

# AI/ML: Preliminaries & Overview



Fall 2018



## Windows

A fatal exception 0E has occurred at 0028:C562F1B7 in VXD ctpci9x(05)  
+ 00001853. The current application will be terminated.

- \* Press any key to terminate the current application.
- \* Press CTRL+ALT+DEL again to restart your computer. You will lose any unsaved information in all applications.

Press any key to continue \_

LOL

A fatal exce  
+ 00001853.

\* Press an  
\* Press CT  
lose any

ctpci9x(05)

will

Press any key to continue \_

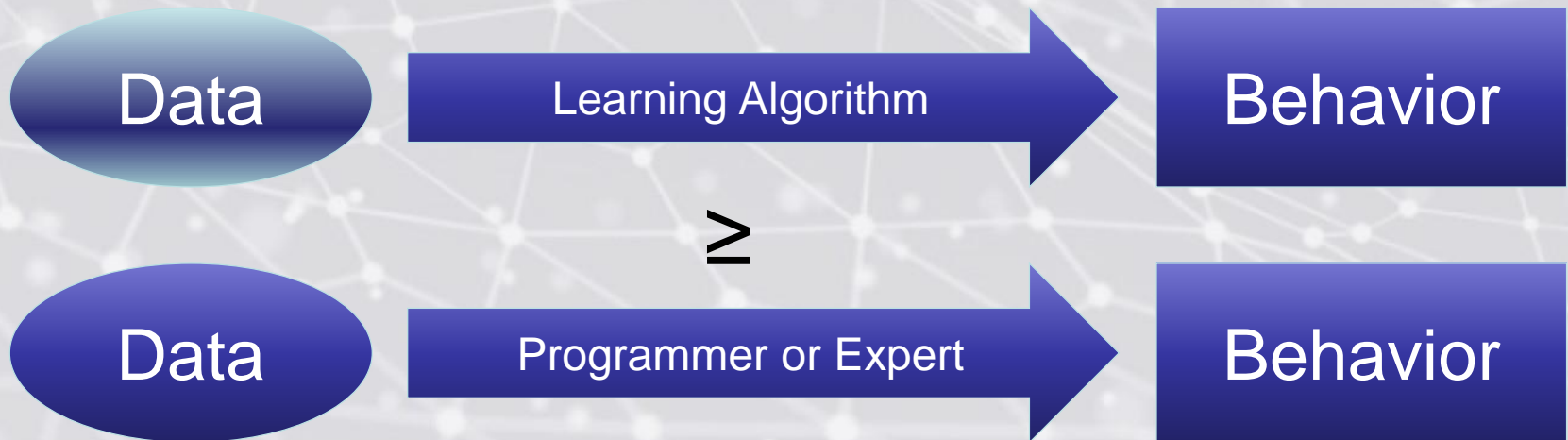
# What is machine learning?

- Textbook definitions of “machine learning”:
  - Detecting patterns and regularities with a good and generalizable approximation (“model” or “hypothesis”)
  - Execution of a computer program to optimize the parameters of the model using training data or past experience.

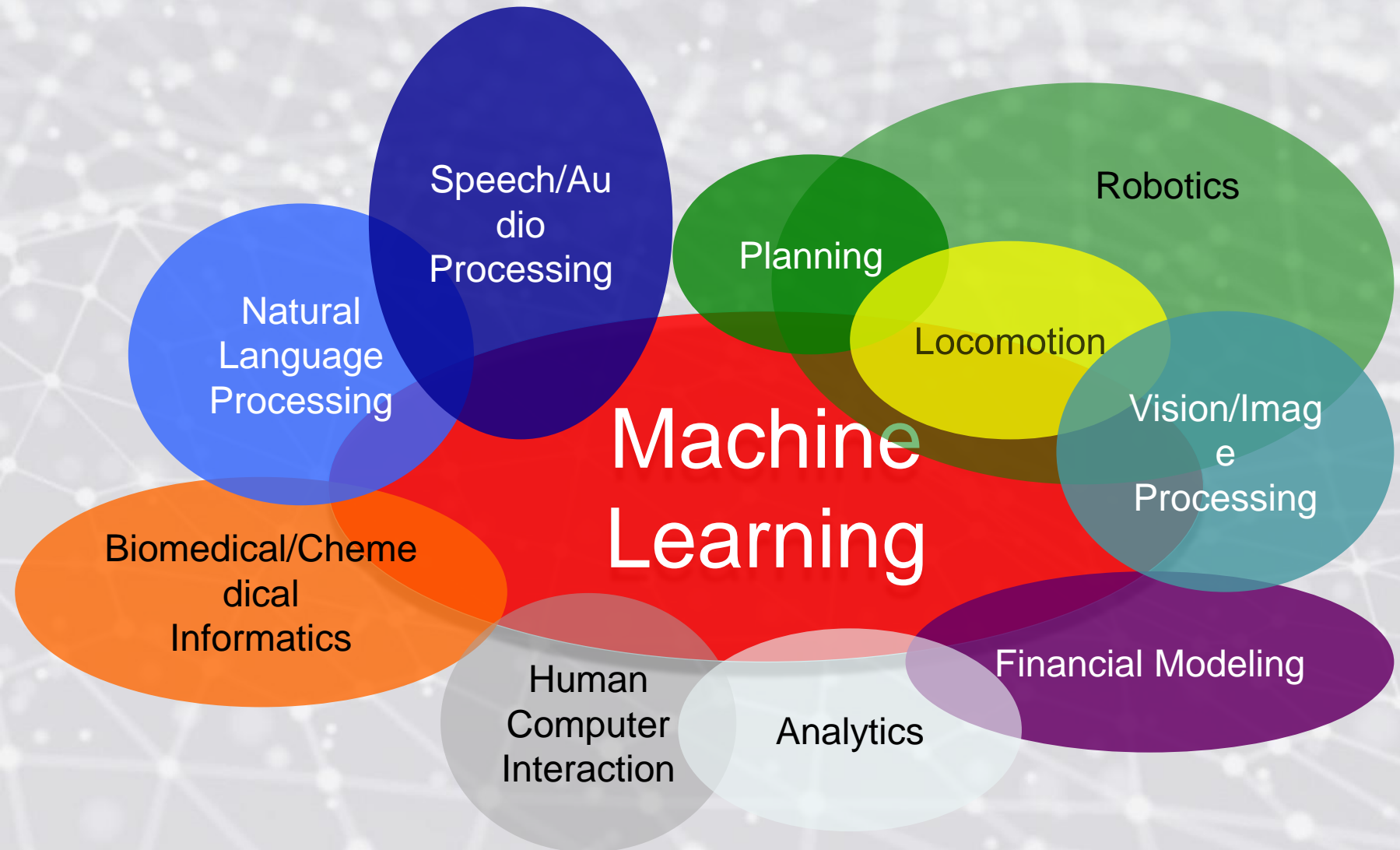


# Machine Learning

- Automatically identifying patterns in data
- Automatically making decisions based on data
- Hypothesis:



# Machine Learning in Computer Science



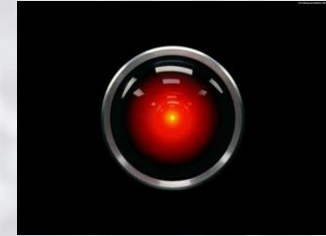
# Major Tasks

- Regression
  - Predict a numerical value from “other information”; Output is a real value (e.g., “\$35/share”)
- Classification
  - Predict a categorical value; Output is one of a number of classes (e.g., ‘A’)
- Clustering
  - Identify groups of similar entities
- Optimization



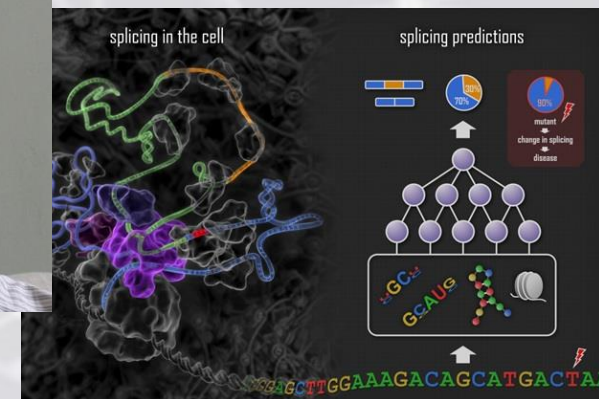
# A Small Subset of Machine Learning Applications

- (\*) Speech Recognition
- (\*) NLP (natural language processing); machine translation.
- (\*) Computer Vision
- (\*) Medical Diagnosis
- (\*) Autonomous Driving
- (\*) Statistical Arbitrage
- (\*) Signal Processing
- (\*) Recommender Systems
- (\*) ~~World Domination~~
- (\*) Fraud Detection
- (\*) Social Media
- (\*) Data Security
- (\*) Search
- (\*) A.I. & Robotics
- (\*) Genomics
- (\*) Computational Creativity
- (\*) Hi Scores



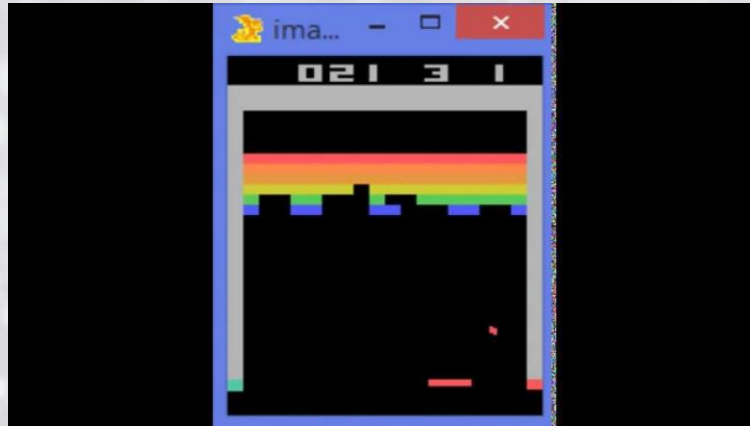
## Big Data meets Machine Learning in the Car

- Real world is a Big Data problem
- Driving in human world required intelligent perception of the world





# A Small Subset of Machine Learning Applications



- <https://www.youtube.com/watch?v=V1eYniJ0Rnk>



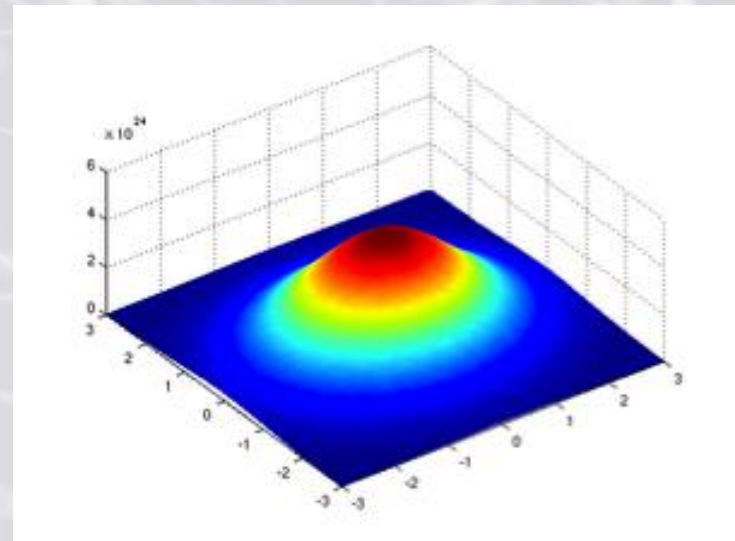
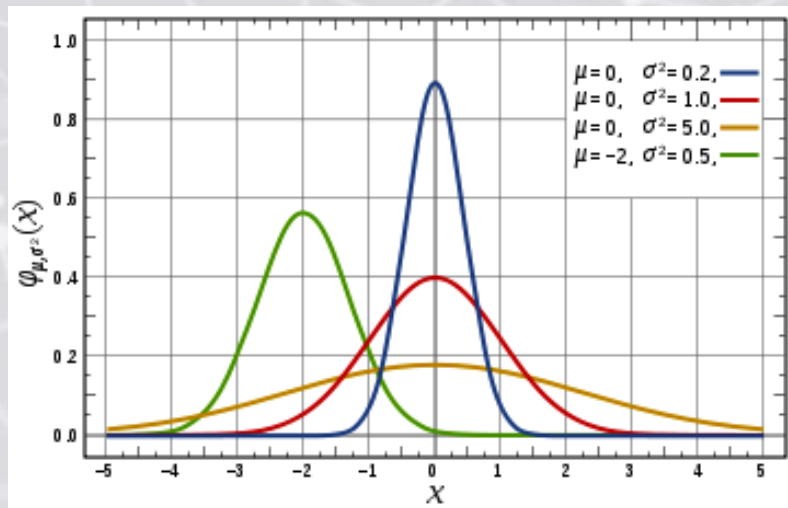
- <https://www.youtube.com/watch?v=SCE-QeDfXtA>

# Mathematical Necessities

- Probability
- Statistics
- Calculus
  - Vector Calculus
- Linear Algebra
- Algorithms

