Announcements

Assignments

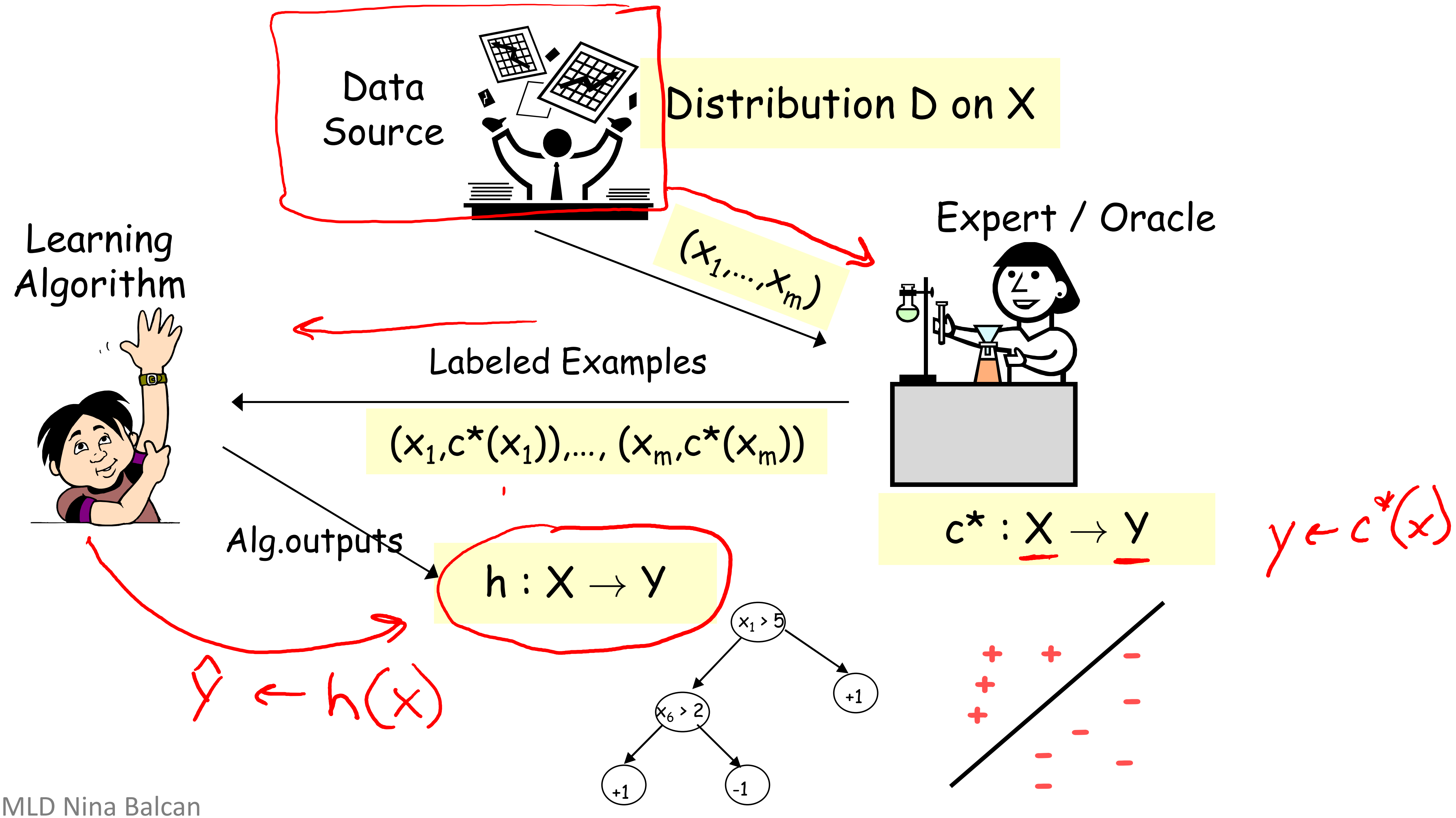
- HW10 (programming + “written”)
  - Due Thu 4/30, 11:59 pm

Introduction to Machine Learning

Learning Theory

Instructor: Pat Virtue

Model for Supervised Learning



Slide credit: CMU MLD Nina Balcan

Optimal Classification Function

Find the best $h(x) \to \hat{y}$ by searching in the space of hypothesis functions $h \in \mathcal{H}$.

