Machine Learning

Lecture 2: Empirical Risk Minimization

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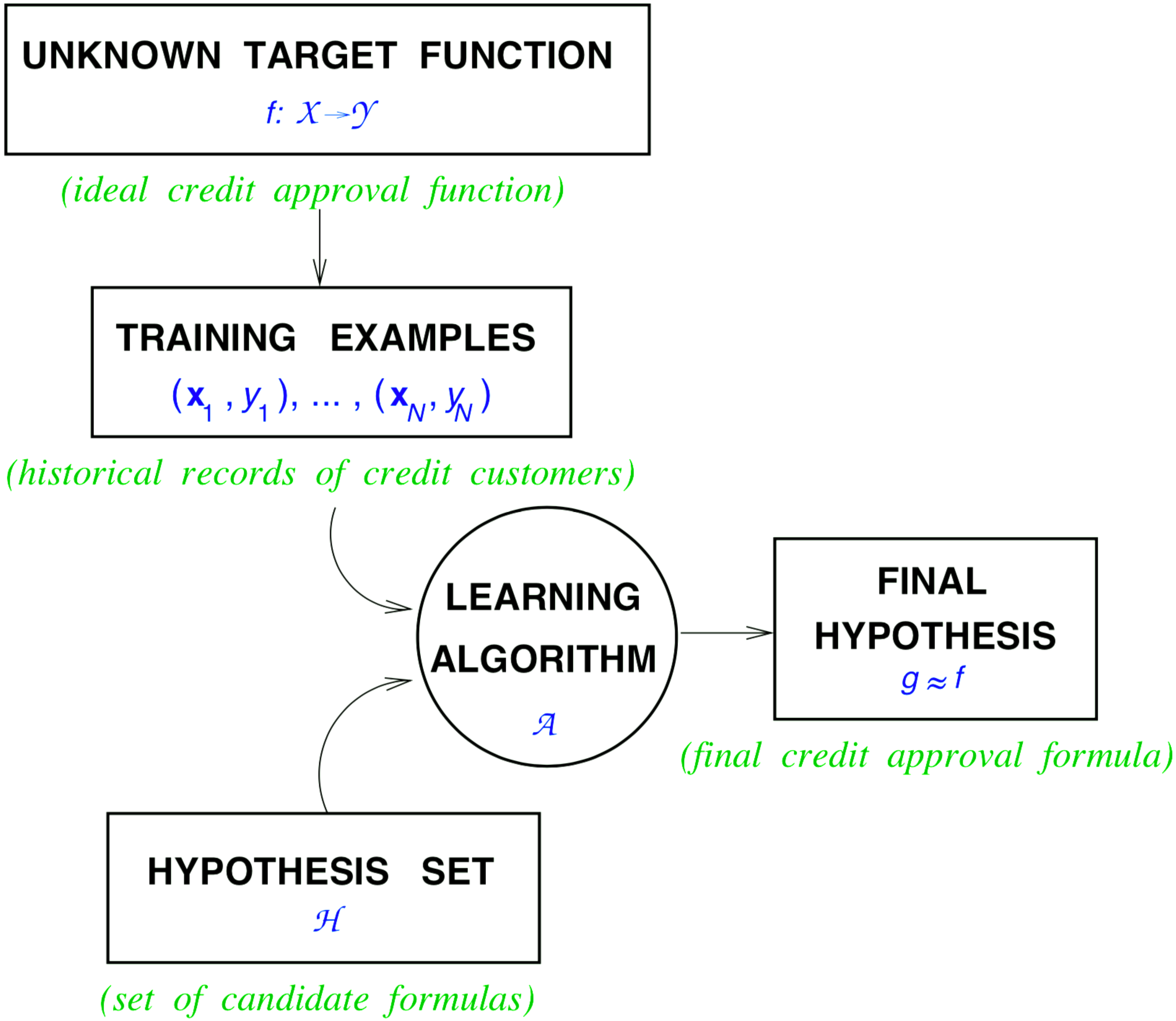
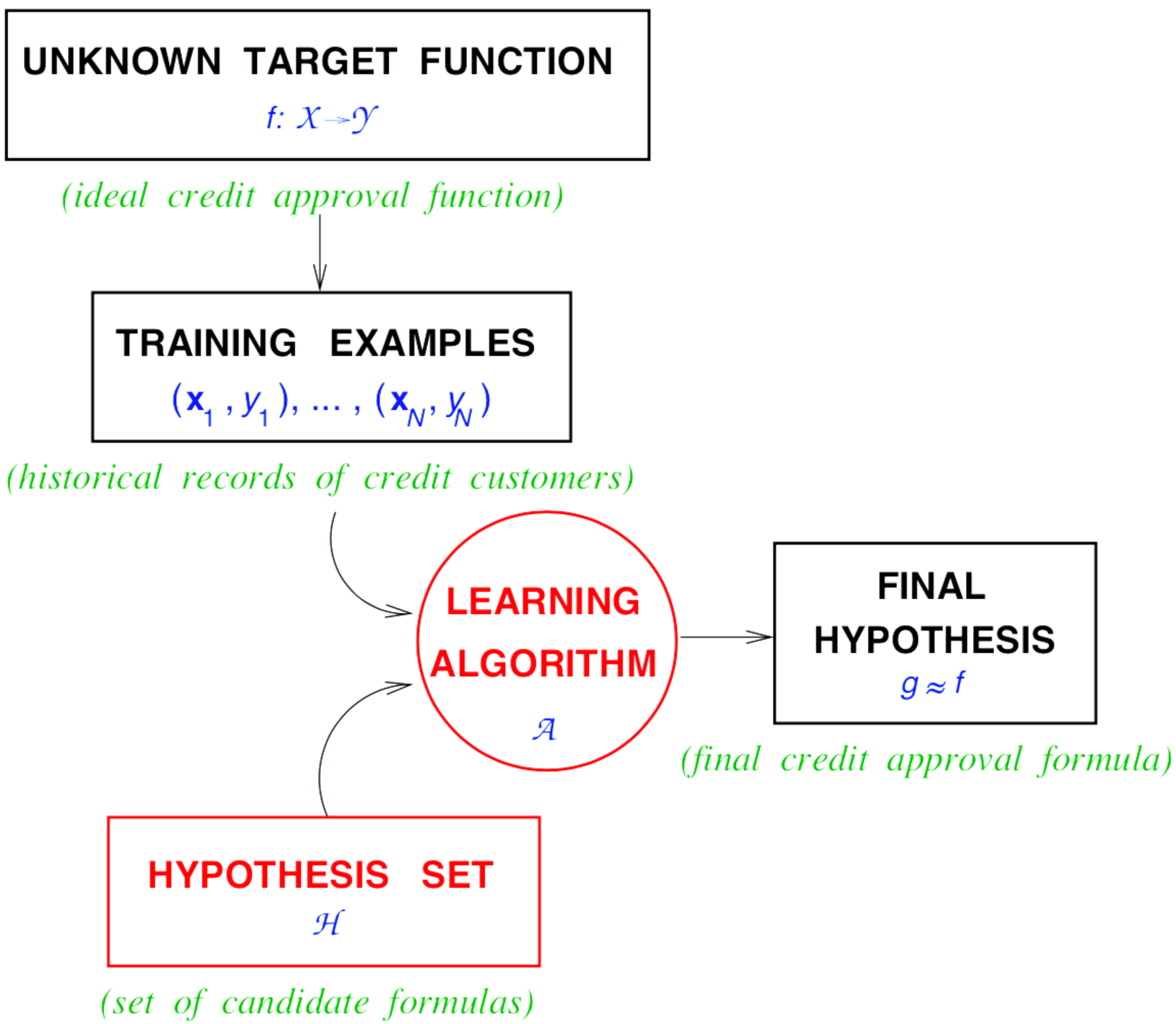
本节内容

