Machine Learning: Lecture #1

Jennifer Ngadiuba (Fermilab)
University of Pavia, May 8-12 2023

Overview of the lectures

- **Day 1:**
  - Introduction to Machine Learning fundamentals
  - Linear Models
- **Day 2:**
  - Neural Networks
  - Deep Neural Networks
  - Convolutional Neural Networks
- **Day 3:**
  - Recurrent Neural Networks
  - Graph Neural Networks (part 1)
- **Day 4:**
  - Graph Neural Networks (part 2)
  - Transformers
- **Day 5:**
  - Unsupervised learning
  - Autoencoders
  - Generative Adversarial Networks
  - Normalizing Flows

Hands on sessions each day will closely follow the lectures topics

Lectures are adapted from M. Kagan's courses

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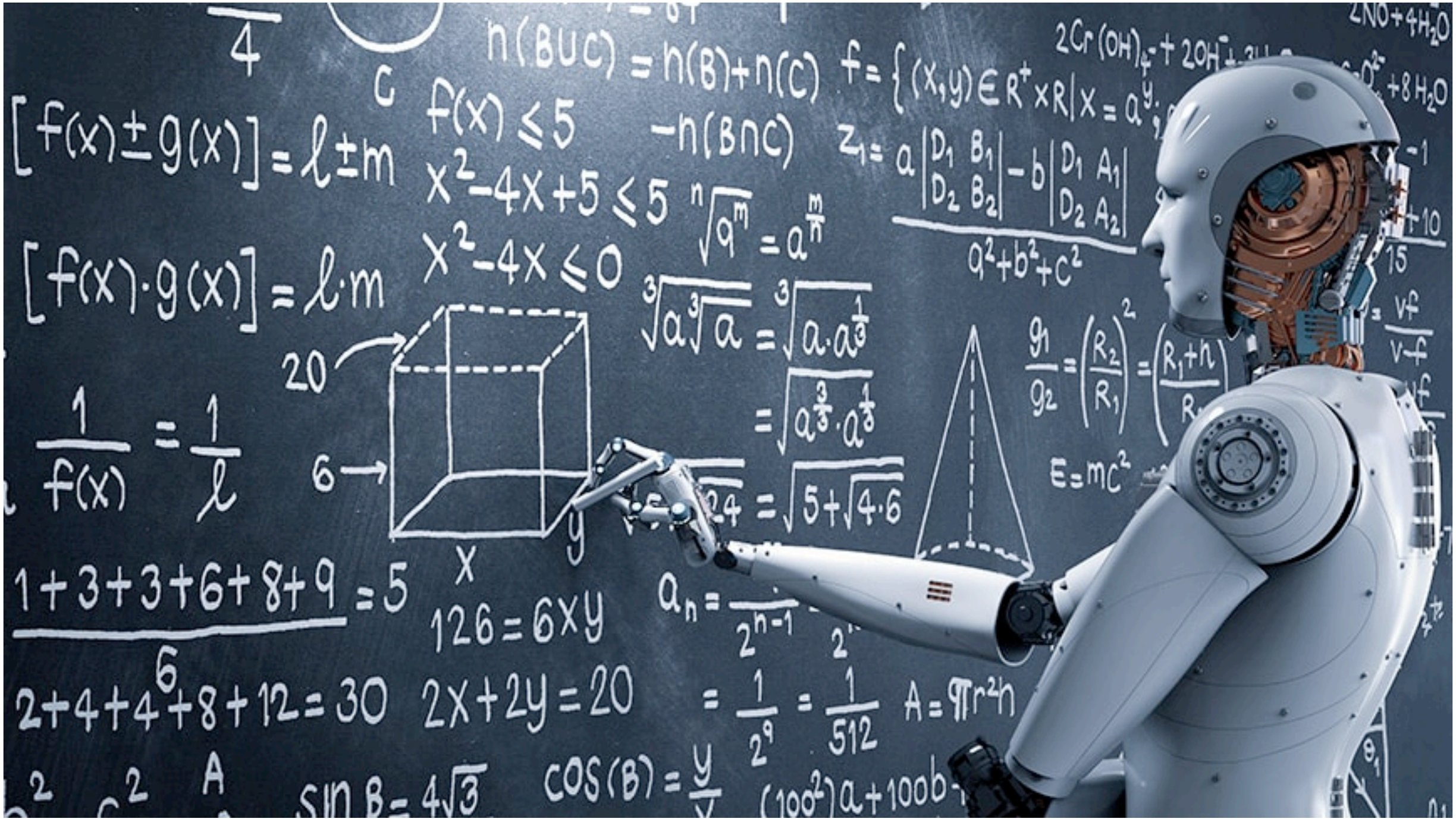
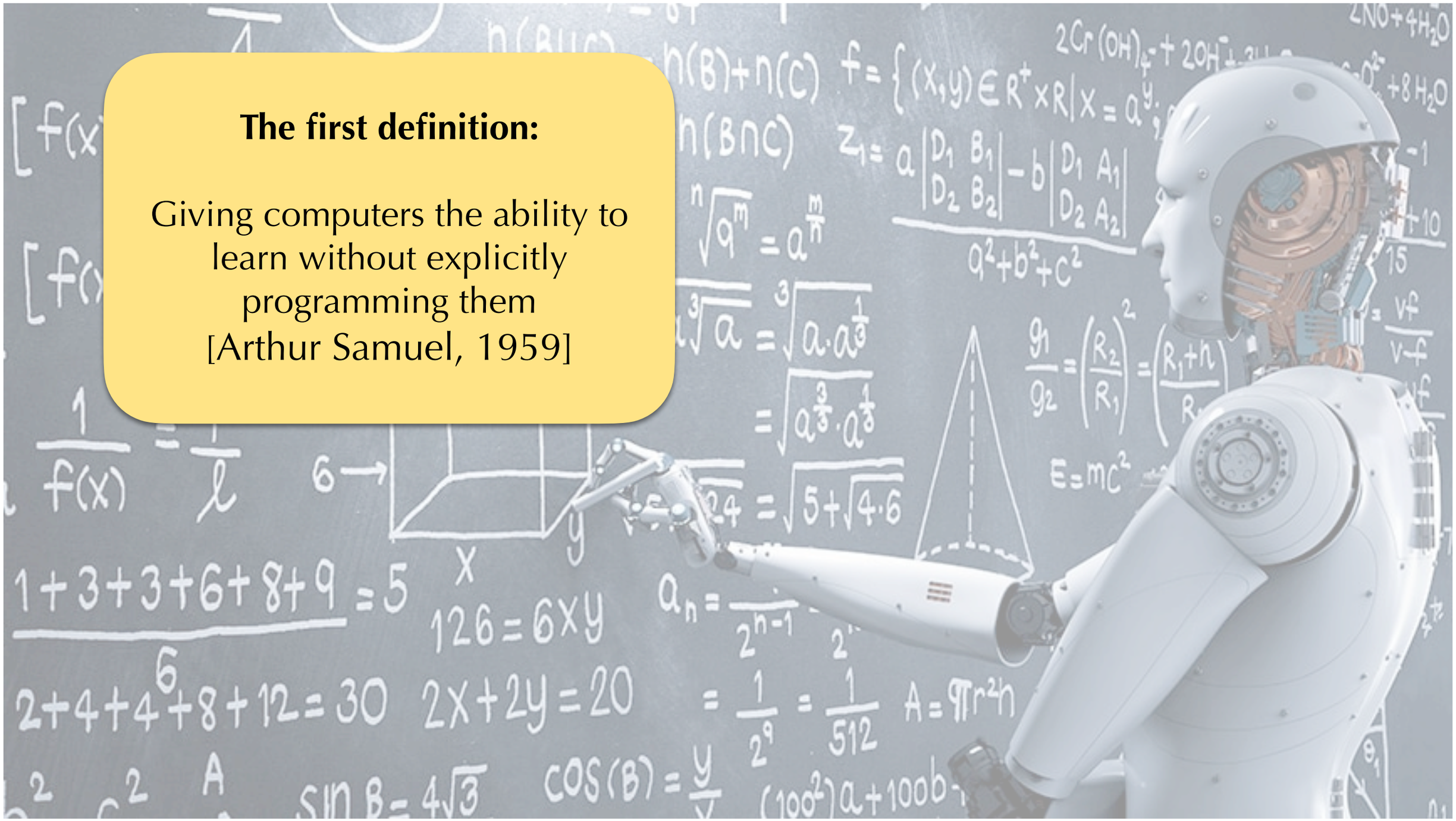


What is machine learning?



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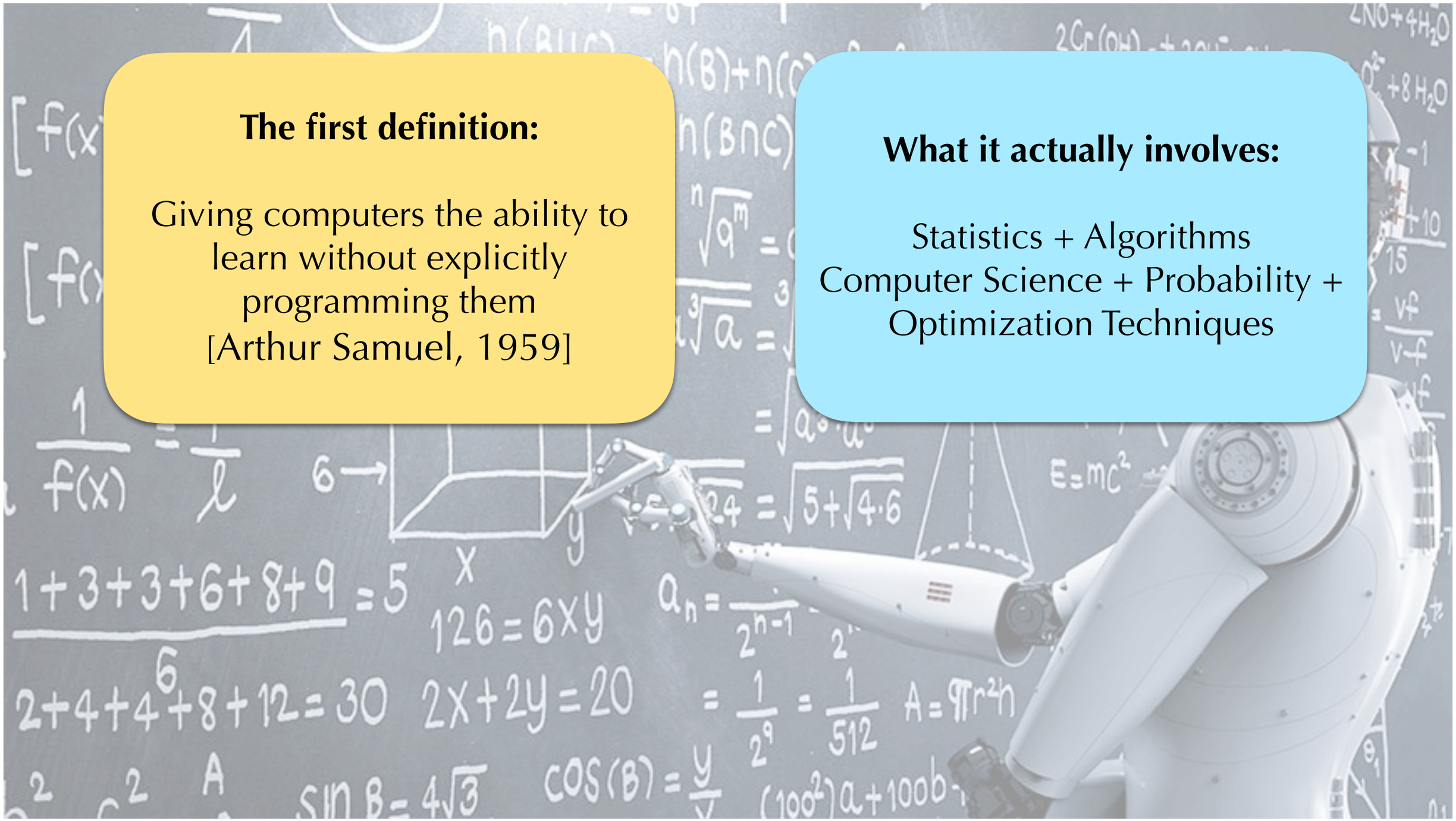

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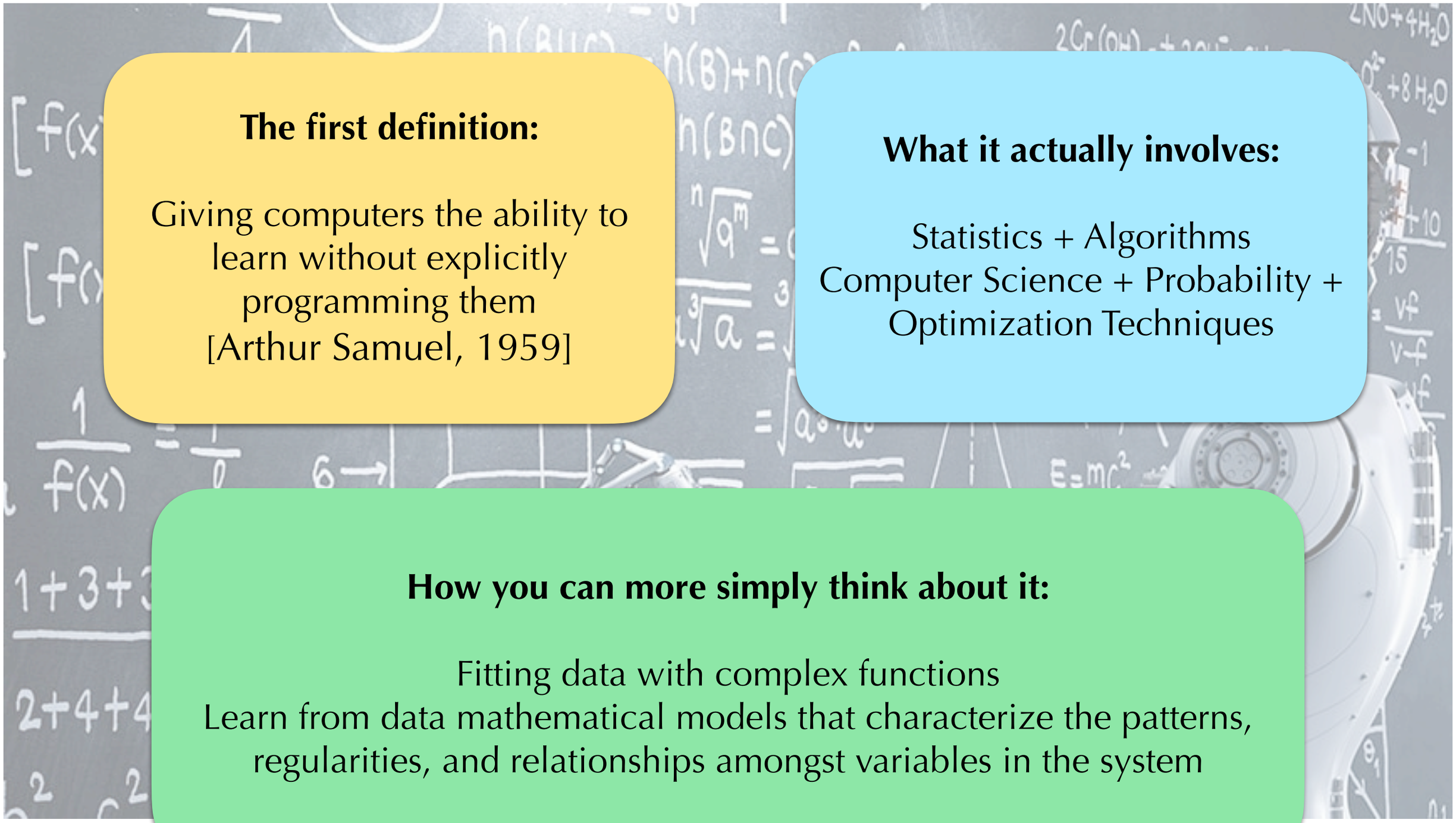


The first definition:

Giving computers the ability to learn without explicitly programming them
[Arthur Samuel, 1959]

What it actually involves:

Statistics + Algorithms
Computer Science + Probability +
Optimization Techniques

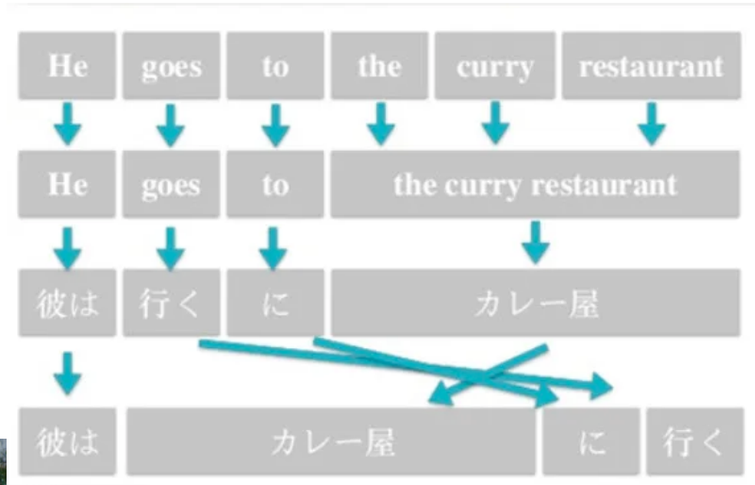
How you can more simply think about it:

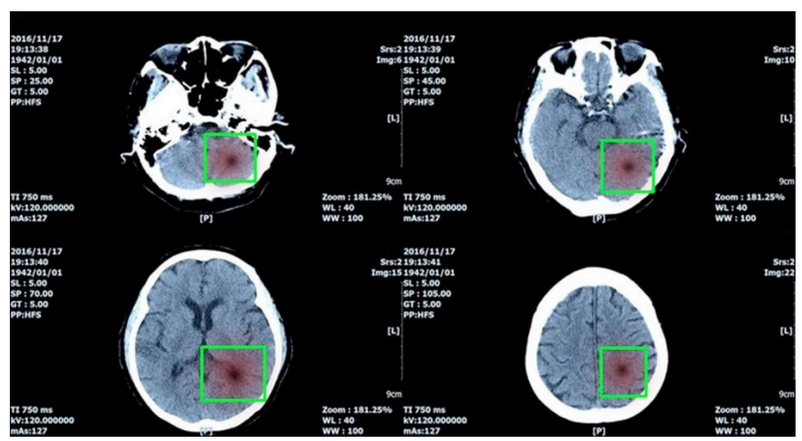
Fitting data with complex functions
Learn from data mathematical models that characterize the patterns, regularities, and relationships amongst variables in the system

What is machine learning?

Where is ML used?

- Natural Language Processing:
  speech and handwriting recognition
- Object recognition and computer vision
- Fraud detection
- Financial market analysis
- Search engines
- Spam and virus detection
- Medical diagnosis
- Robotics control
- Automation: energy usage,
  systems control, video games, self-driving cars
- Advertising
- Data science
- ….

