Artificial Intelligence csc 665

Machine Learning II

4.16.2024

- Search: make decisions by looking ahead
- Logic: deduce new facts from existing facts
- Constraints: find a way to satisfy a given specification
- Probability: reason quantitatively about uncertainty
- Learning: make future predictions from past observations

Framework: empirical risk minimization

Goal: reproduce a mapping from inputs to outputs given a training set of example input-output pairs.

- Representation: How will we model the relationship between inputs and outputs?
- Cost: How will we evaluate whether we're successfully modeling the input-output relationship?
- **Optimizer:** How will we find the best possible (costminimizing) model among all possible choices given our representation?

Modeling

Inference

ERM, mathematically

Goal: approximate a function $f: \mathcal{X} \to \mathcal{Y}$ from features to labels given a training set of examples $(x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_n, f(x_n)).$

- **Representation:** The hypothesis class \mathcal{H} consisting of all possible candidates to approximate f. E.g. the set of all linear functions $\mathcal{H} = \{x \mapsto wx + b \mid w, b \in \mathbb{R}\}.$
- Cost: A function $C: \mathcal{H} \to \mathbb{R}$ that scores elements of the hypothesis class (higher cost is worse). Often the sum of pointwise costs on the data set, i.e. $\sum_{i=1}^{n} c(h(x_i), f(x_i))$ for some function $c: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$. E.g. squared error $c(\hat{y}, y) = (\hat{y} y)^2$.
- **Optimizer:** An algorithm for finding a hypothesis $h \in \mathcal{H}$ that minimizes C(h). \mathcal{H} is usually infinite, so you can't check all hypotheses. E.g. gradient descent.

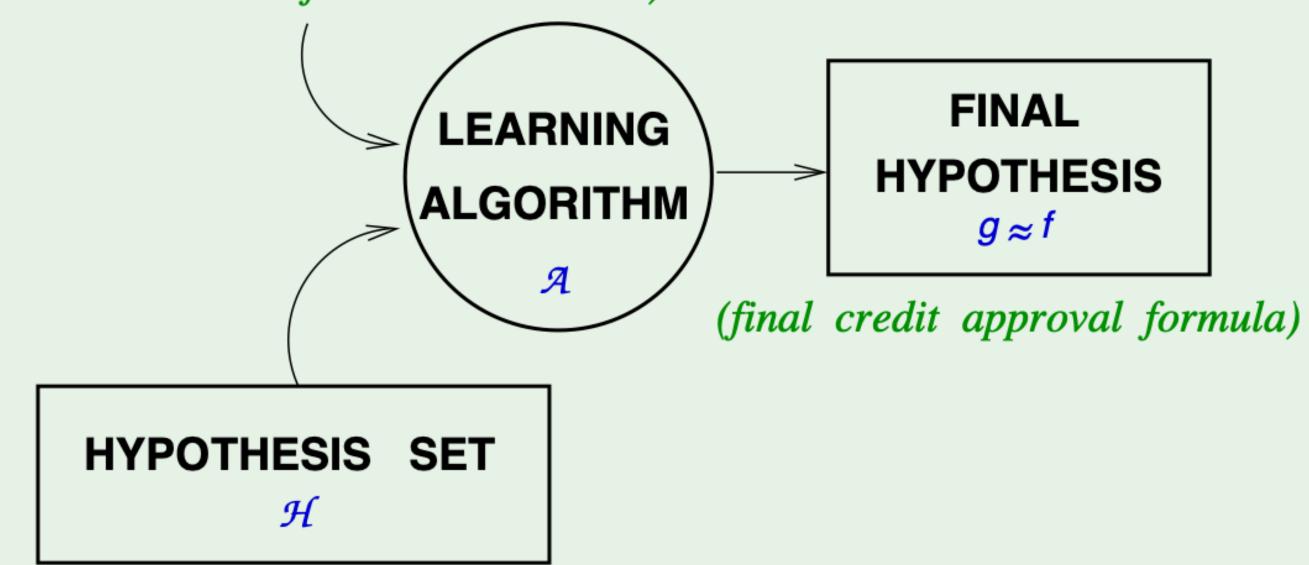
UNKNOWN TARGET FUNCTION

(ideal credit approval function)

