CS189/CS289A
Introduction to Machine Learning
Lecture 4: Decision Theory

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January 29, 2015

Outline

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- Decision theory

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    - Loss functions

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  - Probabilistic assumptions

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Loss Functions

The Prediction Problem

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$$(x_1, y_1), \ldots, (x_n, y_n),$$

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$$\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}.$$

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Aim: $\ell(f(x), y)$ small.

Example: Classification

Loss Functions

Example: Classification

If all mistakes are equally bad, we could define

$$\ell(\hat{y}, y) = 1[\hat{y} \neq y] = \begin{cases} 1 & \text{if } \hat{y} \neq y, \\ 0 & \text{otherwise.} \end{cases}$$

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$\ell(\hat{y}, y)$	$\hat{y} = 0$	$\hat{y} = 1$	$\hat{y} = 2$	$\cdots$	$\hat{y} = 9$
$y = 0$					
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$y = 1$	1	0	1	$\cdots$	1
$y = 2$	1	1	0		1
$\vdots$	$\vdots$	$\vdots$		$\ddots$	$\vdots$
$y = 9$	1	1	1	$\cdots$	0

Example: Spam Classification

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We might be more concerned about some errors than others:

Loss Functions

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$y = \text{Ham}$	100	0

Loss Functions

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Outcomes are in $\mathcal{Y} = \mathbb{R}$, we might choose the quadratic loss function, $\ell(\hat{y}, y) = (\hat{y} - y)^2$.

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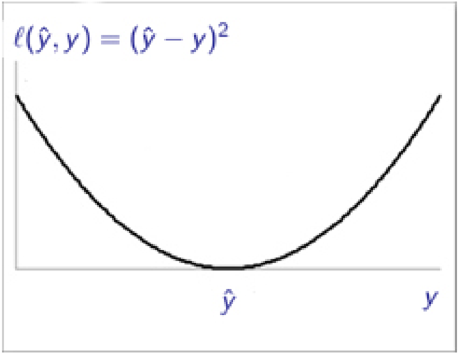

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Probabilistic assumptions for prediction problems

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- A common formulation: Assume that they are randomly chosen, and have the same probability distribution.

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  (Think about the MNIST digits data versus your handwriting.)

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Detour: Joint and conditional distributions

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$P(X, Y)$

Detour: Joint and conditional distributions

$$P(X, Y) = P(Y)P(X|Y)$$

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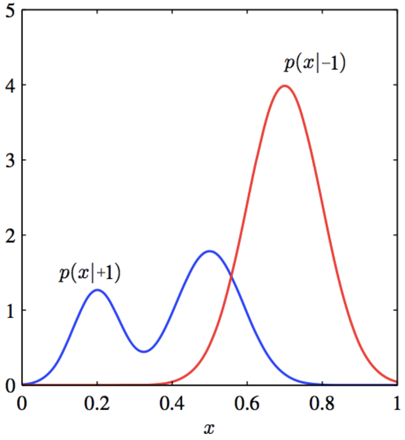
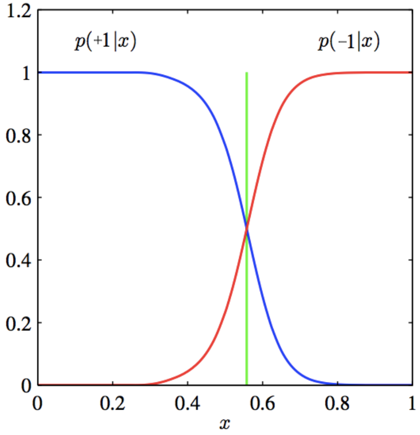
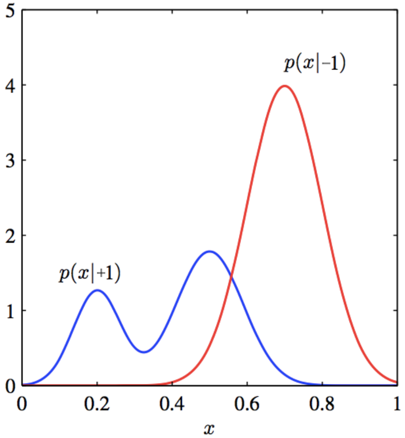


