

Statistical Machine Learning

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Decision Theory (for Supervised Learning Problems)

Goal:

- Understand existing algorithms
- Develop new algorithms with specific (optimal?) properties

For this, we'll have to rely on mathematics. Forget about the implementation, data etc... for now.

Notation

We treat all quantities of interest as *random variables*:

- input: random variable, X , taking values $x \in \mathcal{X}$
(we treat \mathcal{X} as if it is continuous, but discrete works analogously)
- output: random variable, Y , taking values and $y \in \mathcal{Y}$.
- joint probability distribution/density $p(X = x, Y = y)$.
- we write $p(x, y)$ for of $p(X = x, Y = y)$,
 $p(y|x)$ instead of $p(Y = y|X = x)$, etc.

Classification

First first look at classification, $\mathcal{Y} = \{1, \dots, M\}$, or $\mathcal{Y} = \{-1, +1\}$.

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Definition (Generalization error)

Let $c : \mathcal{X} \rightarrow \mathcal{Y}$ be a decision rule. The *generalization error*, \mathcal{R} , of c is the probability of c making a wrong prediction, i.e.

$$\mathcal{R}(c) := \Pr_{(x,y) \sim p(x,y)} \{c(x) \neq y\}.$$

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Definition (Bayes Classifier, Bayes Risk)

The prediction rule that minimizes the generalization error, with

$$c^* := \underset{c: \mathcal{X} \rightarrow \mathcal{Y}}{\operatorname{argmin}} \mathcal{R}(c)$$

is called **Bayes classifier**. The value $\mathcal{R}(c_{\text{Bayes}})$ is called the **Bayes risk**.

Lemma

The Bayes classifier has the decision rule

$$c(x) := \underset{y \in \mathcal{Y}}{\mathbf{argmax}} p(y|x) \quad \text{for any } x \in \mathcal{X}.$$

Proof. We show: no classifier has lower generalization error than the Bayes classifier...

In binary classification we can write c^* in closed form:

Lemma

For $\mathcal{Y} = \{-1, +1\}$, the Bayes classifier is given by

$$c^*(x) = \text{sign} \left[\log \frac{p(x, +1)}{p(x, -1)} \right],$$

as well as

$$c^*(x) = \text{sign} \left[\log \frac{p(+1|x)}{p(-1|x)} \right].$$

Proof: Exercise...

Should we use c^* to decide for every problem?

- c^* is optimal when trying to *minimize the number of wrong decision*.
- That's often a good strategy, but not always.

Reminder

To evaluate a learning task, we use *loss function* $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$.

$\ell(y, \bar{y})$ is the loss incurred when predicting \bar{y} if the correct answer is y .

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Example: Doctor's dilemma

There's a shadow on the X-ray. Should you diagnose cancer?

x : X-ray image. $y \in \{\text{yes, no}\}$: cancer

- $\ell(\text{yes, yes}) = 0$ (you did your job well)
- $\ell(\text{yes, no}) = 1000$ (the cancer gets worse, the patient could die)
- $\ell(\text{no, yes}) = 1$ (the patient is upset until further test are made)
- $\ell(\text{no, no}) = 0$ (you did your job well)

Common: one outcome is rare, but has high loss if mispredicted

Instead of minimizing the error probability, minimize the *expected loss*!

Definition

The classifier of minimal expected ℓ -risk is given by

$$c_{\ell}^*(x) := \mathbf{argmin}_{y \in \mathcal{Y}} \mathbb{E}_{\bar{y} \sim p(\bar{y}|x)} \ell(\bar{y}, y).$$

Lemma

For $\mathcal{Y} = \{-1, +1\}$, and $\ell(y, \bar{y})$ given by the table

$y \setminus \bar{y}$	-1	+1
-1	a	b
+1	c	d

the risk w.r.t. ℓ is minimized by the decision rule

$$c_{\ell}^*(x) = \mathbf{sign} \left[\log \frac{p(x, +1)}{p(x, -1)} + \log \frac{c - d}{b - a} \right],$$

or equivalently
$$c_{\ell}^*(x) = \mathbf{sign} \left[\log \frac{p(+1|x)}{p(-1|x)} + \log \frac{c - d}{b - a} \right].$$

Proof: Exercise.

Observation

The *generalization error* is the *risk* for 0/1-loss, i.e. $\ell(y, y') = \mathbb{1}[y \neq y']$.

Question: What's the best classifier for a fully known problem?

Question answered. We have identified the optimal classifiers!