# Why do we need so much math?

- Probability Density Functions allow the evaluation of how likely a data point is under a model.
  - Want to identify good PDFs. (calculus)
  - Want to evaluate against a known PDF. (algebra)

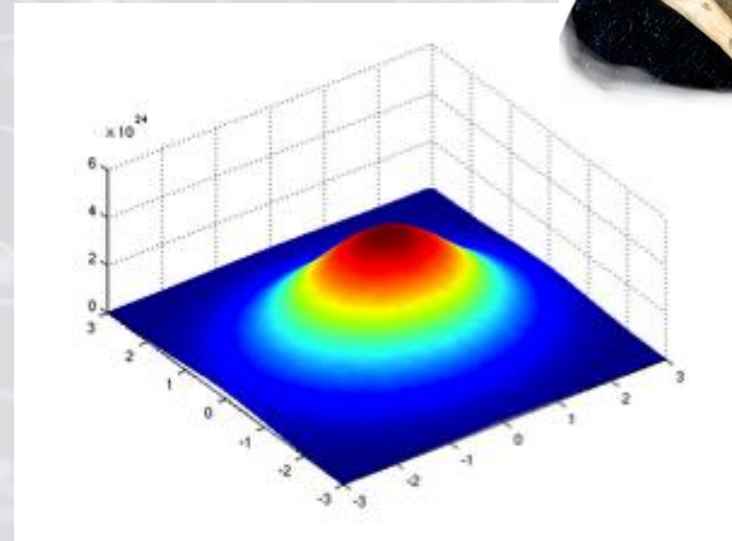
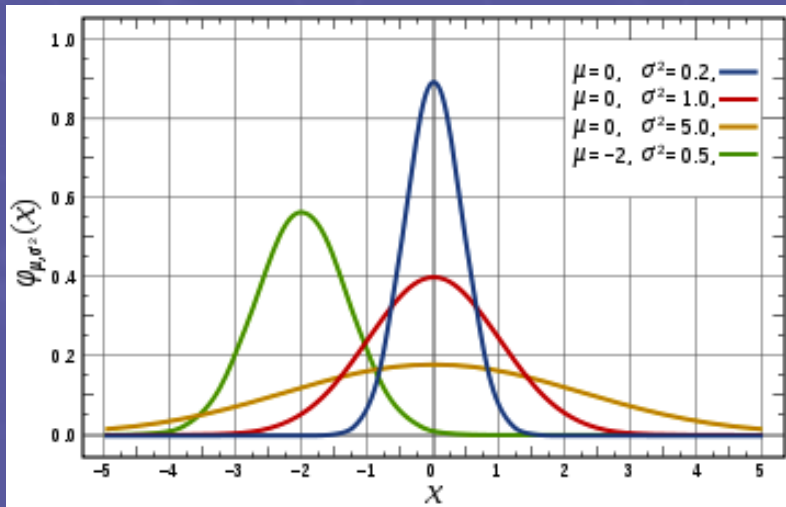




# Gaussian Distributions

- We use Gaussian Distributions all over the place.

$$N(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ -\frac{1}{2\sigma^2} (x - \mu)^2 \right\}$$

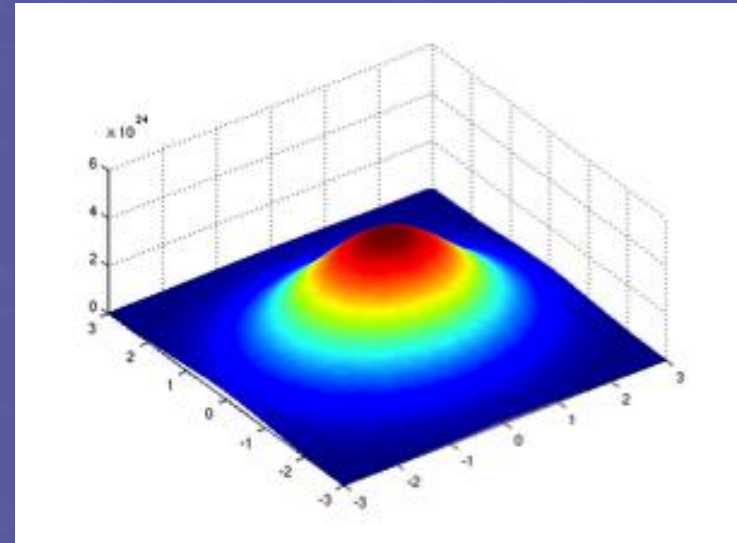
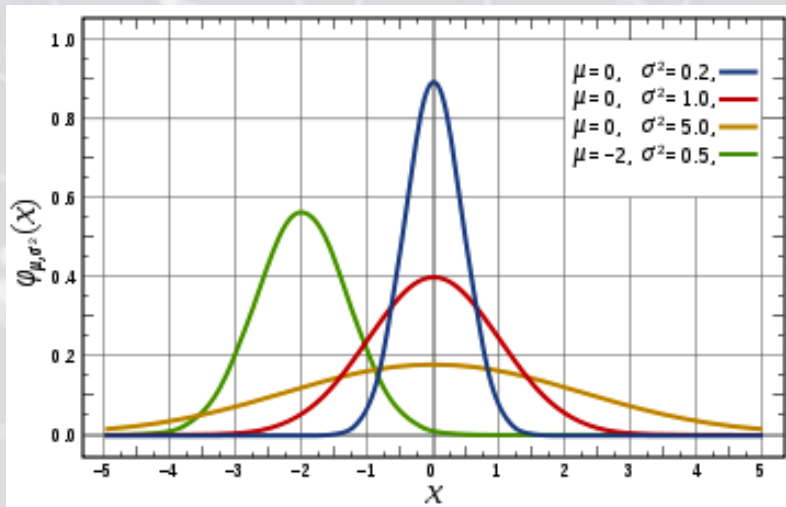




# Gaussian Distributions

- We use Gaussian Distributions all over the place.

$$N(x; \mu, \Sigma) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right\}$$



# Types of Machine Learning Methods

- **Supervised**
  - provide explicit training examples with correct answers
    - e.g. neural networks with back-propagation
- **Unsupervised**
  - no feedback information is provided
    - e.g., unsupervised clustering based on similarity
- **“Semi-supervised”**
  - some feedback information is provided but it is not detailed
    - e.g., only a fraction of examples are labeled
    - e.g., reinforcement learning: reinforcement signal is single-valued assessment of current state

# Data Data Data

- “There’s no data like more data”
- All machine learning techniques rely on the availability of data to learn from.
- There is an ever increasing amount of data being generated, but it’s not always easy to process.
- Is all data equal?
- (Good) Data (can) trump a choice of model!

# Key Ingredients for Any Machine Learning Method

- **Features** (or “attributes”)
- Underlying **Representation** for “hypothesis”, “model”, or “target function”
- **Hypothesis space**
- **Learning method**
- **Data:**
  - **Training data**
    - Used to train the model
  - **Validation (or Development) data**
    - Used to select model hyperparameters, to determine when to stop training, or to alter training method
  - **Test data**
    - Used to evaluate trained model
- **Evaluation method**



## Assumption of all ML methods

### **Inductive learning hypothesis:**

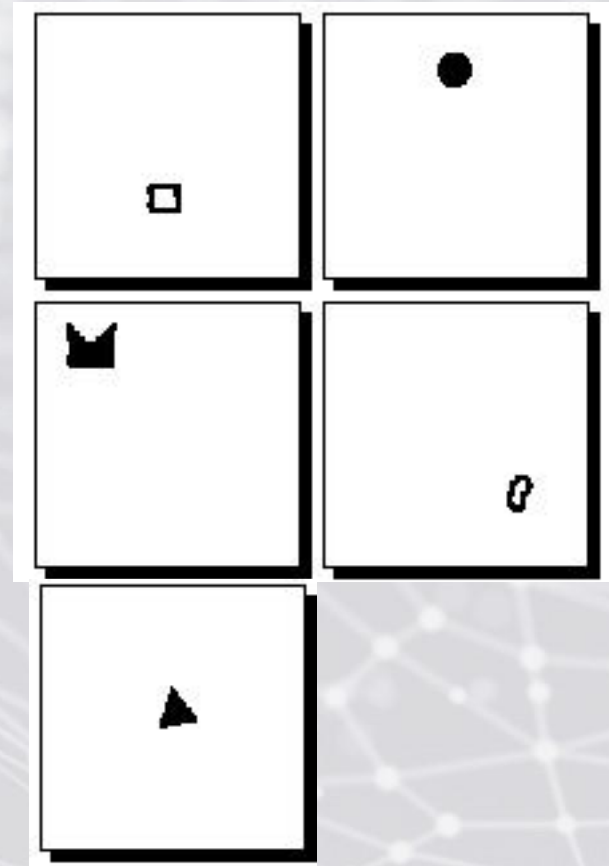
Any hypothesis that approximates target concept well over sufficiently large set of training examples will also approximate the concept well over other examples outside of the training set.

Q: What is the difference between “induction” and “deduction”?

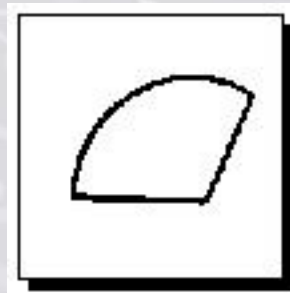
Training Examples: Class 1



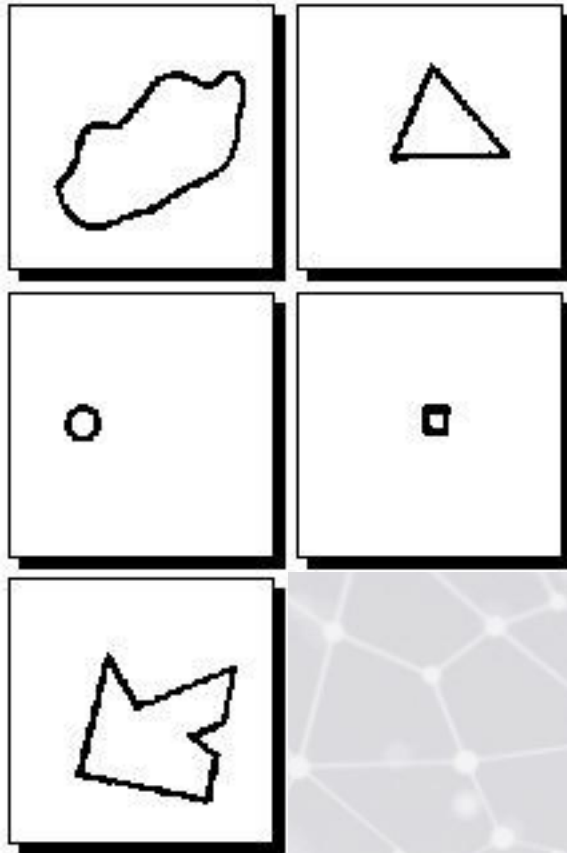
Training Examples: Class 2



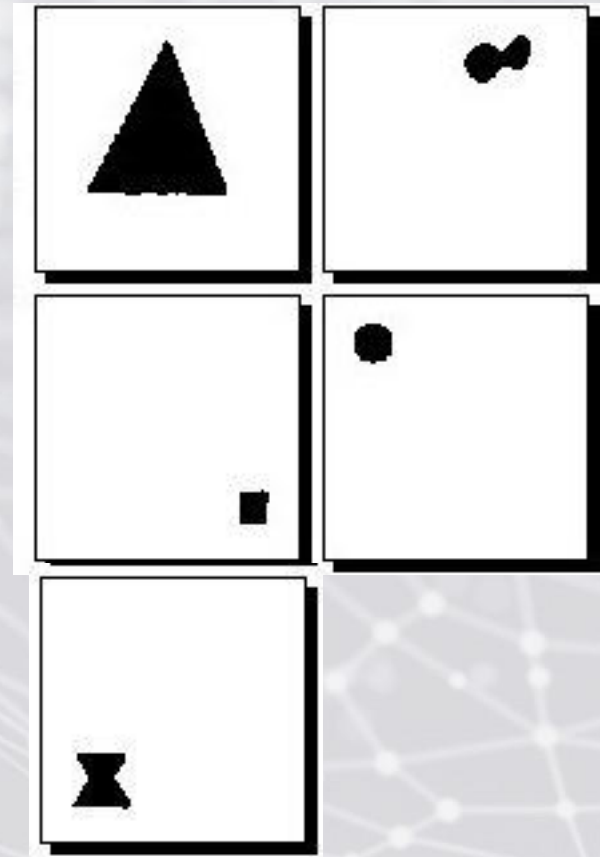
Test example: Class = ?