TRAINING EXAMPLES

$$(\mathbf{x}_{1}, y_{1}), \dots, (\mathbf{x}_{N}, y_{N})$$

(historical records of credit customers)

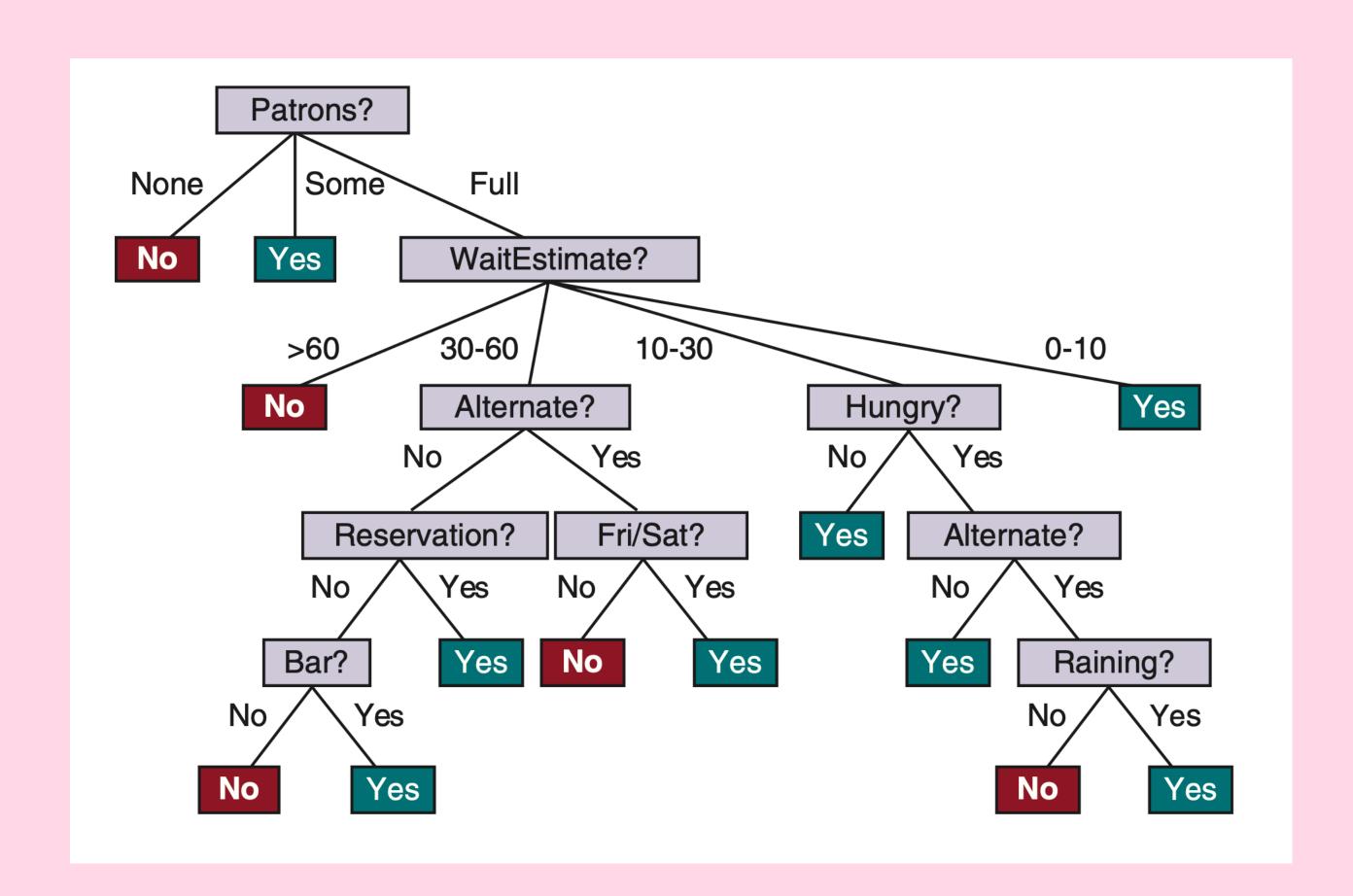


(set of candidate formulas)

