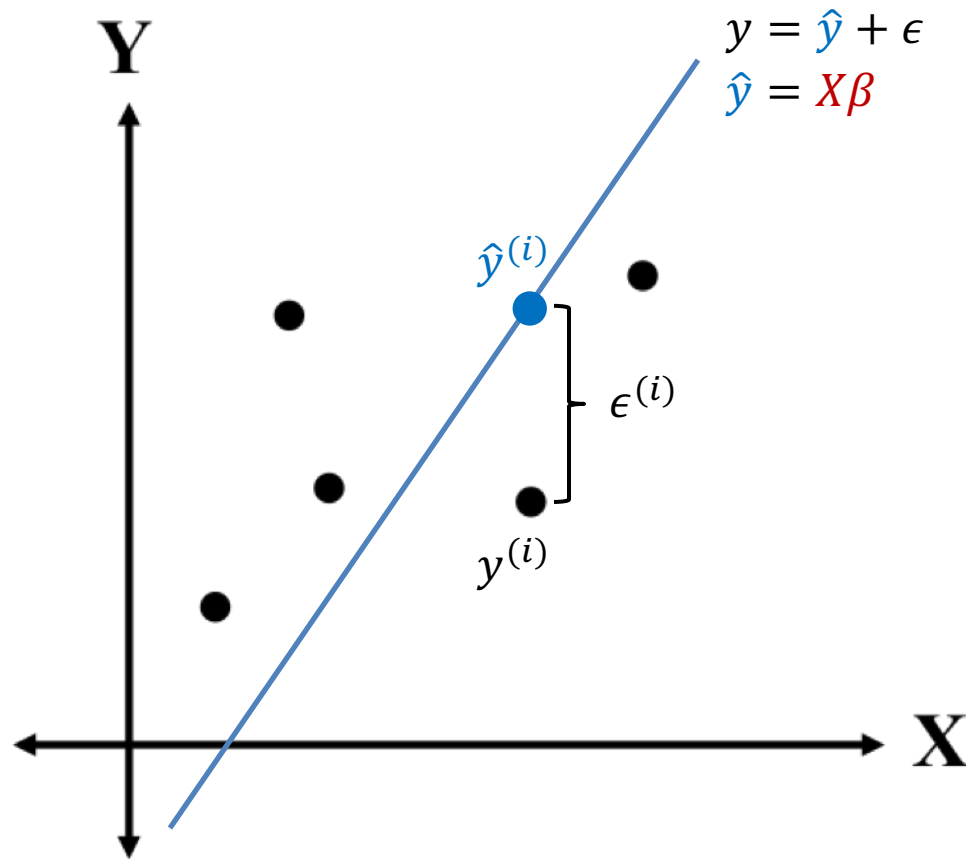
$x_j^{(i)}$: the jth predictor of the ith data point

$y^{(i)}$: response of the ith data point

$\hat{y}^{(i)}$: estimated response of the ith data point

$$X = [\mathbf{1} \quad x_1 \quad \cdots \quad x_p] = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_p^{(1)} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_1^{(n)} & \cdots & x_p^{(n)} \end{bmatrix}$$

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

$$\hat{y} = X\beta = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(n)} \end{bmatrix}$$

More about multiple linear regression -- https://www.stat.cmu.edu/~cshalizi/mreg/15/lectures/14/lecture-14.pdf