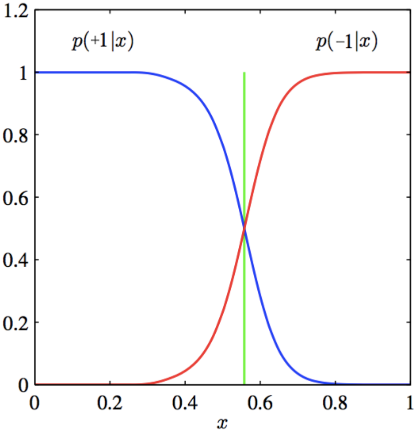


Detour: Joint and conditional distributions

$$P(X, Y) = P(Y)P(X|Y) = P(X)P(Y|X).$$

$P(X \in S \text{ and } Y = 1)$





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$$P(X, Y) = P(Y)P(X|Y) = P(X)P(Y|X).$$
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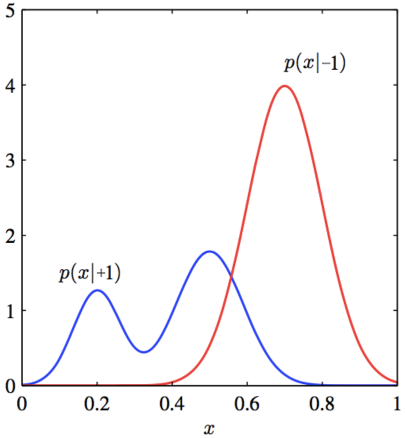
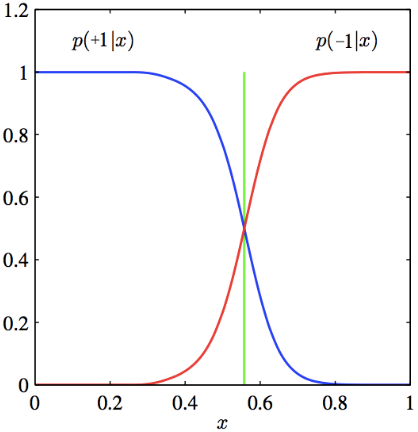
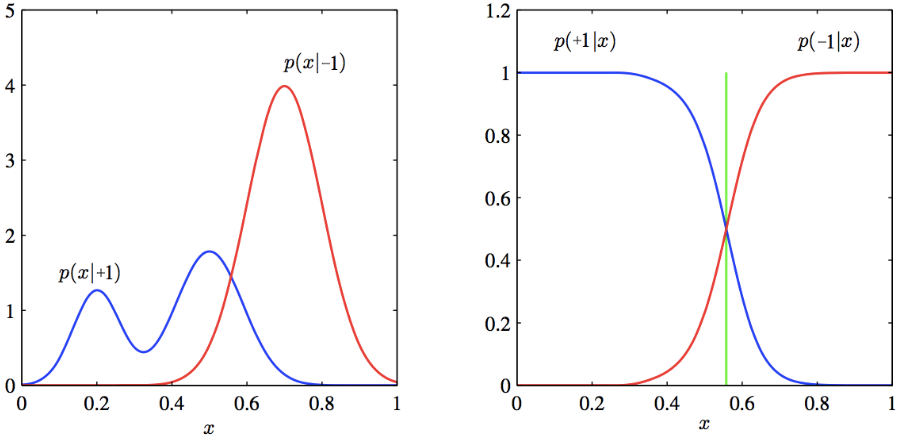




Detour: Joint and conditional distributions

$$\begin{aligned} P(X, Y) &= P(Y)P(X|Y) &= P(X)P(Y|X). \\ P(X \in S \text{ and } Y = 1) &= P(Y = 1)P(X \in S|Y = 1) &= P(X \in S)P(Y = 1|X \in S). \end{aligned}$$



Detour: Joint and conditional distributions

Bayes Theorem

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$$P(Y = +1|X) =$$

Detour: Joint and conditional distributions

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$$P(Y = +1|X) = \frac{P(X|Y = +1)P(Y = +1)}{}.$$

