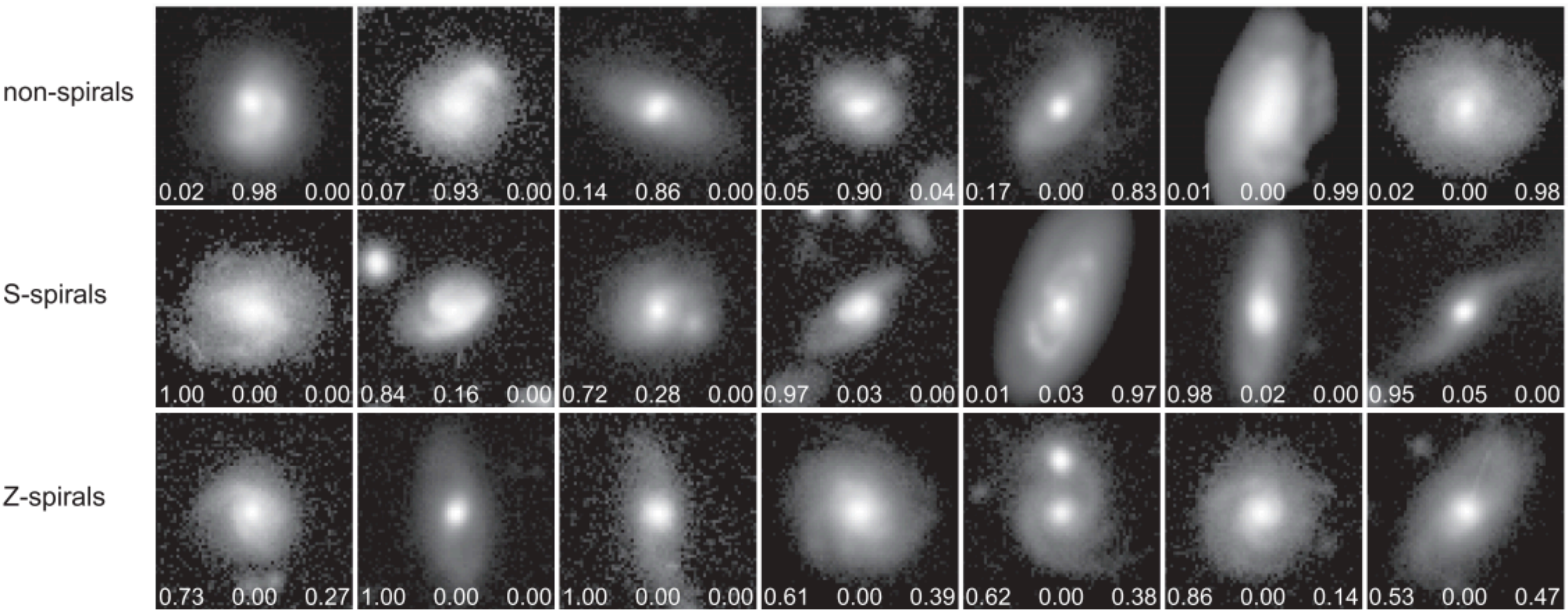
When Models Meet Data

Liang Zheng
Australian National University
liang.zheng@anu.edu.au

Spin parity of spiral galaxies II: a catalogue of 80 k spiral galaxies using big data from the Subaru Hyper Suprime-Cam survey and deep learning
(Tosaki et al., Monthly Notices of the Royal Astronomical Society, 2020)