Modeling

Hypothesis class: decision trees

- Internal nodes test a particular feature and branch based on the feature value
- Leaf nodes correspond to label predictions
- Decision trees are highly expressive
- Small trees can be easy to interpret, and mimic algorithms people might use to make decisions



Inference

Evaluating decision trees

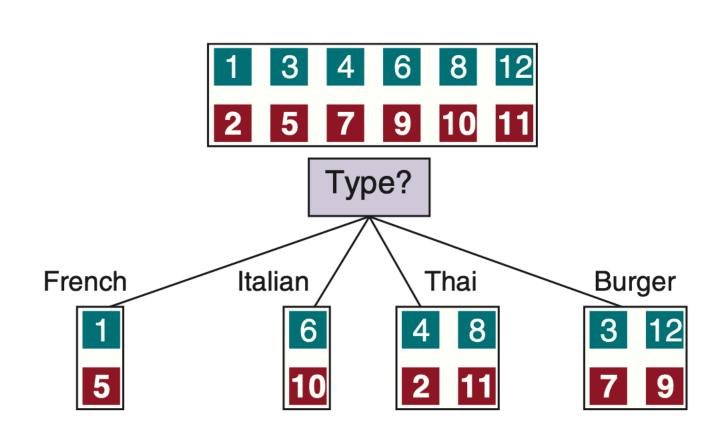
- How do we know if a decision tree is fitting the data well?
- One simple cost function: the proportion of misclassified examples $C(h) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \{h(x_i) \neq f(x_i)\}.$ Also known as the *classification error rate*.
- The term inside the sum is often called 0-1 loss

Example: waiting for a restaurant

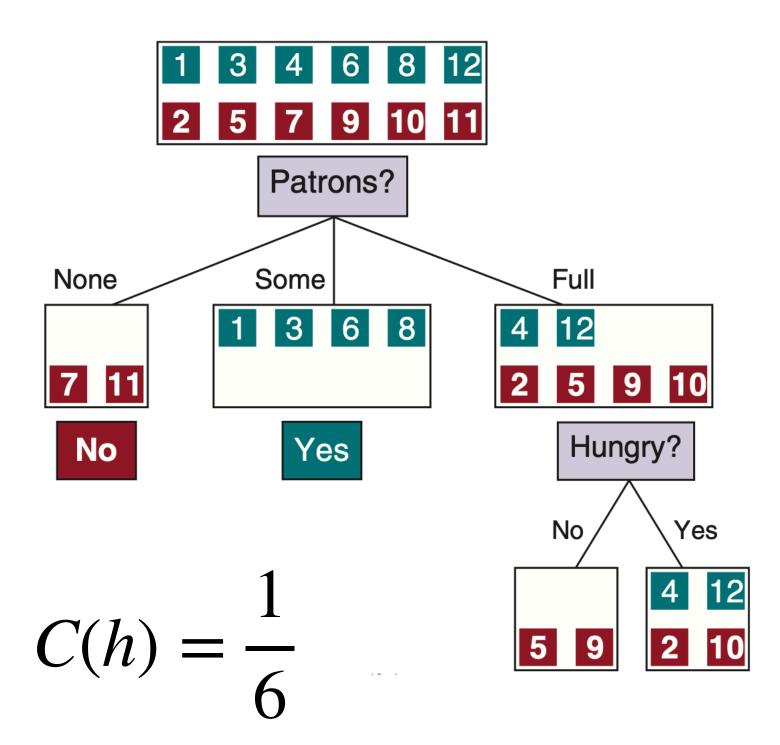
Example	Input Attributes										Output
P	$\overline{\ \ \ }$ Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
\mathbf{x}_1	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0–10	$y_1 = Yes$
\mathbf{x}_2	Yes	No	No	Yes	Full	\$	No	No	Thai	<i>30–60</i>	$y_2 = No$
\mathbf{x}_3	No	Yes	No	No	Some	\$	No	No	Burger	0–10	$y_3 = Yes$
\mathbf{x}_4	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10–30	$y_4 = Yes$
\mathbf{x}_5	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	$y_5 = No$
\mathbf{x}_6	No	Yes	No	Yes	Some	<i>\$\$</i>	Yes	Yes	Italian	0–10	$y_6 = Yes$
X 7	No	Yes	No	No	None	\$	Yes	No	Burger	0–10	$y_7 = No$
X 8	No	No	No	Yes	Some	<i>\$\$</i>	Yes	Yes	Thai	0–10	$y_8 = Yes$
X 9	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	$y_9 = No$
\mathbf{x}_{10}	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10–30	$y_{10} = No$
\mathbf{x}_{11}	No	No	No	No	None	\$	No	No	Thai	0–10	$y_{11} = No$
\mathbf{x}_{12}	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30–60	$y_{12} = Yes$