$\mathcal{H}_\theta$ $g(x^T\theta)$

g, f^o

Optimal classifier:

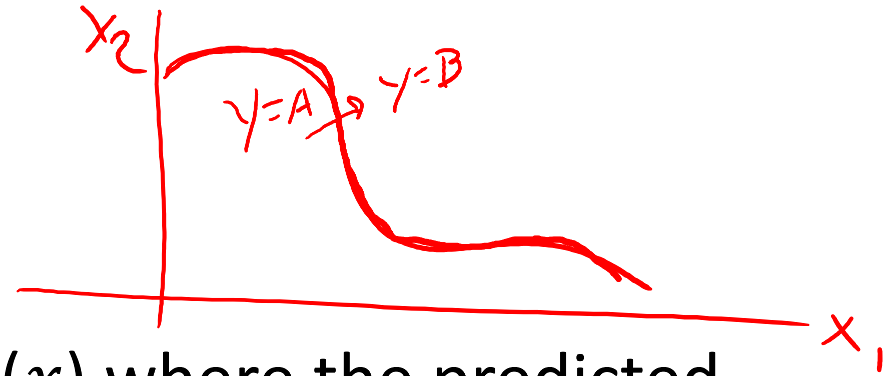
labels input

$$h^*(x) = \underset{y}{\operatorname{argmax}}\, P(Y = y \mid X = x)$$

But why?

$P(x \mid y)P(y)$

Optimal Decision Boundaries



Decision boundary

- The set of points in the domain of the input (x) where the predicted classification changes

Two class decision boundary

- So far, we have decided to let the decision boundary be all x such that:

$$p(Y = 0 \mid X = x) \;=\; p(Y = 1 \mid X = x)$$

- What assumptions are we making here?
  - This assumes that the cost of predicting it wrong is the same for both classes

Optimal Classification Function

Find the best $h(x) \to \hat{y}$ by searching in the space of hypothesis functions $h \in \mathcal{H}$.

Optimal classifier:

$$h^*(x) = \underset{y}{\operatorname{argmax}}\, P(\,Y = y \mid X = x\,)$$

But why?

Goal: find a prediction function $h^*: \mathcal{X} \to \mathcal{Y}$ that minimizes the expected loss for randomly drawn test data (X, Y)

$$h^* = \underset{h}{\operatorname{argmin}}\, \mathbb{E}_{XY}\left[\underline{L\big(Y, h(X)\big)}\right]$$

$L(y, \hat{y})$ is the loss or cost of predicting $\hat{y}$ when the true value is y.

Loss Functions

R(h)

$$h^* = \underset{h}{\operatorname{argmin}}\ \mathbb{E}_{XY}\big[L\big(Y, h(X)\big)\big]$$

Loss function:

$L: \underbrace{\mathcal{Y} \times \mathcal{Y}} \to \mathbb{R}$

Classification:

- Two-class, 0,1 loss

pred

True	$\hat{y}=0$	$\hat{y}=1$
$y=0$	0	1
$y=1$	1	0

- Two-class, arbitrary loss

$y=0$	0	1
SPAM $y=1$	100	0

NOT

False positives and false negatives:

pred

	$\hat{y}=0$	$\hat{y}=1$
$y=0$	TN	FP
$y=1$	FN	TP

Loss Functions

$$h^* = \underset{h}{\operatorname{argmin}}\, \mathbb{E}_{XY}\big[L\big(Y, h(X)\big)\big]$$

