

# Model Evaluation

Choosing the **best** model

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# Which model is better?

- Task: Predict a store's daily ice cream sales based on outside temperature.
- We only have recorded data from 10 days:

Day		1	2	3	4	5	6	7	8	9	10
$x$	Temperature (in °C)	12	33.9	30.1	14.1	4.6	7.3	3.1	29.2	21.1	27.2
$y$	Ice Cream Sales (in \$)	182.2	445.1	394	167.7	53.7	66.8	114.8	344.2	179.5	267.7

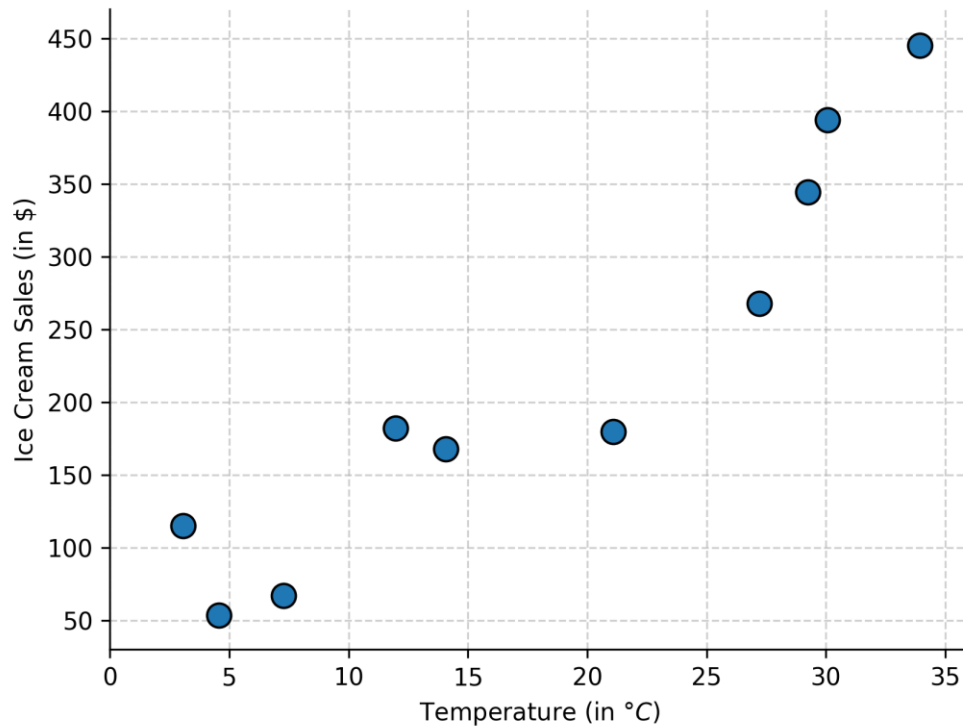
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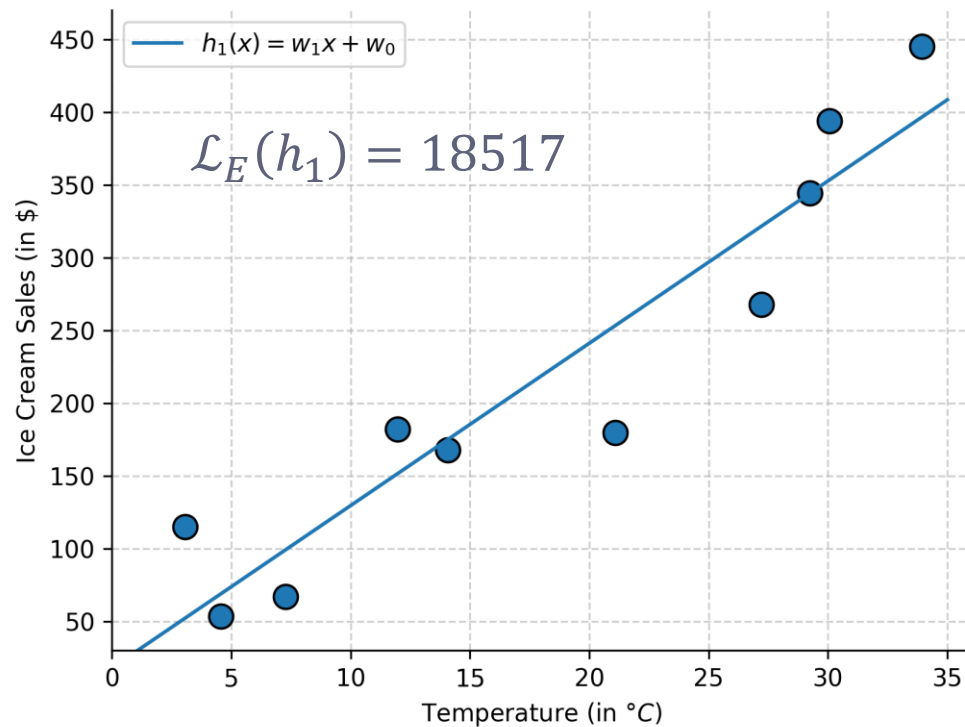
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- We must compare two models:
  - $h_1(x) = w_1x + w_0$
  - $h_2(x) = w'_5x^5 + w'_4x^4 + \dots + w'_1x + w_0$

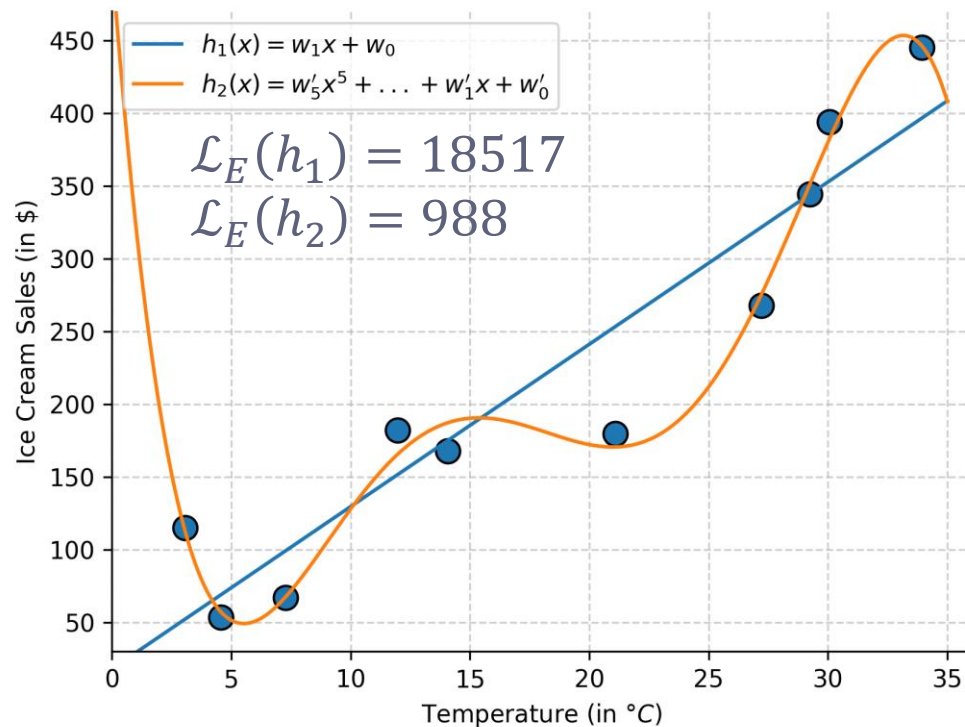
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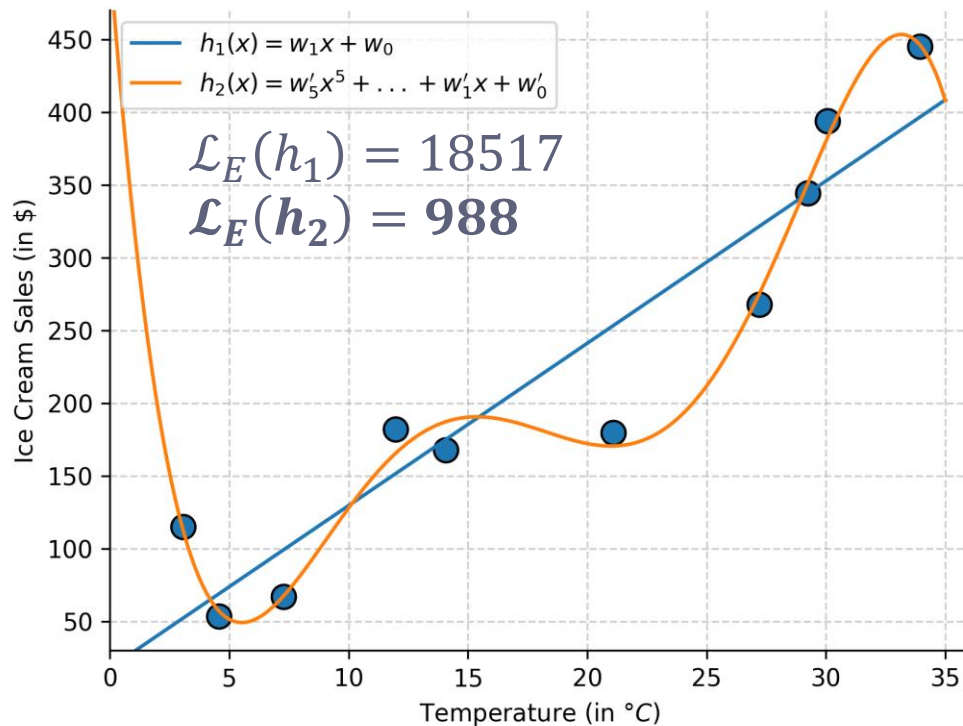