- Hypothesis class
- Joint Distribution of Data
- Expected Risk Minimization
- Empirical Risk Minimization

Components of learning



Components of learning



Two solution components of the learning problem:

- The Hypothesis Set:
  $\mathscr{H} = \{h\}, \quad g \in \mathscr{H}$
- The learning algorithm $\mathscr{A}$

Together, they are referred to as the learning model.

Data and Labels

- In learning we seek a mapping from the initial data $\mathscr{X}$ (the domain of abstract input objects) to some label set $\mathscr{Y}$ (anything we want to predict)
- Hypothesis: $h : \mathscr{X} \to \mathscr{Y}$
- Example: in character recognition, $\mathscr{X}$ consists of possible images of letters and $\mathscr{Y}$ consists of the twenty-six letters of the Latin alphabet.
- Note: For simplicity we will use binary labels $\{+1, -1\}$. Whether something is the letter "G" (+1) or not the letter "G" (−1), or whether given image contains a face (+1) or does not contain a face (−1).

Joint Distribution

- Joint distribution $p_{X,Y}(x, y)$

- Future data is coming from some unknown source joint distribution $p_{X,Y}$ over input objects and their corresponding labels, which we write as the joint distribution $p_{X,Y}$, where $X \in \mathscr{X}, Y \in \mathscr{Y}$

- Example: Character recognition source distribution would assign much more probability to ("image containing a circular shape", "O") than to ("image containing a circular shape", "T"). (why?)

Conditional Probability

- Conditional distribution $p_{Y|X}(y\,|\,x)$

- We can define course joint distribution as really having two components

$$p_{XY}(x,y) = p_{Y|X}(y\,|\,x) \cdot p_X(x)$$

- where $p_{Y|X}(y\,|\,x)$ is the conditional probability of the label random variable Y given the appearance random variable and $p_X(x)$ is marginal probability of the input image.

- Example: In character recognition we may have

$$p_{Y|X}(Y = \text{"A"} \mid X = \text{A}) = 0.9$$
$$p_{Y|X}(Y = \text{"O"} \mid X = \text{O}) = 0.6$$
$$p_{Y|X}(Y = \text{"a"} \mid X = \text{a}) = 0.4$$

Training Set and Test Set

- A training set is a set data used to discover potentially predictive relationship.
- A test set is a set of data used to assess the strength and utility of a predictive relationship
- Random split

1	-1	5	7	14	19	39	40	51	63	67	73	74	76
2	-1	3	6	17	22	36	41	53	64	67	73	74	76
3	-1	5	6	17	21	35	40	53	63	71	73	74	76
4	-1	2	6	18	19	39	40	52	61	71	72	74	76
5	-1	3	6	18	29	39	40	51	61	67	72	74	76
6	-1	4	6	16	26	35	45	49	64	71	72	74	76
7	1	5	7	17	22	36	40	51	63	67	73	74	76
8	1	2	6	14	29	39	42	52	64	67	72	75	76
9	1	4	6	16	19	39	40	51	63	67	73	75	76
10	1	3	6	18	20	37	40	51	63	71	73	74	76
11	1	2	11	15	19	39	40	52	63	68	73	74	76
12	-1	1	6	15	19	39	42	55	62	67	72	74	76
13	-1	2	6	17	24	38	42	50	64	71	73	74	76
14	1	3	6	15	25	38	40	48	63	68	73	74	76
15	-1	1	7	16	22	36	42	56	62	67	73	74	76
16	-1	2	6	16	22	36	42	54	66	67	73	74	76
17	-1	3	6	14	21	35	40	50	63	67	73	74	76
18	1	4	7	18	29	39	41	51	66	67	72	74	76
19	1	3	6	16	32	39	40	52	63	67	73	74	76
20	-1	5	6	18	22	36	43	49	66	71	72	74	76
21	-1	3	9	14	26	35	40	56	63	71	73	74	76
22	1	5	10	17	19	39	40	47	63	67	73	74	76
23	-1	1	6	16	22	36	42	48	62	67	73	74	76
24	1	5	16	20	37	40	63	68	73	74	76	82	93
25	-1	3	6	18	22	36	41	51	64	67	73	74	76
26	-1	4	6	16	22	36	40	48	63	67	73	74	76
27	-1	1	10	16	24	38	42	59	64	67	73	74	76
28	-1	1	6	18	20	37	42	50	62	71	73	74	76
29	-1	4	6	18	19	39	41	51	62	67	73	74	77
30	-1	2	9	14	20	37	40	55	62	67	73	74	76
31	-1	1	11	18	20	37	40	49	63	71	73	74	76
32	-1	4	6	17	21	35	42	54	66	67	73	74	76
33	-1	1	6	17	20	37	42	54	62	67	73	74	76
34	-1	1	6	18	22	36	46	55	61	67	72	74	76
35	1	2	6	14	20	37	40	50	63	67	73	74	76
36	-1	4	7	18	24	38	40	52	63	67	73	74	76
37	-1	2	6	18	26	35	40	54	63	67	73	74	76