Loss function:

$L: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$

Classification:

- Two-class, 0,1 loss
- Two-class, arbitrary loss

	A	B	C	D
A				
B				
C				
D				

Regression: $L(y, h(x)) = (y - h(x))^2$

Expected Value

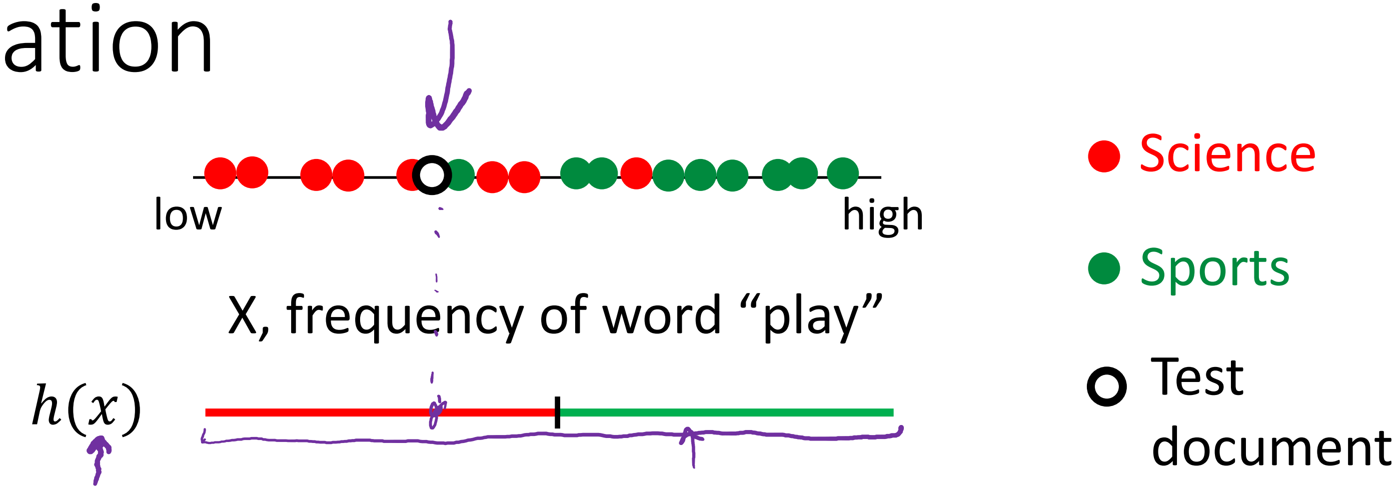
Quick review

$g(Z)$

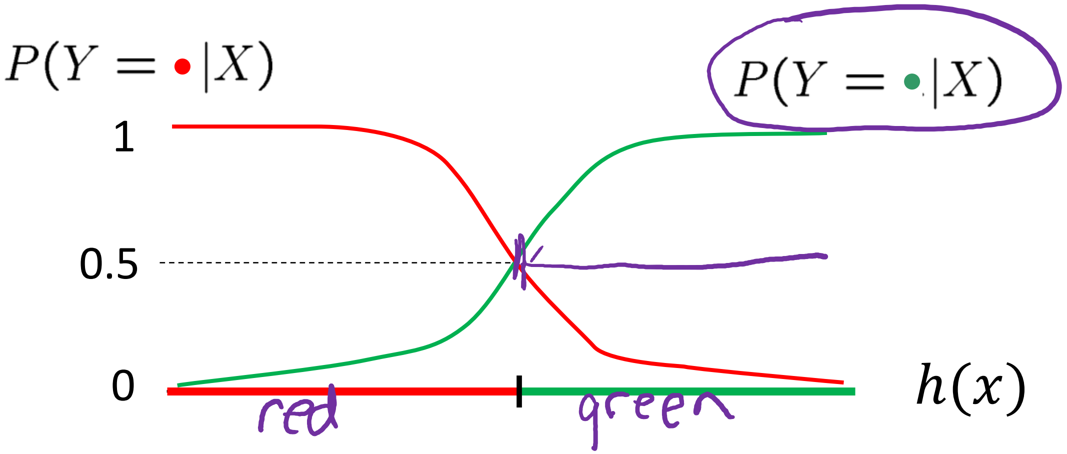
$$E[g(Z)] = \sum_{z \in Z} p(z)\, g(z)$$