Evaluating decision trees

$$C(h) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \{ h(x_i) \neq f(x_i) \}$$



$$C(h) = \frac{1}{2}$$

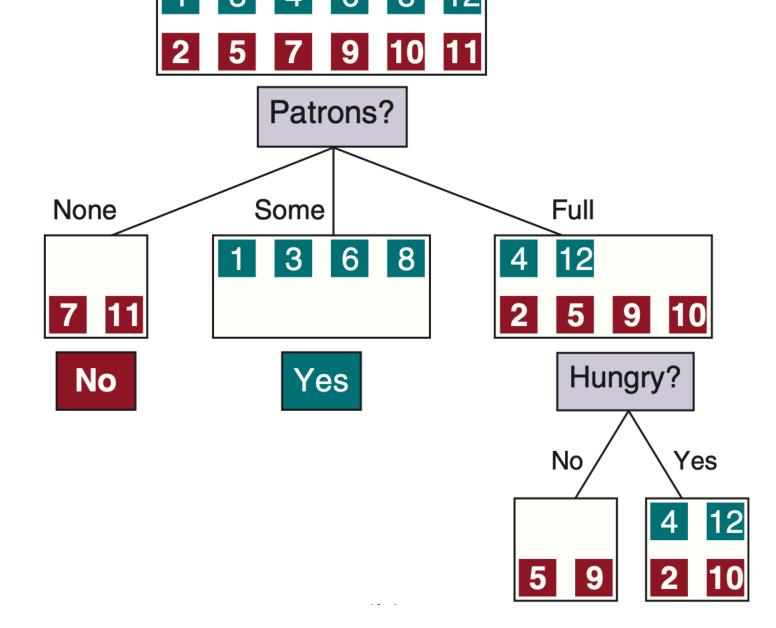


Fitting decision trees

- Want a decision tree with small misclassification rate on the training set
- Want a small tree (why?)
- How many possible decision trees are there?
- For categorical features, number of trees is finite but combinatorially large; impossible to try them all
- Finding the smallest possible tree that is perfectly consistent with the training data is an NP-hard problem
- Need to rely on heuristics to build the tree

Heuristic fitting algorithm

- Pick the feature with the most discriminative power, i.e. the one that separates the training examples into groups that are as pure as possible
- For each child node of this internal node:
 - If all the examples have the same class,
 done
 - Otherwise,* recurse



^{*}Ignoring some edge cases: no examples in a child node, no more features left to use

Restaurant problem via ERM

Goal: approximate $f: \mathcal{X} \to \mathcal{Y}$ given $(x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_n, f(x_n)).$

- Representation: Hypothesis class ${\mathcal H}$
- Cost: A function $C: \mathcal{H} \to \mathbb{R}$ that scores hypotheses, often the sum of pointwise costs, i.e. $\sum_{i=1}^{n} c(h(x_i), f(x_i))$ for some function $c: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$.
- Optimizer: An algorithm for finding an $h \in \mathcal{H}$ that minimizes C(h).

 \mathcal{X} is the set of all possible combinations of feature values (hungry, raining, restaurant type, etc.). $\mathcal{Y} = \{0,1\}$.