Detour: Joint and conditional distributions

Bayes Theorem

$$P(Y=+1|X) = \frac{P(X|Y=+1)P(Y=+1)}{P(X|Y=+1)P(Y=+1) + P(X|Y=-1)P(Y=-1)}.$$

Bayes Theorem

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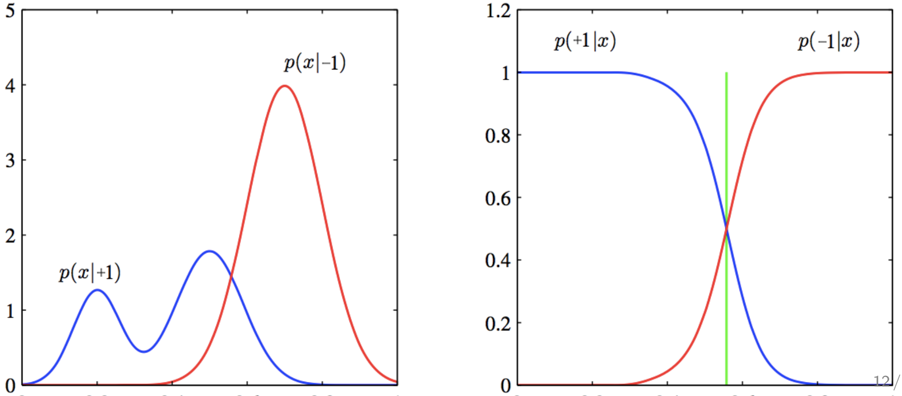

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2. A *good prediction* means small expected loss:
   The aim is to choose f with small *risk*,

$$R(f) = \mathbb{E}\ell(f(X), Y).$$

Risk

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Example: Pattern classification

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Risk is misclassification probability:

Risk

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$$R(f) = \mathbb{E}\ell(f(X), Y) \qquad .$$

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$$R(f) = \mathbb{E}\ell(f(X), Y) = \mathbb{E}1[f(X) \neq Y] \qquad .$$

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- Notation: Capital letters denote random variables.

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- The probability distribution models the relative frequency of different (X, Y) pairs.
- It is crucial that the distribution of the training points (X_i, Y_i) is the same as that of the subsequent (X, Y) pair.

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Minimizing Risk in Classification

Two-class classification: $\mathcal{Y} = \{-1, +1\}$

$$
\begin{aligned}
R(f) &= \mathbb{E}\ell(f(X), Y) \\
&= \mathbb{E}\mathbb{E}[\ell(f(X), Y)|X]
\end{aligned}
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Minimizing Risk in Classification

Two-class classification: $\mathcal{Y} = \{-1, +1\}$

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Minimizing Risk in Classification

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&= \mathbb{E}\left[\ell(f(X), +1)P(Y = +1|X) + \ell(f(X), -1)P(Y = -1|X)\right] \\
&= \mathbb{E}\left[1[f(X) = -1]P(Y = +1|X) + 1[f(X) = +1]P(Y = -1|X)\right].
\end{aligned}
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\end{aligned}
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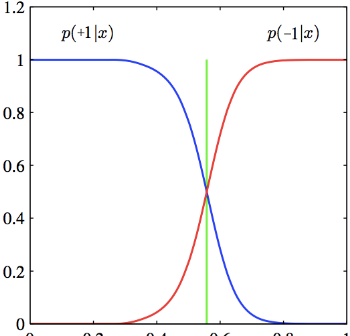

Minimizing Risk in Classification

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Optimizing our choice for each X, we see that risk is minimized when $f = f^*$:

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(How does f^* change if we have a different ℓ? c.f. the spam loss.)

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Excess risk

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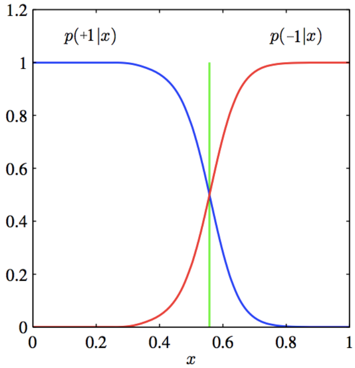

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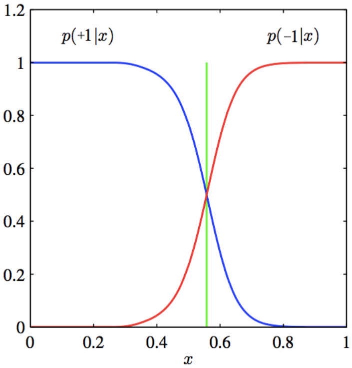