We can model a non-linear relationship using polynomial functions with degree k. The example below uses one predictor x_1.
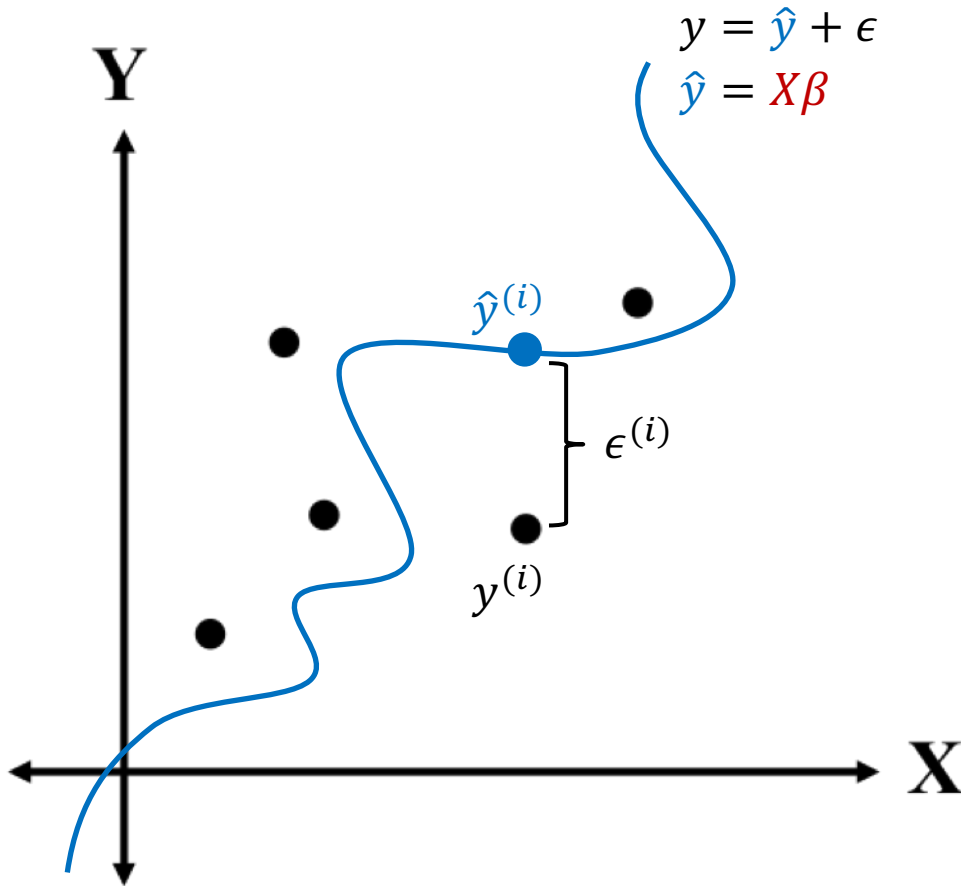
$y = \hat{y} + \epsilon$

$\hat{y} = X\beta$

y: true response (in vector form)

$\hat{y}$: estimated response (in vector form)

X: predictors/features (in matrix form)
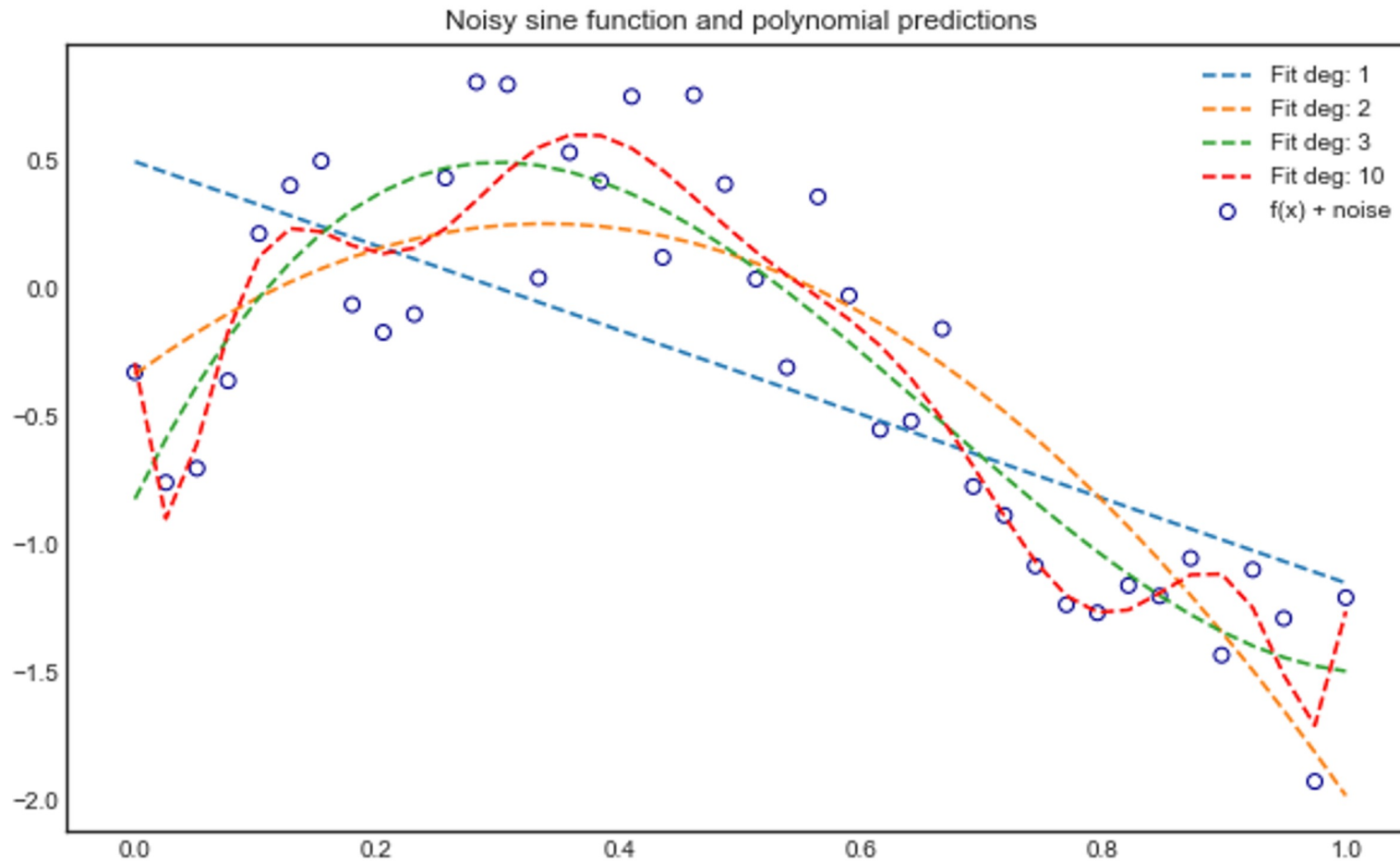
β: coefficient (in vector form)

