Risks and Bayes Optimal Prediction

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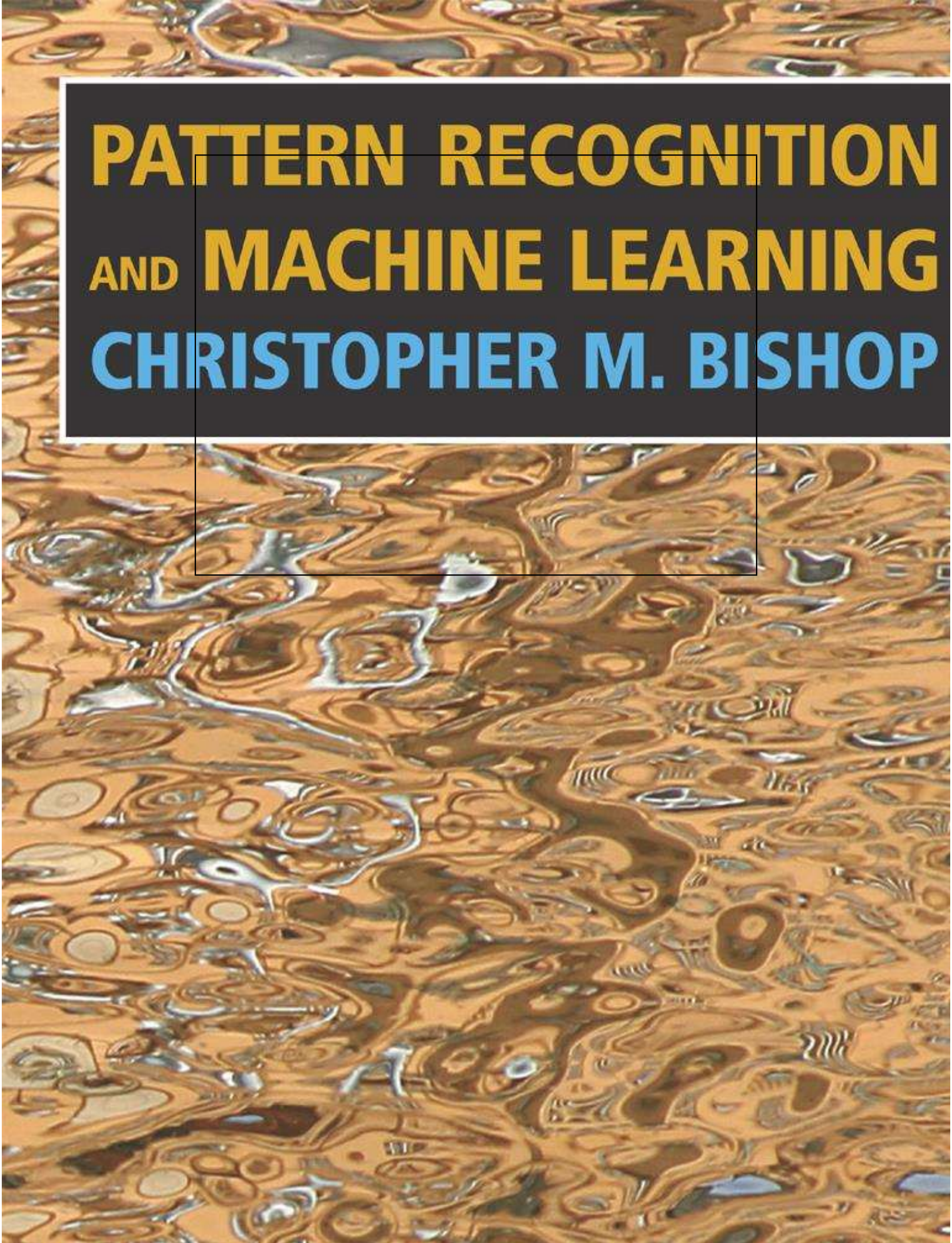
Office Hour: Thursday 3-4pm

