

Data Science

Lecture 2-2: Data Science Fundamentals (Modeling)



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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).

◆◆◆◆◆◆◆◆◆◆ 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

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 ◆◆◆◆◆◆◆◆◆◆



Spam

Number of special characters = 34

Number of digits = 22

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.



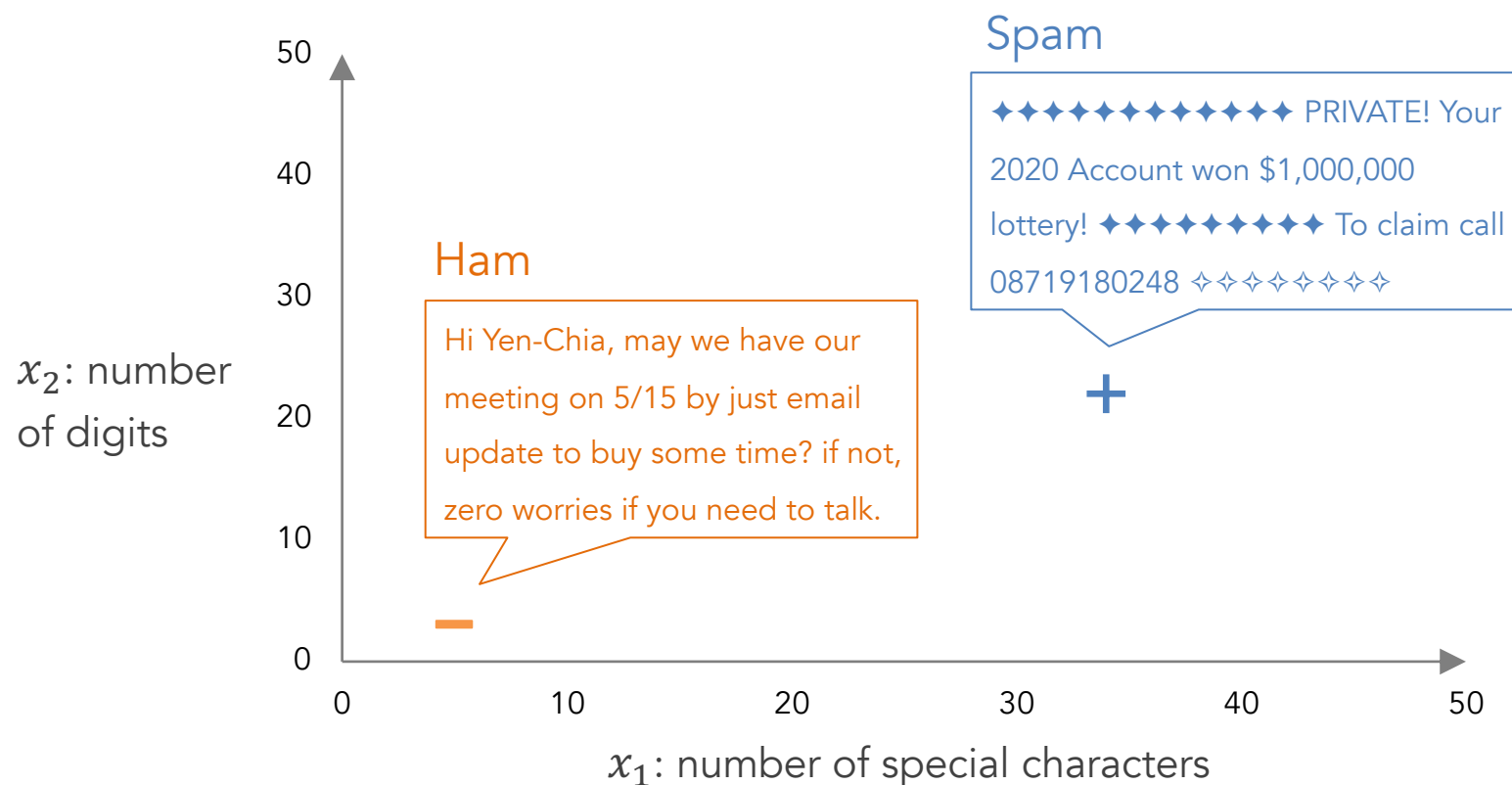
Ham

Number of special characters = 5

Number of digits = 3

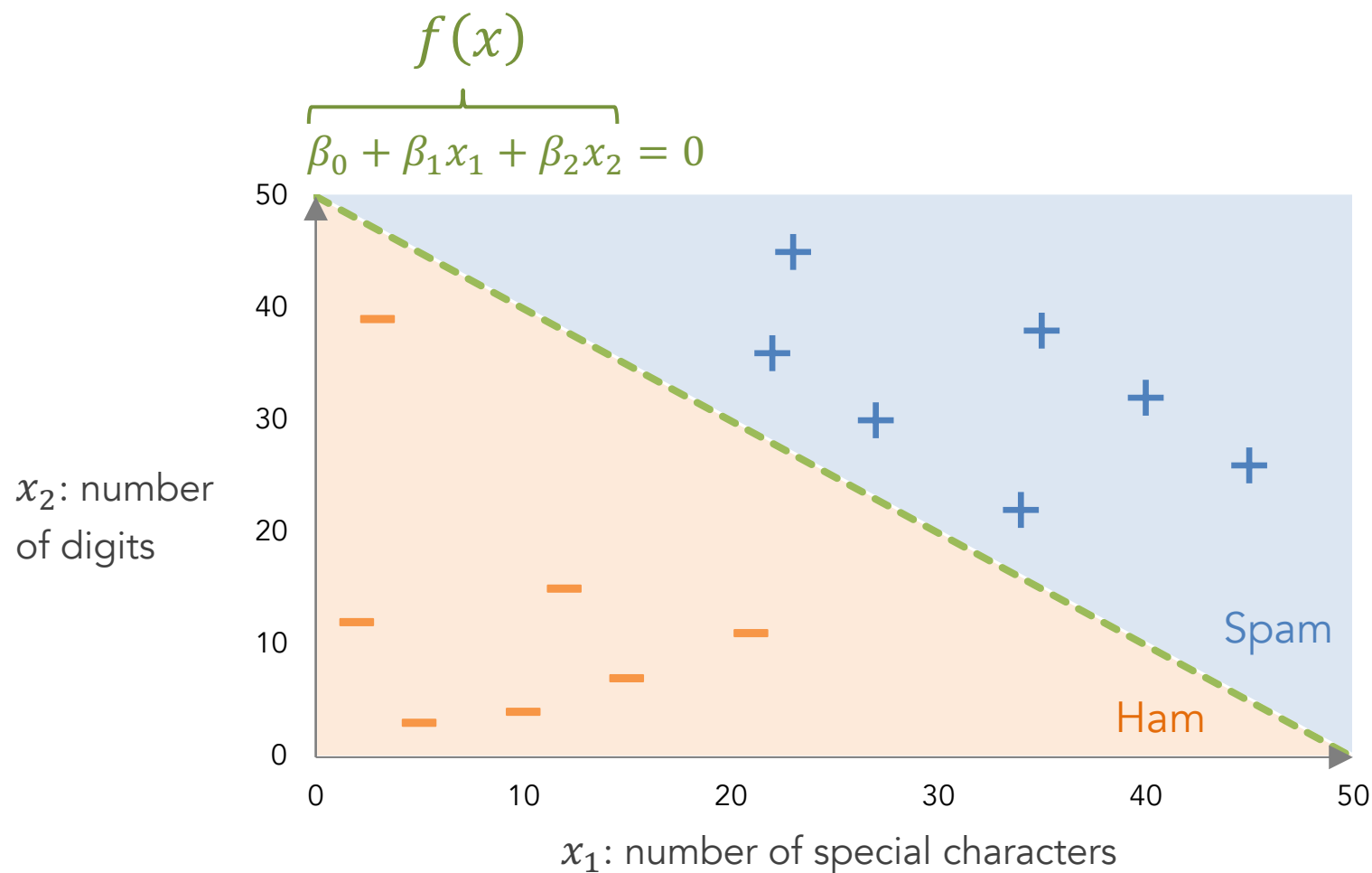
Classification

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).

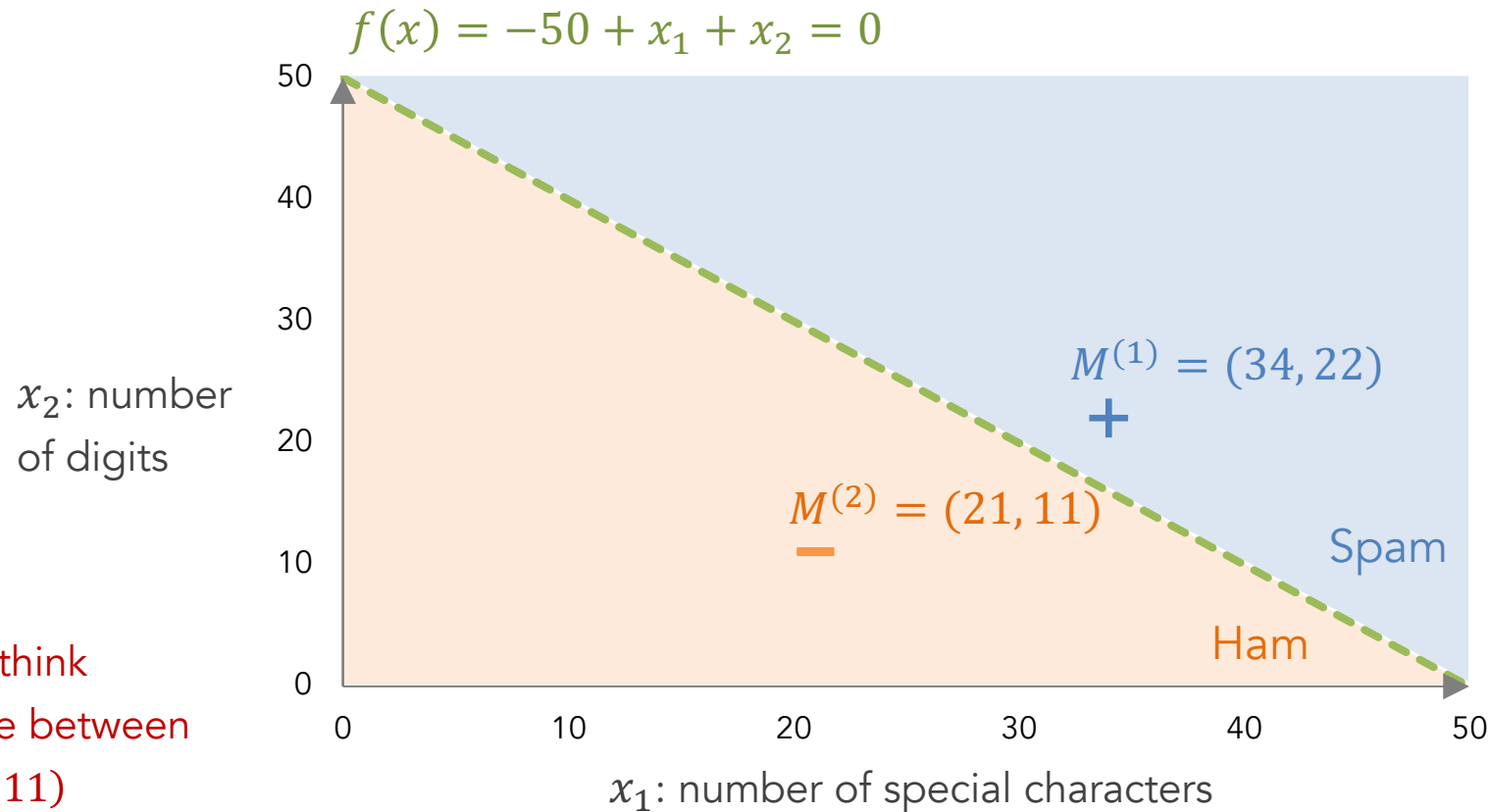


Classification

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



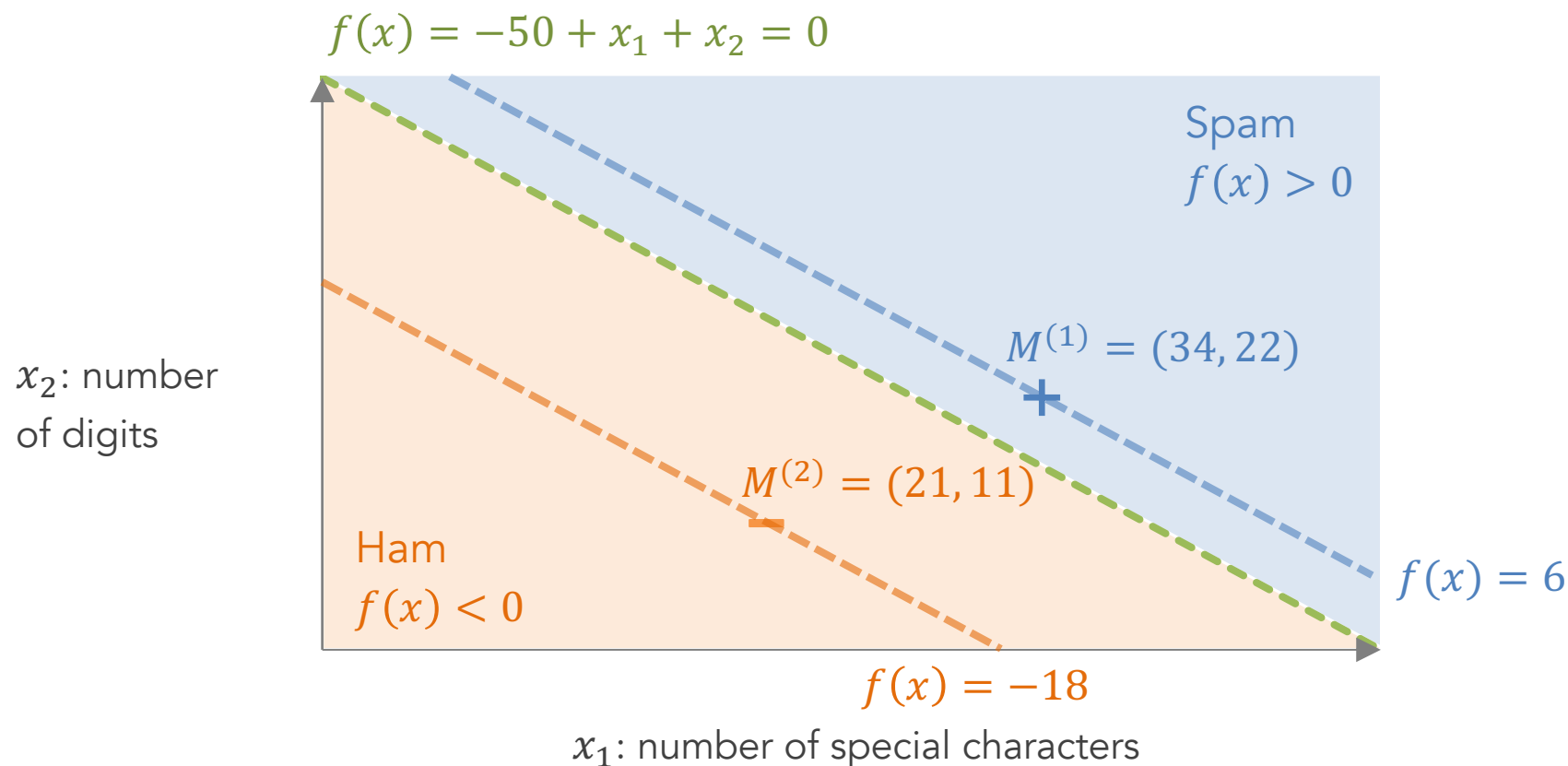
Exercise 2.1: Given a classifier $f(x) = -50 + x_1 + x_2$ and two messages $M^{(1)}$ and $M^{(2)}$, explain how the model classifies the message as spam or ham mathematically. $M^{(1)}$ has 34 special characters and 22 digits. $M^{(2)}$ has 21 special characters and 11 digits.