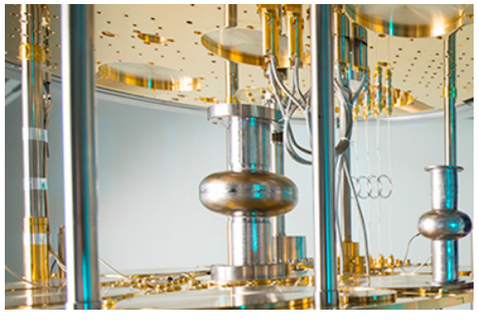




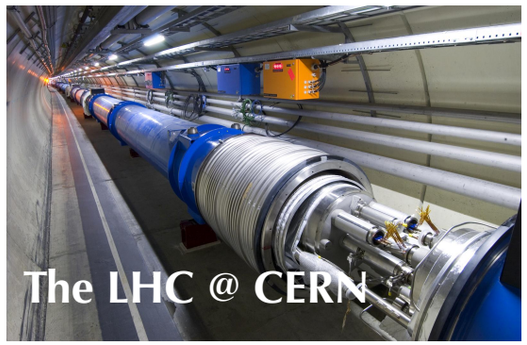
ML for science

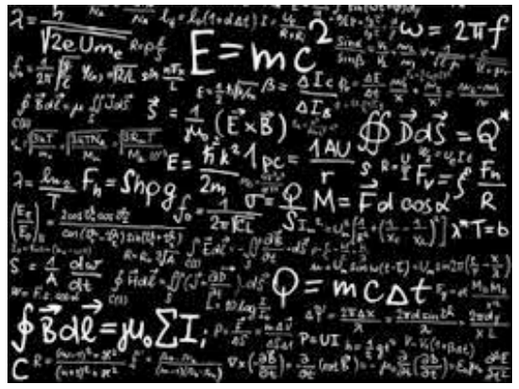
- Classify physics processes/objects
- Compress granular sensor data to lower dimension interpretable features
- Simulation
- Experiment control
- …

Astrophysics & cosmology

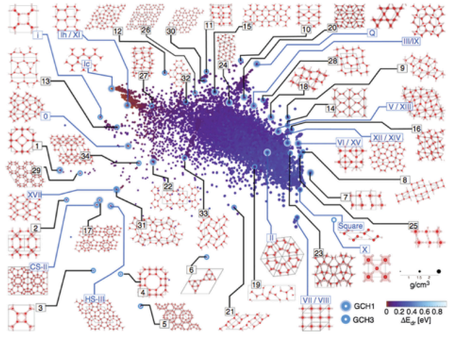


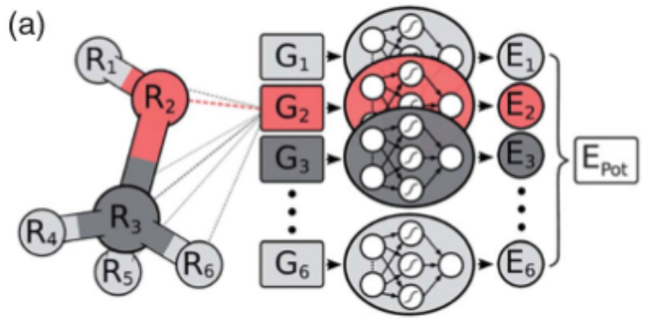
Quantum Information Science





Particle Physics





Chemistry & Materials

Review from G. Carleo et al: [Rev. Mod. Phys. 91, 045002]

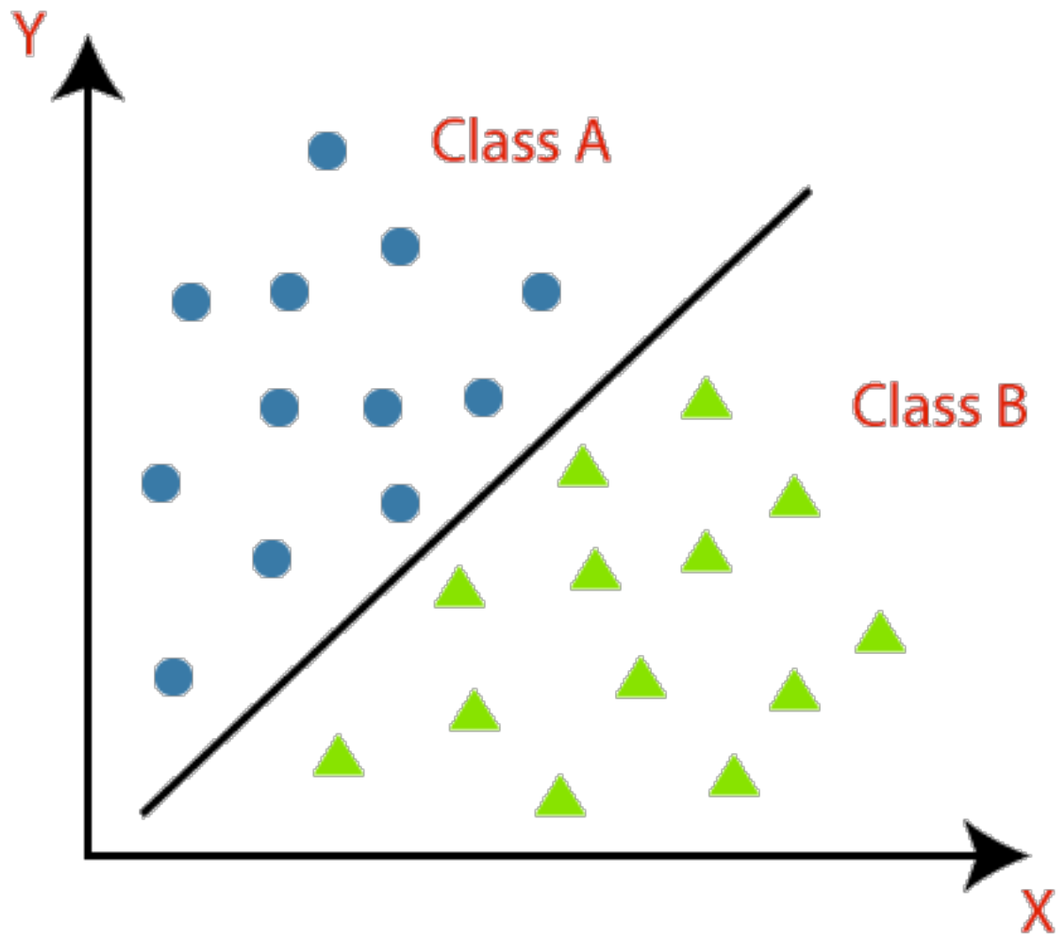
Machine learning: models

- Key element in machine learning
  is a **mathematical model**

  - A mathematical characterization of system(s) of interest

  - Chosen model depends on the task and available data

Classification



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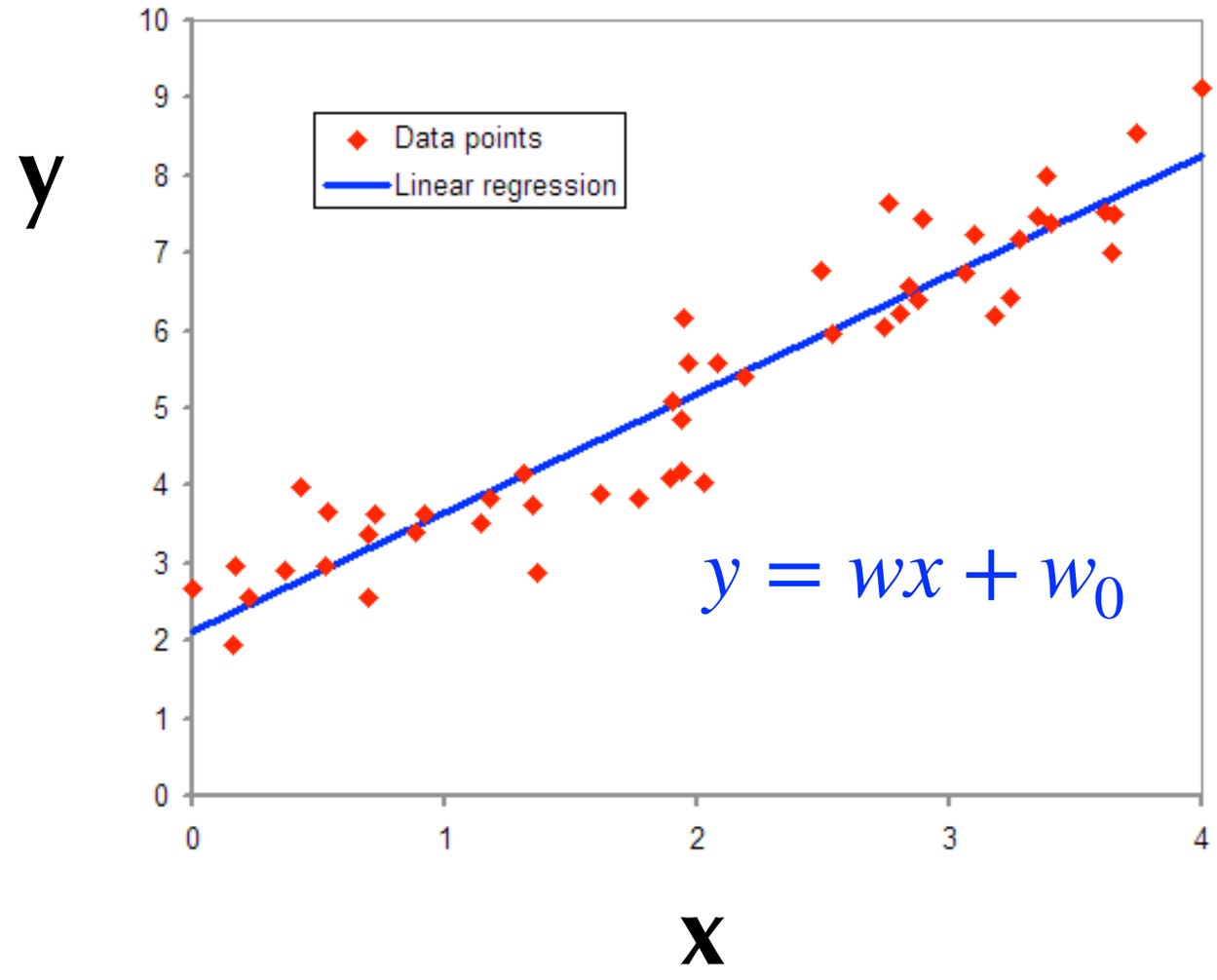
Regression



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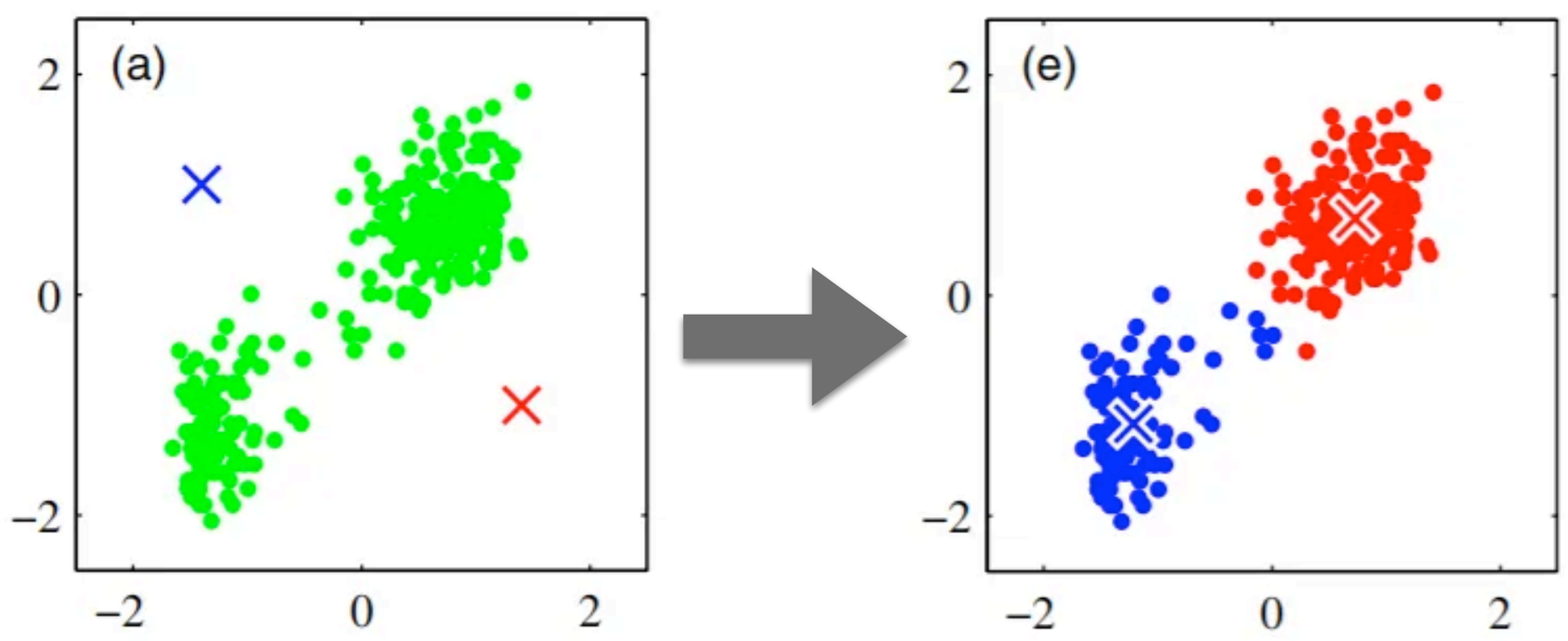
Clustering



Machine learning: models

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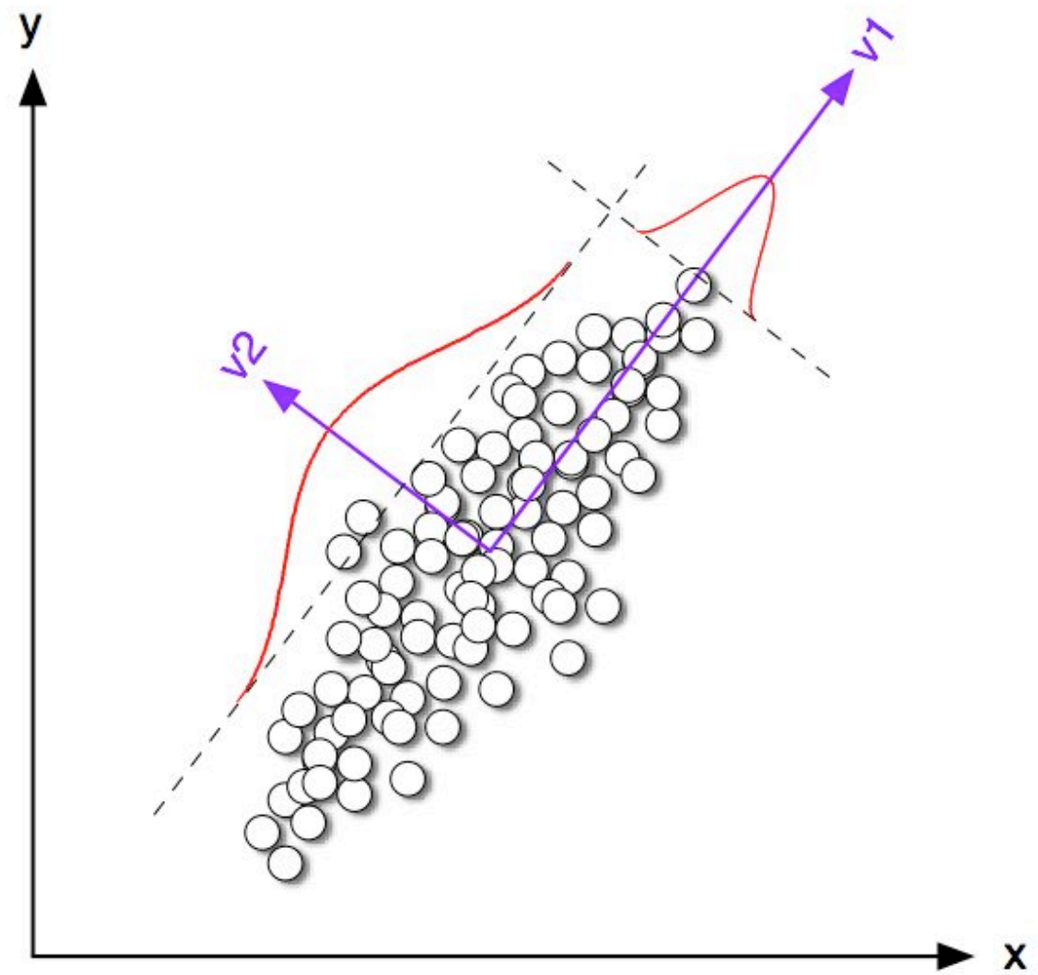
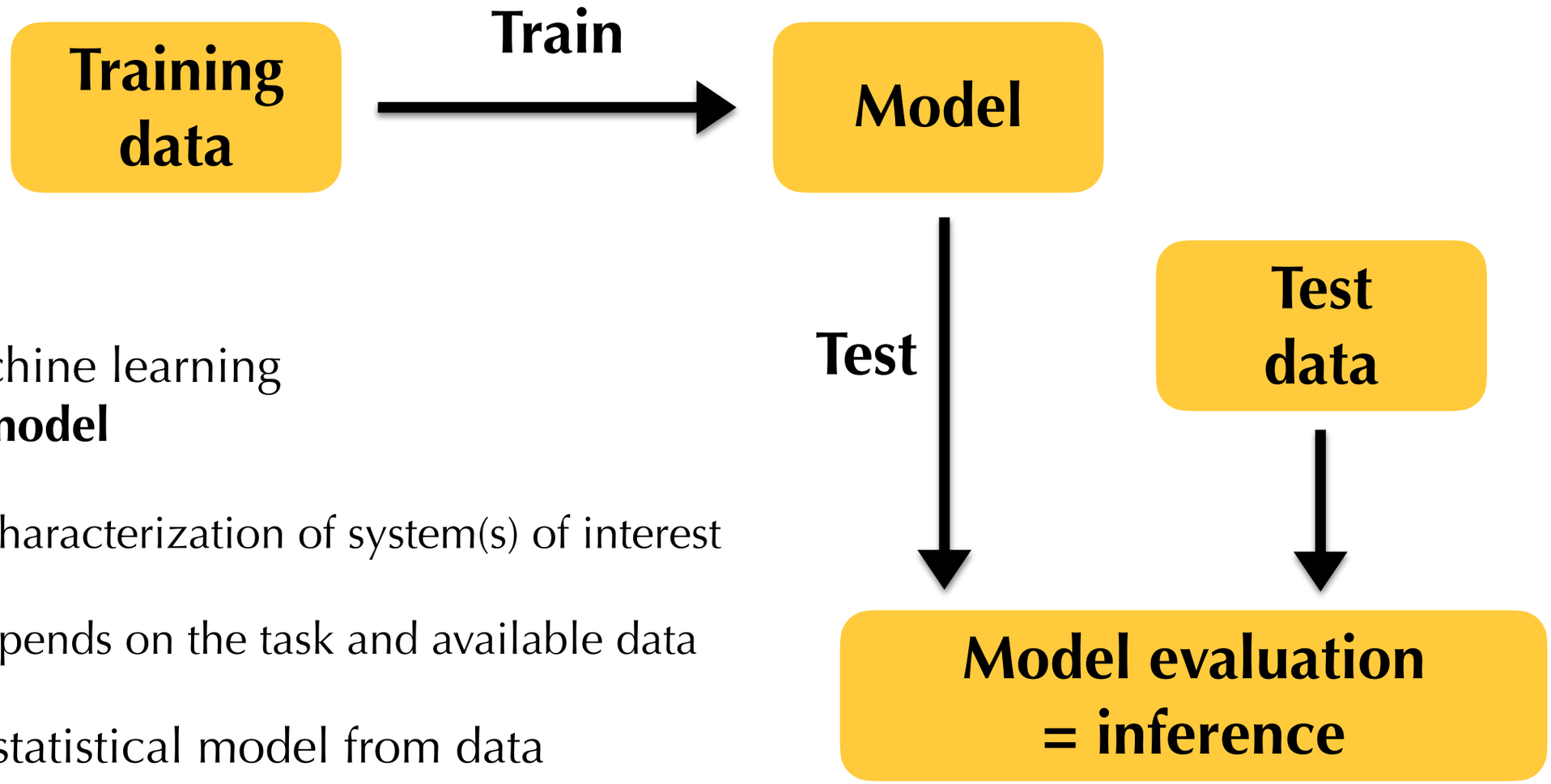
Dimensionality Reduction