Office: GA 18

PATTERN RECOGNITION AND MACHINE LEARNING

CHRISTOPHER M. BISHOP



Binary Classification

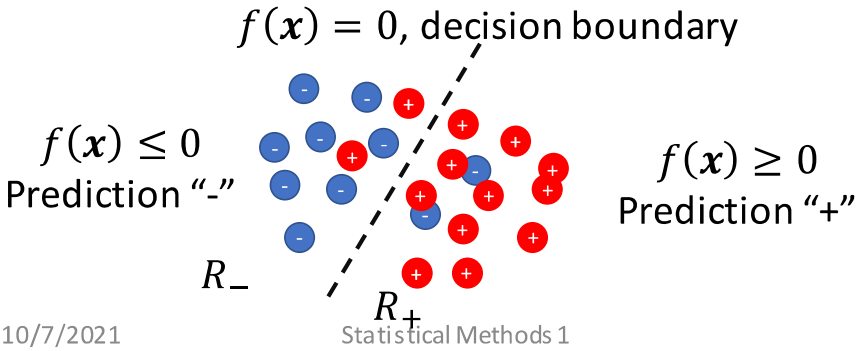
- Sometimes, we need to make discrete decisions
  - In contrast to regression which only predicts a continuous value.
  - e.g., given X-ray image of a person, we decide whether this person is a sick or not.

- **Output**: $y \in \{+1, -1\}$, class label.
  - A binary decision of class, e.g., "normal" or "patient"
- **Input**: $\boldsymbol{x} \in R^d$
  - The input, such as an X-ray image of a person.

- **Task**: Given $\boldsymbol{x}$ make a prediction y
- We want to make as little mistakes as possible.

Binary Classification

- Rather than fit a function like we did in regression, in binary classification, we look for a decision boundary, which separates space of $\boldsymbol{x}$ into two areas R_+ and $R\_$.
- A decision boundary is defined by a function $f(\boldsymbol{x})$



False Positive and False Negative

- What is the best $f(\boldsymbol{x})$ given a dataset D?
- To answer this question, we need to know what are the mistakes we can make in a binary classification.
  - False positive (FP): an $\boldsymbol{x}$ should have been labelled "-1", but is labelled "+1".
  - False negative (FN): an $\boldsymbol{x}$ should have been labelled "+1", but is labelled "-1".
  - **Similarly,** we can define True Positive (TP) and True Negative (TN).