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

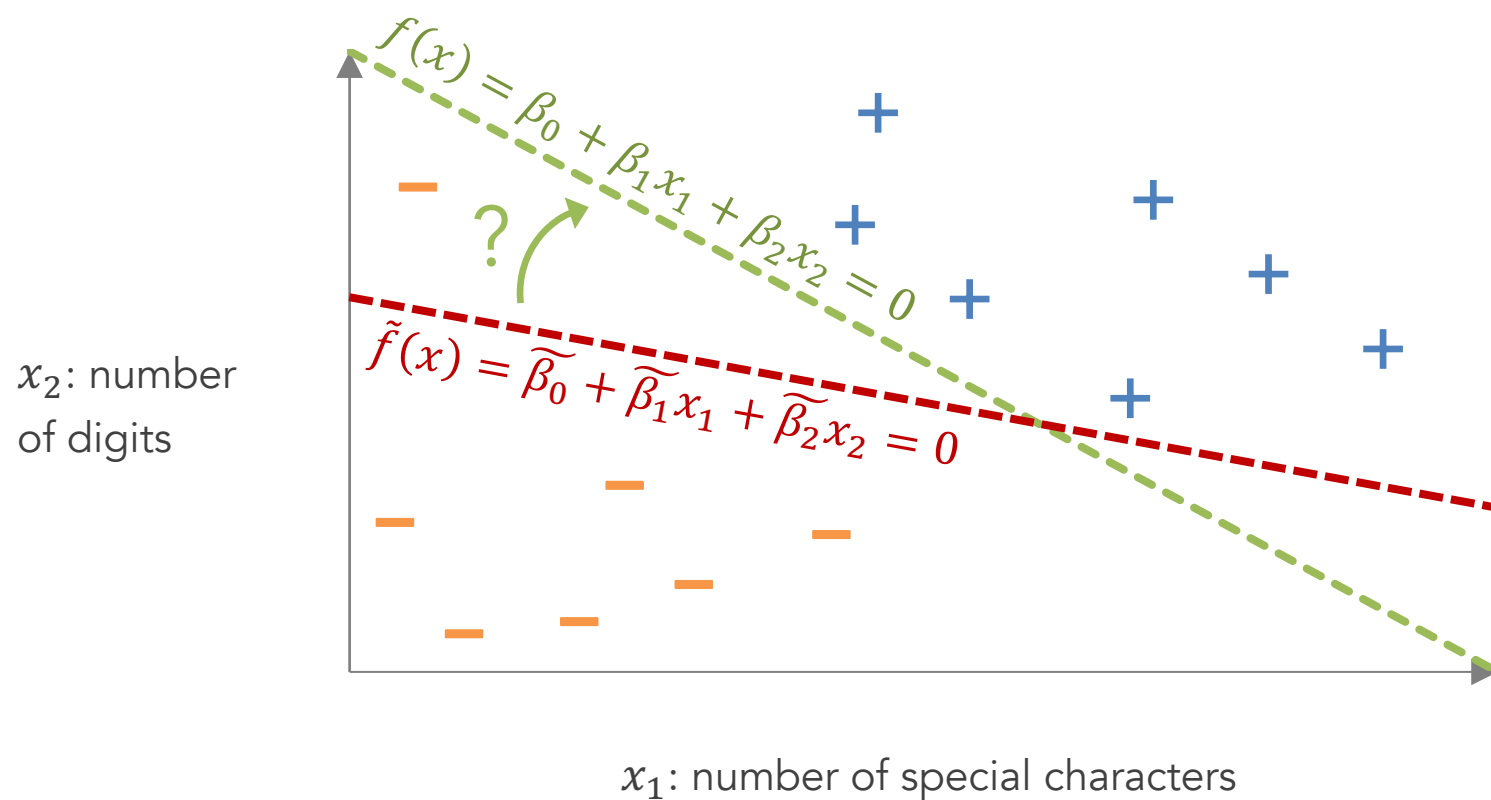
Classification

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

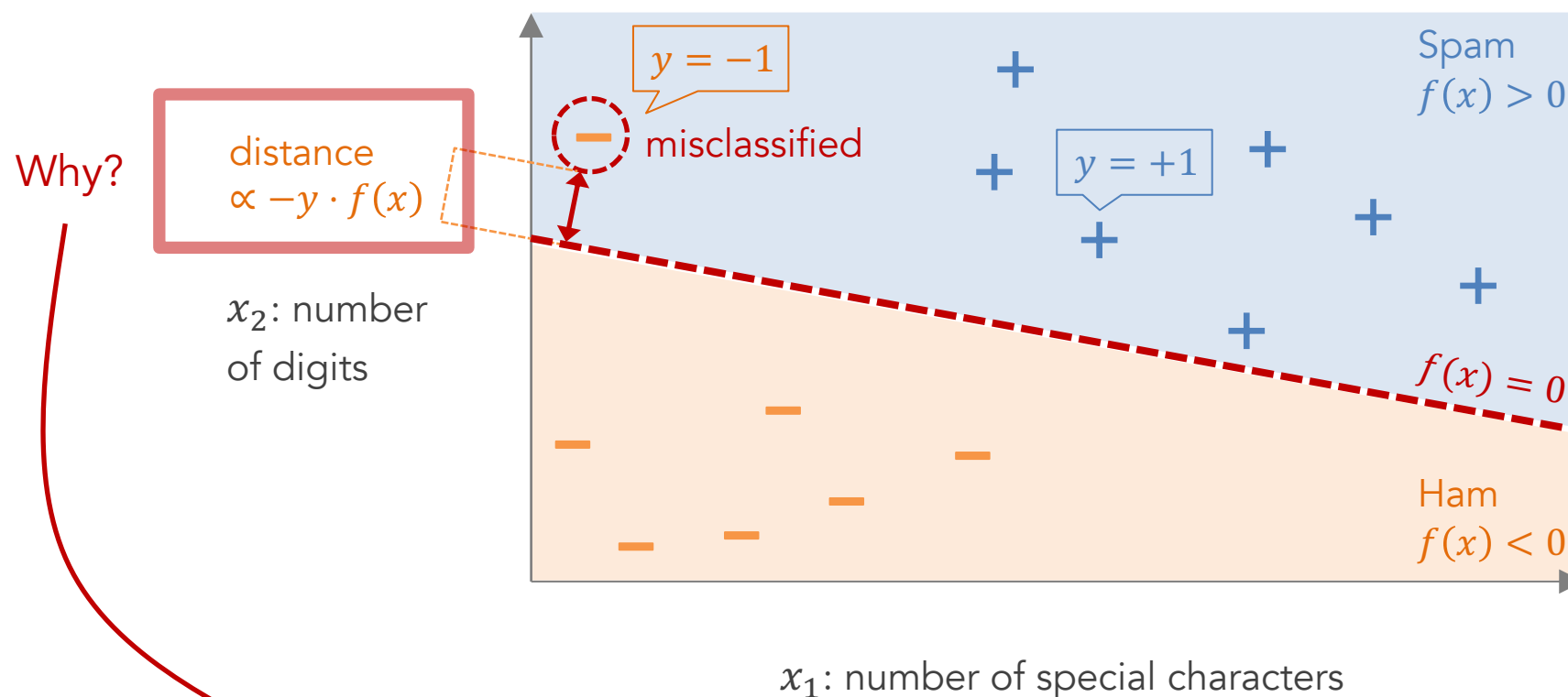
To find a good function f , we start from some f and **train it** until satisfied. We need something to tell us **which direction and magnitude** to update.



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 .

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

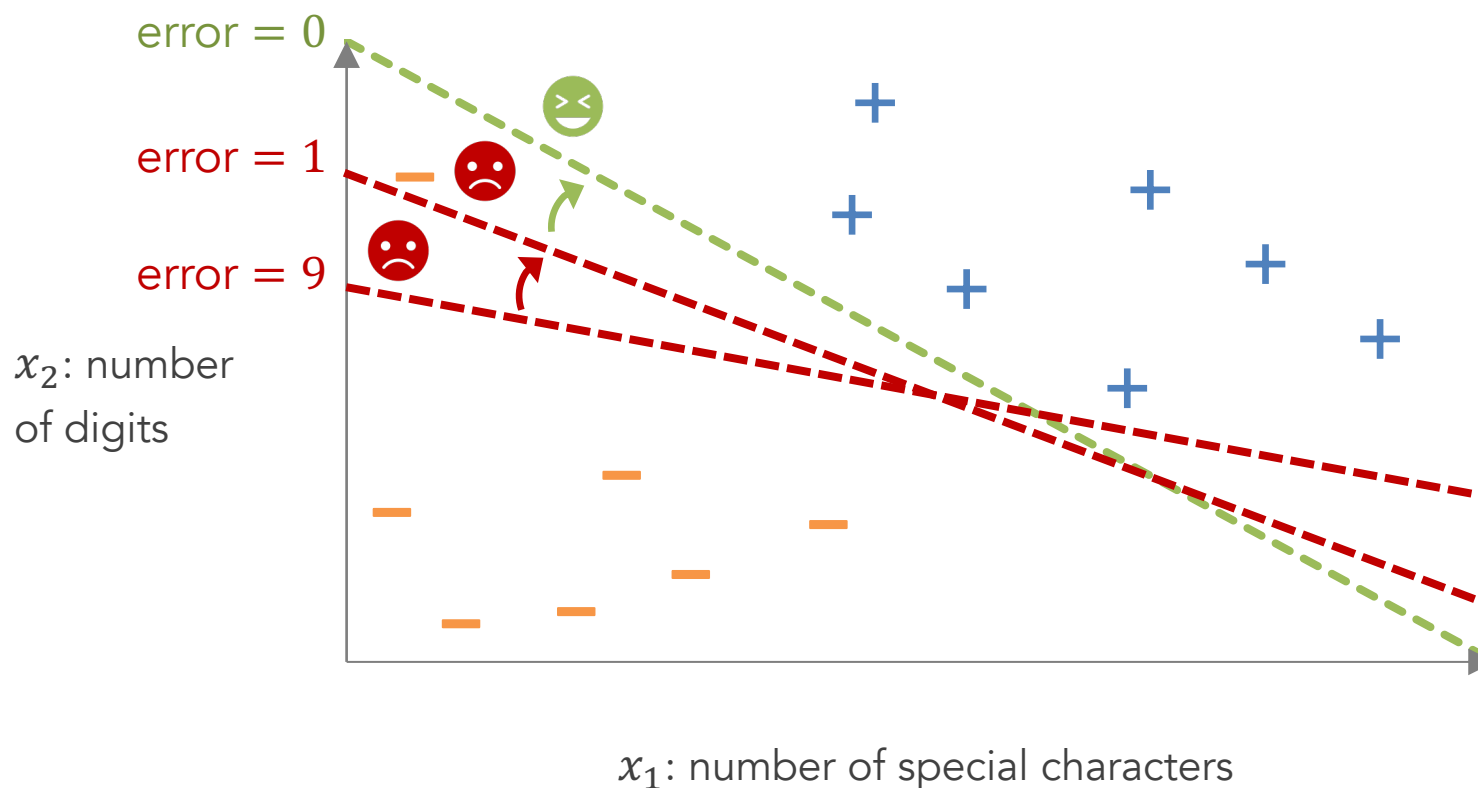


Distance from point to plane: https://mathinsight.org/distance_point_plane

Classification

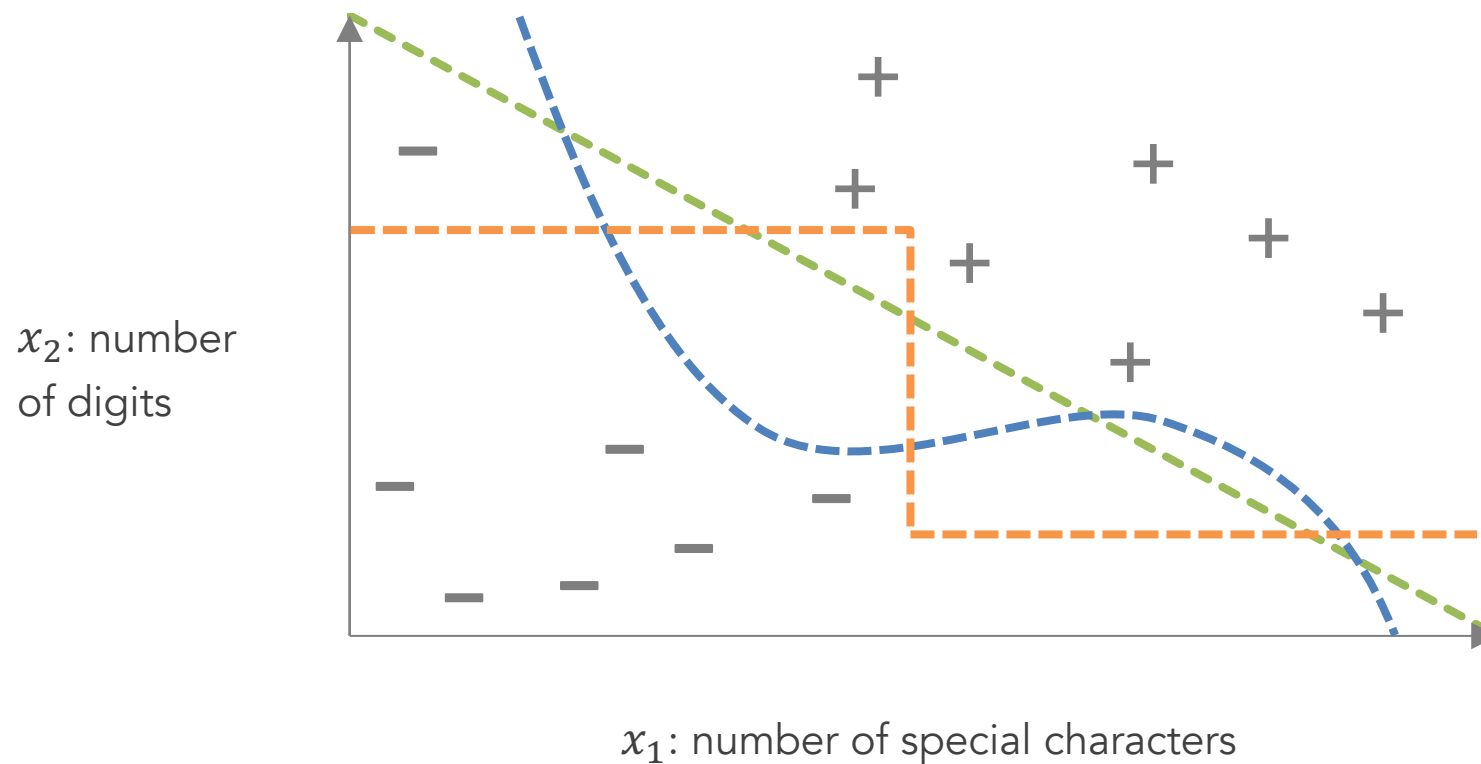
We can use gradient descent (an optimization algorithm) to **minimize the error** to train the model f iteratively. This example is the Perceptron algorithm.