$$X = [\mathbf{1} \quad x_1 \quad (x_1)^2 \quad \cdots \quad (x_1)^k]$$

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$$

$$\hat{y} = X\beta = \beta_0 + \beta_1 x_1 + \beta_2 (x_1)^2 + \cdots + \beta_k (x_1)^k$$

Here is an example of applying linear and polynomial regression to the data that is created using a sine function with some random noise.


Noisy sine function and polynomial predictions

Legend:
- Fit deg: 1
- Fit deg: 2
- Fit deg: 3
- Fit deg: 10
- f(x) + noise

Using too complex/simple models can lead to overfitting/underfitting, which means the model fits the training set well but generalizes poorly on the test set.
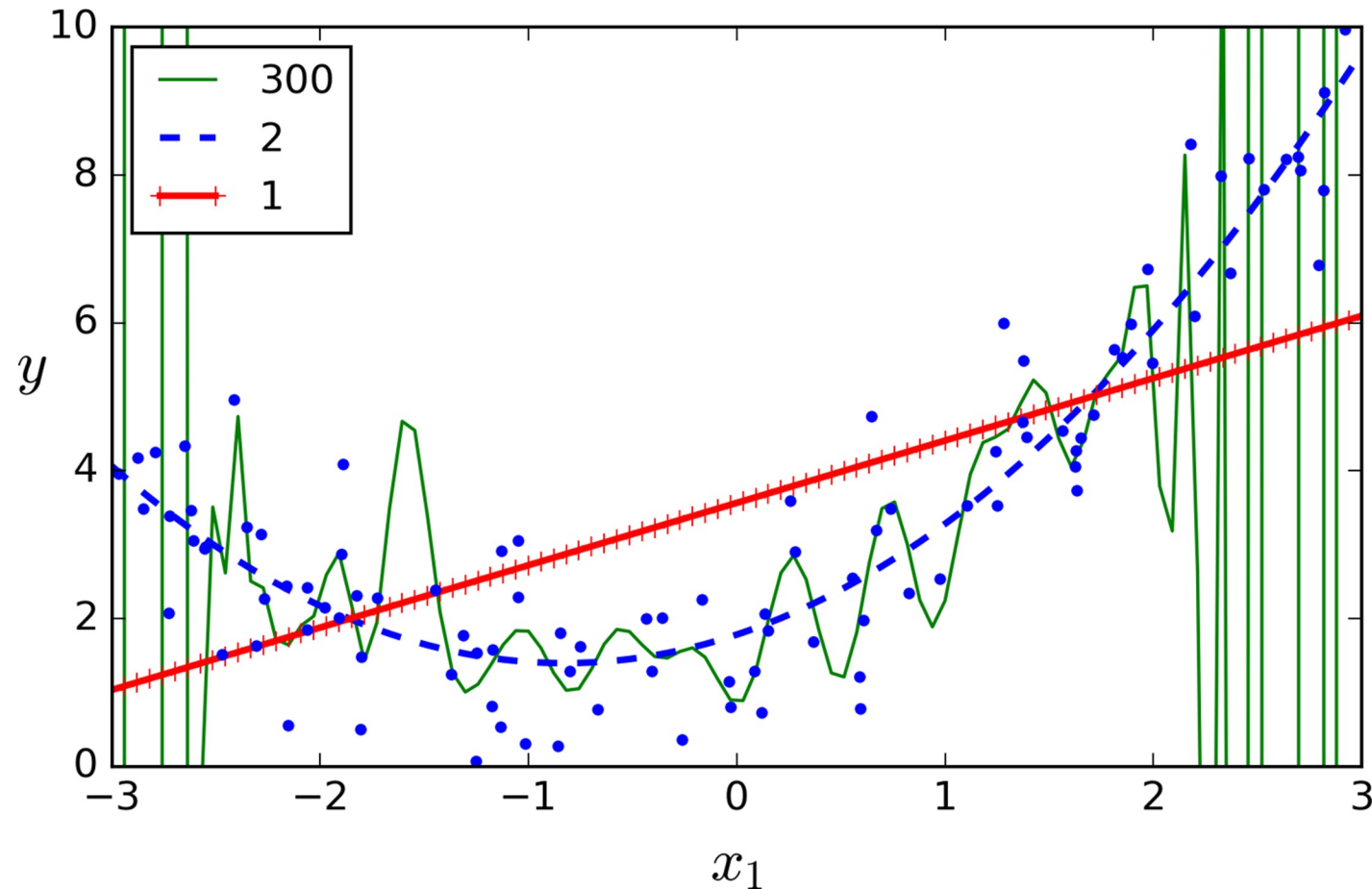
To evaluate regression models, one common metric is the coefficient of determination (R-squared, R^2). There exist other metrics such as AIC (Akaike's Information Criterion) that is based on likelihood, which is not covered in this lecture.
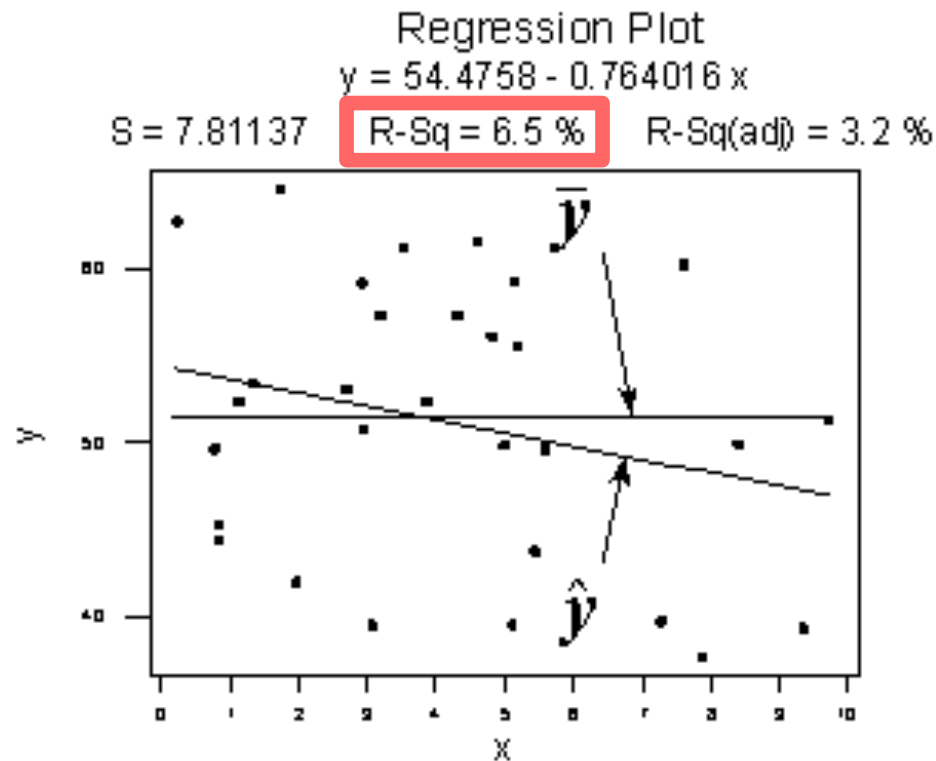

