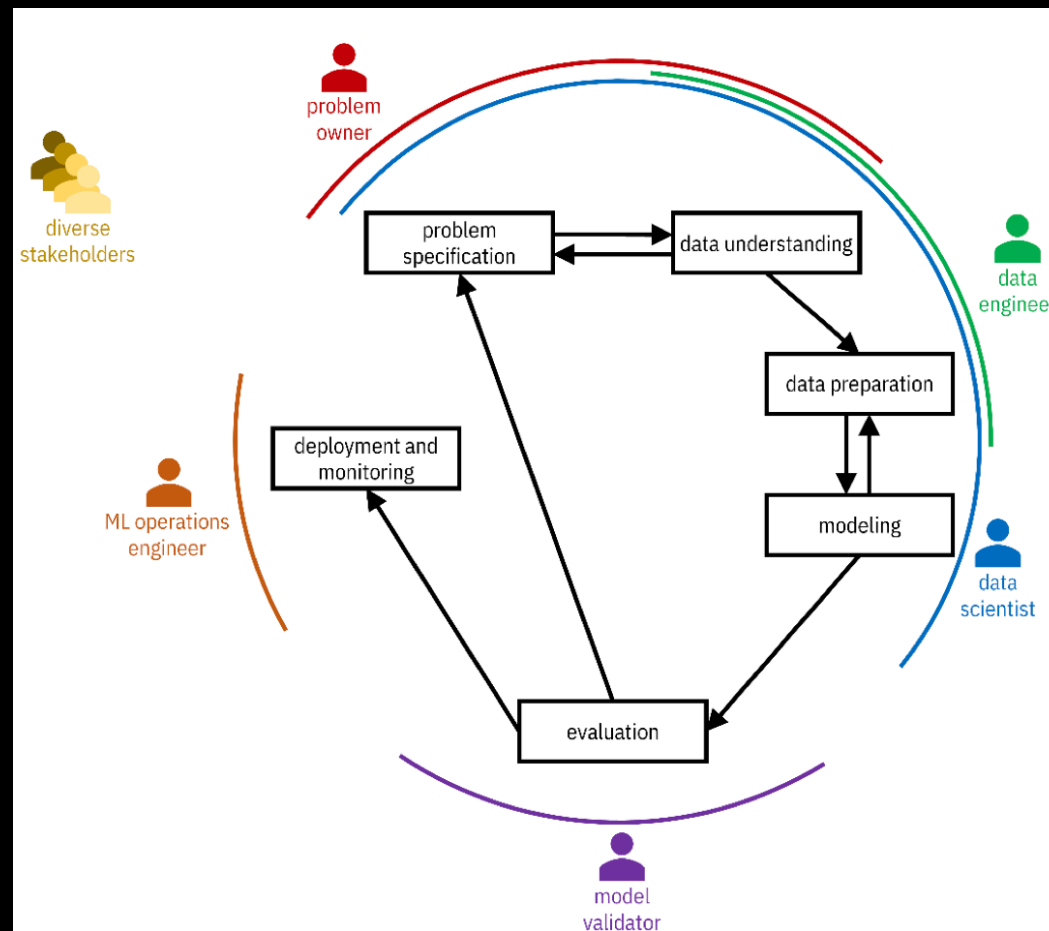


# Machine Learning for Design

