Data Science

Lecture 2-2: Data Science Fundamentals (Modeling)

UNIVERSITY OF AMSTERDAM

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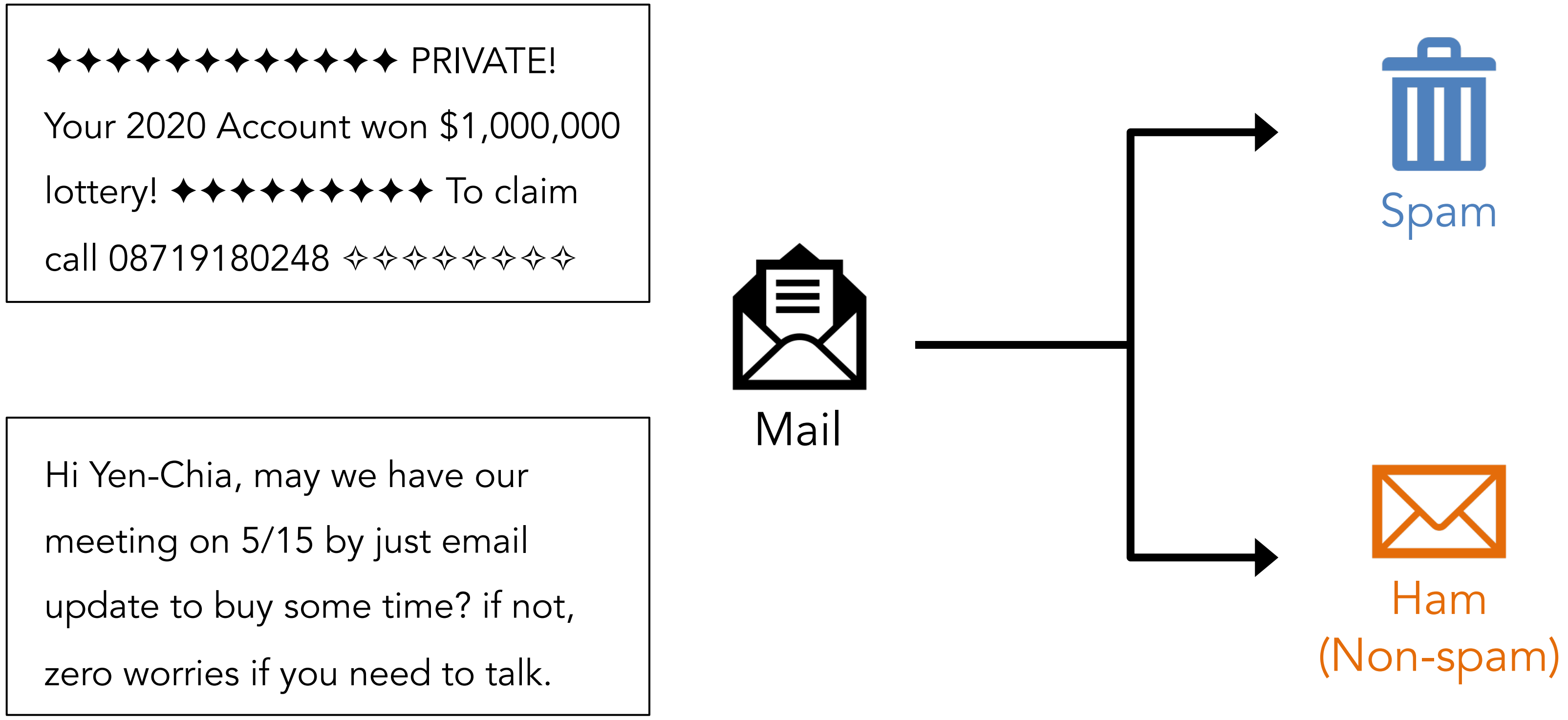
Date: Sep 2025

This lecture introduces classification and regression techniques for modeling data.

Classification 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)

Classification

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

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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

Classification

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

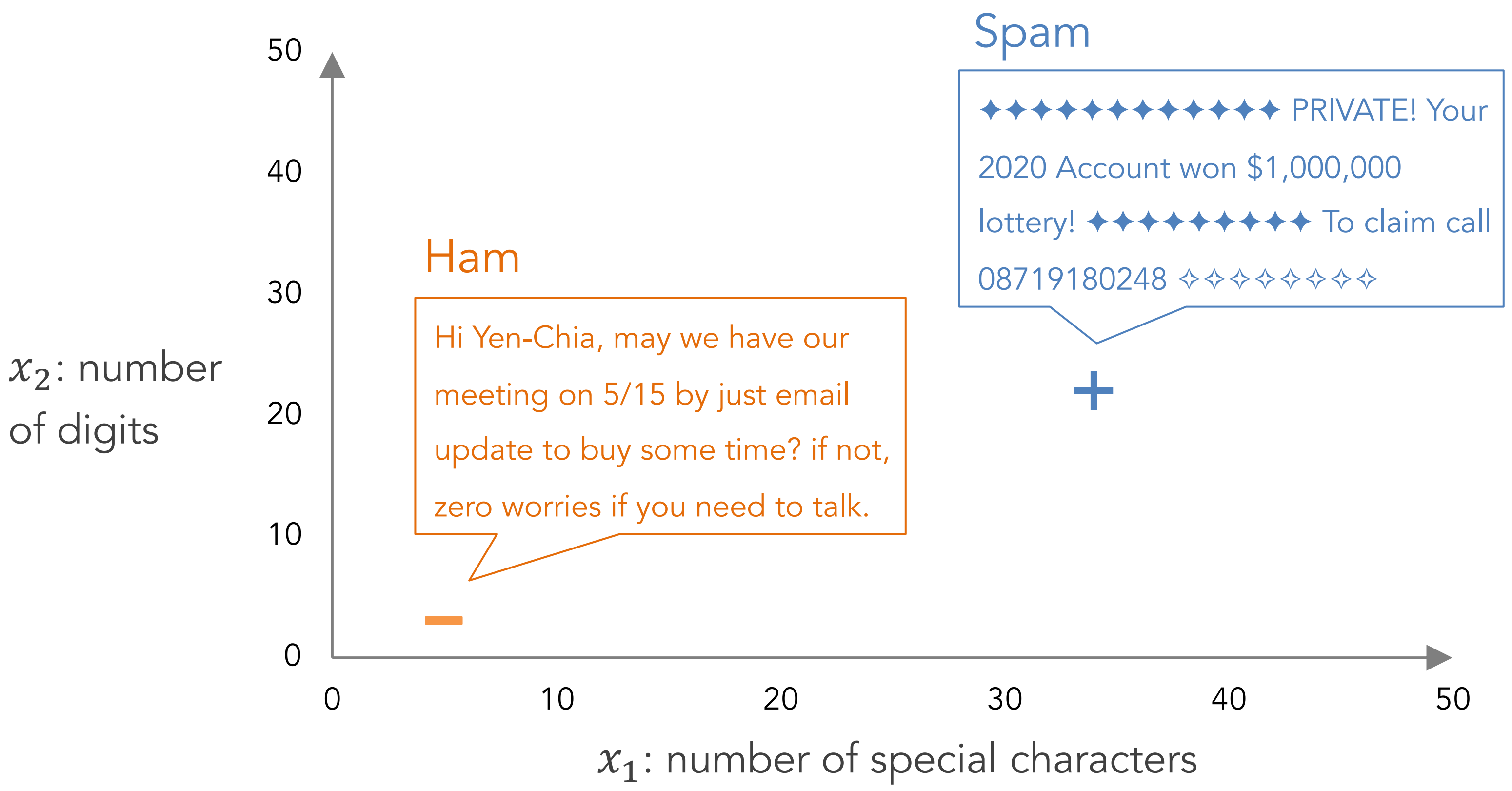
Hi Yen-Chia, may we have our meeting on 5/15 by just email update to buy some time? if not, zero worries if you need to talk.

Number of special characters = 5
Number of digits = 3

Ham

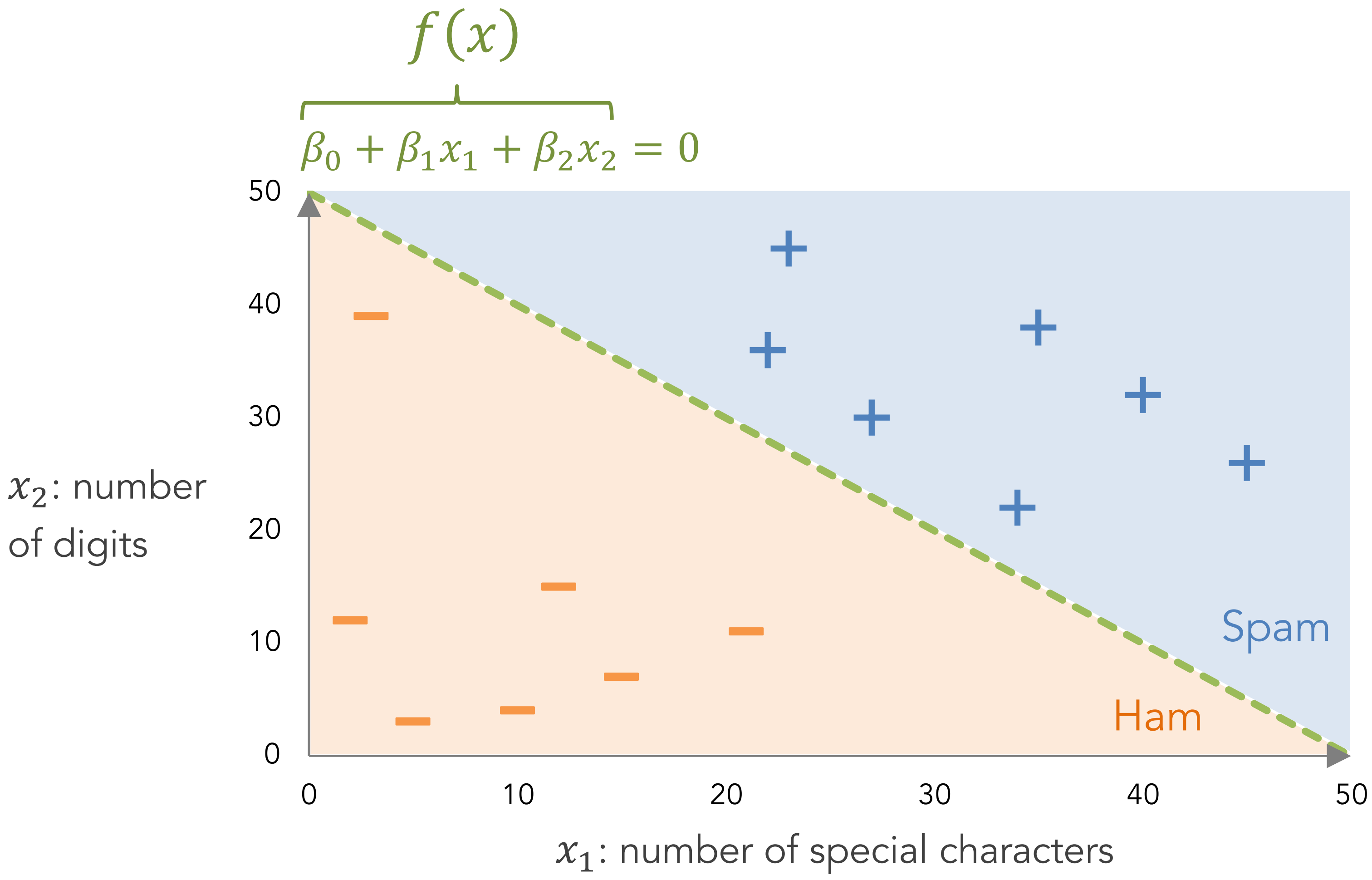
Classification

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

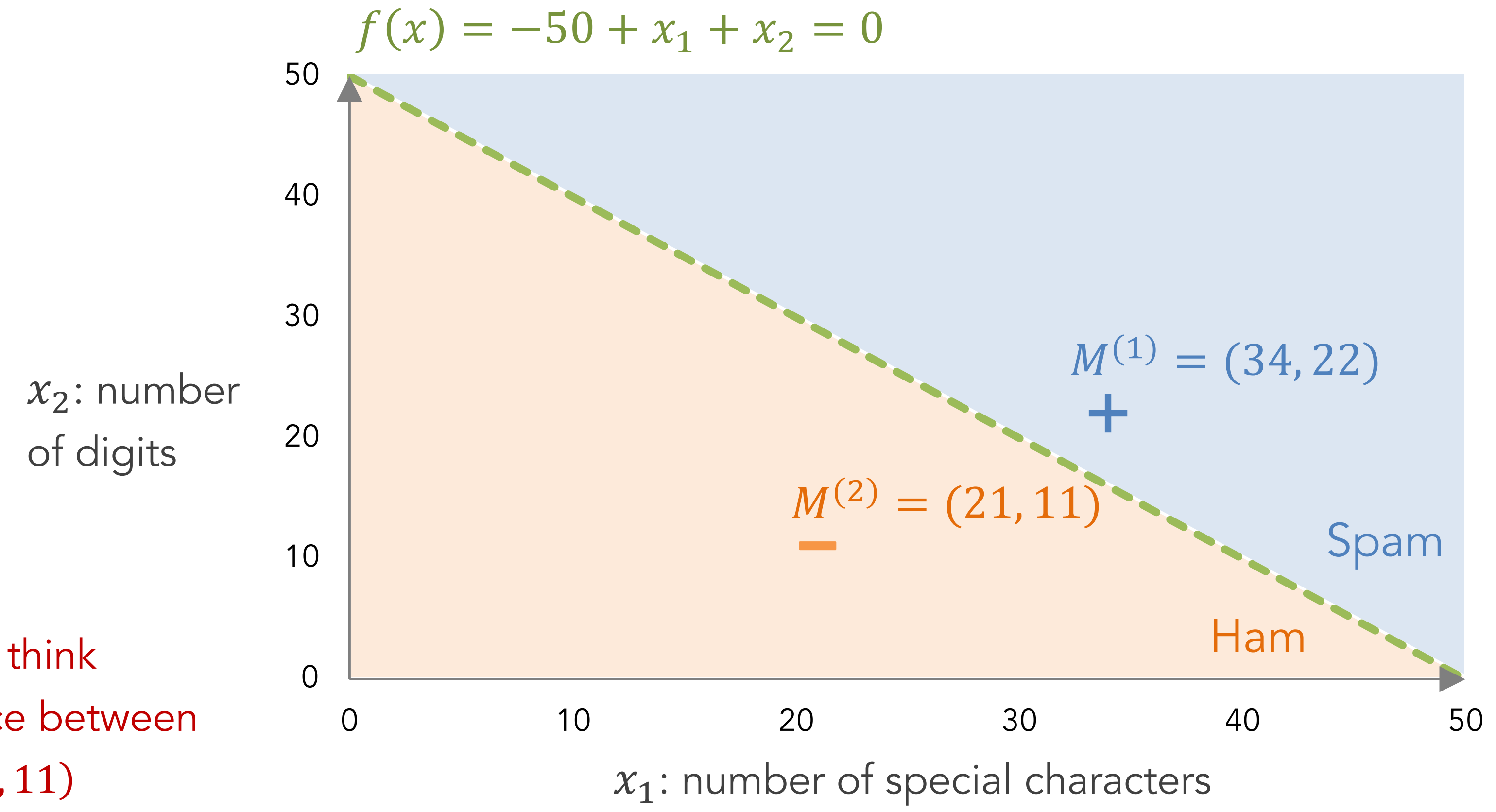


Classification

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 $x = \{x_1, x_2\}$.



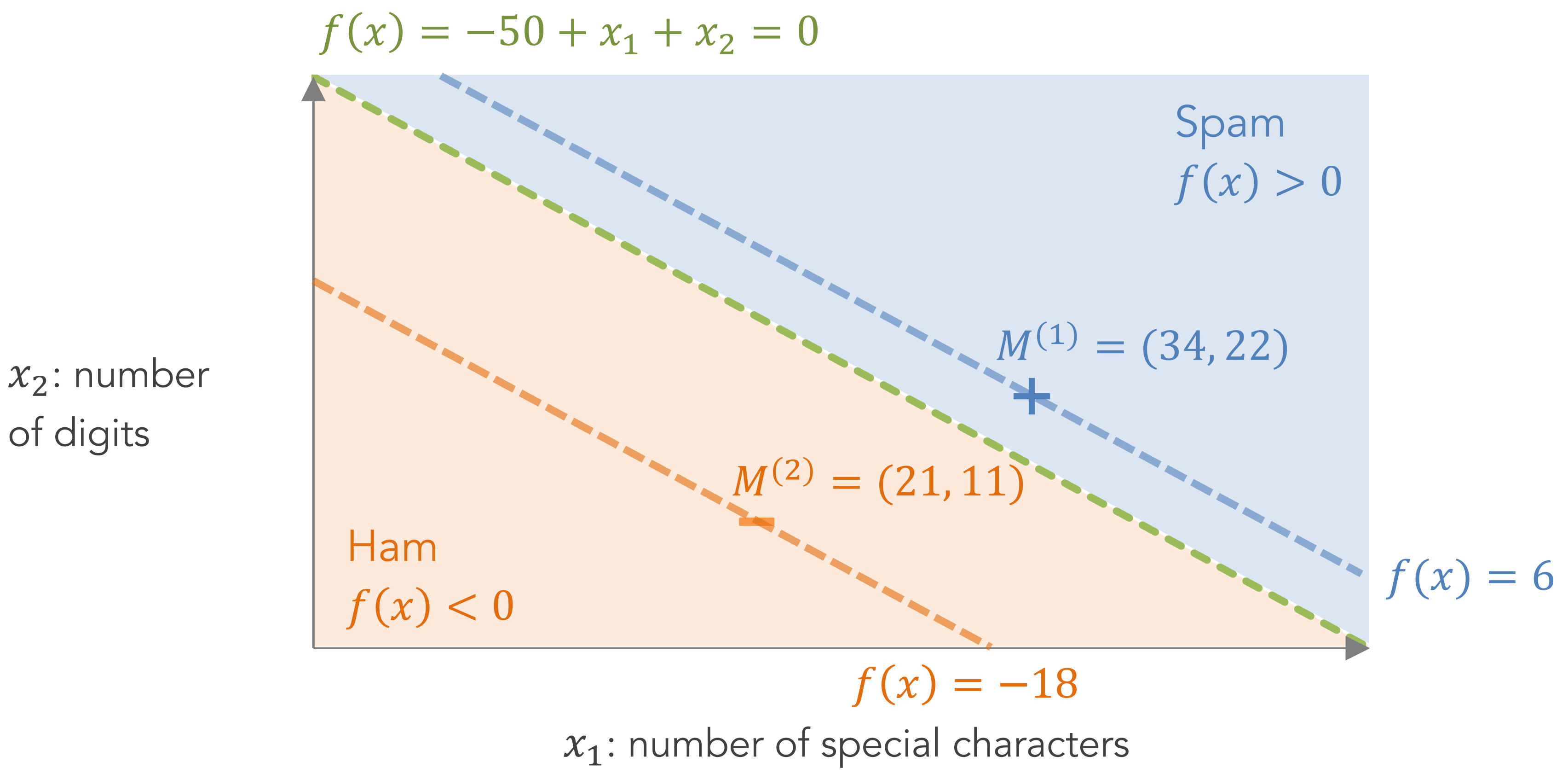
Exercise 2.1: Given a classifier $f(x) = -50 + x_1 + x_2$ and two messages $M^{(1)}$ and $M^{(2)}$, explain how the model classifies the message as spam or ham mathematically. $M^{(1)}$ has 34 special characters and 22 digits. $M^{(2)}$ has 21 special characters and 11 digits.