False Positive and False Negative

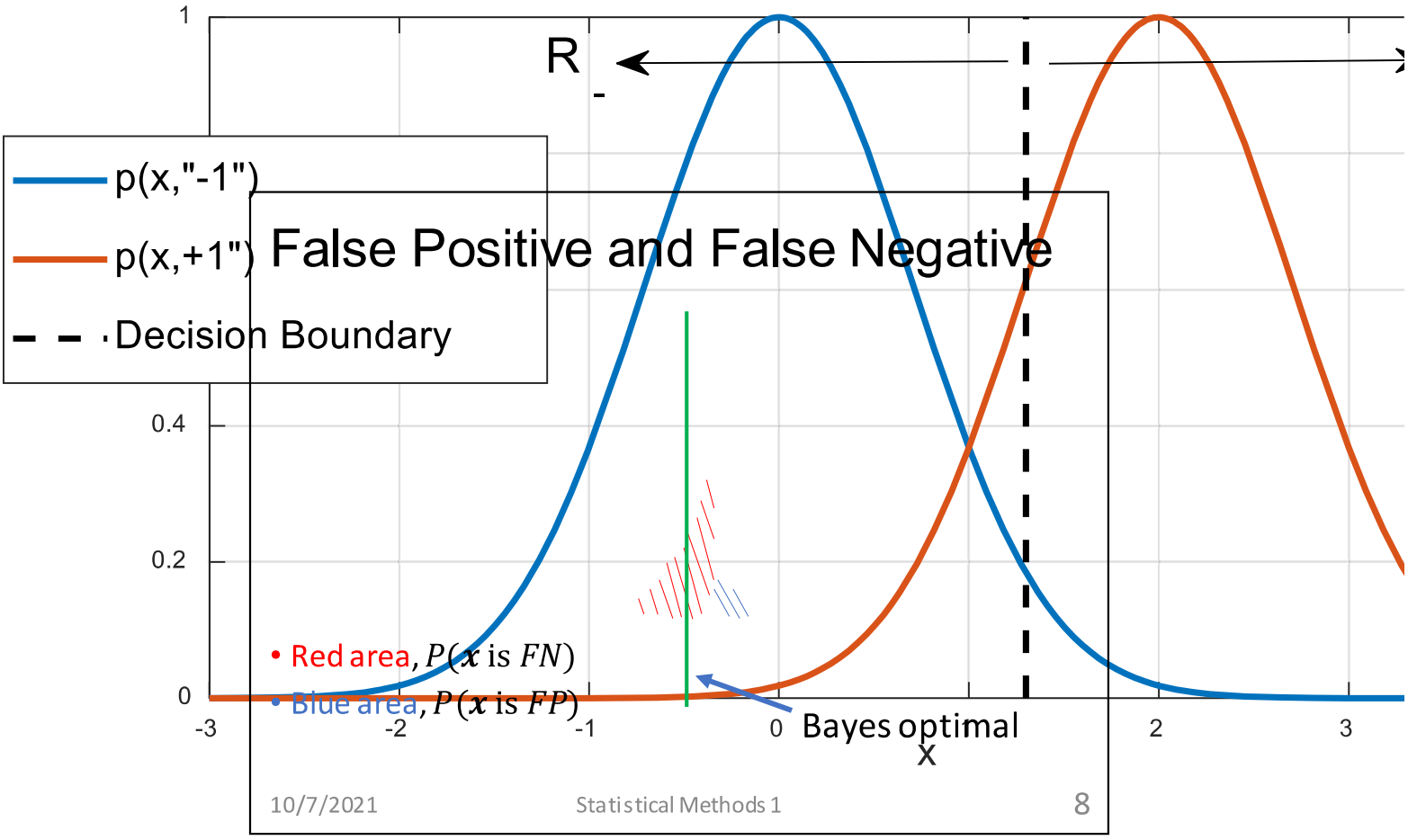
- Let us look at this problem from a probabilistic perspective:
- Probability density of "+" data: $p(\boldsymbol{x}|y = "+1")$
- Probability density of "-" data: $p(\boldsymbol{x}|y = "-1")$
- Probability of class itself, $p(y = +1)$ and $p(y = -1)$.
- What is the probability of making mistakes given areas R_+ and R_- create by a decision function $f(x)$?
- $$P(\boldsymbol{x} \text{ is } FP \text{ or } FN|f) = \int_{R_+} p(\boldsymbol{x}, y = "-1")\mathrm{d}\boldsymbol{x} + \int_{R_-} p(\boldsymbol{x}, y = "+1")\mathrm{d}\boldsymbol{x}$$
- Prove: $P(FP \text{ or } FN|f)$ is minimized when
- $f(\boldsymbol{x}) = p(\boldsymbol{x}, y = +1) - p(\boldsymbol{x}, y = -1)$.

Bayes Optimal Classifier

- $f(\boldsymbol{x}) = p(\boldsymbol{x}, y = +1) - p(\boldsymbol{x}, y = -1)$
- In literatures, this f is referred as Bayes optimal classifier.

- However, this only serves as an idealized optimal classifier.
- In reality, we do not have access to $p(\boldsymbol{x}, y)$ but only data points $D = \{(x_i, y_i)\}_{i=1}^{n}$.
  - Infer joint distribution $p(\boldsymbol{x}, y)$ from data is usually very hard.
  - We will see two different strategies later which can be used to ease the difficulty.