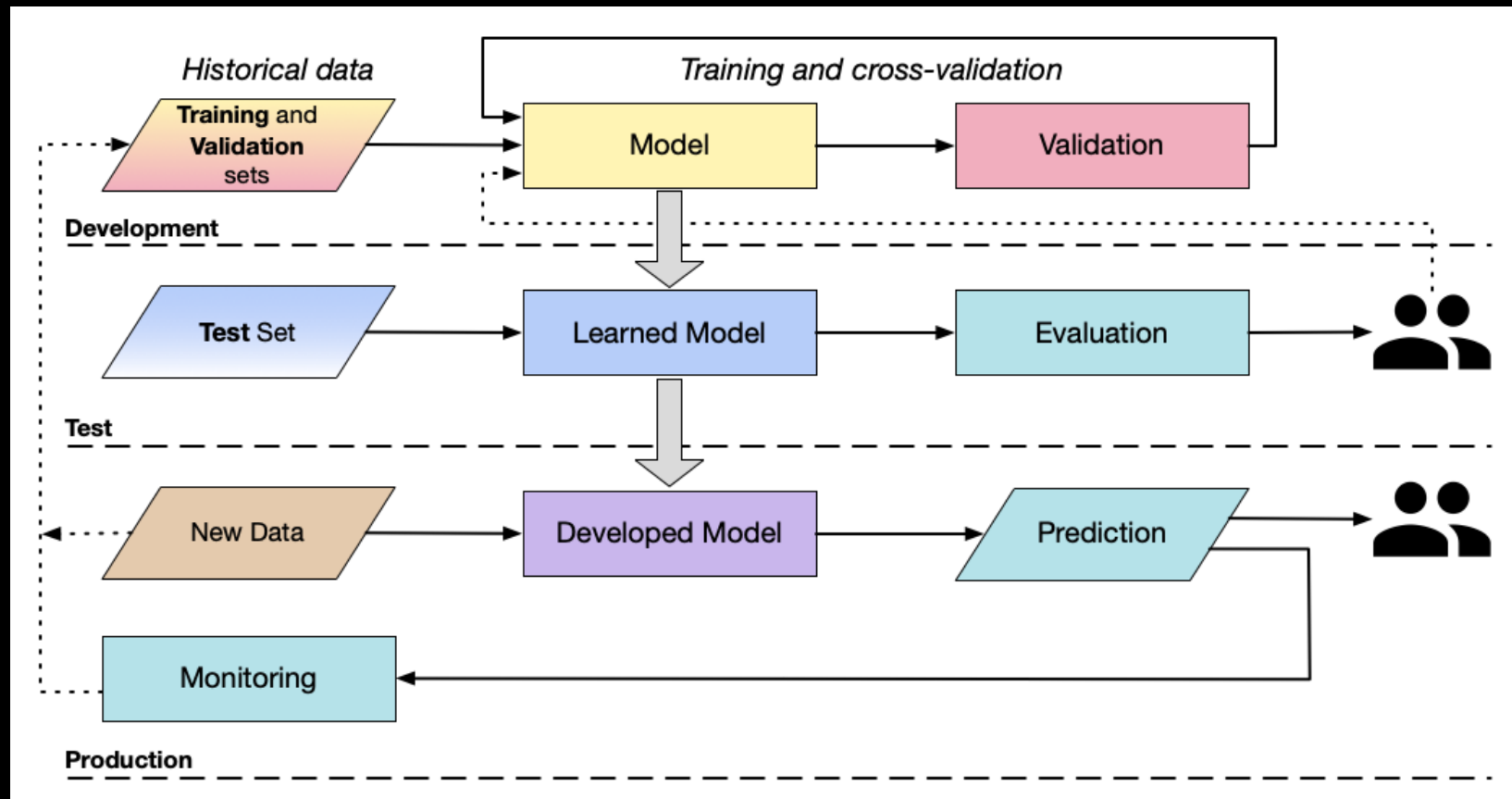
Lecture 5 - Part *a*  
Training and Evaluation

