When Models Meet Data

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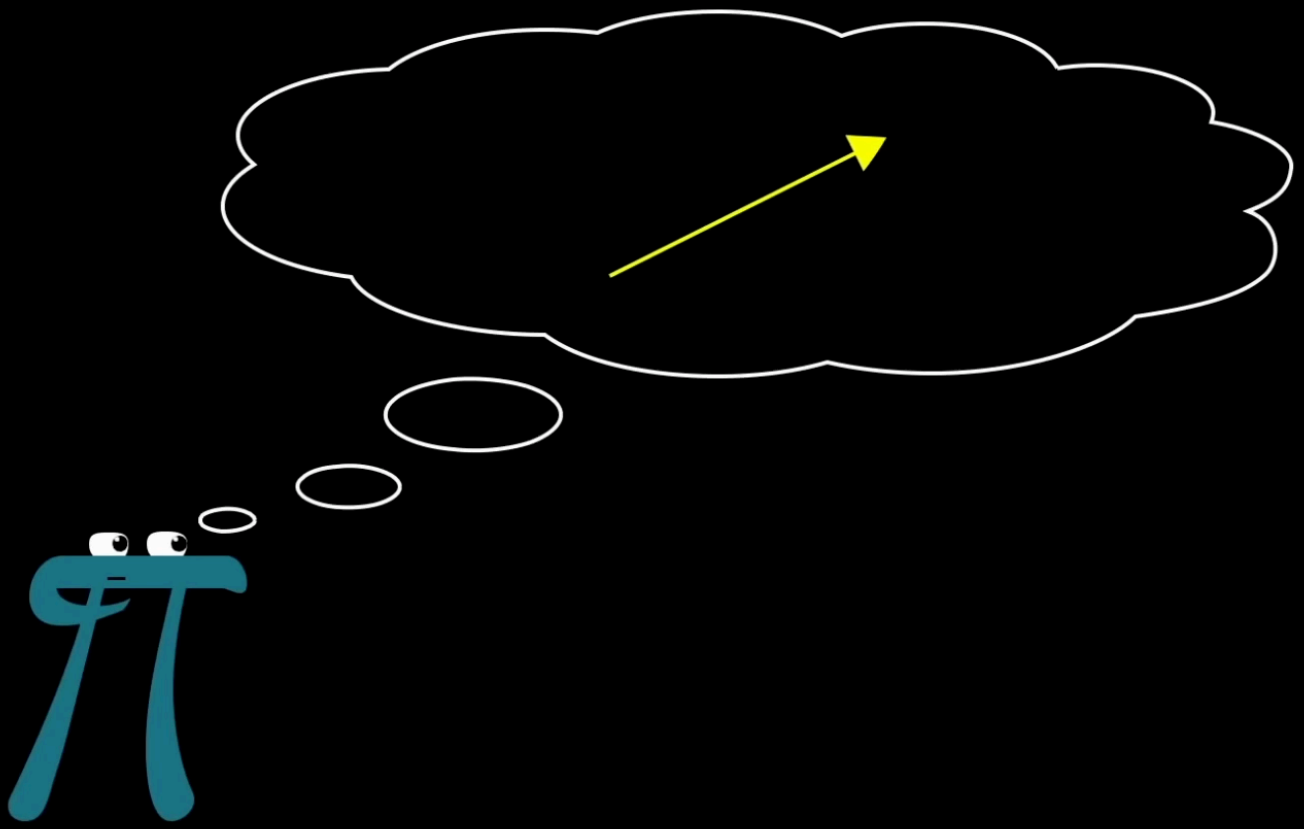
Outline

- Gram-Schmidt Orthogonalization
- Models learning from data
- Model meets data: finding parameters
- Empirical Risk Minimisation

Think of individual vectors as arrows



Credit: 3blue1brown

3.8.3 Gram-Schmidt Orthogonalization

- Consider a basis of $\mathbb{R}^2$

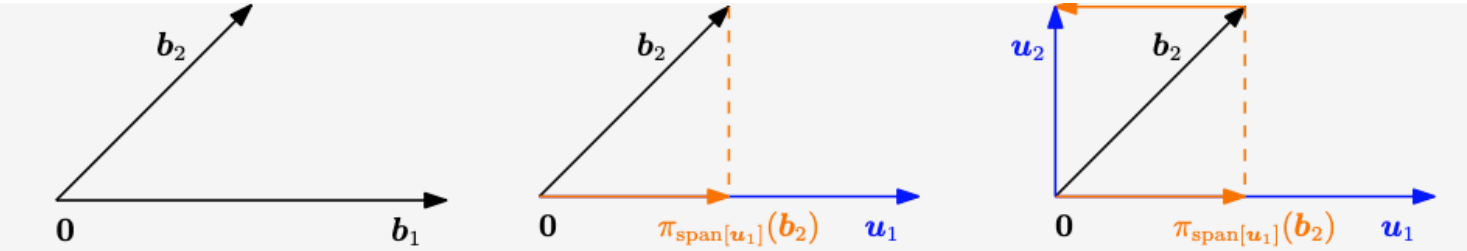
$$\boldsymbol{b}_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix} \qquad \boldsymbol{b}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

- Using the Gram-Schmidt method, we construct an orthogonal basis $(\boldsymbol{u}_1, \boldsymbol{u}_2)$ of $\mathbb{R}^2$ as follows (using dot product).

$$\boldsymbol{u}_1 := \boldsymbol{b}_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$$

$$\boldsymbol{u}_2 := \boldsymbol{b}_2 - \pi_{\text{span}[\boldsymbol{u}_1]}(\boldsymbol{b}_2) = \boldsymbol{b}_2 - \frac{\boldsymbol{u}_1 \boldsymbol{u}_1^{\mathrm{T}}}{\|\boldsymbol{u}_1\|^2} \boldsymbol{b}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- We immediately see that $\boldsymbol{u}_1, \boldsymbol{u}_2$ are orthogonal, i.e., $\boldsymbol{u}_1^{\mathrm{T}} \boldsymbol{u}_2 = 0$



(a) Original non-orthogonal basis vectors $\boldsymbol{b}_1, \boldsymbol{b}_2$.

(b) First new basis vector $\boldsymbol{u}_1 = \boldsymbol{b}_1$ and projection of $\boldsymbol{b}_2$ onto the subspace spanned by $\boldsymbol{u}_1$.

(c) Orthogonal basis vectors $\boldsymbol{u}_1$ and $\boldsymbol{u}_2 = \boldsymbol{b}_2 - \pi_{\text{span}[\boldsymbol{u}_1]}(\boldsymbol{b}_2)$.

3.8.3 Gram-Schmidt Orthogonalization

- Constructively transform basis $(\boldsymbol{b}_1, \cdots, \boldsymbol{b}_n)$ of an n-dim vector space V into an orthogonal/orthonormal basis $(\boldsymbol{u}_1, \cdots, \boldsymbol{u}_n)$ of V.

$\text{span}[\boldsymbol{b}_1, \cdots, \boldsymbol{b}_n] = \text{span}[\boldsymbol{u}_1, \cdots, \boldsymbol{u}_n]$

- The process iterates as follows

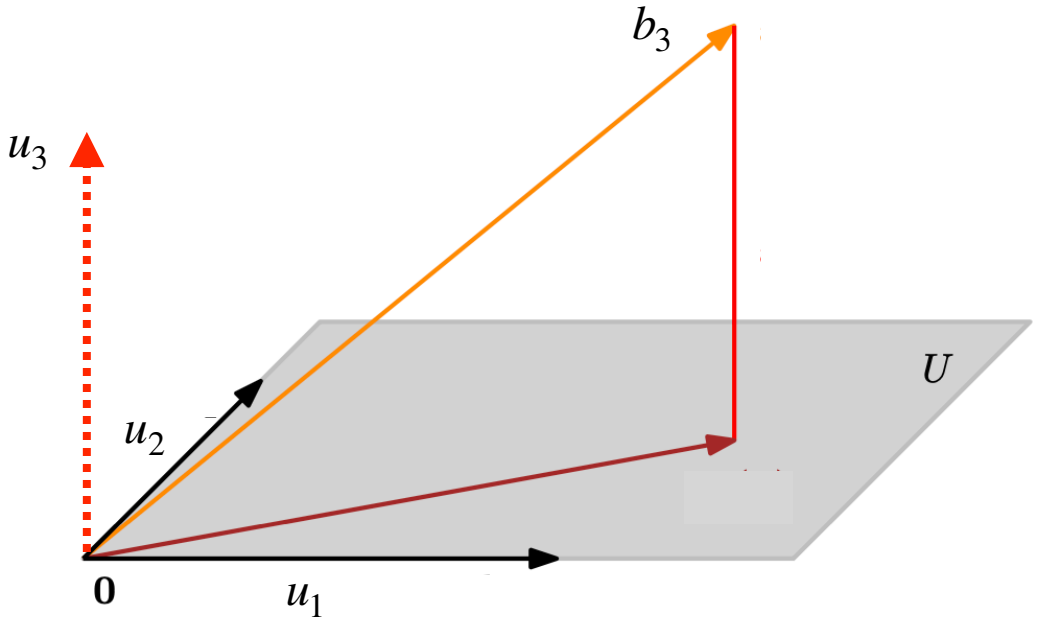
$$\boldsymbol{u}_1 := \boldsymbol{b}_1$$