Joint probability completely characterize the data generating source. Using limited data points to infer such a strong result is usually hard.


False Positive and False Negative
p(x,"-1")
p(x,+1")
Decision Boundary
R -
• Red area, $P(\boldsymbol{x}$ is $FN)$
• Blue area, $P(\boldsymbol{x}$ is $FP)$
Bayes optimal
X
1
0.4
0.2
0
-3
-2
-1
0
2
3
10/7/2021
Statistical Methods 1
8

Risks in Decision Making

- Making wrong decisions may have different **loss.**
- **We might weight FP and FN differently.**

- For example, diagnosing a patient as healthy (FN) is certainly riskier than diagnosing a healthy person as a patient (FN).
  - The patient may miss his/her treatment.
  - Treating a healthy person is usually less dangerous.

Patient Treatment Loss Matrix

- Imagine we can quantify the cost of decision making using a **loss matrix**.
- $\boldsymbol{L} =$

$$\begin{array}{c} \\ \text{patient} \\ \text{normal} \end{array} \begin{array}{c} \begin{array}{cc} \text{patient} & \text{normal} \end{array} \\ \begin{bmatrix} 0 & 1000 \\ 1 & 0 \end{bmatrix} \end{array}$$

- It says, if we label a patient as a normal person, the cost is 1000 times as labelling a normal person as patient.
  - We pay no price for correct labelling.
- Giving this loss matrix, how to make a good cost-sensitive decision?

Risk Minimization

- To make a good decision, we need to minimize the **expected loss of making a wrong decision**.

- Suppose output is $y \in \{\text{normal}, \text{patient}\}$, and input is $\boldsymbol{x}$
- Given $\boldsymbol{x}$, a decision is $y_0 \in \{\text{normal}, \text{patient}\}$
- Then the optimal decision is given by

$$\text{argmin}_{y_0} \mathbb{E}_{p(y|\boldsymbol{x})}[L(y, y_0) \,|\boldsymbol{x}]$$

- Where L is a function whose value is determined by $\boldsymbol{L}$.
  - e.g. $L(y = \text{normal}, y_0 = \text{patient}) = 1$

The dataset is random, so we do not really care about an individual decision is right or wrong. Instead, we care the expected loss.

Risk Minimization

- As y is a discrete variable, we can write down $\mathbb{E}_{p(y|\boldsymbol{x})}[L(y, y_0)\,|\boldsymbol{x}] = \sum_{y\in\{+1,-1\}} p(y|\boldsymbol{x}) L(y, y_0)$
- The expectation is a **weighted sum of** $L(y, y_0)$**,** weighted by $p(y|\boldsymbol{x})$.

- **Problem**: we cannot compute this weighted sum, as
- We have no idea what is $p(y|\boldsymbol{x})$.
- We can infer it from using a dataset D.

inferring $p(y|\boldsymbol{x})$ is usually much easier than inferring $p(y, \boldsymbol{x})$, the full joint probability

Inference of $p(y|\boldsymbol{x})$

- Replace $p(y|\boldsymbol{x})$ with $p(y|\boldsymbol{x}, D)$!
- The decision is now given by
- $\text{argmin}_{y_0} \mathbb{E}_{p(y|\boldsymbol{x},D)}[L(y, y_0) \,|\boldsymbol{x}]$
- Problem: How to get $p(y|\boldsymbol{x}, D)$?
  - MLE, MAP, Full Probabilistic Approach blablabla…

Calculate $p(y|\boldsymbol{x}, D)$

- In classification tasks, there are two schools of thoughts on how to obtain $p(y|\boldsymbol{x}, D)$, both have pros and cons.
- A **straightforward** approach.
  - Infer $p(y|\boldsymbol{x}, D)$ directly.
- An **indirect** approach: $p(y|\boldsymbol{x}, D) \propto p(\boldsymbol{x}|y, D)p(y)$.
  - Infer $p(\boldsymbol{x}|y, D)$ using D.
  - $p(y = +1)$ and $p(y = -1)$ is just the proportion of pos/neg samples.
- The inference of $p(y|\boldsymbol{x}, D)$ or $p(\boldsymbol{x}|y, D)$ can be done using MLE, MAP or full probabilistic methods, we will touch this later.