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



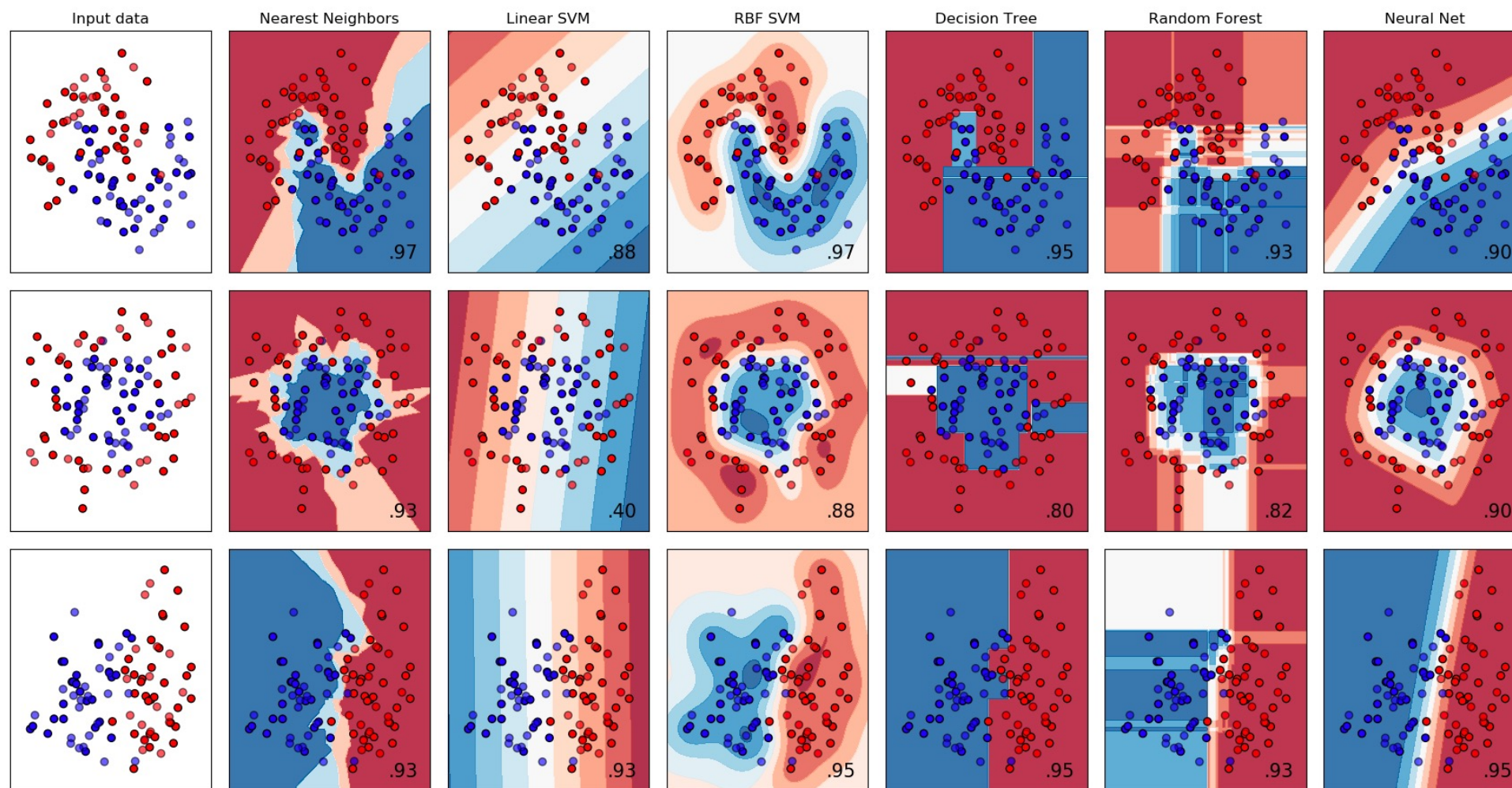
Classification

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



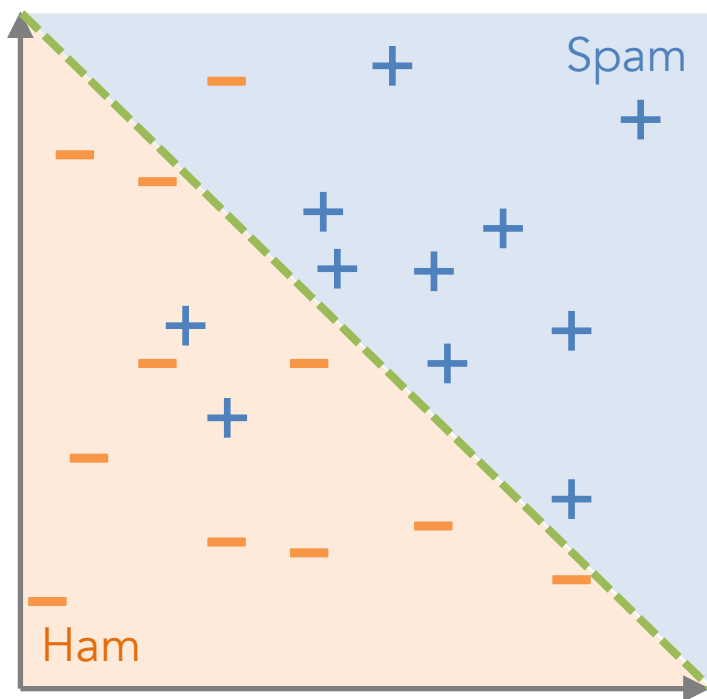
Classification

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



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.



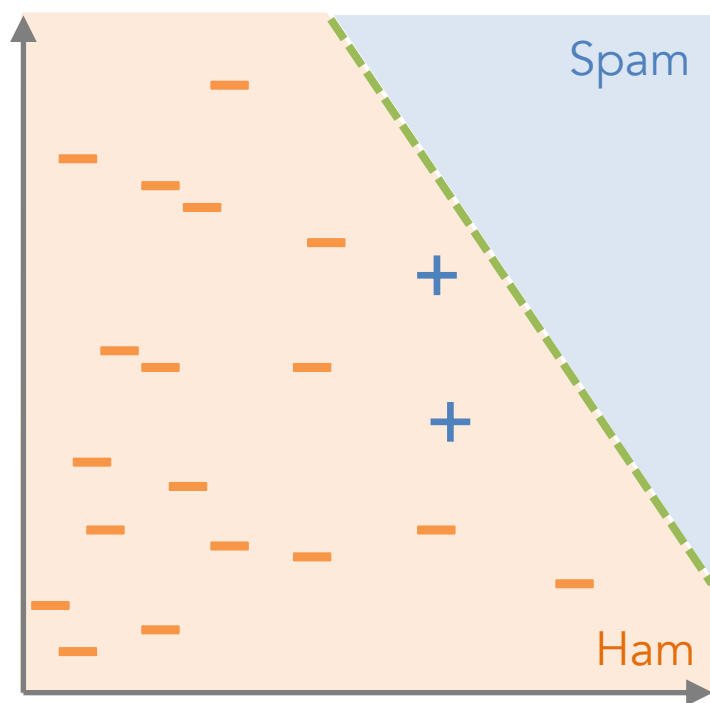
Accuracy for all data

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

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

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

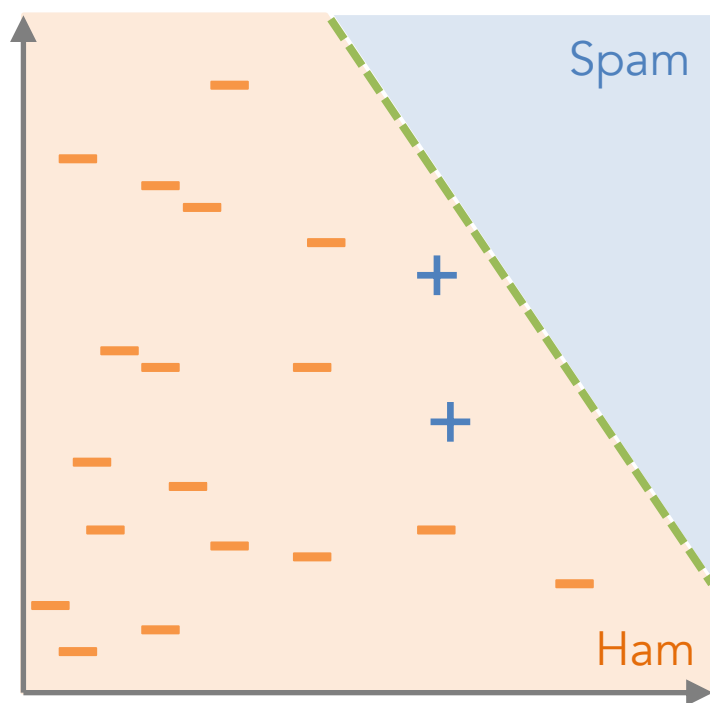
Accuracy for all data

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

$$= \frac{18}{20} = 0.9 \quad \text{☹️}$$

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.



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

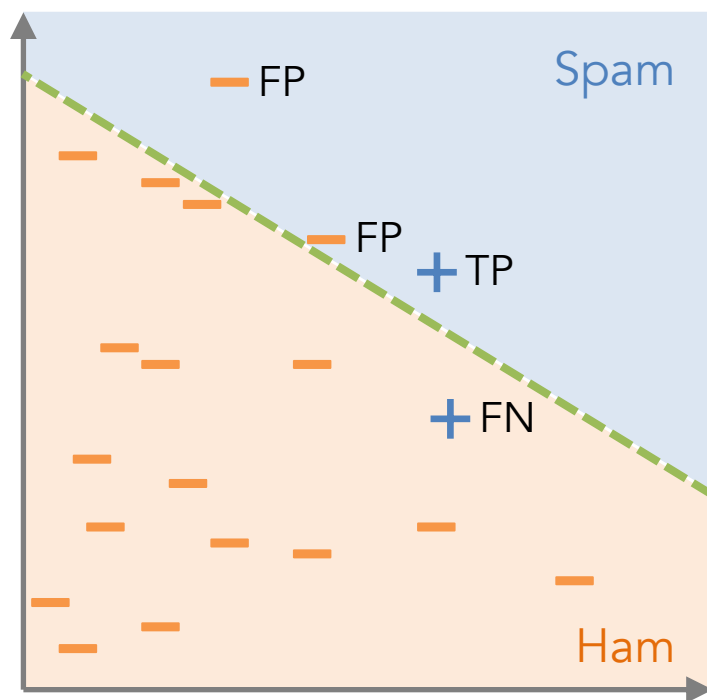
(true positive rate, recall, sensitivity)

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

(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.



TP = 1 (True Positive)

FP = 2 (False Positive)

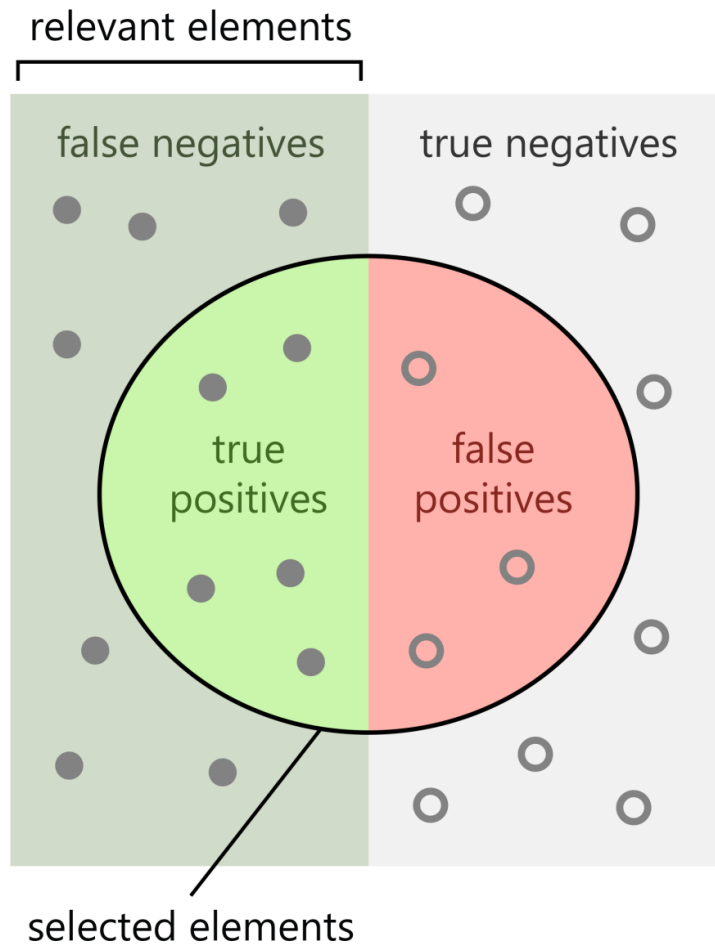
FN = 1 (False Negative)

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

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

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?

$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

How many relevant items are selected?

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

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

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?

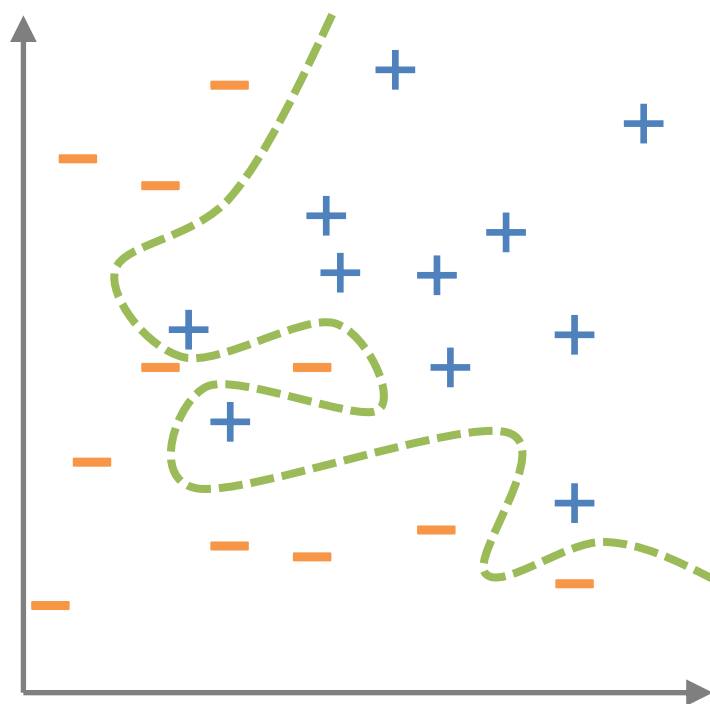
$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

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

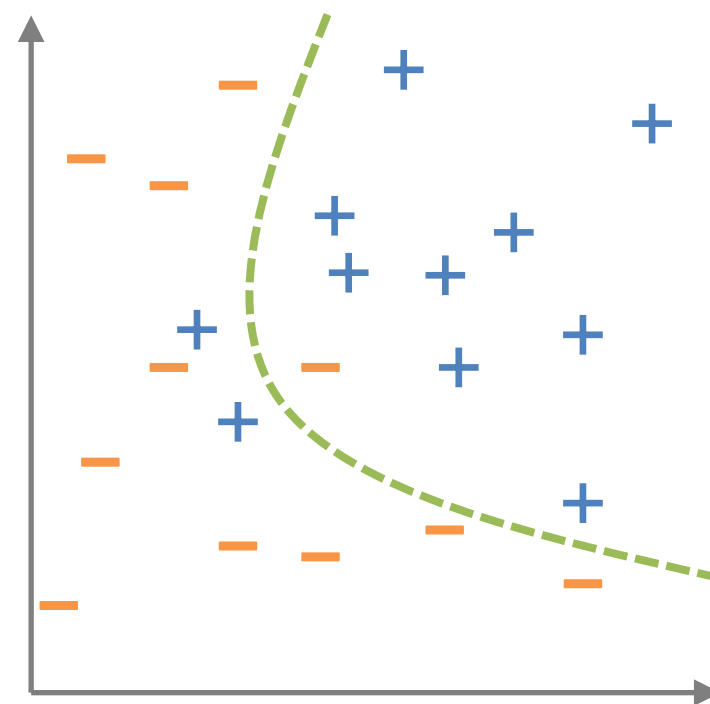
$$F = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

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?



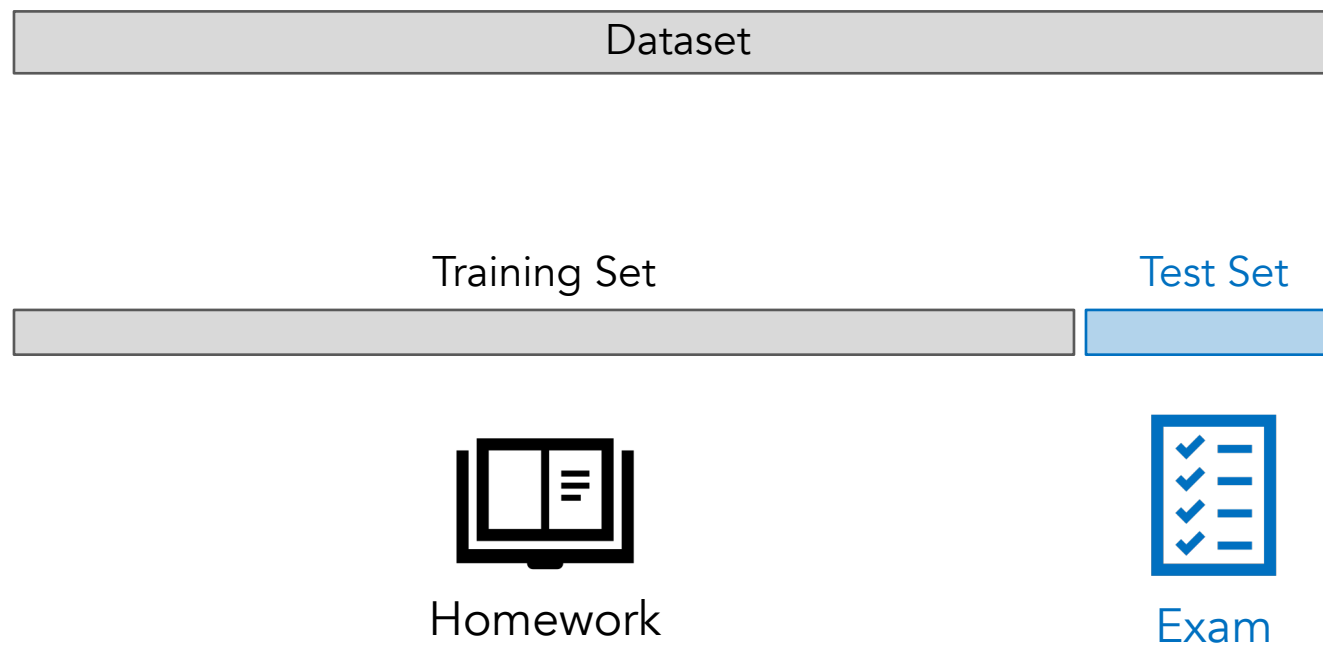
Model A



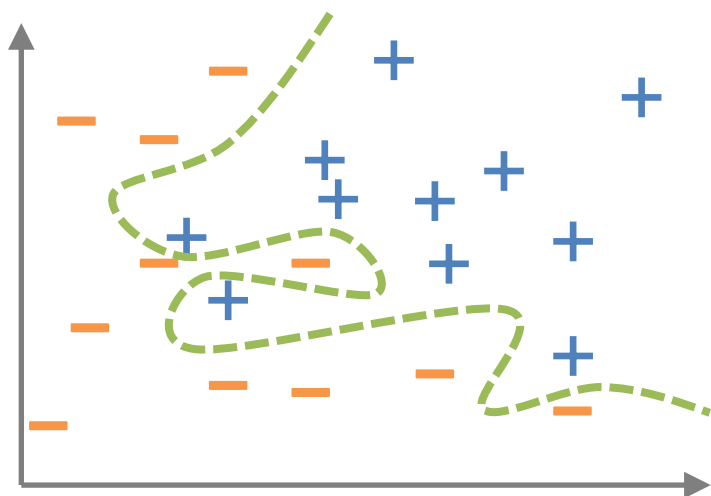
Model B

Model Training

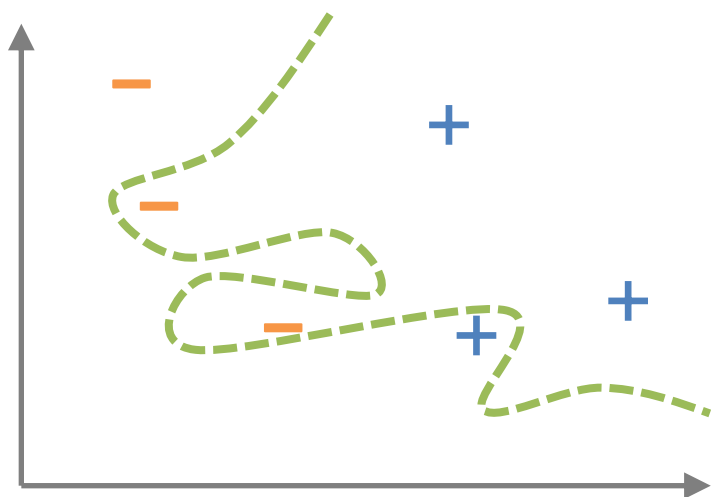
To choose models, we need a **test set**, which contains data that the models **have not yet seen before** during the training phase.