Total sum of squares (SS_{tot})
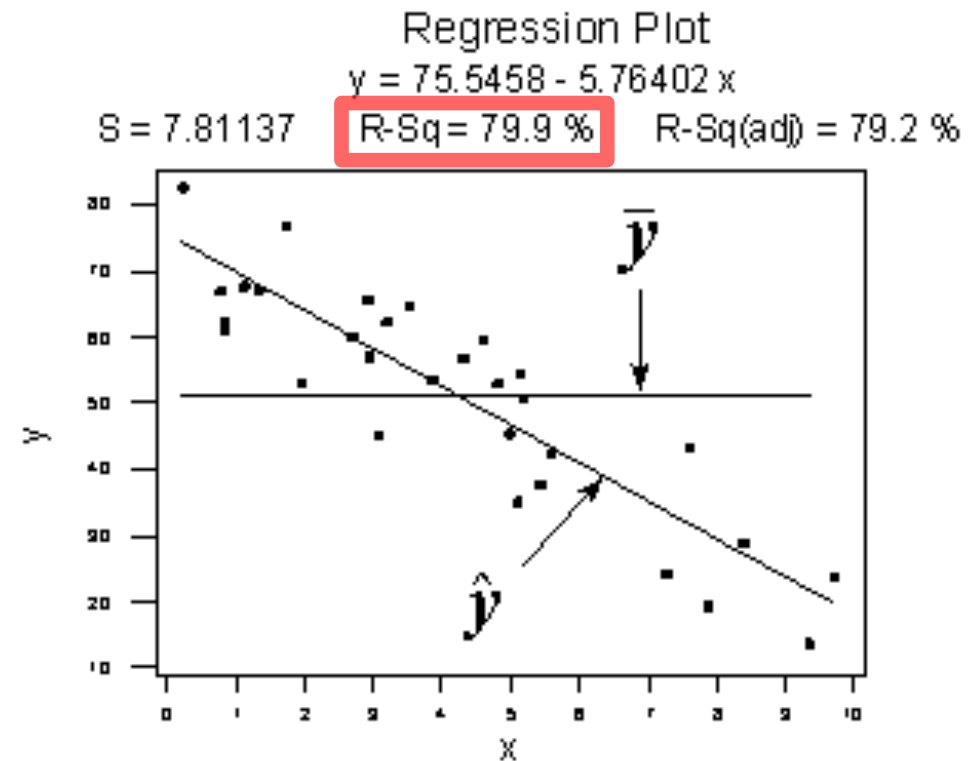
Residual sum of squares (SS_{res})
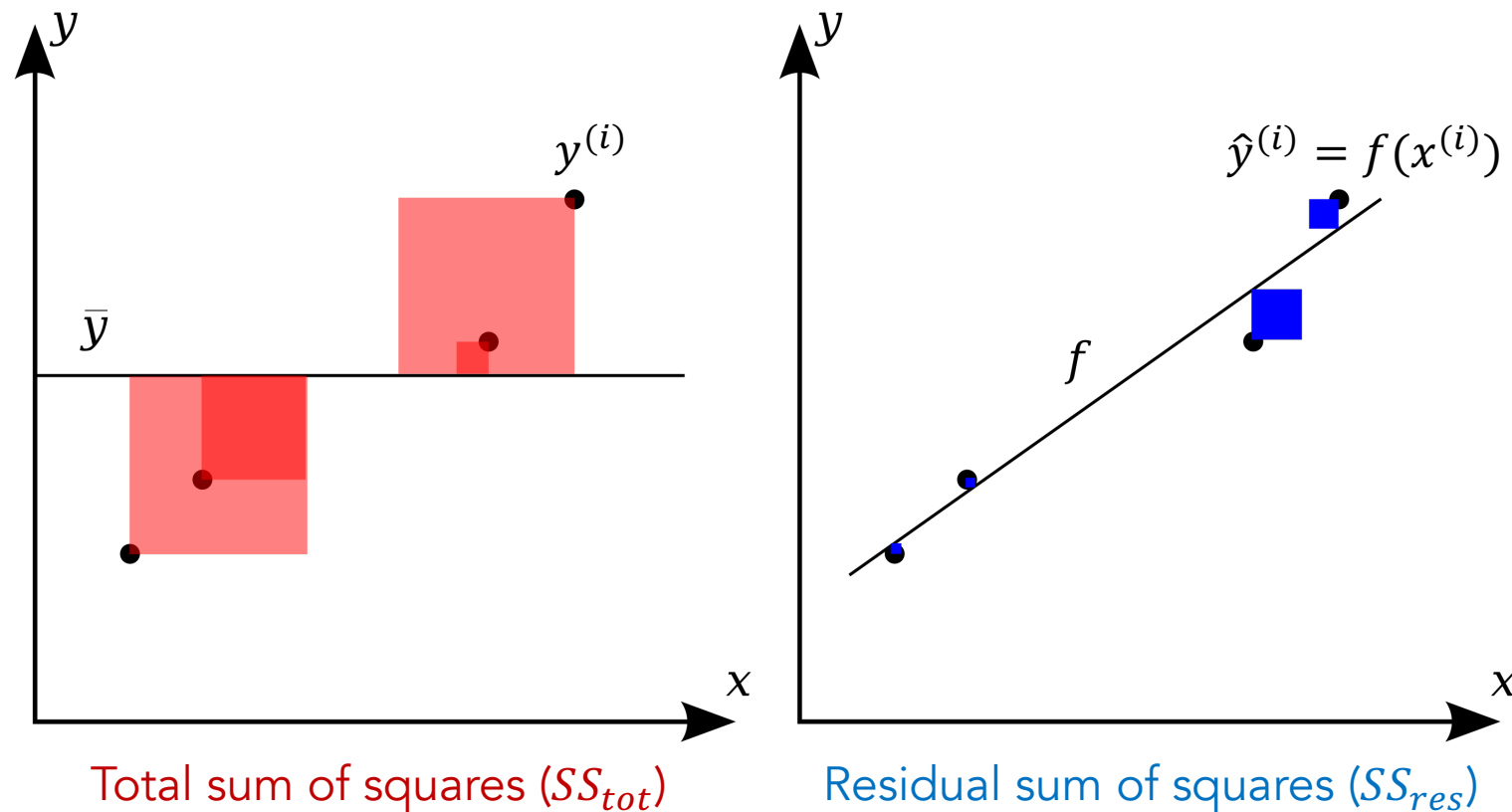
Unexplained Variation