Hypothesis and loss (cost/risk) function

- Hypothesis h: A hypothesis (a predictor) h is a function from $\mathscr{X}$ to $\mathscr{Y}$, $h : \mathscr{X} \to \mathscr{Y}$

- Loss function $\text{loss}(h(x), y)$: How we can evaluate the performance of h on a given (input, label) pair (x, y)

- Example: If the label $h(x)$ does not match the provided label y, we incur a loss of 1 and if the prediction $h(x)$ does match the provided label y, we incur 0 loss.

- The loss function that represents this measure of performance is called the 01 loss and defined as

$$\text{loss}(h(x), y) = \begin{cases} 1 & \text{if } h(x) \neq y \\ 0 & \text{if } h(x) = y \end{cases}$$

Hypothesis class/set/space

- Define $\mathscr{H}$ as a set of predictors, written as $\mathscr{H} = \{h : \mathscr{X} \to \mathscr{Y}\}$.
- Example: Consider binary labels, so the label set is $\mathscr{Y} = \{+1, -1\}$. In addition, we may consider $\mathscr{X} = \mathbb{R}^2$
- Some specific examples of hypothesis classes:
  $\mathscr{H} = \{\text{sign}(w^T x + b) \mid w \in \mathbb{R}^2, b \in \mathbb{R}\}$
  $\mathscr{H} = \{ \sum_{i=1}^{2} x_i \leq \theta \mid \theta \in \mathbb{R}_+\}$
- In a learning problem, we restrict hypotheses in a certain class.

Expected risk/loss/cost

- Expected Risk $R[h]$
- How well we expect to do (on average) over the entire (admittedly known) source joint distribution $p_{X,Y}(x, y)$?
- The expected risk $R[h]$ of a hypothesis h on that distribution, measures the performance of this hypothesis by evaluating its expected loss over pairs (x, y) drawn from the distribution

$$\boxed{R[h] = \mathbb{E}_{(X,Y)\sim p_{X,Y}}[\text{loss}(h(x), y)] = \sum_{X,Y} p(x, y)\text{loss}(h(x), y)}$$

- Note that the randomness comes from the data...
- Other terms with the same meaning are *expected loss, generalization error, or source-distribution risk*

Additional property of expected risk

- A predictor h is "good" on a particular source joint distribution if it has low risk $R[h]$ on that distribution

- The expected risk $R[h]$ is the probability that the predictor h will incorrectly predict the label for any pair (x, y) drawn at random from the source joint distribution:

$$R[h] = \mathbb{E}_{(X,Y)\sim p_{X,Y}}[\text{loss}(h(x), y)] = \mathbb{P}_{(X,Y)\sim p_{X,Y}}\{h(X) \neq Y\}$$

- This equivalence between the risk and the probability of incorrect label prediction holds only for this 0,1 loss

- We will be assuming that the source joint distribution is fixed

The Learning Process (Ideal Case)

Learning from a function from examples! Given

- Domain $\mathscr{X}, \mathscr{Y}$
- The target function f. (unknown)
- $\mathscr{H}$: Hypothesis set; the set of all possible hypotheses
- Extrapolated observed ys over all $x \in \mathscr{H}$
- Final hypothesis (your predictor/model): $g \approx f$
- Ideal case: g is obtained by minimizing $R[h]$

$$g = \arg\min_{h} \quad R[h], \quad h \in \mathscr{H}$$

Expected risk minimizer

$$g = \arg\min_{h \in \mathscr{H}} \mathbb{E}_{(X,Y)\sim p_{X,Y}}[\text{loss}(h(x), y)]$$

- We want to find a predictor that minimizes the expected loss on the true joint distribution, but⋯
- We do not have complete knowledge of the true source joint distribution
- We should choose our predictor to minimize the expected loss on what we do have access to
- We hope that this predictor will do well on the true source joint distribution (However⋯)

Empirical risk minimizer

- The expected loss of a predictor h on a particular observed sample data set $\mathscr{D} = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ could also be referred to as the empirical risk

$$\hat{R}_{\mathcal{D}}[h] = \frac{1}{m}\sum_{i=1}^{m}[\mathsf{loss}(h(x_i), y_i)] = \frac{1}{m}\sum_{i=1}^{m}\{h(x_i) = y_i\}$$