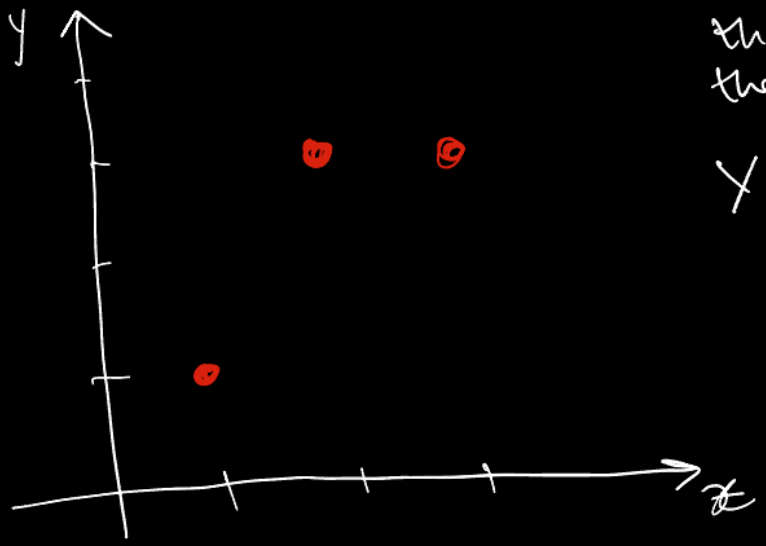
$$\boldsymbol{u}_k := \boldsymbol{b}_k - \pi_{\text{span}[\boldsymbol{u}_1, \cdots, \boldsymbol{u}_{k-1}]}(\boldsymbol{b}_k), \quad k = 2, \cdots, n$$

- The kth basis vector $\boldsymbol{b}_k$ is projected onto the subspace spanned by the first $k-1$ constructed orthogonal vectors $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_{k-1}$.
- This projection is then subtracted from $\boldsymbol{b}_k$ and yields a vector $\boldsymbol{u}_k$ that is orthogonal to the $(k-1)$-dim subspace spanned by $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_{k-1}$
- If we normalize $\boldsymbol{u}_k$, we obtain an ONB where $\|\boldsymbol{u}_k\| = 1$ for $k = 1, \cdots, n$.

3.8.3 Gram-Schmidt Orthogonalization

- Choose one direction as your first $\boldsymbol{u}_1 := \boldsymbol{b}_1$
- Project $\boldsymbol{b}_k$ onto the subspace spanned by the first $k-1$ constructed orthogonal vectors $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_{k-1}$.
- Subtract the projection from $\boldsymbol{b}_k$ and yields a vector $\boldsymbol{u}_k$ that is orthogonal to the $(k-1)$-dim subspace spanned by $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_{k-1}$
- Normalize $\boldsymbol{u}_k$, we obtain an ONB where $\|\boldsymbol{u}_k\| = 1$ for $k = 1, \cdots, n$.





Is there a line that goes through the 3 points?

$y = mx + b$

Let's choose 3 points: $(1,1)$, $(2,3)$, $(3,3)$

$(1,1)$: $m \times 1 + b = 1$

$(2,3)$: $m \times 2 + b = 3$ $\Rightarrow$ $\underbrace{\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} m \\ b \end{bmatrix}}_{u} = \begin{bmatrix} 1 \\ 3 \\ 3 \end{bmatrix} = v.$

$(3,3)$: $m \times 3 + b = 3$

But we can solve $A\tilde{u} = p$, where p is closest vector to v that lies in $C(A)$. And get values for m, b.

Check your understanding

(A) Orthogonal projections are linear projections.

(B) The result will no longer change when applying orthogonal projection multiple times (>1).

(C) Given a subspace to project on, orthogonal projection gives the minimum information loss (l_2).

(D) Gram-Schmidt Orthogonalization outputs the same number of basis vectors as the input.

(E) Projections allow us to visualize better and understand high-dimensional data.

Check your understanding

(A) Orthogonal projections are linear projections. YES

(B) The result will no longer change when applying orthogonal projection multiple times (>1). YES

(C) Given a subspace to project on, orthogonal projection gives the minimum information loss (l_2). YES

(D) Gram-Schmidt Orthogonalization outputs the same number of basis vectors as the input. YES

(E) Projections allow us to visualise better and understand high-dimensional data. YES

Further resources for Linear Algebra to hone the intuition

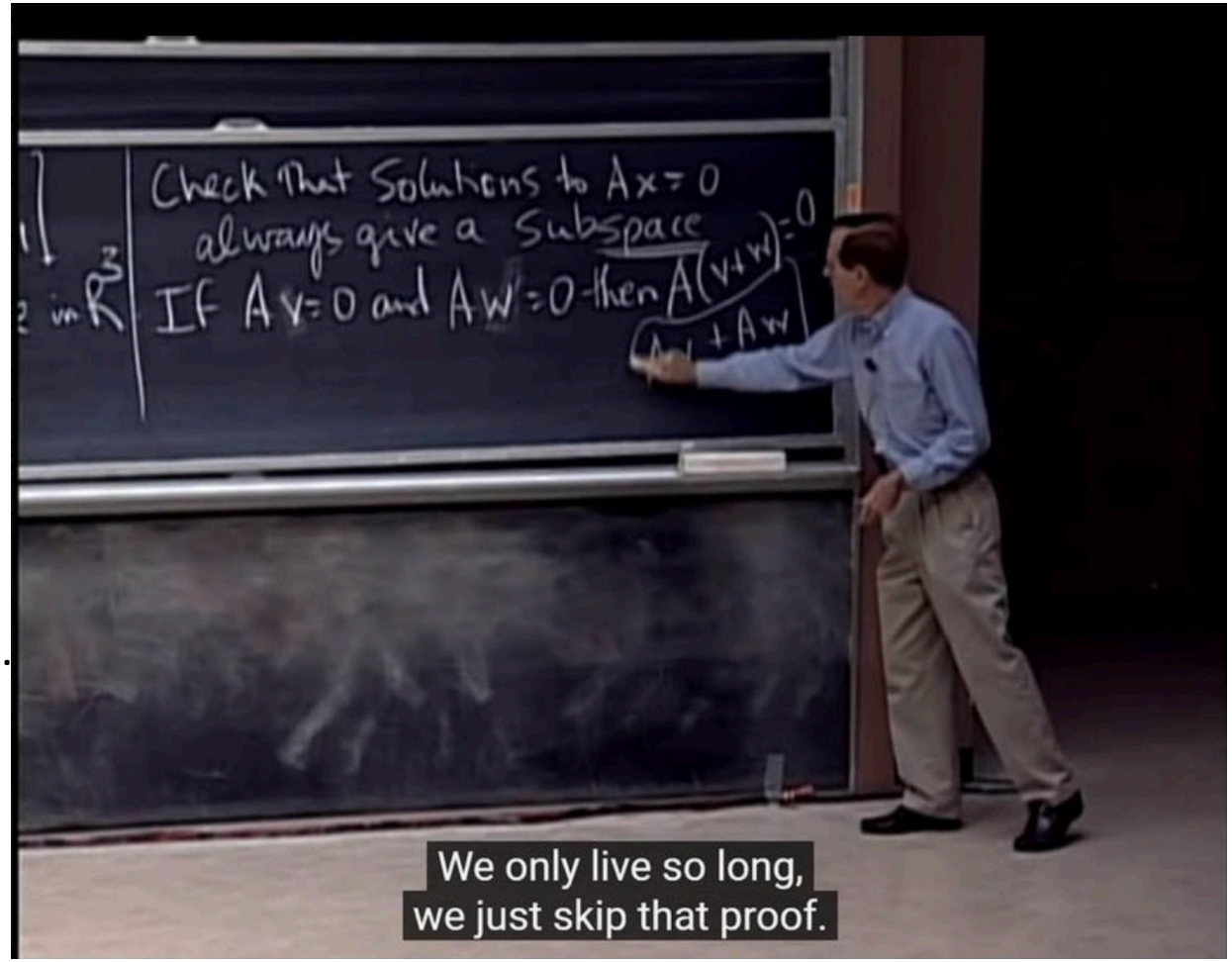
Prof Gilbert Strang MIT course on Linear Algebra