$$E[g(Z)] = \int_{\mathbb{R}} f(z)\, g(z)\, dz$$

Binary Classification



Model X and Y as random variables



For a given x, $h(x)$ = label Y which is more likely

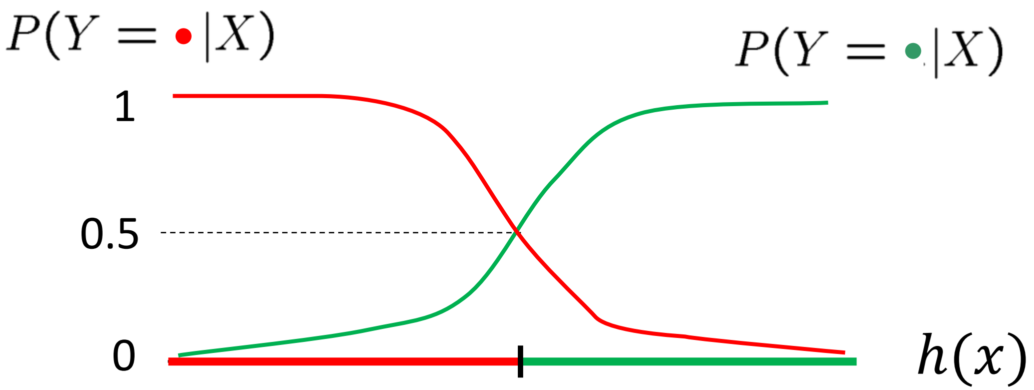
$$h(x) = \underset{Y=y}{\arg\max}\, P(Y = y|X = x)$$

Optimal Classification Function

$$h^*(x) = \underset{y \in \{0,1\}}{\operatorname{argmax}}\, P(\,Y = y \mid X = x\,)$$

$$h^* = \underset{h \in \mathcal{H}}{\operatorname{argmin}}\, \mathbb{E}_{XY}\big[L\big(Y, h(X)\big)\big]$$

Start with arbitrary two-class loss $L(y, \hat{y})$



Optimal Classification Function

Expected loss is also called risk:

$$R(h) = \mathbb{E}_{XY}\left[L\big(Y, h(X)\big)\right]$$

$$h^* = \underset{h}{\operatorname{argmin}}\, R(h)$$

$$= \underset{h}{\operatorname{argmin}}\, \mathbb{E}_{XY}\left[L\big(Y, h(X)\big)\right]$$