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

$$SS_{res} = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

$$SS_{tot} = \sum_i \left(y^{(i)} - \bar{y}\right)^2$$

Figure Source -- https://en.wikipedia.org/wiki/Coefficient_of_determination

For simple/multiple linear regression, R^2 equals the square of Pearson correlation coefficient r between the true y and the estimated $\hat{y} = f(X)$.

Lower Correlation

Higher Correlation

More about the Coefficient of Determination -- https://online.stat.psu.edu/stat501/lesson/1/1.5

R^2 increases as we add more predictors (because the optimization always want to decrease the residual sum of squares) and thus is not a good metric for model selection. We need the adjusted R^2, which considers the number of predictors.

$$R^2_{adj} = 1 - \frac{SS_{res}/df_{res}}{SS_{tot}/df_{tot}}$$

$df_{res} = n - p - 1$

$df_{tot} = n - 1$

$$SS_{res} = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

$$SS_{tot} = \sum_i \left(y^{(i)} - \bar{y}\right)^2$$
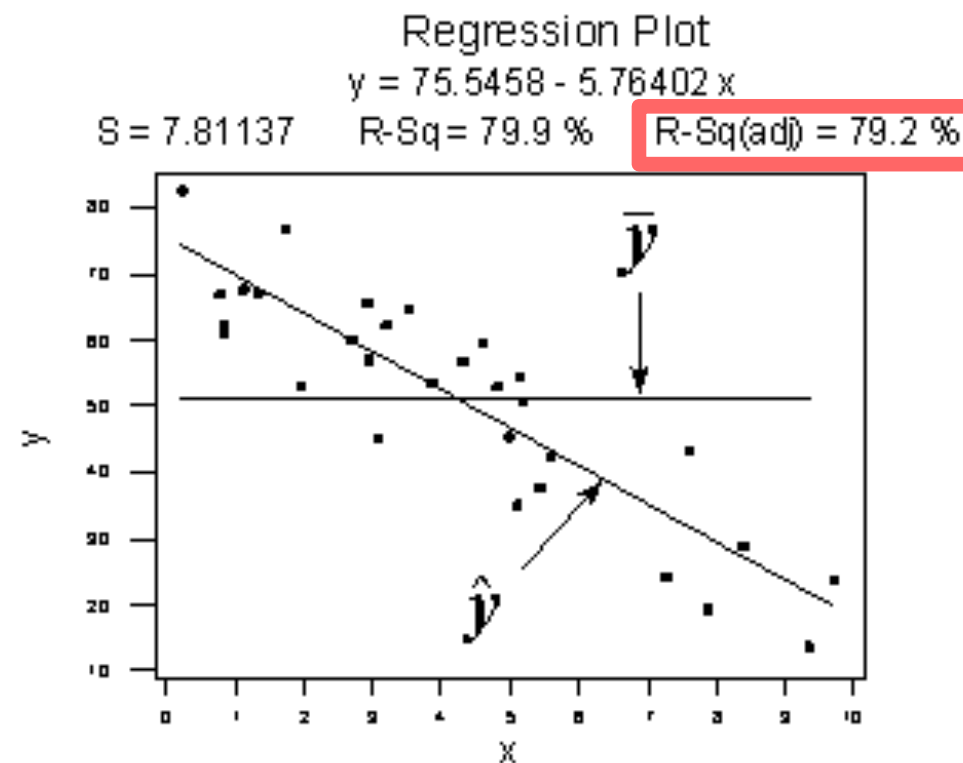
p: number of features/predictors