3blue1brown Chapter I

Linear Algebra done right - Axler

Linear Algebra - Serge Lang
Linear Algebra - Shilov

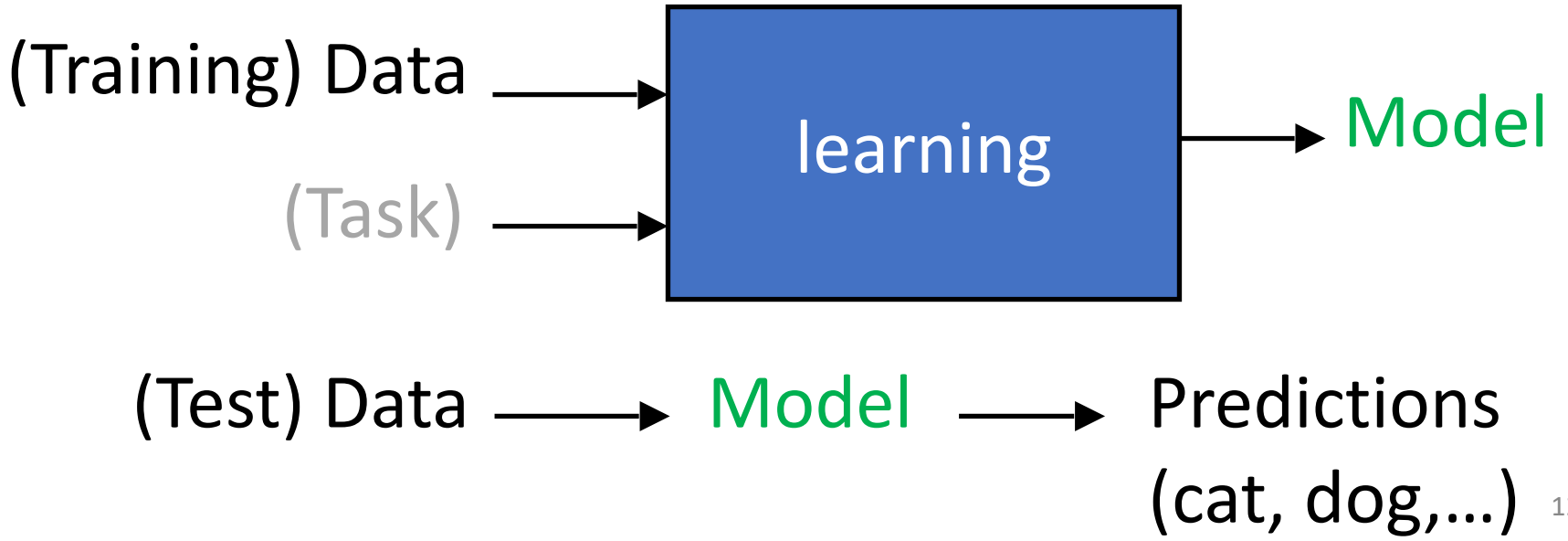
Deep Learning Book - Bengio et al.



8.1 Data, Models, and Learning

- A machine learning system has three major components:
- Data, models, learning

- A model is obtained by learning from the training data
- A prediction is made by applying a learned model on test data



8.1 Data, Models, and Learning

- We aim to learn good models.
- How is good defined? We need to have performance metrics on the test data. Examples include:
- Classification accuracy
- Distance from the ground truth
- Test time (efficiency)
- Model size
- ……
- New performance metrics are constantly being proposed by the machine learning community.

8.1.1 Data as Vectors

- Data, read by computers, should be in a numerical format.
- See the tabular format below

Name	Gender	Degree	Postcode	Age	Annual salary
Aditya	M	MSc	W21BG	36	89563
Bob	M	PhD	EC1A1BA	47	123543
Chloé	F	BEcon	SW1A1BH	26	23989
Daisuke	M	BSc	SE207AT	68	138769
Elisabeth	F	MBA	SE10AA	33	113888

- Row: an instance
- Column: a particular feature
- Apart from tabular format, machine learning can be applied to many types of data, e.g., genomic sequences, text and image contents of a webpage, and social media graphs, citation networks...

- We convert the table into numerical format

Name	Gender	Degree	Postcode	Age	Annual salary
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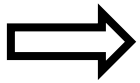

Gender ID	Degree	Latitude (in degrees)	Longitude (in degrees)	Age	Annual Salary (in thousands)
-1	2	51.5073	0.1290	36	89.563
-1	3	51.5074	0.1275	47	123.543
+1	1	51.5071	0.1278	26	23.989
-1	1	51.5075	0.1281	68	138.769
+1	2	51.5074	0.1278	33	113.888

- Gender is quantized to -1 and +1
- Degree from BS, MS to PhD: 1, 2, 3
- Postcode corresponds to Latitude and Longitude on the map
- Name is removed because of privacy and because it does not contain useful information for the machine learning system. (exceptions? See [1])

[1] Chen et al., What's in a Name? First Names as Facial Attributes. CVPR 2013

Figure 4: The top-3 predicted names for some face images. The correct prediction is highlighted in green, while the actual first name is shown in red if it is not ranked within the top-3 predictions. The first 2 rows give some good examples where our top-3 predictions include the actual name, and the bottom 2 rows are randomly selected from our test set. Even when our predictions are wrong, reasonable names are predicted (e.g., appropriate gender or age).

- We use N to denote the number of examples in a dataset and index the examples with lowercase $n = 1, \cdots, N$

Gender ID	Degree	Latitude (in degrees)	Longitude (in degrees)	Age	Annual Salary (in thousands)
-1	2	51.5073	0.1290	36	89.563
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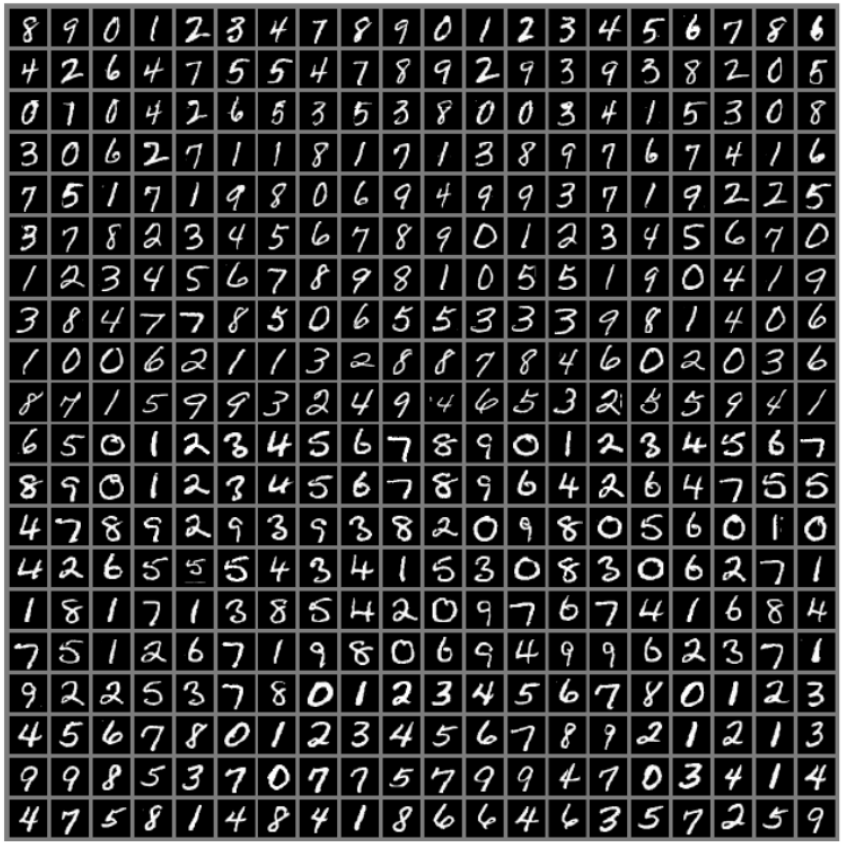
+1	2	51.5074	0.1278	33	113.888