Machine learning: models

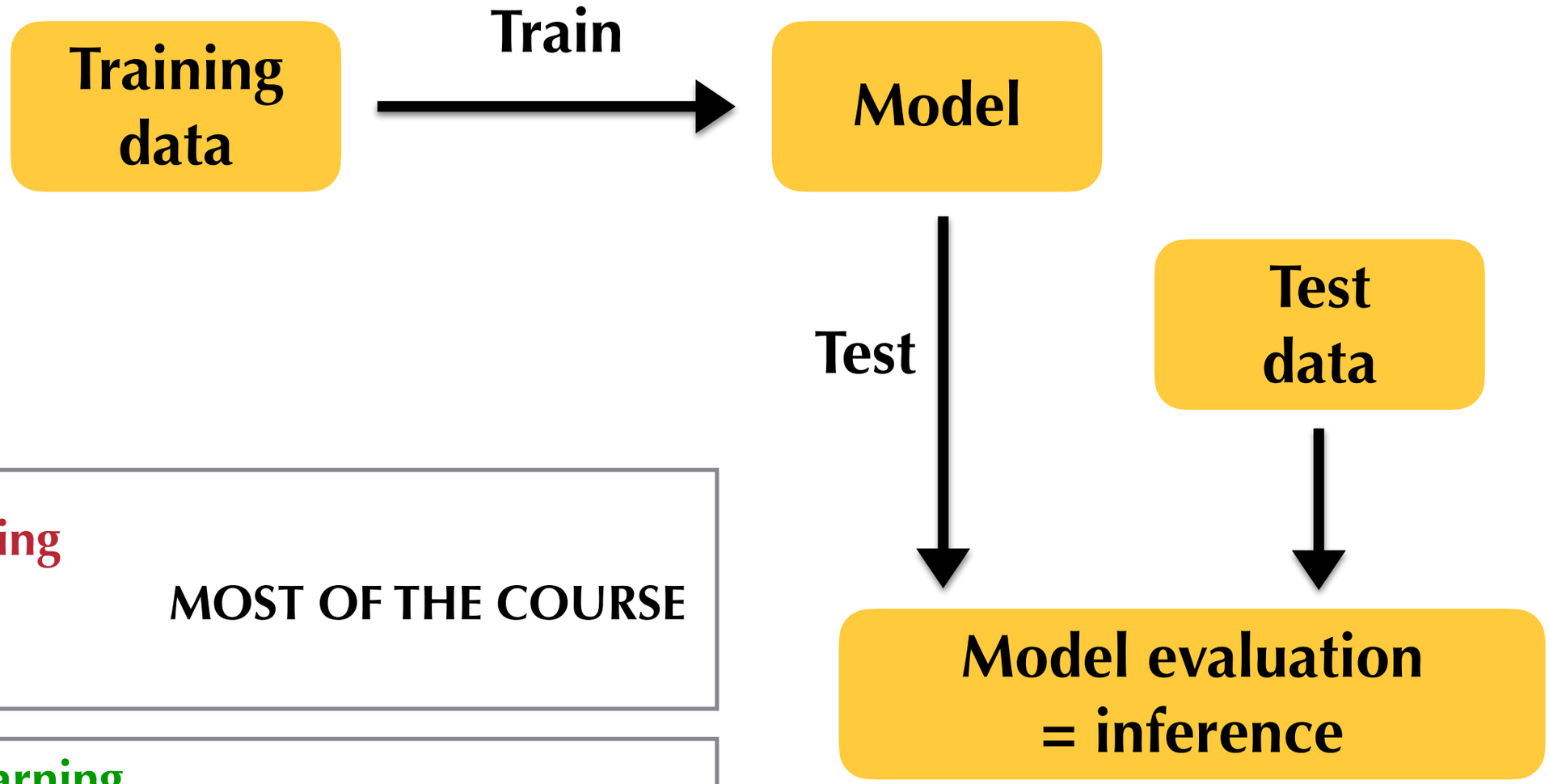
- Key element in machine learning is a **mathematical model**
  - A mathematical characterization of system(s) of interest
  - Chosen model depends on the task and available data
- **Learning:** estimate statistical model from data

Machine learning: models



- Key element in machine learning is a **mathematical model**
  - A mathematical characterization of system(s) of interest
  - Chosen model depends on the task and available data
- **Learning:** estimate statistical model from data
- **Prediction and Inference:** using statistical model to make predictions on new data points and infer properties of system(s)

Types of learning



- **Supervised learning** — MOST OF THE COURSE
  - classification
  - regression
- **Unsupervised learning** — LAST DAY
  - clustering
  - dimensionality reduction
- **Reinforcement learning** — NOT COVERED

Notation

Notation

- $\mathbf{X} \in \mathbb{R}^{\mathbf{m}\times\mathbf{n}}$ Matrices in bold upper case
- $\mathbf{x} \in \mathbb{R}^{\mathbf{n}}$ Vectors in bold lower case
- $x \in \mathbb{R}$ Scalars in lower case, non bold
- $\mathcal{X}$ Sets are upper case cursive
- $\{\mathbf{x}_i\}_{i=1,\ldots,m}$ Sequence of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$
- $y \in \mathbb{I}^k$ / $\mathbb{R}^k$ Labels represented as
  a) integers for classes or
  b) real numbers for regression
- Variables = features = inputs
- Data point $\mathbf{x} = \{x_1, \ldots, x_n\}$ has n features
- Typically use affine coordinates: $y = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 \longrightarrow \mathbf{w}^{\mathrm{T}}\mathbf{x}$
  $\longrightarrow \mathbf{w} = \{w_0, \ldots, w_n\}$
  $\longrightarrow \mathbf{x} = \{x_0, \ldots, x_n\}$

Probability review

- $p(x, y)$ Joint distribution of two variables
- $p(x) = \int p(x, y) dy$ Marginal distribution
- $p(y \mid x) = \frac{p(x, y)}{p(x)}$ Conditional probability
- $p(y \mid x) = \frac{p(x \mid y) p(y)}{p(x)}$ Bayes theorem
- $\mathbf{E}[f(x)] = \int f(x) p(x) dx$ Expected value
- $p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2} \frac{(x-\mu)^2}{\sigma^2}\right)$ Normal distribution $N(\mu, \sigma)$

Supervised Learning

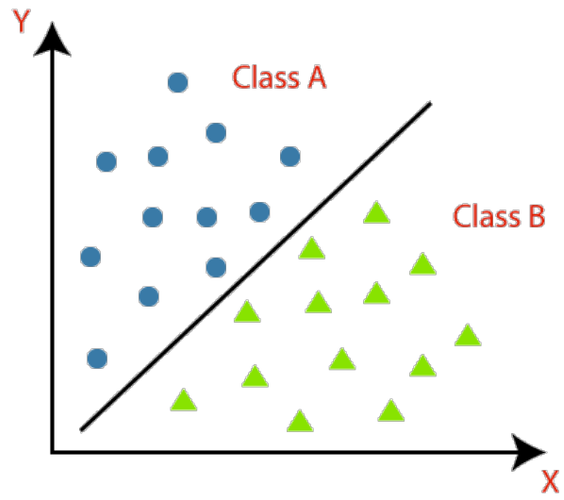
Supervised learning

- Given **N** examples with features $\{x_i \in \mathcal{X}\}$ and targets $\{y_i \in \mathcal{Y}\}$, learn function mapping $h(x) = y$

  - **Classification:** $\mathcal{Y}$ is a finite set of labels (i.e. classes)

$\mathcal{Y} = \{0,1\}$ for binary classification,
encoding classes, e.g. Higgs boson (1) vs background (0)

$\mathcal{Y} = \{c_1, c_2, \ldots, c_n\}$ for multi-class classification
represent with **"one-hot-vector"**: $y_i = (0,0,...,1,\ldots 0)$
where k^{th} element is 1 and all others zero for class c_k



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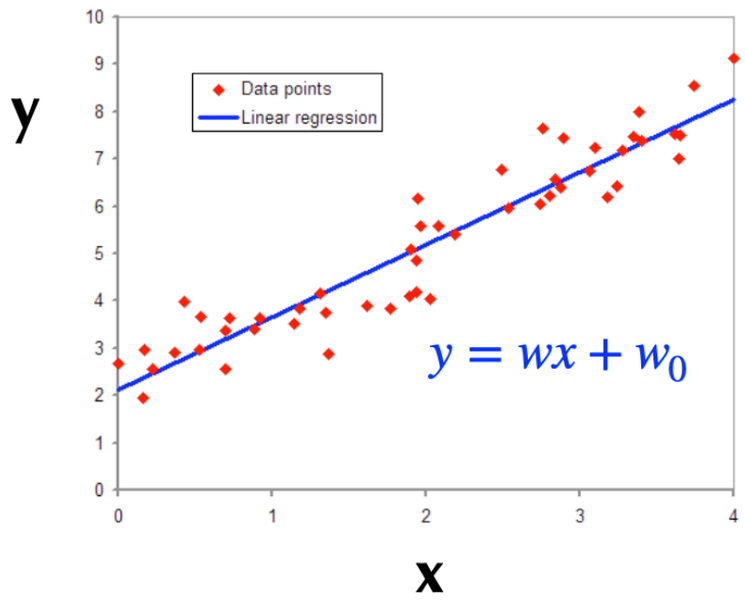
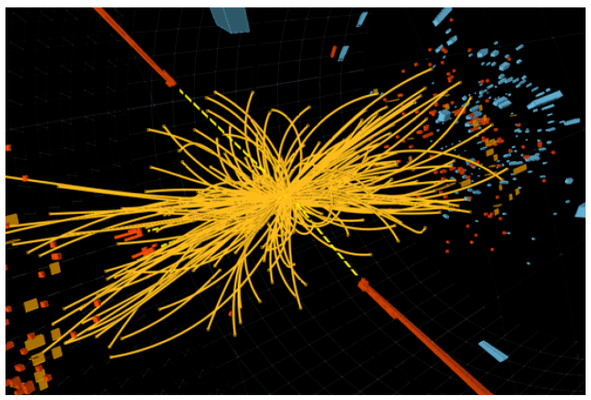
  - **Regression:** $\mathcal{Y}$ is a real number
    (eg., the truth mass of the SM Higgs boson)

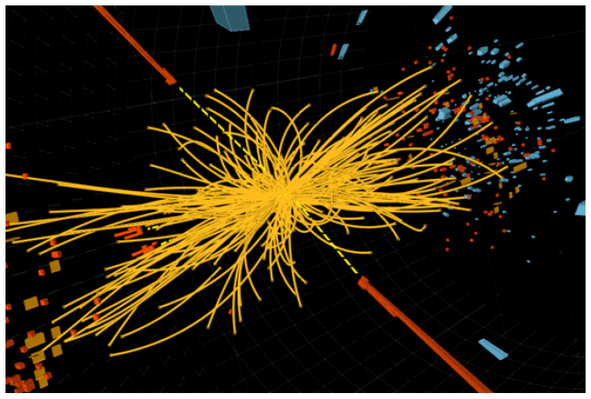


Supervised Learning: how does it work?



True labels:
Higgs = 1
Background = 0

Supervised Learning: how does it work?



h(**x**;**w**)
function with
adjustable
parameters

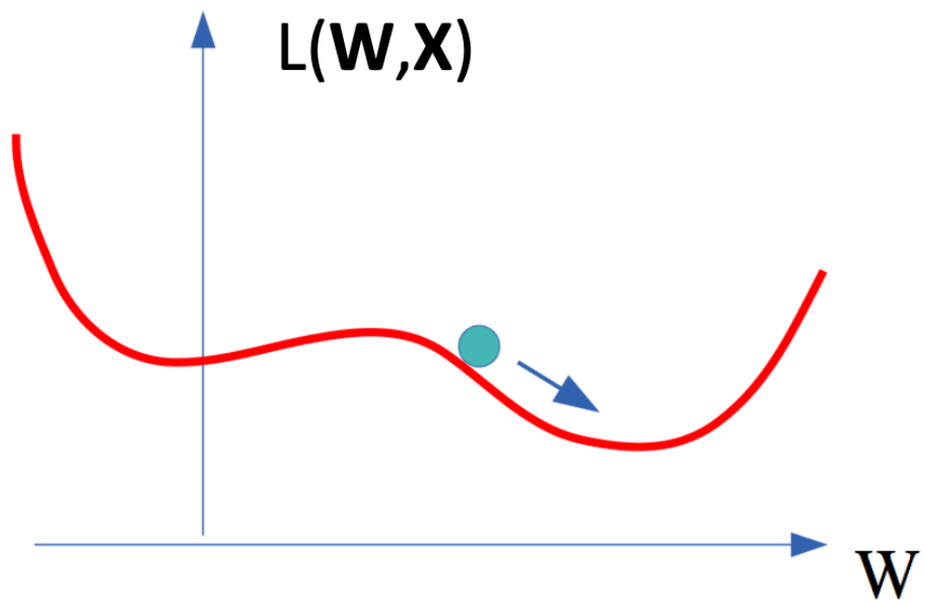
Loss
function

Compare
prediction
with true
label

Loss

True labels:
Higgs = 1
Background = 0

- Design function with adjustable parameters
- Design a Loss function



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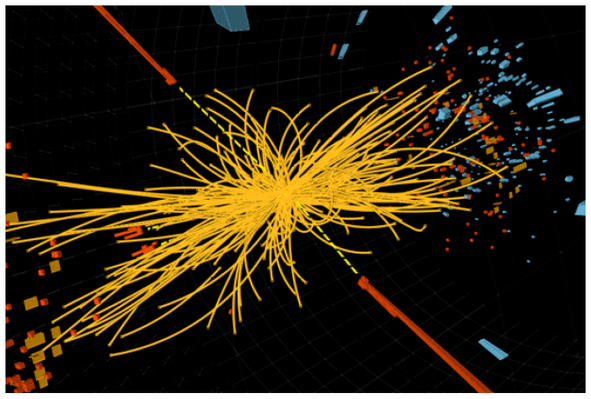

h(**x**;**w**)
function with
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Loss
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Compare
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True labels:
Higgs = 1
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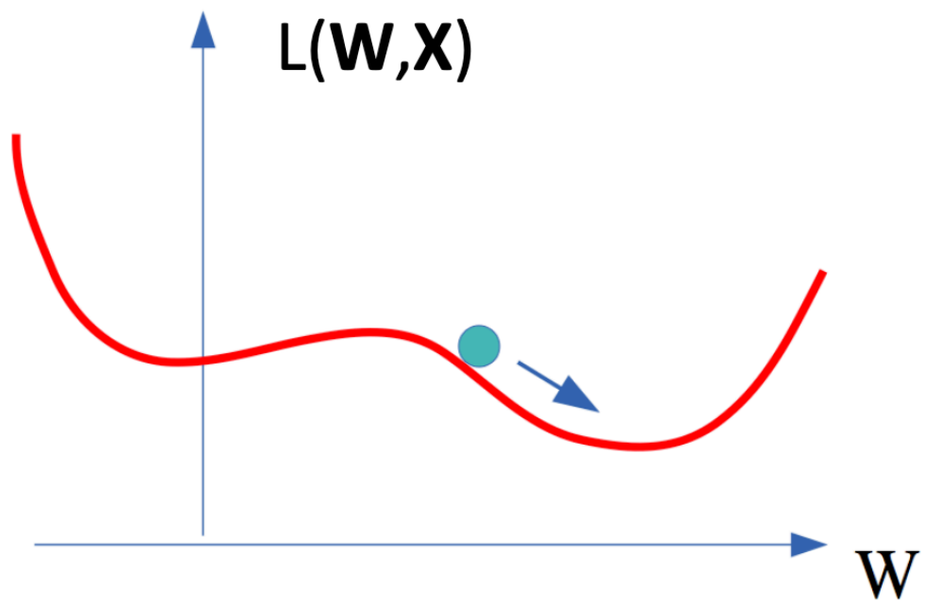
- Design function with adjustable parameters
- Design a Loss function
- Find best parameters which minimize the loss
  - Use a labeled training-set to compute loss
  - Adjust parameters to reduce loss function
  - Repeat until parameters stabilize



- Estimate final performance on test dataset (independent from training set)

Empirical risk minimization

$$\arg\min_{\mathbf{w}} \underbrace{\frac{1}{N}\sum_{i=1}^{N} L(h(\mathbf{x}_i;\mathbf{w}),y_i)}_{\text{Average expected loss}} + \underbrace{\lambda\Omega(\mathbf{w})}_{\text{Model regularization}}$$

- Framework to design learning algorithms
  - L(...) is a **loss function** comparing prediction h(...) with target y
  - Ω(**w**) is a **regularizer**, penalizing certain values of **w**
    - λ controls how much we penalize, and is a **hyperparameter** that we have to tune
    - more on this later
- **Learning is cast as an optimization problem**

Example loss functions

- **Square error loss**

  - often used in regression

$$L(h(\mathbf{x};\mathbf{w}),y) = \big(h(\mathbf{x};\mathbf{w}) - y\big)^2$$

- **Cross entropy**

  - with y ∈ {0,1}

  - often used in classification

$$L(h(\mathbf{x};\mathbf{w}),y) = -\,y\log h(\mathbf{x};\mathbf{w}) - (1-y)\log(1-h(\mathbf{x};\mathbf{w}))$$

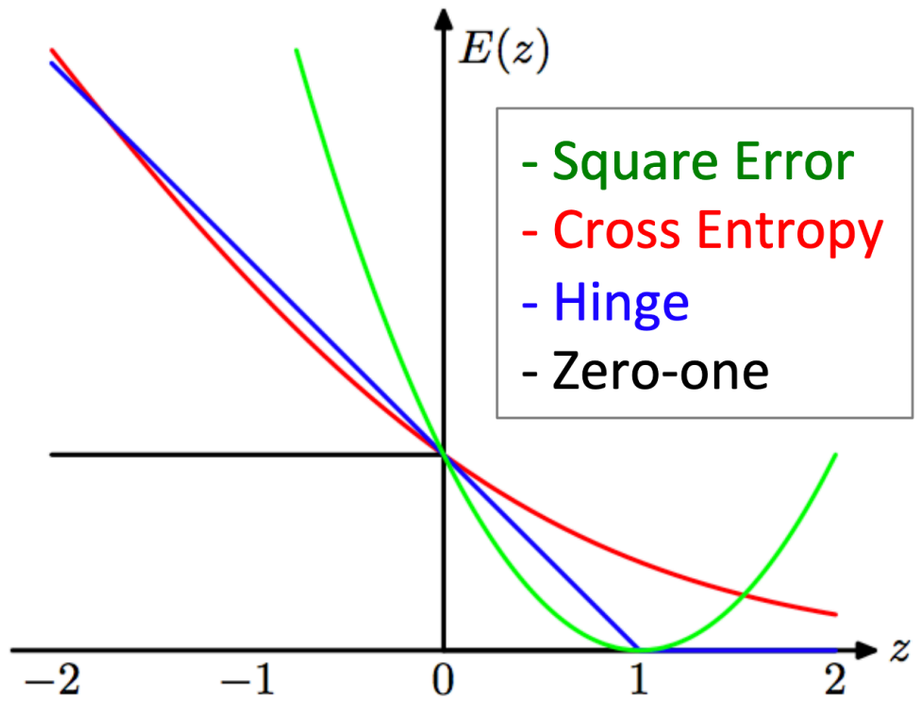
- **Hinge Loss** *(not in this course)*

  - with y ∈ {-1,1}

$$L(h(\mathbf{x};\mathbf{w}),y) = \max(0, 1 - yh(\mathbf{x};\mathbf{w}))$$

- **Zero-One loss** *(not in this course)*

  - with h(**x**; **w**) predicting label



Can be derived from probability theory — trust me at the moment but ask me if interested!