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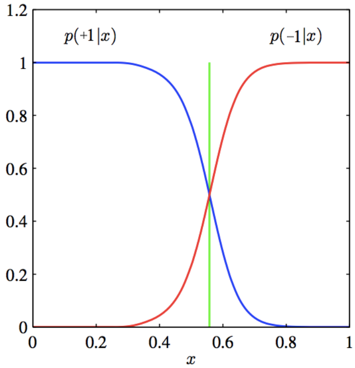

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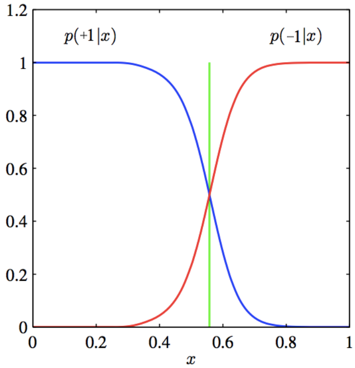

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That is, the excess risk of a decision rule (above the Bayes risk) can be quantified in terms of a certain distance from f^*.

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That is, the excess risk of a decision rule (above the Bayes risk) can be quantified in terms of a certain distance from f^*.

(Not quite a distance: differences between functions at an x with $P(Y = +1|x) = 1/2$ have no influence on the risk.)

Outline

- Decision theory
  - Loss functions
  - Probabilistic assumptions
  - Risk
  - Bayes decision rule
  - Excess risk
  - **Risk, Bayes decision rule, excess risk in regression**
- Three approaches to estimating a classifier:
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Risk

Example: Regression with squared loss

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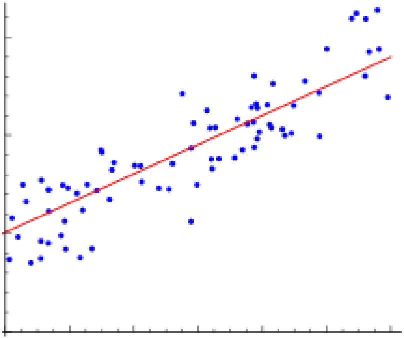

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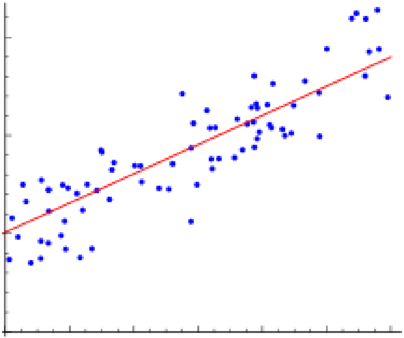

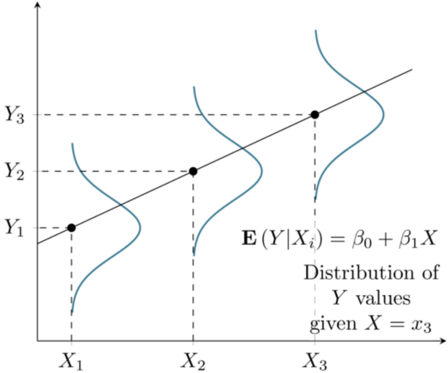

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Bias-variance decomposition

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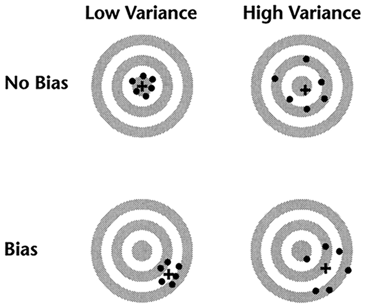

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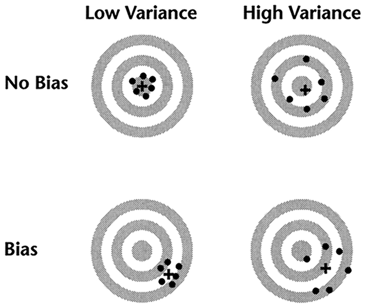