☹️ Model A

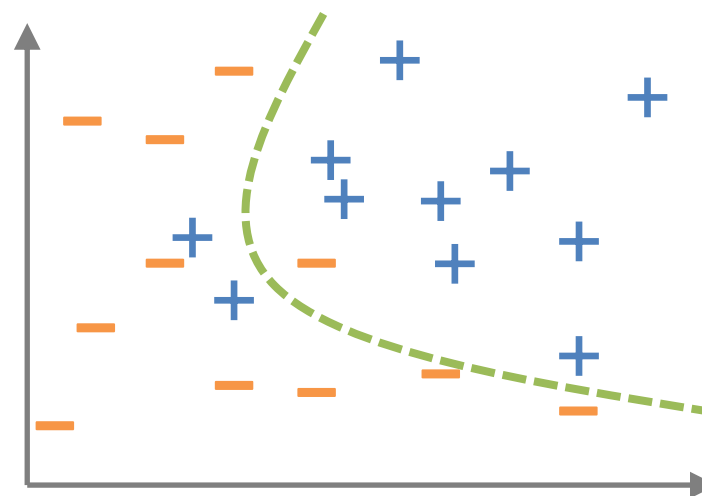


Training Accuracy = 1

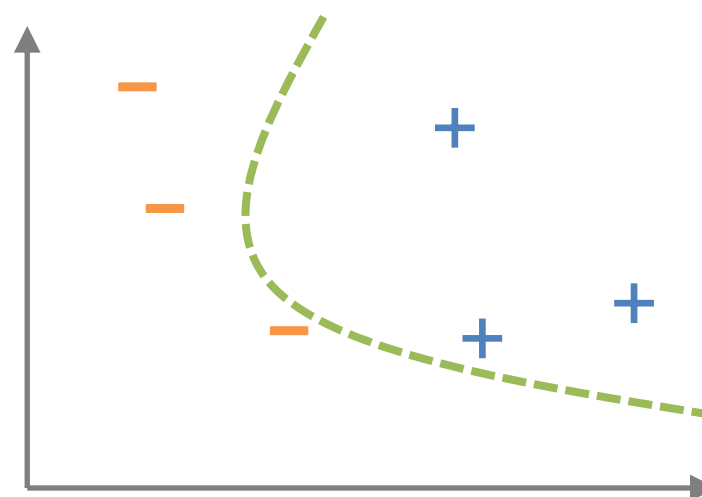


Testing Accuracy = 0.5

😊 Model B



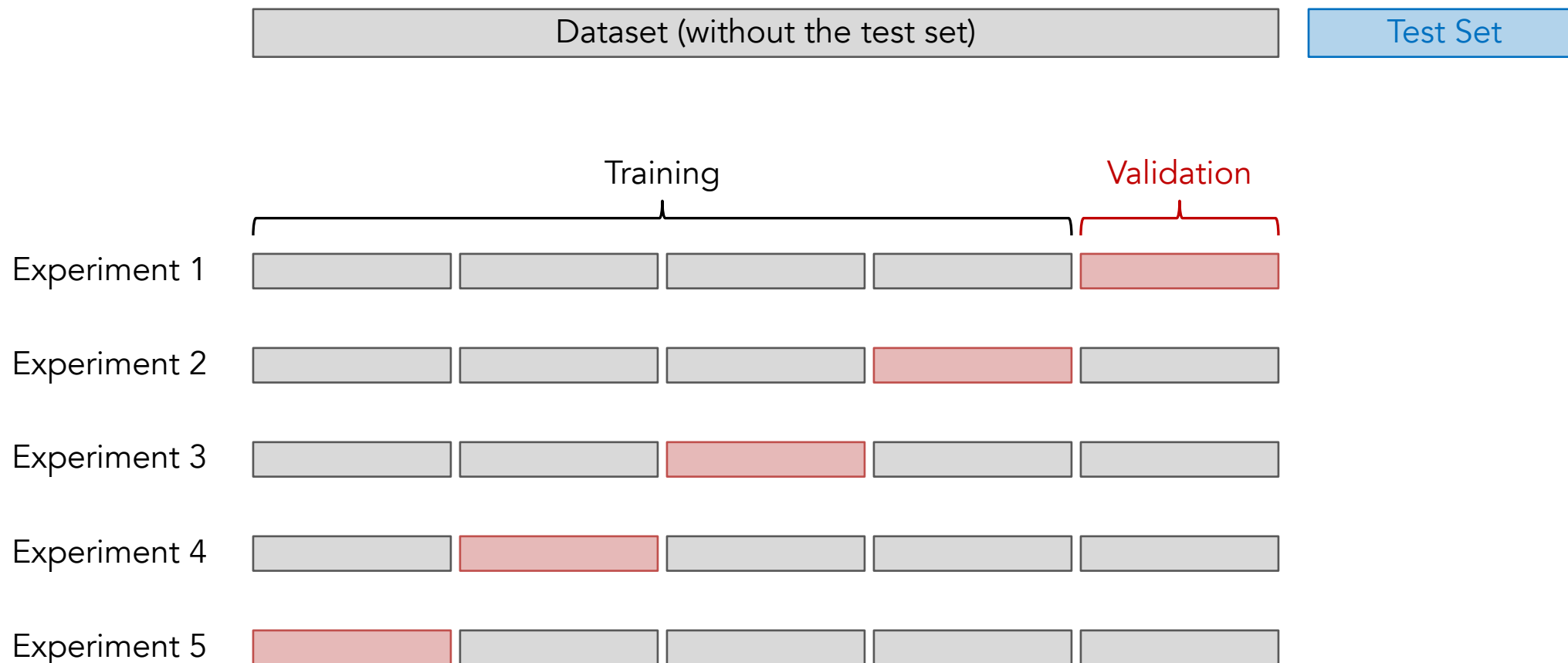
Training Accuracy = 0.86



Testing Accuracy = 1

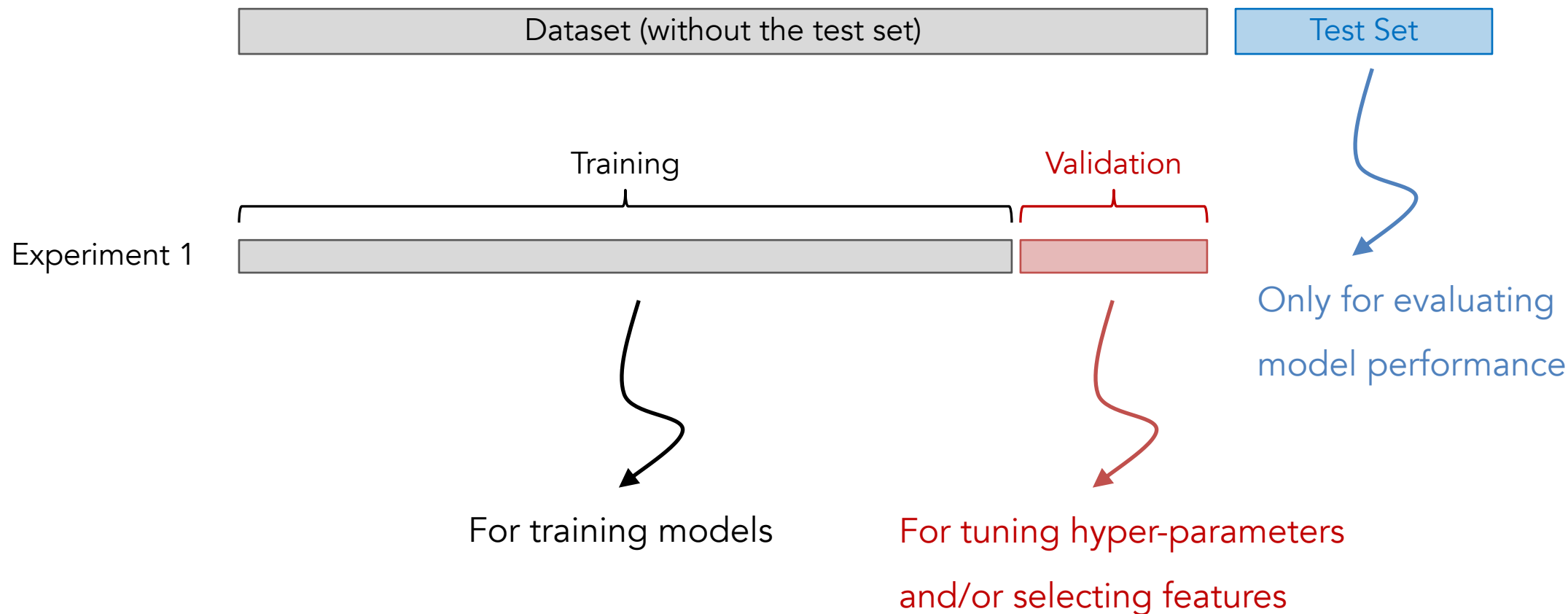
Model Training

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.



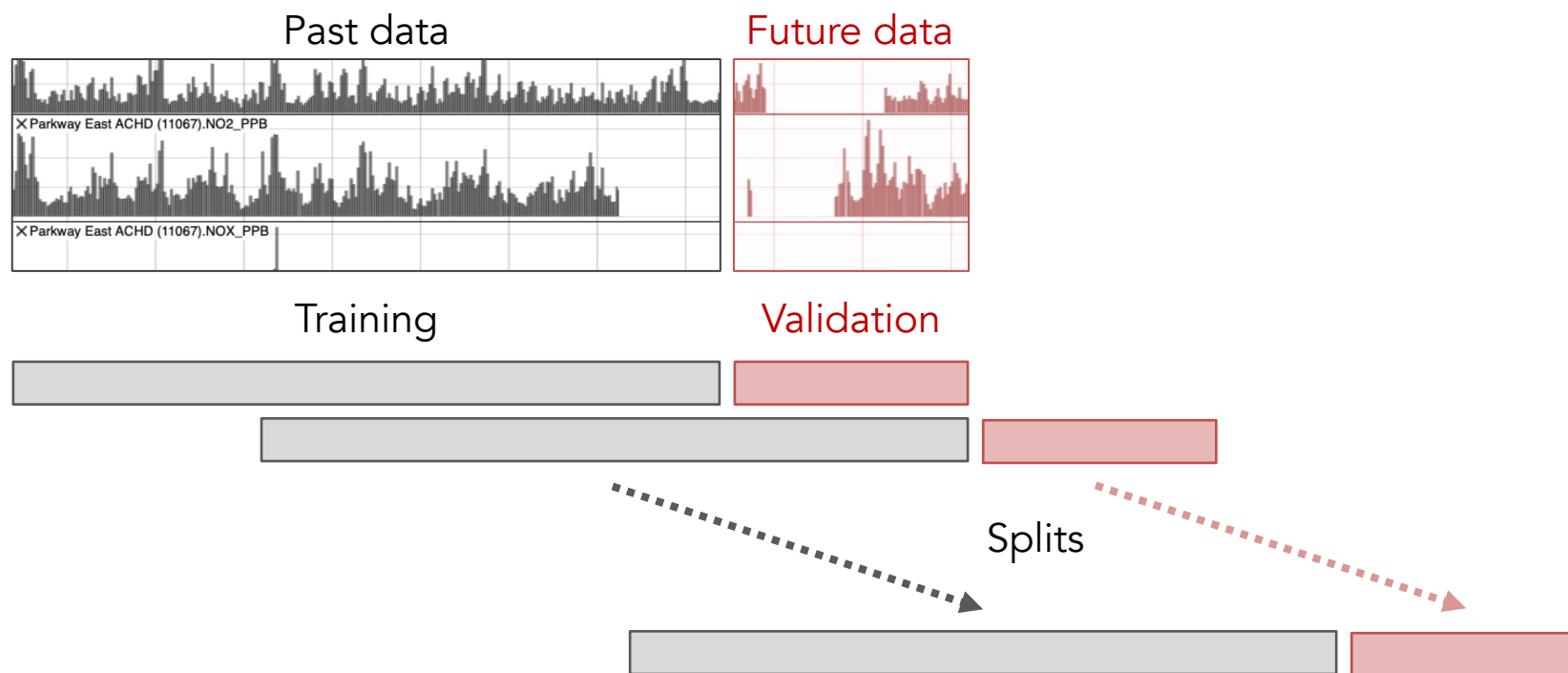
Model Training

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.



Model Training

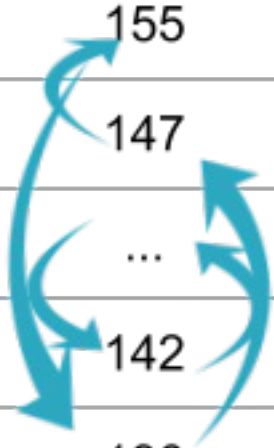
For time-series data, it is better to do the split for cross-validation **based on the order of time intervals**, which means we only use data in the past to predict the future, but not the other way around.



Feature Selection

To select features, we need to know their importances. One way to compute feature importance is to first **shuffle a feature randomly** and then measure the decrease in model performance (i.e., permutation importance).