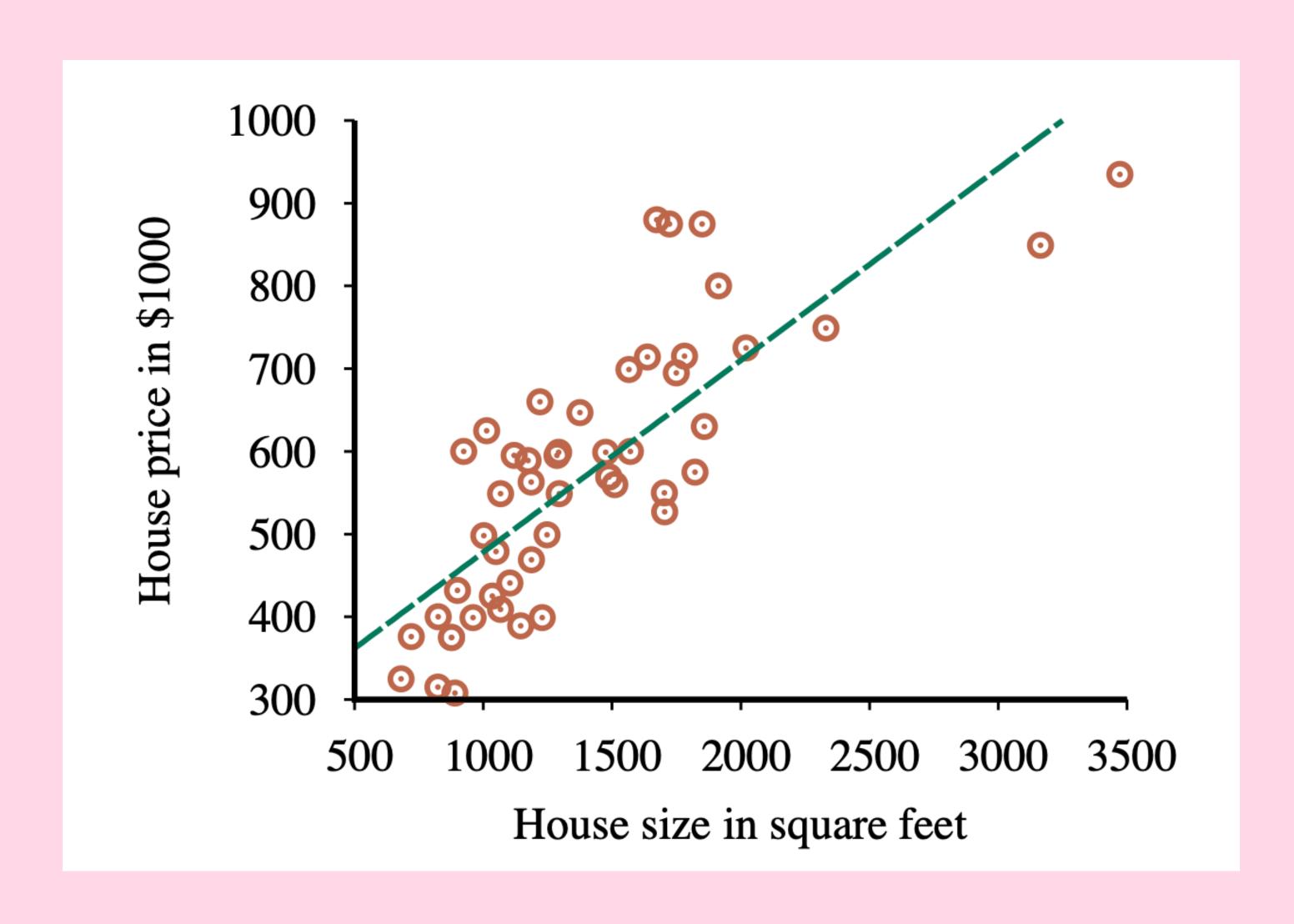
 ${\mathcal H}$ is the set of all possible decision trees.

$$C(h) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1} \{ h(x_i) \neq f(x_i) \}$$