For classification tasks only. The reasoning here in general does not apply to regression tasks.

Discriminative vs. Generative

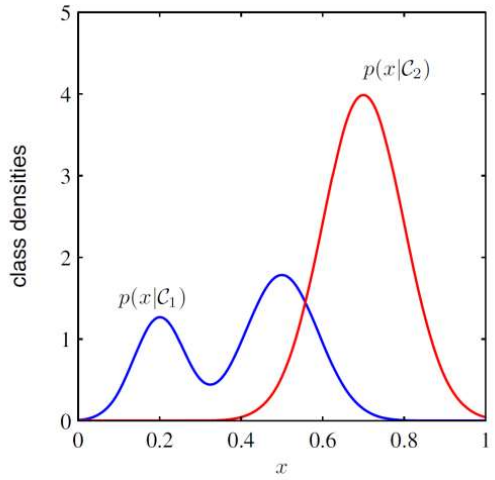
- Straightforward approach models $p(y|\boldsymbol{x})$ with $p(y|\boldsymbol{x};\boldsymbol{w})$.
  - This is called **discriminative** approach.
  - $p(y|\boldsymbol{x})$ only tells the difference between pos/neg.
  - It does not allow us to simulate new $\boldsymbol{x}$ given a class y.
- Indirect approach models $p(\boldsymbol{x}|y)$ with $p(\boldsymbol{x}|y;\boldsymbol{w})$ instead.
  - This is called **generative** approach.
  - $p(\boldsymbol{x}|y)$ can "generate" new input $\boldsymbol{x}$ given an output y.
  - Learning a $p(\boldsymbol{x}|y)$ with a high dim. $\boldsymbol{x}$ can still be difficult.

The probability space of p(y|x) is only binary, but the probability space of p(x|y) is a much bigger space.

If your tasks is only to classify data points, making discrete decisions, usually the discriminative approach is your best bet.

Learning p(x|y) requires you to model and infer a high dimensional distribution on x, which usually suffers from the curse of dimensionality.

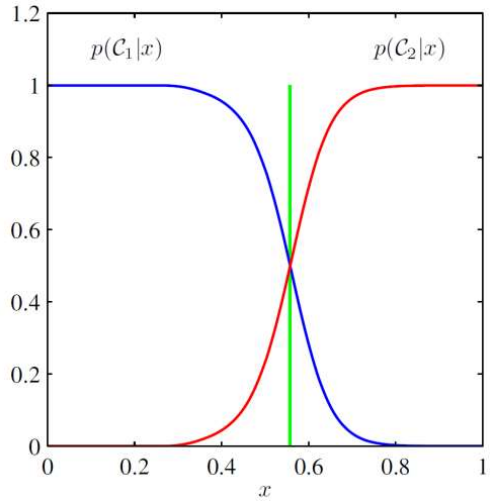
Class Densities: $p(\boldsymbol{x}|y)$



- PRML, Figure 1.27

It tells you how x is distributed at the interval [0,1]

Class-Posterior Probability: $p(y|\boldsymbol{x})$



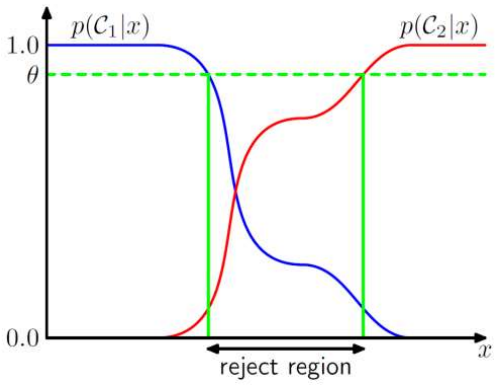
- PRML, Figure 1.27

They look very differently from class densities, as they are probabilities of binary variables.