Hint: calculate and think about the difference between $f(34, 22)$ and $f(21, 11)$

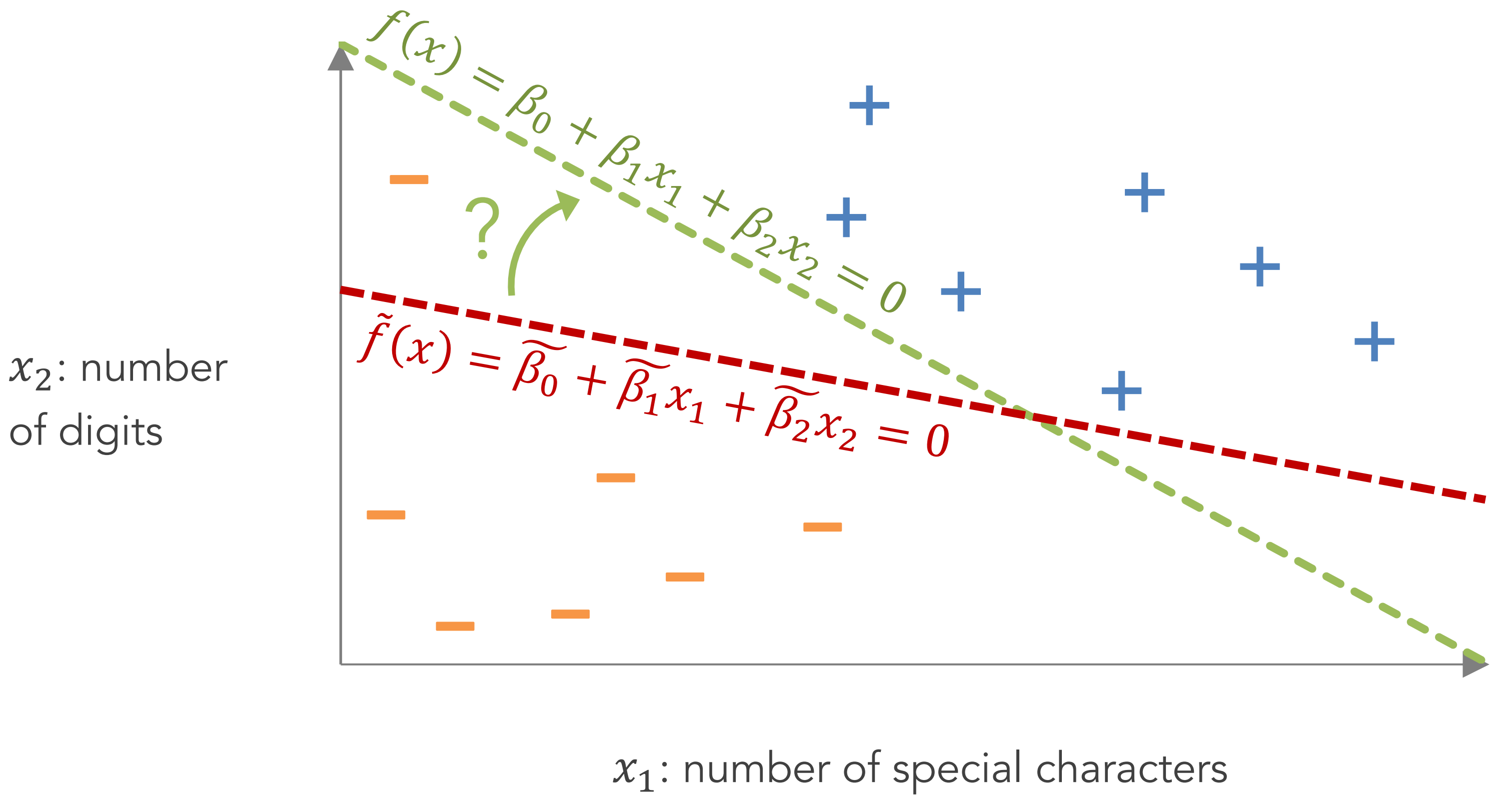
Classification

We can plug the features $x = \{x_1, x_2\}$ into the classifier equation $f(x)$ to determine if it is spam or ham by checking if $f(x)$ is larger or smaller than zero. The intuition is to shift the linear classifier to the position that matches the features.



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.



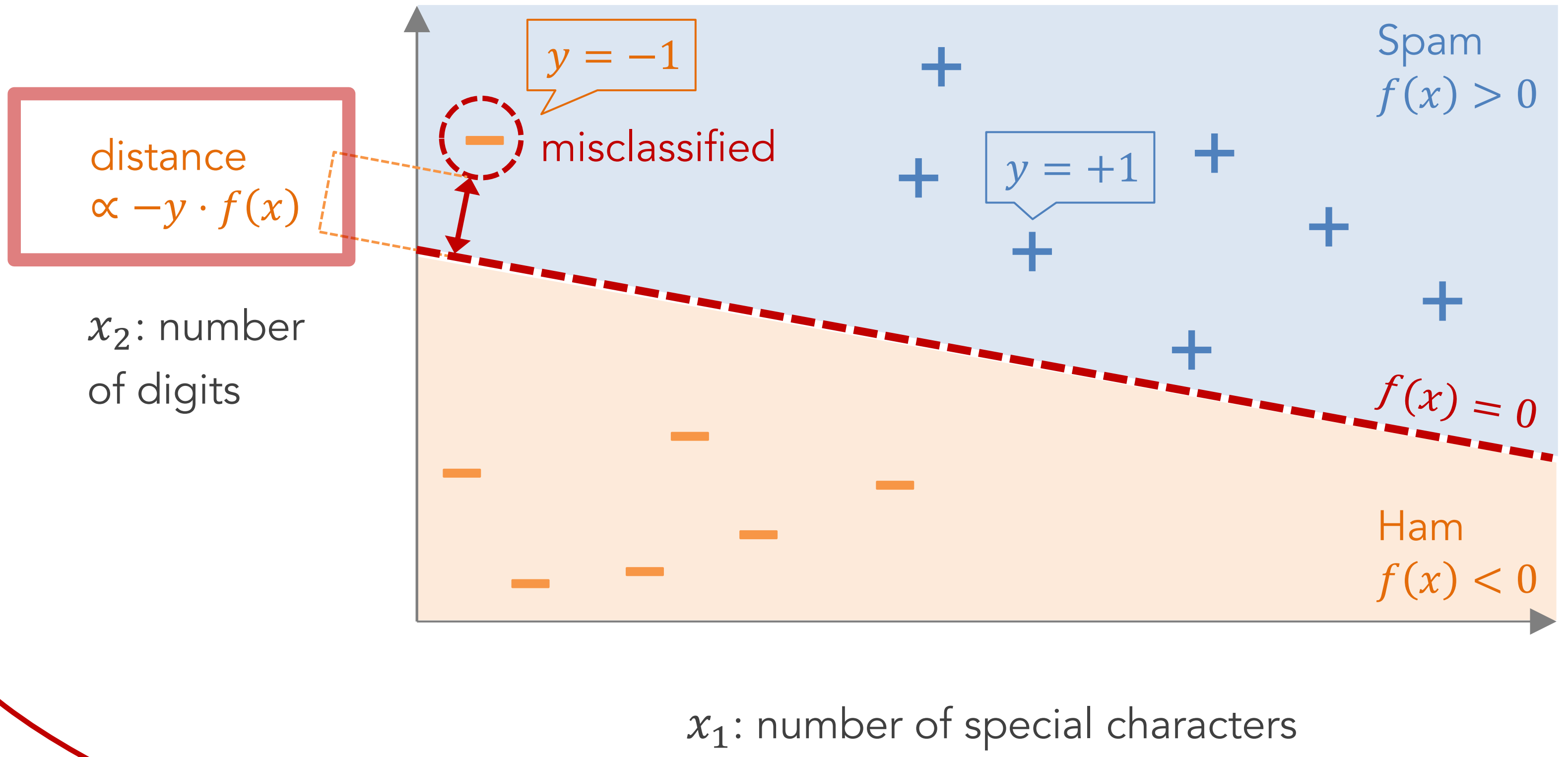
$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 = 0$
?
$\tilde{f}(x) = \widetilde{\beta_0} + \widetilde{\beta_1} x_1 + \widetilde{\beta_2} x_2 = 0$
x_2: number of digits
x_1: number of special characters

Classification

First, we need an error metric (i.e., cost or objective function). For example, we can use the sum of distances between the misclassified points and line f.

$$\text{error} = \sum -y \cdot f(x) \quad \text{for each misclassified point } x = \{x_1, x_2\}$$

Why?

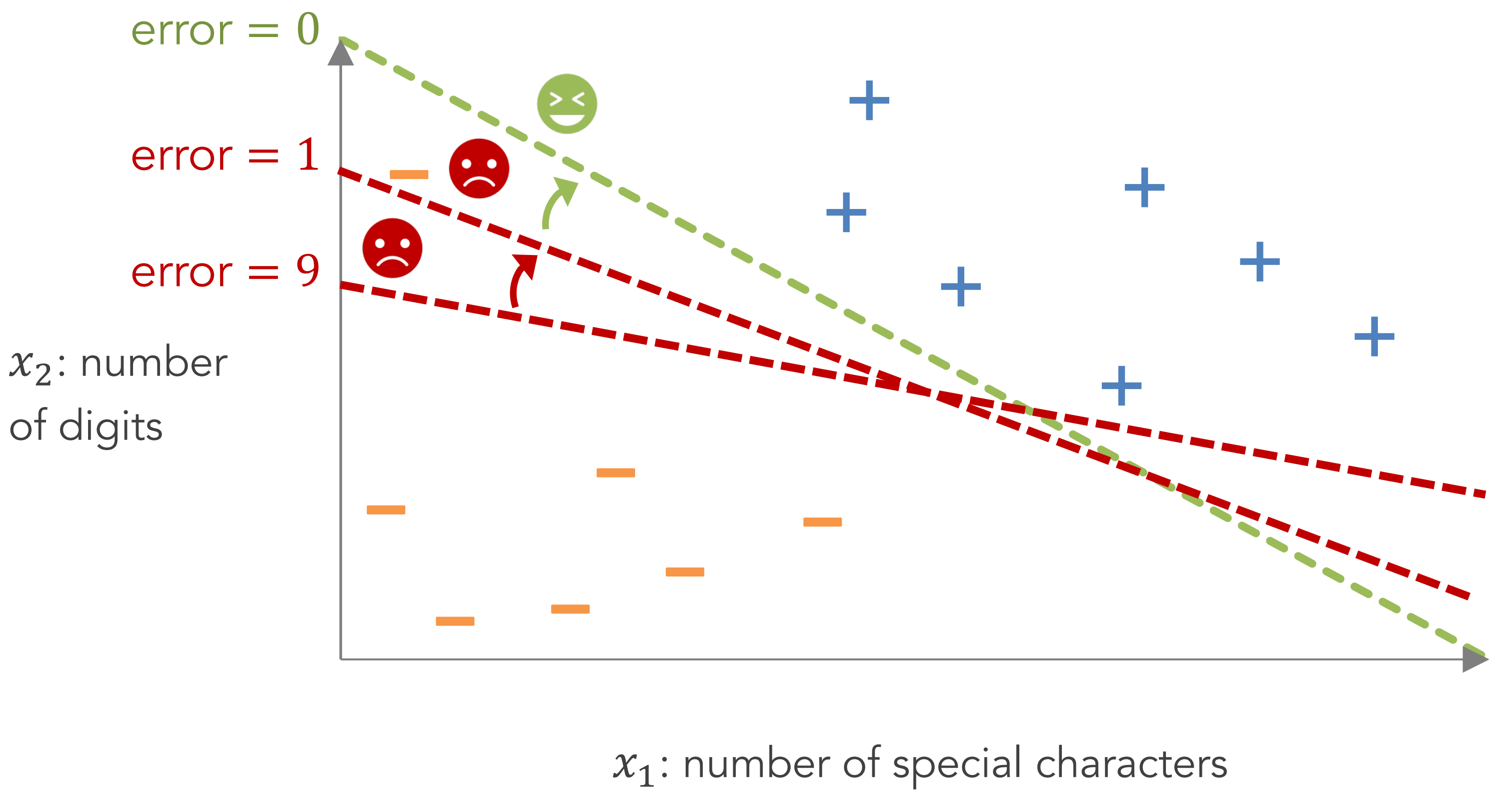


Distance from point to plane: https://mathinsight.org/distance_point_plane

Classification

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

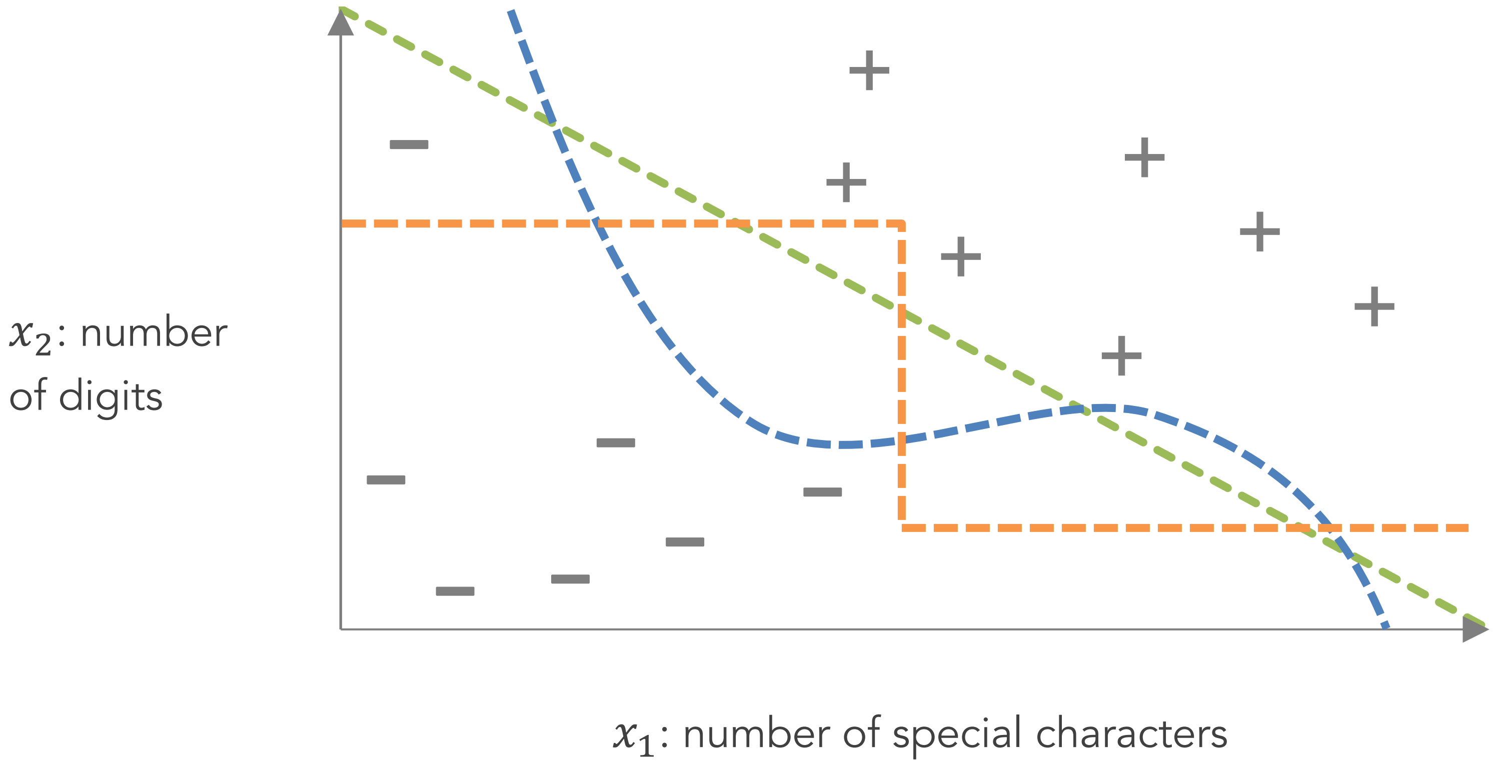
minimize error = $\sum -y \cdot f(x)$ for each misclassified point $x = \{x_1, x_2\}$