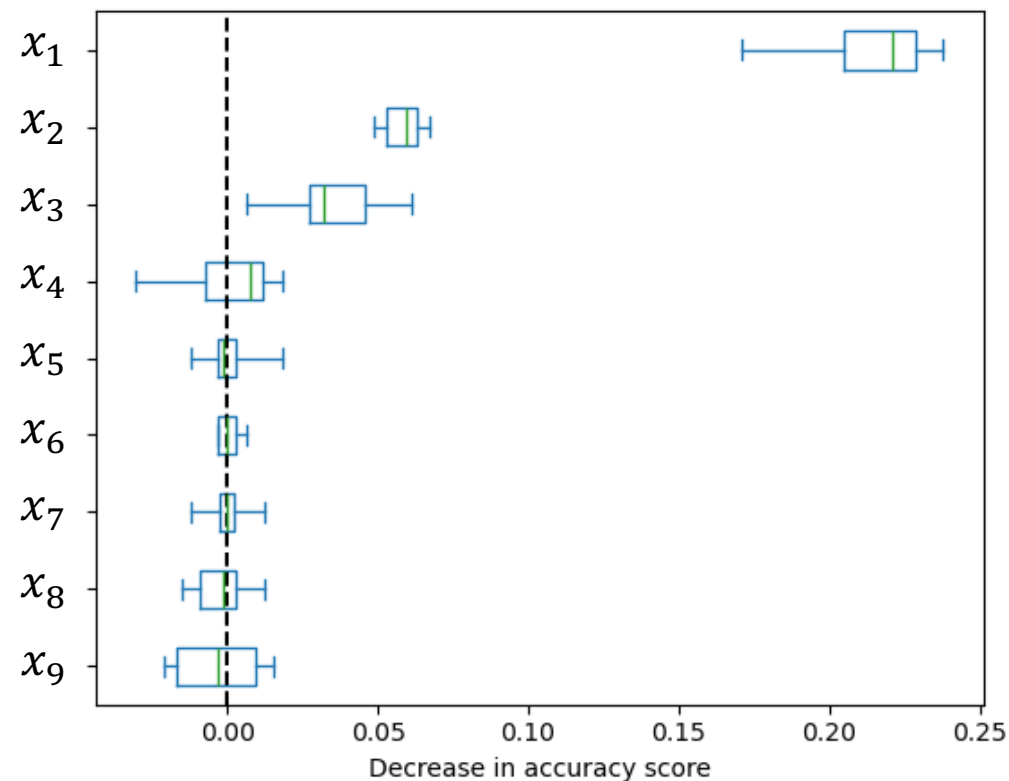
Height at age 20 (cm)	Height at age 10 (cm)	...	Socks owned at age 10
182	155	...	20
175	147	...	10
...
156	142	...	8
153	130	...	24



Feature Selection

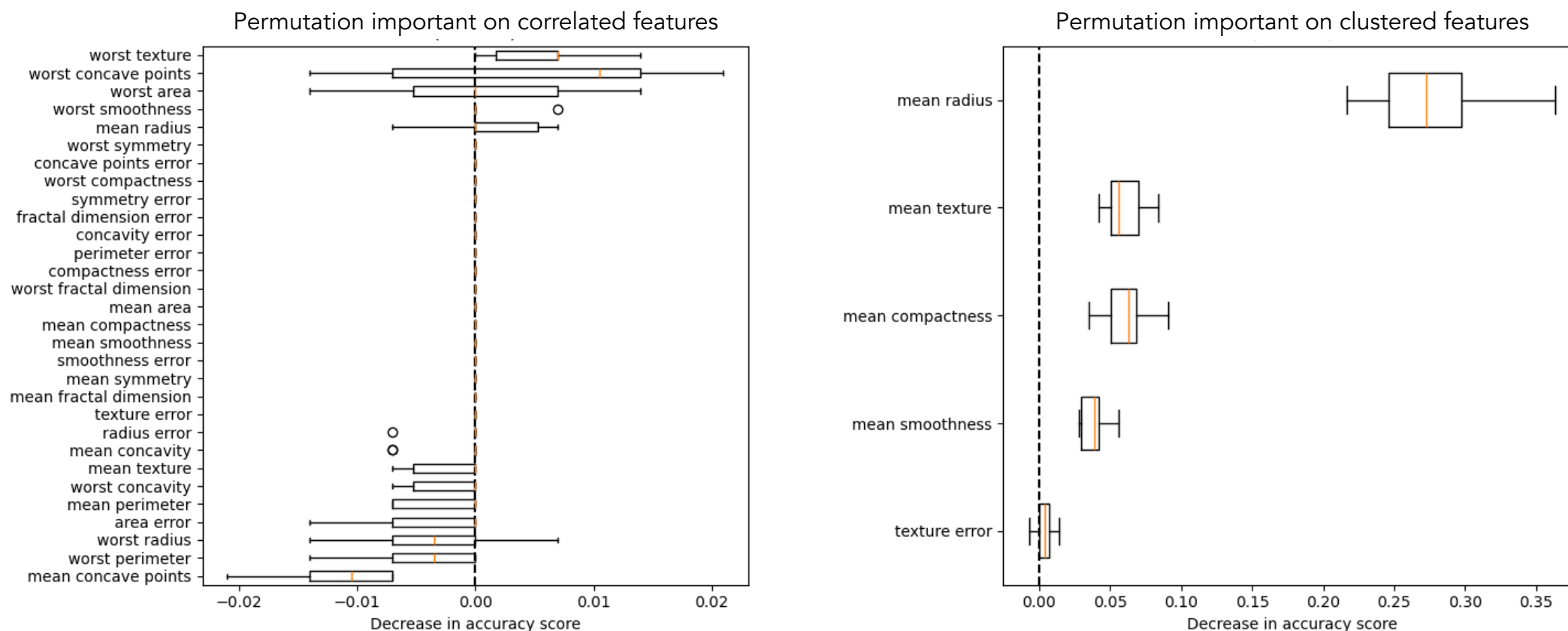
One way to select features is to **recursively eliminate** the feature with the lowest permutation importance score.

We repeat the permutation and compute the decrease of model performance for multiple times. Why?



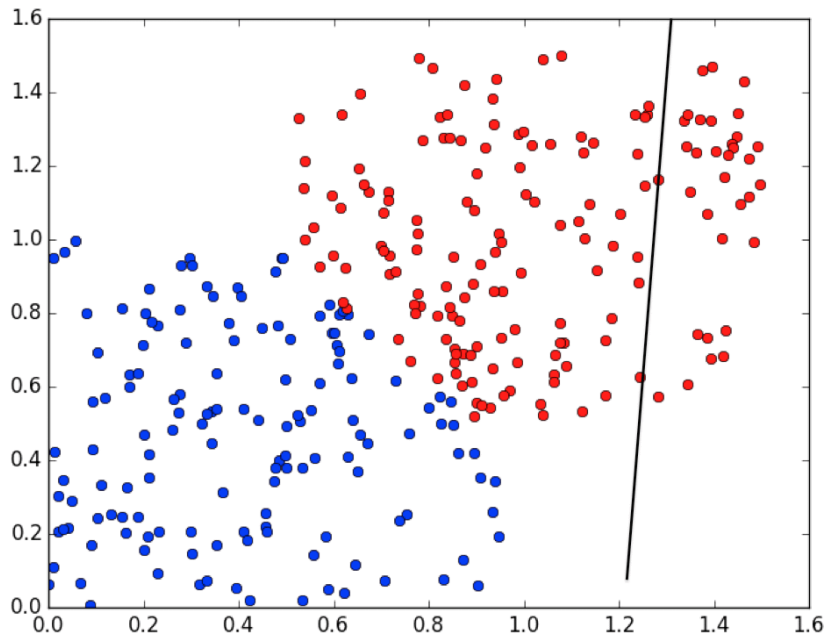
Feature Selection

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.

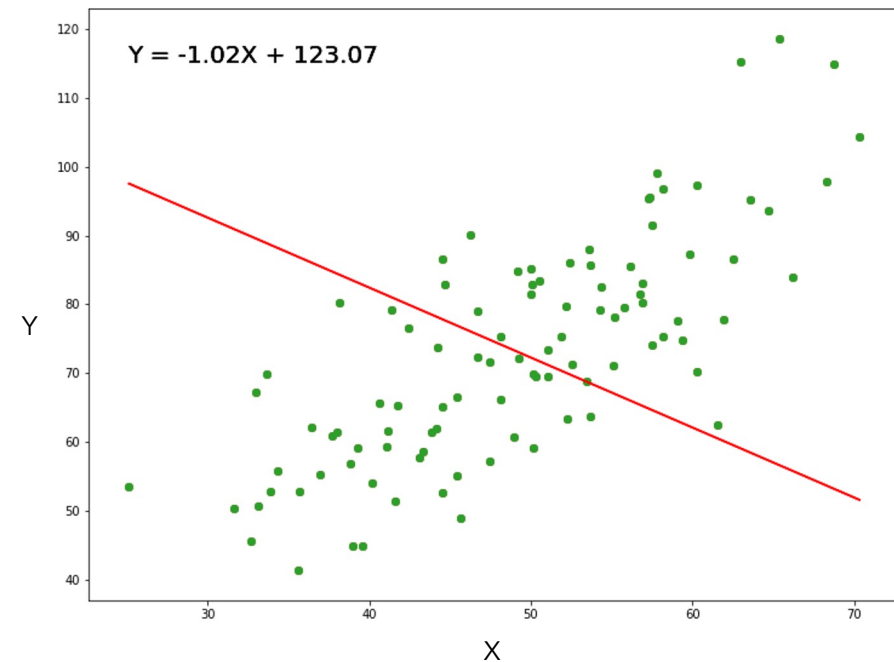


Regression

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



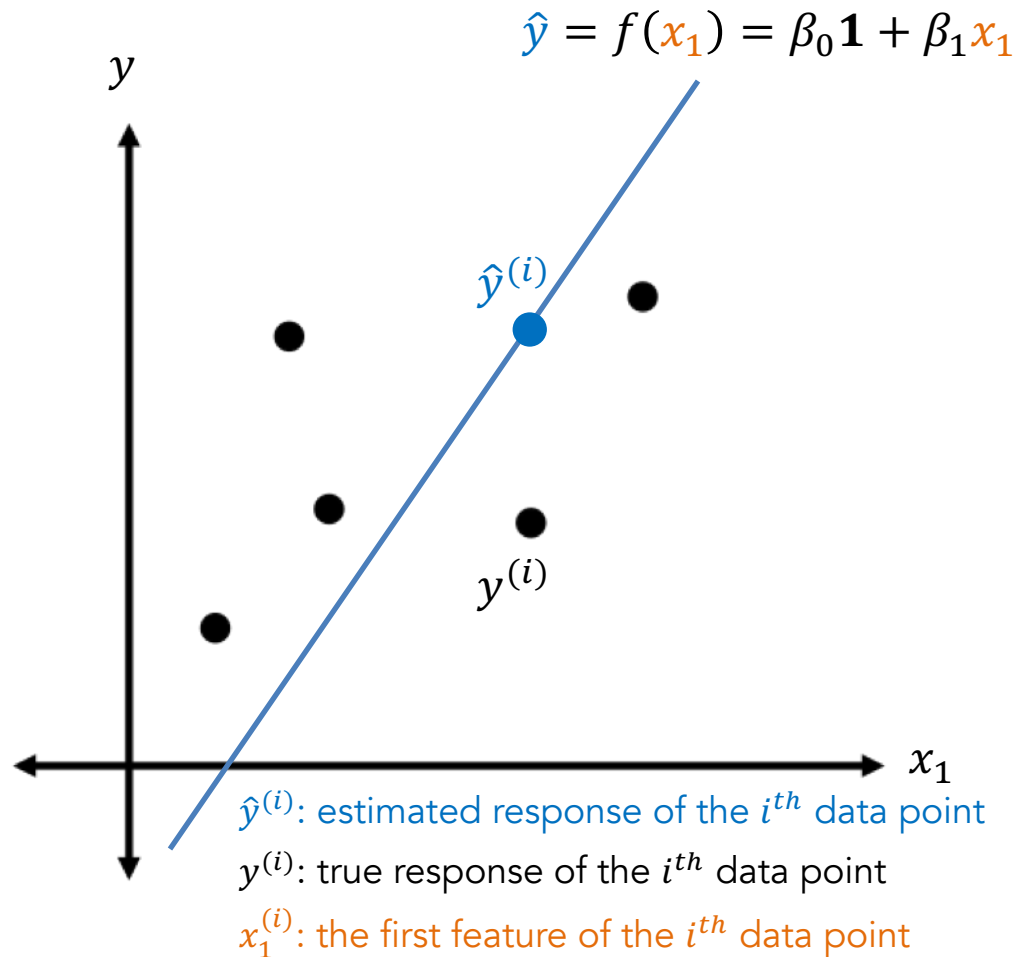
- [Classification] How can we fit a function that separates data points into different groups?



- [Regression] How can we fit a function that maps features (input) to a continuous variable (output)?

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.



y : true response

\hat{y} : estimated response

x_1 : predictor/feature

β_0 and β_1 : intercept and slope

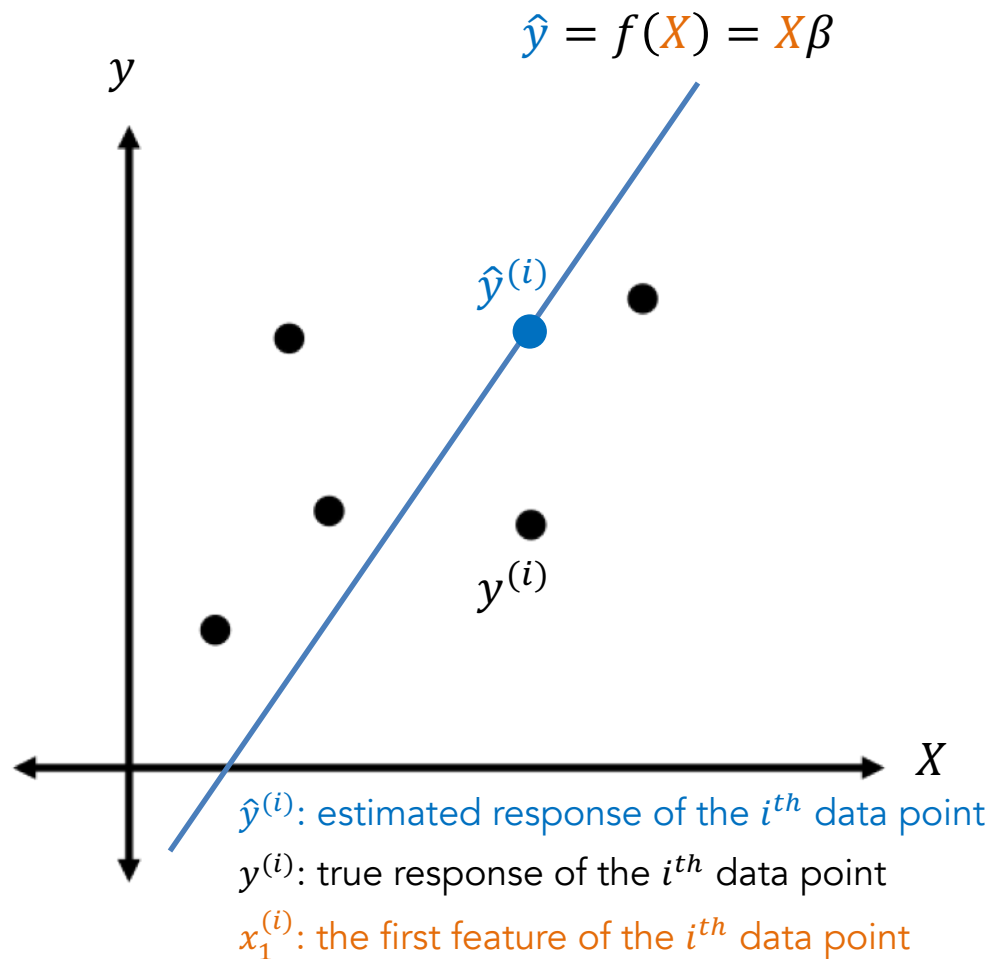
$$\begin{bmatrix} \hat{y}^{(1)} = f(x_1^{(1)}) = \beta_0 \cdot 1 + \beta_1 \cdot x_1^{(1)} \\ \vdots \\ \hat{y}^{(n)} = f(x_1^{(n)}) = \beta_0 \cdot 1 + \beta_1 \cdot x_1^{(n)} \end{bmatrix}$$

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

\hat{y} $\mathbf{1}$ 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.



y : true response (vector)

\hat{y} : estimated response (vector)

X : predictor/feature (matrix)

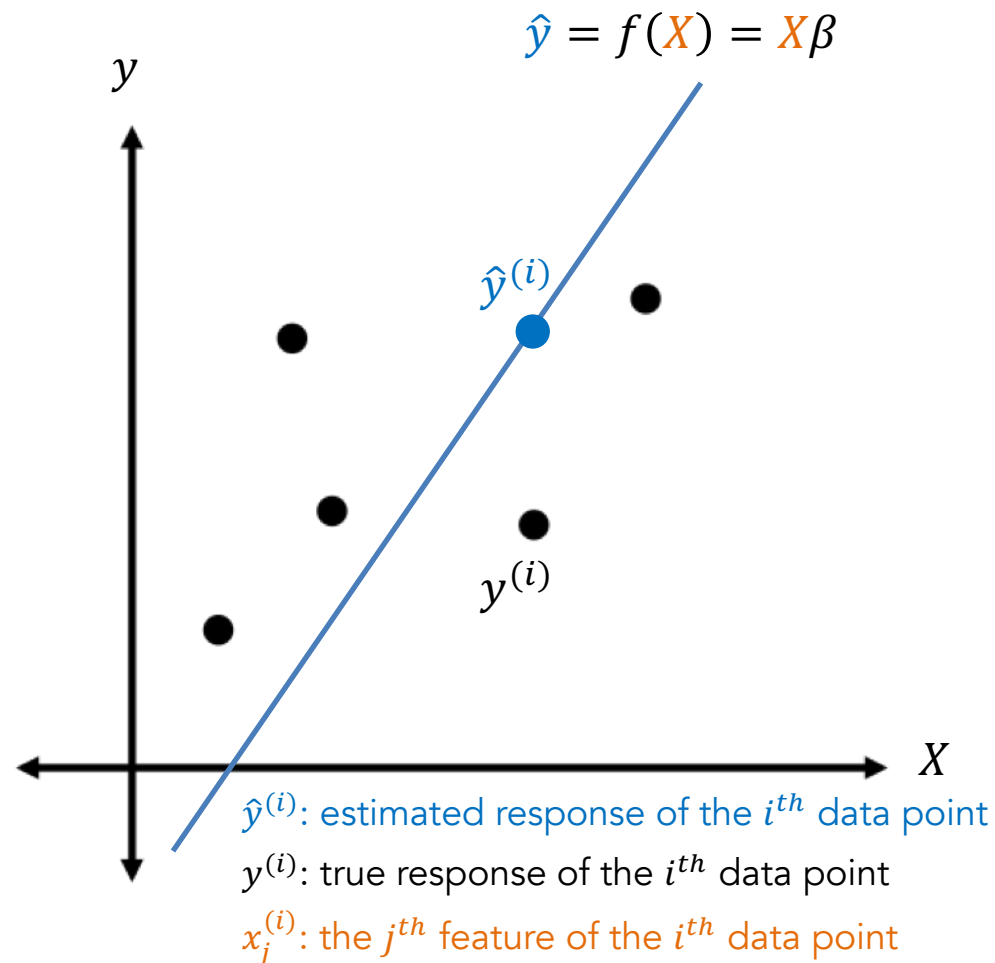
β : coefficients (vector)

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

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

Regression

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



y : true response (vector)

\hat{y} : estimated response (vector)

X : predictor/feature (matrix)

β : coefficients (vector)

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

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

We use the vector and matrix forms to simplify equations.