R^2_{adj}: adjusted value of R^2

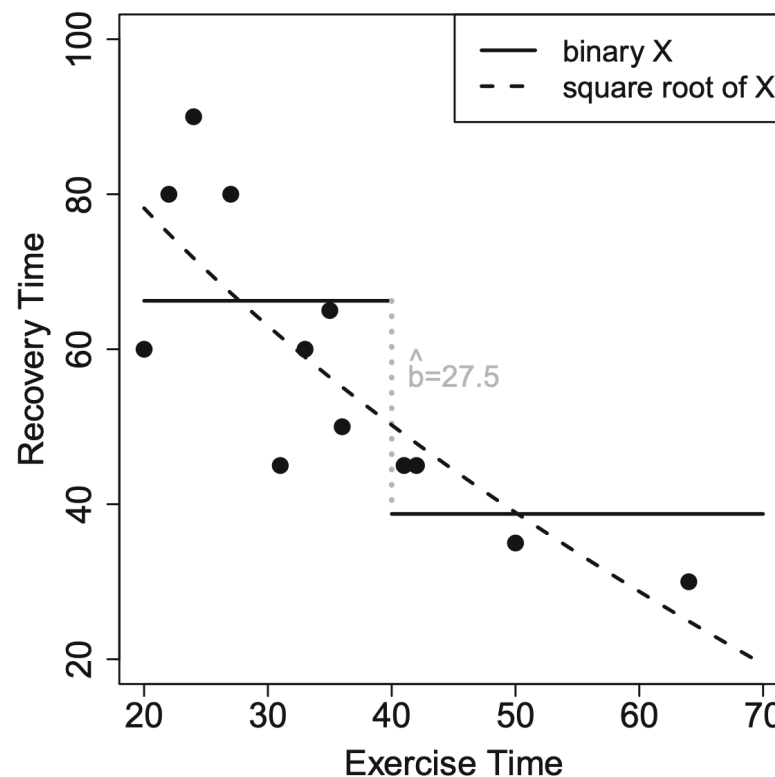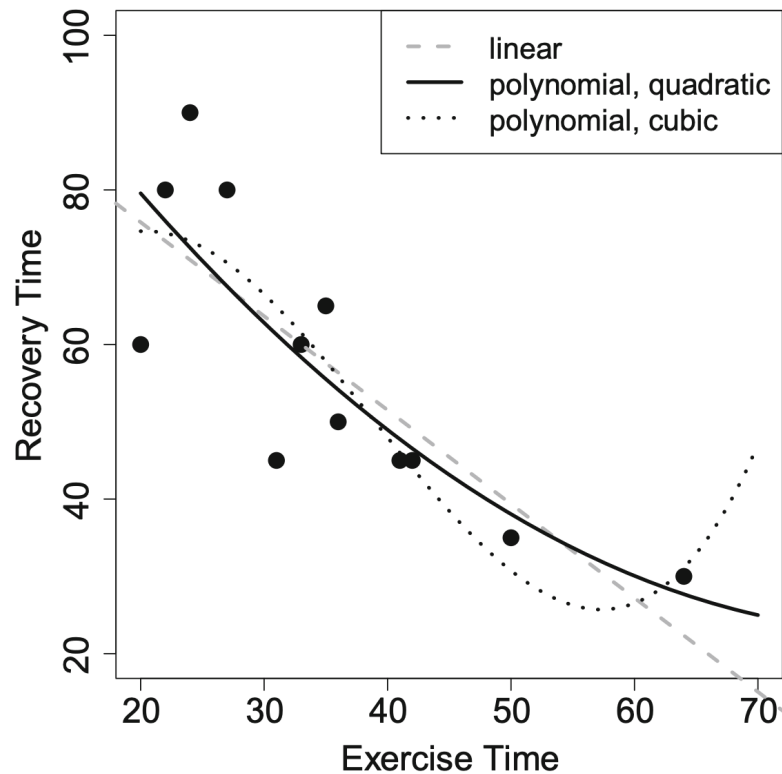df_{res}: residual degree of freedom

df_{tot}: total degree of freedom

SS_{res}: residual sum of squares

SS_{tot}: total sum of squares

Regression Plot
y = 75.5458 - 5.76402 x
S = 7.81137   R-Sq = 79.9 %   R-Sq(adj) = 79.2 %

More about the adjusted Coefficient of Determination -- https://online.stat.psu.edu/stat501/lesson/10/10.3

In the example below, R^2 is larger for the model with more predictors (i.e., the cubic model that has three predictors). The adjusted R^2, which considers the number of predictors (model complexity), favors the the square-root model.