In the real world, $p(x, y)$ is unknown, but we have a training set \mathcal{D} . There's at least 3 approaches:

Definition

Given a training set \mathcal{D} , we call it

- a **generative probabilistic approach**:

if we use \mathcal{D} to build a model $\hat{p}(x, y)$ of $p(x, y)$, and then define

$$c(x) := \operatorname{argmax}_{y \in \mathcal{Y}} \hat{p}(x, y) \quad \text{or} \quad c_\ell(x) := \operatorname{argmin}_{y \in \mathcal{Y}} \mathbb{E}_{\bar{y} \sim \hat{p}(x, \bar{y})} \ell(\bar{y}, y).$$

- a **discriminative probabilistic approach**:

if we use \mathcal{D} to build a model $\hat{p}(y|x)$ of $p(y|x)$ and define

$$c(x) := \operatorname{argmax}_{y \in \mathcal{Y}} \hat{p}(y|x) \quad \text{or} \quad c_\ell(x) := \operatorname{argmin}_{y \in \mathcal{Y}} \mathbb{E}_{\bar{y} \sim \hat{p}(\bar{y}|x)} \ell(\bar{y}, y).$$

- a **decision theoretic approach**: if we use \mathcal{D} to directly search for a classifier c in a hypothesis class \mathcal{H} .

Setting

We are given

- a **training set** of examples $\mathcal{D} = \{(x^1, y^1), \dots, (x^n, y^n)\}$,
(note: rather a multi-set, elements can occur more than once)

Assumption:

- \mathcal{D} are *independent and identically distributed (i.i.d.)* samples from the unknown distribution $p(x, y)$.

Shorthand notation,

- $\mathcal{D}^X := \{x^1, \dots, x^n\}$, input part of \mathcal{D} ,
- $\mathcal{D}^Y := \{y^1, \dots, y^n\}$, output part of \mathcal{D} ,
- $\mathcal{D}_y := \{(x^i, y^i) \in \mathcal{D} : y^i = y\}$, all examples of label y .

Let's use \mathcal{D} to form an estimate of $p(x, y)$.

Definition

There's (at least) three approaches:

- **parametric estimate:**
 - ▶ fix a model class $p(x, y; \theta)$,
 - ▶ estimate parameters $\hat{\theta}$ such that $p(x, y; \hat{\theta}) \approx p(x, y)$.
 - ▶ the size of θ is independent of how large \mathcal{D} is
- **non-parametric estimate:**
 - ▶ estimate any $\hat{p}(x, y) \approx p(x, y)$
 - ▶ the number of parameters/complexity of $\hat{p}(x, y)$ can grow with $|\mathcal{D}|$
- hybrids of the two

If \mathcal{X} and \mathcal{Y} are *finite*, we can represent any $p(x, y)$ as a table of values.

To simplify notation, we look at arbitrary $z \in \mathcal{Z}$ (think: $z = (x, y)$):

Definition (Empirical estimate)

Let z^1, \dots, z^n be samples from $p(z)$, then we call

$$\hat{p}_n(z) := \frac{1}{n} \sum_{i=1}^n \mathbb{I}[z^i = z]$$

the empirical estimate of $p(z)$.

Theorem (Convergence of the empirical estimate)

Let z^1, z^2, \dots be i.i.d. samples from $p(z)$. For every possible value $z \in \mathcal{Z}$

$$\Pr \left\{ \lim_{n \rightarrow \infty} \hat{p}_n(z) = p(z) \right\} = 1.$$

Proof.

Every textbook on statistics: *law of large numbers* (strong version). \square

The curse of dimensionality

Setting:

Let $\mathcal{Z} = \mathcal{Z}_1 \times \cdots \times \mathcal{Z}_d$, i.e. data decomposes into d non-trivial "features", "attributes", or "dimensions". Let $m_j := |\mathcal{Z}_j| \geq 2$ for $j = 1, \dots, d$.

Lemma

*The number of samples needed to estimate $\hat{p}(z)$ **grows exponentially in d** (unless we made additional assumptions).*

Proof.

$\hat{p}(z)$ has $|\mathcal{Z}| = \prod_{j=1}^d m_j \geq 2^d$ entries. Without further assumptions, each entry can be set arbitrarily, independently, except for the one constraint that they must sum to 1. Each sample influences only one bin, so we need at least $2^d - 1$ samples (in practice, many times that, of course). □

Example (Dating agency table)

TRAINING	eyes	height	handsome	sex	soccer	date?
Apu	blue	tall	yes	male	no	yes
Bernice	brown	short	yes	female	no	no
⋮						
Itchy	brown	short	no	male	yes	yes

Could we estimate $p(x, y)$ here?