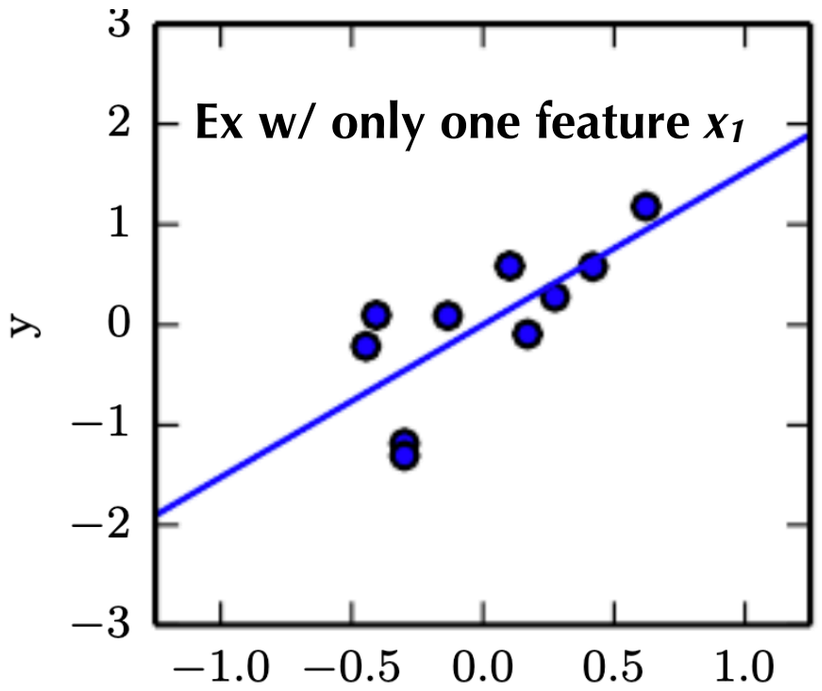
Linear Regression

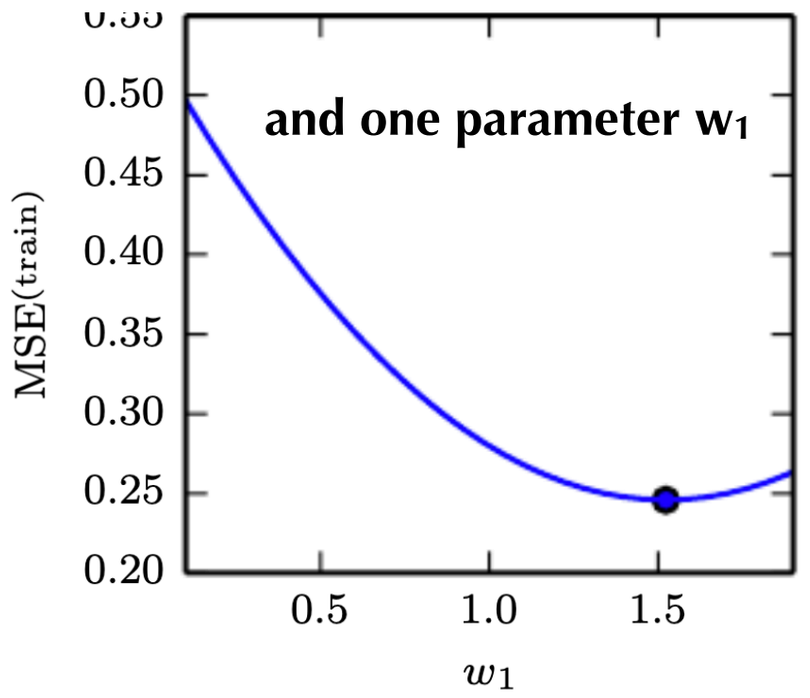
Linear regression

- Set of input / output pairs $D = \{x_i, y_i\}_{i=1,\ldots,n}$ where n is number of examples
  - $\mathbf{x}_i \in \mathbb{R}^m$ (m = number of features)
  - $y_i \in \mathbb{R}$ (just one target per example)
- Assume a **linear model**: $\hat{y} = h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x}$
- To find parameters w of h that best fit the data we chose the **Mean Squared Error (MSE)*** as performance metric (or loss function)

$$\mathscr{L}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h(\mathbf{x}_i; \mathbf{w}))^2$$

- Find $\mathbf{w}^* = \mathrm{argmin}_{\mathbf{w}}\mathscr{L}(\mathbf{w})$





** equivalent to the least square method — this is not the only method possible and other metrics can be used*

Linear regression: matrix form

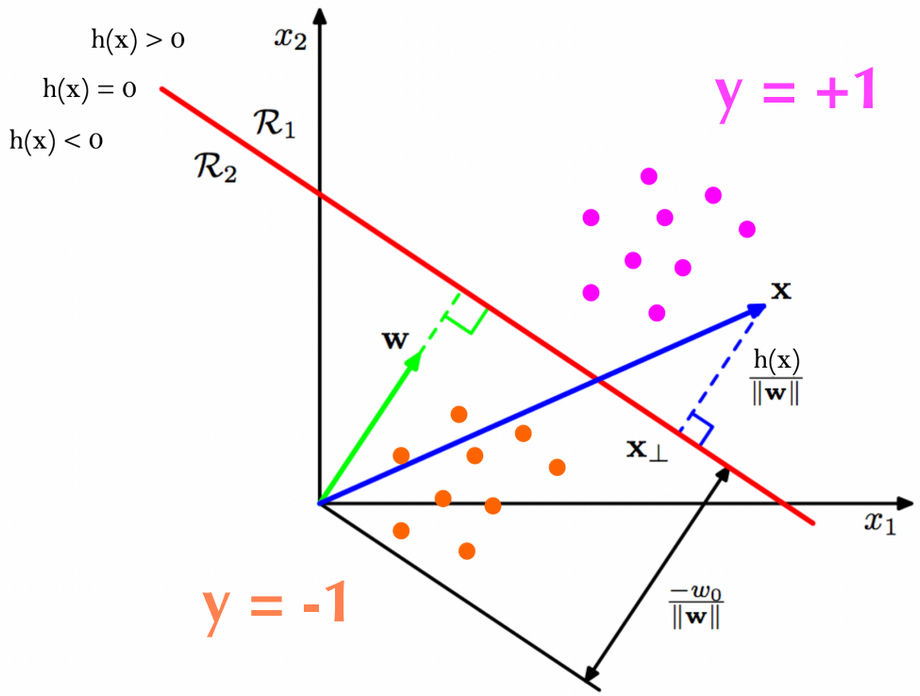
- Set of input / output pairs $D = \{x_i, y_i\}_{i=1,\ldots,n}$ where n is number of examples
  - Design matrix $\mathbf{X} \in \mathbb{R}^{n \times m}$ (m = number of features)
  - Target vector: $\mathbf{y} \in \mathbb{R}^n$ (just one target per example)
- Rewrite linear model as: $\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,m} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,m} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix} \longrightarrow \hat{\mathbf{y}} = \mathbf{X}\mathbf{w}$ predicted vector
- Rewrite loss as: $\mathscr{L}(\mathbf{w}) = ||\mathbf{y} - \mathbf{X}\mathbf{w}||^2 = \frac{1}{n}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$
- Minimization solved by computing gradient: $\nabla_{\mathbf{w}} \mathscr{L}(\mathbf{w}) = 2(\mathbf{y} - \mathbf{X}\mathbf{w})\mathbf{X} = 0$
- The solution can be solved *analytically**: $\mathbf{w}* = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$

** not always possible or most efficient (we come back to this later)*

Linear Classification

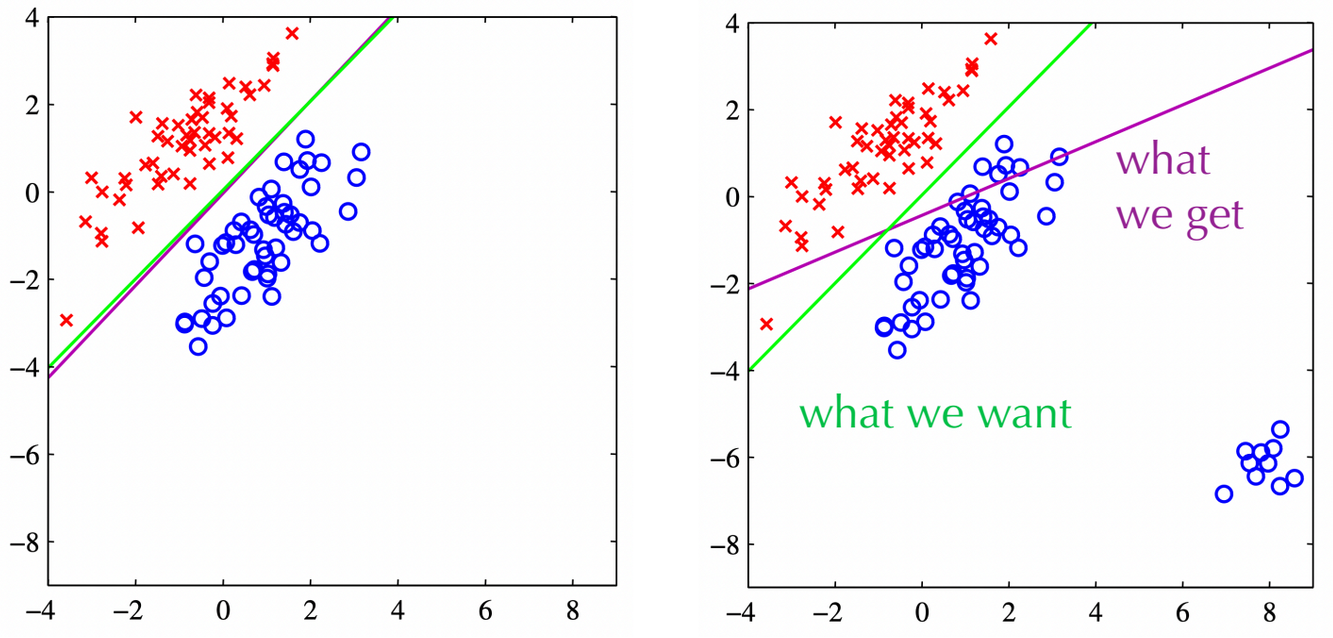
Linear classification

- Task: learn a function to **separate different classes of data** — for two classes we call this "binary classification":
  - $\mathbf{x}_i \in \mathbb{R}^m$
  - $y_i \in \{-1, 1\}$ — we call these "true labels"
- Assume **linear discriminant function:** $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x}$
- **Decision boundary** defined by hyperplane $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} = 0$
  - boundary is perpendicular to weight vector $\mathbf{w}$



- Classifier score for point $\mathbf{x}_i = h(\mathbf{x}_i; \mathbf{w})$ → make predictions:
  - class = 0 if $h(\mathbf{x}_i; \mathbf{w}) < 0$
  - class = 1 if $h(\mathbf{x}_i; \mathbf{w}) \geq 0$

Linear classification

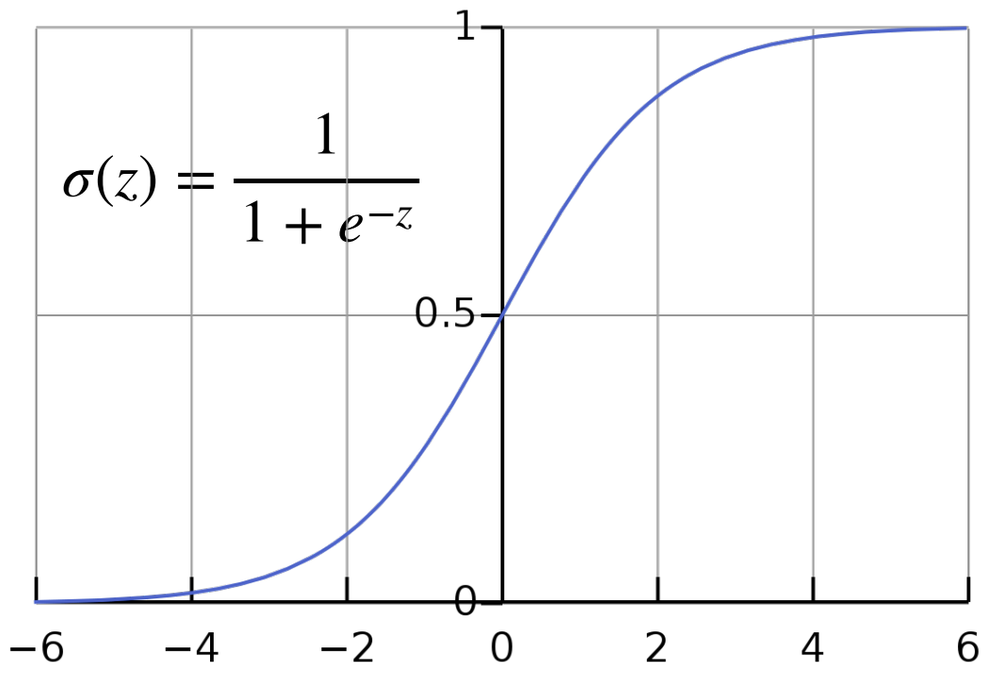


$$\mathscr{L}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h(\mathbf{x}_i;\mathbf{w}))^2$$

- As for regression we can apply the least square method to find the decision boundary
  - penalized even when predict class correctly
  - very sensitive to outliers
- The MSE is not the right loss function to use for classification task

Logistic regression

- Set of input/out pairs $\mathscr{D} = \{\mathbf{x}_i, y_i\}_{i=1,\ldots,n}$
  - $\mathbf{x}_i \in \mathbb{R}^m$
  - $y_i \in \{0,1\}$
- Assume linear discriminant function: $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x}$
- Convert the distance from the boundary into a probability that a point belongs to a class or the other → **sigmoid function***

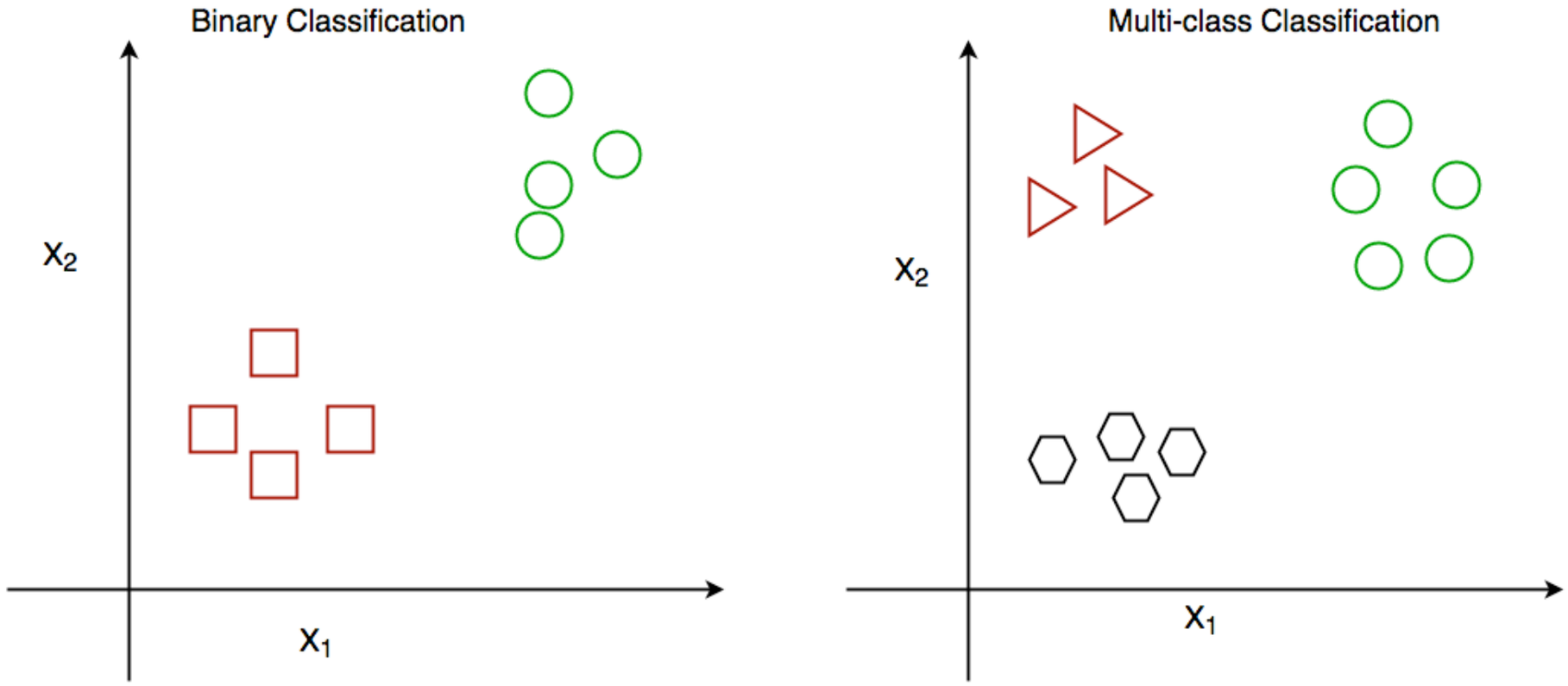


$$p(y = 1 \mid \mathbf{x}) \equiv p_i = \frac{1}{1 + e^{-h(\mathbf{x};\mathbf{w})}} = \frac{1}{1 + e^{-\mathbf{w}^{\mathrm{T}}\mathbf{x}}}$$

- The further from boundary $\mathbf{w}^{\mathrm{T}}\mathbf{x} = 0$ the more certain about a class
- Class decision rule: choose class 0 if pi < 0.5, else choose class 1

**nb, not a random choice — see generalized linear models*

Multi-class classification



- **Softmax** → multi-class generalization of logistic sigmoid function
  - have N classes $\{c_1, \ldots, c_N\}$ per each example $\mathbf{x}_i$ where $\mathbf{x}_i$ belongs to just one class k
  - model target $\mathbf{y}_i = \{0,...,0,1,0,...0\}$ → set 1 for element k_{th}

$$p(c_k \mid \mathbf{x}) = \frac{e^{\mathbf{w}_k^{\mathrm{T}}\mathbf{x}}}{\sum_{j=1}^{N} e^{\mathbf{w}_j^{\mathrm{T}}\mathbf{x}}}$$

Logistic regression

- We now write $p(y \mid \mathbf{x})$ as Bernoulli random variable:

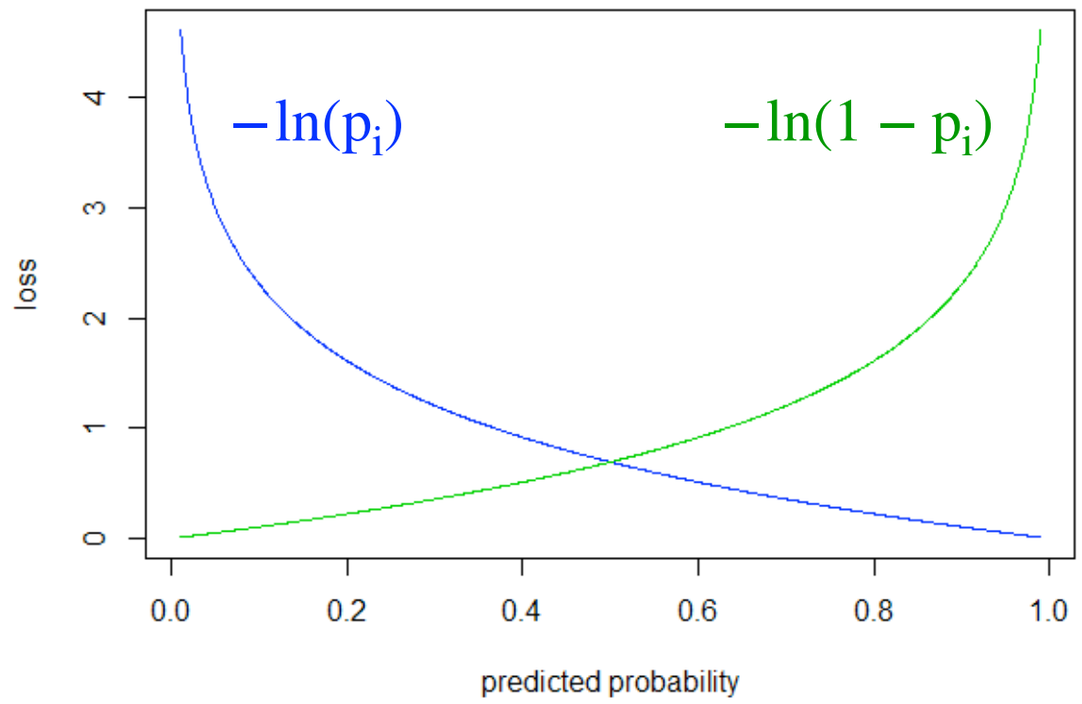
$$p(y_i = y \mid \mathbf{x}_i) = (p_i)^{y_i}(1 - p_i)^{1-y_i} = \begin{cases} p_i & \text{if } y_i = 1 \\ 1 - p_i & \text{if } y_i = 0 \end{cases}$$

- Negative log-likelihood

$$-\ln\mathscr{L} = -\ln\prod_{\mathrm{i}} (\mathrm{p_i})^{\mathrm{y_i}}(1 - \mathrm{p_i})^{1-\mathrm{y_i}}$$

$$= -\sum_{i} y_i \ln(\mathrm{p_i}) + (1 - \mathrm{y_i})\ln(1 - \mathrm{p_i})$$

binary cross entropy loss function!