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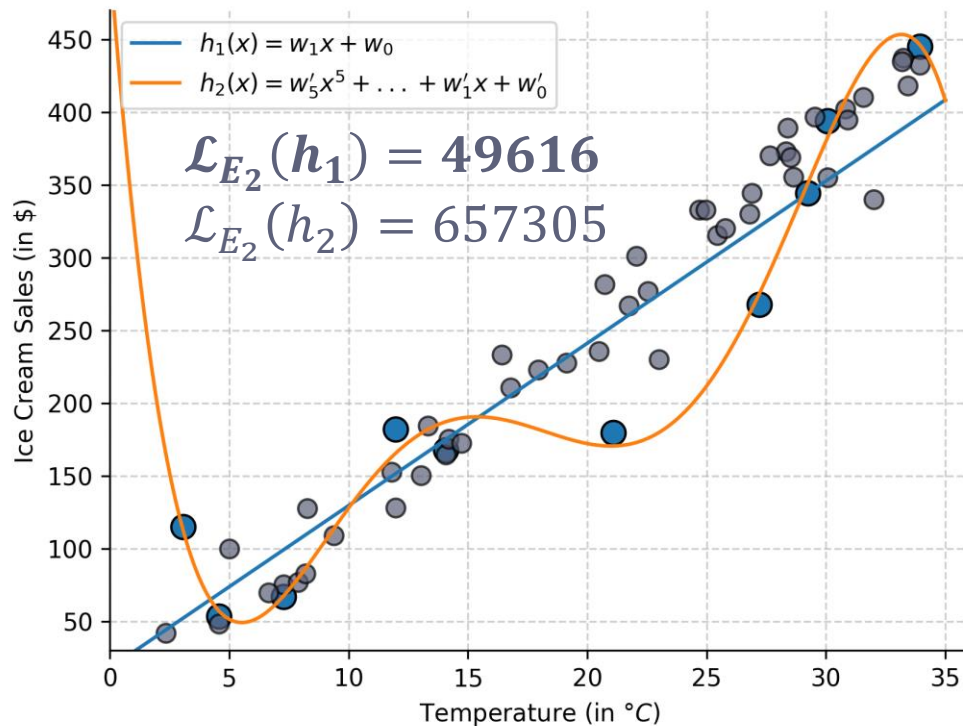
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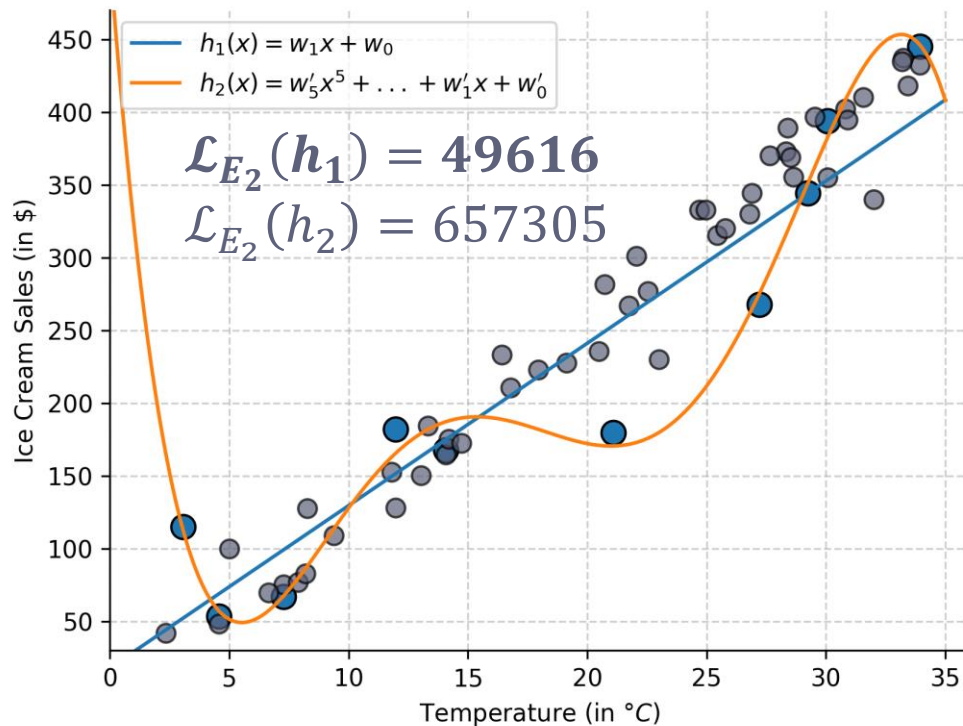


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In practice, we don't always get to do this.