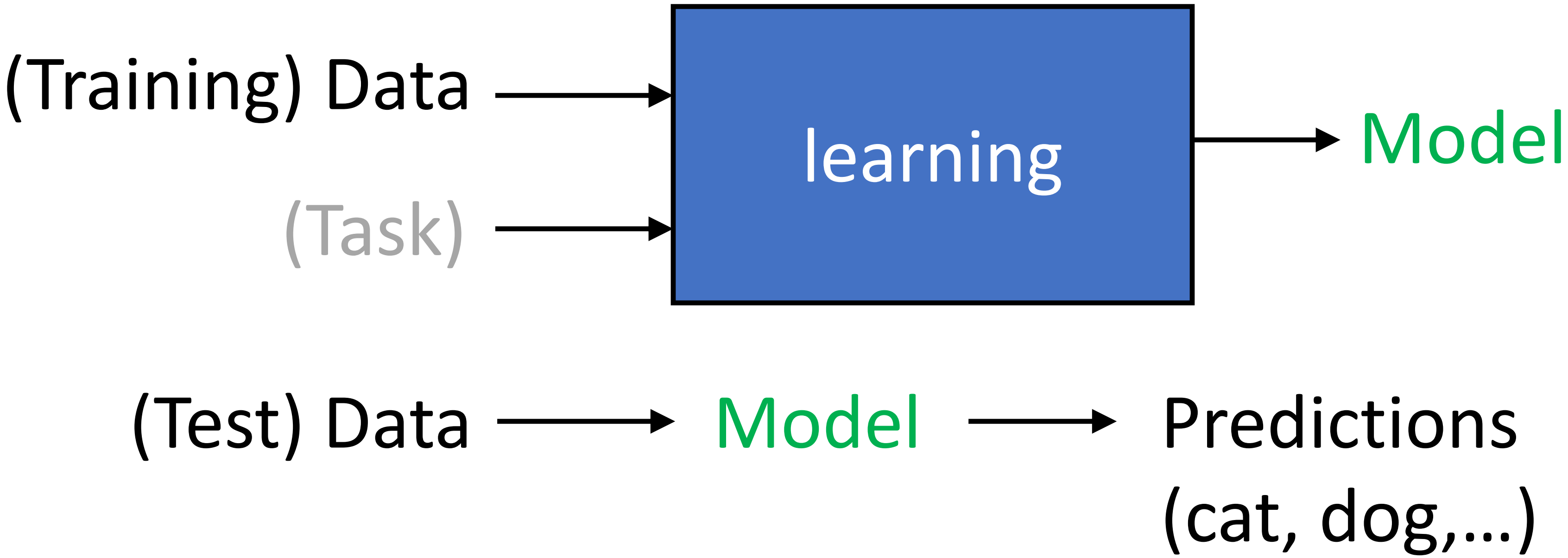
- 560,000 galaxies have been detected in the images captured by the Subaru Telescope
- an accuracy of 97.5%
- it identified spirals in about 80,000 galaxies



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
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

⇨

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
-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

- 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

- Consider the problem of predicting annual salary from age

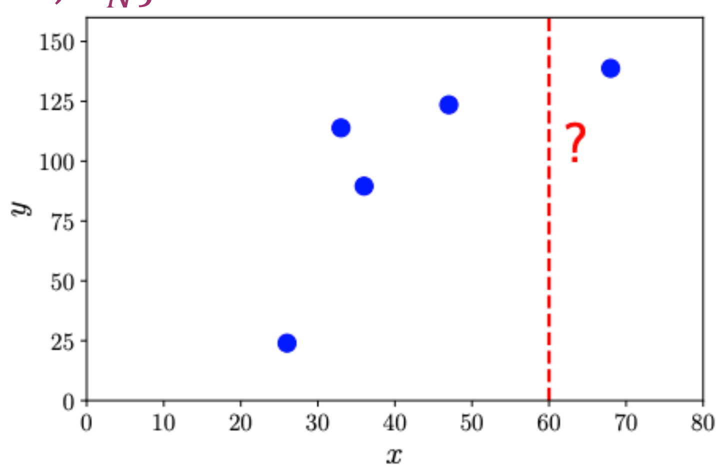
D columns

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
-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

- 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 $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$
- 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,

