Probabilistic modeling

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CMPSCI 689: Machine Learning

3 March 2015

5 March 2015

Administrivia

- Mini-project 1 due Thursday, March 05
- Turn in a hard copy
  - In the next class
  - Or in CS main office reception area by 4:00pm (mention 689 hw)
- Clearly write your name and student id in the front page
- Late submissions:
  - At most 48 hours at 50% deduction (by 4:00pm March 07)
  - More than 48 hours get zero
  - Submit a pdf via email to the TA: xiaojian@cs.umass.edu

Overview

- So far the models and algorithms you have learned about are relatively disconnected
- Probabilistic modeling framework unites the two
- Learning can be viewed as statistical inference
- Two kinds of data models
  - Generative
  - Conditional
- Two kinds of probability models
  - Parametric
  - Non-parametric

Classification by density estimation

- The data is generated according to a distribution D

$$(\mathbf{x}, y) \sim D(\mathbf{x}, y)$$

- Suppose you had access to D, then classification becomes simple:

$$\hat{y} = \arg\max_{y} D(\hat{\mathbf{x}}, y)$$

- This is the Bayes optimal classifier which achieves the smallest expected loss among all classifiers

$$\epsilon(\hat{y}) = \mathbb{E}_{(\mathbf{x},y)\sim\ D}\left[\ell(y, \hat{y})\right]$$: expected loss of a predictor

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

- Unfortunately, we don't have access to the distribution

Classification by density estimation

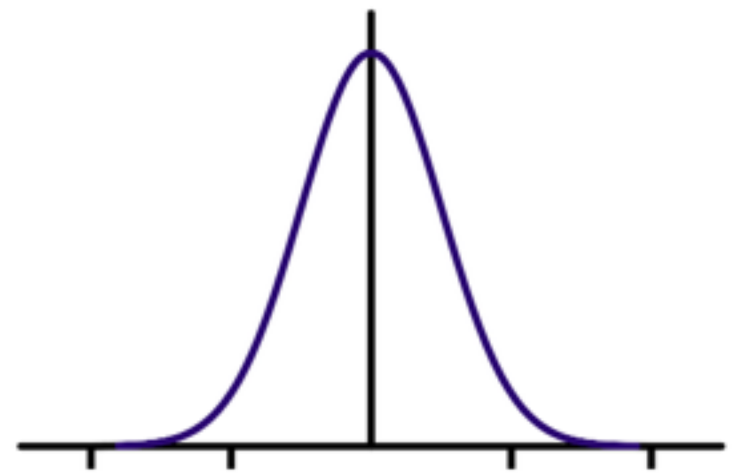
- This suggests that one way to learn a classifier is to estimate D

Training data

$$(\mathbf{x}_1, y_1) \sim D$$
$$(\mathbf{x}_2, y_2) \sim D$$
$$\ldots$$
$$(\mathbf{x}_n, y_n) \sim D$$

$$\xrightarrow{\text{Estimation}} \hat{D}$$

parametric distribution



Gaussian: $N(\mu, \sigma^2)$

Estimate the parameters of the distribution

- We will assume that each point is independently generated from D
  - A new point doesn't depend on previous points
  - Commonly referred to as the i.i.d assumption or independently and identically distributed assumption

Statistical estimation

- **Coin toss:** observed sequence {H, T, H, H}
- Probability of H: β
- What is the value of β that best explains the observed data?
- Maximum likelihood principle (MLE): pick parameters of the distribution that maximize the likelihood of the observed data
- Likelihood of data:

$$\begin{aligned} p_\beta(\text{data}) &= p_\beta(\text{H,T,H,H}) \\ &= p_\beta(\text{H})p_\beta(\text{T})p_\beta(\text{H})p_\beta(\text{H}) \qquad \text{i.i.d data} \\ &= \beta \times (1-\beta) \times \beta \times \beta \\ &= \beta^3(1-\beta) \end{aligned}$$

- Maximize likelihood:

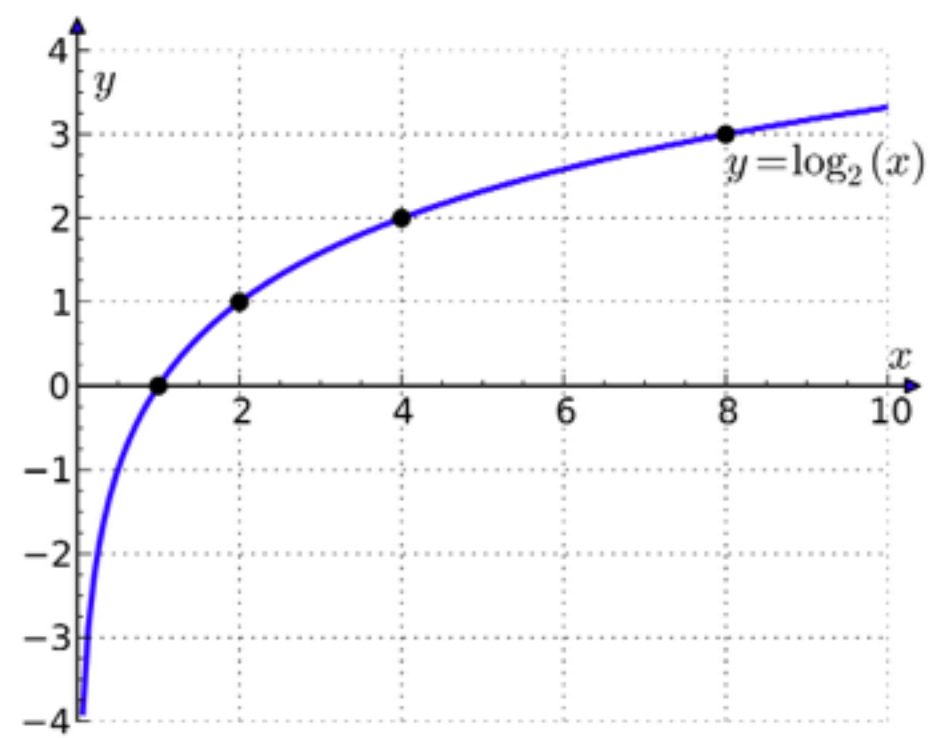
$$\frac{dp_\beta(\text{data})}{d\beta} = \frac{d\beta^3(1-\beta)}{d\beta} = 3\beta^2(1-\beta) + \beta^3(-1) = 0 \quad \Longrightarrow \quad \beta = \frac{3}{4}$$