{Whiteboard derivation}

Optimal Classification Function

$$h^*(x) = \underset{y \in \{0,1\}}{\text{argmax}}\, P(Y = y \mid X = x)$$

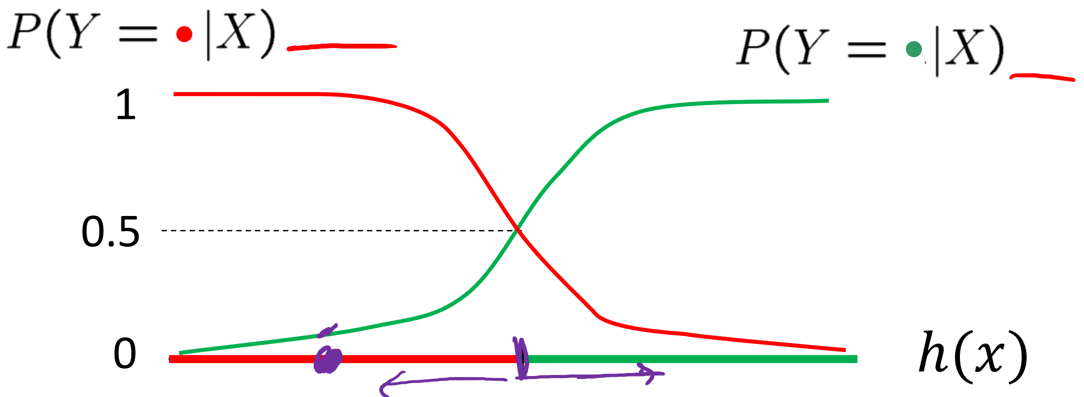
$$h^* = \underset{h}{\text{argmin}}\, \mathbb{E}_{XY}\left[L\big(Y, h(X)\big)\right]$$

Start with arbitrary two-class loss $L(y, \hat{y})$

$$h^*(x) = \begin{cases} 1 & \text{if} \quad P(Y=0 \mid x)L(0,1) + P(Y=1 \mid x)L(1,1) \\ & \quad \le P(Y=0 \mid x)L(0,0) + P(Y=1 \mid x)L(1,0) \\ 0 & \text{otherwise} \end{cases}$$

Two-class, 0, 1 loss

$$h^*(x) = \begin{cases} 1 & \text{if} \quad P(Y=0 \mid x) \\ & \quad \le P(Y=1 \mid x) \\ 0 & \text{otherwise} \end{cases}$$



Optimal Classification Function

$$h^*(x) = \underset{y \in \{0,1\}}{\operatorname{argmax}} P(Y = y \mid X = x)$$

$$h^* = \underset{h}{\operatorname{argmin}} \mathbb{E}_{XY}\left[L\big(Y, h(X)\big)\right]$$

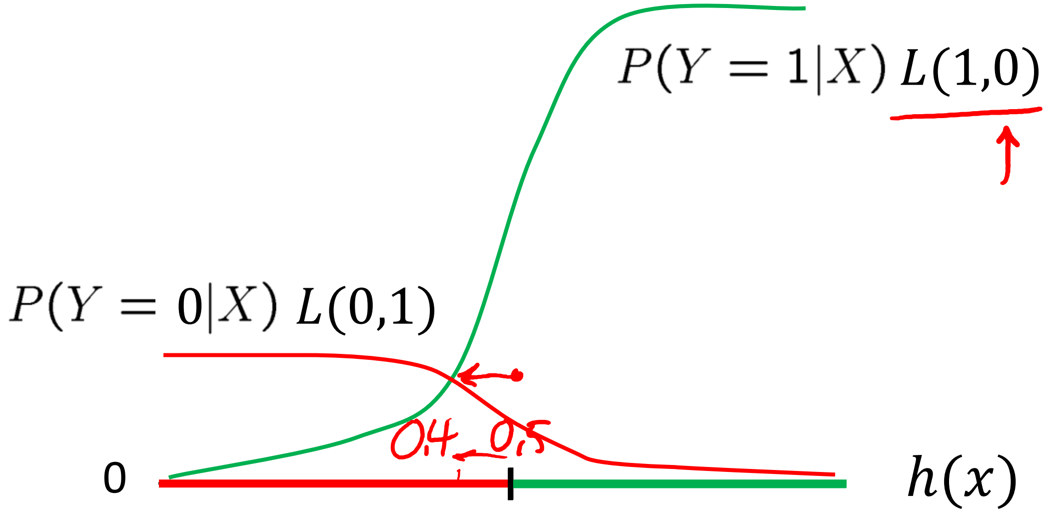
0	.1
100	0

Start with arbitrary two-class loss $L(y, \hat{y})$

$$h^*(x) = \begin{cases} 1 & \text{if} \quad P(Y = 0 \mid x)L(0,1) + \cancel{P(Y = 1 \mid x)L(1,1)} \\ & \quad \leq \cancel{P(Y = 0 \mid x)L(0,0)} + P(Y = 1 \mid x)L(1,0) \\ 0 & \text{otherwise} \end{cases}$$