# Data Splitting Strategies

# Training – Test split

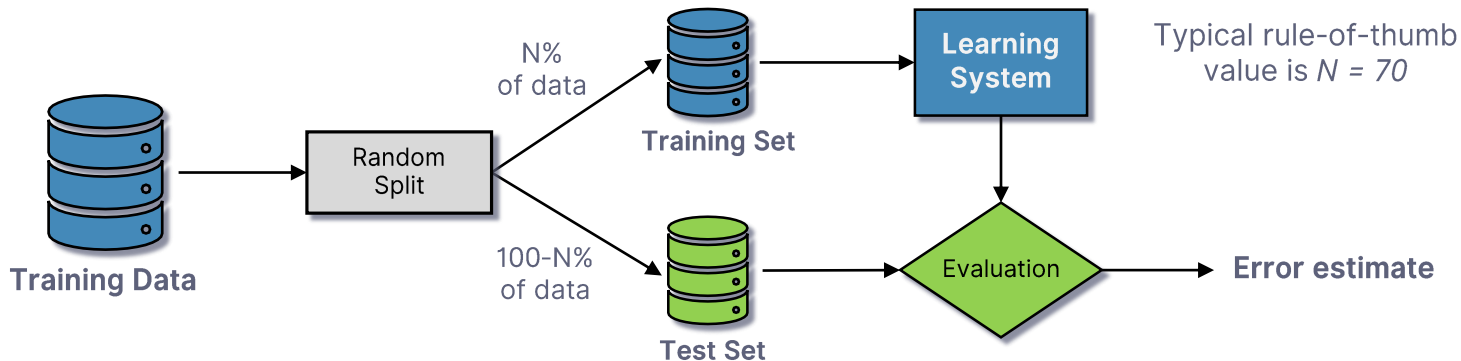
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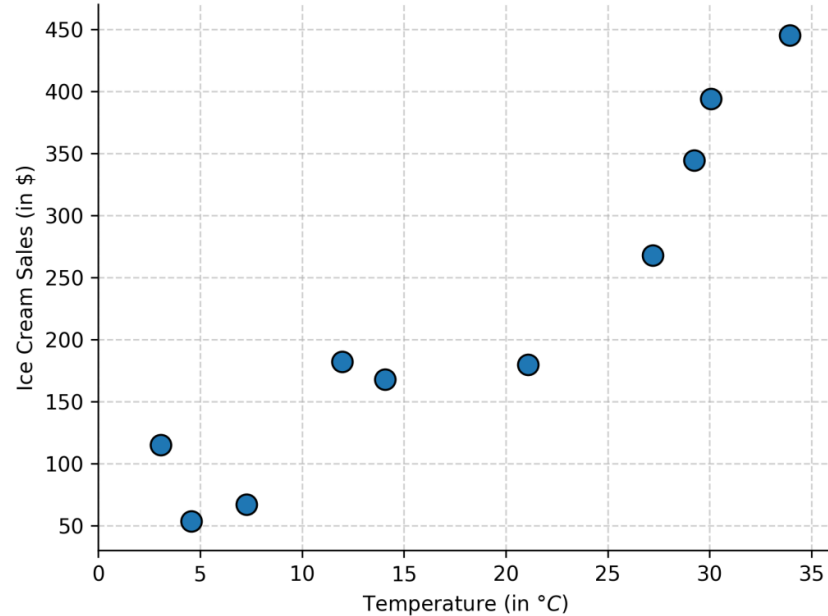
- In practice, we don't get to see the *true distribution* and we don't always get access to *more samples* to evaluate on.
- As we have seen, training error is a very optimistic estimate of true error.
  - It will almost always be lower than true error.
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- As we have seen, training error is a very optimistic estimate of true error.
  - It will almost always be lower than true error.
  - It will favor more complex models, which tend to overfit.
- One possibility to improve the estimate is the **Hold-out method**:

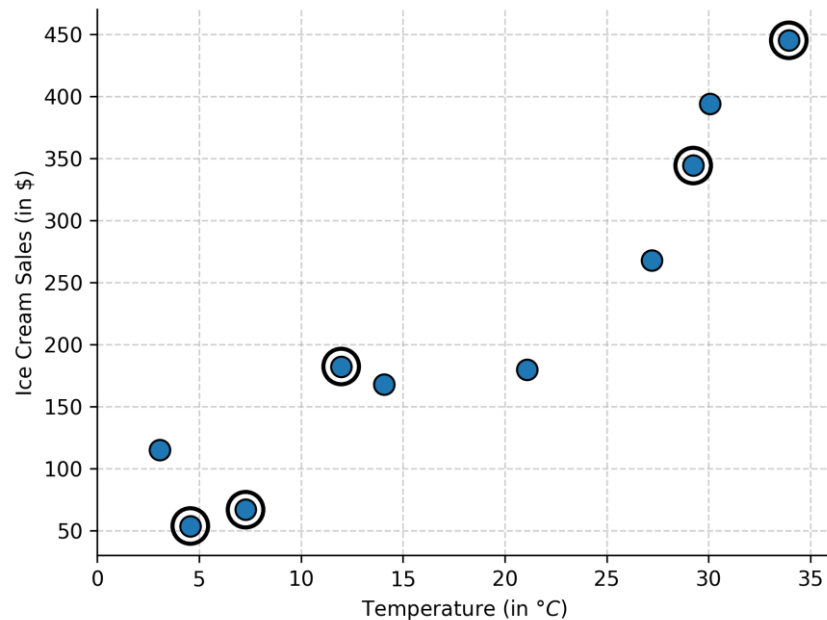


# Training – Test split



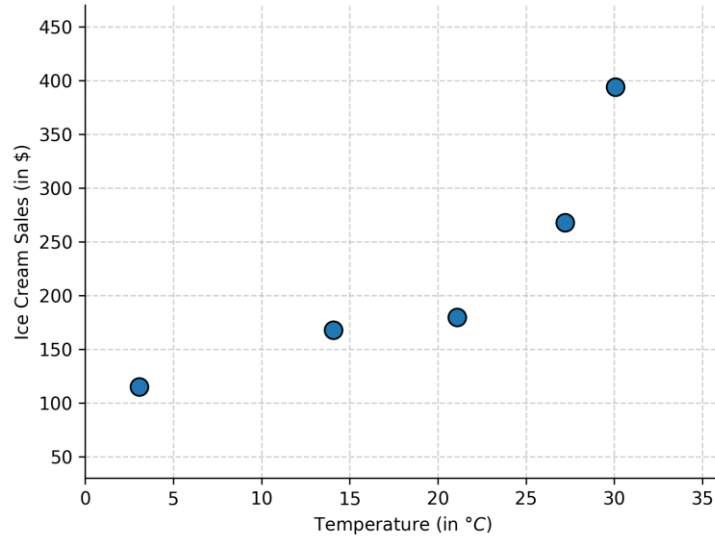
# Training – Test split

Randomly select some points from the training data.