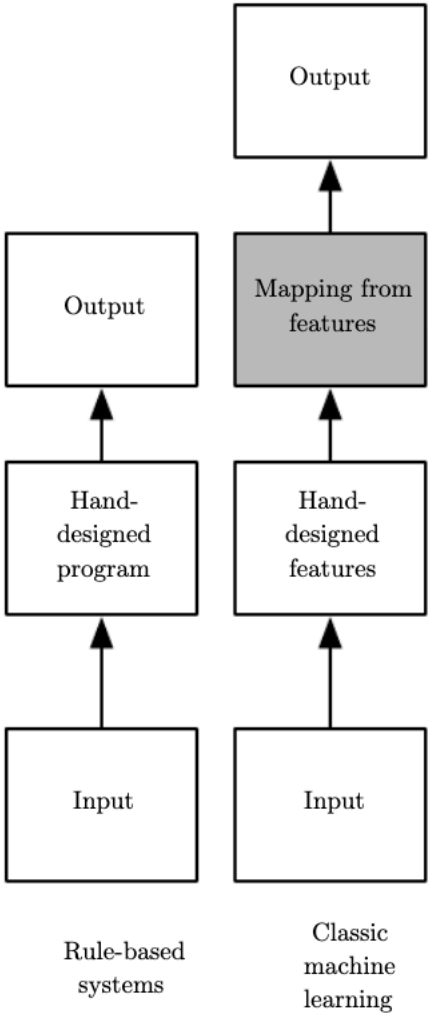
- Each row is a particular individual $\boldsymbol{x}_n$ referred to as an example or data point in machine learning
- The subscript n refers to the fact that this is the nth example out of a total of N examples in the dataset
- Each column represents a particular feature of interest about the example, and we index the features as $d = 1, \cdots, D$
- Each example is a D-dimensional vector

Shaded = learning from data

Classical Machine Learning vs Representation Learning



MNIST dataset, ~70k images



- Consider the problem of predicting annual salary from age

D columns

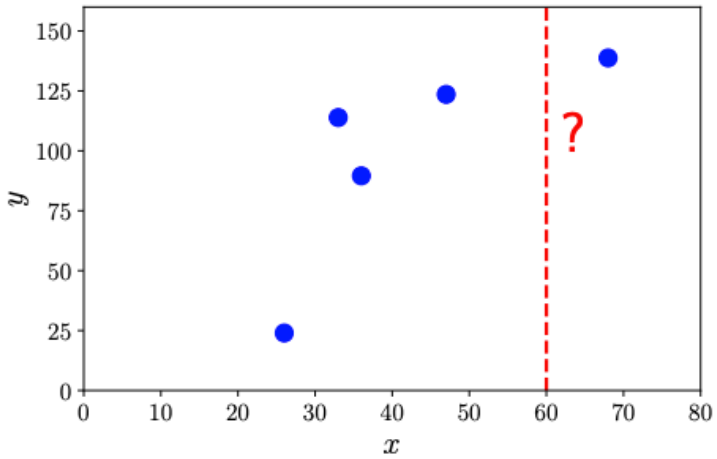
Gender ID	Degree	Latitude (in degrees)	Longitude (in degrees)	Age	Annual Salary (in thousands)
-1	2	51.5073	0.1290	36	89.563
-1	3	51.5074	0.1275	47	123.543
+1	1	51.5071	0.1278	26	23.989
-1	1	51.5075	0.1281	68	138.769
+1	2	51.5074	0.1278	33	113.888

N rows

- A supervised learning algorithm
- We have a label y_n (the salary) associated with each example $\boldsymbol{x}_n$ (e.g., age).
- A dataset is written as a set of example-label pairs $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$
- The table of examples $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ are concatenated and written as $X \in \mathbb{R}^{N \times D}$

We are interested in:

What is the salary (y) at age 60 ($x = 60$)?



x: age

y: salary

8.1.2 Models as Functions

- Once we have data in an appropriate vector representation, we can construct a predictive function (known as a predictor).
- Here, a model means a predictor.
- A predictor is a function that, when given a particular input example (in our case, a vector of features), produces an output.

- For example,

$$f: \mathbb{R}^D \rightarrow \mathbb{R}$$

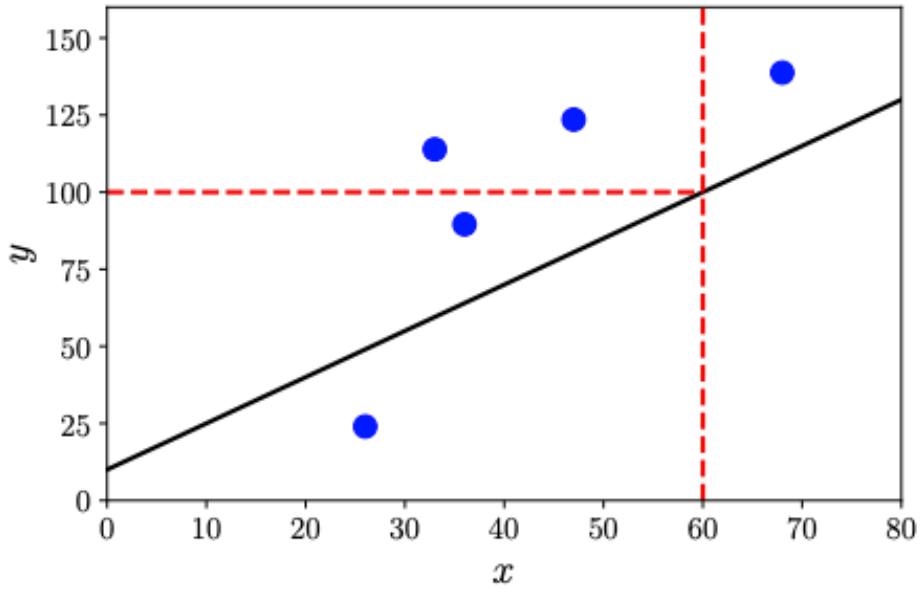
where the input $\boldsymbol{x}$ is a D-dimensional vector, and the output is a real-valued scalar. That is, the function f is applied to $\boldsymbol{x}$, written as $f(\boldsymbol{x})$ and returns a real number.

8.1.2 Models as Functions

- We mainly consider the special case of linear functions

$$f(\boldsymbol{x}) = \boldsymbol{\theta}^T \boldsymbol{x} + \theta_0$$

- Example: predicting salary $f(\boldsymbol{x})$ from age $\boldsymbol{x}$.

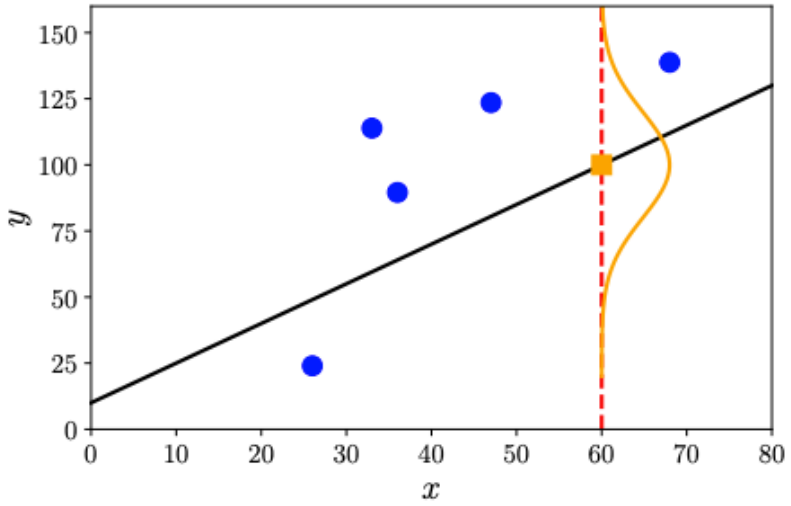


Black and solid diagonal line is an example predictor.