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

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

Vector

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

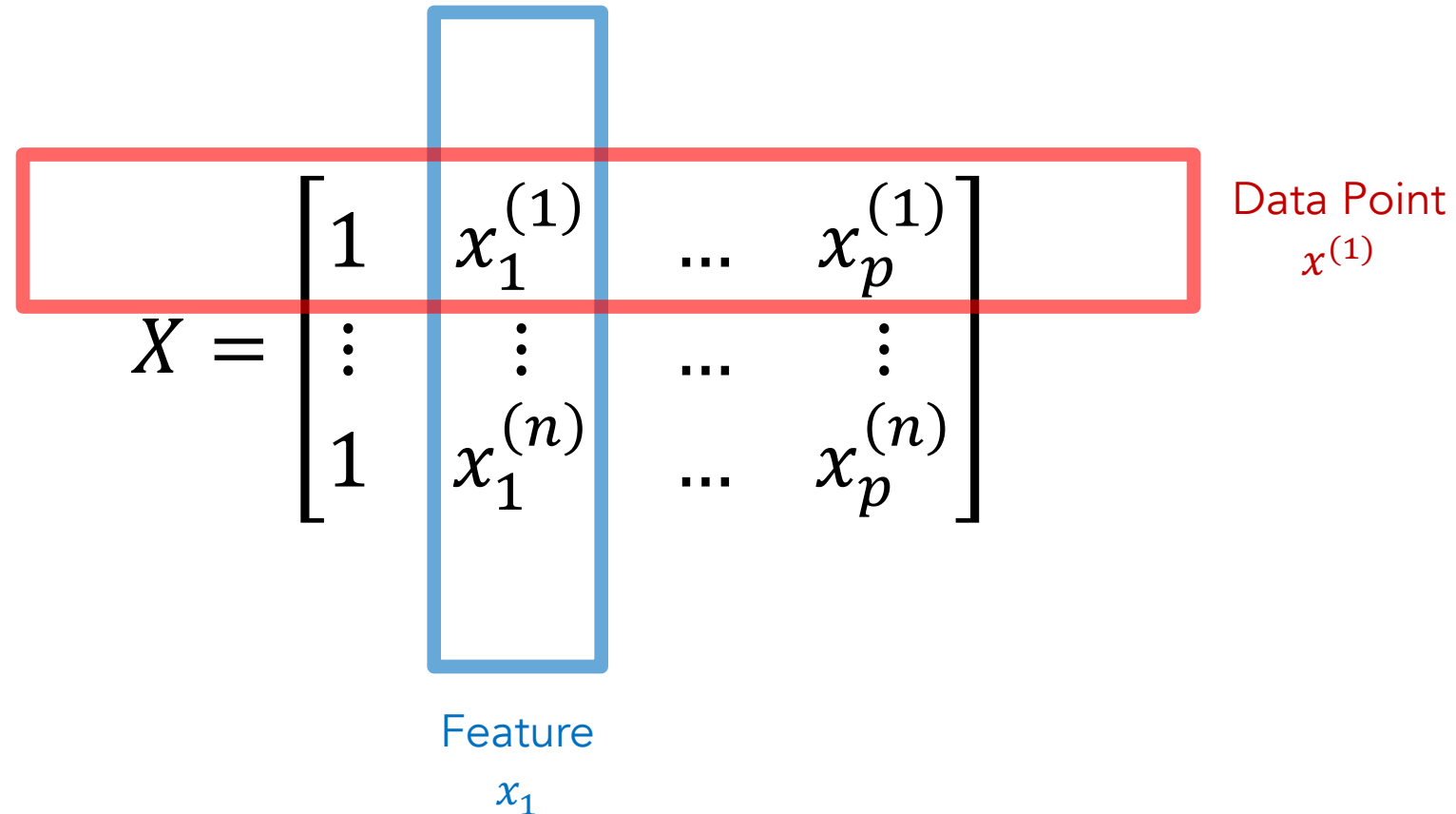
Regression

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

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

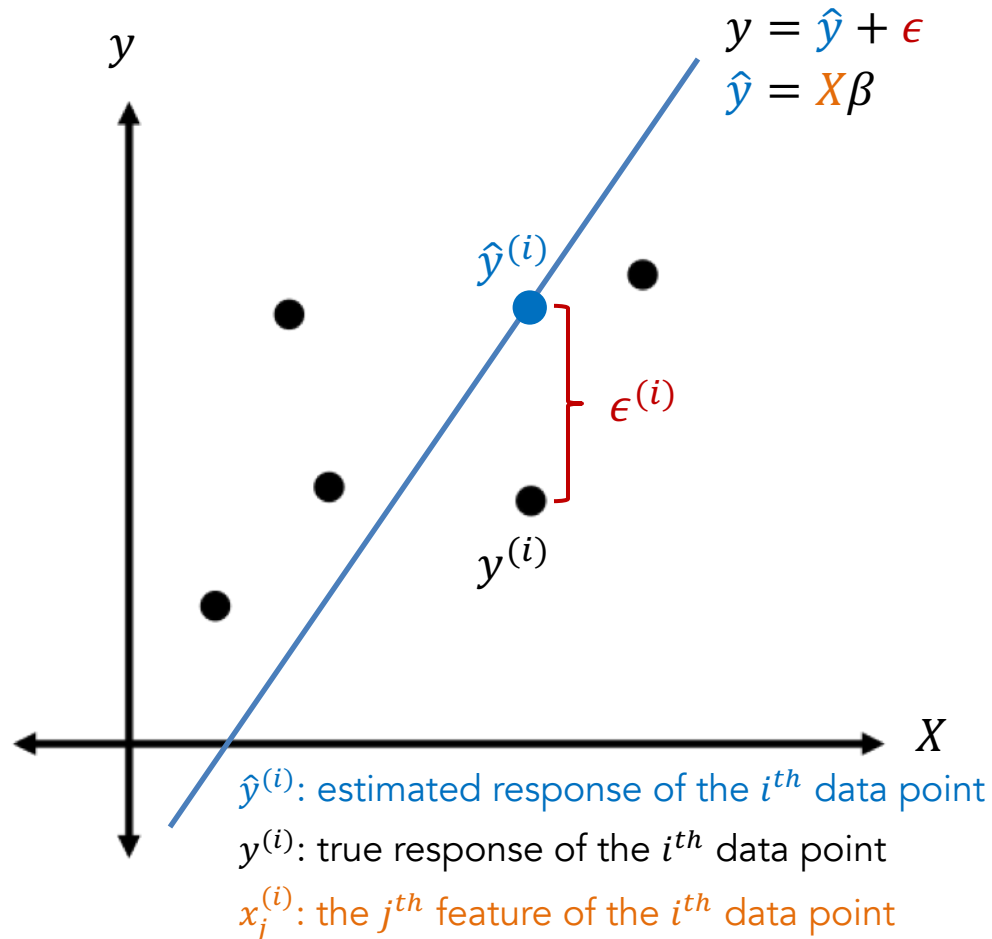
Feature
 x_1

Data Point
 $x^{(1)}$

The diagram shows the feature matrix X as a grid of values. A blue vertical rectangle highlights the first column, which contains the values 1, x1^(1), ..., x1^(n). Below this rectangle is the label 'Feature x1'. A red horizontal rectangle highlights the first row, which contains the values 1, x1^(1), ..., xp^(1). To the right of this rectangle is the label 'Data Point x^(1)'. The matrix is enclosed in large square brackets, and the elements are separated by commas and ellipses to indicate the continuation of the matrix.

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.



y : true response (vector)

\hat{y} : estimated response (vector)

X : predictor/feature (matrix)

β : coefficients (vector)

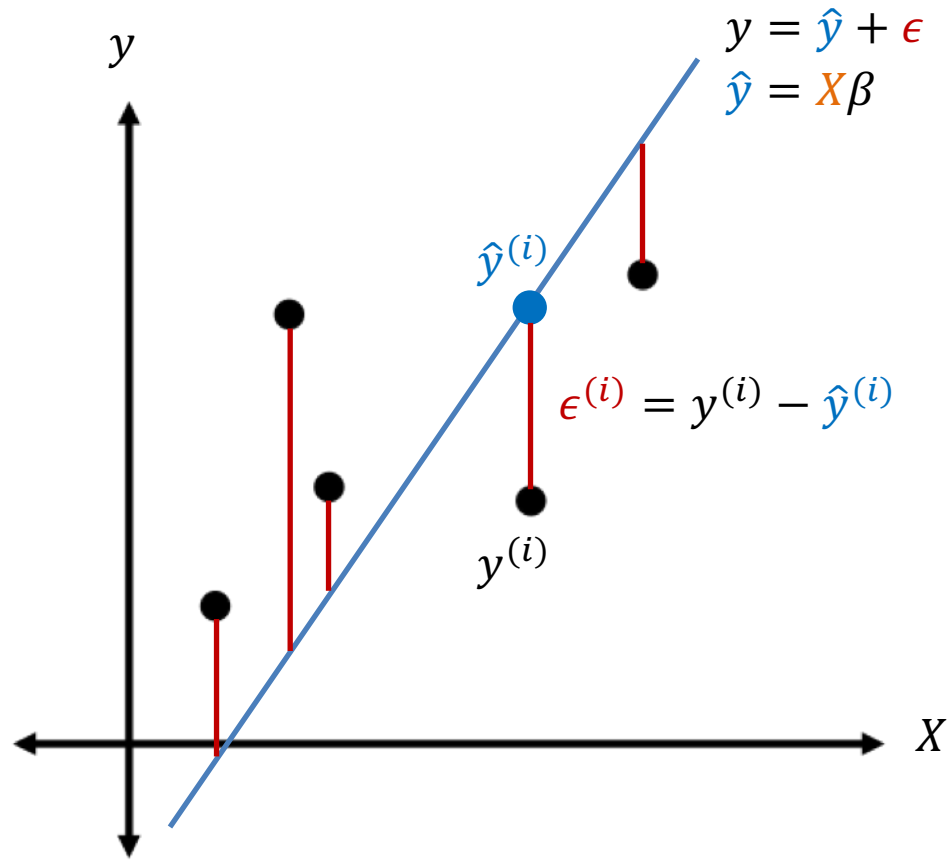
ϵ : error/noise/residual (vector)

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

X β

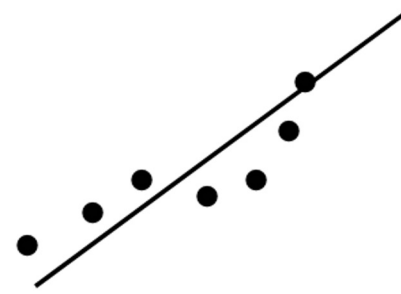
Regression

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 .