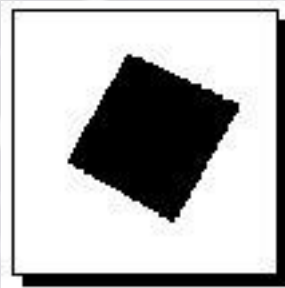
Training Examples: Class 1



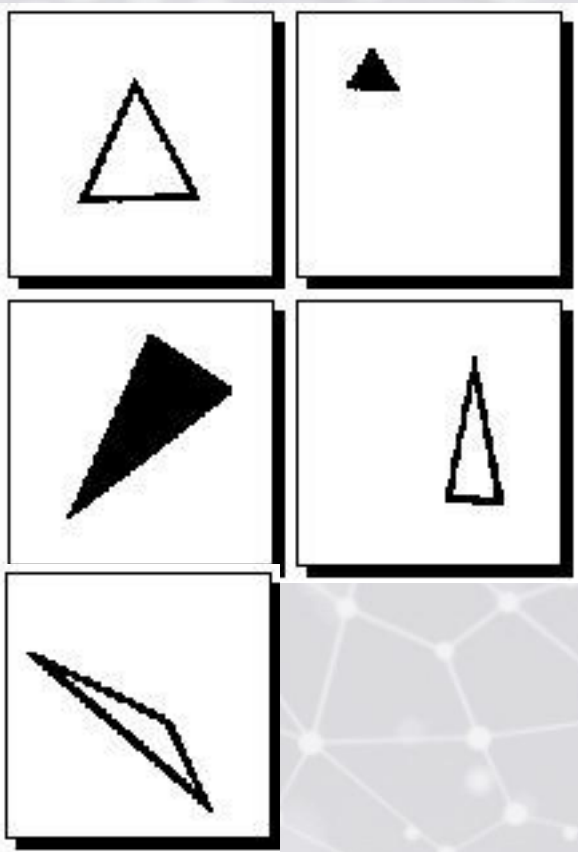
Training Examples: Class 2



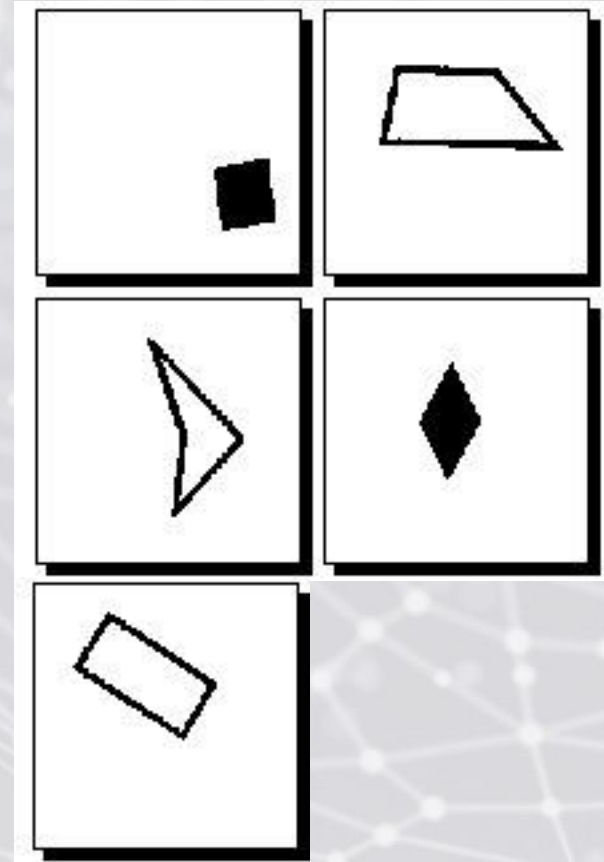
Test example: Class = ?



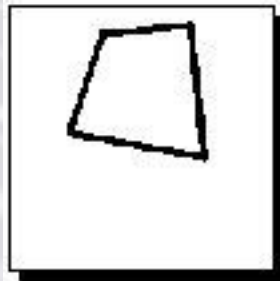
Training Examples: Class 1



Training Examples: Class 2

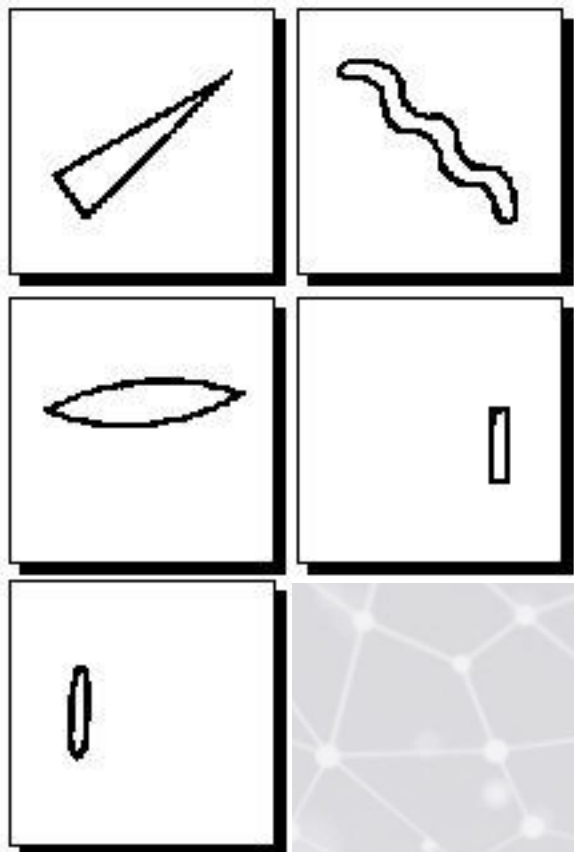


Test example: Class = ?





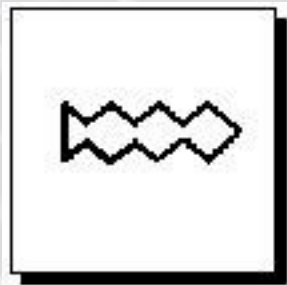
Training Examples: Class 1



Training Examples: Class 2

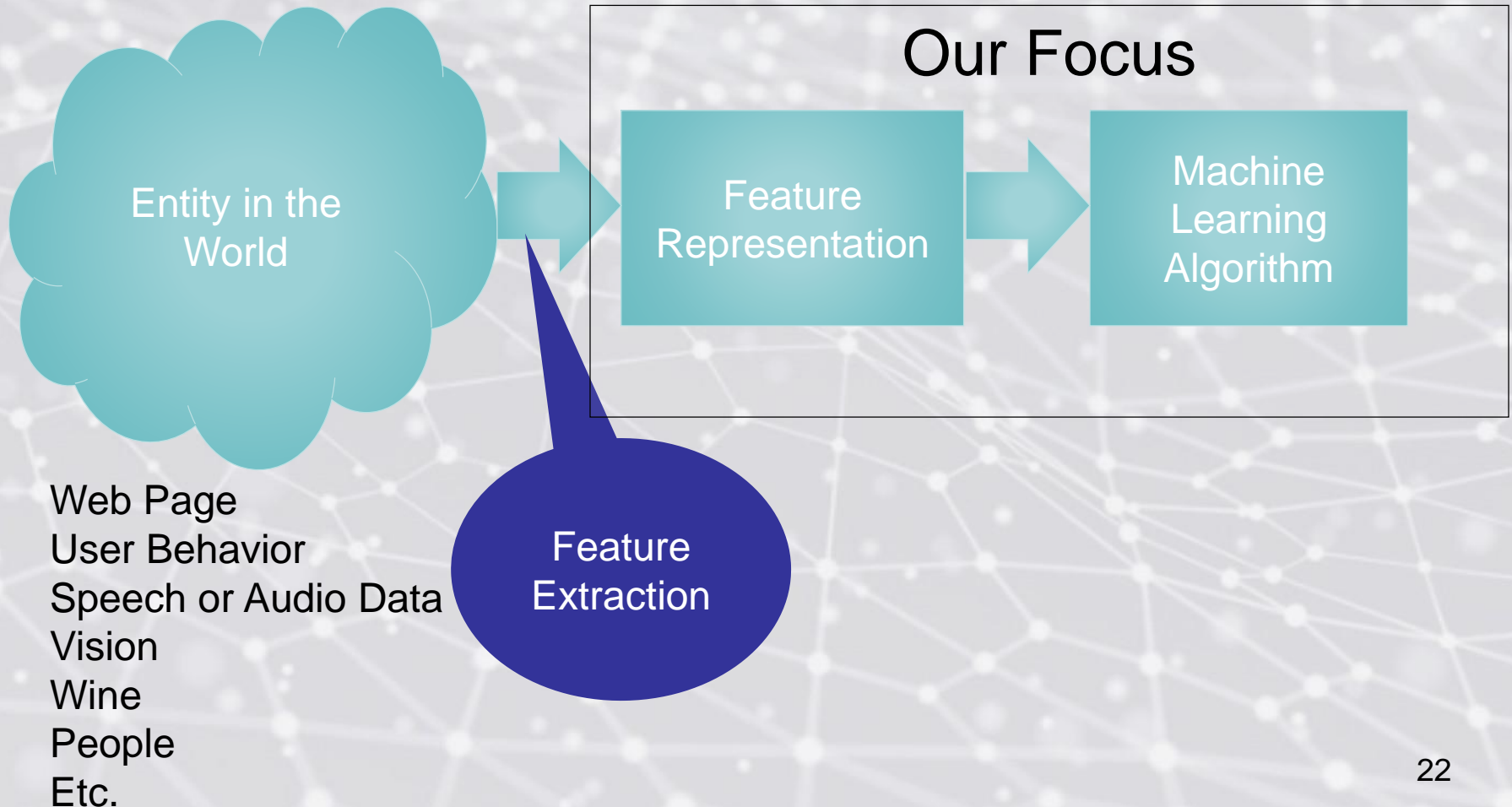


Test example: Class = ?



# Feature Representations

- How do we view data?



# Feature Representations

Height	Weight	Eye Color	Gender
66	170	Blue	Male
73	210	Brown	Male
72	165	Green	Male
70	180	Blue	Male
74	185	Brown	Male
68	155	Green	Male
65	150	Blue	Female
64	120	Brown	Female
63	125	Green	Female
67	140	Blue	Female
68	165	Brown	Female
66	130	Green	Female

# Classification

- Identify which of  $N$  classes a data point,  $\mathbf{x}$ , belongs to.
- $\mathbf{x}$  is a column vector of features.

$$\vec{x} = \begin{pmatrix} x_0 \\ x_1 \\ \dots \\ x_{n-1} \end{pmatrix} \quad \text{OR} \quad \vec{x} = \begin{pmatrix} f_0(x) \\ f_1(x) \\ \dots \\ f_{m-1}(x) \end{pmatrix}$$



# Target Values

- In **supervised** approaches, in addition to a data point,  $\mathbf{x}$ , we will also have access to a target value,  $\mathbf{t}$ .