Rosenblatt's Perceptron Learning Algorithm: section 4.5.1 in book https://hastie.su.domains/ElemStatLearn/

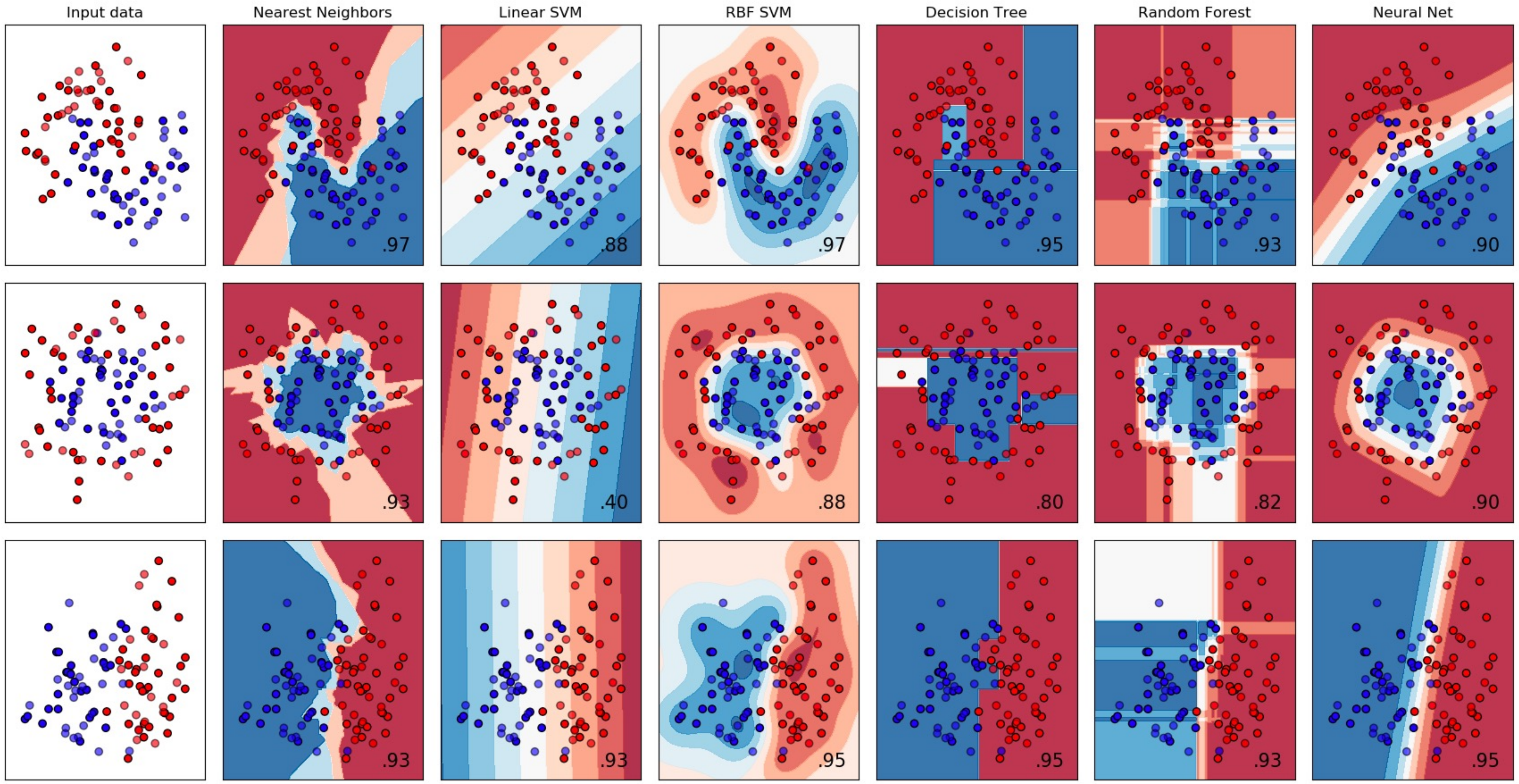
Classification

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



Classification

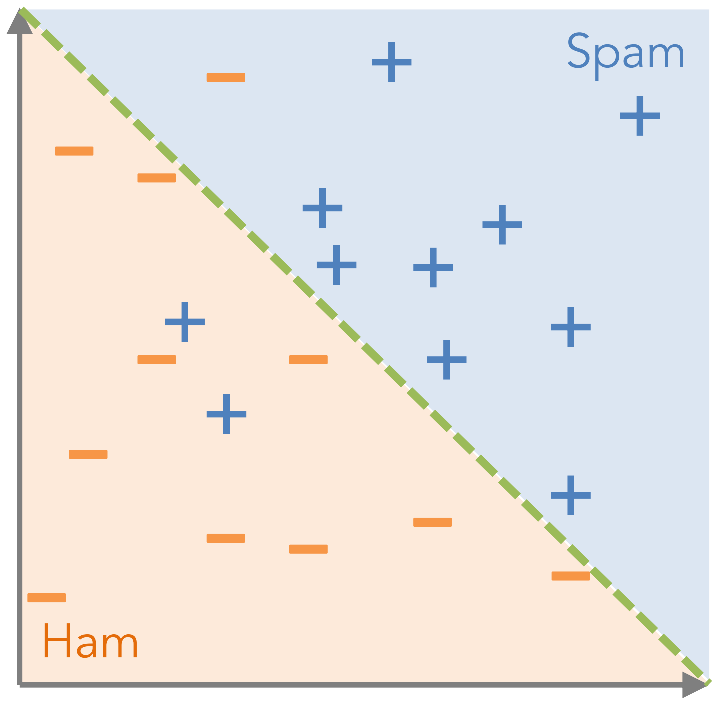
Depending on the needs, we can train different models (using different loss functions) with various shapes of decision boundaries.



Retrieved from https://scikit-learn.org/stable/auto_examples/#classification

Classification

To evaluate our classification model, we need to compute evaluation metrics to measure and quantify model performance, such as the accuracy of all data.



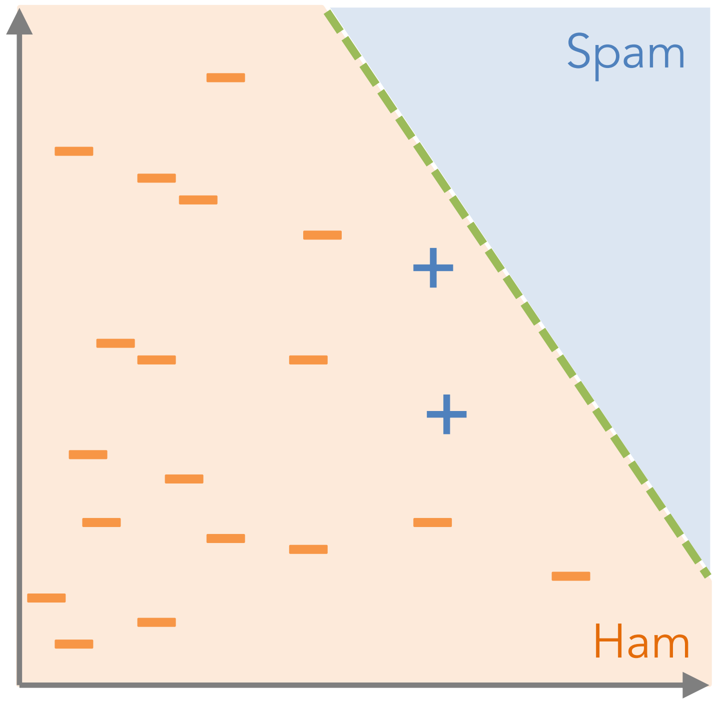
Accuracy for all data

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

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

Classification

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



Classify all data as non-spam

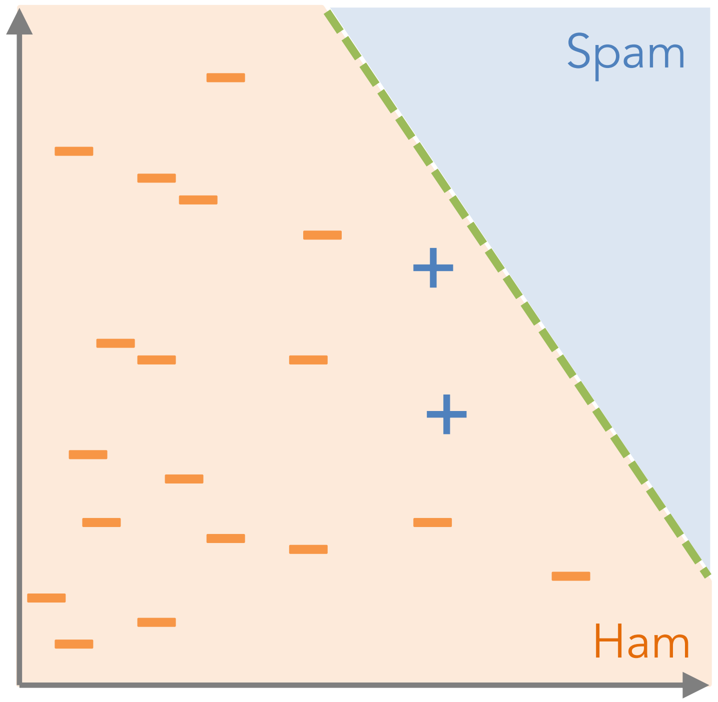
Accuracy for all data

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

$$= \frac{18}{20} = 0.9$$ 😕

Classification

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

$$\text{Accuracy for spam} = \frac{0}{2} = 0$$

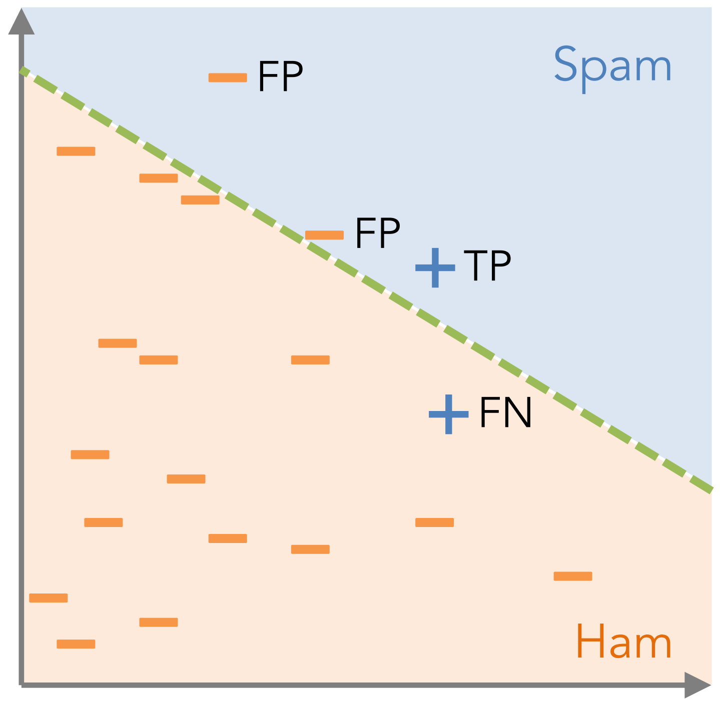
(true positive rate, recall, sensitivity)

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

(true negative rate, specificity)

Classification

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.



$\text{TP} = 1$ (True Positive)

$\text{FP} = 2$ (False Positive)

$\text{FN} = 1$ (False Negative)

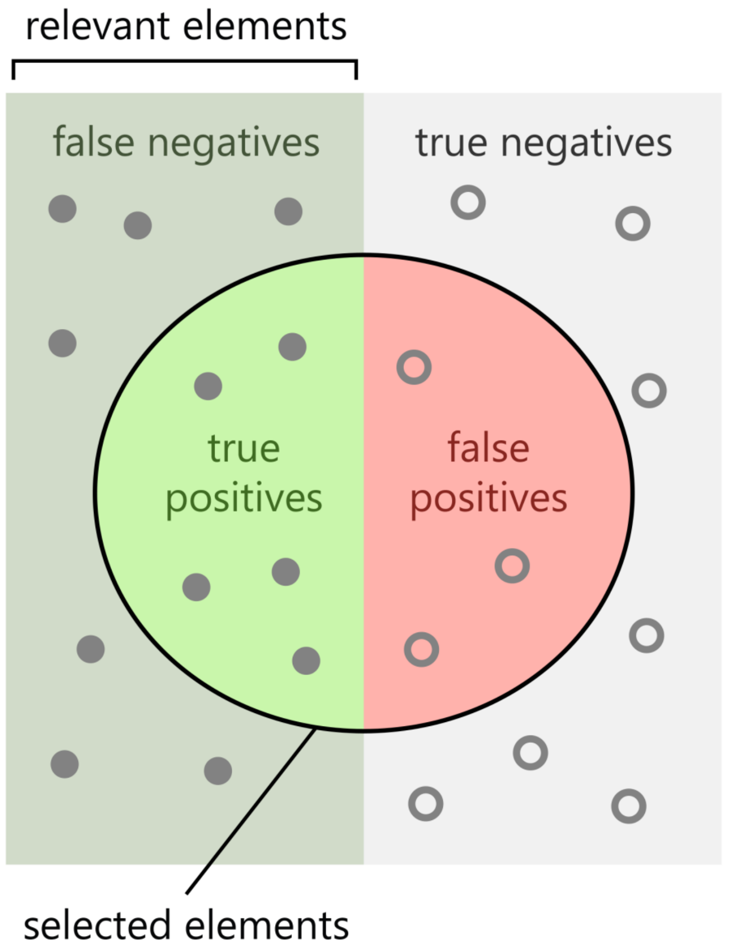
$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} = 0.33$$

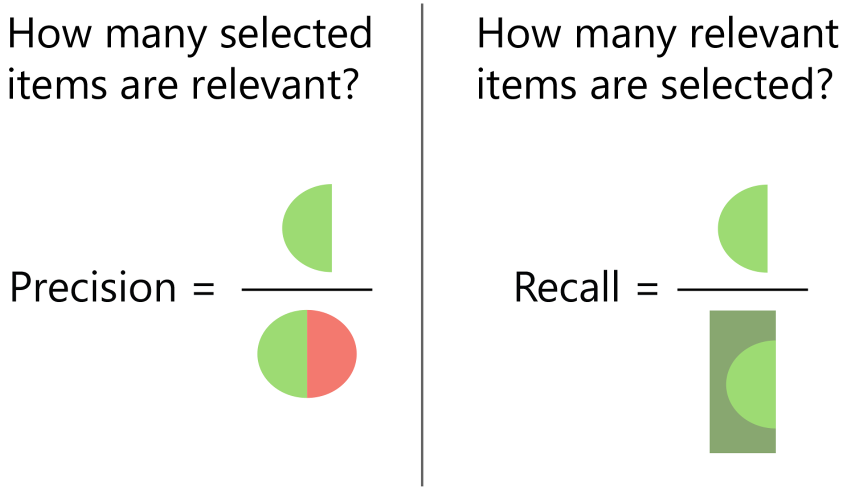
$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} = 0.5$$

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

Classification

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.




How many selected items are relevant?
Precision =
How many relevant items are selected?
Recall =

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

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

Exercise 2.2: Suppose that we fit a binary classification model in identifying spam and ham (i.e., non-spam). Spam is the positive label, and ham is the negative label.

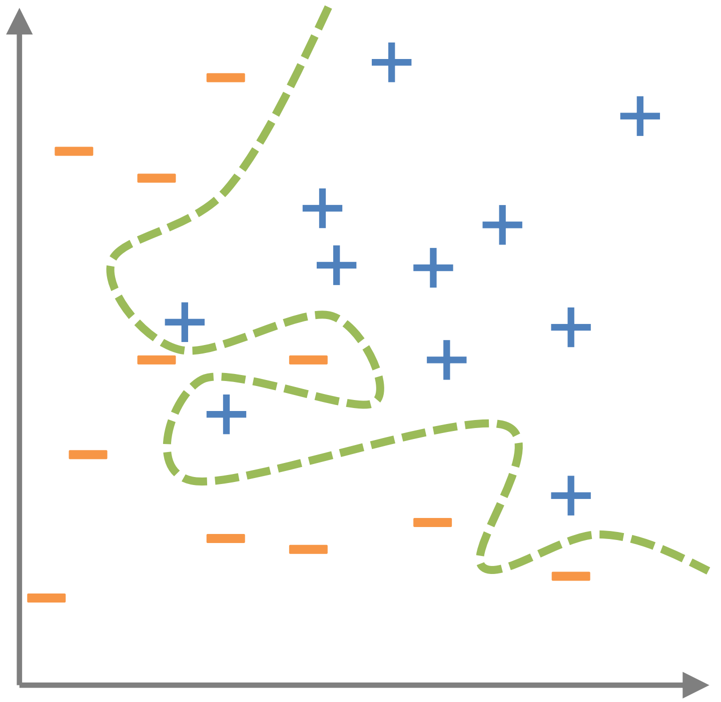
- 40 samples are predicted as spam, and they are indeed spam in reality
- 20 samples are predicted as spam, but it turns out that they are not spam in reality
- 60 samples are predicted as ham, but it turns out that they are spam in reality
- 80 samples are predicted as ham, and they are indeed ham in reality

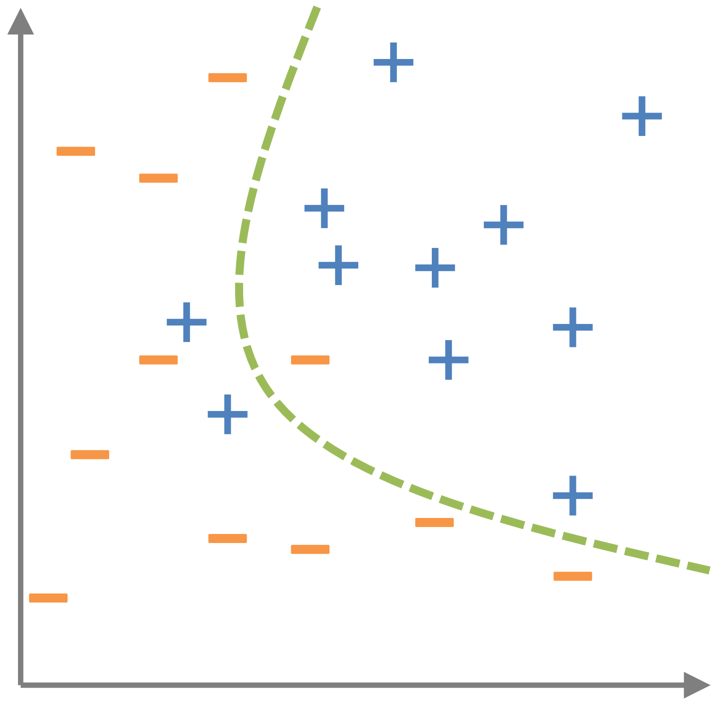
What are the precision, recall, and f-score (F) of the model?