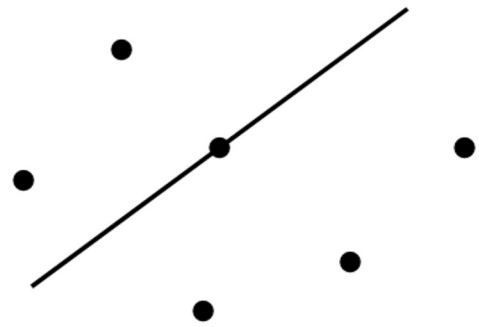


$$\epsilon \sim iid N(0, \sigma^2)$$

Small σ^2

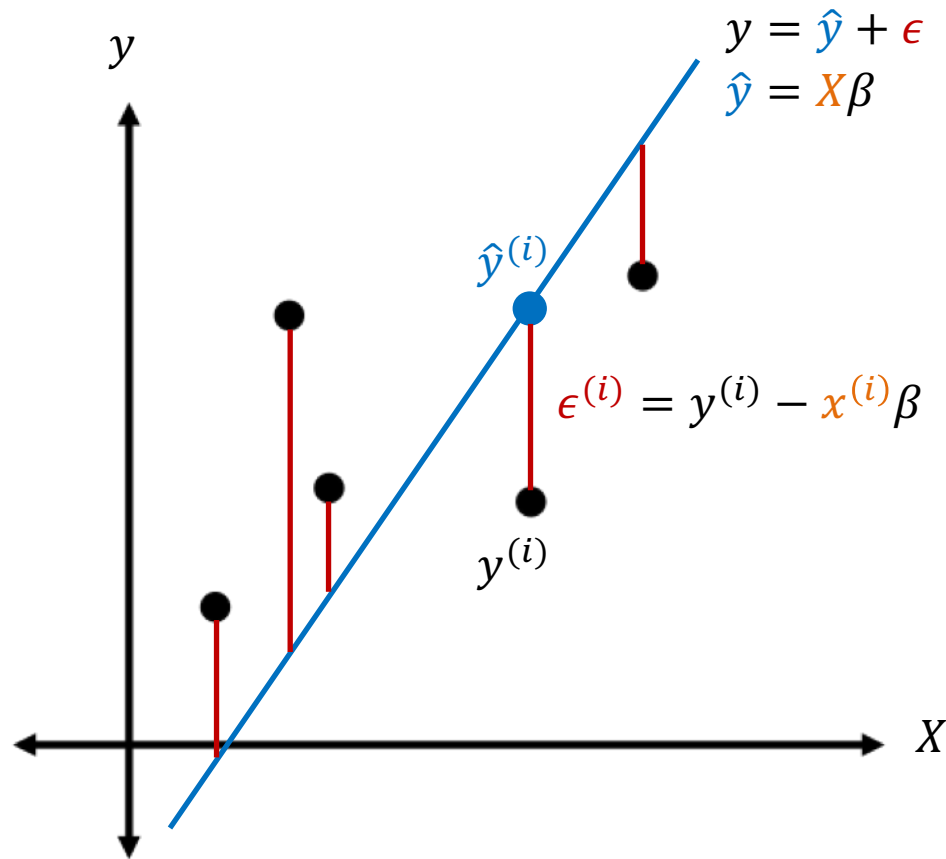


Large σ^2

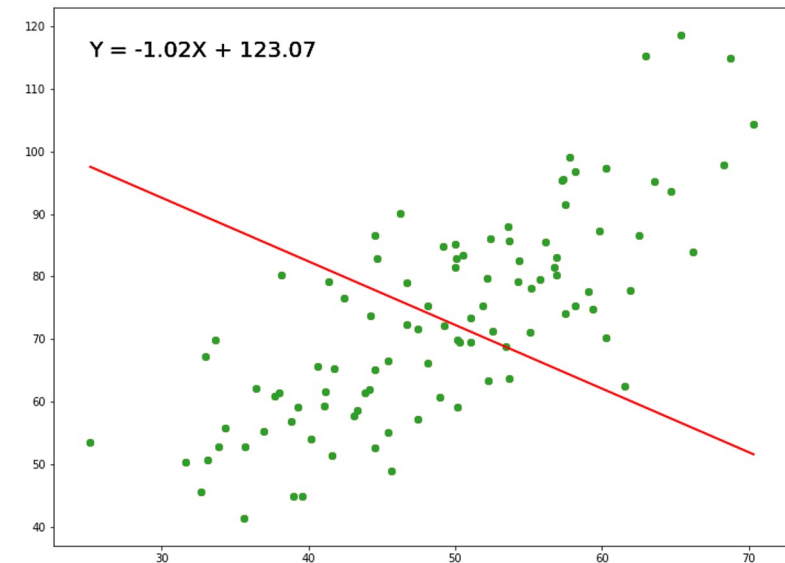


Regression

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

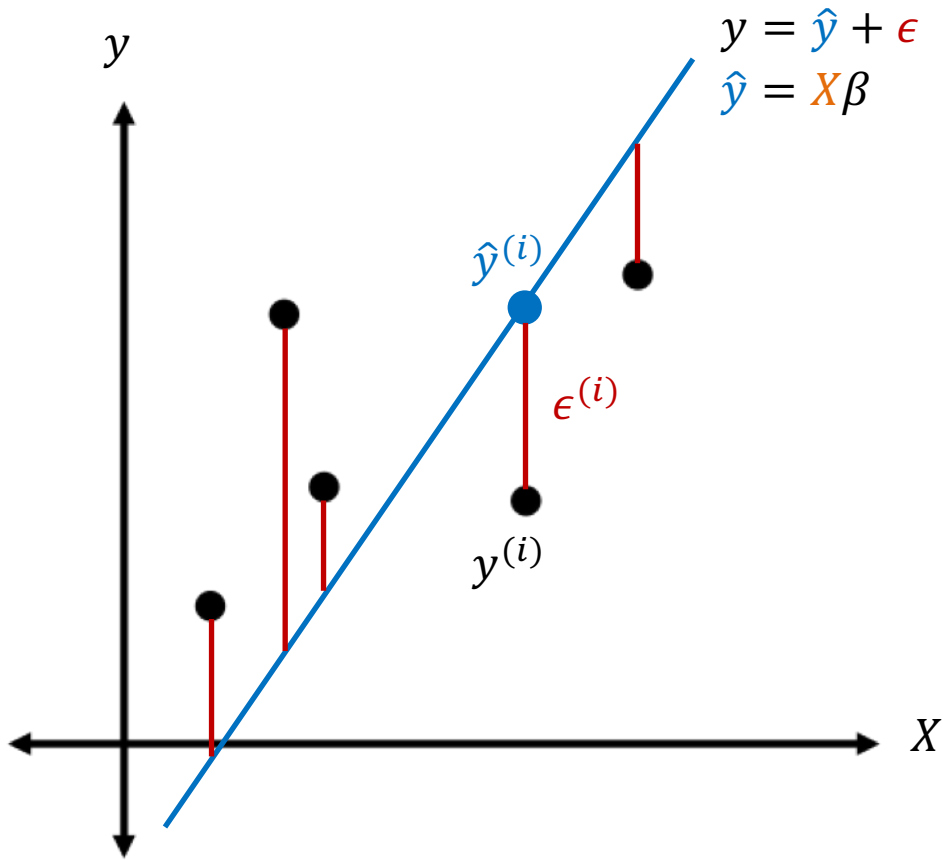


$$\begin{aligned}\text{MSE} &= \min_{\beta} \frac{1}{n} \sum_{i=1}^n (\epsilon^{(i)})^2 = \min_{\beta} \frac{1}{n} \sum_{i=1}^n (y^{(i)} - x^{(i)}\beta)^2 \\ &= \min_{\beta} \frac{1}{n} (y - X\beta)^T (y - X\beta)\end{aligned}$$



Regression

Recall that we use the mean squared error: $\text{MSE} = \min_{\beta} \frac{1}{n} \sum_{i=1}^n (\epsilon^{(i)})^2$



Q1: Why using the “squared error” and not just the original error?

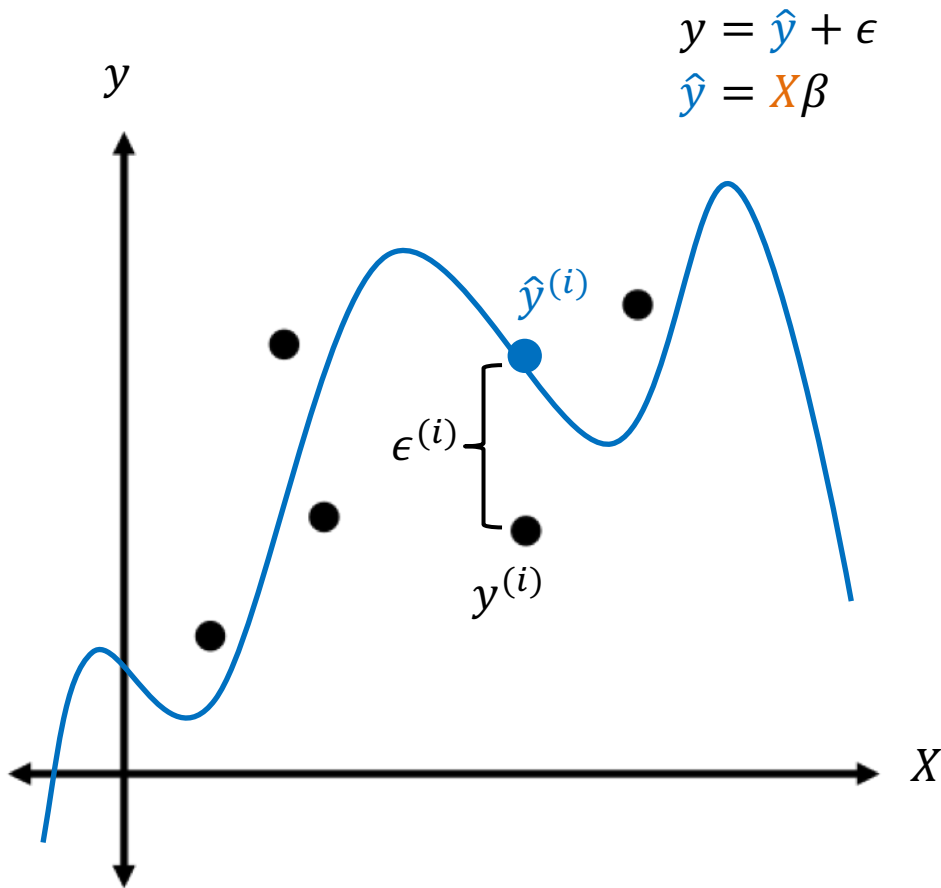
$$\text{ME} = \min_{\beta} \frac{1}{n} \sum_{i=1}^n \epsilon^{(i)}$$

Q2: Why using the “mean of squared errors” and not the “sum of squared errors”?

$$\text{SE} = \min_{\beta} \sum_{i=1}^n (\epsilon^{(i)})^2$$

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)

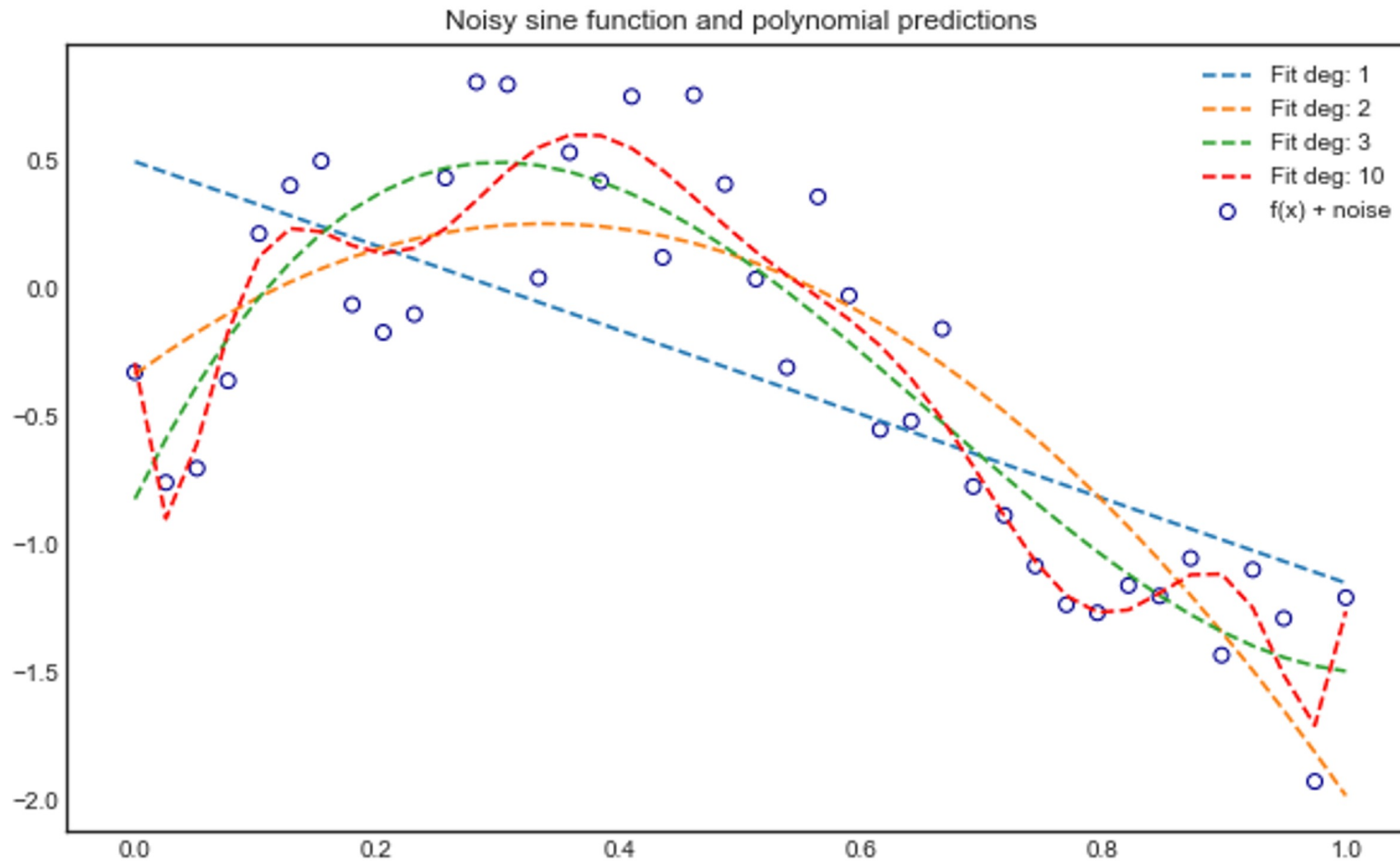
$$X = [\mathbf{1} \quad x_1 \quad (x_1)^2 \quad \cdots \quad (x_1)^k]$$

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

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

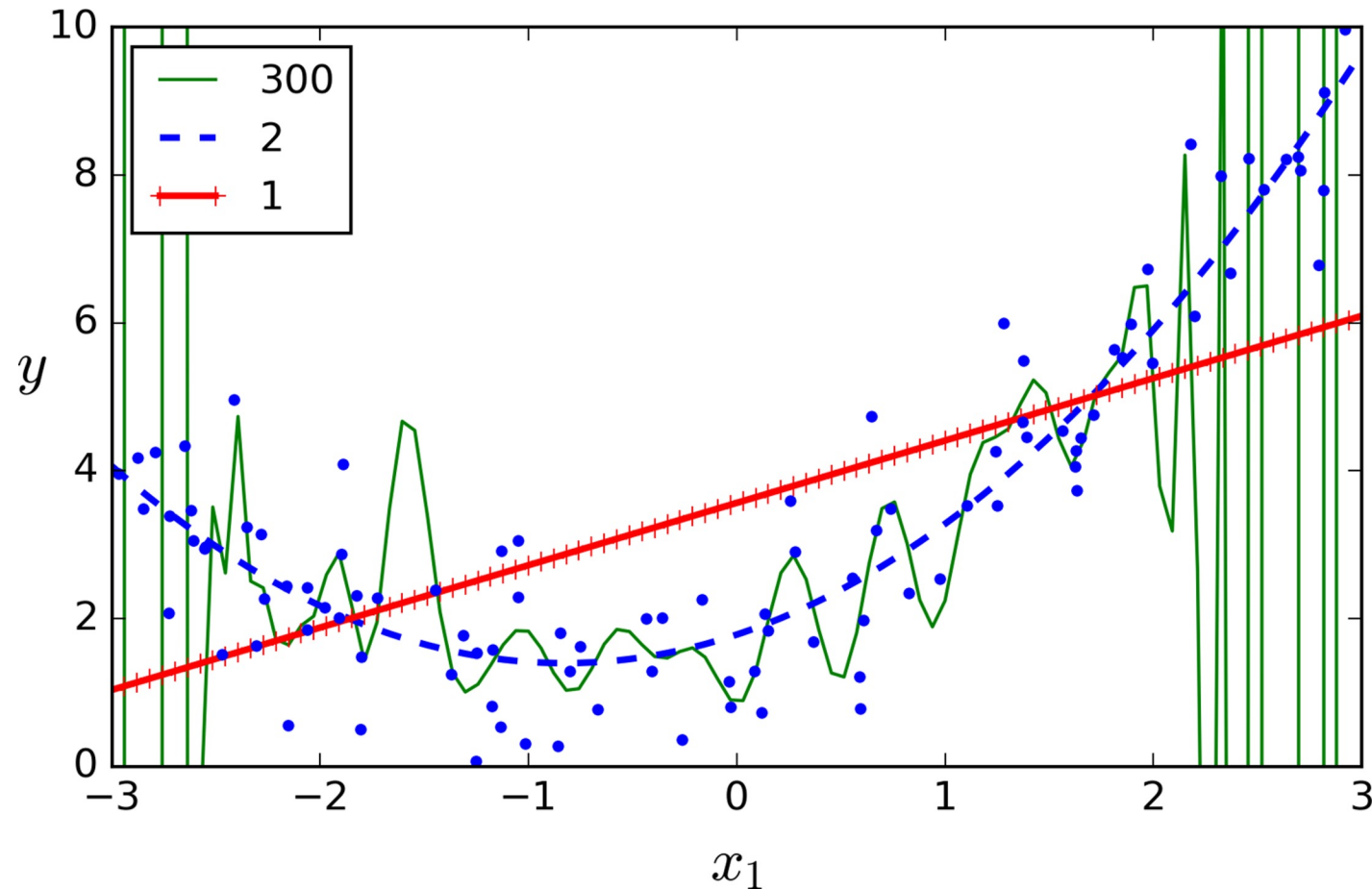
Regression

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



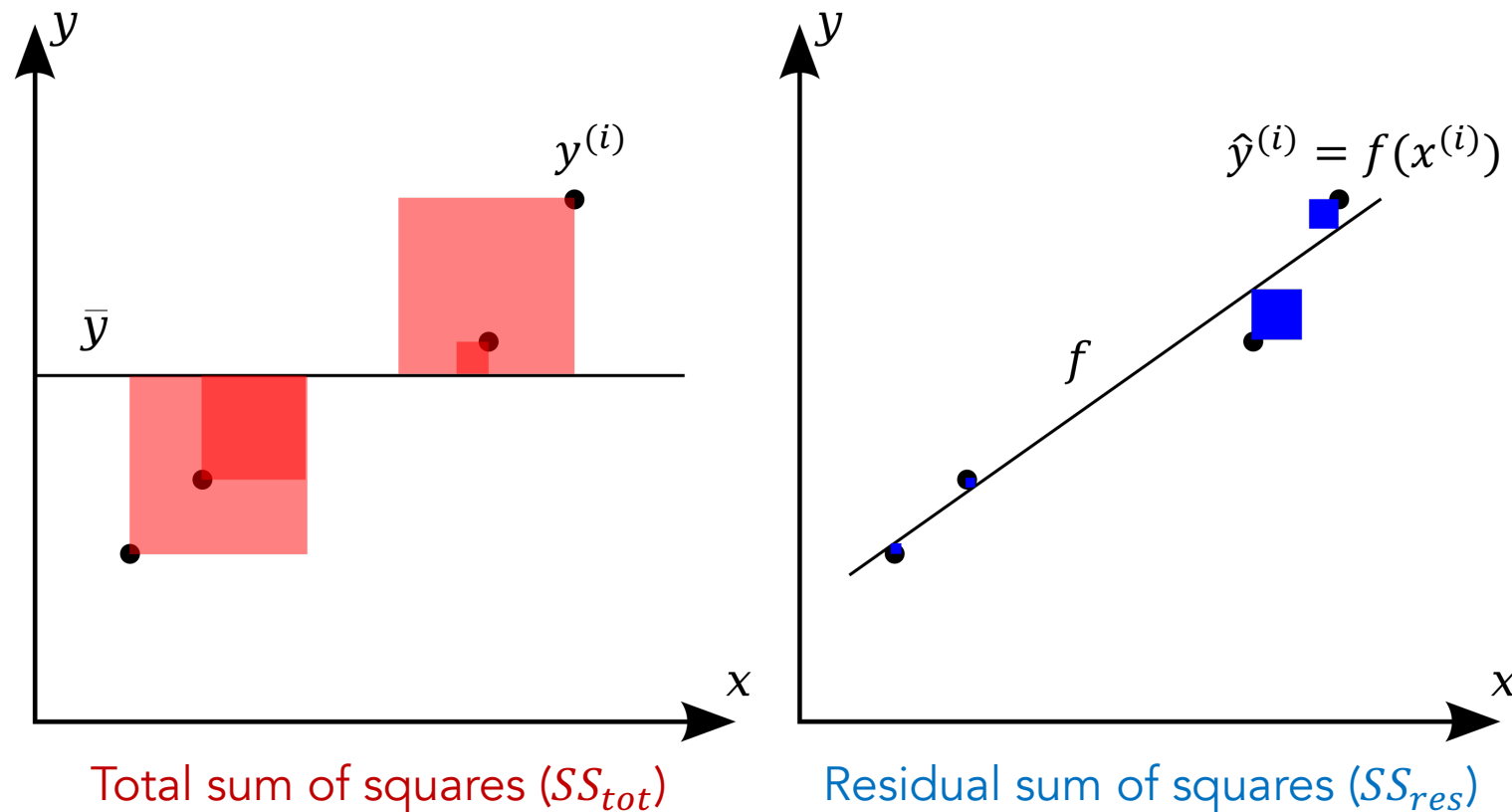
Regression

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.