## Goal of Classification

Identify a function  $y$ , such that  $y(\mathbf{x}) = \mathbf{t}$

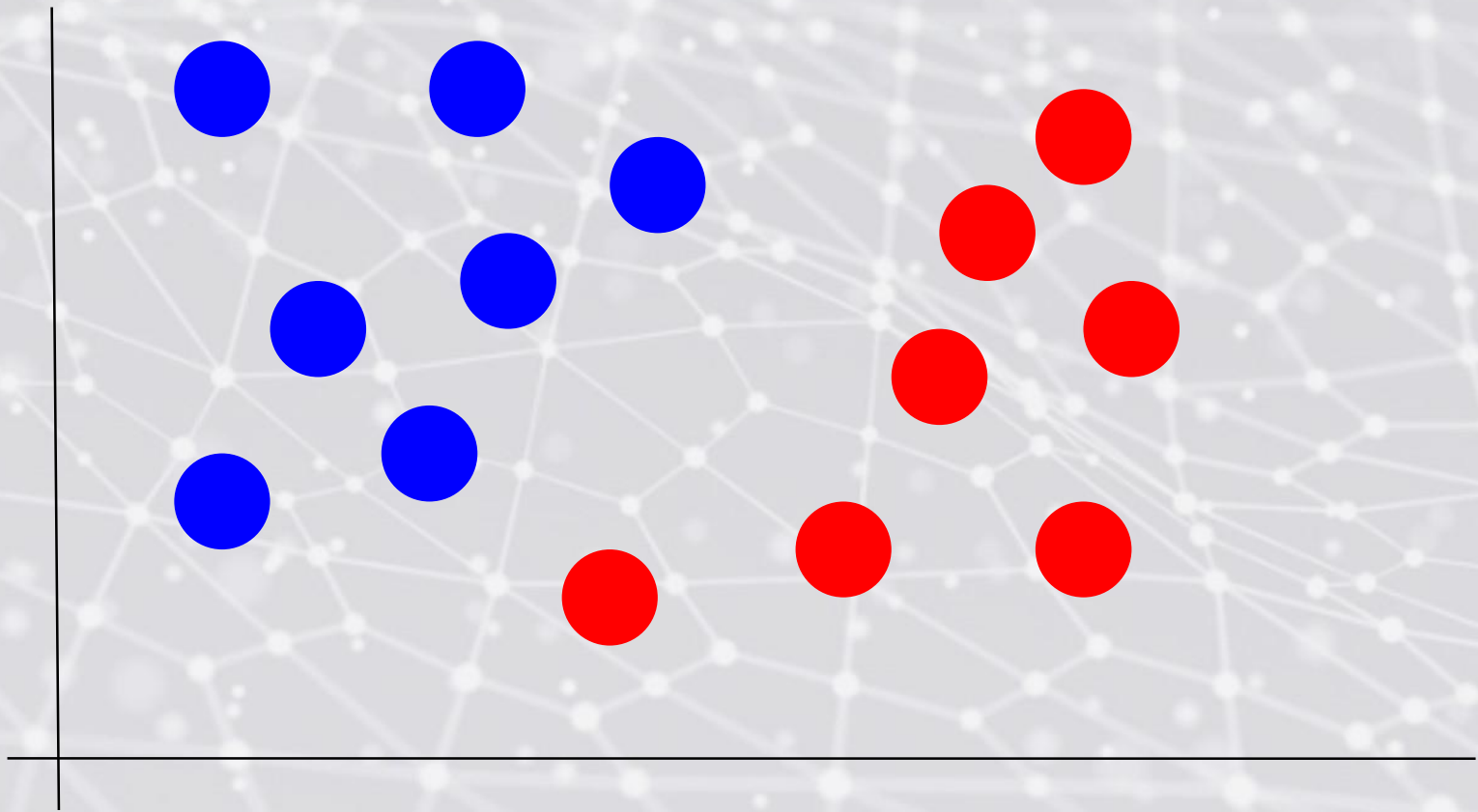
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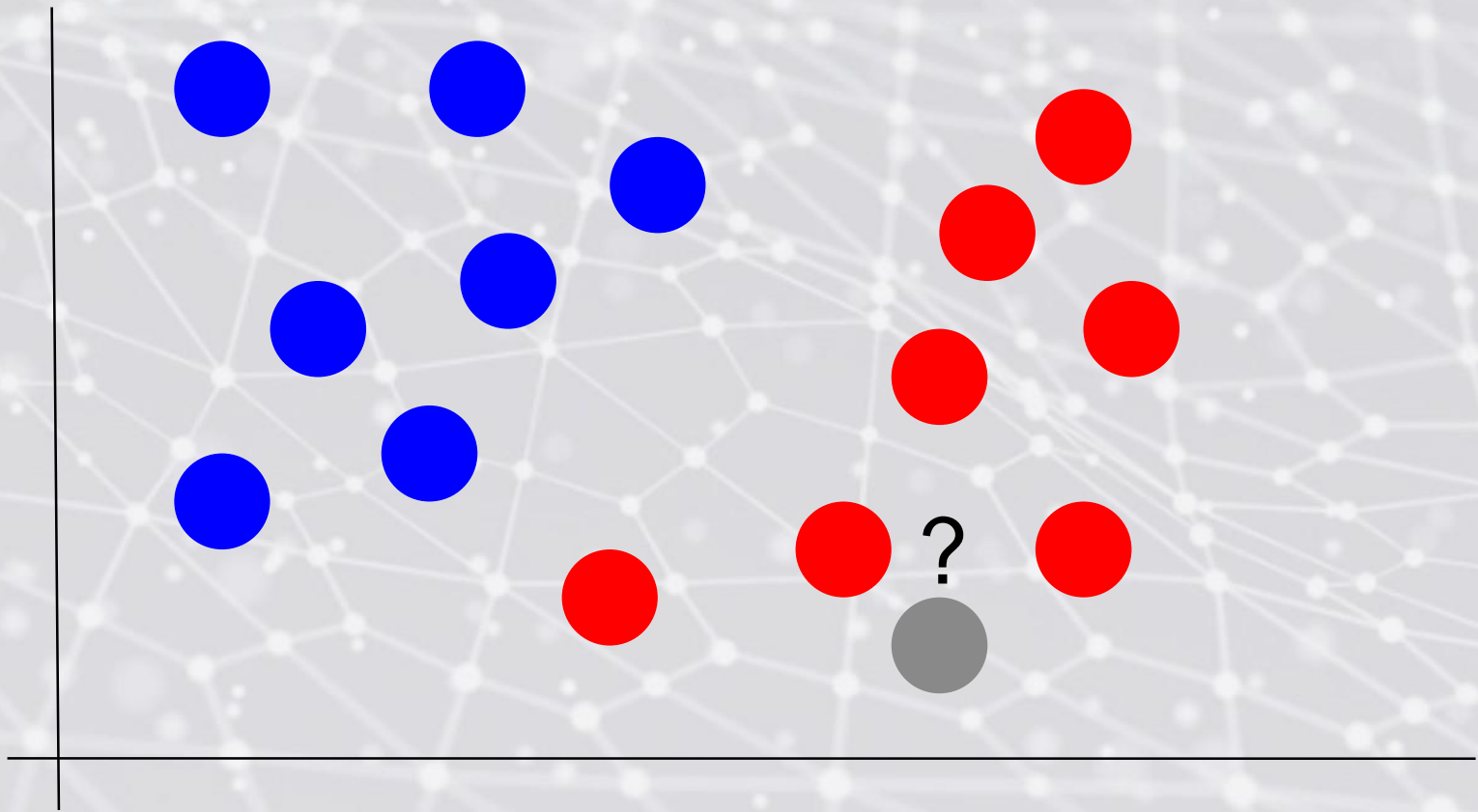
$$\vec{x}_0 = \begin{pmatrix} 66 \\ 170 \\ Blue \end{pmatrix}$$

