# When Models Meet Data

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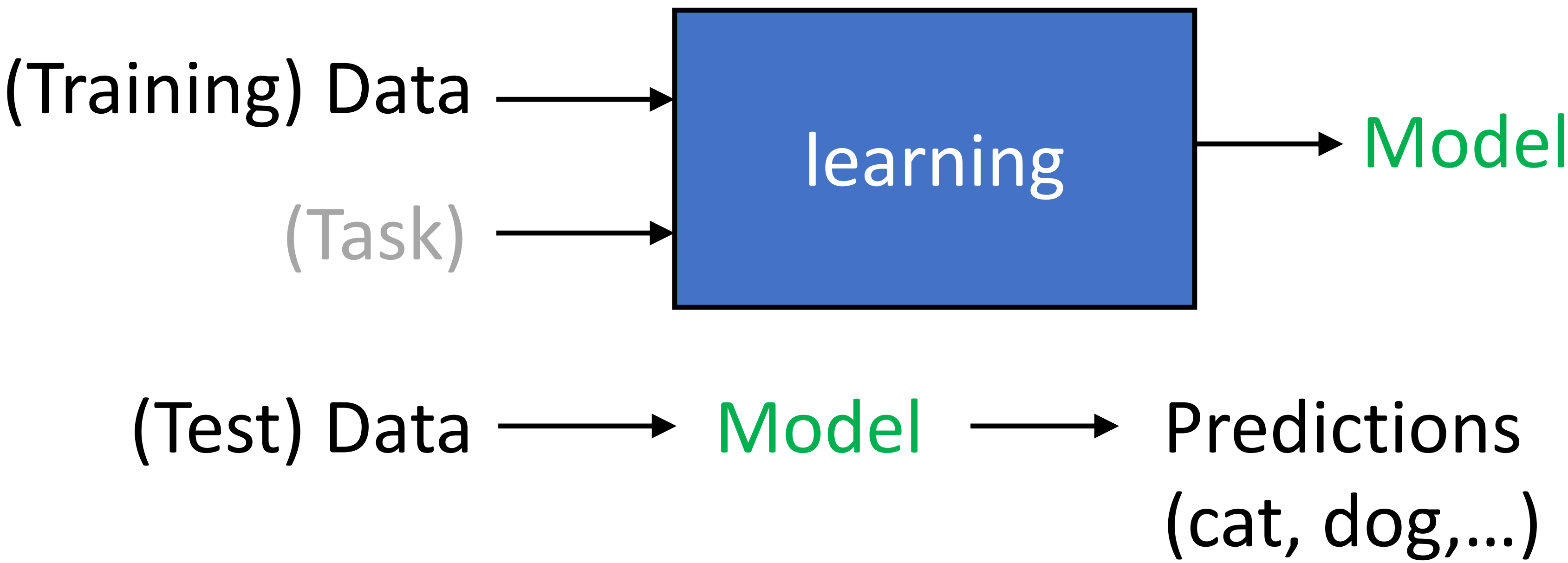
# 8.1 Data, Models, and Learning

- 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

accuracy

- 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 |
|---|---|---|---|---|---|
| Aditya | M | MSc | W21BG | 36 | 89563 |
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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

- 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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- Each row is a particular individual $\boldsymbol{x}_n$ $1-5$ referred to as an example or data point in machine learning
- The subscript $n$ refers to the fact that this is the $n$th 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

- Consider the problem of predicting annual salary from age

$D$ columns

$N$ rows

| 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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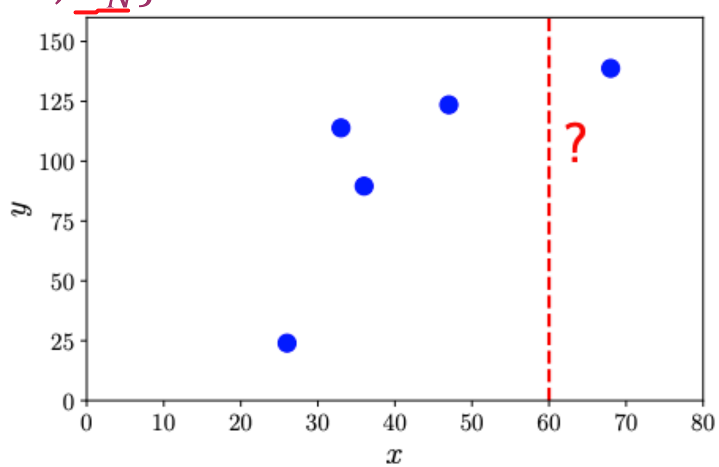
- A supervised learning algorithm
- We have a label $y_n$ (the salary) associated with each example $\boldsymbol{x}_n$ (age).
- A dataset is written as a set of example-label pairs $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n), \dots, (\boldsymbol{x}_N, y_N)\}$
- The table of examples $\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ 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,