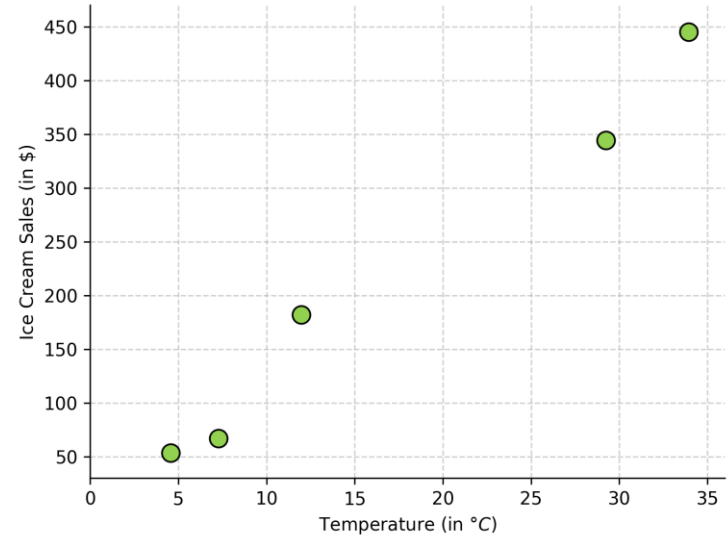


# Training – Test split

Training Set



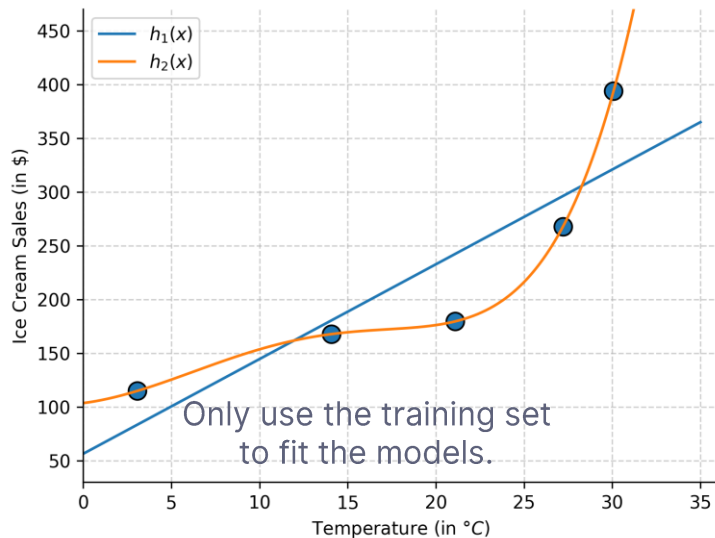
Test Set



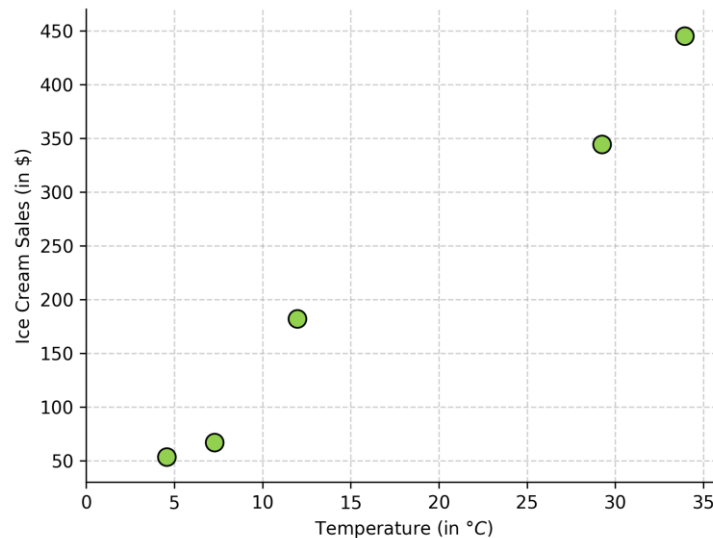


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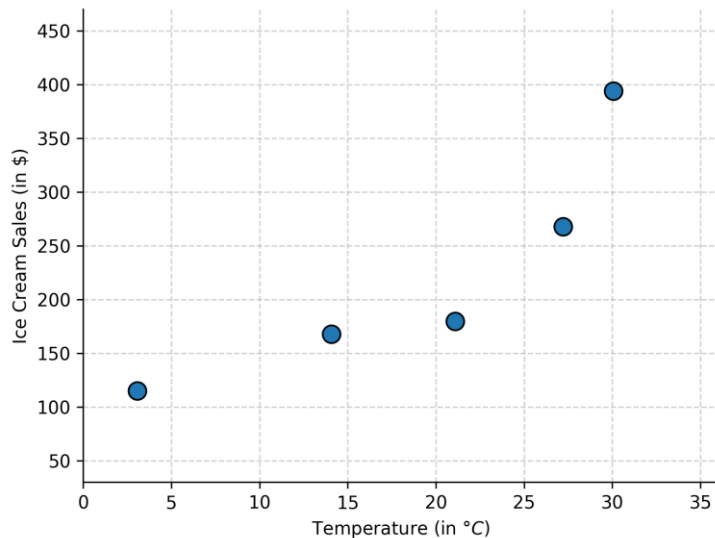


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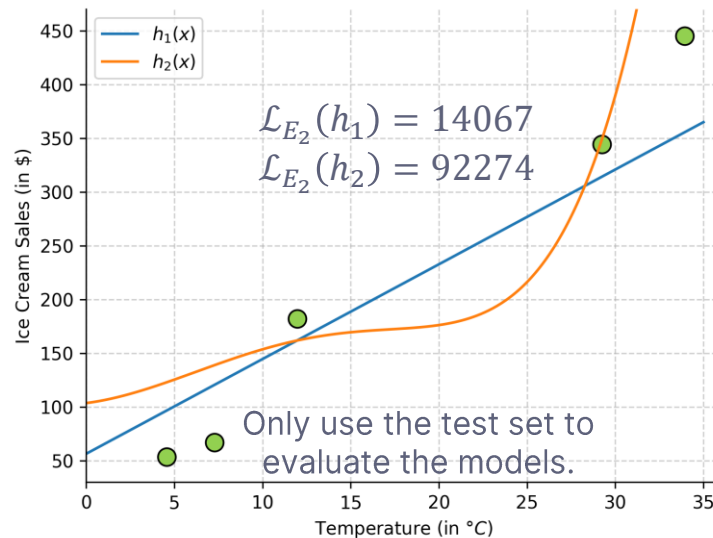


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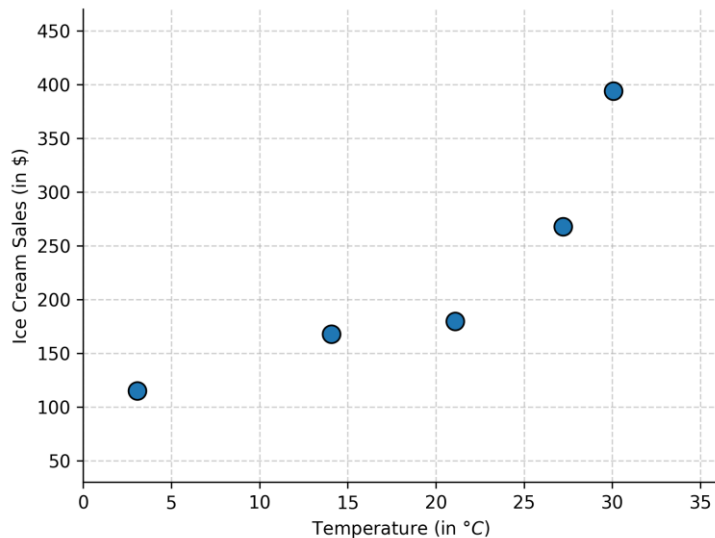
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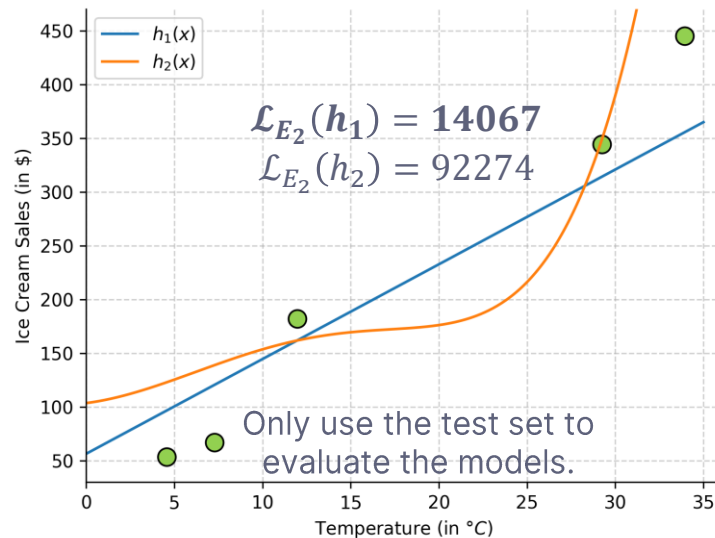
# Training – Test split

We can conclude that  $h_1$  is a better model for this task, without seeing any additional points.

Training Set



Test Set



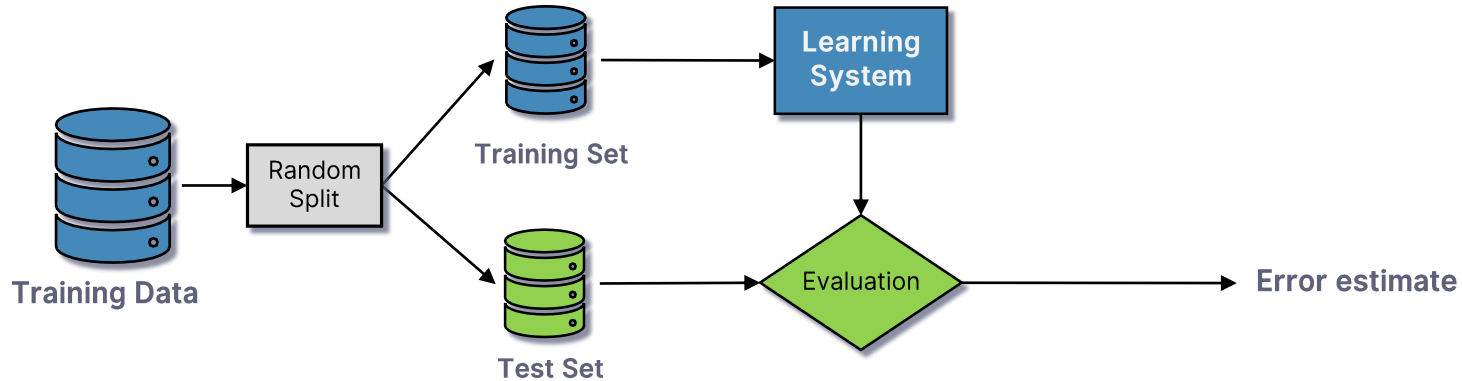
# Problems with using a single train-test split

- Some algorithms have *hyperparameters*, which control the training process.
  - e.g. Parameter  $\lambda$  in Ridge Regression
- Repeatedly using the same train – test sets when trying different hyperparameters can “*wear out*” the test set.
  - Overfitting in hyperparameter space.