- $|\mathcal{X} \times \mathcal{Y}| = 96$, $p(x, y)$ has 95 free parameters
- We have 9 samples.
- **Most possible combinations we have never seen!**

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Bayes classifier from $\hat{p}(x, y)$: $c(x) := \mathbf{argmax}_{y \in \mathcal{Y}} \hat{p}(x, y)$

- $\hat{p}(\text{Apu}, \text{yes}) = \frac{1}{9}$, $\hat{p}(\text{Apu}, \text{no}) = 0$, $\rightarrow c(\text{Apu}) = \text{yes}$,
- $\hat{p}(\text{Jimbo}, \text{yes}) = 0$, $\hat{p}(\text{Jimbo}, \text{no}) = 0$, $\rightarrow c(\text{Jimbo}) = ???$,

No clue about previously unseen patterns \rightarrow very little generalization

Definition

Let $\mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_d$. The *Naive Bayes (NB)* estimate of $p(x, y)$ is

$$\hat{p}_{\text{NB}}(x, y) := \hat{p}(y) \prod_{j=1}^d \hat{p}_j(x_j|y),$$

where

- $\hat{p}(y)$ is an estimate of $p(y)$,
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Lemma

The number of free parameters in $p_{\text{NB}}(x, y)$ grows linear with d .

Proof.

$p_{\text{NB}}(x, y)$ has $|\mathcal{Y}|[1 + \sum_{j=1}^d (m_j - 1)] - 1$ degrees of freedom. □

Definition

The *Naive Bayes* classifier is given by

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A Naive Bayes classifier needs much fewer examples for 'training' than one based on a full probability table.

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Remark

Even for $n \rightarrow \infty$, we likely won't have $\hat{p}_{NB}(x, y) \nearrow p(x, y)$!

So, most likely, **the NB model is wrong** as a density estimate.

But that doesn't mean it doesn't work for making decisions!

In fact, NB is *very successful*, e.g. in Spam filtering (text classification).

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"All models are wrong, but some are useful." (George E. P. Box, 1979)

Parametric models for finite domains

Both models we saw so far are *parametric*:

For finite $z \in \mathcal{Z}$, $p(z)$ is *multinomial* distribution:

- $|\mathcal{Z}|$ parameters: θ_z for $z \in \mathcal{Z}$ with $p(Z = z) = \theta_z$
- parameters fulfill
 - ▶ $\theta_z \geq 0$
 - ▶ $\sum_z \theta_z = 1$

Similar for Naive Bayes model:

- $\hat{p}(y)$ is multinomial for $y \in \mathcal{Y}$, parameter $\theta_y \in \mathbb{R}^{|\mathcal{Y}|}$,
 - ▶ $\hat{p}(y) = \theta_y$ with $\theta_y \geq 0$, $\sum_{y \in \mathcal{Y}} \theta_y = 1$,
- $\hat{p}(x_j|y)$ is multinomial for $x_j \in \mathcal{X}_j$, parameters $\theta_{x_j}^j$
 - ▶ $\hat{p}(x_j|y) = \theta_{x_j}^y$ with $\theta_{x_j}^y \geq 0$, $\sum_{x_j \in \mathcal{X}_j} \theta_{x_j}^y = 1$, for all $y \in \mathcal{Y}$

We set parameters as $\theta_z = \frac{1}{n} \sum_{i=1}^n \mathbb{1}[z^i = z]$? Why?

Let $\hat{p}(z; \theta)$ be a parametric model with parameter $\theta \in \Theta$.

Let $\mathcal{D} = \{z^1, \dots, z^n\}$ be i.i.d. samples from $p(z)$.

Definition (Parameter estimation)

There's (at least) two main approaches to set θ :

Maximum Likelihood (ML) Estimation:

Which parameter value makes it most likely that we observed \mathcal{D} ?

$$\theta_{ML} = \underset{\theta \in \Theta}{\operatorname{argmax}} p(z^1, \dots, z^n; \theta) = \underset{\theta \in \Theta}{\operatorname{argmax}} \prod_i p(z^i; \theta)$$

Bayesian Parameter Estimation:

Treat θ as a random variable itself. What's its most likely value given \mathcal{D} ?

$$\begin{aligned} \theta_{Bayes} &= \underset{\theta \in \Theta}{\operatorname{argmax}} p(\theta \mid z^1, \dots, z^n) \\ &= \underset{\theta \in \Theta}{\operatorname{argmax}} p(\theta)p(z^1, \dots, z^n \mid \theta) = \underset{\theta \in \Theta}{\operatorname{argmax}} p(\theta) \prod_i p(z^i; \theta) \end{aligned}$$

where $p(\theta)$ is a *prior* distribution over the possible parameter values.