$$t_0 = Male$$

# Graphical Example of Classification

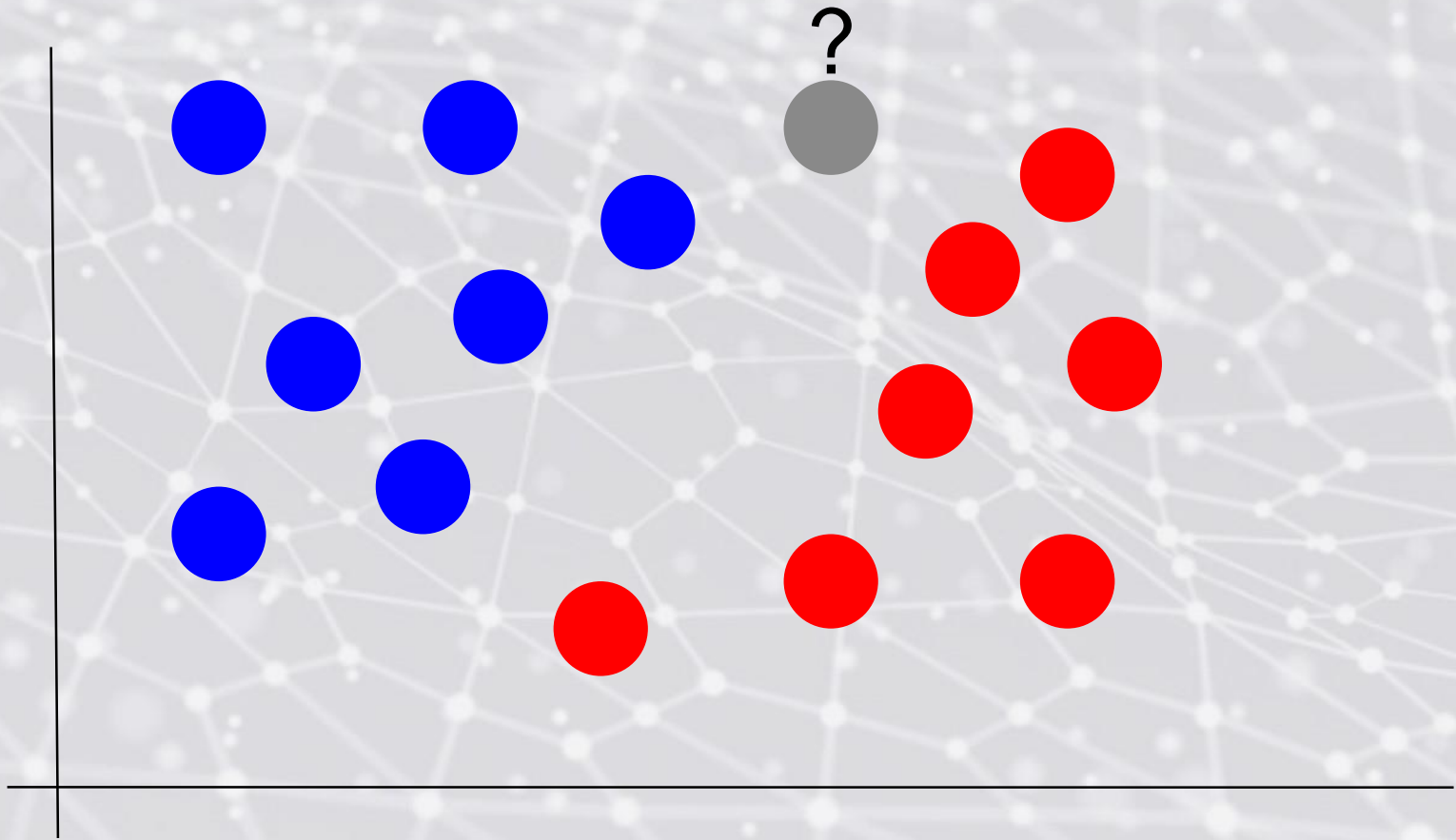


# Graphical Example of Classification

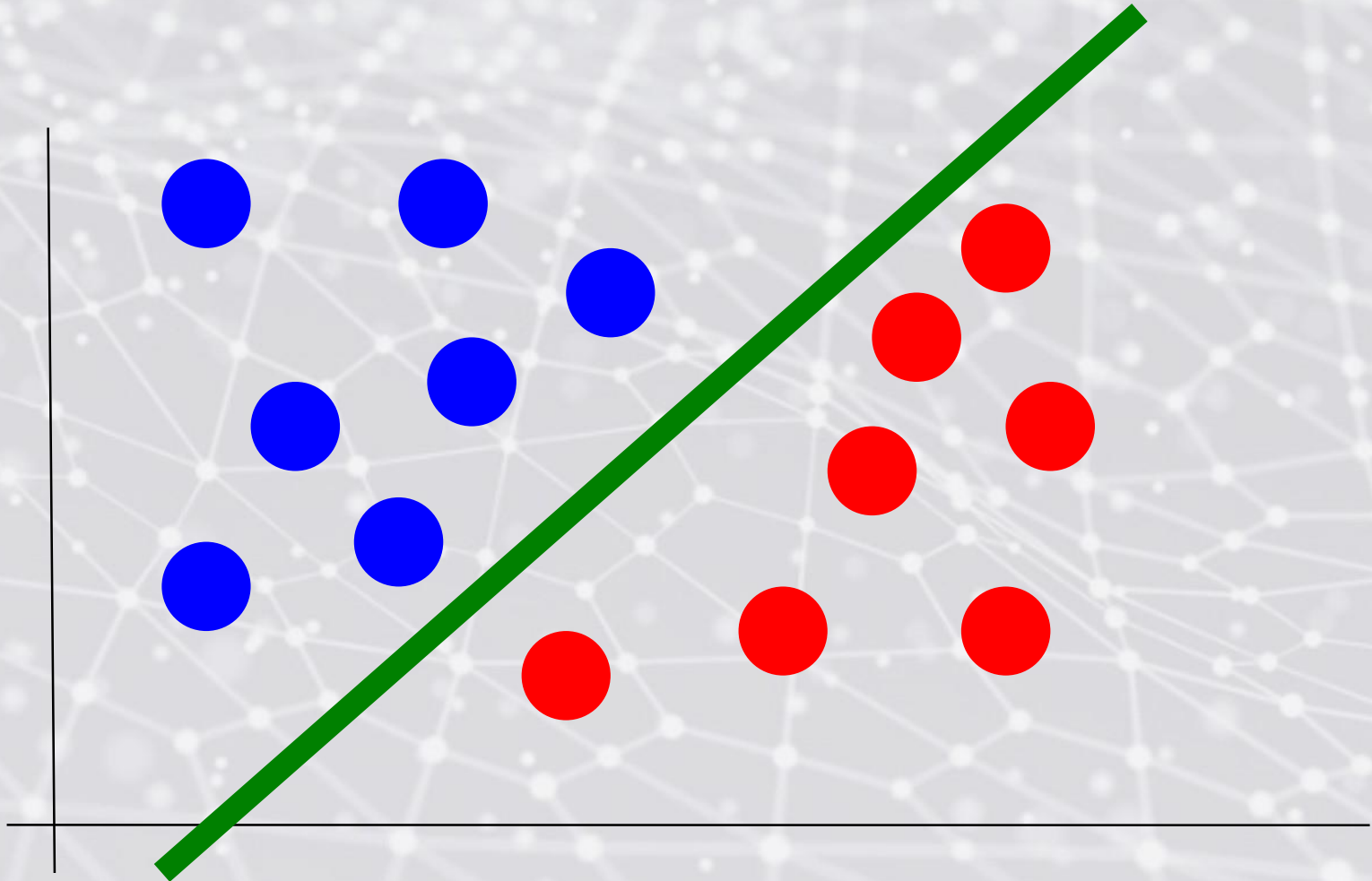




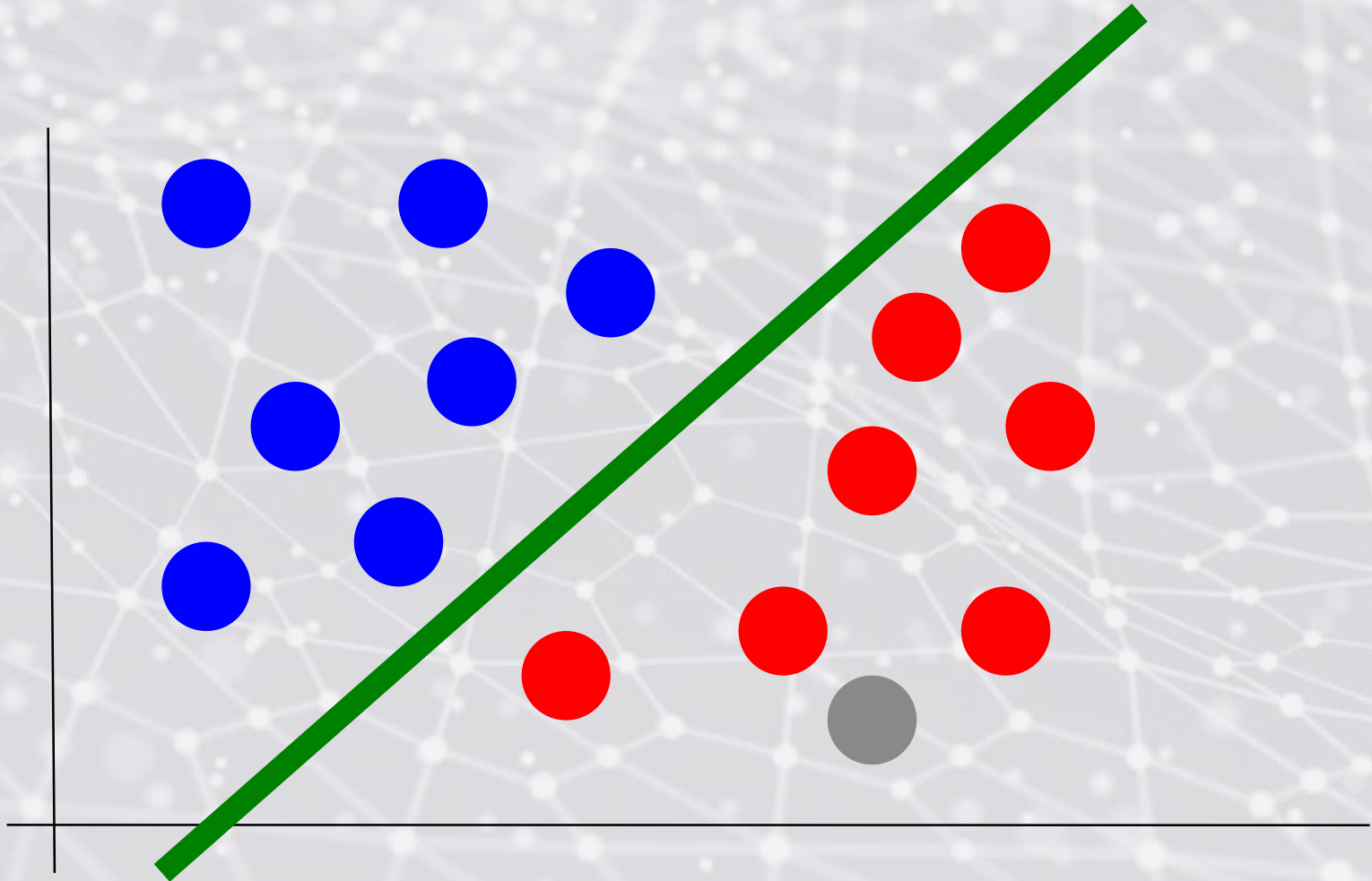
# Graphical Example of Classification



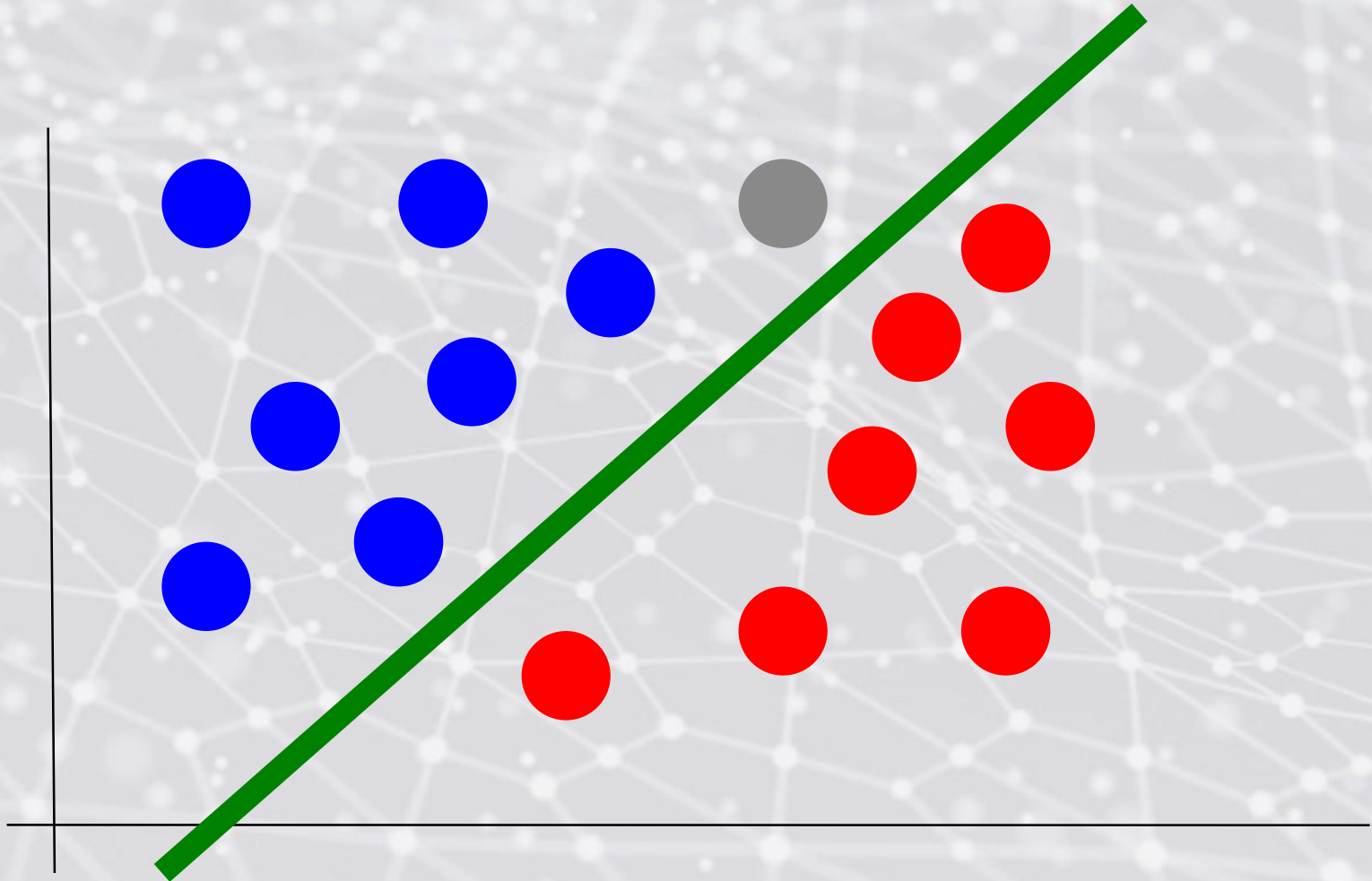
# Graphical Example of Classification



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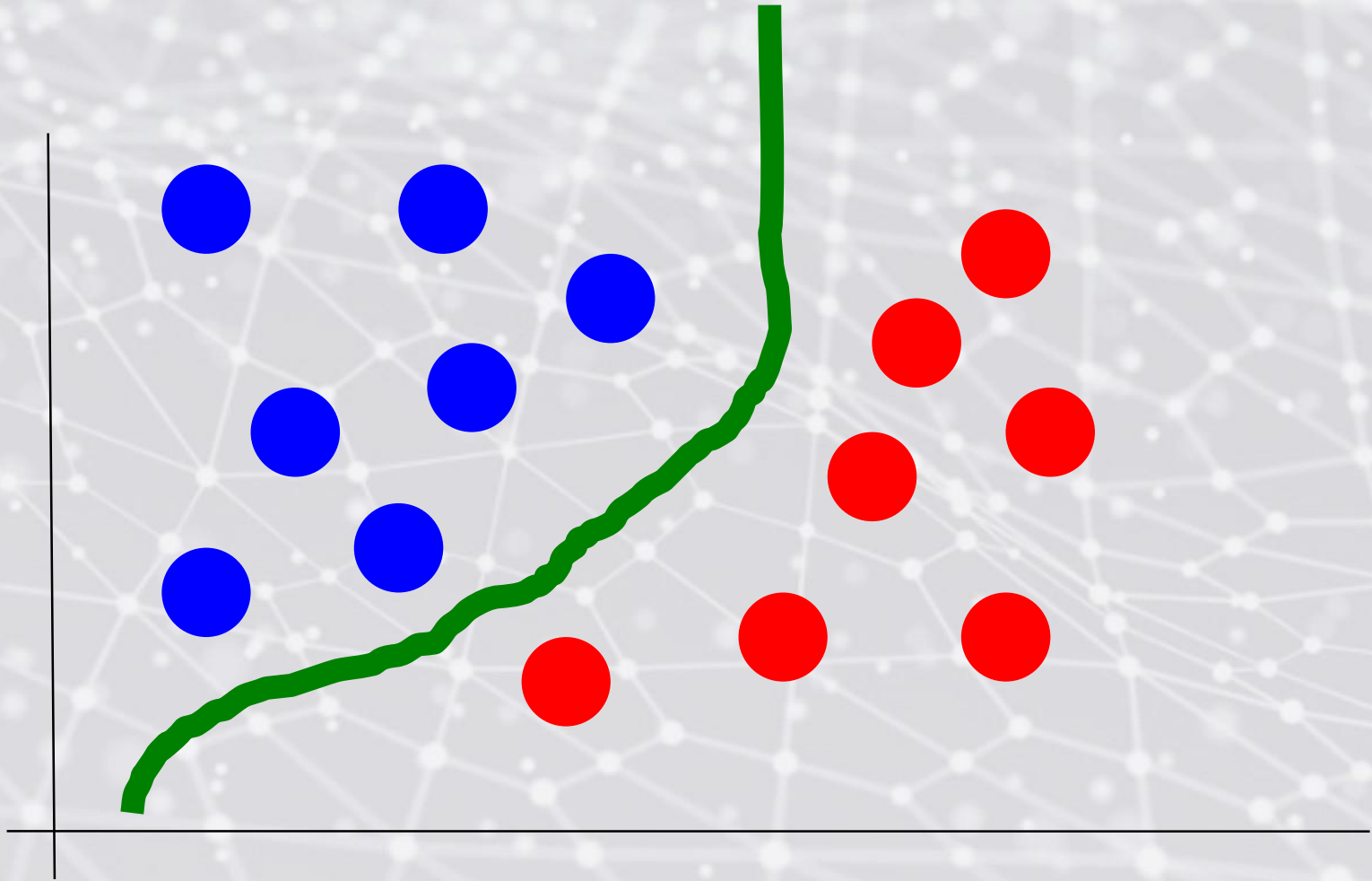


# Graphical Example of Classification





# Decision Boundaries



# Regression

- Regression is a **supervised** machine learning task.
  - So a target value, **t**, is given.
- Classification: nominal **t**  $t \in \{c_0, \dots, c_{N-1}\}$
- Regression: continuous **t**  $t \in \mathbb{R}$