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- Negative log-likelihood

$$\begin{aligned} -\ln\mathscr{L} &= -\ln\prod_i (p_i)^{y_i}(1 - p_i)^{1-y_i} \\ &= -\sum_i y_i \ln(p_i) + (1 - y_i)\ln(1 - p_i) \\ &= \sum_i \ln(1 + e^{-\mathbf{w}^T\mathbf{x}}) + (1 - y_i)\ln(1 + e^{\mathbf{w}^T\mathbf{x}}) \end{aligned}$$

binary cross entropy loss function!

- No analytic solution to $\mathbf{w}^* = \text{argmin}_{\mathbf{w}} - \ln\mathscr{L}$

- How to solve for $\mathbf{w}$?

- Many numerical optimization methods to solve — we'll learn today about the most popular **Gradient Descent** method

Gradient Descent

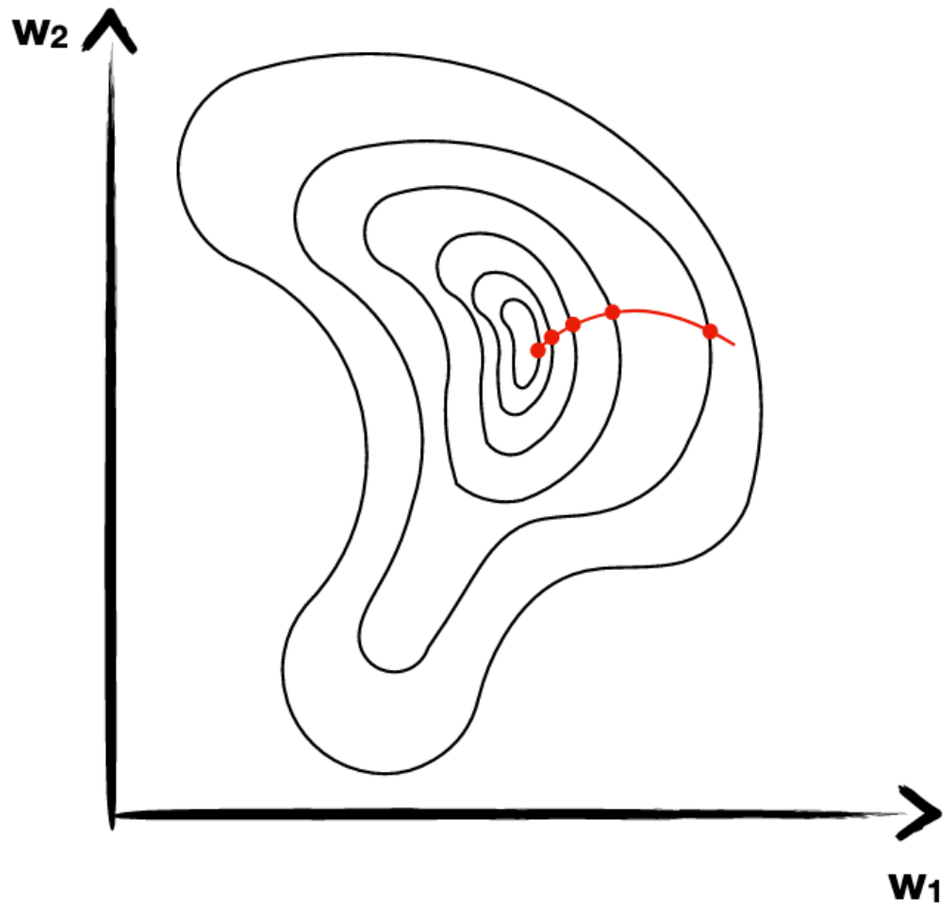
Gradient Descent

- Start from a random point
- Compute the gradient of the loss wrt the model parameters (i.e. "how should the weight be updated to decrease the loss?")

$$\nabla_{\mathbf{w}} \mathscr{L}(\mathbf{w})$$

- Make a step of size **η** (the **learning rate**) towards the gradient direction
- Update the parameters of the model accordingly

$$\mathbf{w}' \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathscr{L}(\mathbf{w})$$

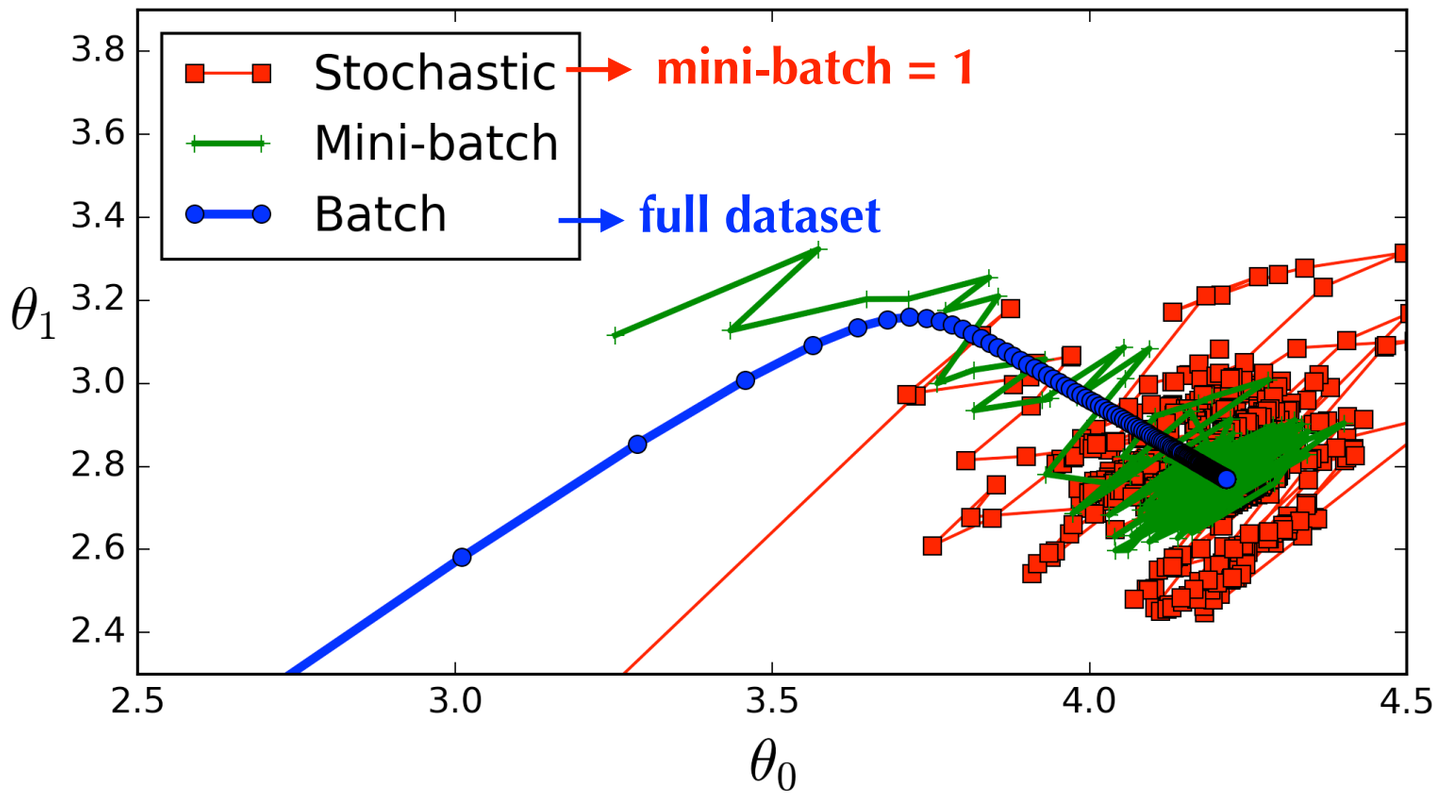


- Effective, but computationally expensive (gradient over entire dataset)

$$\nabla_{\mathbf{w}} \mathscr{L}(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} \nabla_{\mathbf{w}} \mathscr{L}(\mathbf{x}_i, y_i; \mathbf{w})$$

Stochastic Gradient Descent

- Make the minimization more computationally efficient
  - compute gradient on a small batch of examples (faster & parallelizable but noisy)
  - better scalability come at the cost of (sometimes) not converging to optimal point
  - increase robustness with larger batches at acceptable increased computational cost



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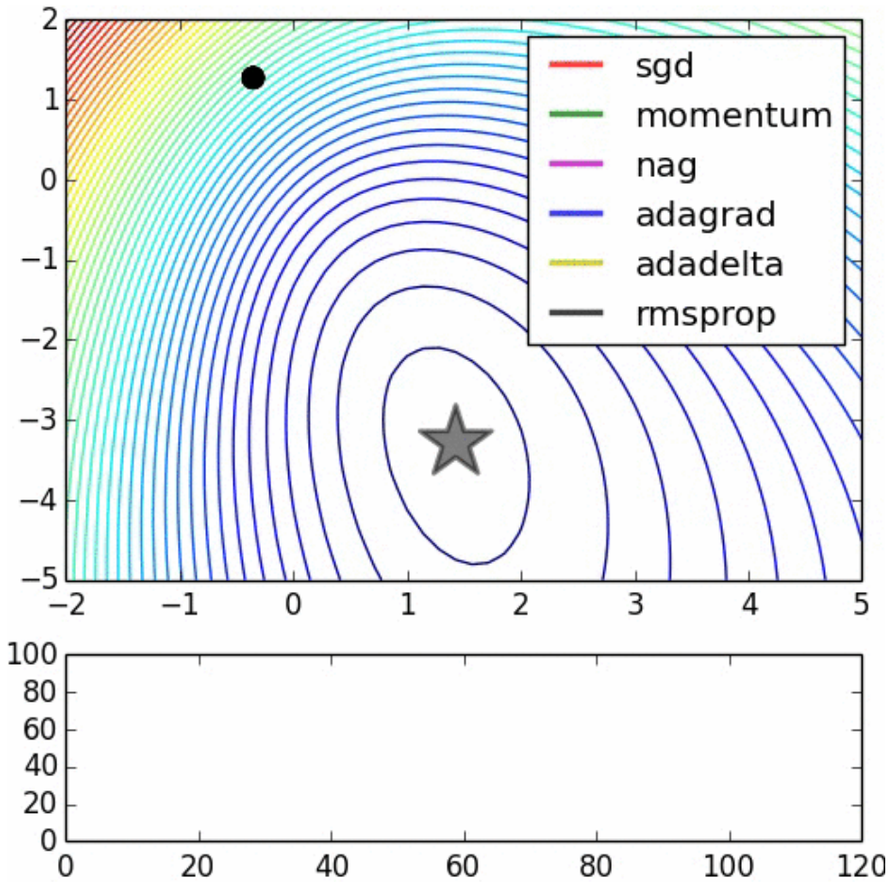

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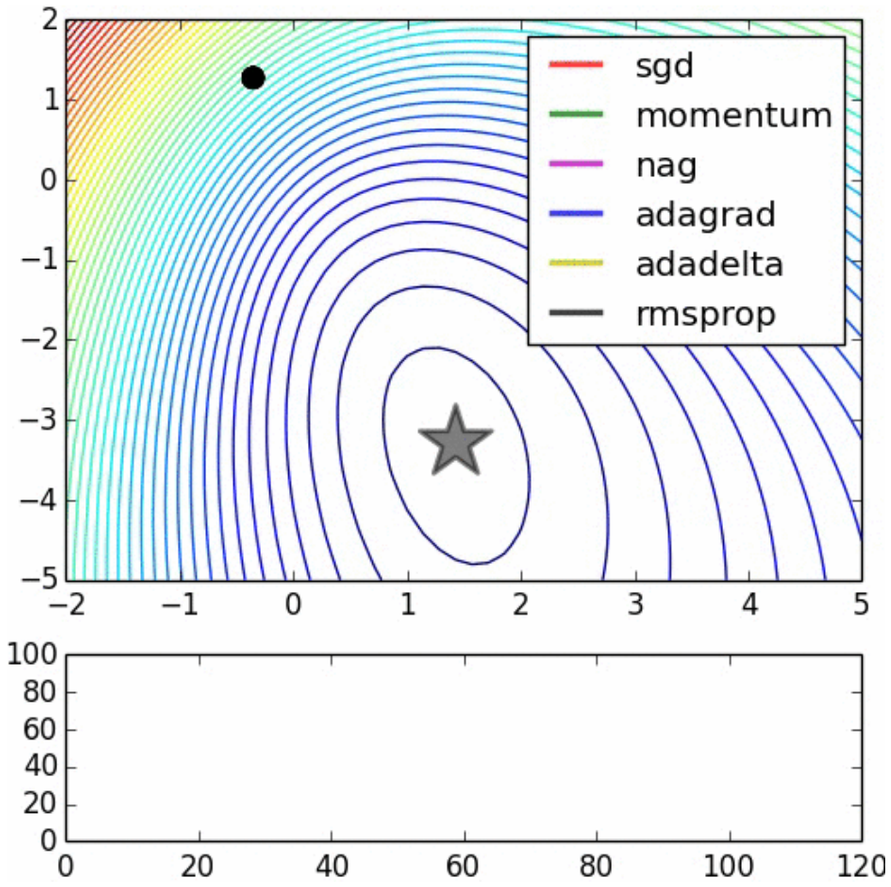

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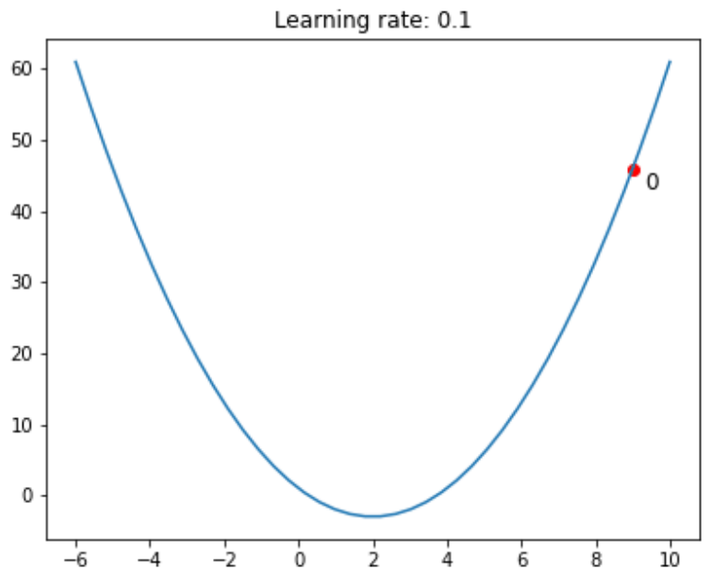
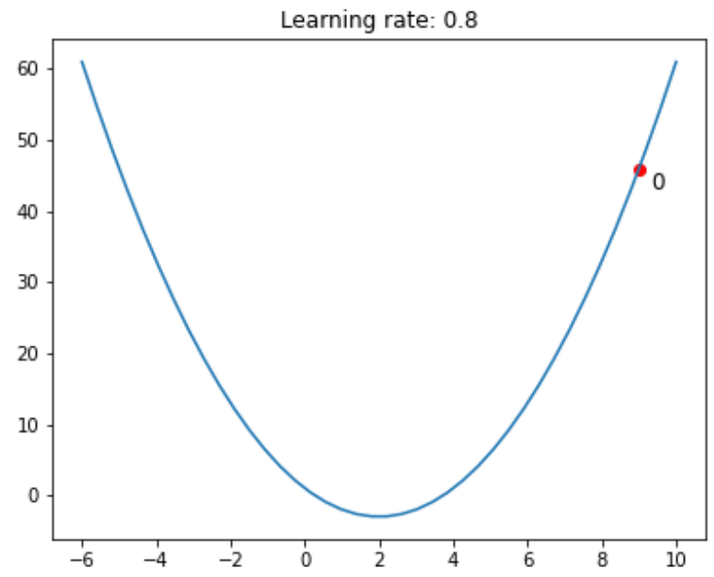
- Too small a learning rate, convergence very slow
- Too large a learning rate, algorithm diverges