"Optimize" via the heuristic fitting algorithm

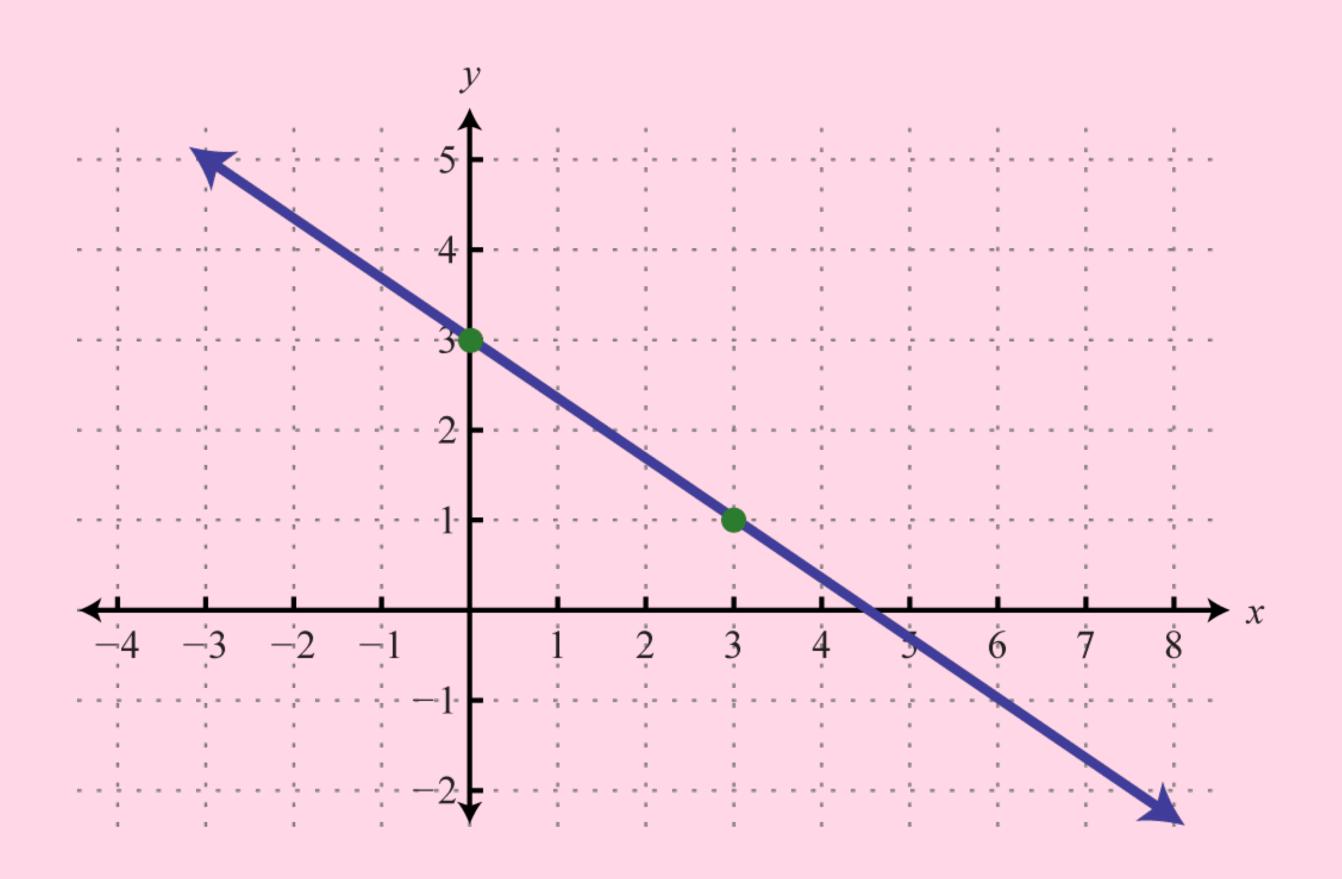
Modeling

Example: predicting housing prices



Representation: linear models

- Hypothesis class: the set of all linear functions $\mathbb{R} \to \mathbb{R}$
- Every one of these functions has the form $h(x) = w_1 x + w_0$
- E.g. $w_0 = 3$ and $w_1 = -2/3$ on the right
- Straight lines are simple and easy to interpret: as x increases by 1 unit, y increases by w_1 units.
- Every hypothesis $h \in \mathcal{H}$ can be identified by a pair of numbers (w_0, w_1) .