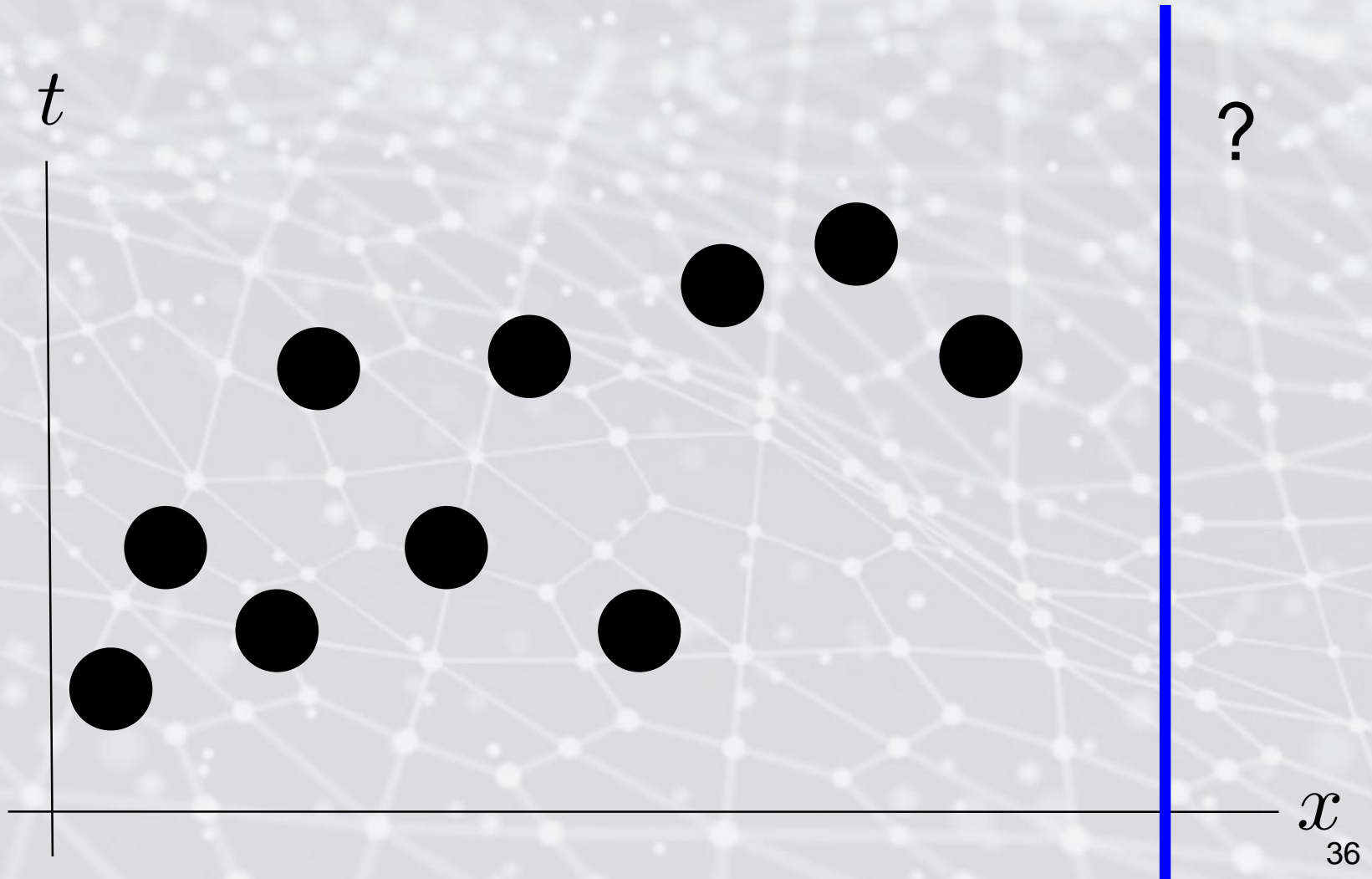
## Goal of Classification

Identify a function  $y$ , such that  $y(\mathbf{x}) = \mathbf{t}$

# Differences between Classification and Regression

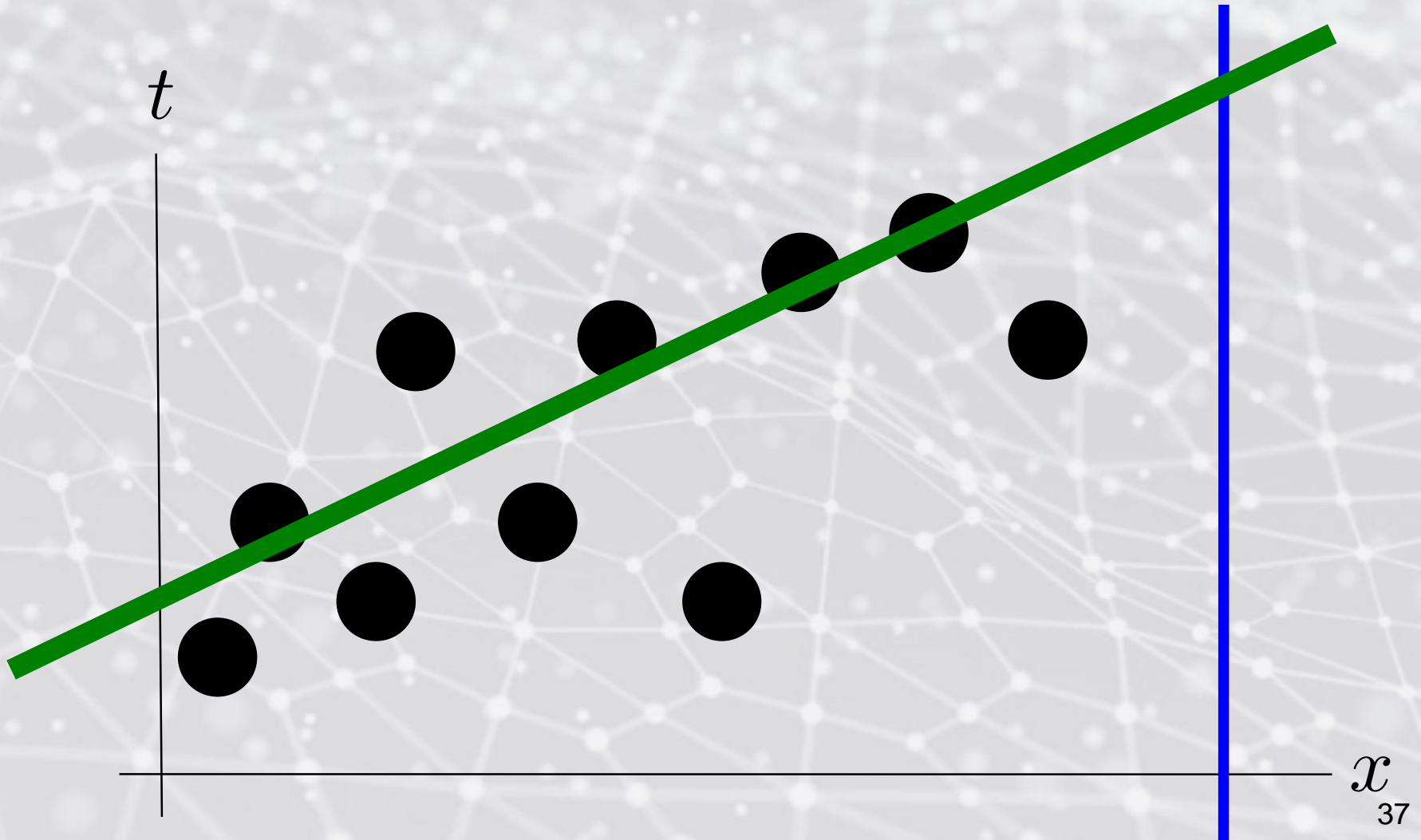
- Similar goals: Identify  $y(\mathbf{x}) = \mathbf{t}$ .
- What are the differences?
  - The form of the function,  $y$  (naturally).
  - Evaluation
    - Root Mean Squared Error
    - Absolute Value Error
    - Classification Error
    - Maximum Likelihood
  - Evaluation drives the optimization operation that learns the function,  $y$ .