$f(60) = 100$

8.1.3 Models as Probability Distributions

- The observed data is usually a combination of the true underlying data and noise, i.e., $\tilde{x} = x + n$
- We wish to reveal x from $\tilde{x}$
- So we would like to have predictors that express some sort of uncertainty, e.g., to quantify the confidence we have about the value of the prediction for a particular test data point.



Example function (black solid diagonal line) and its predictive uncertainty at $x = 60$ (drawn as a Gaussian).

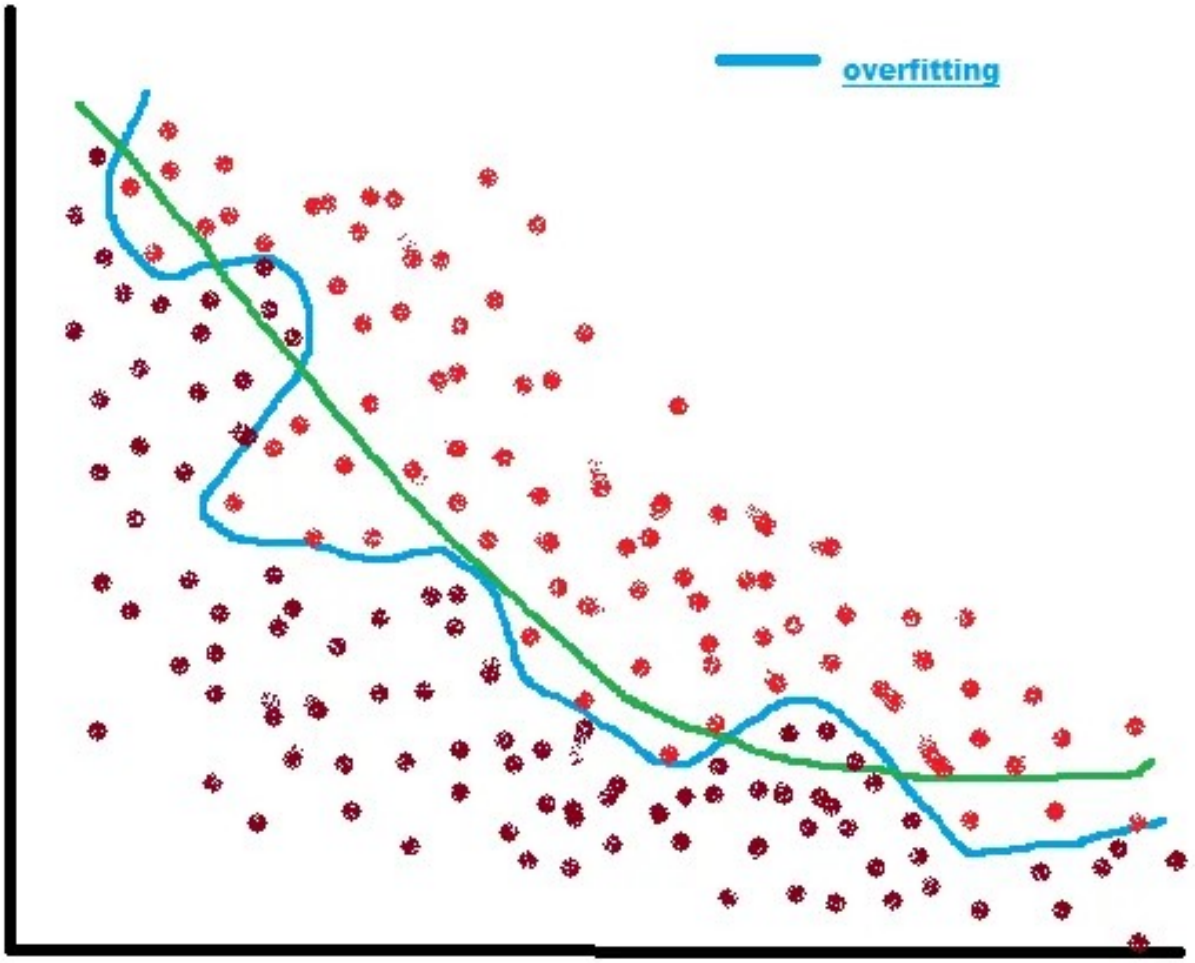
- Instead of considering a predictor as a single function, we could consider predictors to be probabilistic models.
- We will learn probability in later lectures

8.1.4 Learning is Finding Parameters

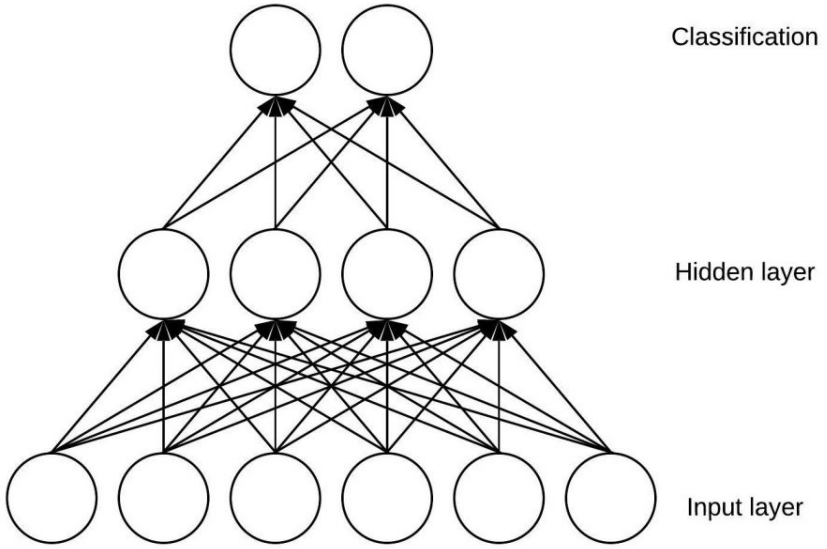
- The goal of learning is to find a model and its corresponding parameters such that the resulting predictor will perform well on unseen data.
- 3 algorithmic phases when discussing machine learning algorithms
- Prediction or inference
- Training or parameter estimation
- Hyperparameter tuning or model selection

- Prediction phase: we use a trained predictor on previously unseen test data
- The training or parameter estimation phase: we adjust our predictive model based on training data. We will introduce the empirical risk minimization for finding good parameters.
- We use cross-validation to assess predictor performance on unseen data.
- We also need to balance between fitting well on training data and finding "simple" explanations of the phenomenon. This trade-off is often achieved using regularization.

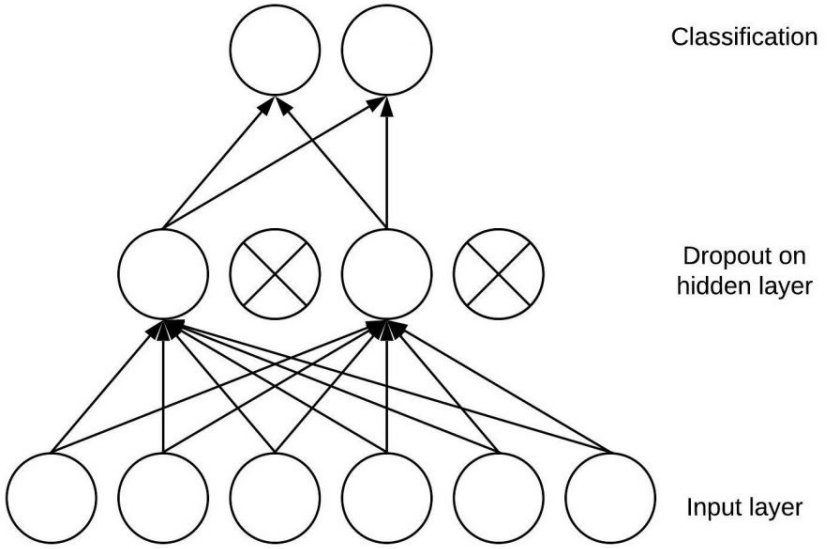
Regularization helps with overfitting.



Regularization in neural networks: dropout.