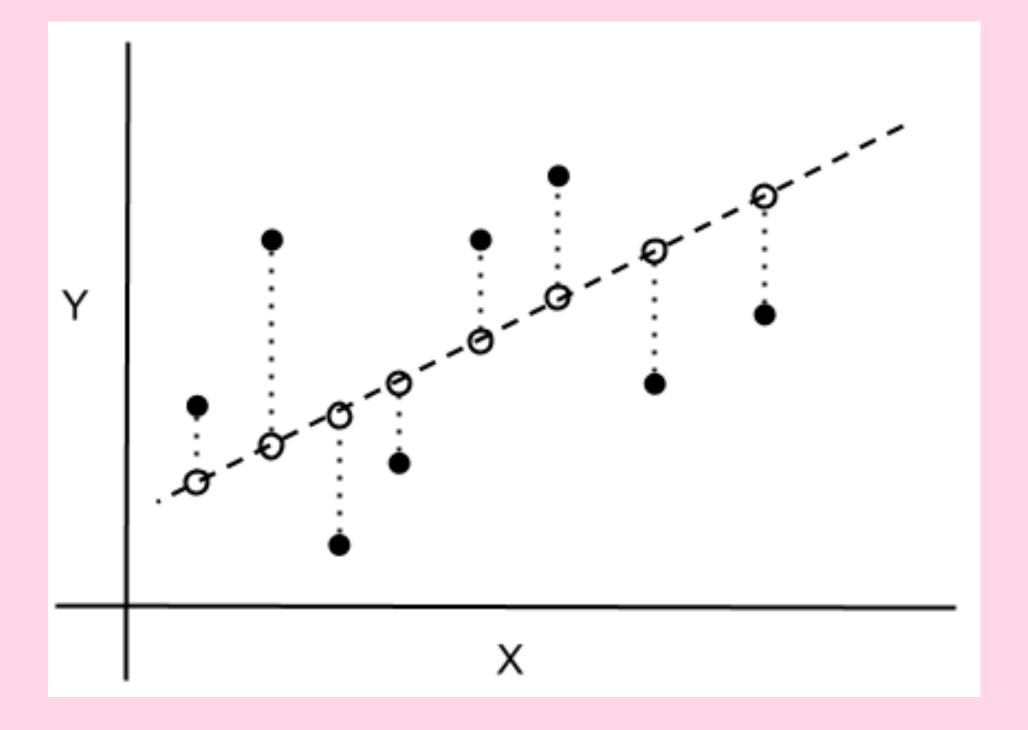


Cost: squared error

- How do we know if a line is a good fit to the data?
- Add up squared errors between predictions and labels.

$$C(h) = \sum_{i=1}^{n} (y_i - h(x_i))^2$$
$$= \sum_{i=1}^{n} (y_i - (w_1 x_i + w_0))^2$$

• Sometimes called ℓ_2 loss, because this is the squared ℓ_2 norm of the residual vector $y - \hat{y}$.



Optimizer: calculus

- How do we find the values of w_0 and w_1 that minimize $C(w_0, w_1)$?
- Because \mathcal{H} is simple, we can optimize directly with calculus!

[calculus on board]

Optimizer: calculus

- How do we find the values of w_0 and w_1 that minimize $C(w_0, w_1)$?
- Because ${\mathcal H}$ is simple, we can optimize directly with calculus!
- Solutions:

$$w_{0} = \frac{1}{n} \sum_{i=1}^{n} y_{i} - w_{1}x_{i}$$

$$w_{1} = \frac{n \sum_{i} x_{i}y_{i} - \left(\sum_{i} x_{i}\right)\left(\sum_{i} y_{i}\right)}{n \sum_{i} x_{i}^{2} - \left(\sum_{i} x_{i}\right)^{2}}$$

• Solution is unique because the cost function is convex in the parameters