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} \qquad \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \qquad \text{F} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precisio} + \text{Recall}}$$

Classification

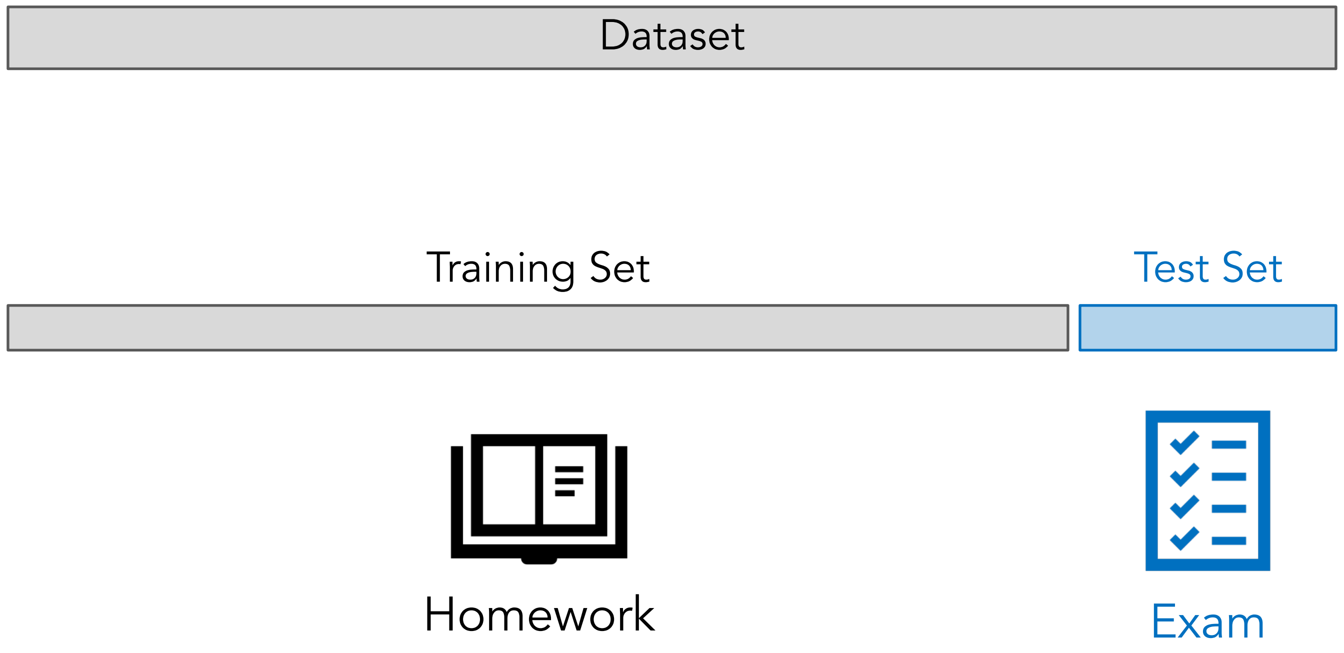
We can train different types of models. But how do we know which one is better? Can we just pick an evaluation metric to determine which model is good?


Model A

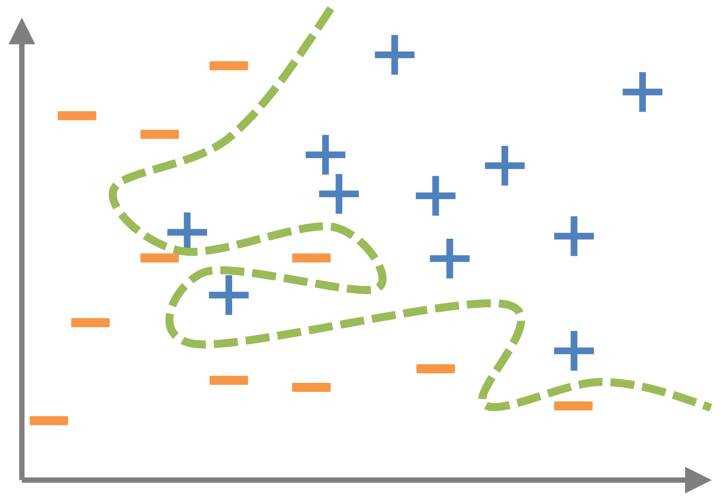

Model B

Model Training

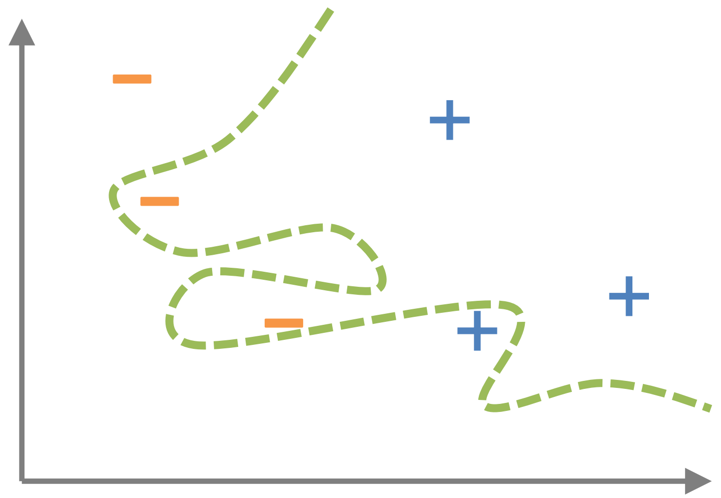
To choose models, we need a test set, which contains data that the models have not yet seen before during the training phase.



😟 Model A

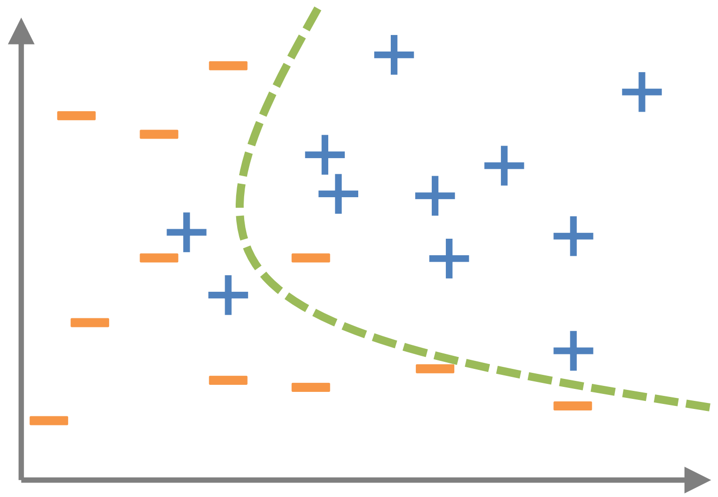


Training Accuracy = 1

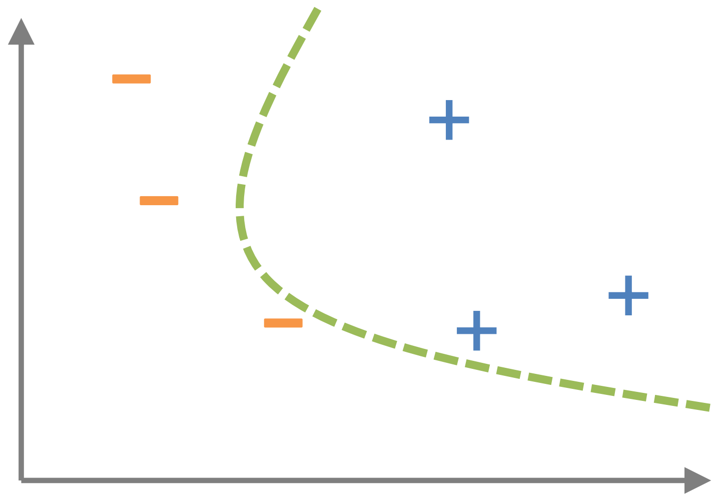


Testing Accuracy = 0.5

😆 Model B



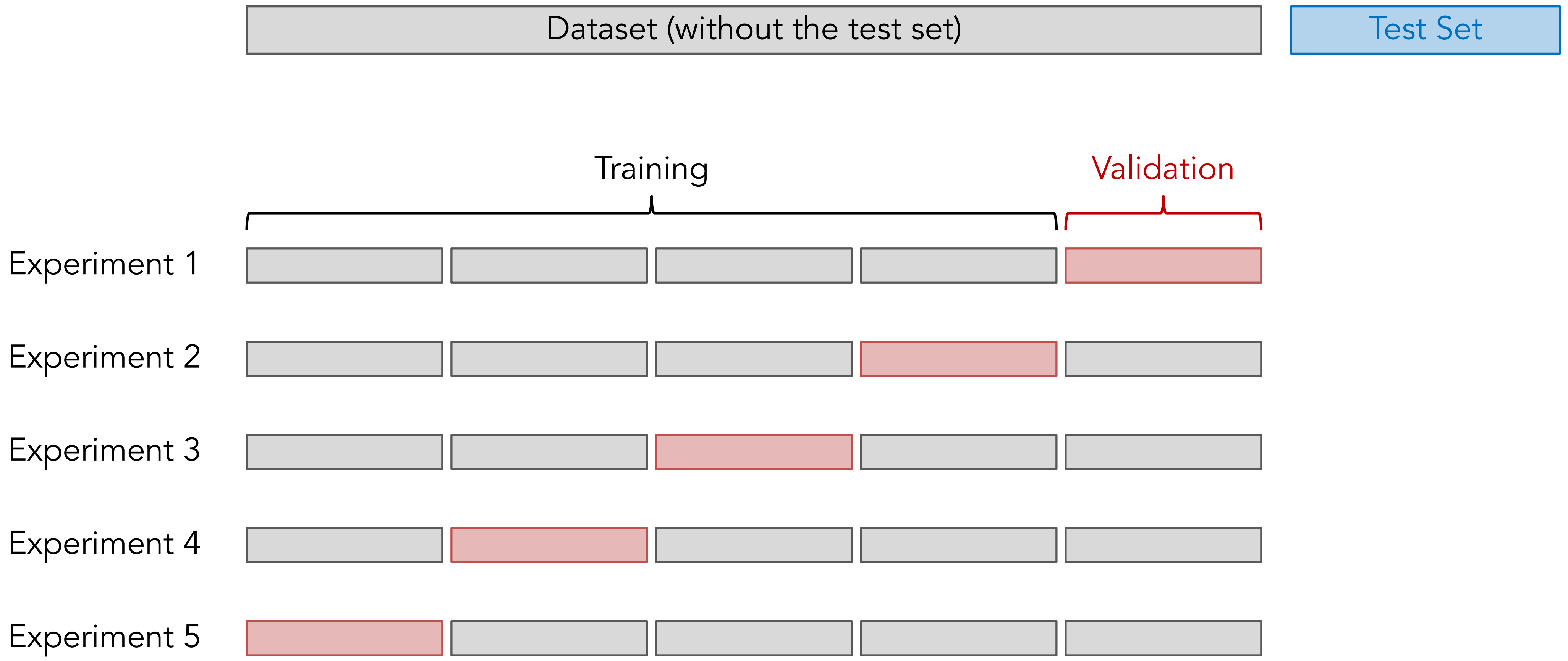
Training Accuracy = 0.86



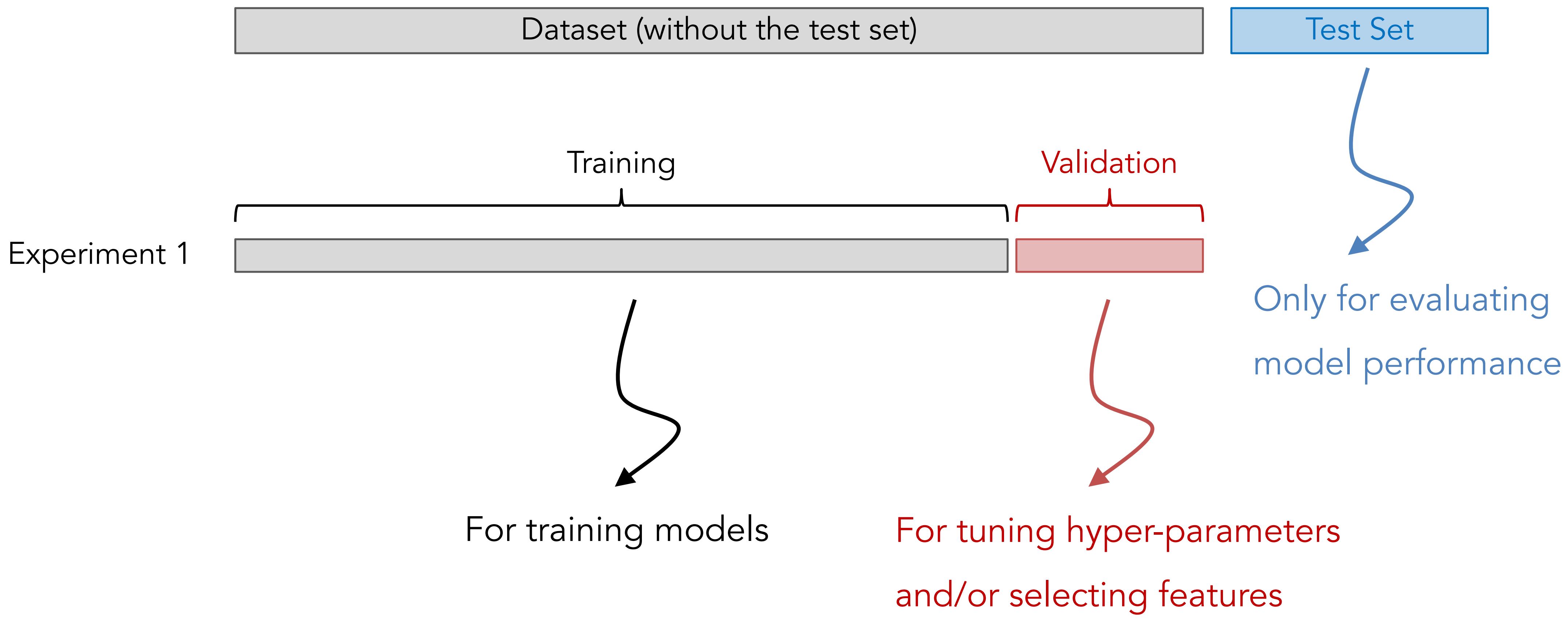
Testing Accuracy = 1

Model Training

To tune hyper-parameters or select features for a model, we use cross-validation to divide the dataset into folds and use each fold for validation.



Model Training You should not use the test set to tune hyper-parameters or select features, which will lead to information leakage. The test set is used to do an unbiased check of generalization performance after all modeling decisions are made.


Dataset (without the test set)
Test Set
Training
Validation
Experiment 1
Only for evaluating model performance
For training models
For tuning hyper-parameters and/or selecting features

Model Training

One way to select features is to recursively eliminate the less important ones by using metrics like permutation importance (which means permuting a feature several times and measuring the decrease in model performance).

We repeat the permutation (and compute model performance) for multiple times. Why?