Without Dropout



With Dropout

Credit: Wenkang Wei

- Hyperparameter tuning or model selection
- We need to make high-level modeling decisions about the structure of the predictor. For example
- Number of layers to be used in deep learning
- Number of components in a Gaussian Mixture Model
- Weight of regularization terms

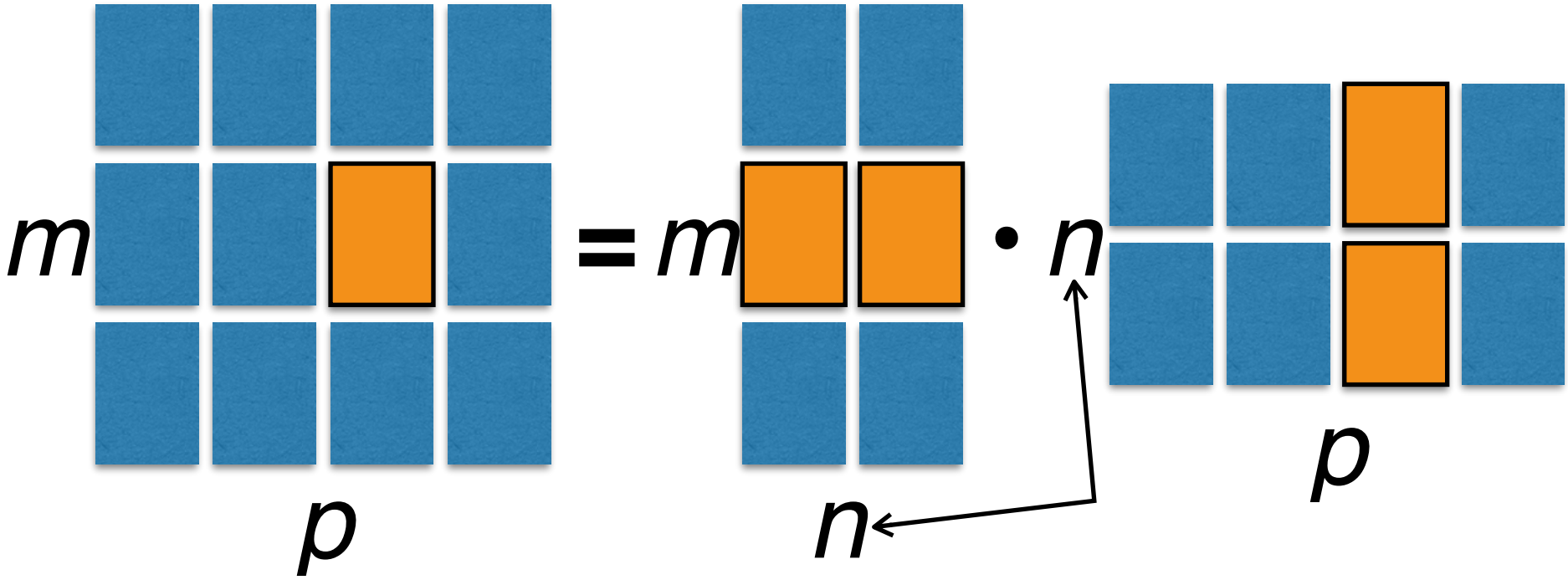
Hyperparameter

- The problem of choosing among different models/hyperparameters is called model selection

- Difference between parameters and hyperparameters
- Parameters are to be numerically optimized ($\sim 10^6$ weights in a deep network)
- Hyperparameters need to use search techniques and validation sets (neural architecture search [2]).

[2] Zoph et al., Neural architecture search with reinforcement learning, Arxiv 2016

Let’s take a break



8.2 Empirical Risk Minimization

- What does it mean to learn?
- Estimating parameters based on training data.
- Four questions will be answered
- What is the set of functions we allow the predictor to take? – Hypothesis class of functions
- How do we measure how well the predictor performs on the training data? -- Loss functions for training
- How do we construct predictors from only training data that performs well on unseen test data? -- regularization
- What is the procedure for searching over the space of models? -- Cross-Validation

8.2.1 Hypothesis Class of Functions

- We are given N examples $\boldsymbol{x}_n \in \mathbb{R}^D$ and corresponding scalar labels $y_n \in \mathbb{R}$.
- Supervised learning: we have pairs $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$
- We want to estimate a predictor $f(\bullet, \boldsymbol{\theta}) : \mathbb{R}^D \to \mathbb{R}$, parametrized by $\boldsymbol{\theta}$
- We hope to be able to find a good parameter $\boldsymbol{\theta}^*$ such that we fit the data well, that is

$$f(\boldsymbol{x}_n, \boldsymbol{\theta}^*) \approx y_n \text{ for all } n = 1, \ldots, N$$

- We use $\hat{y}_n = f(\boldsymbol{x}_n, \boldsymbol{\theta}^*)$ to represent the output of the predictor

Example (least-squares regression)

- When the label y_n is real-valued, a popular choice of function class for predictors is affine functions (linear functions).

$$f(\boldsymbol{x}) = \boldsymbol{\theta}^T \boldsymbol{x} + \theta_0$$

- For more compact representations, we concatenate an additional unit feature $x^{(0)} = 1$ to $\boldsymbol{x}_n$, i.e.,

$$\boldsymbol{x}_n = \left[x_n^{(0)},\ x_n^{(1)}, x_n^{(2)}, \ldots, x_n^{(D)}\right]^{\mathrm{T}} = \left[1,\ x_n^{(1)}, x_n^{(2)}, \ldots, x_n^{(D)}\right]^{\mathrm{T}}$$

- The parameter vector is $\boldsymbol{\theta} = \left[\theta_0, \theta_1, \theta_2, \ldots, \theta_D\right]^T$
- We can write the predictor as follows

$$f\left(\boldsymbol{x}_n, \boldsymbol{\theta}\right) = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{x}_n$$

which is equivalent to the affine model

$$f\left(\boldsymbol{x}_n, \boldsymbol{\theta}\right) = \theta_0 + \sum_{d=1}^{D} \theta_d x_n^{(d)} = \theta_0 x_n^{(0)} + \sum_{d=1}^{D} \theta_d x_n^{(d)} = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{x}_n$$

Example (least-squares regression)

$$f(\boldsymbol{x}_n, \boldsymbol{\theta}) = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{x}_n$$

- The predictor takes the vector of features representing a single example $\boldsymbol{x}_n$ as input and produces a real-valued output,

$$f\colon \mathbb{R}^{D+1} \to \mathbb{R}$$

- $f(\boldsymbol{x}_n, \boldsymbol{\theta}) = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{x}_n$ is a linear predictor
- There are many non-linear predictors, such as the neural networks

8.2.2 Loss Function for Training

- In training, we aim to learn a model that fits the data well.
- To define "fits the data well", we specify a loss function

$$\ell\left(y_n, \hat{y}_n\right)$$

- Input: ground truth label y_n of a training example

  the prediction $\hat{y}_n$ of this training example
- Output: a non-negative number, called loss. It represents how much error we have made on this particular prediction
- To find good parameters θ^*, we need to minimize the average loss on the set of N training examples