Remark

In practice, one almost always uses the log-likelihood, which gives the same θ (since \log is a monotonous function):

$$\theta_{ML} = \underset{\theta \in \Theta}{\operatorname{argmax}} \log \prod_{i=1}^n \hat{p}(x^i; \theta) = \underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{i=1}^n \log \hat{p}(x^i; \theta)$$

and

$$\begin{aligned} \theta_{Bayes} &= \underset{\theta \in \Theta}{\operatorname{argmax}} \log \left[p(\theta) \prod_i p(z^i; \theta) \right] \\ &= \underset{\theta \in \Theta}{\operatorname{argmax}} \log p(\theta) + \sum_i \log p(z^i; \theta) \end{aligned}$$

Example on blackboard.

Definition (Laplace smoothing)

Let z^1, \dots, z^n be i.i.d. samples from $p(z)$. For $\alpha \geq 0$ we call

$$\hat{p}_n(z) := \frac{1}{n + |\mathcal{Z}|\alpha} \left(\alpha + \sum_{i=1}^n \mathbb{I}[z^i = z] \right) \quad (1)$$

the *smoothed empirical estimate* of $p(z)$ (with smoothing parameter α).

Bayesian interpretation:

- Bayesian estimate of parameters θ_z of a multinomial distribution
- Prior on θ : symmetric Dirichlet distribution with parameter α

$$p(\theta) = \frac{1}{B(\alpha)} \prod_{z=1}^{|\mathcal{Z}|} (\theta_z)^{\alpha-1} \quad \text{with} \quad B(\alpha) = \frac{\Gamma(\alpha)^{|\mathcal{Z}|}}{\Gamma(\alpha|\mathcal{Z}|)}$$

Laplace's "rule of succession": $\alpha = 1$. More common: $\alpha < 1$, e.g. $\frac{1}{2}$.

If \mathcal{X} is continuous, $p(x, y)$ is a strange object, mixing continuous and discrete. Instead of modeling $p(x, y)$, we decompose it:

Definition

Let $p(x, y) = p(x|y)p(y)$.

- $p(y)$ are called **class priors**,
- $p(x|y)$, for $y \in \mathcal{Y}$, are called **class conditional densities**.

Remark

$p(y)$ is a discrete probability distribution over $|\mathcal{Y}|$ possible values, i.e.

- $p(y) \geq 0$ for all $y \in \mathcal{Y}$, and $\sum_y p(y) = 1$.

For any fixed $y \in \mathcal{Y}$, $p(x|y)$ is a probability density, i.e.

- $p(x|y) \geq 0$ for all $x \in \mathcal{X}$, and $\int_x p(x|y) dx = 1$.

Most popular parametric model for continuous data is **Gaussian**:

Definition (Gaussian Density Parameter Estimation)

For $x \in \mathbb{R}^d$, let $\hat{p}(x|y; \mu, \Sigma) = \mathcal{G}(x, \mu_y, \Sigma_y)$ with

$$\mathcal{G}(x, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d \det \Sigma_y}} \exp\left(-\frac{1}{2}(x - \mu_y)^\top \Sigma_y^{-1}(x - \mu_y)\right).$$

Given a set $\mathcal{D} = \{(x^1, y^1), \dots, (x^n, y^n)\}$, we estimate all μ_y and Σ_y for $y \in \mathcal{Y}$ using the classical formulas:

$$\mu_y = \frac{1}{n_y} \sum_{\{i: y^i=y\}} x^i \quad \Sigma_y = \frac{1}{n_y} \sum_{\{i: y^i=y\}} (x^i - \mu_y)(x^i - \mu_y)^\top \quad (2)$$

Remark: Alternatively, we can assume a fixed Σ_y and estimate only μ_y , or estimate a single Σ for all classes, or set $\Sigma_y = \sigma_y Id$ and estimate σ , etc.

Example (Gaussian Model of Height Distribution)

We observe the following situation:

- X : height of a person in cm, $Y = \{\text{male, female}\}$.
- $\mathcal{D} = \{(181, \text{m}), (165, \text{f}), (161, \text{f}), (172, \text{m}), (175, \text{m}), (178, \text{f})\}$.