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

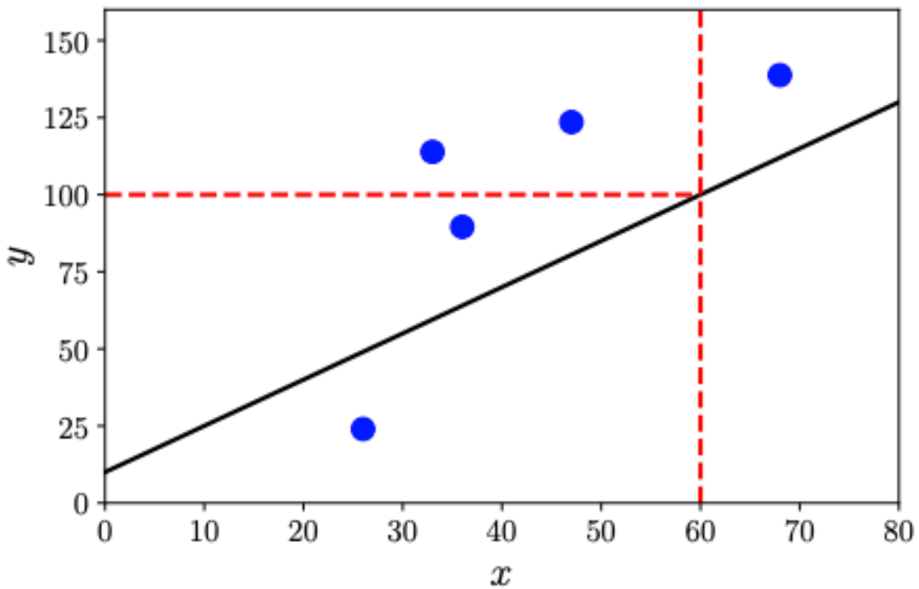
where the input $\boldsymbol{x}$ is a D-dimensional vector, and the output is a real-valued scalar. That is, the function f is applied to $\boldsymbol{x}$, written as $f(\boldsymbol{x})$ and returns a real number.

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 $\boldsymbol{x}$.

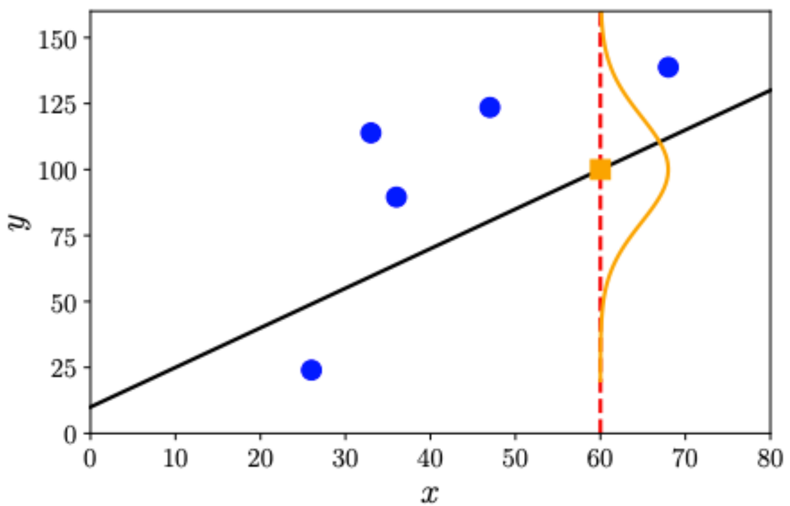


Black and solid diagonal line is an example predictor.

$$f(60) = 100$$

8.1.3 Models as Probability Distributions

- The observed data is usually a combination of the true underlying data and noise, i.e., $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{n}$
- We wish to reveal $\boldsymbol{x}$ from $\tilde{\boldsymbol{x}}$
- 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.

- 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
- 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 $(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)$
- 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

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

- 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.,

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

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

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

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)

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

- 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

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

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

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

  and a label vector

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

- The average loss is given by

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

  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)

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

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

Check your understanding

T
- A machine learning model may contain as few as a couple of parameters

T
- When we use a linear regression modeling, $f(\boldsymbol{x}) = \boldsymbol{\theta}^T \boldsymbol{x} + \theta_0$, we don't have hyperparameters.

F
- Hyperparameters are usually learned through the same way as normal parameters.

T
- It's very hard to know the expected risk, but easier to know the empirical risk

F
- Given a fixed task, we can only use a fixed set of evaluation metrics.