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

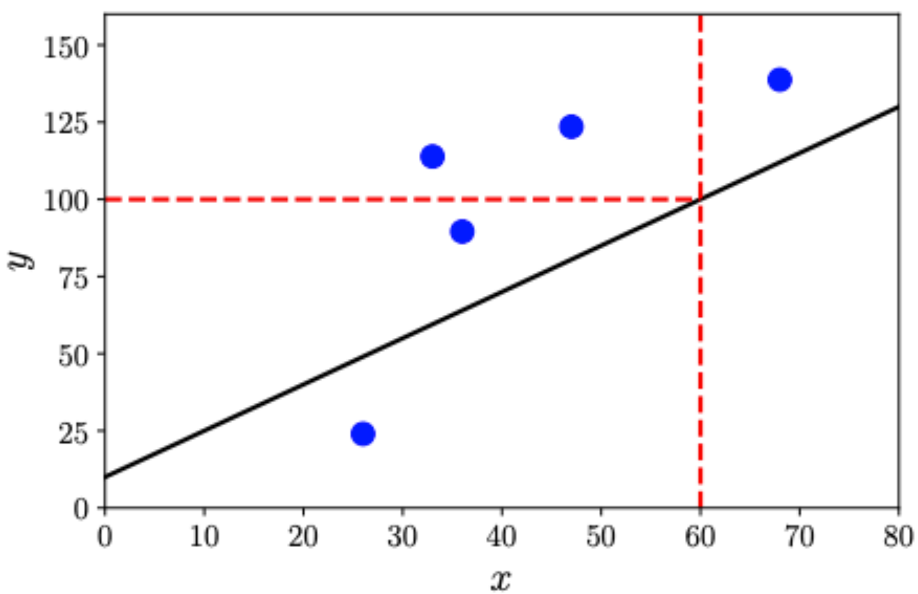
where the input $\boldsymbol{x}$ is a $D$-dimensional vector, and the output is a real-valued scalar. That is, the function $f$ is applied to $\boldsymbol{x}$, written as $f(\boldsymbol{x})$ and returns a real number.

# 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 $\boldsymbol{x}$.

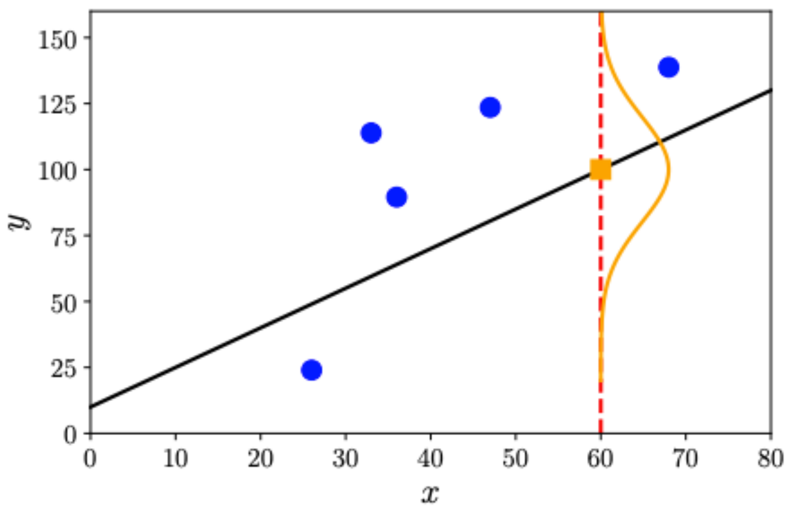



Black and solid diagonal line is an example predictor.

$$f(60) = 100$$

# 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

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- 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.

avoid overfitting

To make the model as simple as possible, otherwise may overfitting

- 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 (neural architecture search [2])

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

# 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

  i.e. models 根据不同的任务选择不同类型的模型，通常根据经验选择
- 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 $f(\cdot, \boldsymbol{\theta}): \mathbb{R}^D \to \mathbb{R}$, 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.,

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

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

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

x, θ ∈D+1

which is equivalent to the affine model

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

# Example (least-squares regression)

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

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

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

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

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

- 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 $\boldsymbol{\theta}^*$, we need to minimize the average loss on the set of $N$ training examples

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

- 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 $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\}$, we use the notation of an example matrix

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

and a label vector

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

- The average loss is given by

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

where $\hat{y}_n = f(\boldsymbol{x}_n, \boldsymbol{\theta})$. 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

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

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

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

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

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

- This equation can be equivalently expressed in matrix form

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

- 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)

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

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

- $\mathbf{R}_{\mathrm{true}}(f)$ 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

# Check your understanding

- A machine learning model may contain as few as a couple of parameters Y
- When we use a linear regression modeling, $f(\boldsymbol{x}) = \boldsymbol{\theta}^T \boldsymbol{x} + \theta_0$, we don't have hyperparameters. This model itself does not, but training process can have
- Hyperparameters are usually learned through the same way as normal parameters. F
- It's very hard to know the expected risk, but easier to know the empirical risk Y
- Given a fixed task, we can only use a fixed set of evaluation metrics. F