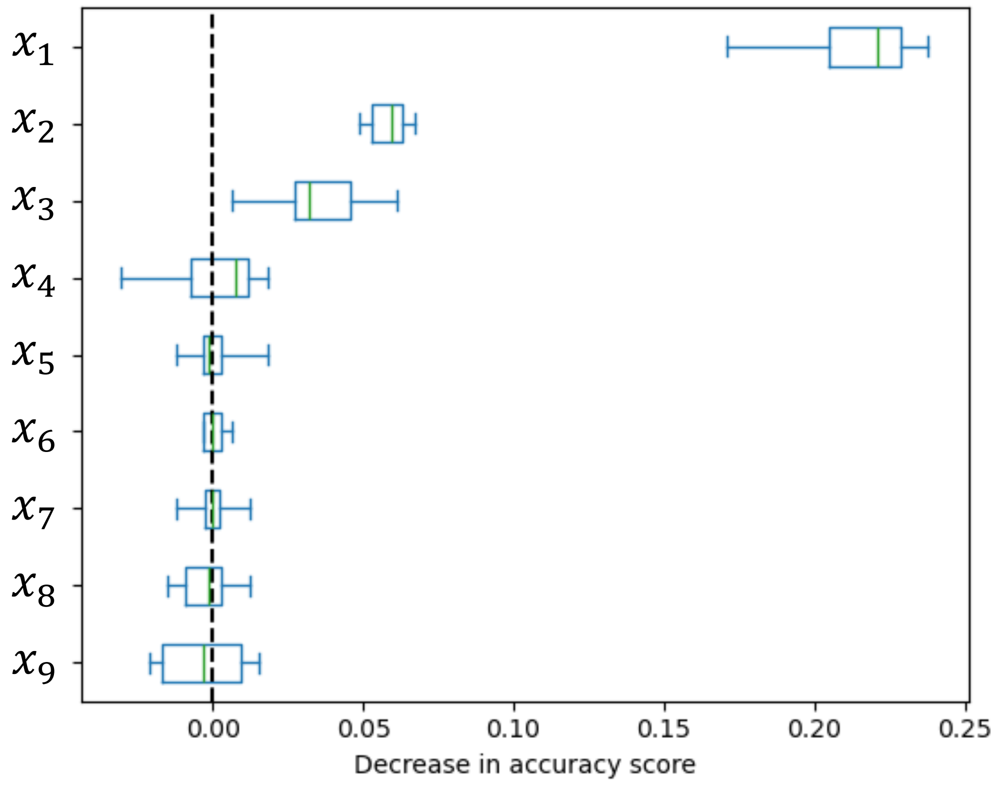
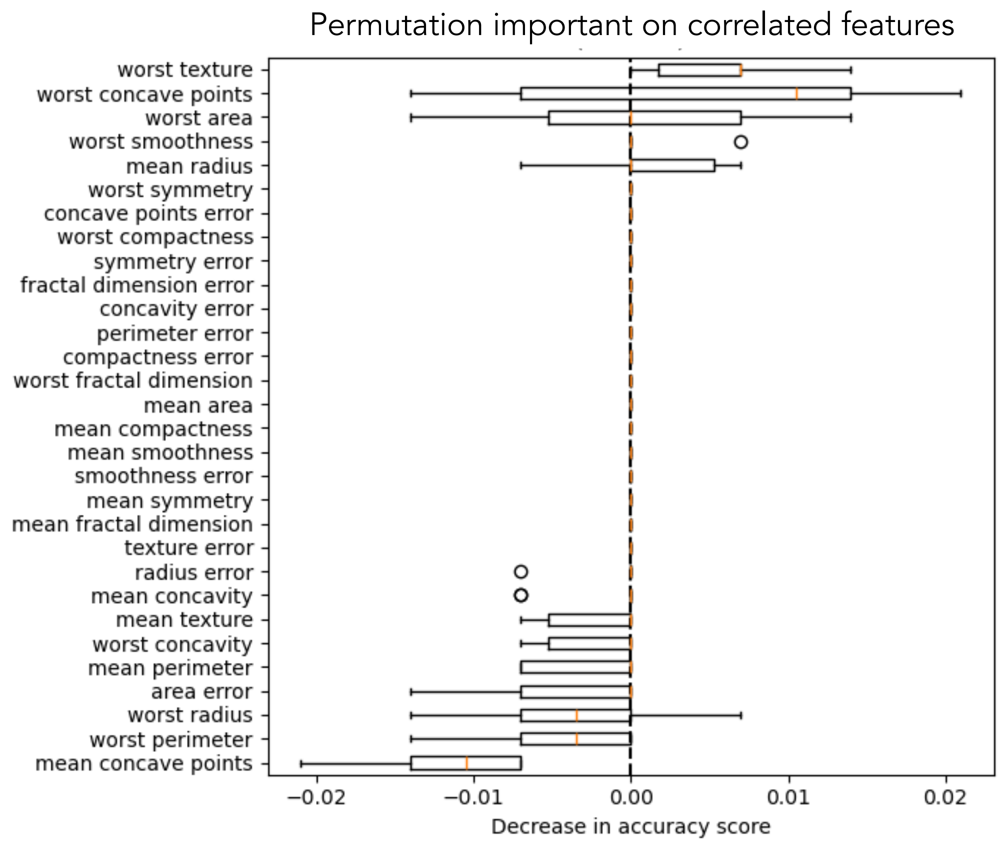


Figure source -- https://scikit-learn.org/1.5/modules/permutation_importance.html

Model Training

If two highly correlated features exist, the model can access the information from the non-permuted feature. Thus, it may appear that both features are not important (which can be false). A better way is to cluster the correlated features first.



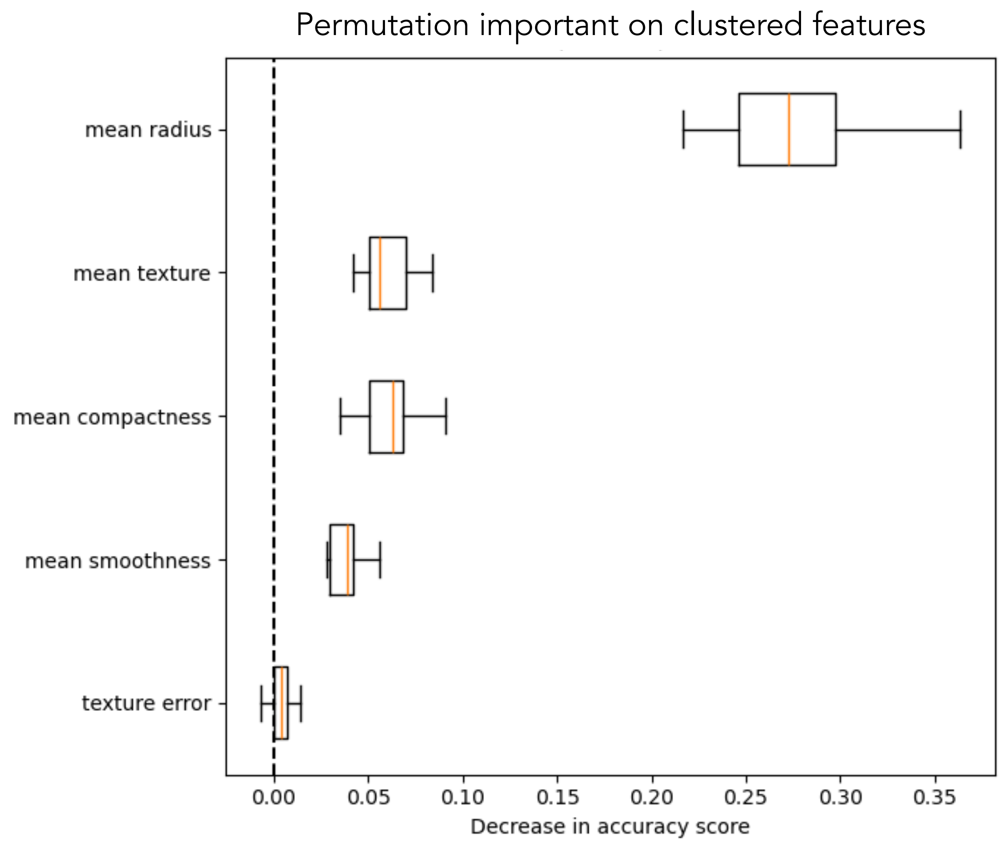
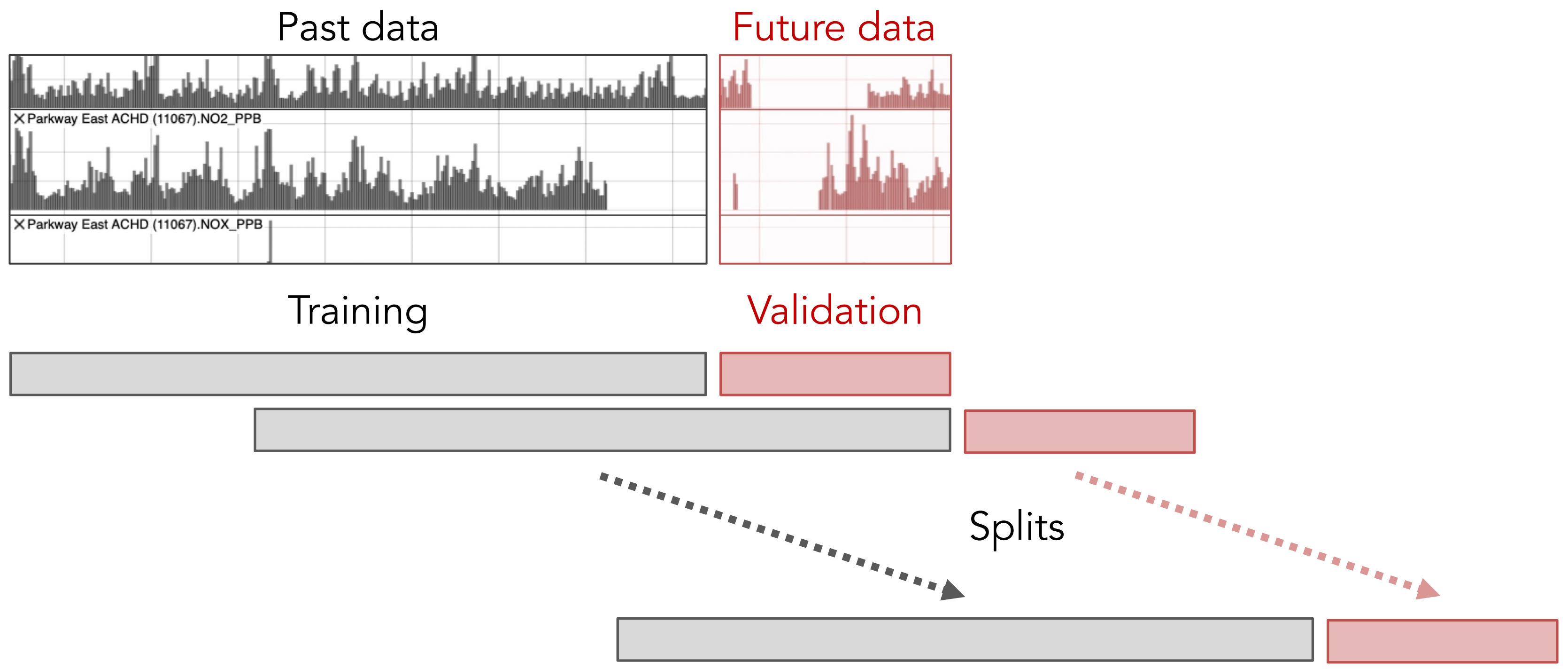


Figure source -- https://scikit-learn.org/1.5/modules/permutation_importance.html

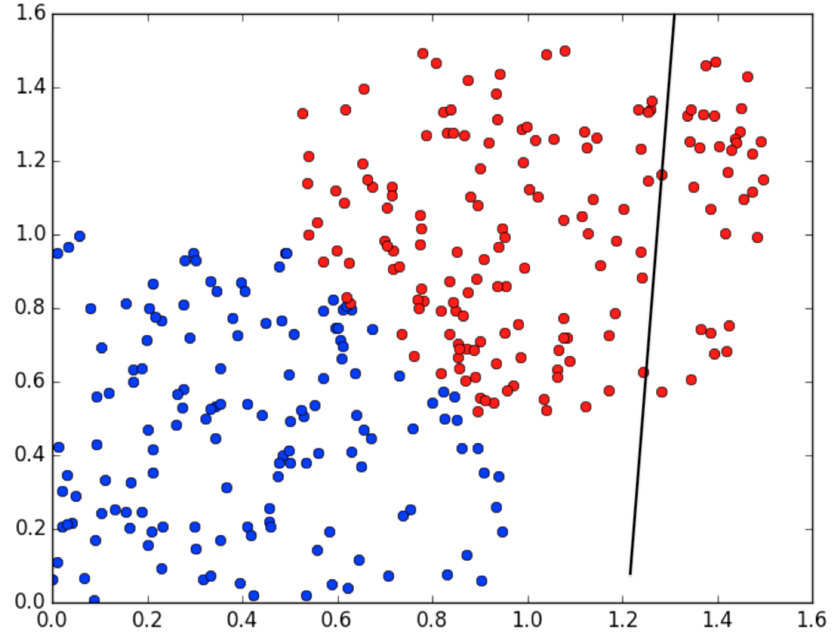
Model Training

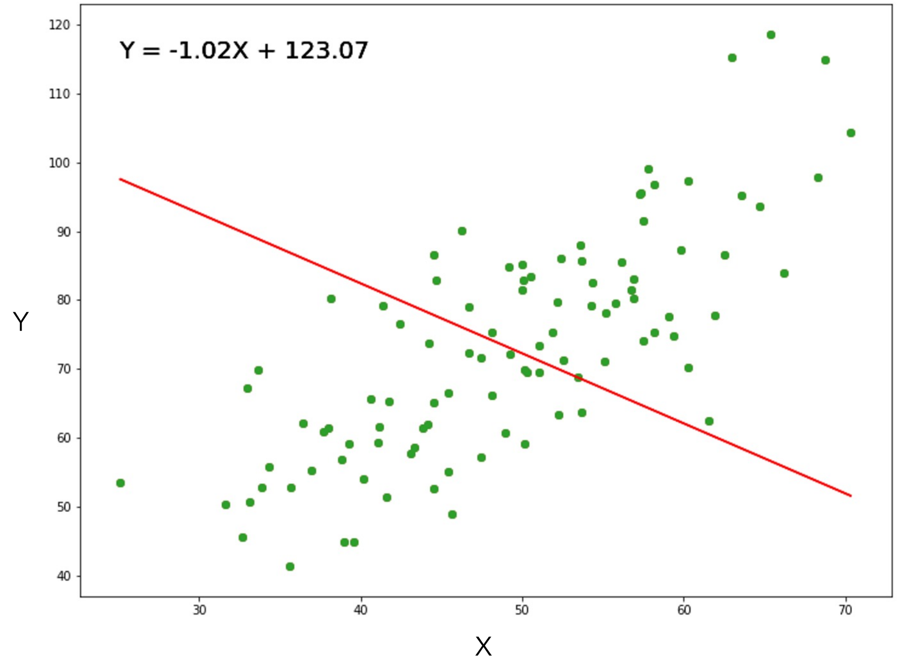
For time-series data, it is better to do the split for cross-validation based on the order of time intervals, which means we only use data in the past to predict the future, but not the other way around.


Past data
Future data
Parkway East ACHD (11067).NO2_PPB
Parkway East ACHD (11067).NOX_PPB
Training
Validation
Splits

Regression

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



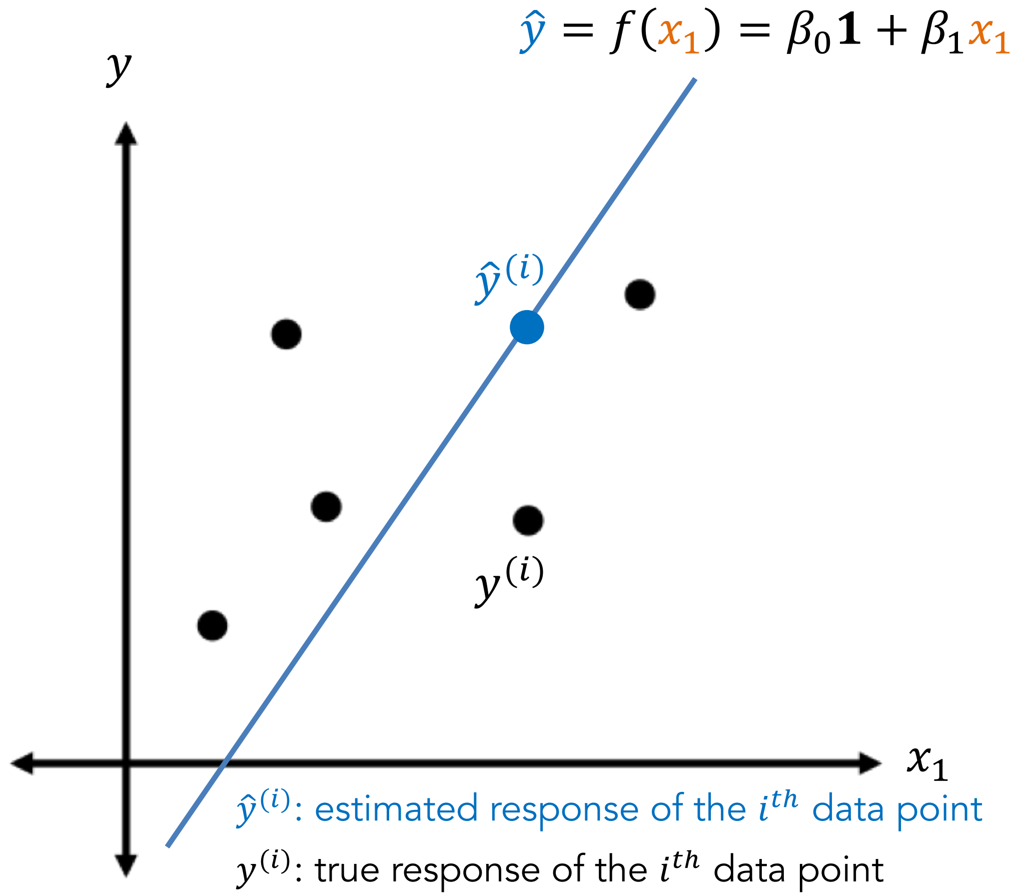


- [Classification] How can we fit a function that separates data points into different groups?
- [Regression] How can we fit a function that maps features (input) to a continuous variable (output)?

Figure source -- https://saichandra1199.medium.com/classification-vs-regression-622b83ff8e90

Regression

Linear regression fits a linear function f that maps x_1 (e.g., the first feature vector of something) to y, which can best describe their linear relationship.