Two-class, weighted loss

$$h^*(x) = \begin{cases} 1 & \text{if} \quad P(Y = 0 \mid x)L(0,1) \\ & \quad \leq P(Y = 1 \mid x)L(1,0) \\ 0 & \text{otherwise} \end{cases}$$



Optimal Classification Function

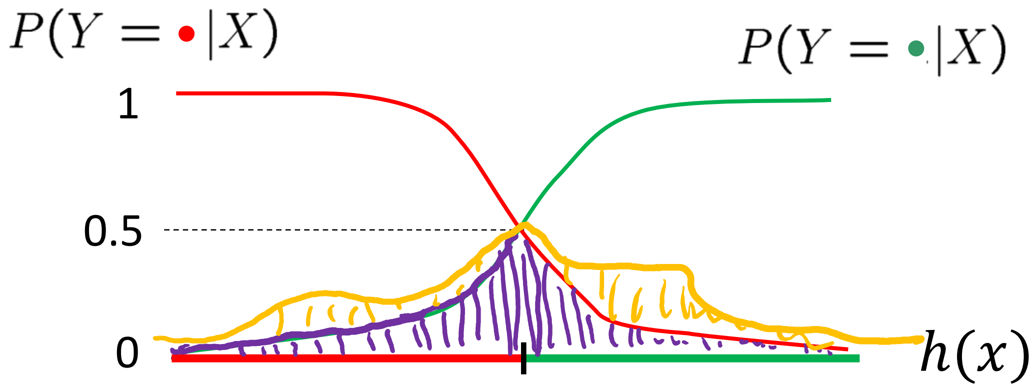
$$h^*(x) = \begin{cases} 1 & \text{if} \quad P(Y=0 \mid x) \le P(Y=1 \mid x) \\ 0 & \text{otherwise} \end{cases}$$

What is the risk of the optimal classifer?

$$R(h^*) = \mathbb{E}_{XY}\left[L\left(Y, h^*(X)\right)\right]$$

$$= \int f(x)\left[p(Y=0 \mid x)\underbrace{L(0, h(x))}_{h(x)} + p(Y=1 \mid x)\underbrace{L(1, h(x))}_{1-h(x)}\right]dx$$

$$R(h^*) > 0$$



$$\underbrace{R(h) - R(h^*)}$$

Risk in Regression

Squared error loss $L(y, h(x)) = (h(x) - y)^2$

$$h^* = \underset{h}{\operatorname{argmin}}\ \mathbb{E}_{XY}\left[L\big(Y, h(X)\big)\right]$$

$$R(h) = E_{XY}\left[L(Y, h(X))\right]$$

$$= \iint (y - h(x))^2 f(dx, dy)$$

$$= E_X\left[E_{Y|X}\left[(Y - h(x))^2 \mid X\right]\right]$$

$$h^*(x) = \underset{\hat{y}}{\operatorname{argmin}}\ E_{Y|X}\left[(Y - \hat{y})^2 \mid X = x\right] \longrightarrow h^*(x) = E\left[Y \mid X = x\right]$$

Optimal Hypothesis Function

Goal: find a prediction function $h^*: \mathcal{X} \rightarrow \mathcal{Y}$ that minimizes the risk, the expected loss for randomly drawn test data $\underbrace{(X, Y)}$

$$h^* = \underset{h}{\operatorname{argmin}}\, R(h) = \underset{h}{\operatorname{argmin}}\, \mathbb{E}_{XY}\left[L\big(Y, h(X)\big)\right]$$

Learning from Training Data

But we want our hypothesis function to generalize well?

- How do we characterize and quantify this trade-off?
- {Back to the whiteboard}