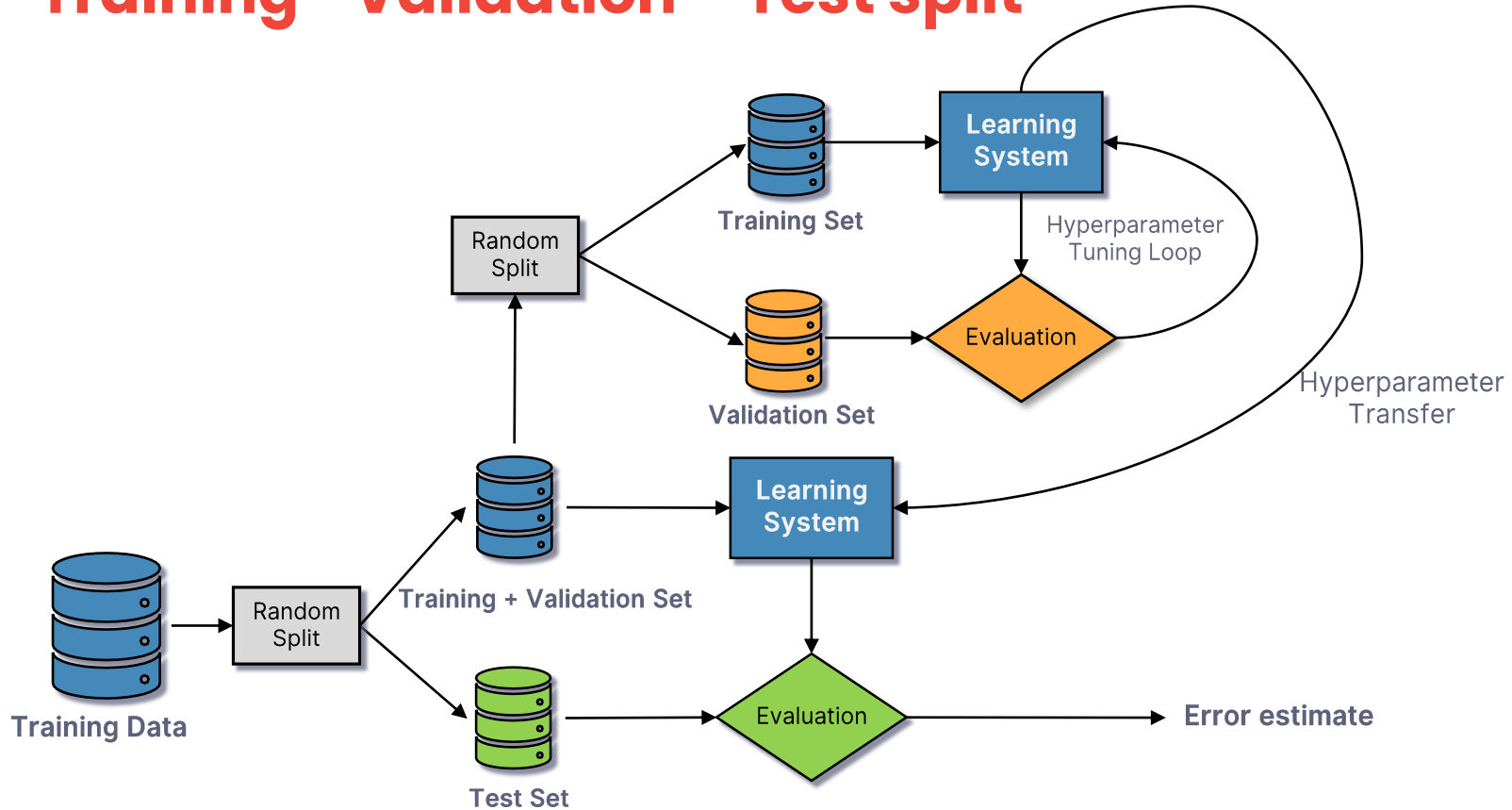
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  - Overfitting in hyperparameter space.
- We can improve the error estimate by using a separate **validation** set for *hyperparameter tuning*

# Training– Validation – Test split



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# K-fold Cross-Validation

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- **K-fold Cross-Validation:**
  - Split the data into k equal parts (a.k.a. *folds*)
  - Repeat the train – test process k times, each time using one fold for testing and the rest for training.
  - Average out the errors.

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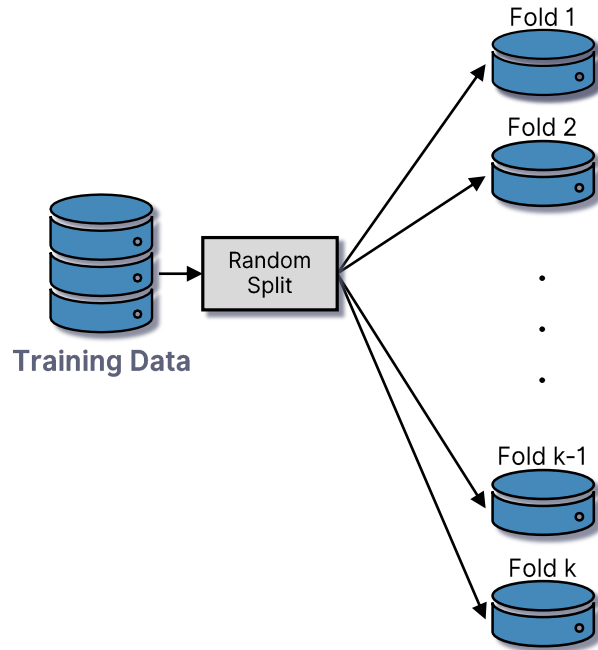
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  - Split the data into k equal parts (a.k.a. *folds*)
  - Repeat the train – test process k times, each time using one fold for testing and the rest for training.
  - Average out the errors.
- Even if we have enough data for a validation set, we can obtain a better estimate of true error this way.
  - If we have enough computing power.