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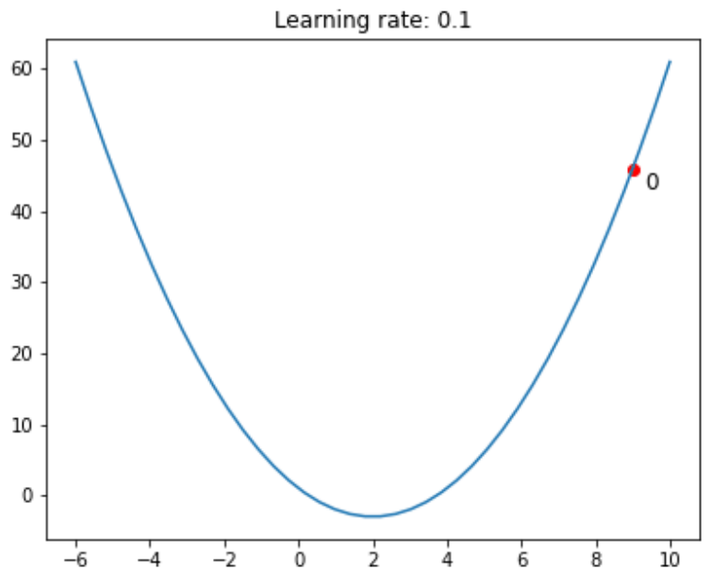
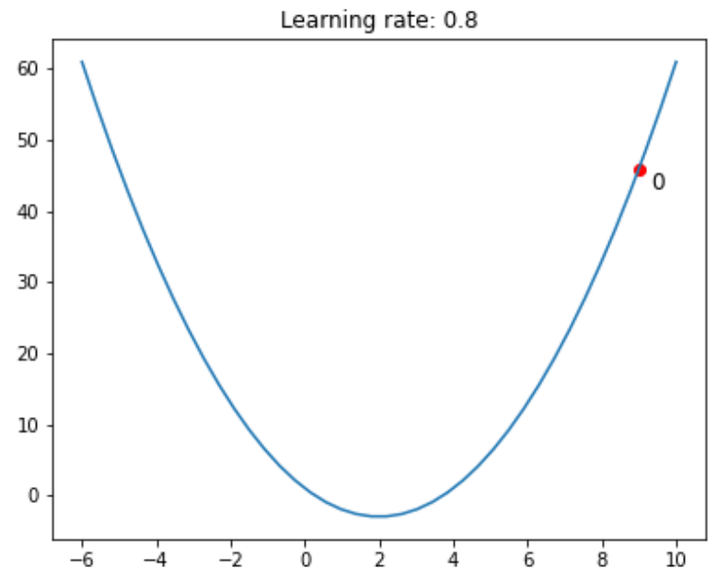
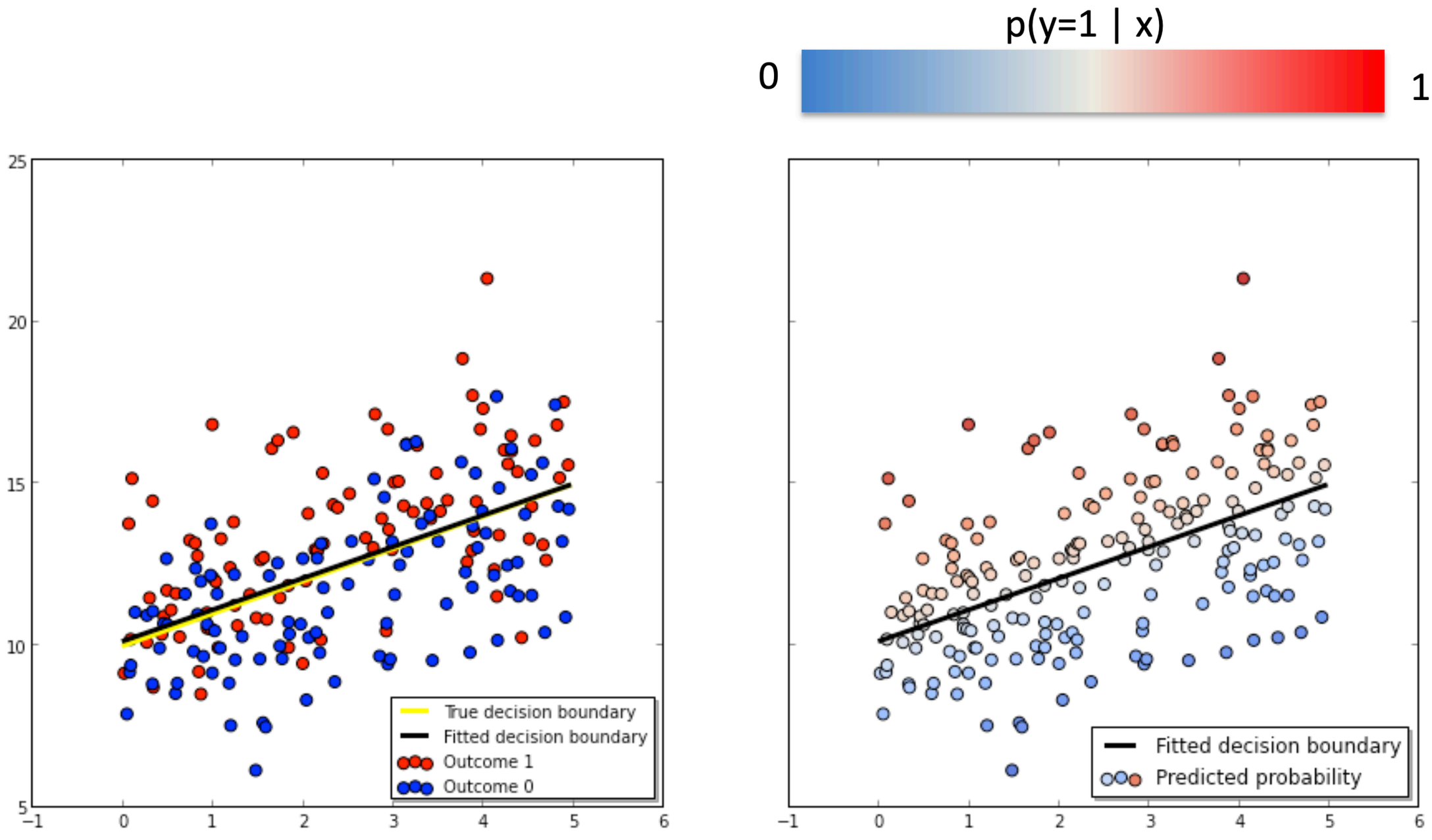


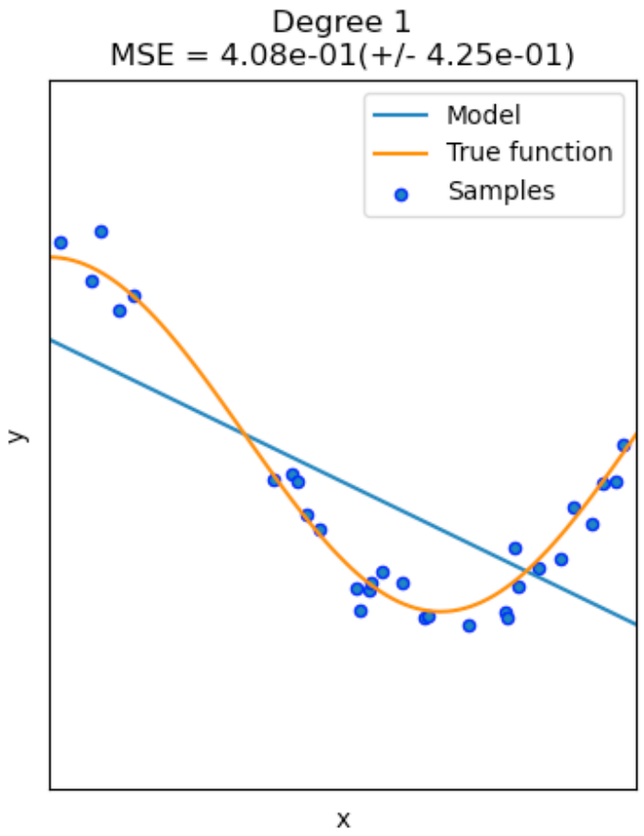


Apply it to logistic regression



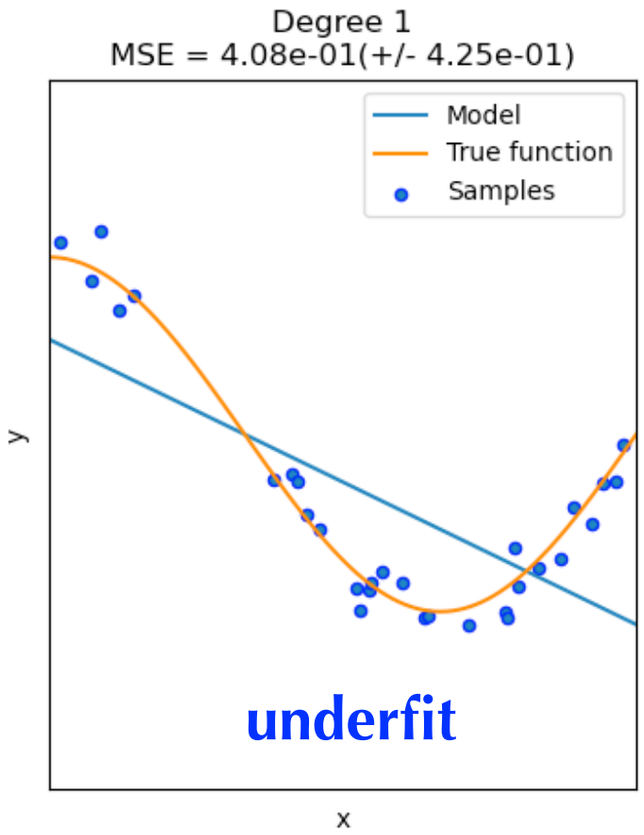
Overfitting

Fooling the linear regression



- What if $\mathbf{x}$ and $\mathbf{y}$ are not linearly correlated?
- Can chose a basis functions $\phi(\mathbf{x})$ to form new features such that $\mathbf{y} = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x})$
  - polynomial basis $\phi(\mathbf{x}) = \{1, \mathbf{x}, \mathbf{x}^2, \mathbf{x}^3, \dots\}$
  - **Linear regression on new features $\phi(\mathbf{x})$**
- **Problem: what basis functions to choose?** (e.g., up to which order polynomial)

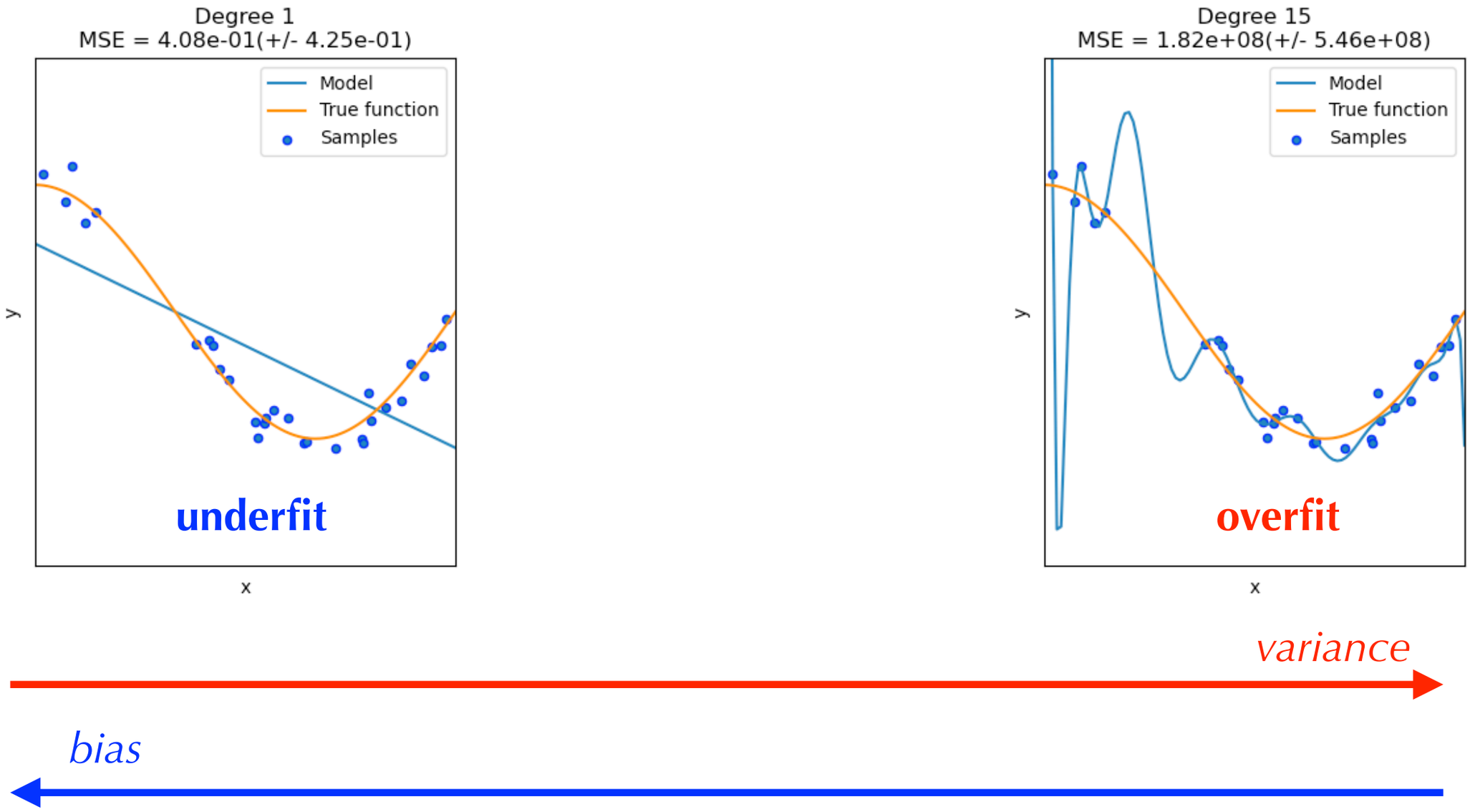
Bias-variance tradeoff



bias ←

- **A too simple model underfits the data:** will deviate from data (high bias) but will not be influenced by peculiarities of the data (low variance) → not enough flexibility

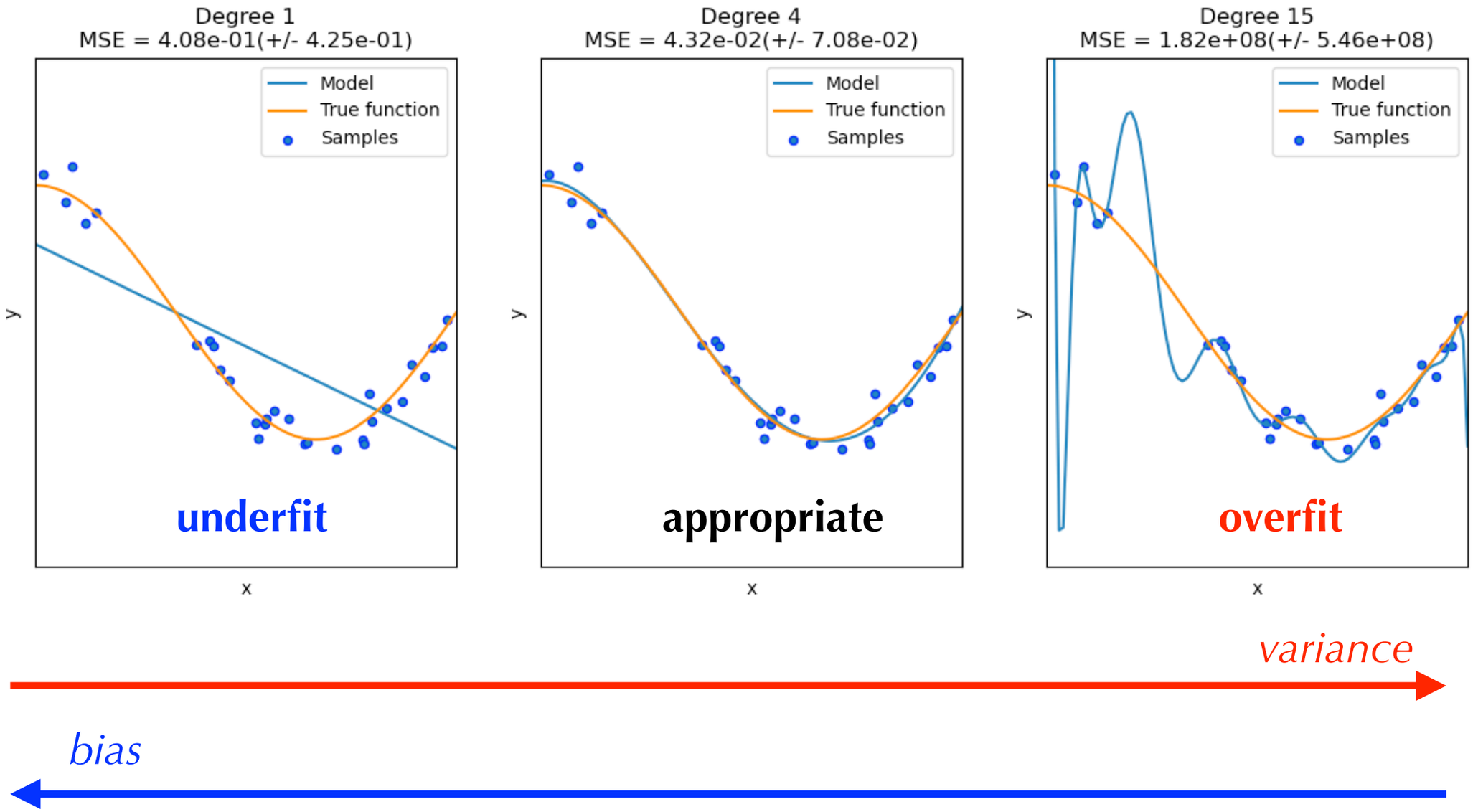
Bias-variance tradeoff



- **A too simple model underfits the data:** will deviate from data (high bias) but will not be influenced by peculiarities of the data (low variance) → not enough flexibility

- **A too complex model overfits the data:** will not deviate systematically from data (low bias) but will be very sensitive to noise in the data (high variance)

Bias-variance tradeoff



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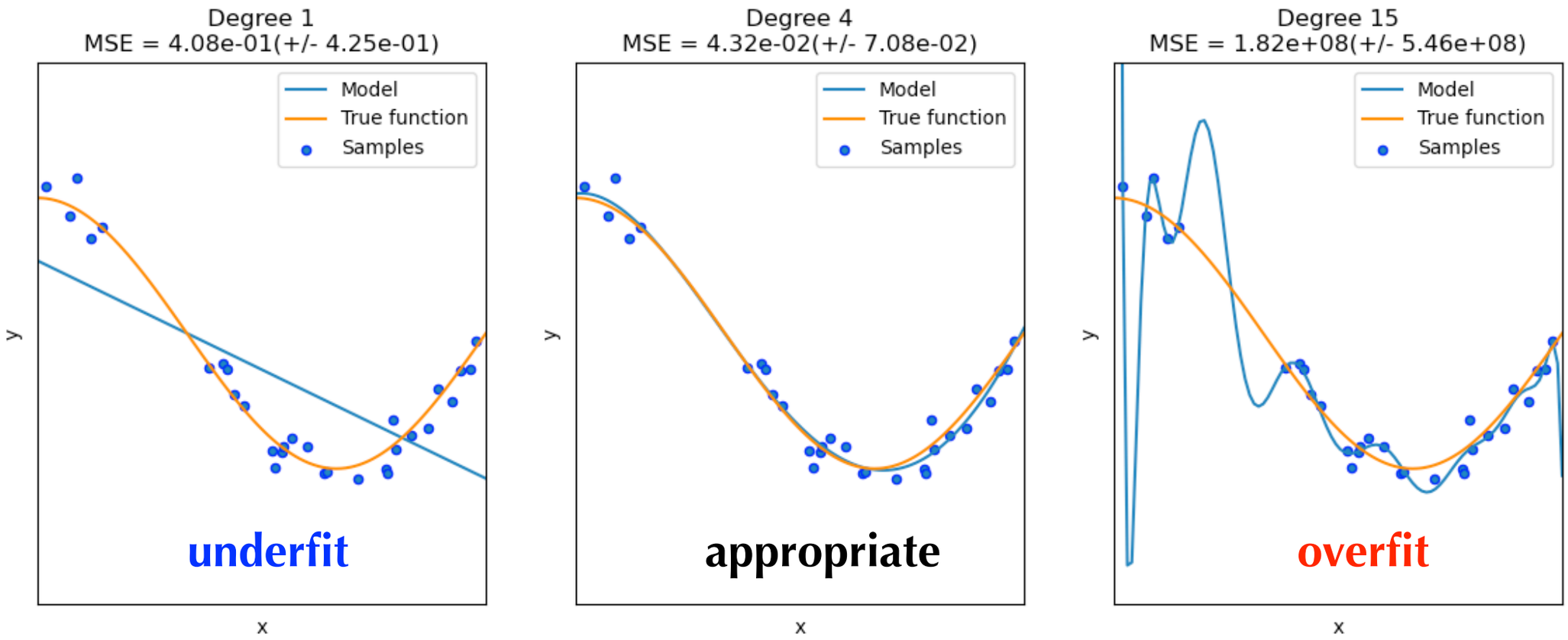
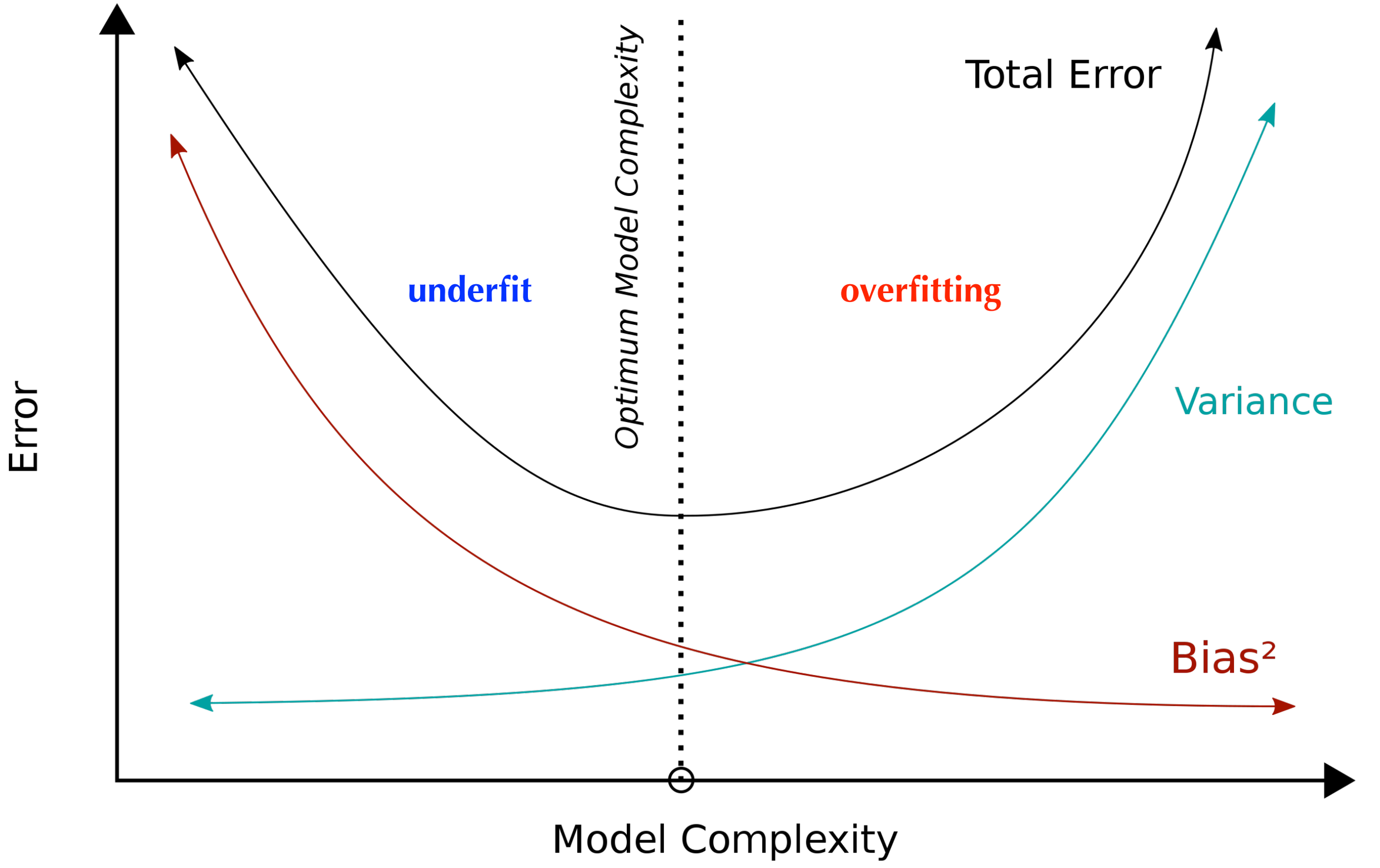