It tells you how likely x is in blue/red class give different x on the horizontal axis.

You can see the class posterior probability looks a lot simpler, cleaner!! This is why, if your task is only classification, discriminative approach is your best bet.

Rejection Option



PRML **Figure 1.26**

We can reject decision making when we find $\max\{p(y=+1|\boldsymbol{x}), p(y=-1|\boldsymbol{x})\}$ is lower than a threshold.

What about Regression?

- Output value of regression is a continuous variable.
  - We cannot have a loss matrix anymore.

- We can use the loss function, such as squared-loss
- $L(y, y_0) = (y - y_0)^2$
- Again, we minimize the expected loss:
- $\hat{y} := \text{argmin}_{y_0} \mathbb{E}_{p(y|\boldsymbol{x})}[L(y, y_0) \,|\boldsymbol{x}]$
  Prove the optimal prediction using squared−loss is
- $\hat{y} := \mathbb{E}_{p(y|\boldsymbol{x})}[y]$.

What about Regression?

- $\hat{y} \coloneqq \mathbb{E}_{p(y|\boldsymbol{x})}[y]$

- We do not have $p(y|\boldsymbol{x})$, but we can infer $p(y|\boldsymbol{x}, D)$.
- $\hat{y} \approx \mathbb{E}_{p(y|\boldsymbol{x}, D)}[y]$
- The optimal prediction with respect to squared-risk function **is calculating the mean** of the inferred $p(y|\boldsymbol{x}, D)$.

$p(y|\boldsymbol{x}, D)$ can be inferred using MLE, MAP or Full Probabilistic approach.

When $p(y|\boldsymbol{x}, D)$ is inferred by MLE, least-squares give the optimal prediction.

Absolute Value Risk Function

- We can use other loss functions, e.g. absolute val. function
  - $L(y, y_0) \coloneqq |y - y_0|$
- **Prove the optimal prediction using absolute value loss is:**
- $\text{argmin}_{y_0} \mathbb{E}_{p(y|\boldsymbol{x})}[\,|y - y_0|\,]$ is the Median of $p(y|\boldsymbol{x})$.

- Median m is defined as a real value such that
- $\int_{-\infty}^{m} p(y|\boldsymbol{x})\, dy = \int_{m}^{+\infty} p(y|\boldsymbol{x})\, dy = \frac{1}{2}$

- Or the "50% percentile".

Computing Lab (1)

- Generate data $y_i = \exp(1.5x_i - 1) + \epsilon_i, \epsilon_i \sim N(0, .64)$.
  - $i = 1 \ldots 200$
- Modify your last week's implementation of least squares to calculate the regularized least squares solution: $\boldsymbol{w}_{\mathrm{LS-R}}$.
- Tuning regularization constant λ and measure the CV error.
- Can you find a λ such that CV error is minimized?

Computing Lab (2)

- Using the same dataset,
- Calculate the predictive probability distribution using the "marginalization trick":
  - $p(\hat{y}|\boldsymbol{x}, D)$
- Plot $\mathbb{E}_{p(\hat{y}|\boldsymbol{x}, D)}[\hat{y}|\boldsymbol{x}]$ on your dataset, as a function of $\boldsymbol{x}$.
- Plot "the tube",
- $\mathbb{E}_{p(\hat{y}|\boldsymbol{x}, D)}[\hat{y}|\boldsymbol{x}] \pm \sqrt{\mathrm{var}_{p(\hat{y}|\boldsymbol{x}, D)}[\hat{y}|\boldsymbol{x}]}$
- How much data does the tube cover (in terms of percentage)?