# Graphical Example of Regression

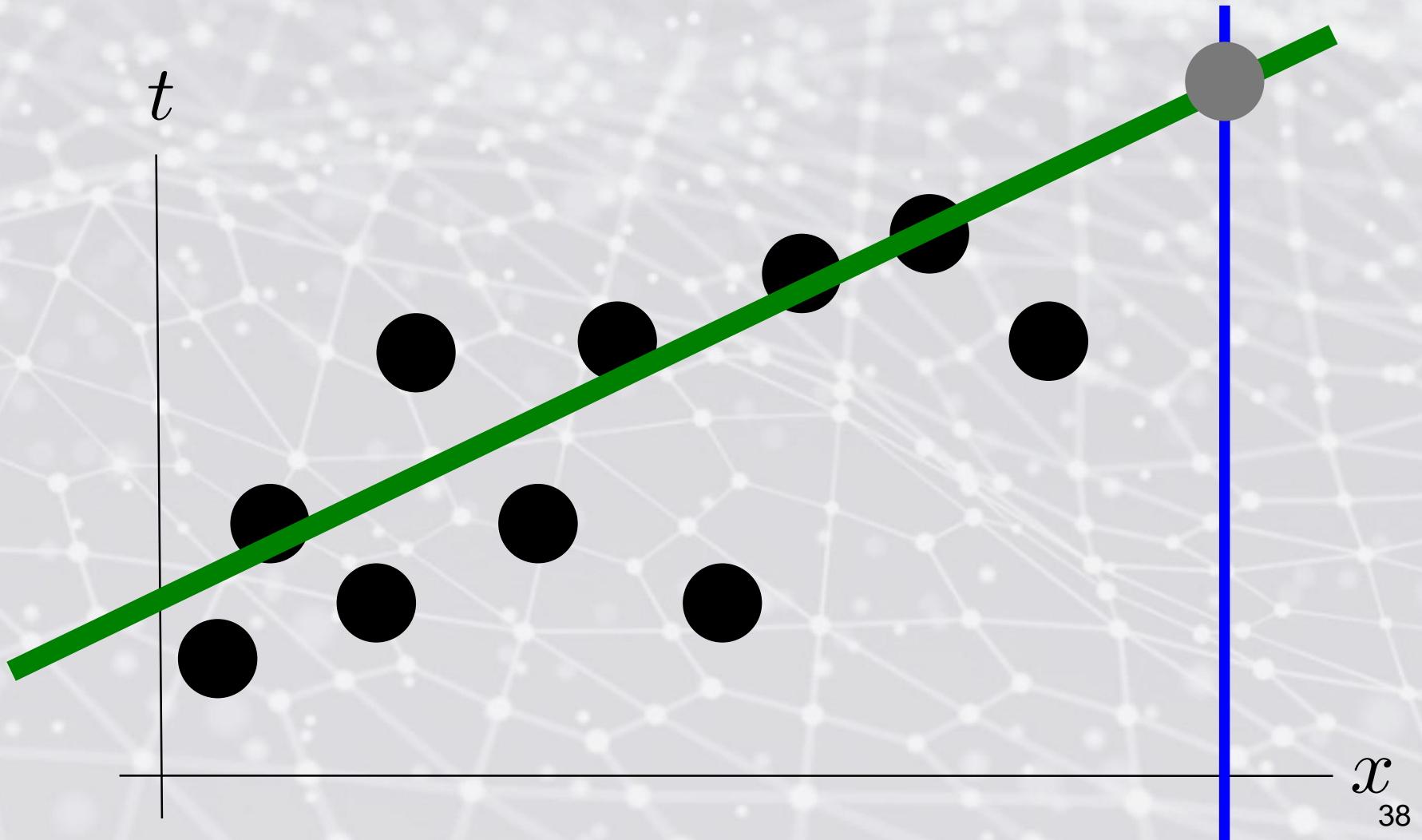




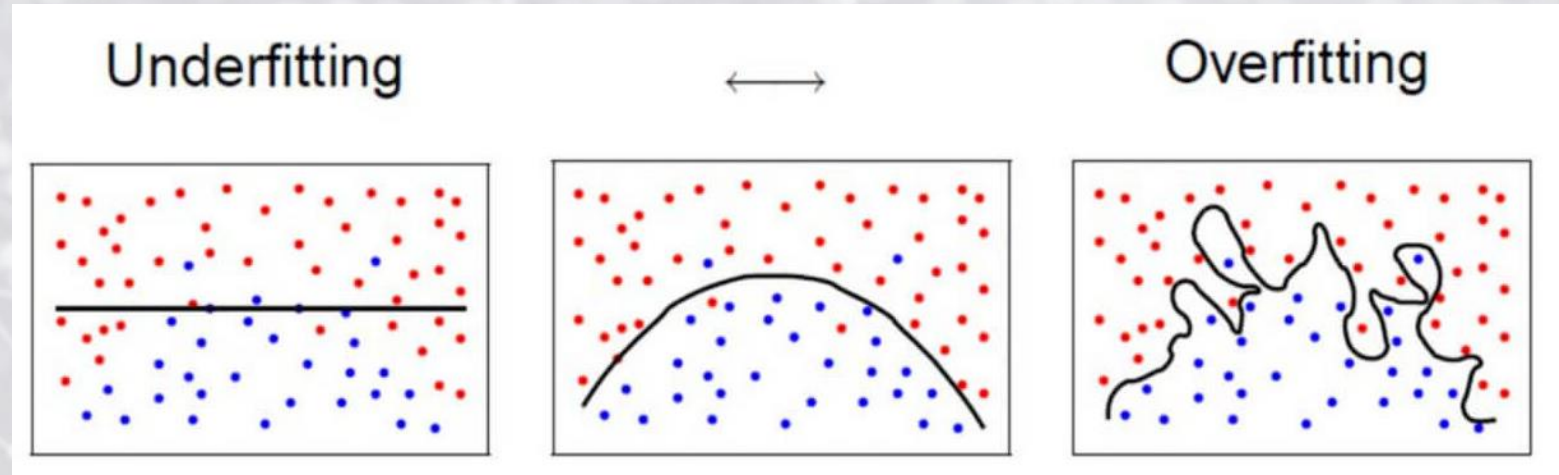
# Graphical Example of Regression



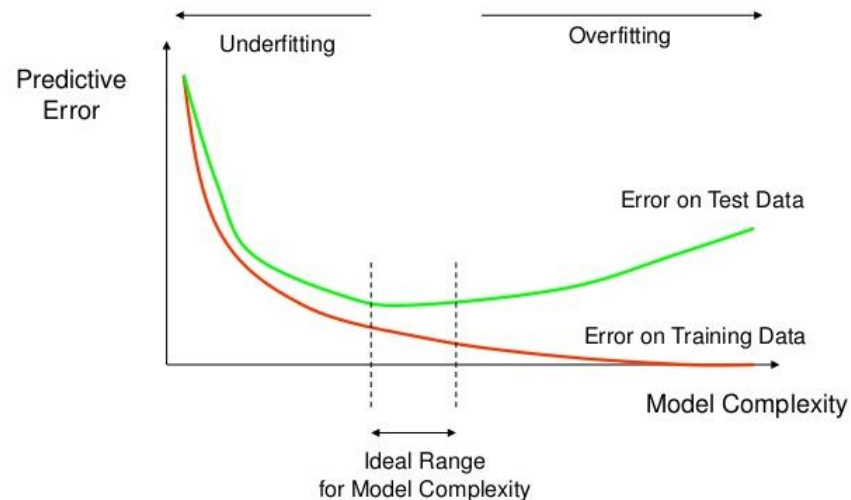
# Graphical Example of Regression



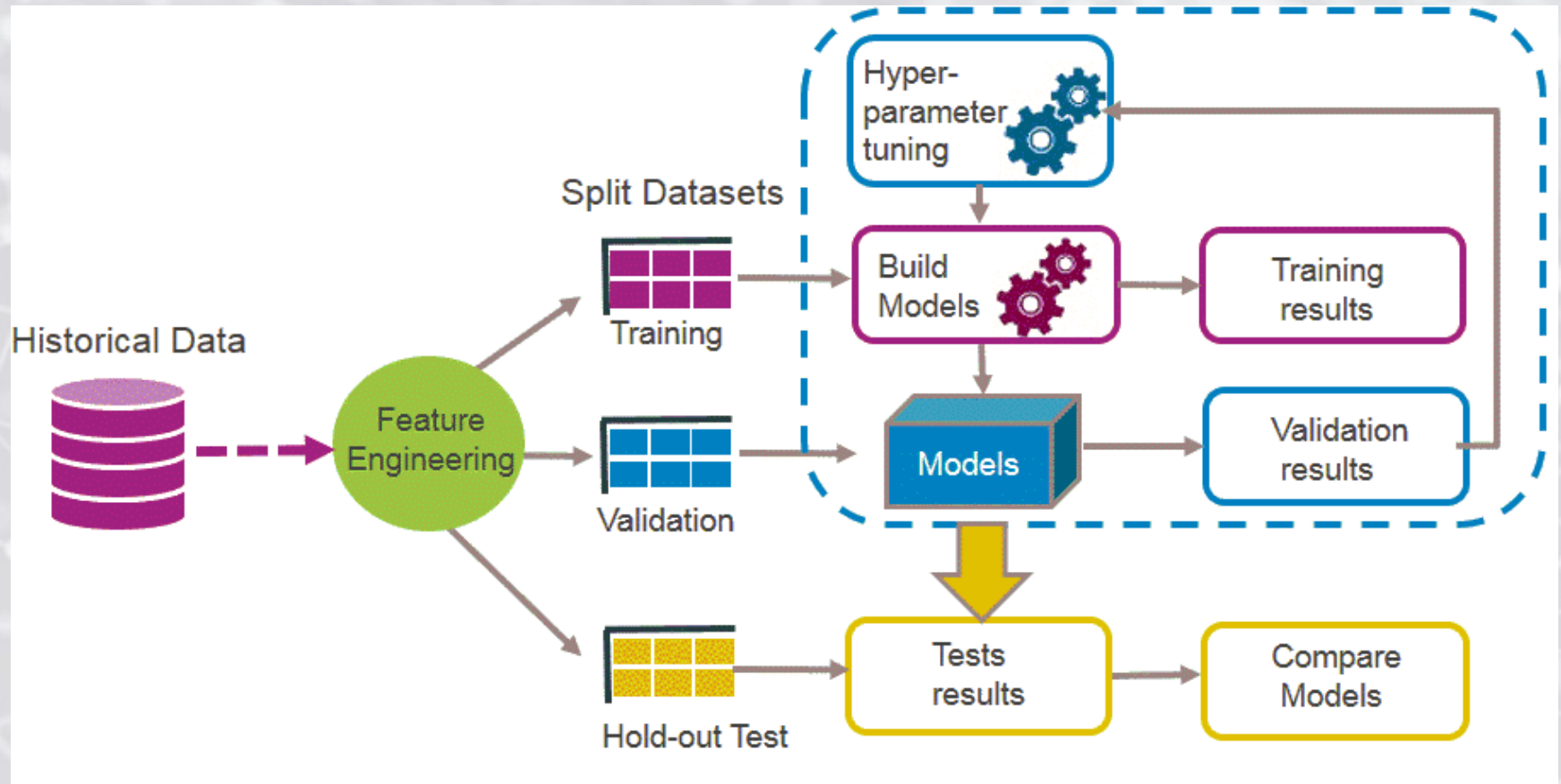
# Generalization Problem in Prediction/Classification



## How Overfitting affects Prediction



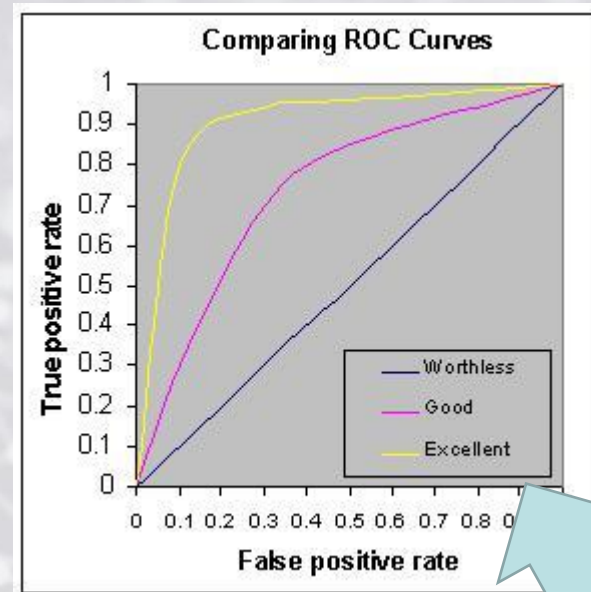
# Common ML Pipeline





# Confusion Matrix, ROC curves, etc.

		Predicted class	
		<i>P</i>	<i>N</i>
Actual Class	<i>P</i>	True Positives (TP)	False Negatives (FN)
	<i>N</i>	False Positives (FP)	True Negatives (TN)



Measure	Formula
Accuracy	$\frac{TP + TN}{TP + TN + FP + FN}$
Misclassification rate (1 – Accuracy)	$\frac{FP + FN}{TP + TN + FP + FN}$
Sensitivity (or Recall)	$\frac{TP}{TP + FN}$
Specificity	$\frac{TN}{TN + FP}$
Precision (or Positive Predictive Value)	$\frac{TP}{TP + FP}$

Area under (the) curve (AUC) is a common metric used to assess/compare classifiers

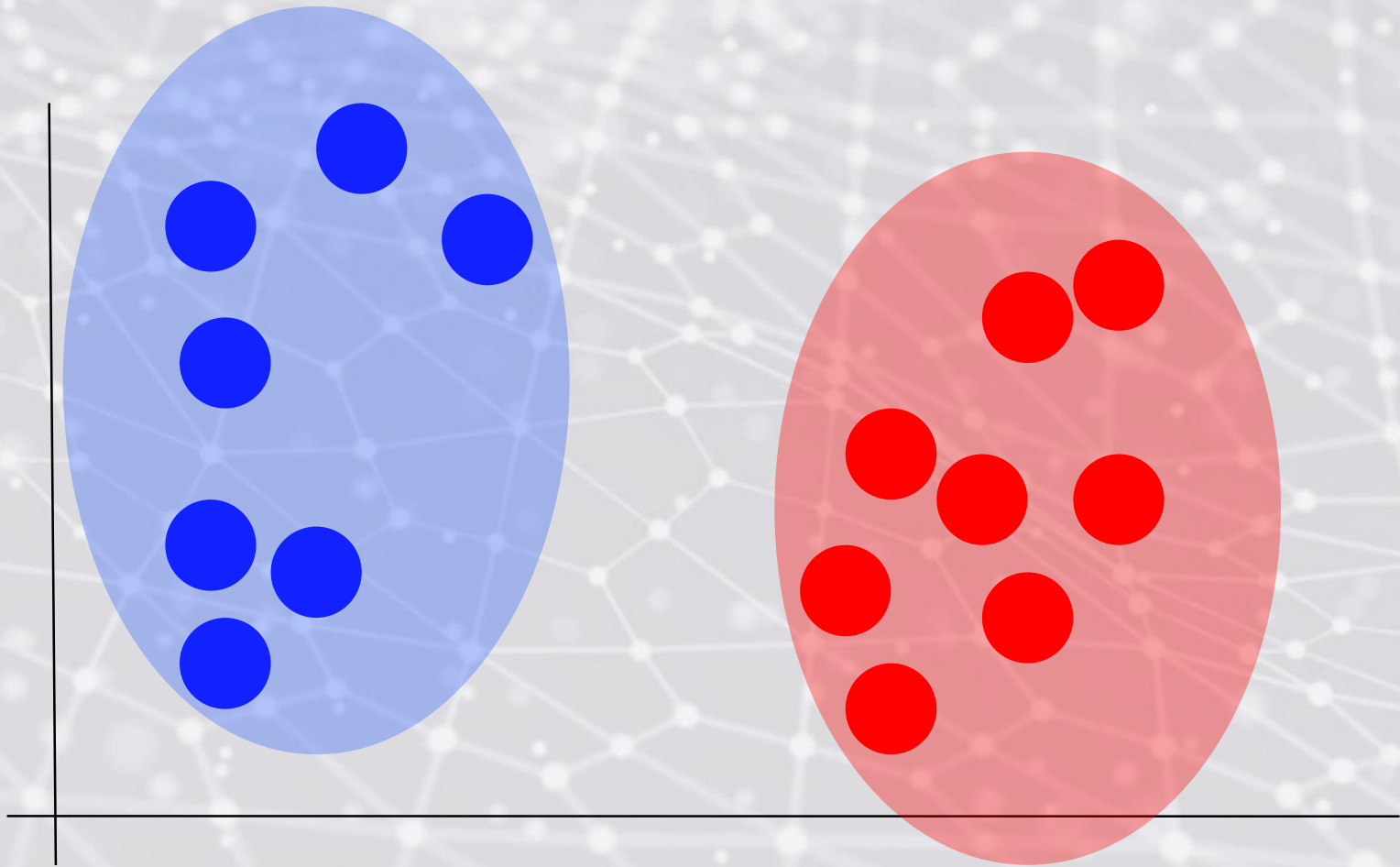
# Clustering

- Clustering is an **unsupervised** learning task.
  - There is no target value to shoot for.
- Identify groups of “similar” data points, that are “dissimilar” from others.
- **Partition** the data into groups (clusters) that satisfy these constraints
  1. Points in the same cluster should be **similar**.
  2. Points in different clusters should be **dissimilar**.