- Usually, the target predictor is found by

$$\hat{h} = \mathsf{arg}\min_{h} \ \hat{R}_{\mathcal{D}}[h], \qquad h \in \mathcal{H}$$

- Parameterize $h(\,\cdot\,;\theta) \iff \theta$

$$\hat{\theta} = \mathsf{arg}\min_{\theta} \ R_{\mathcal{D}}[\theta], \qquad \theta \in \ \Theta$$

Goal of Machine Learning

- The core of machine learning deals with representation and generalization:
- Representation (Explanation) of data instances and functions evaluated on these instances are part of all machine learning systems
- Generalization (Prediction) is the property that the system will perform well on unseen data instances

Notes:

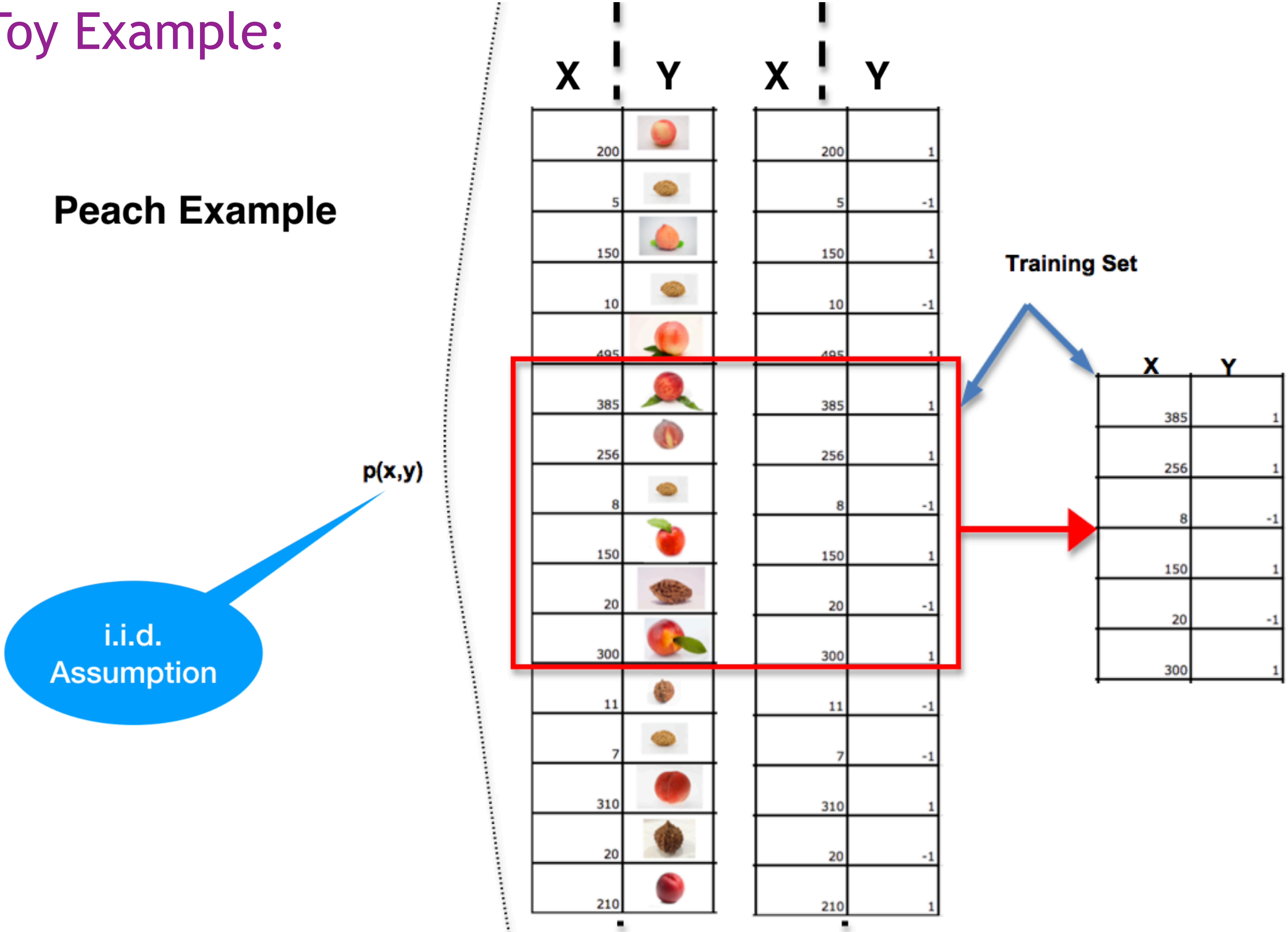
- Are we done with Empirical Risk Minimization?
- Remember the ultimate goal is ***Expected Risk Minimization***
- In Empirical Risk Minimization, we use