- What models allow us to do is to **generalize** to unseen examples
- Different models can have better or worse generalization performance
- **Generalization error** = **systematic error** + **sensitivity to noise**
  (bias) (variance)

Bias-variance tradeoff



Regularization

- A technique that helps avoid overfitting by shrinking the parameter estimates towards zero (i.e., discourages learning a more complex or flexible model)

- A modified loss is introduced, with a penalty term attached to each model parameter

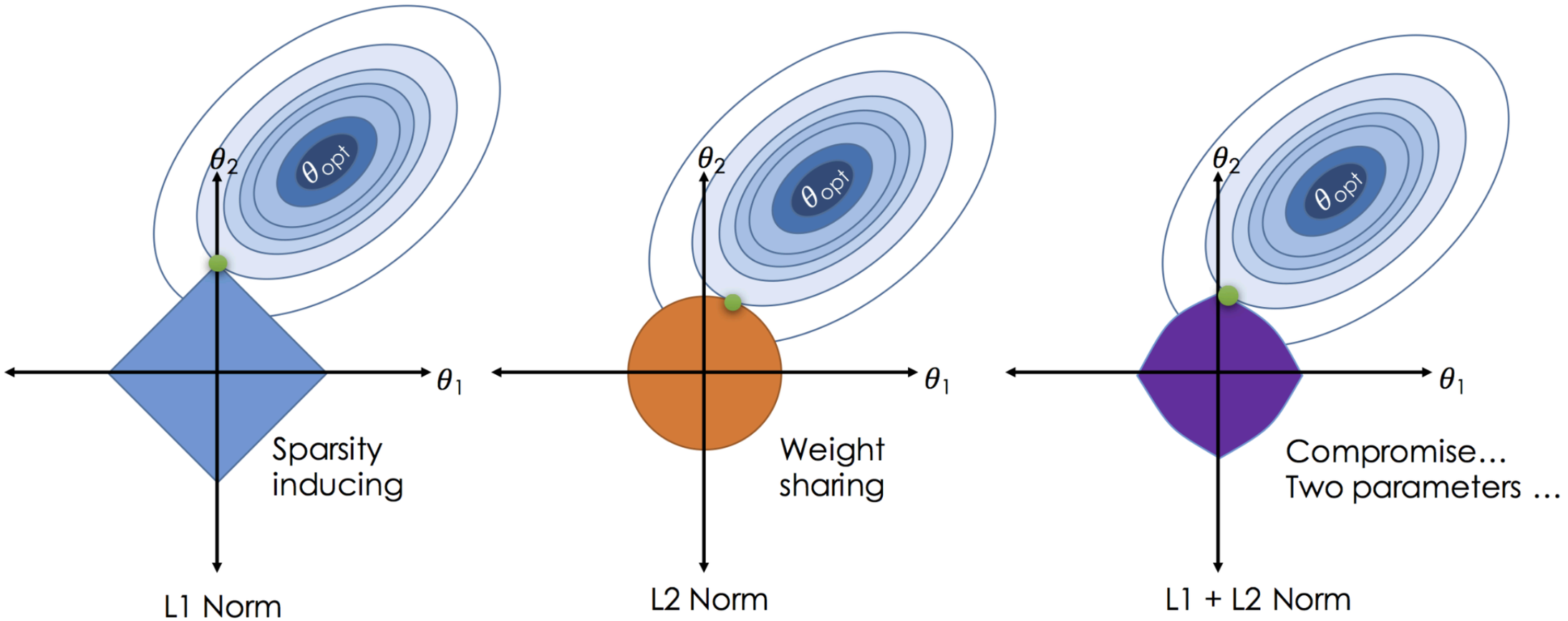
$$\mathcal{L}_{reg} = \mathcal{L}(\mathbf{W}) + \lambda\Omega(\mathbf{W})$$

- Example: L_p regularization $\Omega(\mathbf{W}) = ||\mathbf{W}||^p = \sum_i |w_i|^p$

- The minimization is then a tradeoff between:
  - pushing down the 1st term by taking advantage of the parameters
  - pushing down the 2nd term by switching off the parameters

- The value of λ determines this tradeoff
  - $\lambda \sim 0$: the penalty term has no effect
  - $\lambda \rightarrow +\infty$: the impact of the penalty grows

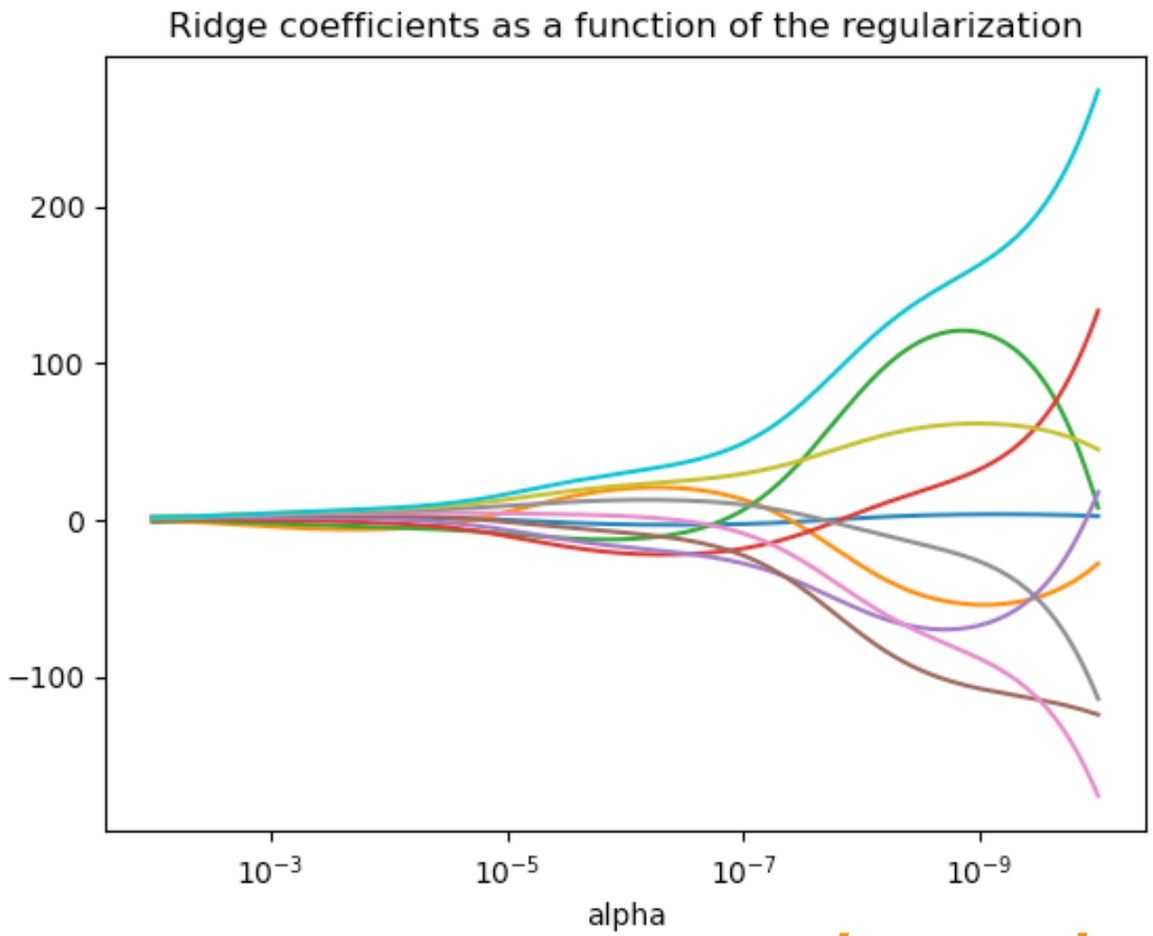
Regularizer types



- **L1 regularization:** $\Omega(\mathbf{w}) = ||\mathbf{w}|| = \sum |w_i|$
  - "Lasso regression" — enforce sparse weights
- **L2 regularization:** $\Omega(\mathbf{w}) = ||\mathbf{w}||^2 = \sum w_i^2$
  - "Ridge regression" — enforce small weights
- **Elastic Net = L1+L2 regularization**

Regularizer types

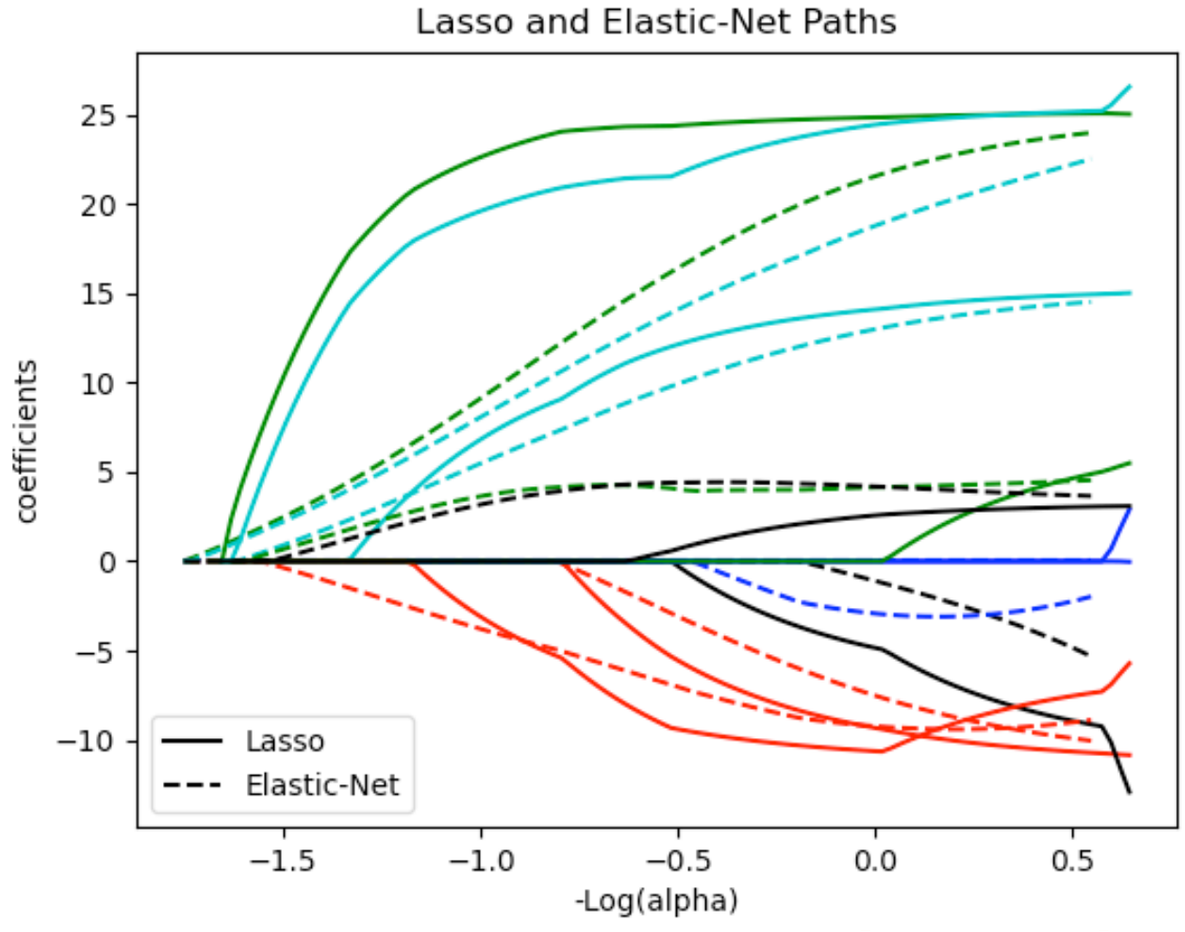
L2 regularization



less penalty

Some parameters switch on while being small

L1 + Elastic Net regularization

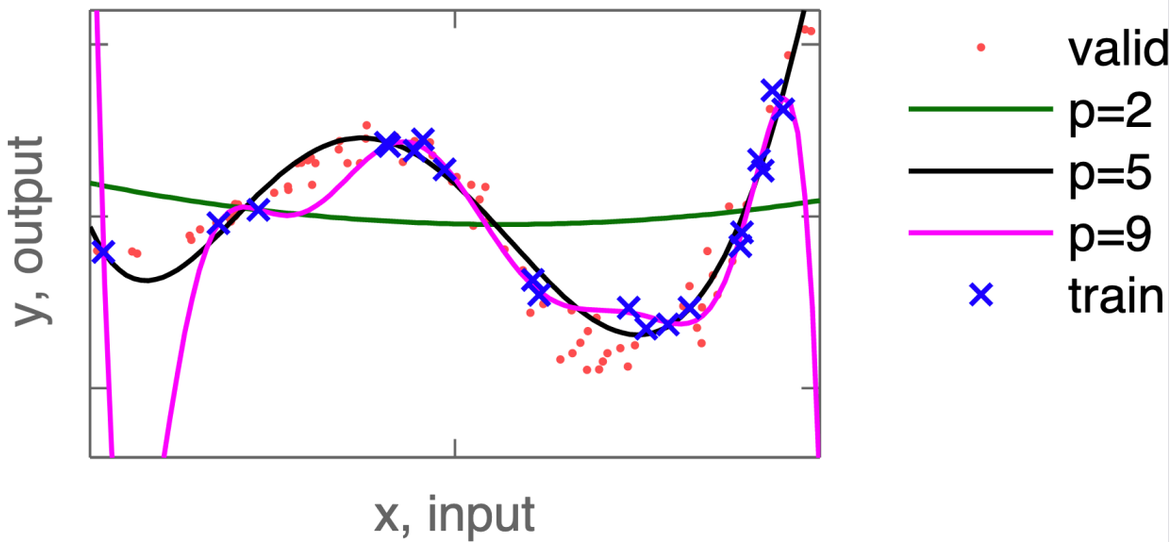


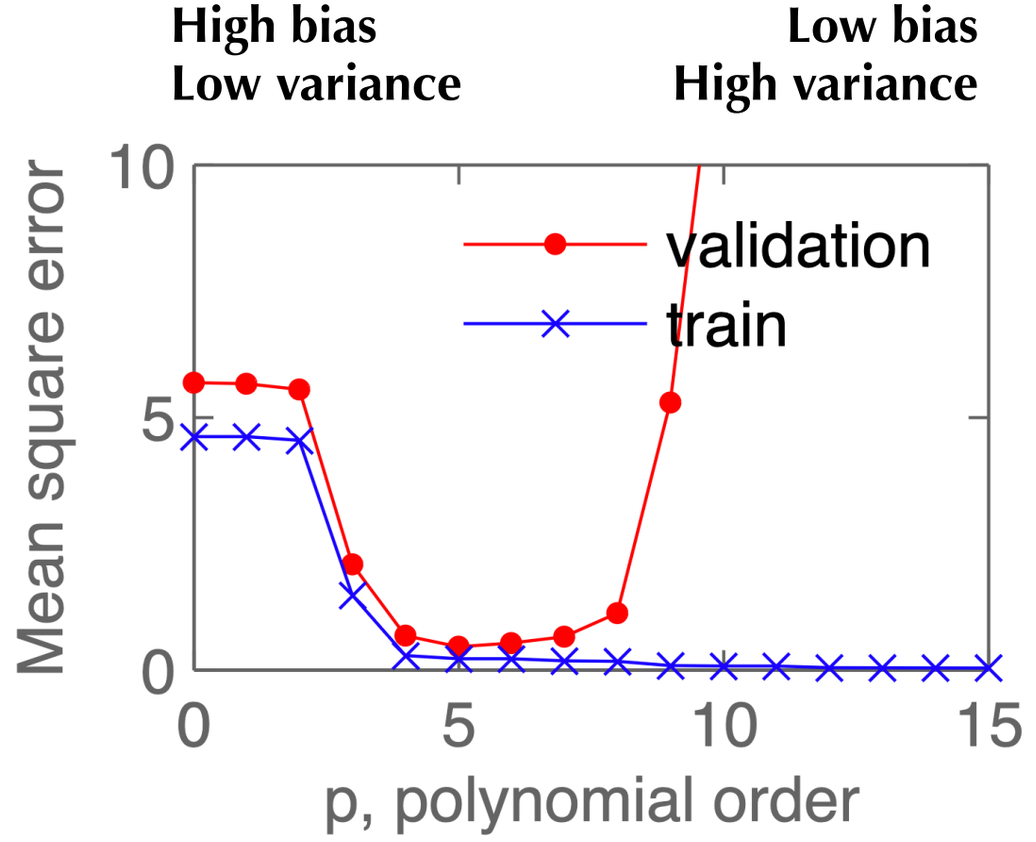
less penalty

Not all parameters switch on

How to monitor generalization?