# K-fold Cross-Validation

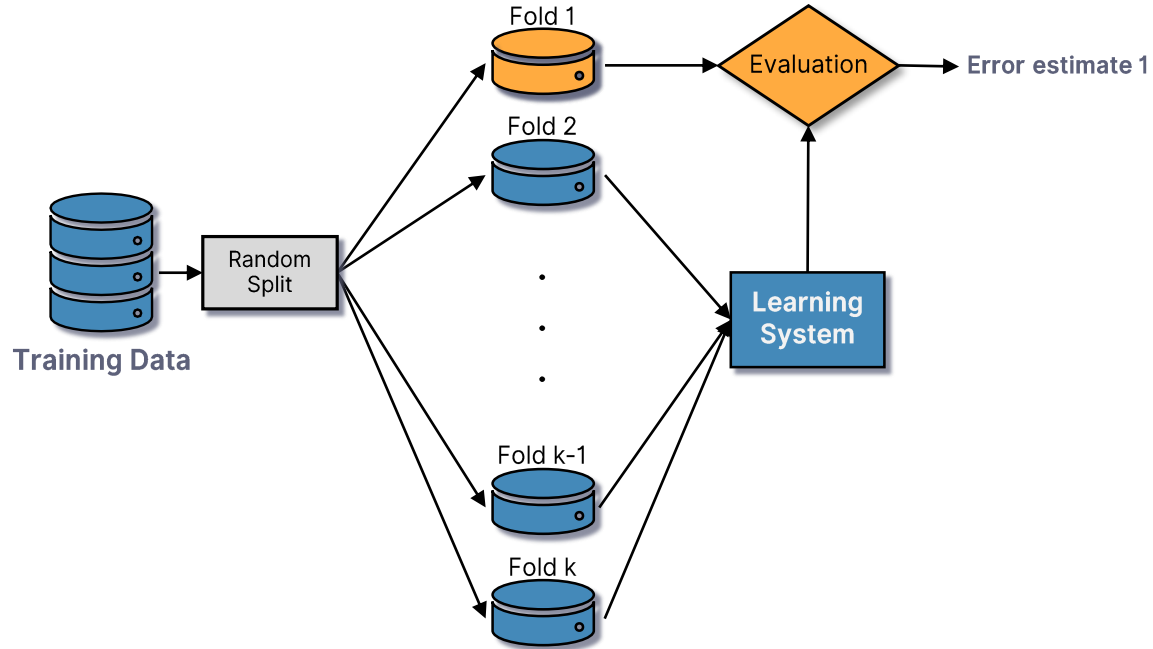


Training Data

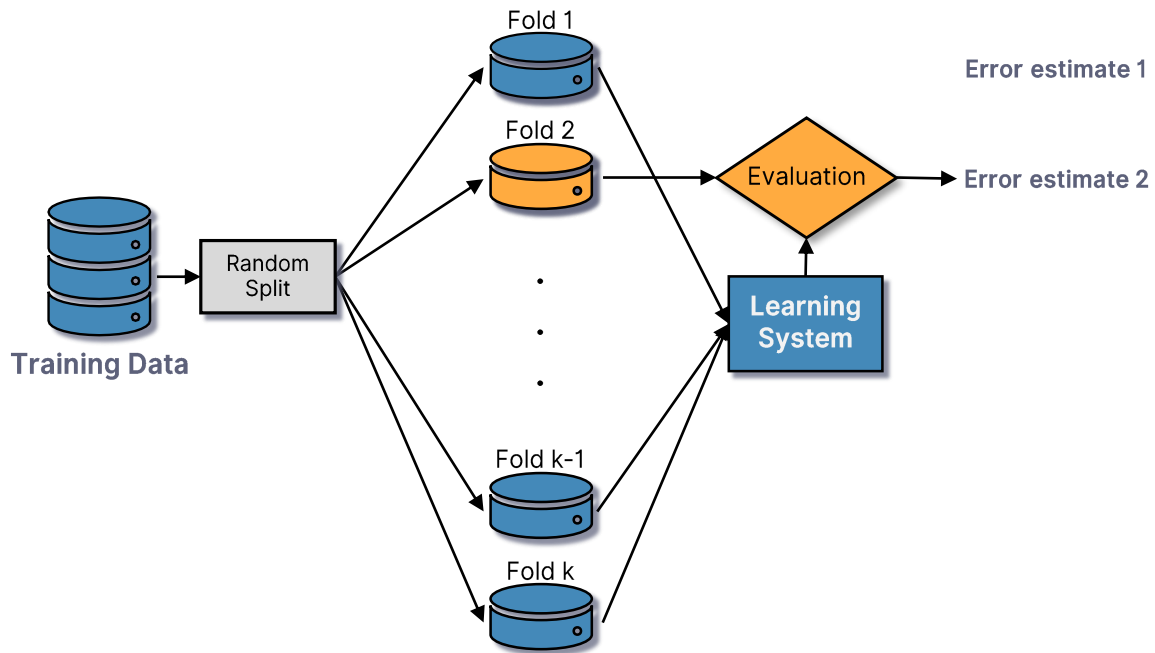
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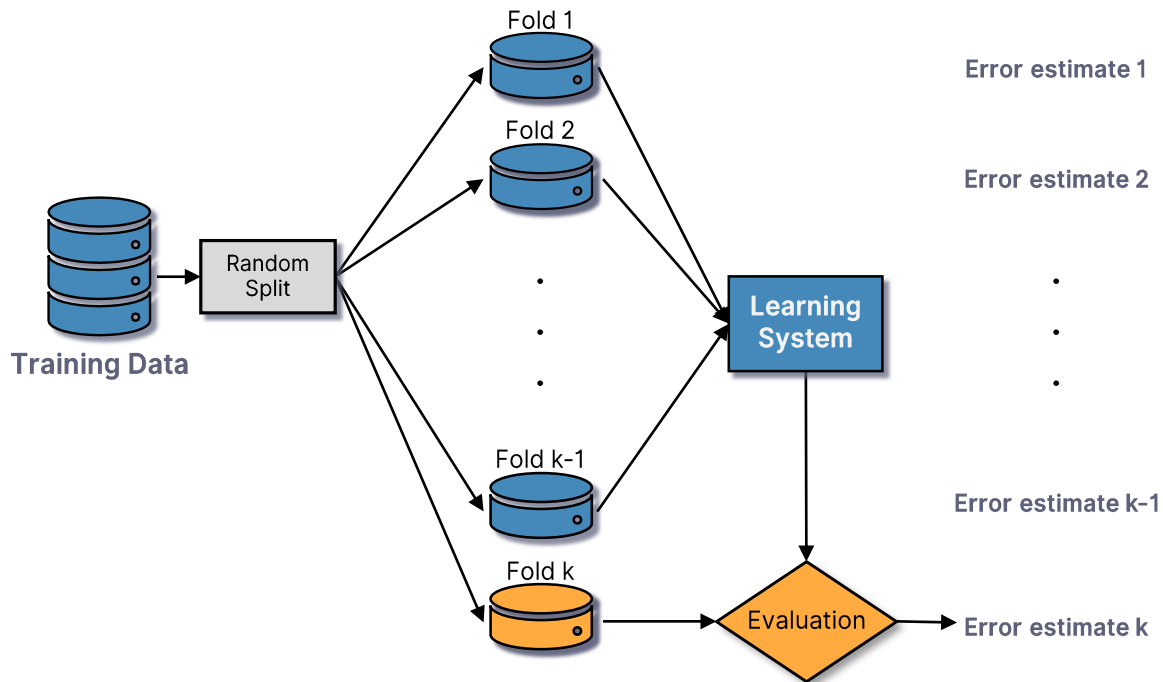
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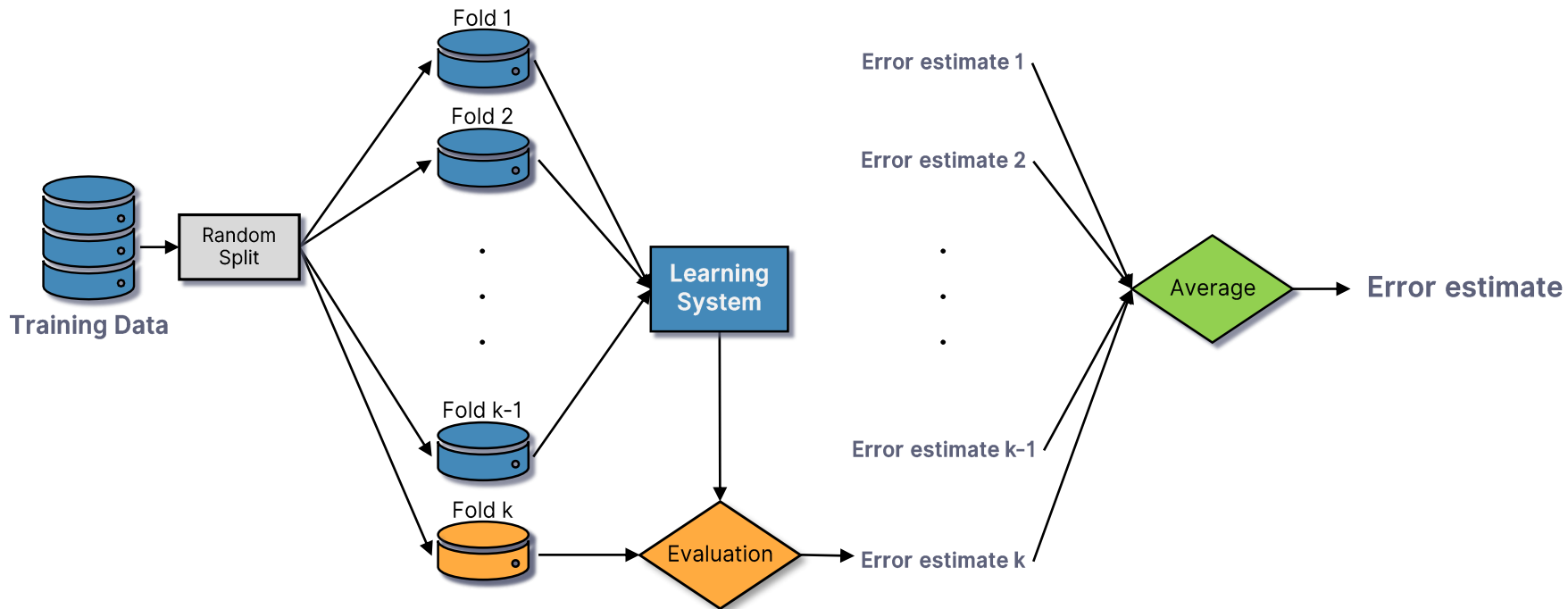
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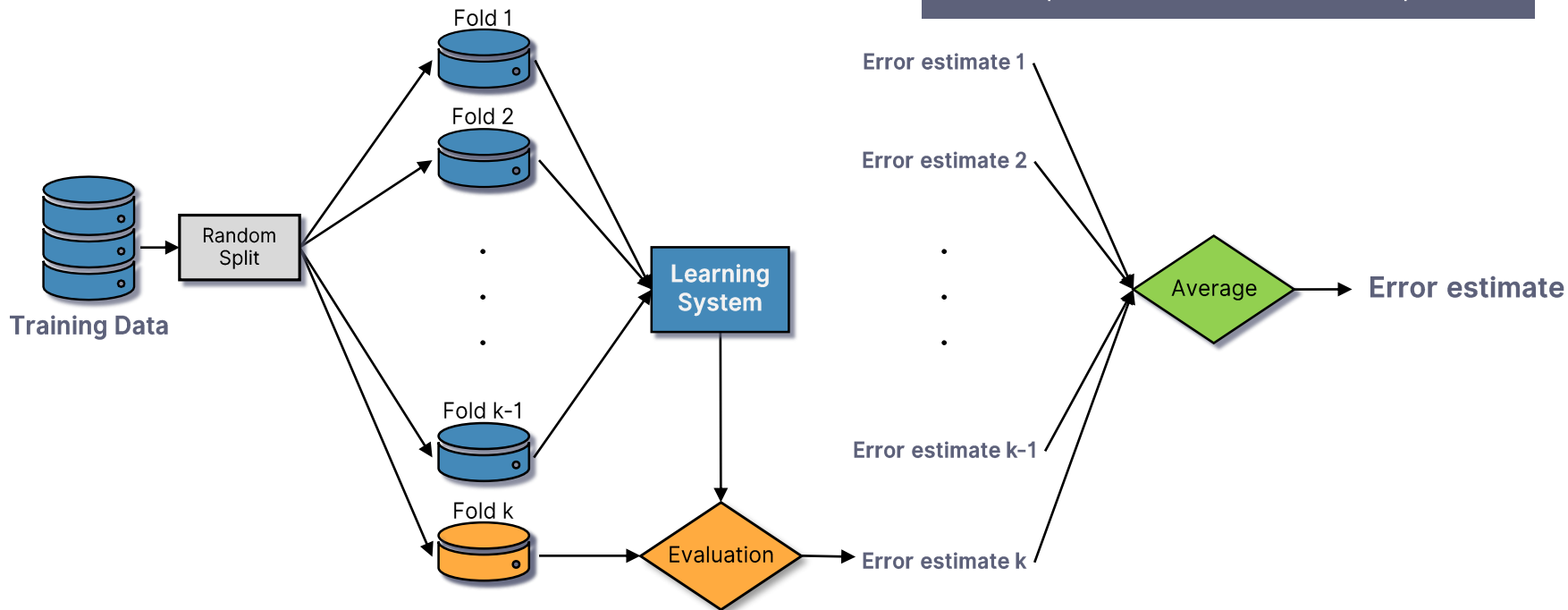