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$$\mathcal{X} = \mathbb{R}^1, \text{ so } \hat{p}(x|y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{1}{2\sigma_y^2}(x - \mu_y)^2\right).$$

$$\mu_{\text{m}} = \frac{1}{3}(181 + 172 + 175) = 176$$

$$\sigma_{\text{m}}^2 = \frac{1}{3}(5^2 + 4^2 + 1^2) = 14$$

$$\mu_{\text{f}} = \frac{1}{3}(161 + 165 + 178) = 168$$

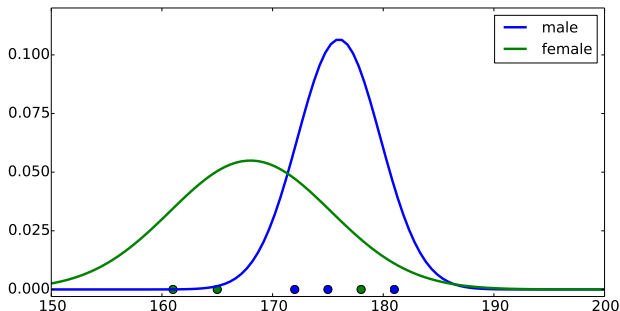
$$\sigma_{\text{f}}^2 = \frac{1}{3}(7^2 + 3^2 + 10^2) \approx 52.7$$

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Lemma

The classical expressions for estimating μ_y and Σ_y for a Gaussian are the maximum likelihood estimates for the parameters of $\hat{p}(x|y; \mu, \sigma)$.

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Proof. With $\mathcal{G}(x; \mu, \Sigma) = \frac{1}{(2\pi \det \Sigma)^{d/2}} \exp\{-\frac{1}{2}(x - \mu)^\top \Sigma^{-1}(x - \mu)\}$, solve $\mu_{ML} = \operatorname{argmax}_{\mu} \mathcal{L}(\mu)$ for $\mathcal{L}(\mu) = \log \sum_{i=1}^n \log \mathcal{G}(x^i; \mu, \Sigma)$.

$$\mathcal{L}(\mu) = \frac{1}{2} \sum_{i=1}^n (x^i - \mu)^\top \Sigma^{-1} (x^i - \mu) - \frac{d}{2} \log 2\pi - \frac{d}{2} \log \det \Sigma$$

$$\nabla_{\mu} L(\mu, \Sigma) = \sum_{i=1}^n \Sigma^{-1} (x^i - \mu) = \Sigma^{-1} \sum_{i=1}^n (x^i - \mu)$$

$$H_{\mu} L(\mu, \Sigma) = -\Sigma^{-1} \preceq 0$$

$$\mu_{ML} = \frac{1}{n} \sum_{i=1}^n x^i \Rightarrow \nabla_{\mu} L(\mu_{ML}, \Sigma) = 0 \Rightarrow \text{maximum of } \mathcal{L}$$

Σ_{ML} analogously, but requires some matrix derivatives.

Classification based on Gaussian models

Let $\hat{p}(x|y; \mu_y, \Sigma_y) = \frac{1}{\sqrt{(2\pi)^d \det \Sigma_y}} \exp(-\frac{1}{2}(x - \mu_y)^\top \Sigma_y^{-1}(x - \mu_y))$.

How to make decisions?

General Bayes classifier:

$$c(x) = \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \left\{ \frac{\hat{p}(y)}{\sqrt{(2\pi)^d \det \Sigma_y}} \exp(-\frac{1}{2}(x - \mu_y)^\top \Sigma_y^{-1}(x - \mu_y)) \right\}$$

For two classes, $\mathcal{Y} = \{+1, -1\}$:

$$\begin{aligned} c(x) &= \operatorname{sign} \left[\log \frac{p(x, +1)}{p(x, -1)} \right] \\ &= \operatorname{sign} \left[(x - \mu_{-1})^\top (\Sigma_{-1})^{-1} (x - \mu_{-1}) \right. \\ &\quad \left. - (x - \mu_{+1})^\top (\Sigma_{+1})^{-1} (x - \mu_{+1}) - \log \frac{\det \Sigma_{+1}}{\det \Sigma_{-1}} \right] \end{aligned}$$

Gaussian Mixture Models (GMMs)