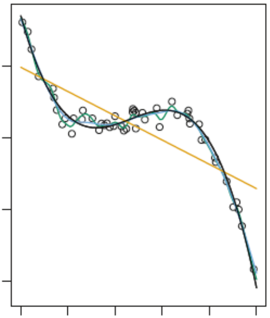

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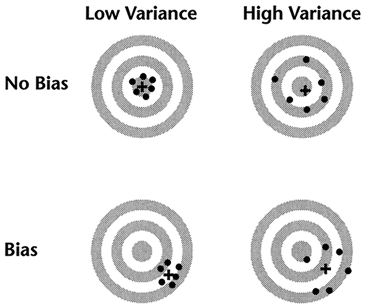

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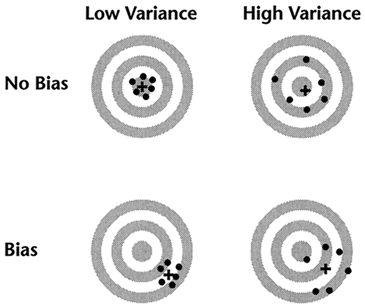

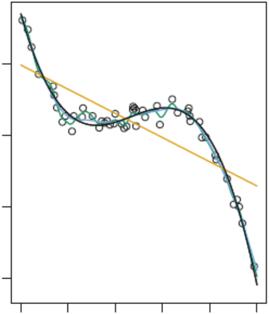

Outline

- Decision theory
    - Loss functions
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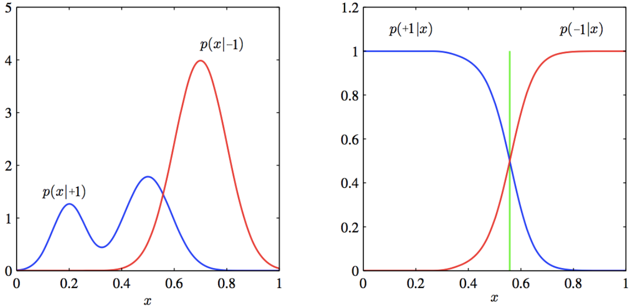

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2. Estimate a model for the joint probability distribution of (X, Y):
   - **(a)** Generative model $\quad P(X, Y) = P(Y)P(X|Y)$
   - **(b)** Discriminative model $\quad P(X, Y) = P(X)P(Y|X)$

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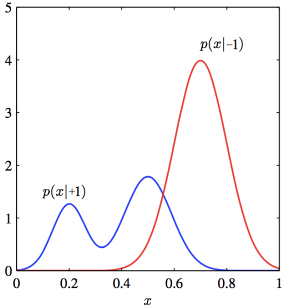

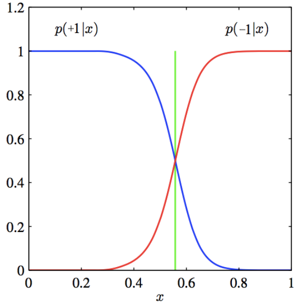

Three approaches to choosing classifiers

Discriminative models

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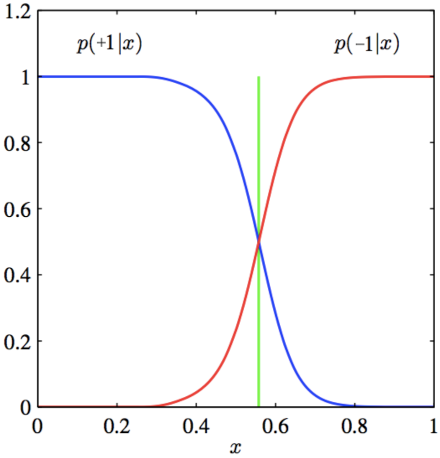
Discriminative models

1. Estimate $P(Y|X)$.



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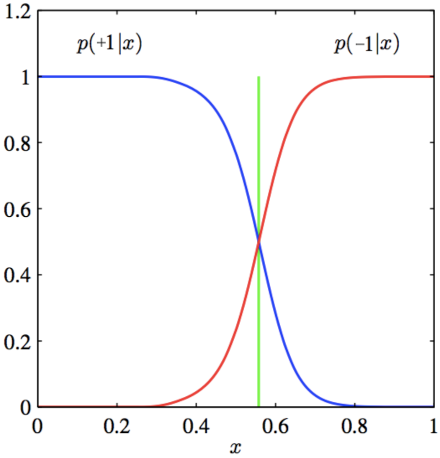
1. Estimate $P(Y|X)$.
2. Pretend that our estimate $\hat{P}(Y|X)$ is actually $P(Y|X)$ and substitute it in the expression for the Bayes rule:



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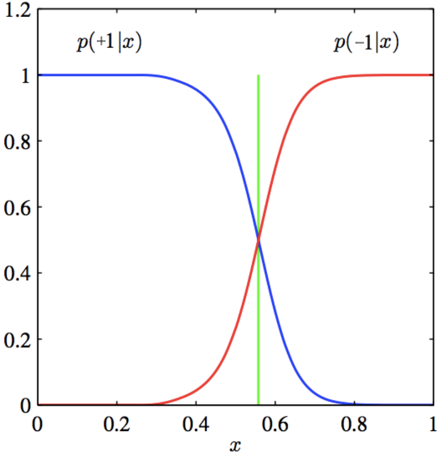
$$\hat{f}(x) = \begin{cases} 1 & \text{if } \hat{P}(Y=1|x) \\ & \quad > \hat{P}(Y=-1|x), \\ -1 & \text{otherwise.} \end{cases}$$



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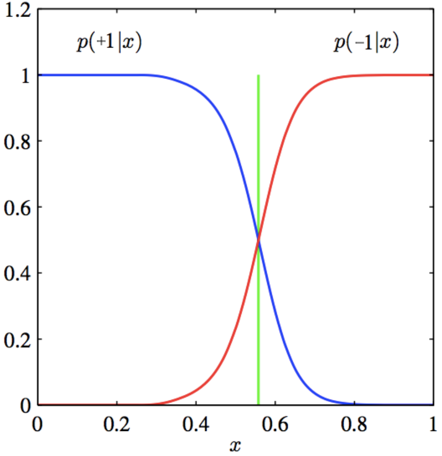
Called a *plug-in estimator*.



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Generative models

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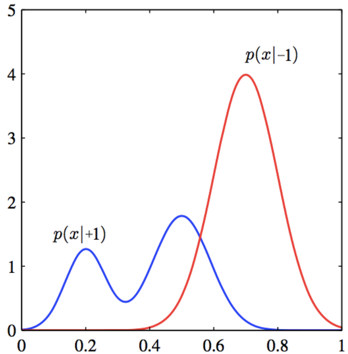
Generative models

1. Estimate $P(Y)$ and $P(X|Y)$.

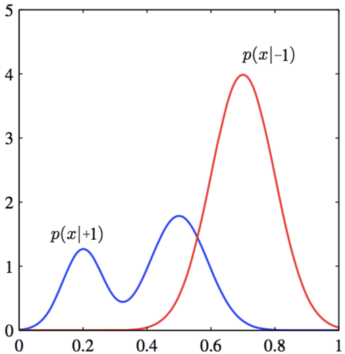


Three approaches to choosing classifiers

Generative models

1. Estimate $P(Y)$ and $P(X|Y)$.
2. Use Bayes theorem:

$$P(Y=+1|X) = \frac{P(X|Y=+1)P(Y=+1)}{P(X|Y=+1)P(Y=+1) + P(X|Y=-1)P(Y=-1)}.$$



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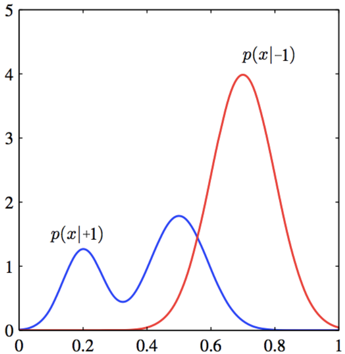
3. Define the plug-in estimator as for a discriminative model.



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3. Choose a classifier directly

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   Estimate $P(X|Y)$.

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   Directly estimate the conditional probability $P(Y|X)$.
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3. Choose a classifier directly:
   By not solving a more difficult problem (e.g., density estimation), we might hope that this approach will do better.

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  e.g. an estimate of $P(X = x)$ can indicate if a point is an outlier.

Outline

- Decision theory
  - Loss functions
  - Probabilistic assumptions
  - Risk
  - Bayes decision rule
  - Excess risk
  - Risk, Bayes decision rule, excess risk in regression
- Three approaches to estimating a classifier:
  generative models, discriminative models, decision rules