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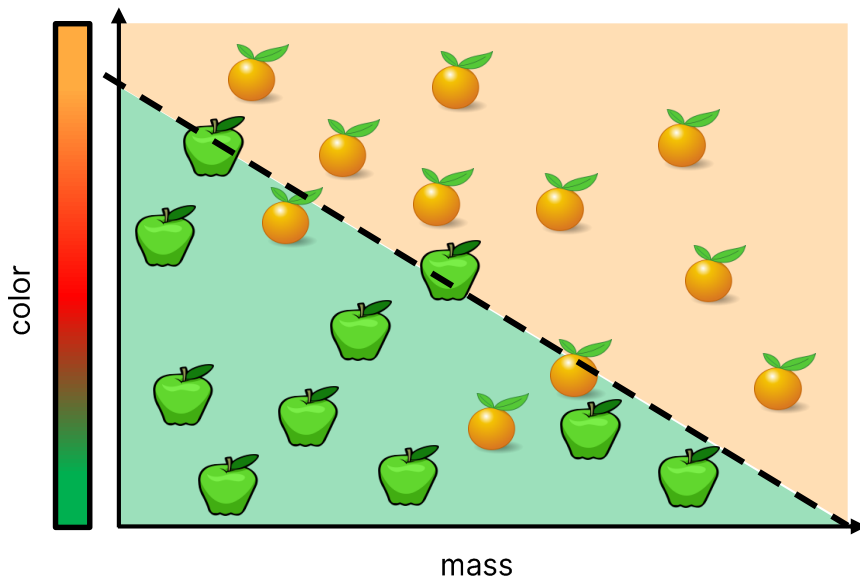
# Summary

- Using training error for performance evaluation is usually a bad idea.
  - It is a very optimistic estimate of true error and it favors models which overfit.
- **Holding out data for testing** gives a much better estimate.
- However, if we use a single test set for *hyperparameter selection*, we might end up reducing the quality of the estimation.
  - Using a separate **validation set** for this is a much better idea.
- If we don't have enough data or if we have enough computing power, **K-fold Cross-Validation** gives an even better estimate.
  - If we use each sample as a fold, we get **Leave-One-Out Cross Validation**





# Performance Metrics for Classification

# Confusion Matrix

- A **confusion matrix** is a table which describes the performance of a classification model by displaying how often classes get confused.