$$\boxed{\sum_{i=1}^{m} \text{loss}(h(x_i), y_i; \theta) \text{ to approximate } \mathbb{E}[\text{loss}(h(x), y)]}$$

- When is this a good approximation (good generalization)?
- What if it's not a good approximation (bad generalization)?

These are key questions we are to answer in this class!!!

Toy Example:



Question: Why we need i.i.d. throughout this course?

Machine Learning Procedures

Hypothesis (Prediction function): $h_\theta(x) = \mathrm{sign}(x - \theta)$, parameterize by θ

Training set

385	1
256	1
8	-1
150	1
20	-1
300	1

$h_{30}(x) = \mathrm{sign}(x - 30)$

1	0
-1	0
1	0
-1	0
1	0
1	0

$h_{200}(x) = \mathrm{sign}(x - 200)$

1	0
-1	0
1	0
-1	0
-1	1
1	0

Loss Function: $\mathrm{loss}(h(x), y) = (h(x) - y)^2$

On average over training set: $\mathrm{loss}(h(x), y) = \frac{1}{m}\sum_{i=1}^{m}(h(x_i) - y_i)^2$
(training error, empirical risk, in-sample error)

$\mathrm{loss}(h_{30}(x), y) = 0 \quad \mathrm{loss}(h_{200}(x), y) = 1/6$

Sample Space $p(x,y)$

200	1	**-1**	1
5	-1	**1**	1
150	1	**1**	0
10	-1	**1**	1
405	1	**1**	0
385	1	**1**	0
256	1	**1**	0
8	-1	**1**	1
150	1	**1**	0
20	-1	**1**	1
300	1	**1**	0
11	-1	**1**	1
7	-1	**1**	1
310	1	**1**	0
20	-1	**1**	1
210	1	**1**	0

⋮

Training Set

$$\theta = 200, \quad h_{200}(x) = \text{sign}(x - 200)$$

Expected loss on the entire sample space:

$$\mathbb{E}[\text{loss}(h(X),\, Y)] = \int \text{loss}(h(x), y) \cdot p(x, y)\;\, d(x, y)$$

(generalization error, expected risk, out-of-sample error)

What is our Hypothesis Set?

$$\mathcal{H} = \{h(x;\theta) \mid 0 \leq \theta \leq 500\}$$

What is the best (optimal) θ value?

- The "key (ultimate) goal" in machine learning is to answer this question.
- Obviously, the "best θ" should be the value minimizing $\mathbb{E}[\text{loss}(h(X;\theta),\, Y)]$.
- This is called *expected risk minimization*

Expected Risk Min v.s. Empirical Risk Min

- Expected Risk Minimization

$$\min_h \ \mathbb{E}[\text{loss}(h(X), Y)] \quad \text{s.t. } h \in \mathcal{H} \quad \rightarrow \quad \text{parameterize...}$$

$$\min_\theta \ \mathbb{E}[\text{loss}(h(X;\theta), Y)] = \min_\theta \int \text{loss}(h(x;\theta), y) \cdot p(x,y) \ d(x,y)$$

However, generally we can't do this….why?

- Empirical Risk Minimization

$$\min_h \ \frac{1}{m}\sum_{i=1}^{m}[\text{loss}(h(x_i), y_i)] \quad \text{s.t. } h \in \mathcal{H} \quad \rightarrow \quad \text{parameterize...}$$

$$\min_\theta \ \frac{1}{m}\sum_{i=1}^{m}[\text{loss}(h(X;\theta), Y)] \quad \text{s.t. } 0 \le \theta \le 500$$