# Previously on ML4D

# CRISP-DM Methodology

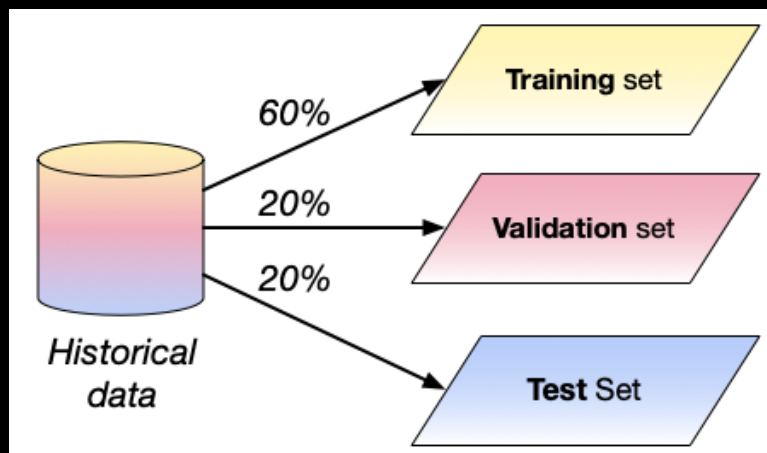


# Model Development Lifecycle



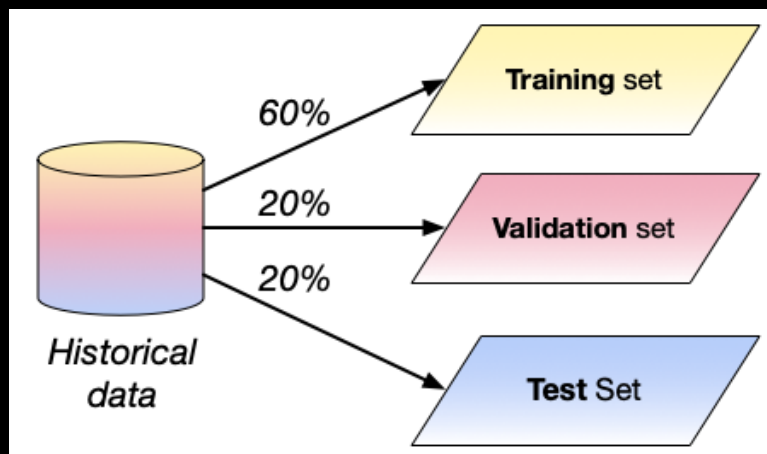
# Dataset Splitting

# Split your data



- **Training** set
  - *train*
- **Validation** set
  - *fine-tune*
- **Test** set
  - *evaluate*

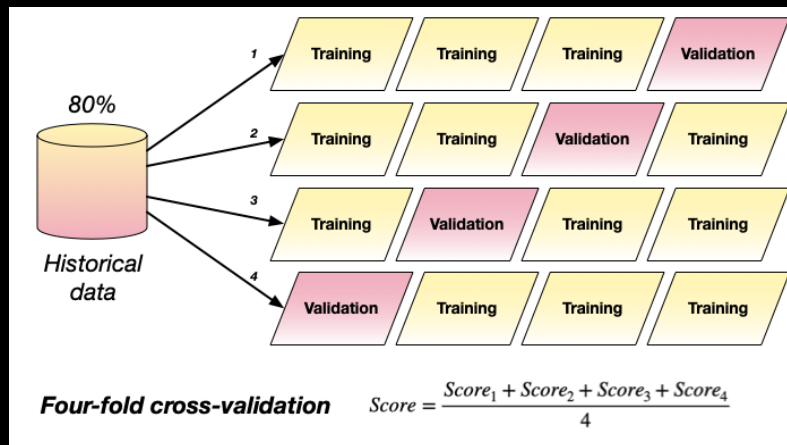
# Avoid leakages



- **Data items**
  - in the *validation* or *evaluation* sets
- **Features**
  - highly correlated to prediction
  - not present in the production environment