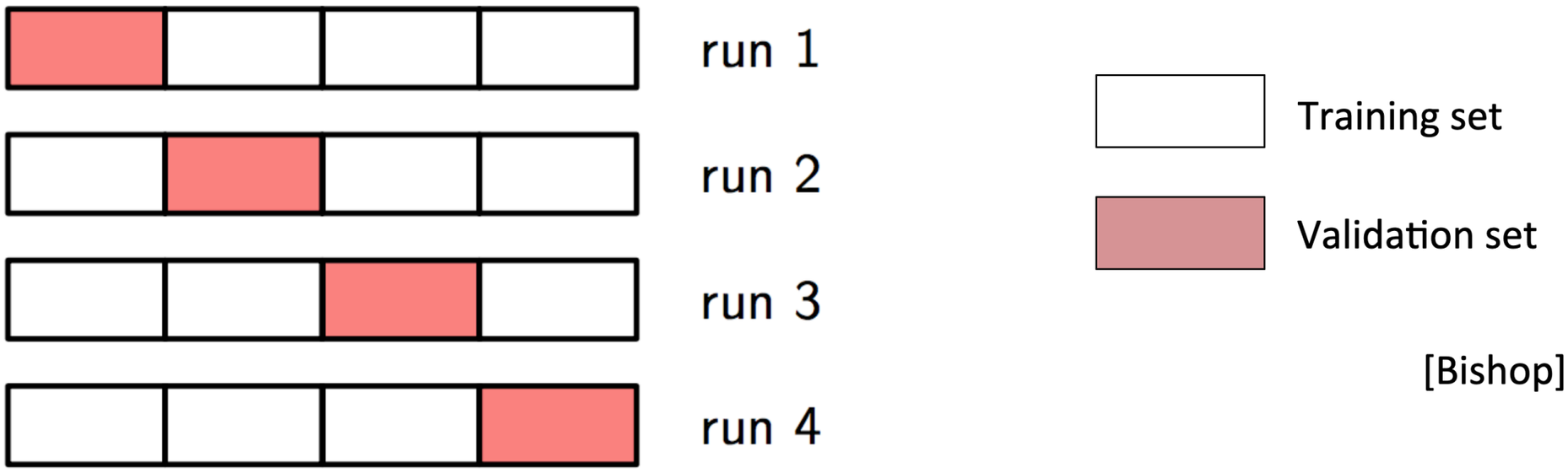
- Split the sample in three parts:
  - **Training:** the biggest chunk — used to fit the model parameters
  - **Validation:** an auxiliary dataset to verify generalization — used to tune parameters
  - **Test:** the dataset for the final independent check after all parameters are fixed — needed since we tune performance on validation set during fitting





Example: 55% training, 20% validation, 25% test

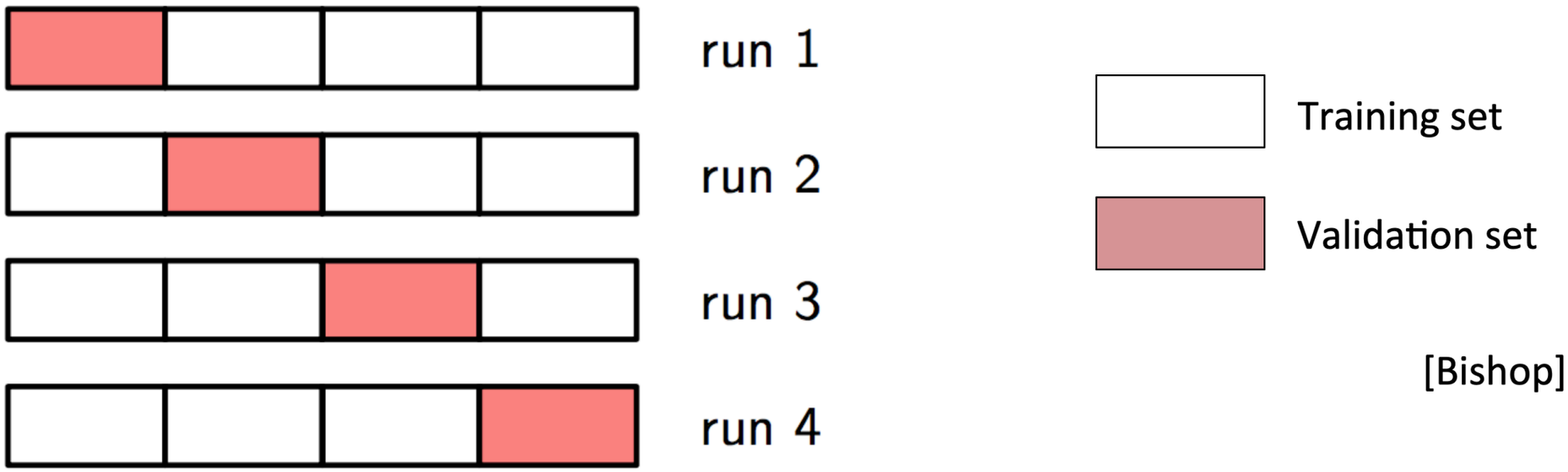
Cross validation to the rescue



[Bishop]

- **How does it work:**
  - Split the dataset in K chunks (called folds)
  - Train on K-1 chunks → obtain K-1 losses
  - Validate averaged K-1 losses on the K chunk for optimization then iterate over K
  - End up with K minimized losses → average them and test on full dataset
- **Allow you to use the full dataset (especially when it's small) while being unbiased**
- **Even when dataset not small, useful technique to estimate variance of expected performance**

Choose number of folds



[Bishop]

- **Too many folds:**
  - **Small bias:** the estimator will be very accurate
  - **Large variance:** due to small split sizes
  - **Costly:** many experiments, large computational time
- **Too few folds:**
  - **Cheap, computationally effective:** few experiments
  - **Small variance:** average over many samples
  - **Large bias:** estimated error rate conservative or smaller than the true error rate

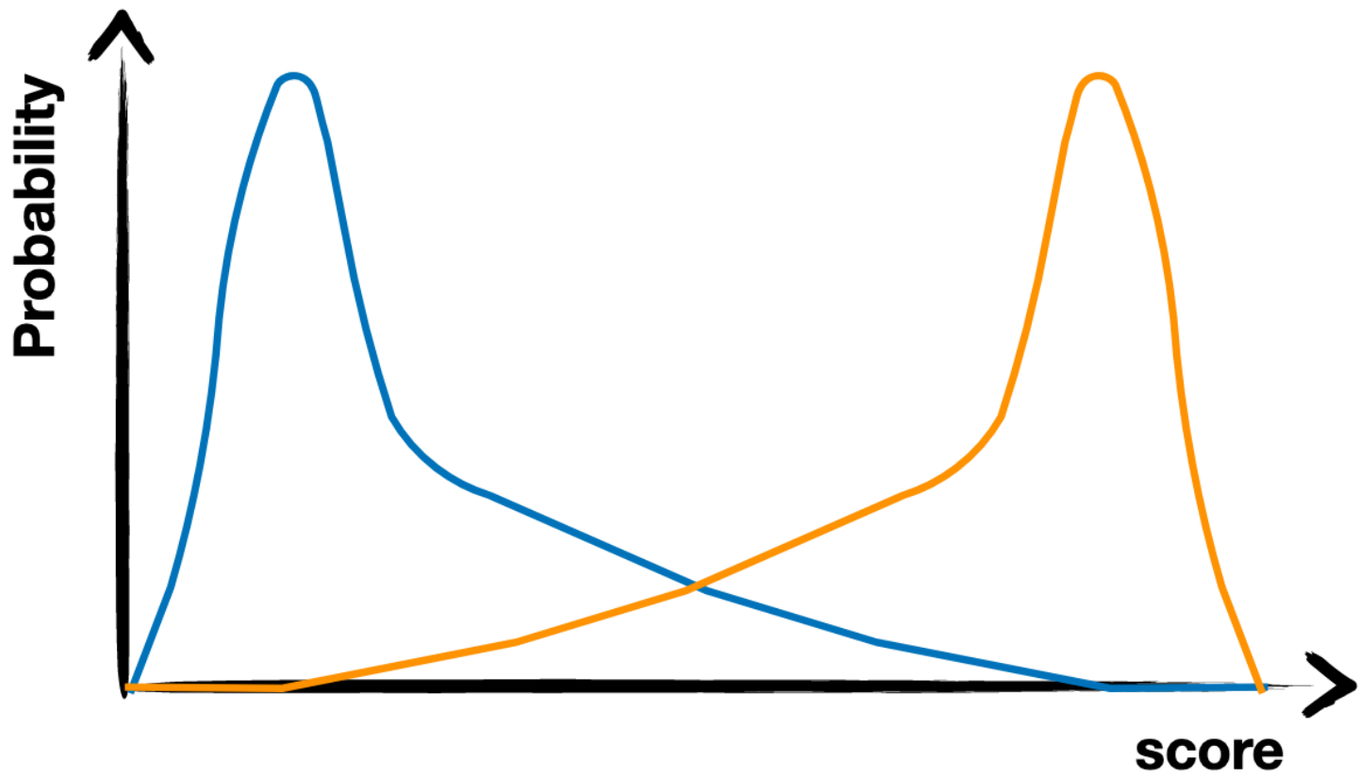
Performance Metrics

Evaluate classifier performance

- Consider a binary classifier:
  its output $\hat{y}$ is a number in the range $\{0,1\}$

  - we call $\hat{y}$ the classifier score

- If well trained, value should be close
  to 0 (1) for class-0 (class-1) examples



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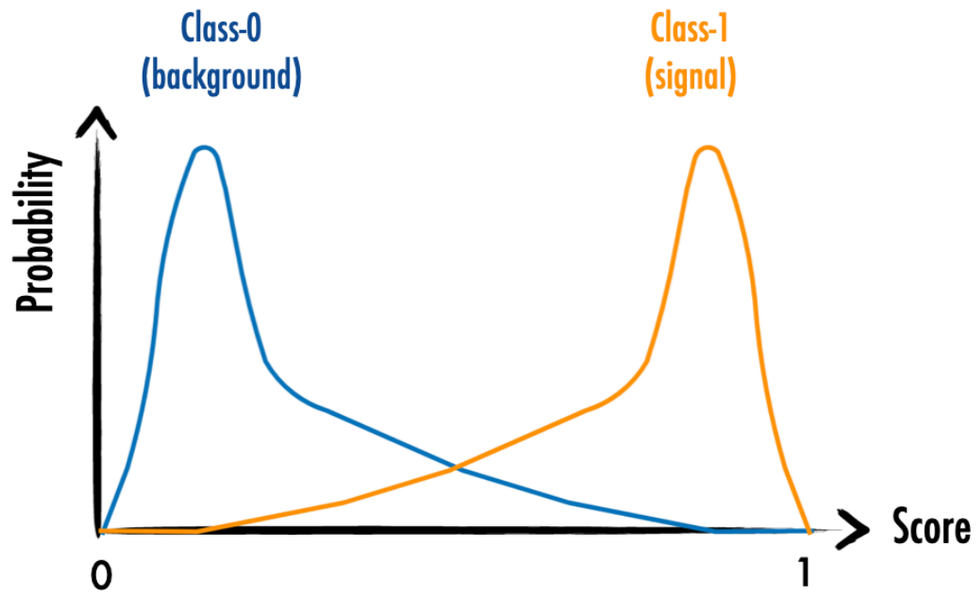
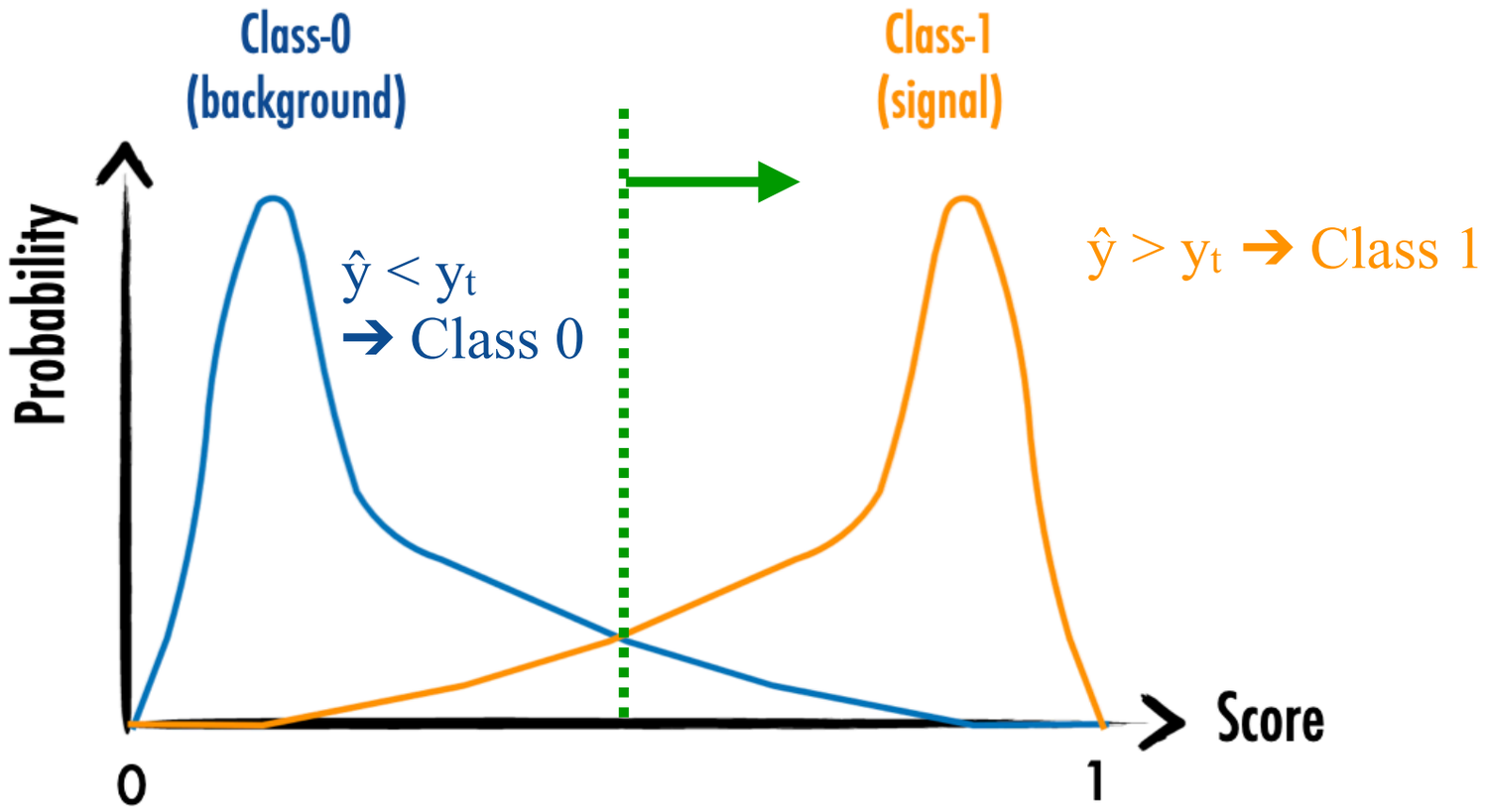
- One usually defines a threshold y_t such that:

  - $\hat{y} > y_t$ ➔ Class 1

  - $\hat{y} < y_t$ ➔ Class 0





Evaluate classifier performance

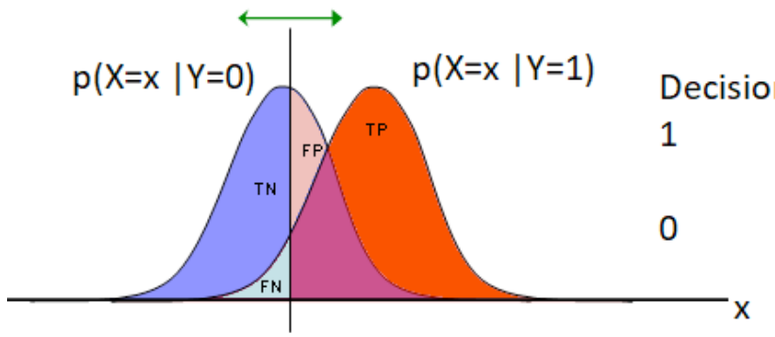
- Given the threshold y_t you can define:

		True classes		
		class 1	**class 0**	
Predicted classes	**class 1**	True Positive (TP)	False Positive (FP)	$\hat{y} > y_t$
	class 0	False Negative (FN)	True Negative (TN)	$\hat{y} < y_t$

- **Rates** are typically more informative:

$$\text{False Positive Rate (FPR)} = \frac{\mathbf{FP}}{\mathbf{FP + TN}}$$

$$\text{True Positive Rate (FPR)} = \frac{\mathbf{TP}}{\mathbf{TP + FN}}$$

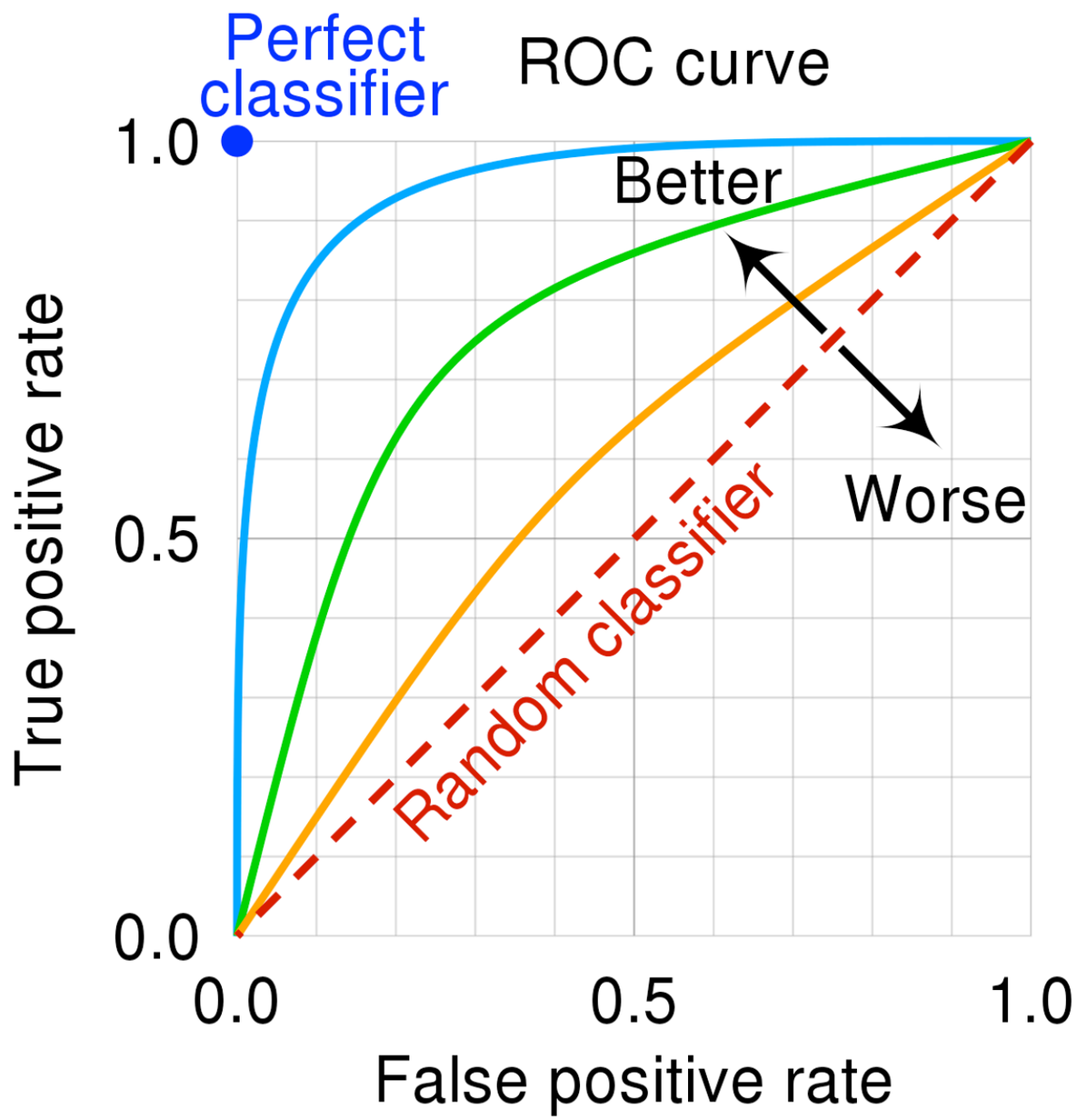


- And **accuracy** can be expressed as:

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

Evaluate classifier performance

- You can plot the rates to obtain the so-called **Receiver Operating Curve (ROC)**
- The **Area Under The Curve (AUC)** can be used to tell how good your model is doing



Summary lecture #1

- Machine learning uses mathematical and statistical models learned from data to characterize patterns and relations between inputs, and use this for inference / prediction
- Machine learning comes in many forms, much of which has probabilistic and statistical foundations and interpretations (i.e. *Statistical Machine Learning*)
- Discussed linear models today
- Tomorrow will be about nonlinear models → **Neural Networks!**
- This afternoon we'll go through **tools for data manipulation** — crucial to make data inputs to the ML tools we'll learn about in the next days