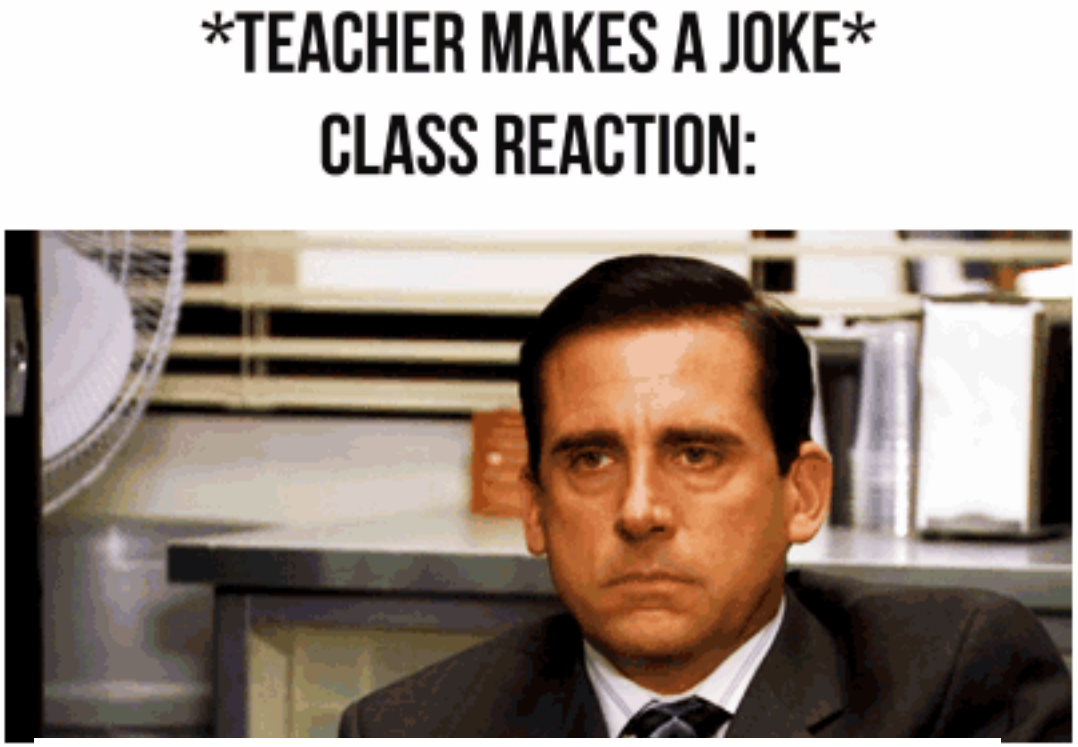
- We usually assume training examples $\left(\boldsymbol{x}_1, y_1\right), \ldots, \left(\boldsymbol{x}_N, y_N\right)$ are independent and identically distributed (i.i.d).

Intuitive example: Learning how to give you the best lecture

5. Which do you prefer?

More Details

Slidesss	60
Blackboard sessions	29
Hybrid for the win	63
Other	3



- Under the i.i.d assumption, the empirical mean is a good estimate of the population mean.
- We can use the empirical mean of the loss on the training data
- Given a training set $\left\{ \left(\boldsymbol{x}_1, y_1 \right), \ldots, \left(\boldsymbol{x}_N, y_N \right) \right\}$, we use the notation of an example matrix

$$\boldsymbol{X} := \left[\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \right]^{\mathrm{T}} \in \mathbb{R}^{N \times D}$$

and a label vector

$$\boldsymbol{y} = \left[y_1, \ldots, y_N \right]^{\mathrm{T}} \in \mathbb{R}^{N}$$

- The average loss is given by

$$\mathbf{R}_{emp}\left(f,\ \boldsymbol{X},\ \boldsymbol{y} \right) = \frac{1}{N} \sum_{n=1}^{N} \ell \left(y_n,\ \hat{y}_n \right)$$

where $\hat{y}_n = f\left(\boldsymbol{x}_n, \boldsymbol{\theta} \right)$. The above equation is called the empirical risk. The learning strategy is called empirical risk minimization.

Example - Least-Squares Loss

- We use the squared loss function

$$\ell\left(y_n, \hat{y}_n\right) = \left(y_n - \hat{y}_n\right)^2$$

- We aim to minimize the empirical risk, which is the average of the losses over the training data.

$$\min_{\theta \in \mathbb{R}^D} \frac{1}{N} \sum_{n=1}^{N} \ell\left(y_n, \hat{y}_n\right) = \min_{\theta \in \mathbb{R}^D} \frac{1}{N} \sum_{n=1}^{N} \left(y_n - f\left(\boldsymbol{x}_n, \boldsymbol{\theta}\right)\right)^2$$

Using the linear predictor $f\left(\boldsymbol{x}_n, \boldsymbol{\theta}\right) = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{x}_n$, we obtain the optimization problem

$$\min_{\theta \in \mathbb{R}^D} \frac{1}{N} \sum_{n=1}^{N} \left(y_n - f\left(\boldsymbol{x}_n, \boldsymbol{\theta}\right)\right)^2$$

- This equation can be equivalently expressed in matrix form

$$\min_{\theta \in \mathbb{R}^D} \frac{1}{N} \left\| \boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta} \right\|^2$$

- This is known as the least-squares problem. There exists a closed-form analytic solution for this by solving the normal equations. We will discuss it in later lectures

- We actually want to find a predictor f that minimizes the expected risk (or the population risk)

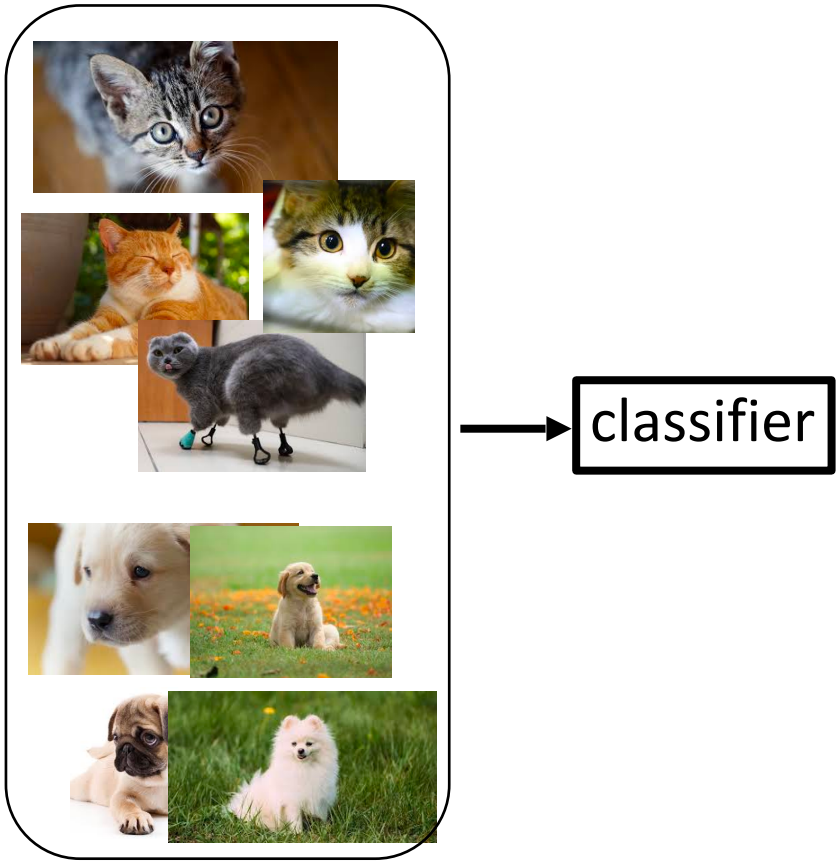
$$\mathbf{R}_{\text{true}}(f) = \mathbb{E}_{x,y}\left[\ell\left(y,\ f(\boldsymbol{x})\right)\right]$$

where y is the ground truth label and $f(\boldsymbol{x})$ is the prediction based on the example $\boldsymbol{x}$.

- $\mathbf{R}_{\text{true}}(f)$ is the true risk, if we can access an infinite amount of data
- The expectation $\mathbb{E}$ is over the infinite set of all possible data and labels.

- Machine learning applications have different types of performance measure.
  - For classification: accuracy, AUC, F1 score, etc.
  - For detection: mean average precision, mIoU, etc.
  - For image denoise/super resolution: SSIM, PSNR, etc.
- In principle, the loss function should correspond to the measure.
- However, there are often mismatches between loss functions and the measures – due to implementation/optimization considerations.

We start with training a classifier



Training data

Deng and Zheng, “Are labels always necessary for classifier accuracy evaluation?” CVPR 2021.

We do a bit testing….