# Cross-validation



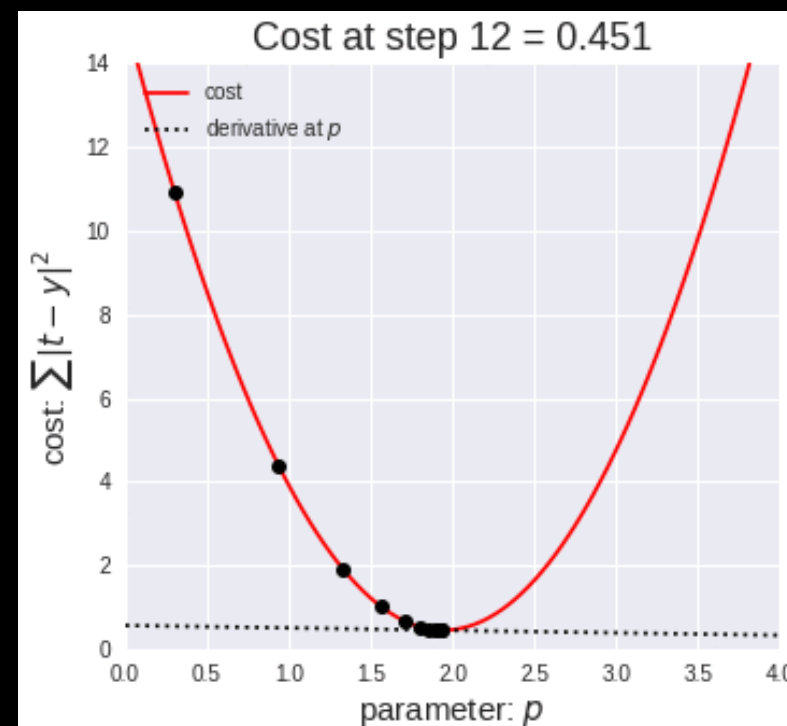
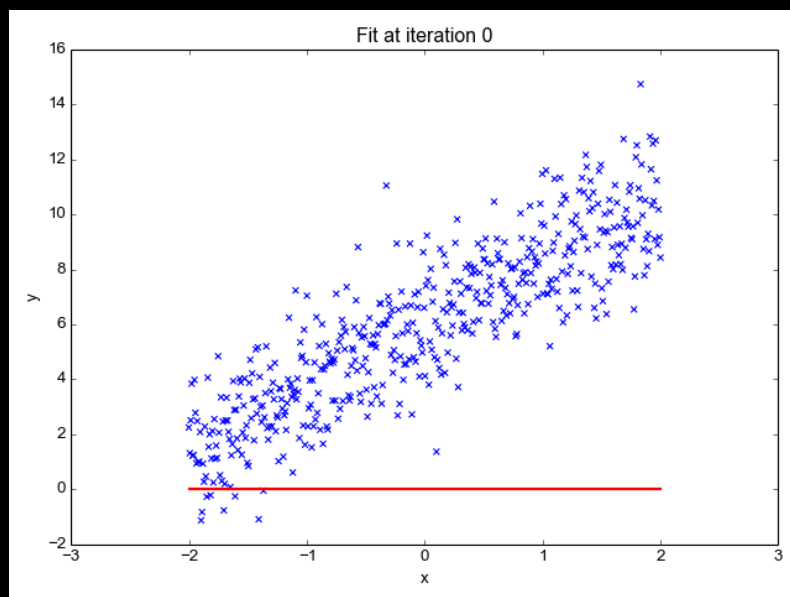
- Cycle training and validation data several times
- Useful when dataset is small
- Split the data into  $n$  portions
- Train the model  $n$  times using  $n - 1$  portions for training
- Average results

# Evaluation

# How to Evaluate?

- **Metric**
  - How to measure errors?
  - Both training and testing
- **Training**
  - How to “help” the ML model to perform well?
- **Testing**
  - How to “help” the ML model to generalise?
- **Experiment**
  - How to pick the best ML model?

# Model Training Process



# Let errors guide you

- Errors are almost inevitable!
- How to measure errors?
- Select an evaluation procedure (a “metric”)

# Errors

- These are the most common questions:
  - *How* is the prediction wrong?
  - *How often* is the prediction wrong?
  - What is the *cost* of wrong predictions?
  - How does the *cost* vary by the wrong prediction type?
  - How can *costs* be minimised?

# Regression

## Mean absolute error



$$MAE = \frac{1}{N} \sum_{j=1}^N |p_j - v_j|$$

Average of the difference between the *training* value ( $v_j$ ) and the *predicted* value ( $p_j$ )



## Mean square error



$$MSE = \frac{1}{2N} \sum_{j=1}^N (p_j - v_j)^2$$

Average of the square of the difference between the *training* value ( $v_j$ ) and the *predicted* value ( $p_j$ )

Square is easier to use during the training process (derivative)

More significant errors are more pronounced

# Classification

## Confusion Matrix

Describes the complete performance of the model

		Actual Class	
		Yes	No
Predicted Class	Yes	50	10
	No	40	100

True Positive (arrow points to 50)