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

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

$x_1^{(i)}$: the first feature of the i^{th} data point

y: true response

$\hat{y}$: estimated response

x_1: predictor/feature

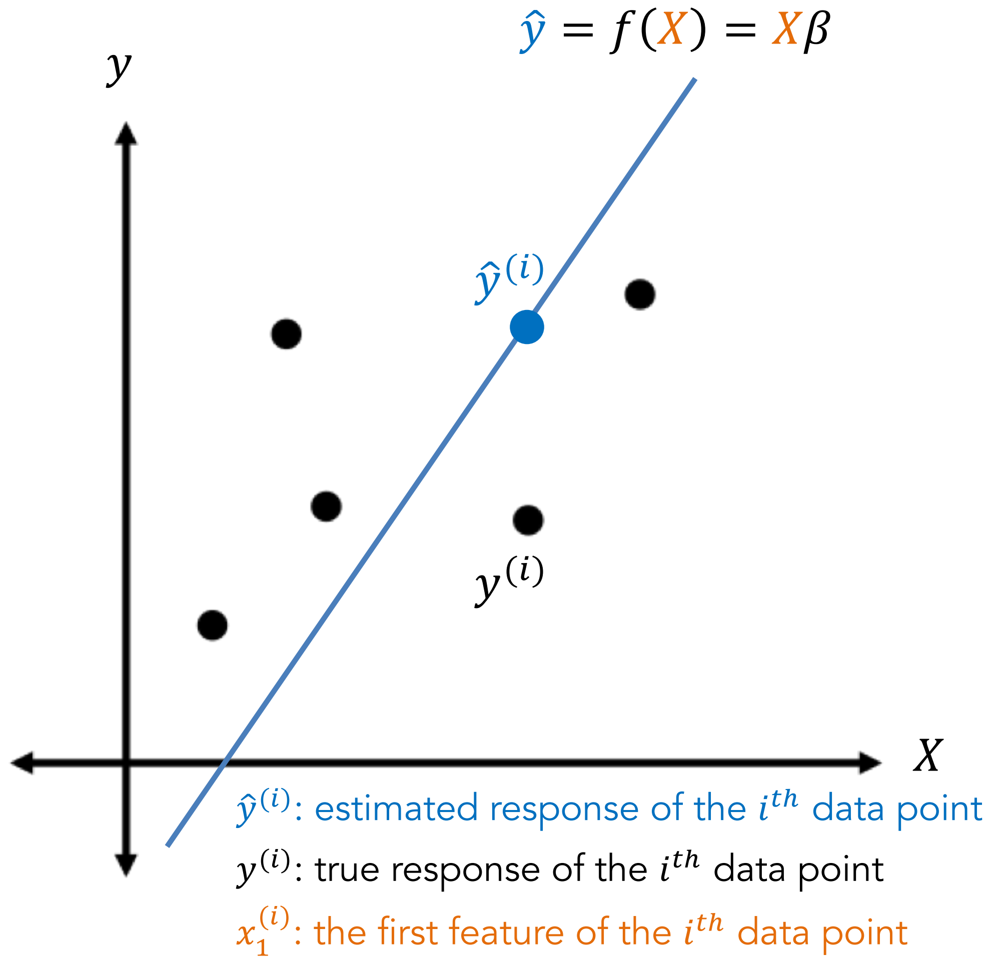
β_0 and β_1: intercept and slope

$$\begin{bmatrix} \hat{y}^{(1)} = f\left(x_1^{(1)}\right) = \beta_0 \cdot 1 + \beta_1 \cdot x_1^{(1)} \\ \vdots \\ \hat{y}^{(n)} = f\left(x_1^{(n)}\right) = \beta_0 \cdot 1 + \beta_1 \cdot x_1^{(n)} \end{bmatrix}$$

$$\underbrace{\boxed{\begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(n)} \end{bmatrix}}}_{\hat{y}} = f\left(\begin{bmatrix} x_1^{(1)} \\ \vdots \\ x_1^{(n)} \end{bmatrix}\right) = \beta_0 \underbrace{\boxed{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}}_{\mathbf{1}} + \beta_1 \underbrace{\boxed{\begin{bmatrix} x_1^{(1)} \\ \vdots \\ x_1^{(n)} \end{bmatrix}}}_{x_1}$$

Regression

We can now create a feature matrix X that includes the intercept term β_0, which gives us a compact form of equation.



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

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

$x_1^{(i)}$: the first feature of the i^{th} data point

y: true response (vector)

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

X: predictor/feature (matrix)

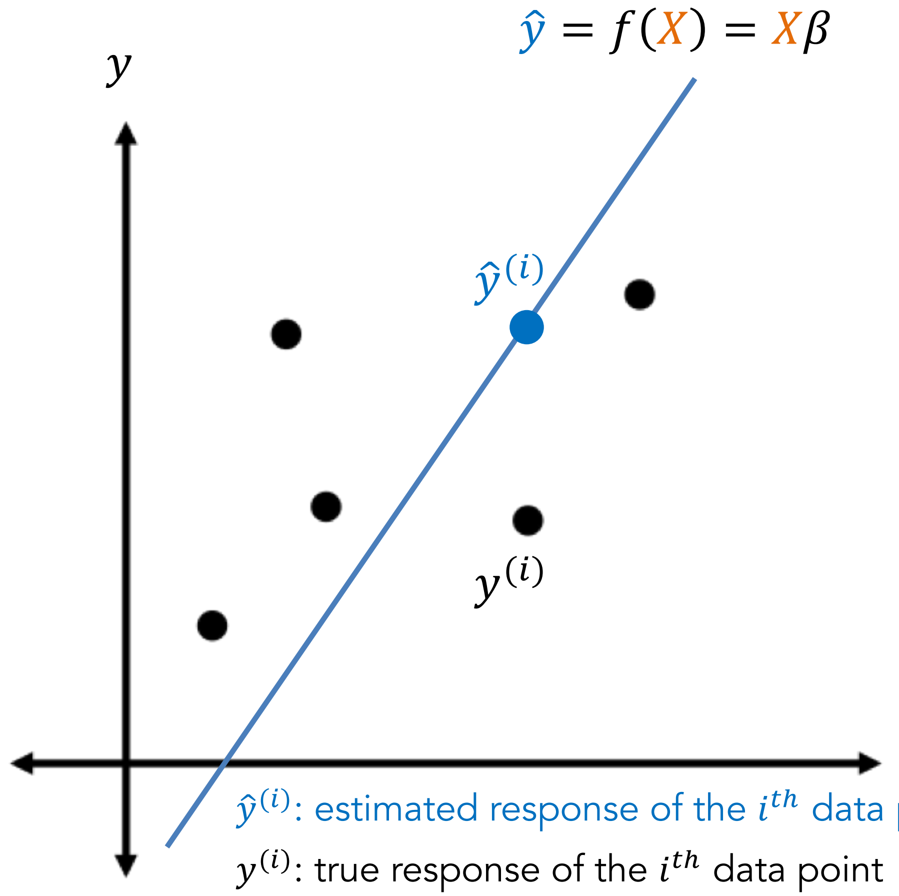
β: coefficients (vector)

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

$$\hat{y} = \beta_0 \mathbf{1} + \beta_1 x_1 = \underbrace{\boxed{\begin{bmatrix} 1 & x_1^{(1)} \\ \vdots & \vdots \\ 1 & x_1^{(n)} \end{bmatrix}}}_{X} \times \underbrace{\boxed{\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}}}_{\beta}$$

Regression

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



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

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

$x_j^{(i)}$: the j^{th} feature of the i^{th} data point

y: true response (vector)

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

X: predictor/feature (matrix)

β: coefficients (vector)

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

$$\hat{y} = f(X) = \underbrace{\boxed{\begin{bmatrix} 1 & x_1^{(1)} & \dots & x_p^{(1)} \\ \vdots & \vdots & \dots & \vdots \\ 1 & x_1^{(n)} & \dots & x_p^{(n)} \end{bmatrix}}}_{X} \times \underbrace{\boxed{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}}}_{\beta}$$

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

We use the vector and matrix forms to simplify equations.

$$X = [\mathbf{1}\quad \overset{\text{Vector}}{\boxed{x_1}}\quad \cdots\quad x_p] = \overset{\text{Matrix}}{\boxed{\begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_p^{(1)} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_1^{(n)} & \cdots & x_p^{(n)} \end{bmatrix}}} \qquad \beta = \begin{bmatrix} \overset{\text{Scalar}}{\boxed{\beta_0}} \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

$$\hat{y} = f(x) = X\beta = [\mathbf{1}\quad x_1\quad \cdots\quad x_p] \times \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \overset{\text{Vector}}{\boxed{\begin{bmatrix} \hat{y}^{(1)} \\ \vdots \\ \hat{y}^{(n)} \end{bmatrix}}}$$

Regression

We can map vector and matrix forms to data directly.

Sum of smell ratings	H2S in PPM	SO2 in PPM	…	Wind direction in DEG	Wind speed in MPH
…	…	…	…	…	…
25	0.019	0.020	…	215.0	3,2
40	0.130	0.033	…	199.0	3.4
45	0.095	0.044	…	184.0	2.9
…	…	…	…	…	…

Vector $\begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$

Vector x_1

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

Regression

We can look at the feature matrix X from two different directions: one represents features, and the other one represents data points.

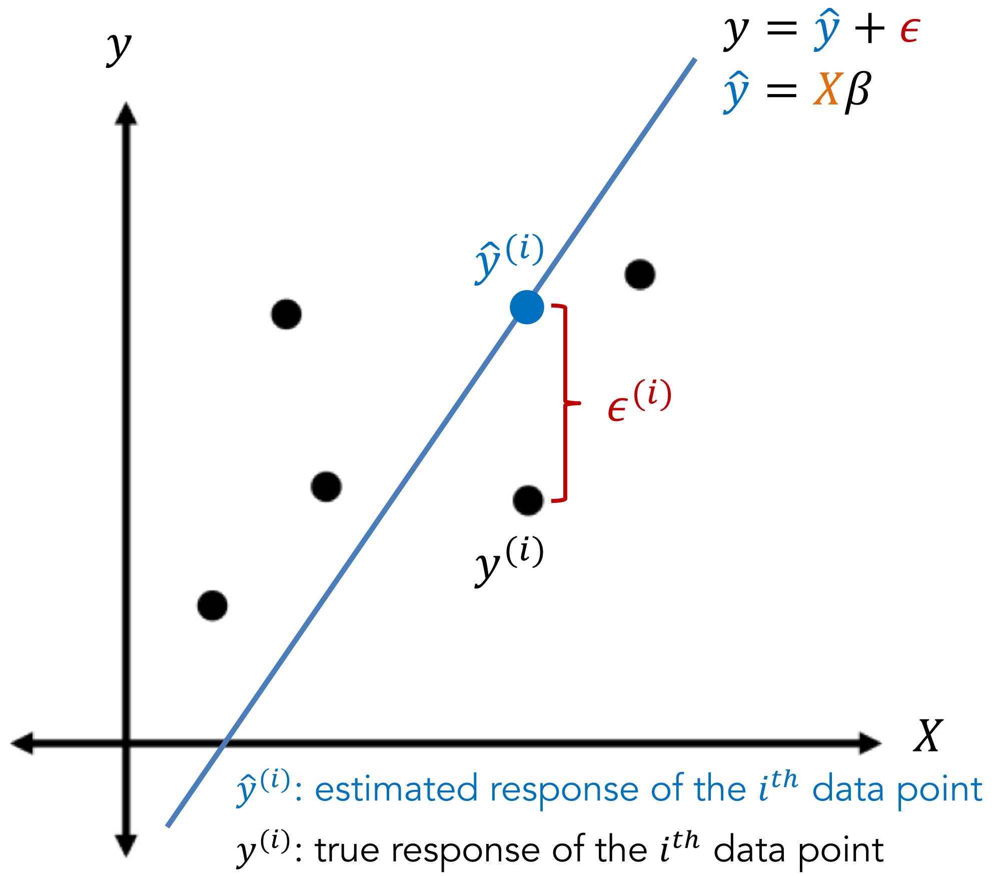
$$X = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_p^{(1)} \\ \vdots & \vdots & \dots & \vdots \\ 1 & x_1^{(n)} & \dots & x_p^{(n)} \end{bmatrix}$$

Data Point
$x^{(1)}$

Feature
x_1

Regression

Finally, we need an error metric between the estimated response $\hat{y}$ and the true response y to know if the model fits the data well.



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

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

$x_j^{(i)}$: the j^{th} feature of the i^{th} data point

y: true response (vector)

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

X: predictor/feature (matrix)

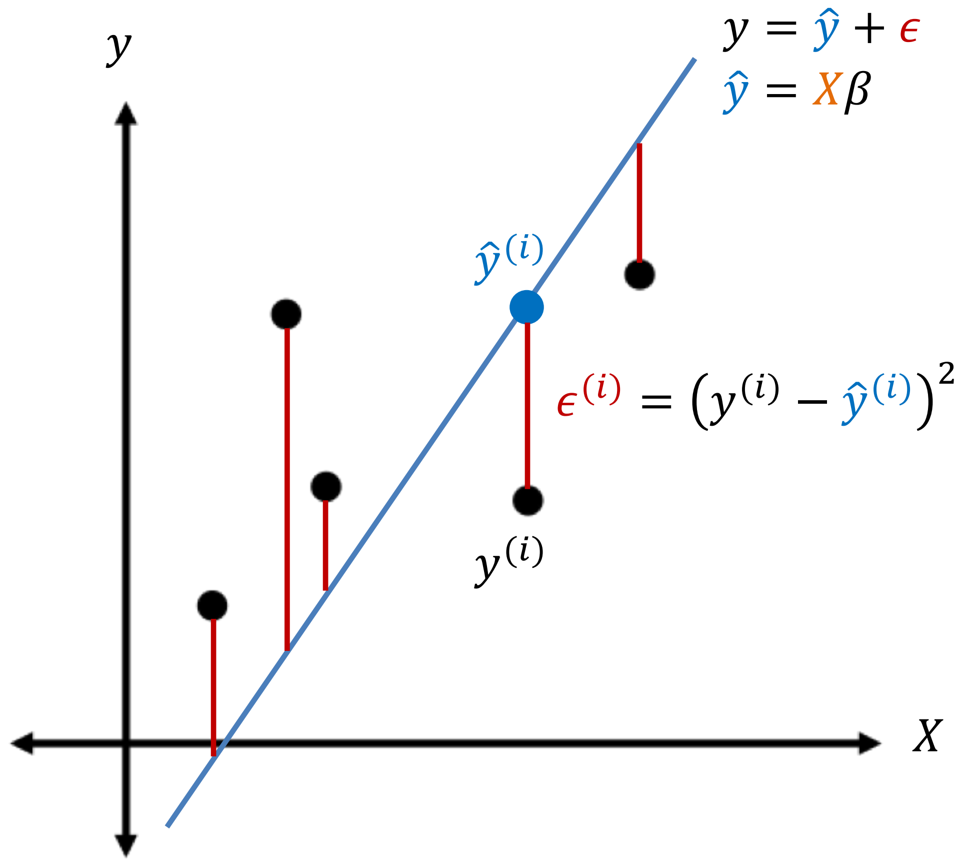
β: coefficients (vector)

ϵ: error/noise/residual (vector)

$$\hat{y} = f(X) = \underbrace{\begin{bmatrix} 1 & x_1^{(1)} & \dots & x_p^{(1)} \\ \vdots & \vdots & \dots & \vdots \\ 1 & x_1^{(n)} & \dots & x_p^{(n)} \end{bmatrix}}_{X} \times \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}}_{\beta}$$

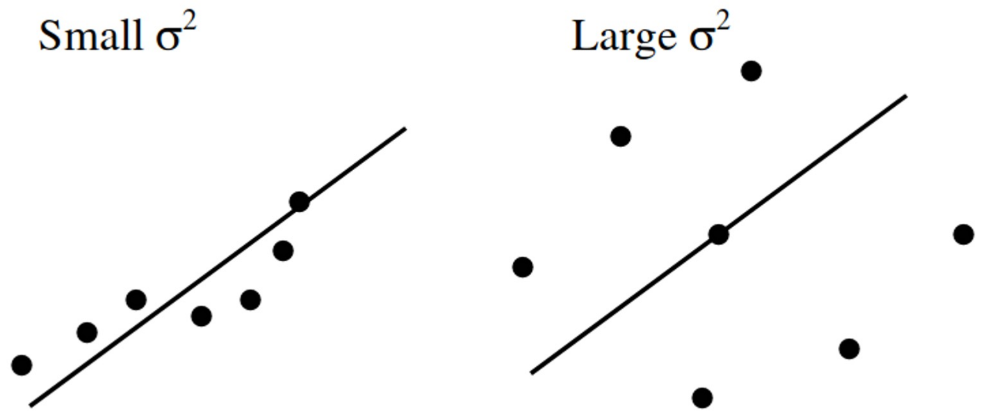
Regression

Usually, we assume that the error ϵ is IID (independent and identically distributed) and follows a normal distribution with zero mean and some variance σ^2.