	R^2	R^2_{adj}
Linear	0.6584	0.6243
Quadratic	0.6787	0.6074
Cubic	0.7151	0.6083
Square root	0.6694	0.6363

This example is from section 11.8 Comparing Different Models in book: Introduction to Statistics and Data Analysis

Be careful when using and explaining R^2 in your findings. A bad R^2 does not always mean no pattern in the data. A good R^2 does not always mean that the function fits the data well. And R^2 can be greatly affected by outliers.
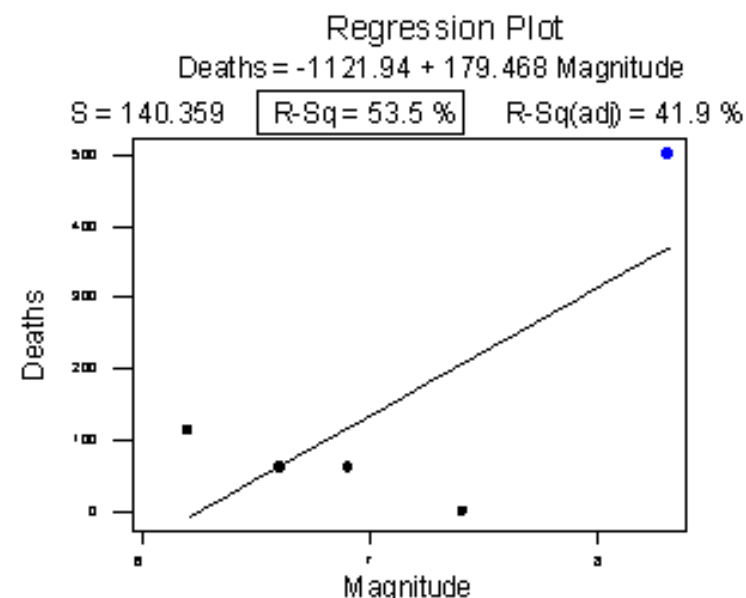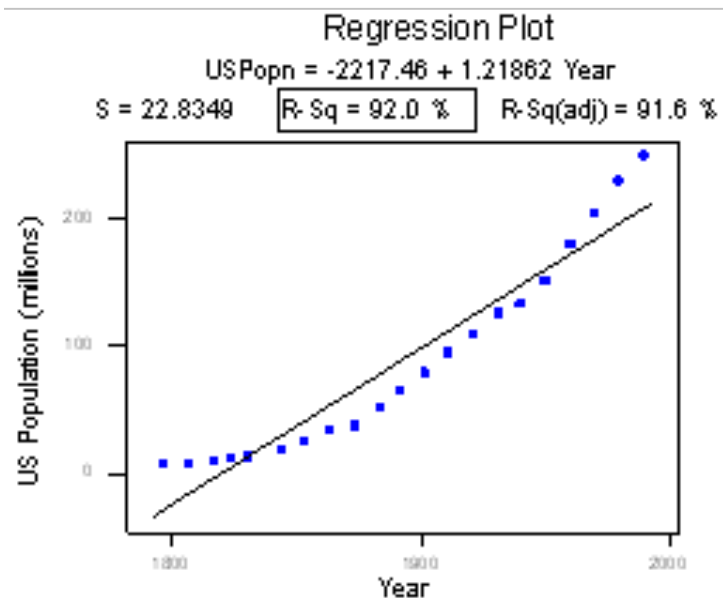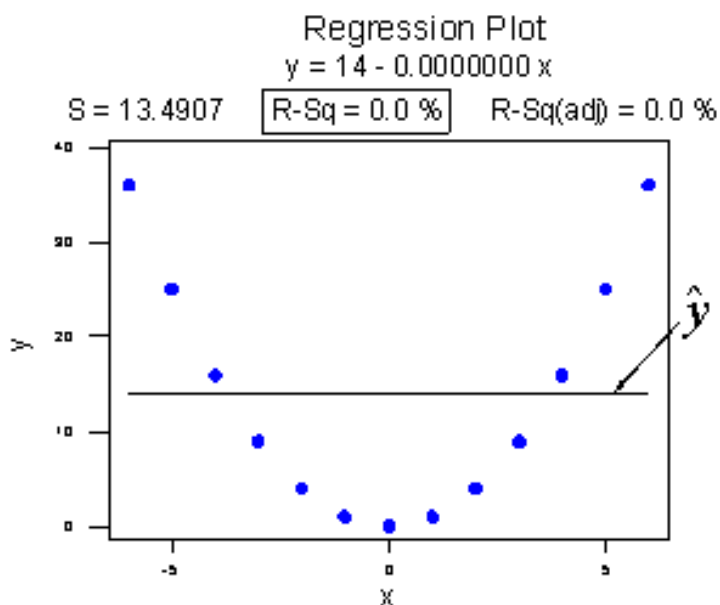
Take-Away Messages

- Classification outputs discrete labels, while regression outputs continuous values.

- Precision, recall, and F-score are common metrics for evaluating classification models.

- R-squared is a common evaluation metric for regression models.

- Feature engineering is an important step for models that do not use deep learning techniques.

- To train and update a model iteratively, you need a loss function to measure errors.

- Generally, it is a good practice to divide datasets into different parts for model training and testing.

- A model can perform extremely well on the training set but badly on the test set (i.e., overfitting).

- Cross-validation is a good technique to prevent overfitting.

Questions?