More flexibility by modeling each class as a **Mixture of Gaussians**

$$\hat{p}(x|y; \pi, \vec{\mu}, \vec{\Sigma}) = \sum_{k=1}^K \pi_k \mathcal{G}(x; \mu_k, \Sigma_k) \quad \text{with } \pi_k \geq 0 \text{ and } \sum_{k=1}^K \pi_k = 1.$$

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No closed form for MLE parameters, but popular iterative algorithm:

Expectation-Maximization (EM) algorithm for GMMs

input x^1, \dots, x^n, K

init $\pi, \vec{\mu}, \vec{\Sigma}$

repeat

$$\hat{\gamma}_{ik} = \pi_k \mathcal{G}(x^i; \mu_k, \Sigma_k), \quad \gamma_{ik} = \hat{\gamma}_{ik} / (\sum_j \hat{\gamma}_{ij}) \quad \text{E-step}$$

$$\pi_k = \frac{1}{n} \sum_{i=1}^n \gamma_{ik}$$

$$\mu_k = \frac{1}{n\pi_k} \sum \gamma_{ik} x^i$$

$$\Sigma_k = \frac{1}{n\pi_k} \sum_i \gamma_{ik} (x^i - \mu_k)(x^i - \mu_k)^\top$$

M-step(s)

until convergence

output $\pi, \vec{\mu}, \vec{\Sigma}$

Definition

Let $K_h(x) : \mathcal{X} \rightarrow \mathbb{R}$ be a (fixed) kernel function, where h is a *bandwidth* parameter. Then

$$\hat{p}(x|y) := \frac{1}{|\{y_i = y\}|} \sum_{\{i:y_i=y\}} K_h(x - x^i)$$

is called a *kernel density estimate (KDE)* of $p(x|y)$.

Alternative name: *Parzen windows estimate*.

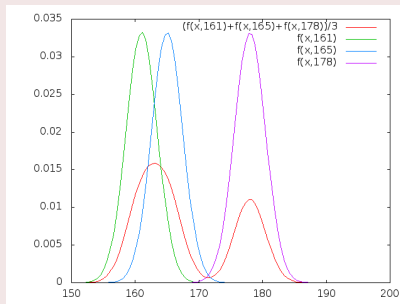
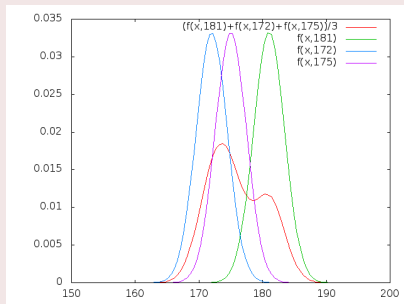
Kernel density estimates are *non-parametric*. The number of terms grows with the number of examples.

Example: Kernel density estimate

Example

- X : height of a person in cm, $Y = \{(\text{male}, \text{female})\}$.
- $\mathcal{D} = \{(181, \text{m}), (165, \text{f}), (161, \text{f}), (172, \text{m}), (175, \text{m}), (178, \text{f})\}$.

For $K_h(x) = \frac{1}{\sqrt{2\pi}h^2} \exp(-\frac{1}{h^2} \|x\|^2)$ (Gaussian with bandwidth h):

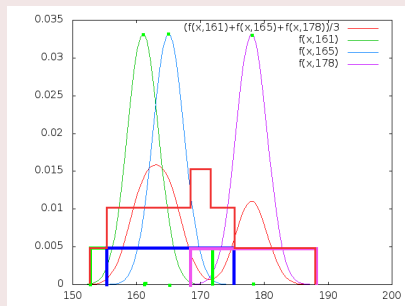
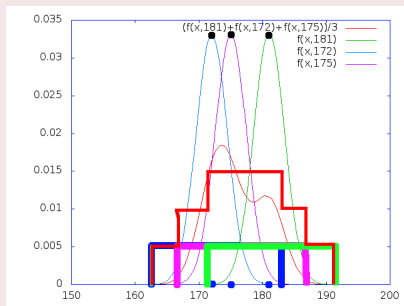


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For $K_h(x) = \frac{1}{2h} \mathbb{I}[|x| < h]$ (Box kernel):



Summary: Generative Models

For generative models, one uses the available data to estimate $p(x, y)$

- either directly, or
- through the decomposition $p(x, y) = p(x|y)p(y)$

Generative models are popular in the natural sciences because they

- model all information in the data
- reflect the data generation process

But: they suffer from **curse of dimensionality!**

- one either needs a *lot* of data,
- or, one must have strong additional assumptions,
- or one must resort to a simple (usually wrong) model.