False Positive - *false alarm!*  
(Type I Error) (arrow points to 10)

True Negative (arrow points to 100)

False Negative - *underestimation*  
(Type II Error) (arrow points to 40)

# Type I and Type II errors

Type I Error



Type II Error



## Accuracy

$$\frac{TP+TN}{TP+TN+FP+FN}$$

The *percentage of times* that a model is correct

The model with the highest accuracy *is not necessarily the best*

Some errors (e.g., False Negative) can be more expensive than others

# Errors are not equal

## FALSE POSITIVES: SELF-DRIVING CARS AND THE AGONY OF KNOWING WHAT MATTERS



According to a preliminary report released by the National Transportation Safety Board last week, Uber's system detected pedestrian Elaine Herzberg six seconds before striking and killing her. It identified her as an unknown object, then a vehicle, then finally a bicycle. (She was pushing a bike, so close enough.) About a second before the crash, the system determined it needed to slam on the brakes. But Uber hadn't set up its system to act on that decision, the NTSB explained in the report. The engineers prevented their car from making that call on its own "to reduce the potential for erratic vehicle behavior." (The company relied on the car's human operator to avoid crashes, which is a whole separate problem.)

Uber's engineers decided not to let the car auto-brake because they were worried the system would overreact to things that were unimportant or not there at all. They were, in other words, very worried about false positives.

LEARN MORE

- Detecting the “Alexa” command?
- Pregnancy detection
  - Cost of “false negatives”?
  - Cost of “false positives”?
- Covid testing
  - Cost of “false negatives”?
  - Cost of “false positives”?
- Law enforcement?

## Precision

$$\frac{TP}{TP+FP}$$

Among the examples we classified as positive, how many did we correctly classify?

## Recall

$$\frac{TP}{TP+FN}$$

Among the positive examples, how many did we correctly classify?



## F1-Score

$$F_1 = 2 * \frac{1}{\frac{1}{P} + \frac{1}{R}}$$

The harmonic mean  
between *precision*  
and *recall*

What is the implicit  
assumption about the  
costs of errors?

## **Sensitivity (true positive rate)**

$$\frac{TP}{FN+TP}$$

Identification of the positively labeled data items

*Same as recall*

## Specificity (false positive rate)

$$\frac{TN}{FP+TN}$$

Identification of the negatively labeled data items

*Not the same as precision*

		Actual Class		
Predicted Class		P	N	
	P	TP	FN	$\rightarrow \text{Sensitivity} = \frac{TP}{FN + TP}$
	N	FP	TN	$\rightarrow \text{Specificity} = \frac{TN}{FP + TN}$
				$\rightarrow \text{Precision} = \frac{TP}{TP + FP}$

## Medical Test Model

- **Recall** and **sensitivity**
    - Among the sick people (positives), how many were correctly diagnosed as sick?
  - **Precision**
    - Among the people diagnosed as sick, how many were sick?
  - **Specificity**
    - Among the healthy people (negatives), how many were correctly diagnosed as healthy?
- \u2028

## Spam Detection Model

- **Recall** and **sensitivity**
  - Among the spam emails (positives), how many were correctly deleted?
- **Precision**
  - Among the deleted emails, how many were spam?
- **Specificity**
  - Among the good emails (negatives), how many were correctly sent to the inbox?

## How to choose a metric?

- Constraint: **high precision**
  - e.g., search engine results (false positive are tolerable)
  - Pick a model with a higher recall
  - **Metric:** *Recall at Precision =  $x\%$*

## How to choose a metric?

- Constraint: **high recall**
  - e.g., medical diagnosis (false negatives are tolerable)
  - Pick a model with a higher precision
  - **Metric:** *Precision at Recall =  $x\%$*



## **Metrics are also designed in a multi-stakeholder context**

- One team builds the mode
  - Data scientists / ML engineers
- Many teams will make use of it
  - e.g., product team, management team

# Machine Learning for Design

Lecture 5 - Part *a*  
Training and Evaluation

## Credits

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