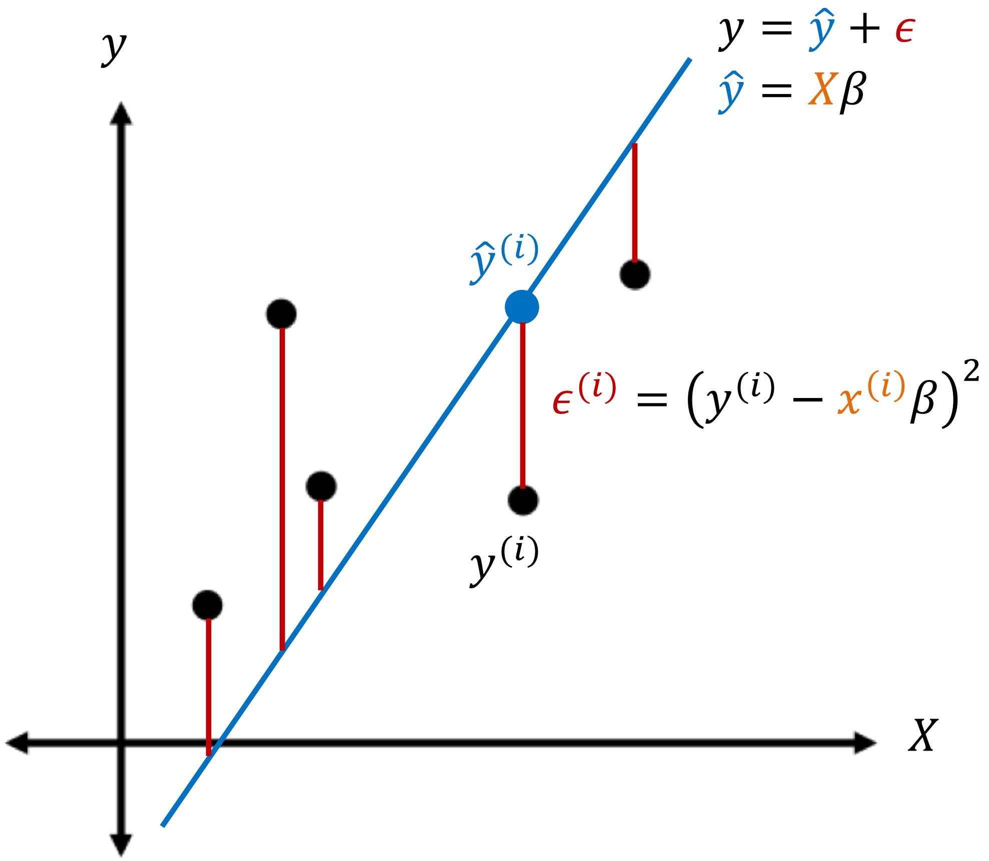
$$\epsilon \sim^{iid} N(0, \sigma^2)$$

$$\text{total errors} = \sum_{i=1}^{n} \epsilon = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$



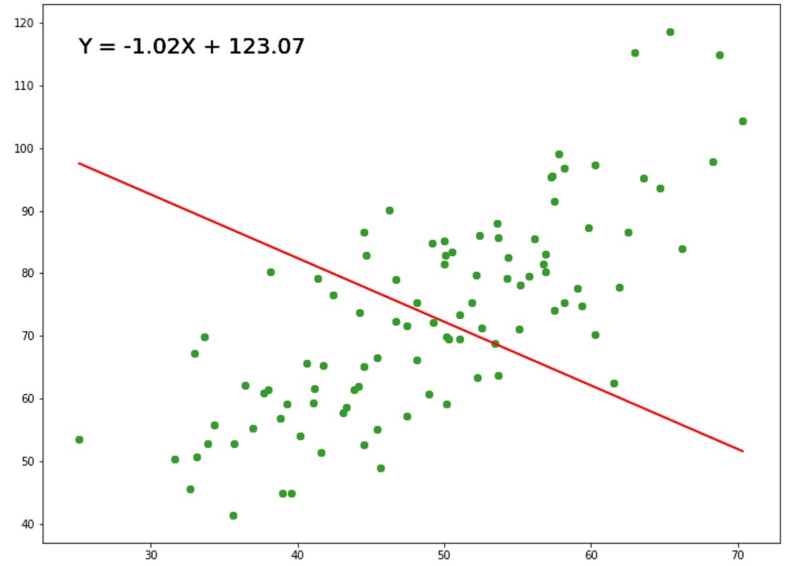
Regression

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



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

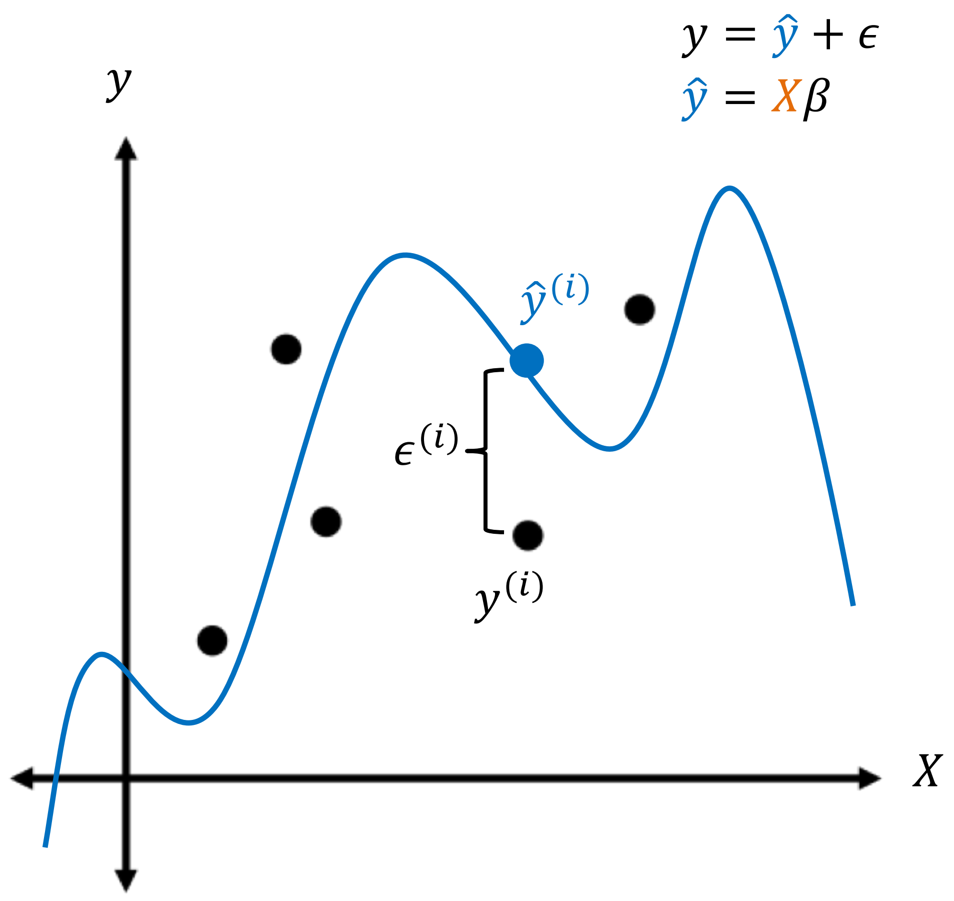
$$= \min_{\beta} (y - X\beta)^T (y - X\beta)$$



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

Regression

We can model a non-linear relationship using polynomial functions with degree k. The example below uses one predictor x_1.



y: true response (vector)

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

X: predictor/feature (matrix)

β: coefficients (vector)

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

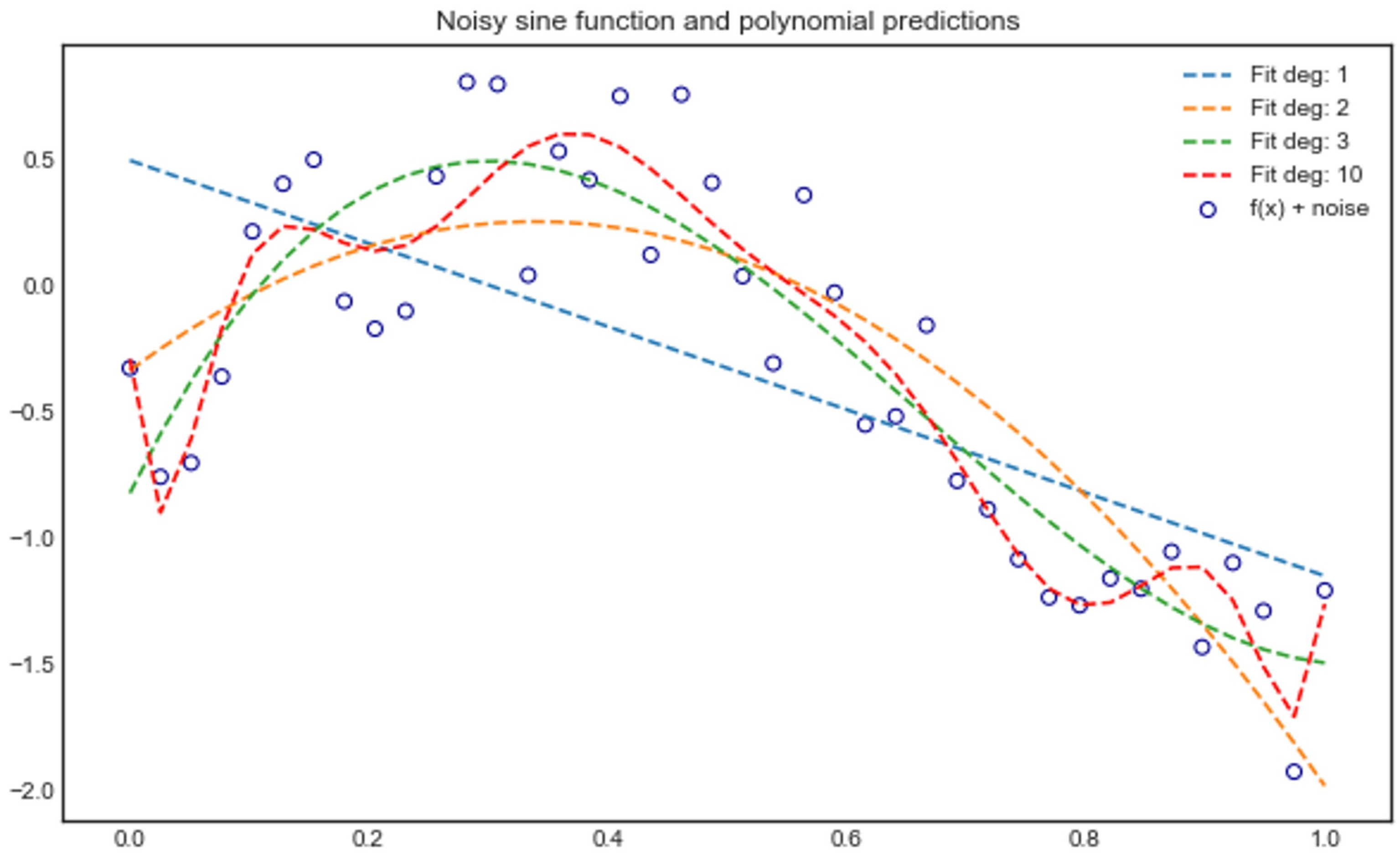
$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$$

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

More about polynomial regression -- https://www.stat.cmu.edu/~cshalizi/mreg/15/lectures/lecture-16.pdf

Regression

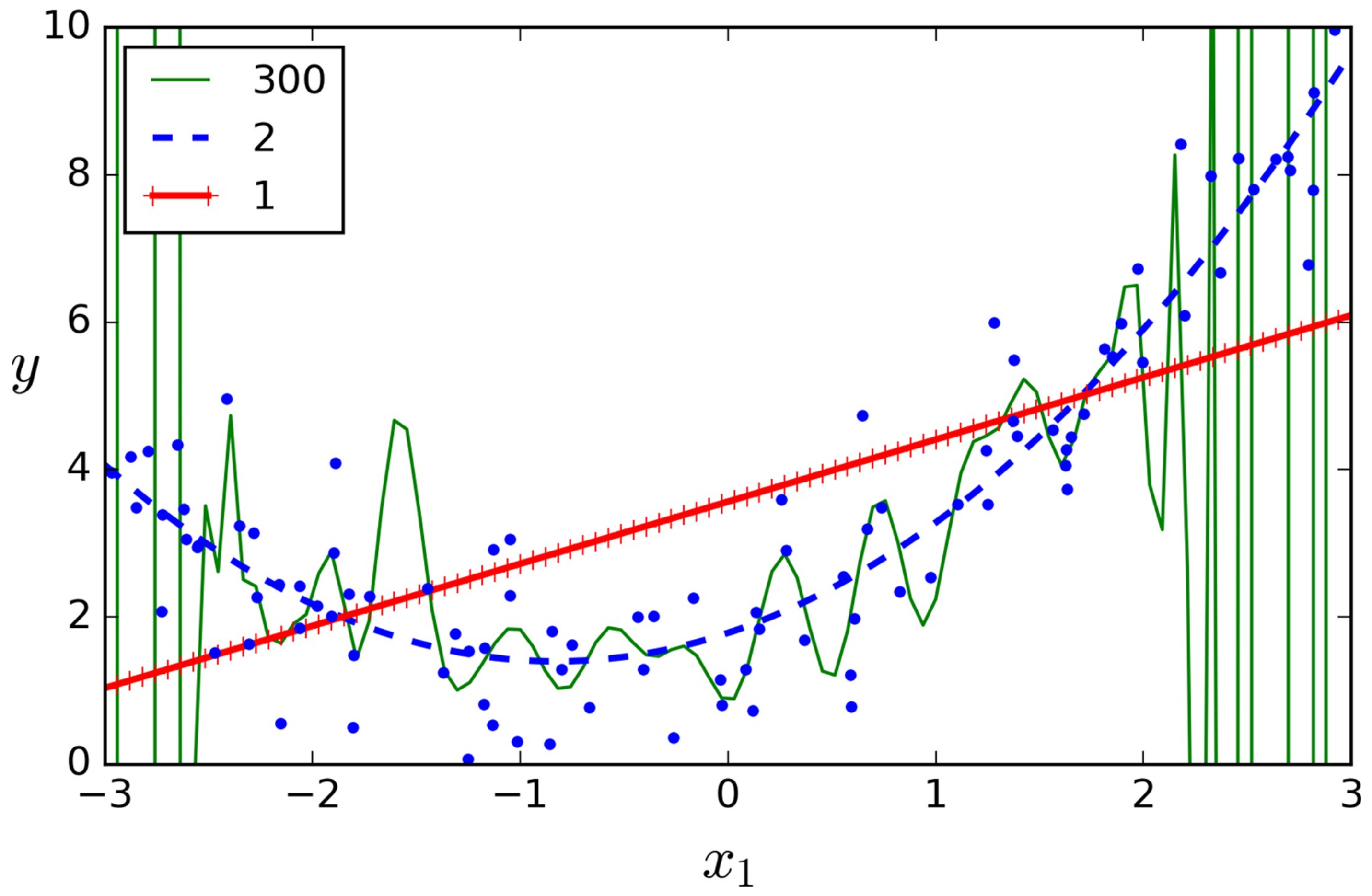
Here is an example of applying linear and polynomial regression to the data that is created using a sine function with some random noise.

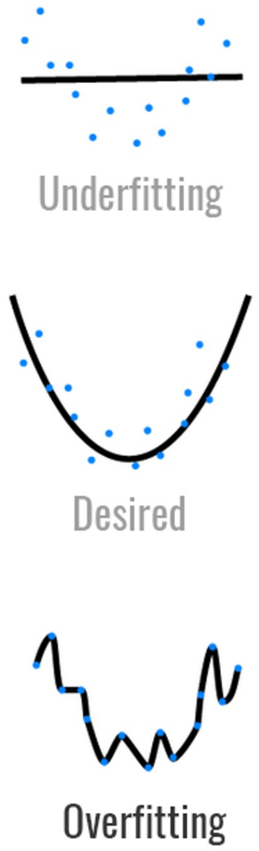


Source -- https://stats.stackexchange.com/questions/350130/why-is-gradient-descent-so-bad-at-optimizing-polynomial-regression

Regression

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.

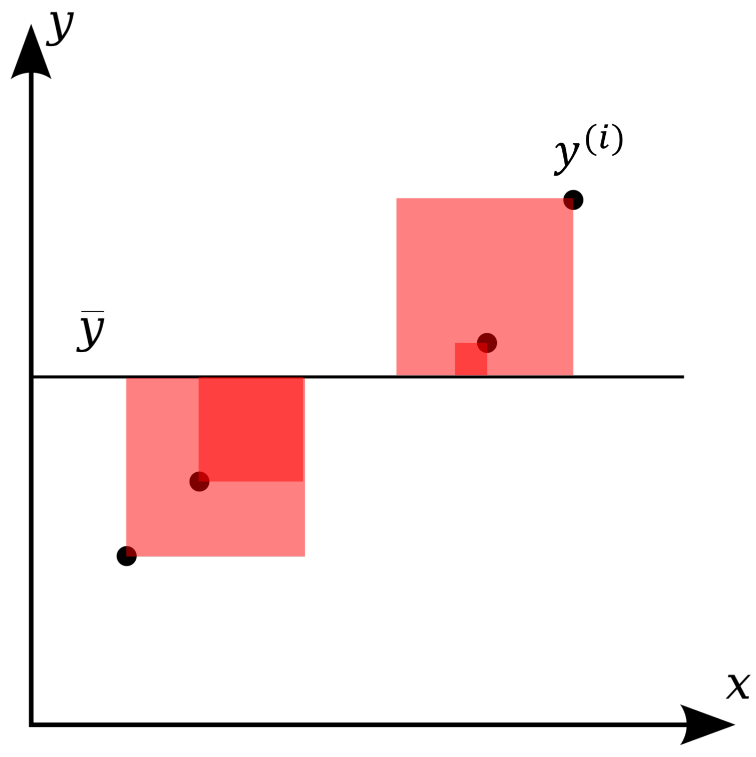




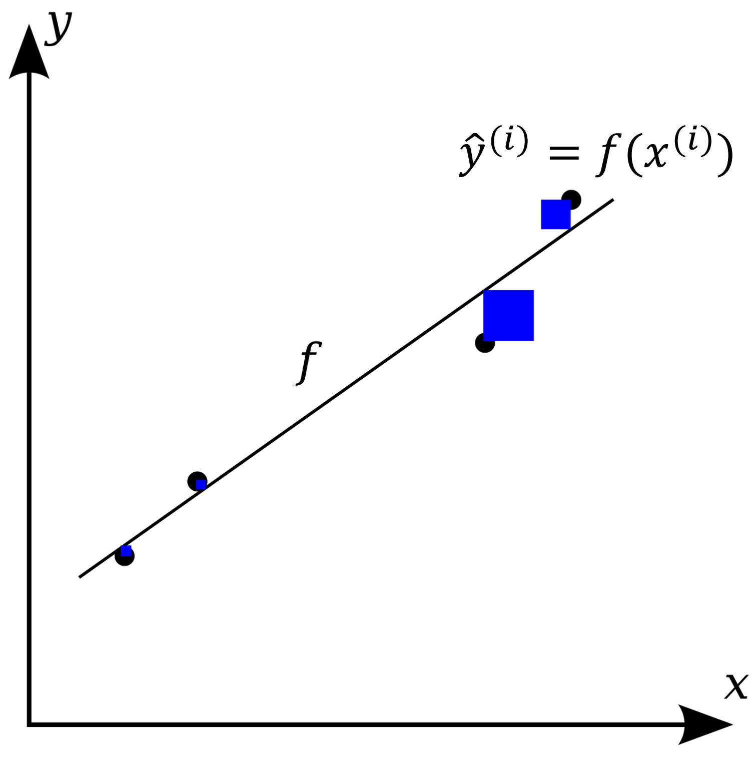
Source -- https://www.oreilly.com/library/view/hands-on-machine-learning/9781491962282/ch04.html