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.

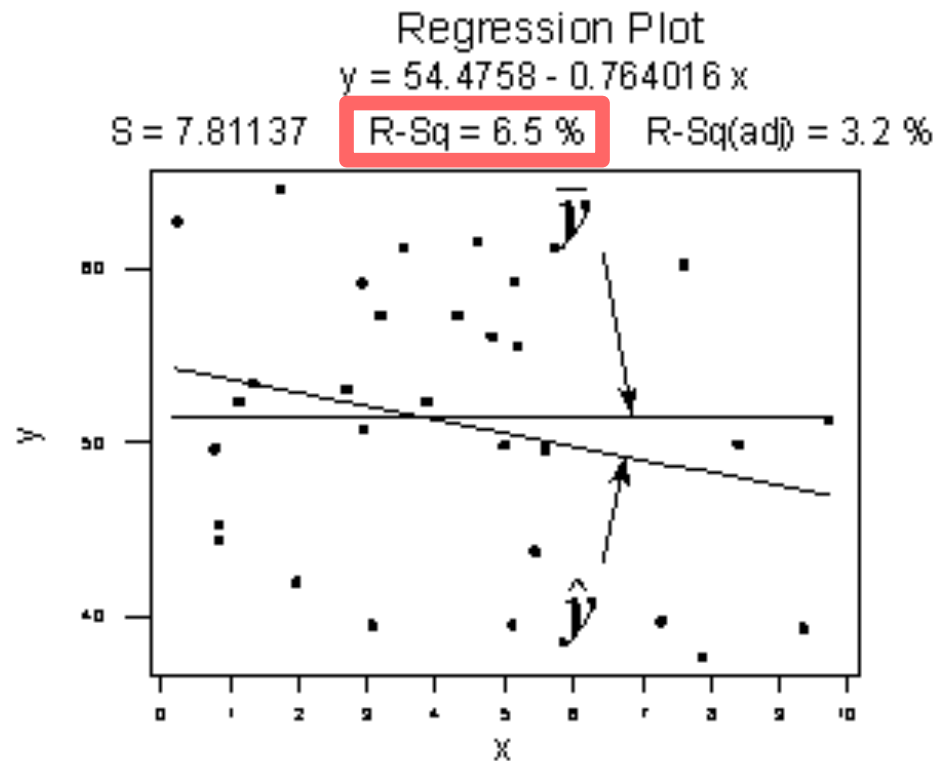


Unexplained Variation

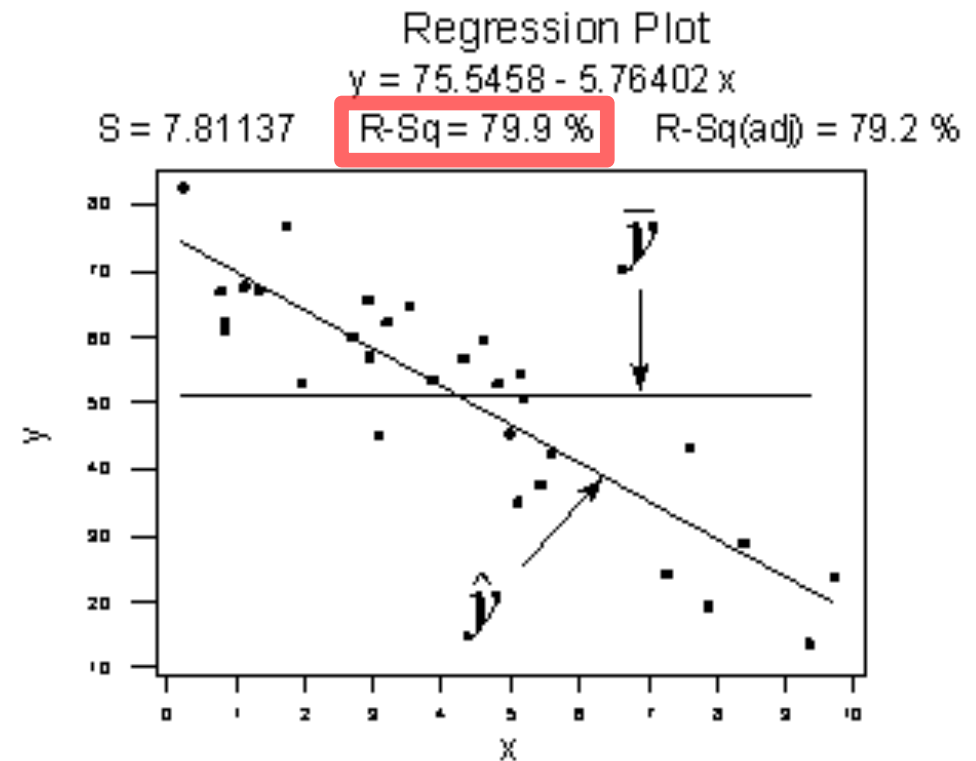
$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$
$$SS_{res} = \sum_i (y^{(i)} - \hat{y}^{(i)})^2$$
$$SS_{tot} = \sum_i (y^{(i)} - \bar{y})^2$$

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

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).

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

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

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

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

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

p : number of features/predictors

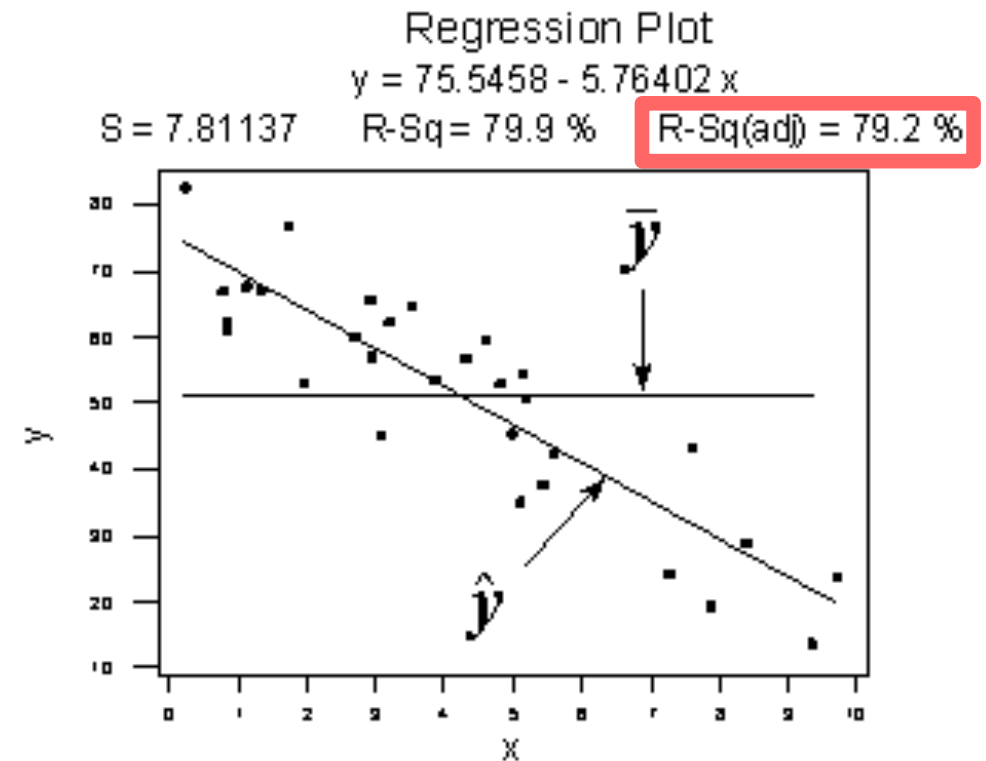
R^2_{adj} : adjusted value of R^2

df_{res} : residual degree of freedom

df_{tot} : total degree of freedom

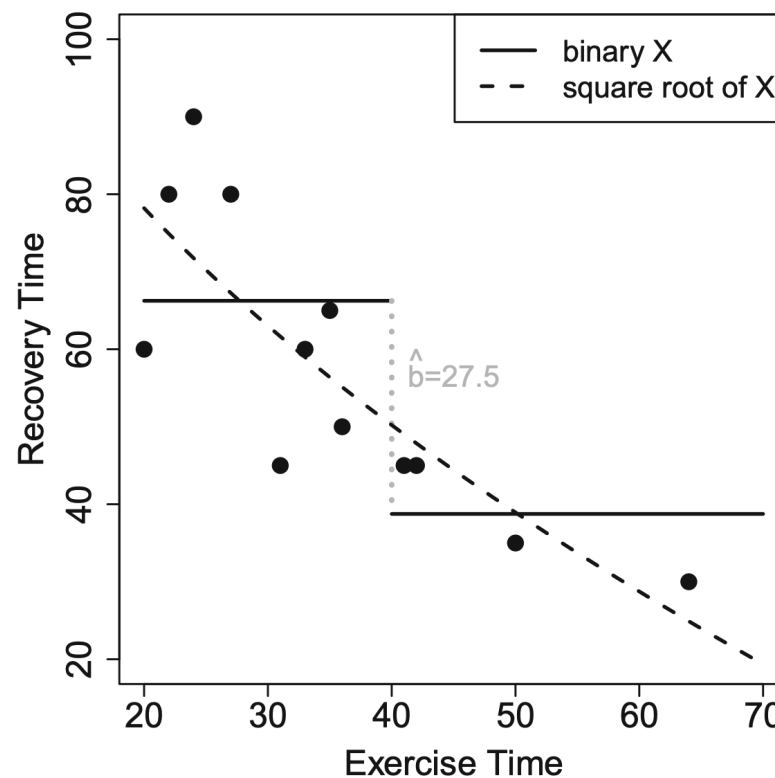
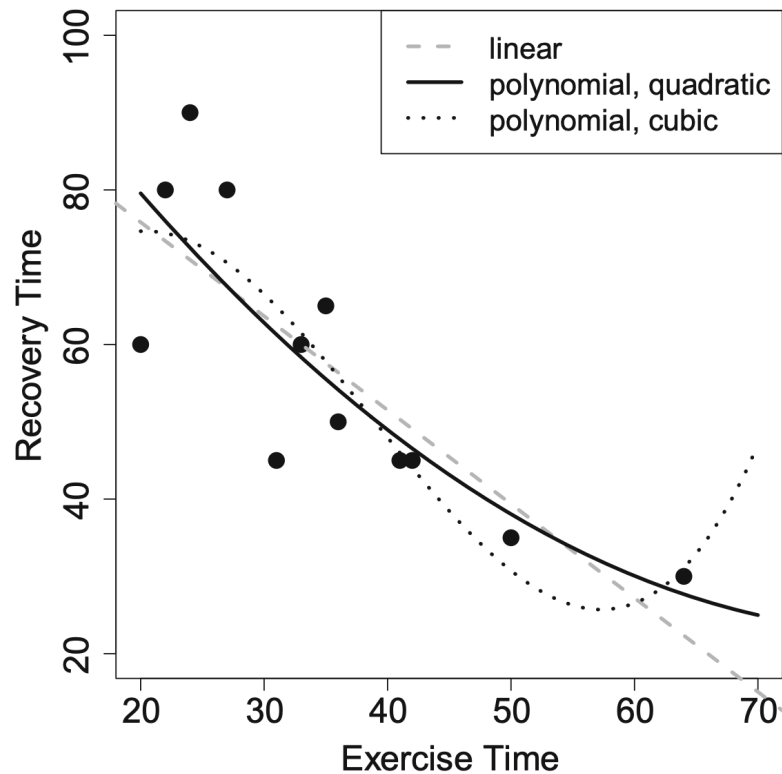
SS_{res} : residual sum of squares

SS_{tot} : total sum of squares



Regression

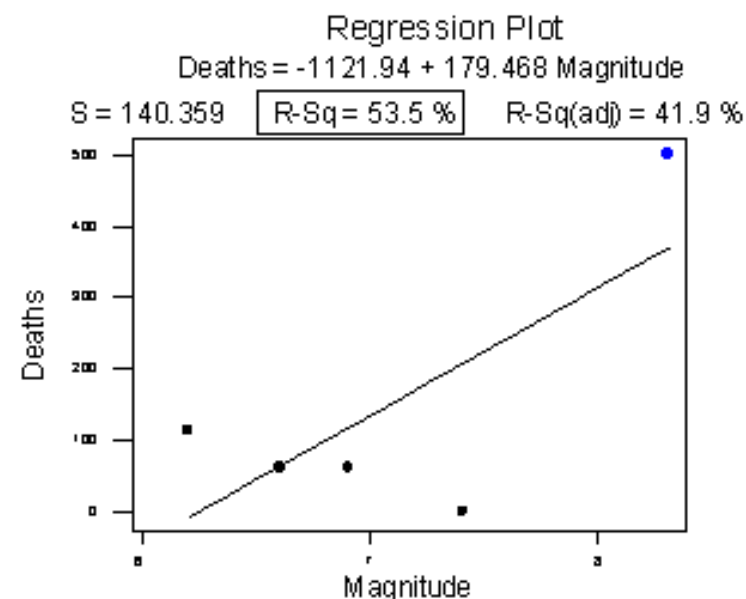
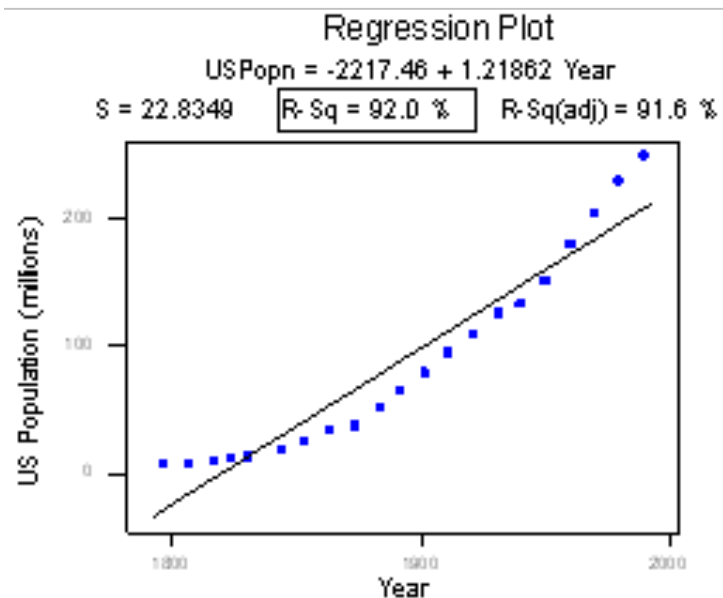
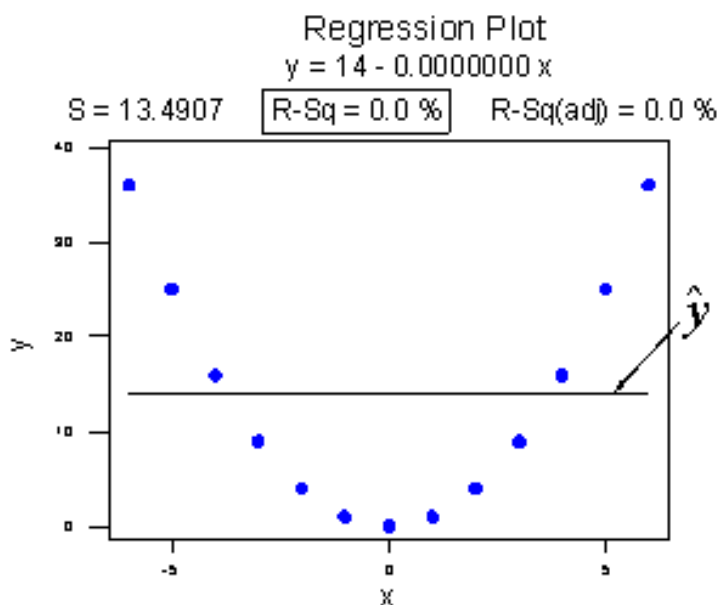
In the example below, R^2 is larger for the model with more predictors (i.e., the **cubic model** that has three predictors). The **adjusted R^2** , which considers the number of predictors (model complexity), favors the **square-root model**.



	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

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?