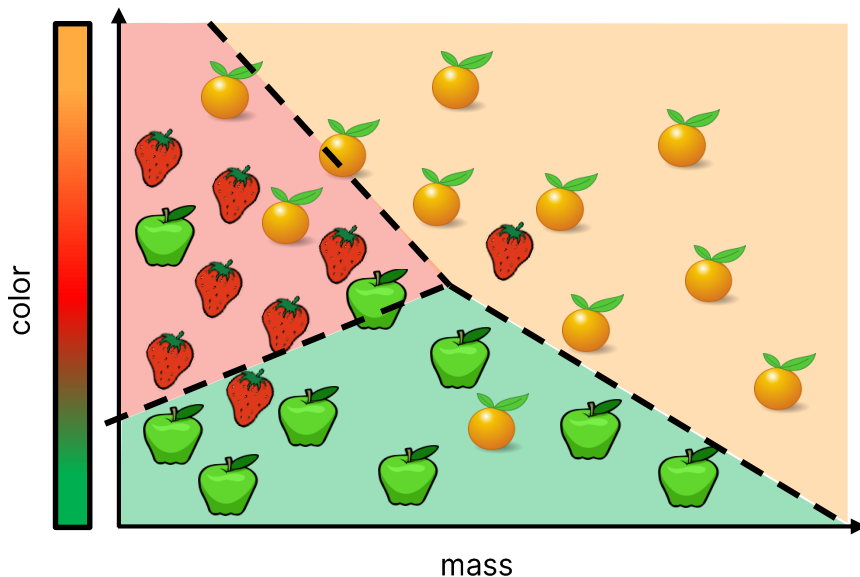
Predicted Labels







		
	9	1
	3	8

Actual Labels

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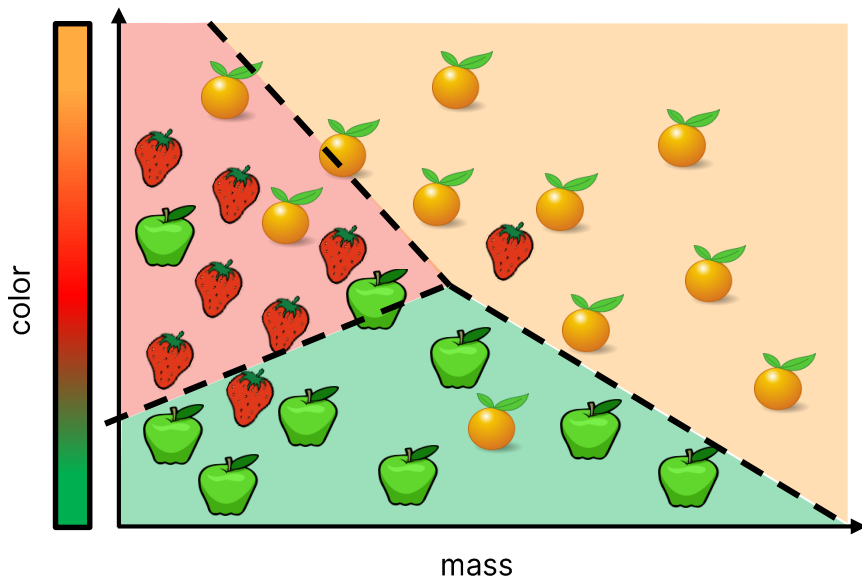


		Predicted Labels		
				
Actual Labels		7	0	2
		1	8	2
		1	1	6

It can be used for any number of classes.

# Accuracy

- **Accuracy** is the fraction (or percentage) of items for which the model predicted the correct class.



$$\text{Accuracy} = \frac{21}{28} = 0.75 = 75\%$$

# Problems with Accuracy

- Imagine that we must train a classifier to detect if a patient has an extremely rare disease.
  - From 1000 patients, only 20 have the disease.
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- Imagine that we must train a classifier to detect if a patient has an extremely rare disease.
  - From 1000 patients, only 20 have the disease.
  - This is not just our dataset, this is the *true distribution*.
- A classifier which predicts that nobody has the disease is 98% accurate.
  - Pretty good, right?
  - Not really... What is the problem?



# Problems with Accuracy

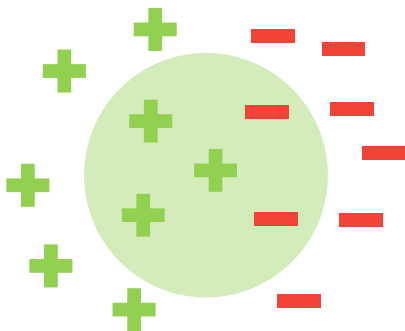
- Accuracy does not capture several aspects:
  - The dataset is very imbalanced.
    - One class is much more common than the other.
  - The 2 classes are conceptually different.
    - One is “*positive*”, it represents what we are looking for.
    - One is “*negative*”, it represent the default state.
  - There are 2 types of errors, which may differ in terms of severity.
    - *Type 1 error (“False Positive”)*
    - *Type 2 error (“False Negative”)*

Depending on the problem, one might more serious than the other.

# Precision and Recall

- When there is a *positive* class or classes are imbalanced, precision and recall are more informative than accuracy.
  - **Precision** is the fraction of *selected* items which are *relevant*.
  - **Recall** is the fraction of *relevant* items which are *selected*.

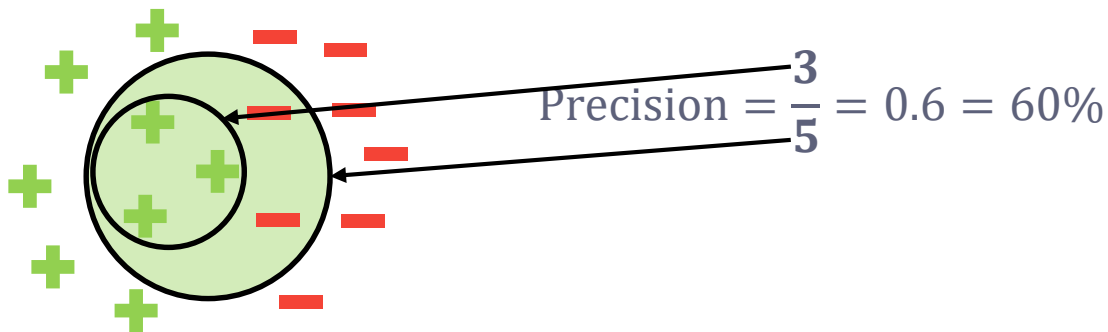
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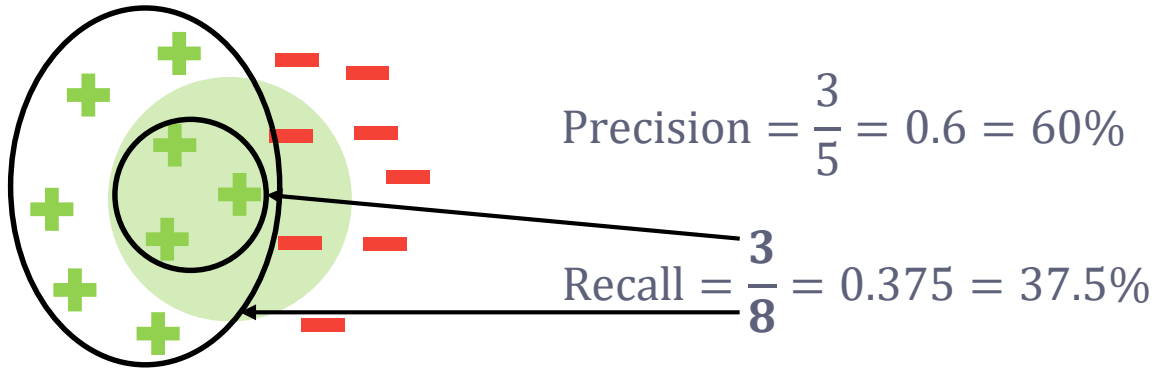
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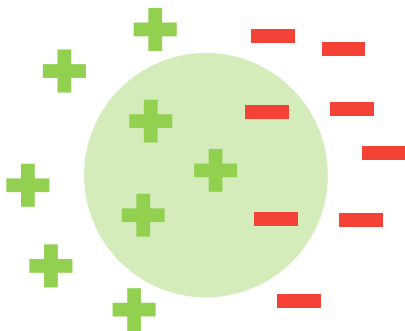
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$$\text{Precision} = \frac{3}{5} = 0.6 = 60\%$$

$$\text{Recall} = \frac{3}{8} = 0.375 = 37.5\%$$

- **F<sub>1</sub> score** is the harmonic mean of precision and recall.

# Summary

		Predicted Labels	
		+	-
Actual Labels	+	TP	FN
	-	FP	TN

Confusion Matrix

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

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

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

$$F_1 = \frac{2}{\frac{1}{\text{Precision}} + \frac{1}{\text{Recall}}} = \frac{2(\text{Precision} * \text{Recall})}{\text{Precision} + \text{Recall}}$$

# Keywords

Training Set

Test Set

Error Estimate

Hyperparameter Tuning

Validation Set

Cross-Validation

K-fold

Leave-One-Out

Confusion Matrix

Accuracy

Precision

Recall

$F_1$  Score