Regression

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

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

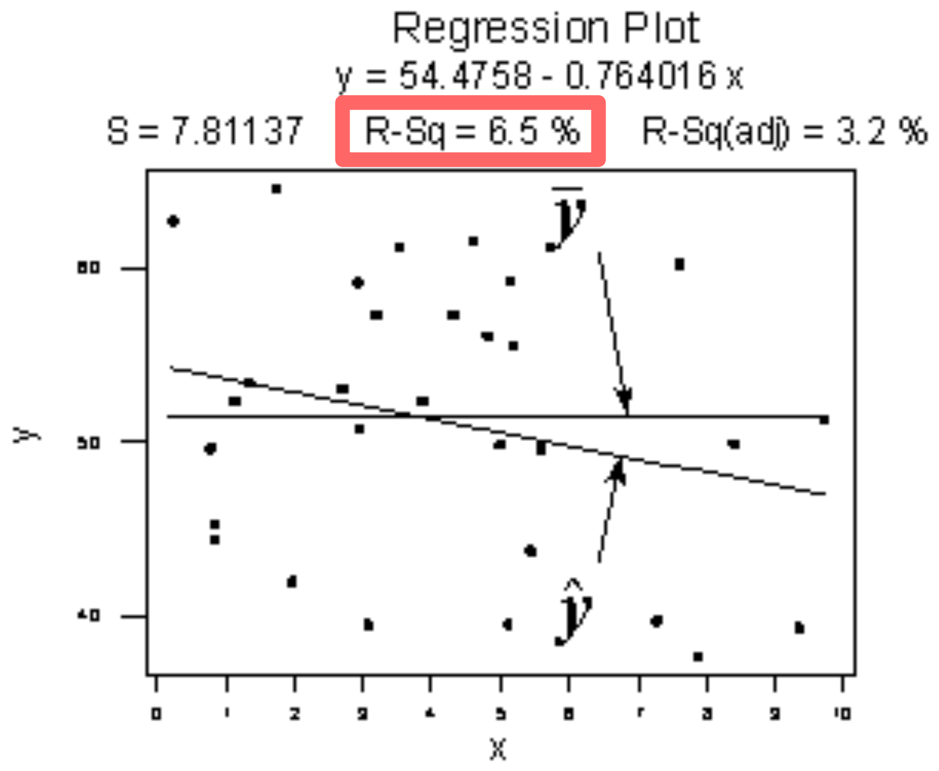
$$SS_{res} = \sum_i \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

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

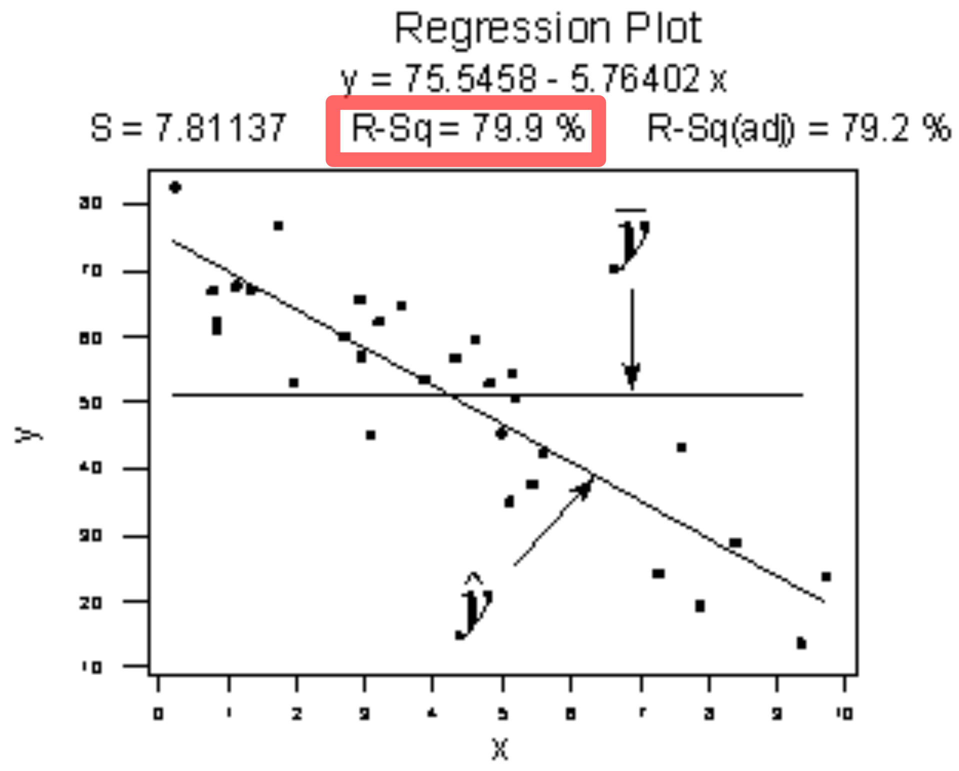
Figure source -- https://en.wikipedia.org/wiki/Coefficient_of_determination

Regression

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

Regression

R^2 increases as we add more predictors (since the optimization wants to decrease the residual sum of squares) and thus is not a good metric for model selection. The adjusted R^2 considers the number of samples (n) and predictors (p).

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

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

$$df_{tot} = n - 1$$

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

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

p: number of features/predictors

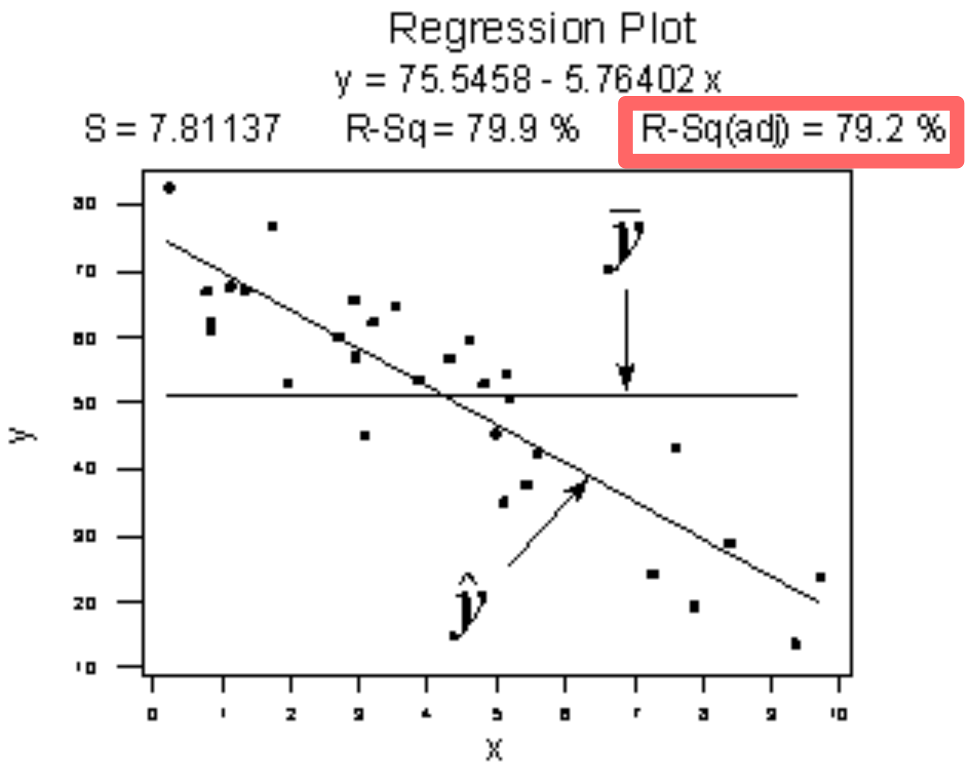
R^2_{adj}: adjusted value of R^2

df_{res}: residual degree of freedom

df_{tot}: total degree of freedom

SS_{res}: residual sum of squares

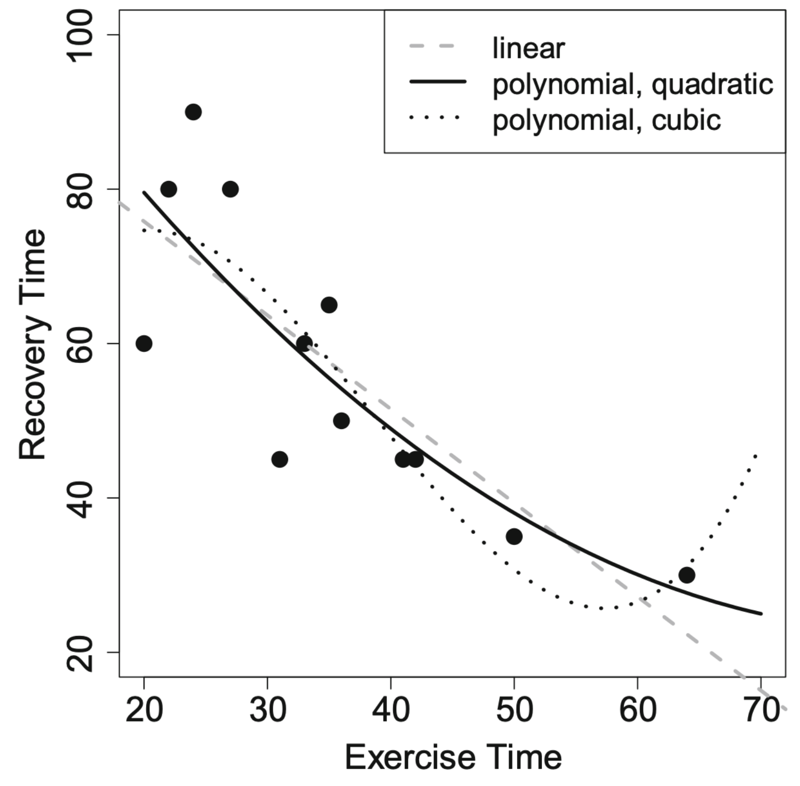
SS_{tot}: total sum of squares

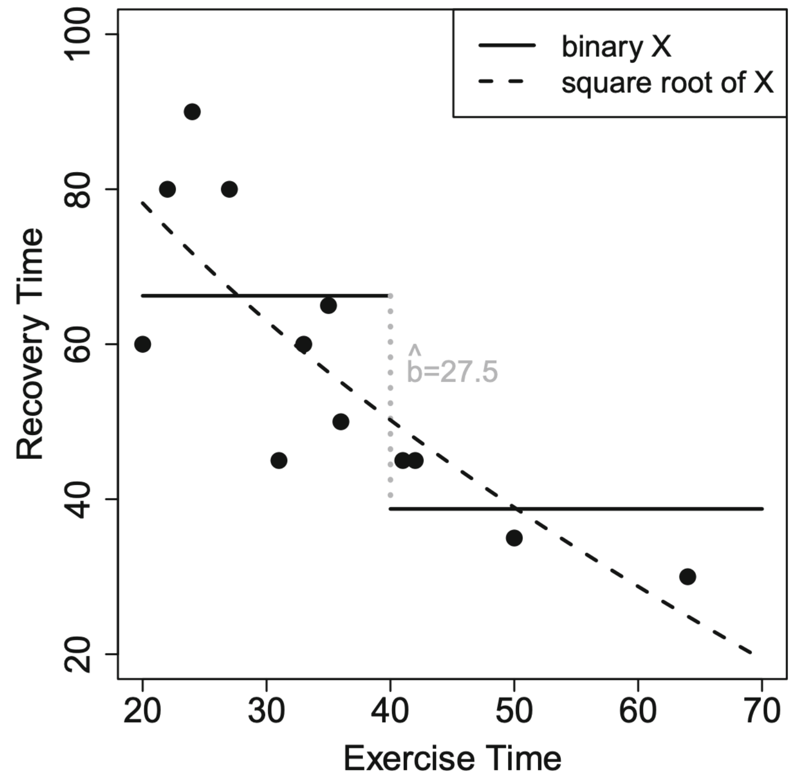


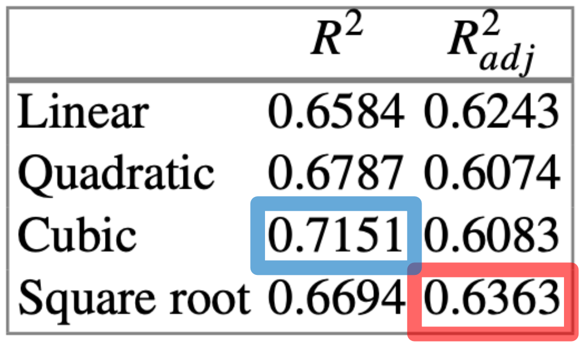
More about the adjusted Coefficient of Determination -- https://online.stat.psu.edu/stat501/lesson/10/10.3

Regression

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.





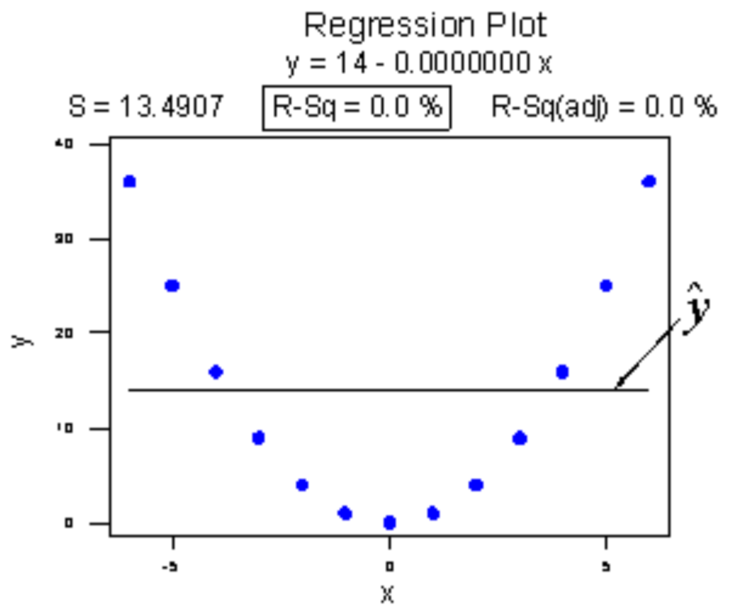


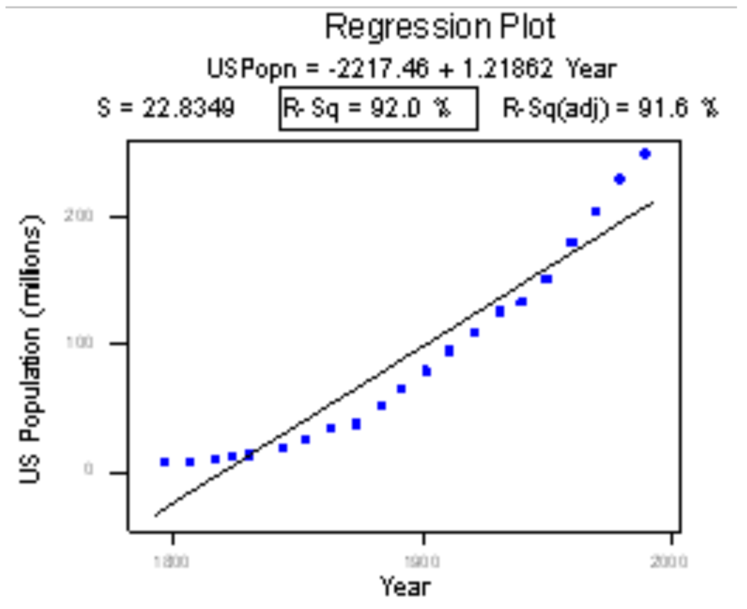
	R^2	R^2_{adj}
Linear	0.6584	0.6243
Quadratic	0.6787	0.6074
Cubic	0.7151	0.6083
Square root	0.6694	0.6363

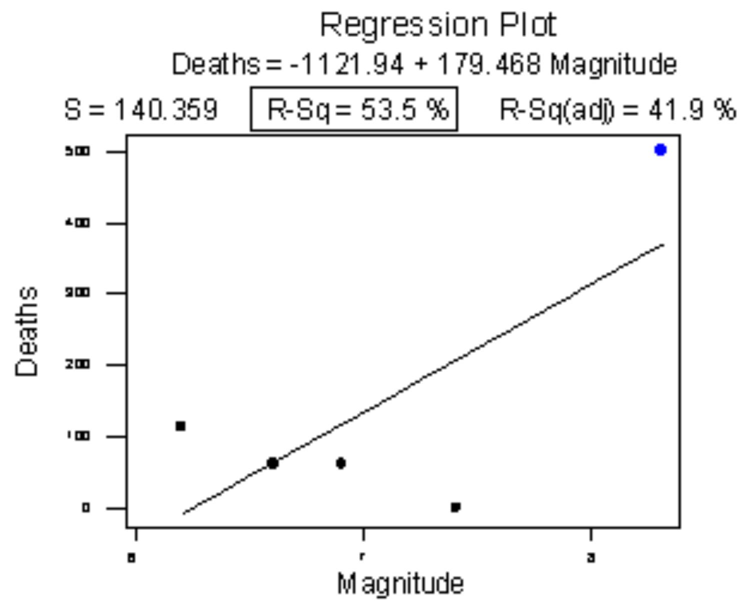
This example is from section 11.8 Comparing Different Models in book: Introduction to Statistics and Data Analysis

Regression

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?