Correct prediction

Testing image → classifier → Dog 0.05, Cat 0.95 → Cat

Prediction result = Ground truth

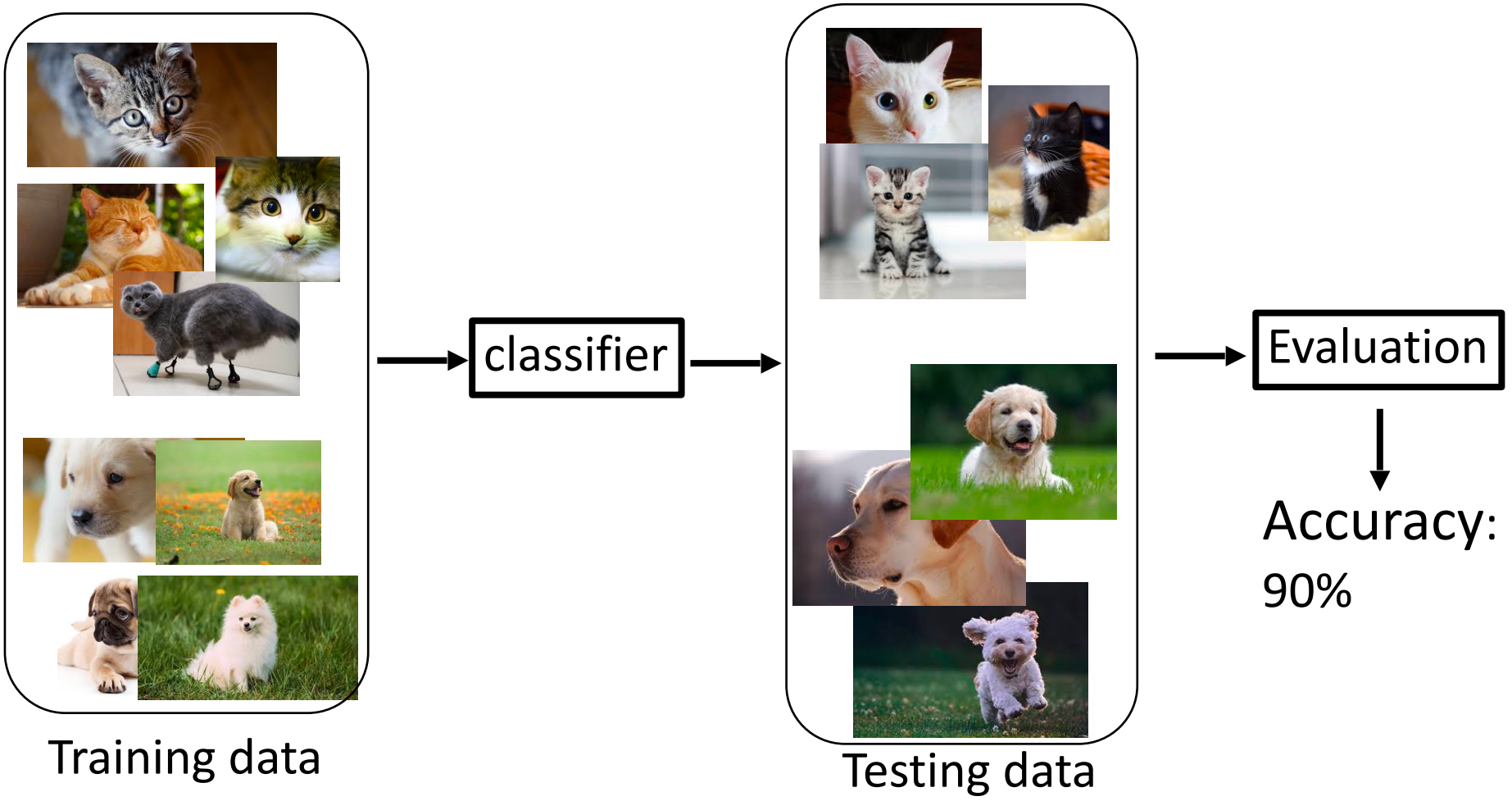
Wrong prediction

Testing image → classifier → Dog 0.85, Cat 0.15 → Cat

Prediction result ≠ Ground truth

Deng and Zheng, “Are labels always necessary for classifier accuracy evaluation?” CVPR 2021.

We now evaluate a model

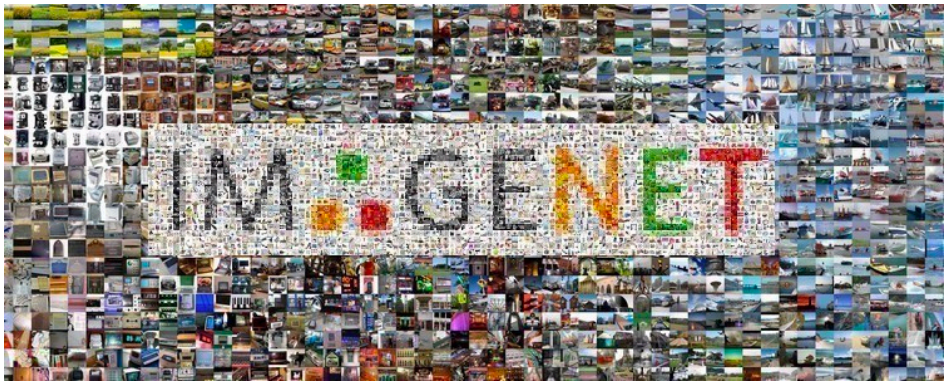


Ground truths provided

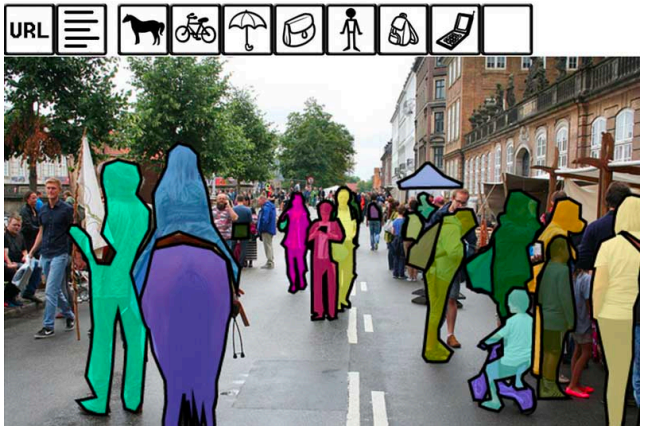
Deng and Zheng, “Are labels always necessary for classifier accuracy evaluation?” CVPR 2021.

Is this way of evaluation feasible?

- Yes



ImageNet



MSCOCO

Ground truths provided

LFW

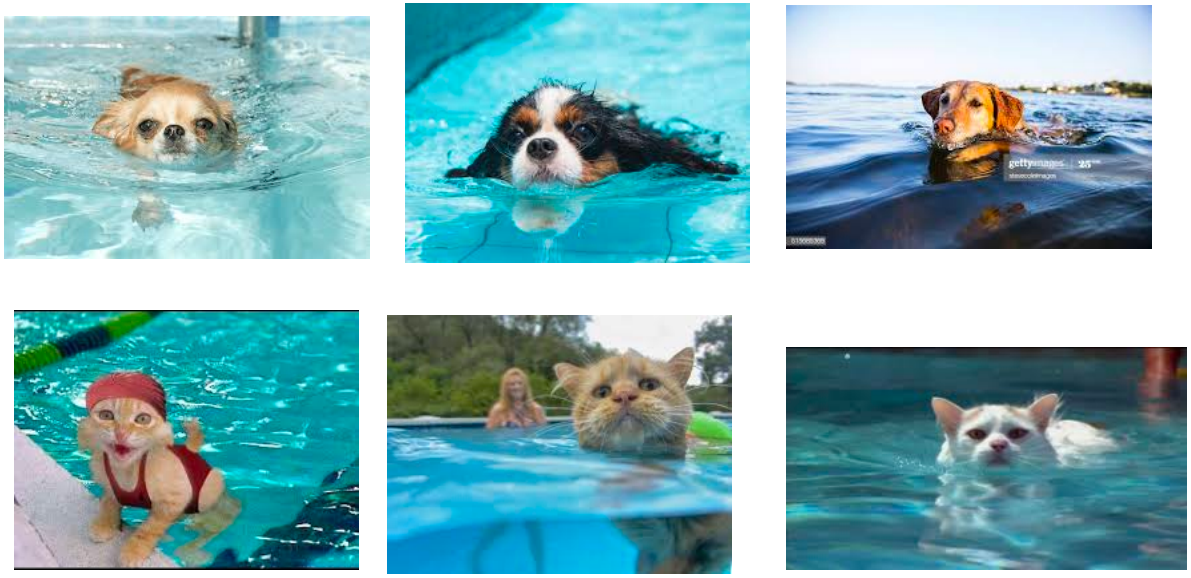
Deng and Zheng, “Are labels always necessary for classifier accuracy evaluation?” CVPR 2021.

Is this way of evaluation feasible?

- No….

We can’t calculate a classifier accuracy!!

Suppose we deploy our cat-dog classifier to a swimming pool



Ground truths not provided

Deng and Zheng, “Are labels always necessary for classifier accuracy evaluation?” CVPR 2021.

Research Bit: finding stars that weren’t born in our Galaxy