# Graphical Example of Clustering

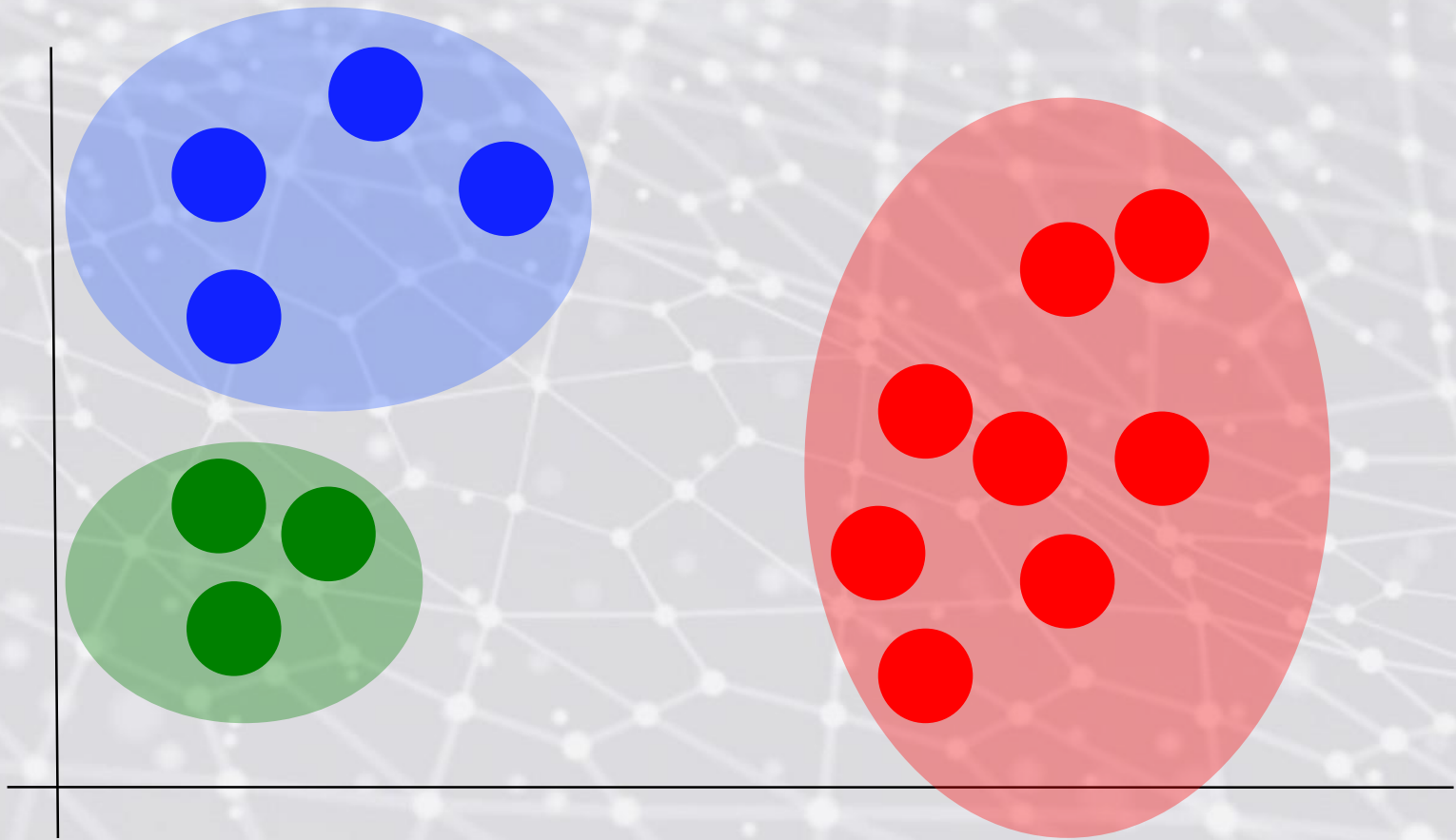


# Graphical Example of Clustering



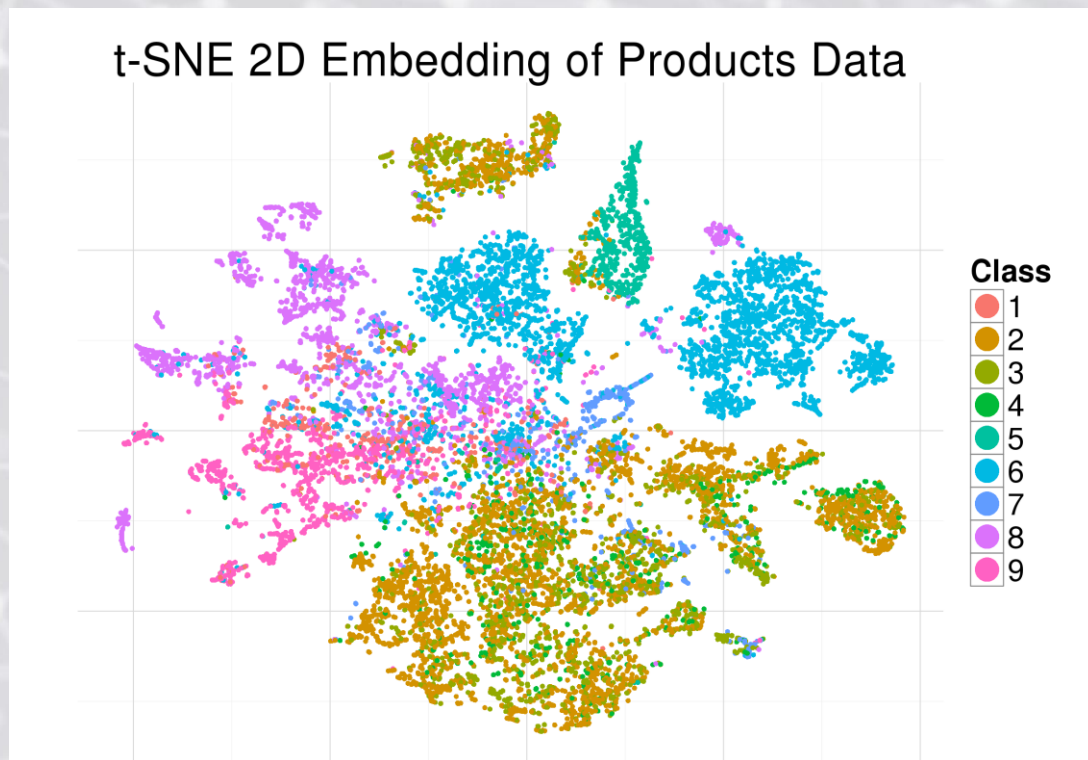


# Graphical Example of Clustering



# MNIST Classification

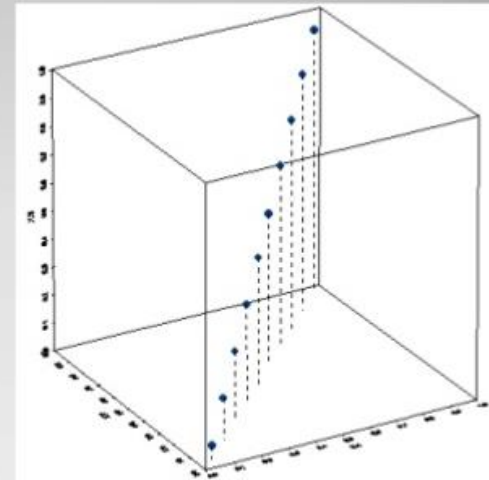
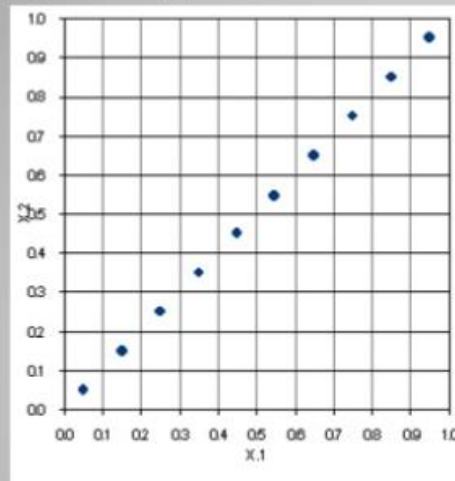
- 60k training/10k test images
- LeCun, Bengio, *et al.* (1998) used SVMs to get error rate of 0.8%.
- More recent research using CNNs (a type of neural network) yields 0.23% error.



# The Curse of Dimensionality

- In ML we are faced with a fundamental dilemma: to maintain a given model accuracy in higher dimensions we need a huge amount of data!
- An exponential increase in data required to densely populate space as the dimension increases.
- Points are equally far apart in high dimensional space (this is counter-intuitive).

Representation of 10% sample probability space  
(i) 2-D (ii) 3-D

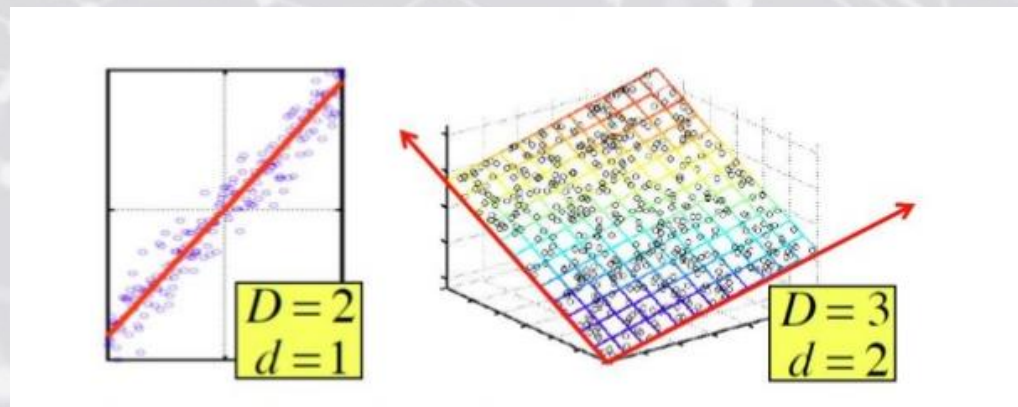


The Number of Points Would Need to Increase Exponentially  
to Maintain a Given Accuracy.  
 $10^n$  samples would be required for a  $n$ -dimension problem.

# Dealing with High Dimensionality

What can we do?

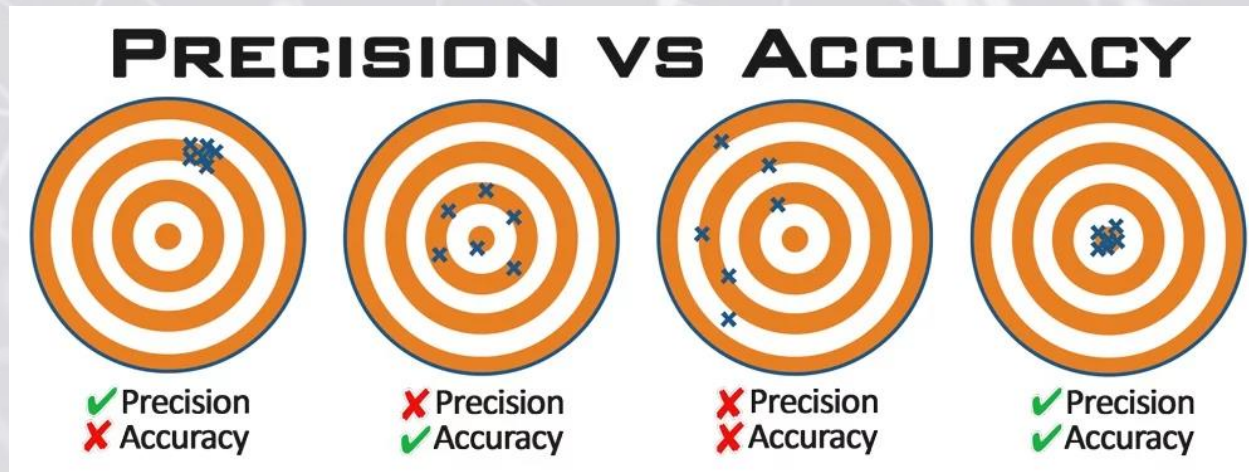
- Use Domain Knowledge
  - Feature engineering
- Make assumptions about dimensions
  - Independence: Count along each dimension separately
  - Smoothness: Propagate class counts to neighboring regions
  - Symmetry: e.g., invariance to order of dimensions
- Perform dimensionality reduction





# Bias-Variance Tradeoff

- Whenever we train any type of ML algorithm/model we are making some model choices, and fitting the parameters of that model.
- The more degrees of freedom (dof) the algorithm has, the more complicated the model that can be fitted (recall: overfitting).
- Note that a model can be “bad” for (2) basic reasons: (1) it is **inaccurate** and doesn't match the data well; (2) it is **not very precise**, meaning that there is a lot of variation in the results.
- (1) is known as **bias**; (2) is **statistical variance**.



# Bias-Variance Tradeoff

- The **MSE** (mean-squared error) decouples to reflect what is known as the bias-variance tradeoff:

$$\begin{aligned}\text{MSE}(\hat{\theta}) &\equiv \mathbb{E}((\hat{\theta} - \theta)^2) = \mathbb{E} \left[ \left( \hat{\theta} - \mathbb{E}(\hat{\theta}) + \mathbb{E}(\hat{\theta}) - \theta \right)^2 \right] \\&= \mathbb{E} \left[ \left( \hat{\theta} - \mathbb{E}(\hat{\theta}) \right)^2 + 2 \left( (\hat{\theta} - \mathbb{E}(\hat{\theta}))(\mathbb{E}(\hat{\theta}) - \theta) \right) + \left( \mathbb{E}(\hat{\theta}) - \theta \right)^2 \right] \\&= \mathbb{E} \left[ \left( \hat{\theta} - \mathbb{E}(\hat{\theta}) \right)^2 \right] + 2\mathbb{E} \left[ (\hat{\theta} - \mathbb{E}(\hat{\theta}))(\mathbb{E}(\hat{\theta}) - \theta) \right] + \mathbb{E} \left[ \left( \mathbb{E}(\hat{\theta}) - \theta \right)^2 \right] \\&= \mathbb{E} \left[ \left( \hat{\theta} - \mathbb{E}(\hat{\theta}) \right)^2 \right] + \underbrace{2(\mathbb{E}(\hat{\theta}) - \theta) \mathbb{E}(\hat{\theta} - \mathbb{E}(\hat{\theta}))}_{=\mathbb{E}(\theta) - \mathbb{E}(\theta) = 0} + \mathbb{E} \left[ \left( \mathbb{E}(\hat{\theta}) - \theta \right)^2 \right] \\&= \mathbb{E} \left[ \left( \hat{\theta} - \mathbb{E}(\hat{\theta}) \right)^2 \right] + \mathbb{E} \left[ \left( \mathbb{E}(\hat{\theta}) - \theta \right)^2 \right] \\&= \text{Var}(\hat{\theta}) + \text{Bias}(\hat{\theta}, \theta)^2\end{aligned}$$

Where:  $\theta := \text{true parameter value}$

$\hat{\theta} := \text{parameter estimate}$

# Bias-Variance Tradeoff

- In pictures...