Log-likelihood

- It is convenient to maximize the logarithm of the likelihood instead
- Log-likelihood of the observed data:

$$\begin{aligned}\log p_\beta(\text{data}) &= \log p_\beta(\text{H,T,H,H}) \\ &= \log p_\beta(\text{H}) + \log p_\beta(\text{T}) + \log p_\beta(\text{H}) + \log p_\beta(\text{H}) \\ &= \log \beta + \log(1-\beta) + \log \beta + \log \beta \\ &= 3\log \beta + \log(1-\beta)\end{aligned}$$

- Maximizing the log-likelihood is equivalent to maximizing likelihood
  - Log is a concave monotonic function
  - Products become sums
  - Numerically stable



Log-likelihood

- Log-likelihood of observing **H**-many heads and **T**-many tails:

$$\log p_\beta(\text{data}) = \text{H} \log \beta + \text{T} \log(1 - \beta)$$

- Maximizing the log-likelihood:

$$\frac{d[\text{H} \log \beta + \text{T} \log(1 - \beta)]}{d\beta} = \frac{\text{H}}{\beta} - \frac{\text{T}}{1 - \beta} = 0$$

$$\implies \beta = \frac{\text{H}}{\text{H} + \text{T}}$$

Rolling a die

- Suppose you are rolling a k-sided die with parameters: $\theta_1, \theta_2, \ldots, \theta_k$
- You observe: $x_1, x_2, \ldots, x_k$
- Log-likelihood of the data:

$$\log p(\text{data}) = \sum_k x_k \log \theta_k$$

- Maximizing the log-likelihood by setting the derivative to zero:

$$\frac{d \log p(\text{data})}{d\theta_k} = \frac{x_k}{\theta_k} = 0 \implies \theta_k = \infty$$

- We need additional constraints:

$$\sum_k \theta_k = 1$$

Lagrangian multipliers

- Constrained optimization:

$$\max_{\theta_1,\theta_2\ldots,\theta_k} \sum_k x_k \log \theta_k$$

subject to: $$\sum_k \theta_k = 1$$

- Unconstrained optimization:

$$\min_{\lambda} \max_{\{\theta_1,\theta_2\ldots,\theta_k\}} \sum_k x_k \log \theta_k + \lambda\left(1 - \sum_k \theta_k\right)$$

  - At optimality: $$\frac{x_k}{\theta_k} = \lambda \implies \theta_k = \frac{x_k}{\lambda}$$

$$\lambda = \sum_k x_k \qquad \theta_k = \frac{x_k}{\sum_k x_k}$$

Naive Bayes

- Consider the binary prediction problem
- Let the data be distributed according to a probability distribution:

$$p_\theta(y, \mathbf{x}) = p_\theta(y, x_1, x_2, \ldots, x_D)$$

- We can simplify this using the chain rule of probability:

$$\begin{aligned} p_\theta(y, \mathbf{x}) &= p_\theta(y) p_\theta(x_1|y) p_\theta(x_2|x_1, y) \ldots p_\theta(x_D|x_1, x_2, \ldots, x_{D-1}, y) \\ &= p_\theta(y) \prod_{d=1}^{D} p_\theta(x_d|x_1, x_2, \ldots, x_{d-1}, y) \end{aligned}$$

- **Naive Bayes** assumption:

$$p_\theta(x_d|x_{d'}, y) = p_\theta(x_d|y), \forall d' \neq d$$

- E.g., The words "free" and "money" are independent given spam

Naive Bayes

- **Naive Bayes** assumption:

$$p_\theta(x_d | x_{d'}, y) = p_\theta(x_d | y), \forall d' \neq d$$

- We can simplify the joint probability distribution as:

$$p_\theta(y, \mathbf{x}) = p_\theta(y) \prod_{d=1}^{D} p_\theta(x_d | x_1, x_2, \ldots, x_{d-1}, y)$$

$$= p_\theta(y) \prod_{d=1}^{D} p_\theta(x_d | y) \qquad \text{// simpler distribution}$$

- At this point we can start parametrizing the distribution

Naive Bayes: a simple case

- **Case:** binary labels and binary features

$$\left.\begin{aligned} p_\theta(y) &= \texttt{Bernoulli}(\theta_0) \\ p_\theta(x_d|y=1) &= \texttt{Bernoulli}(\theta_d^+) \\ p_\theta(x_d|y=-1) &= \texttt{Bernoulli}(\theta_d^-) \end{aligned}\right\}$$ 1+2D parameters

- Probability of the data:

$$p_\theta(y,\mathbf{x}) = p_\theta(y)\prod_{d=1}^{D} p_\theta(x_d|y)$$

$$= \theta_0^{[y=+1]}(1-\theta_0)^{[y=-1]}$$

$$\ldots \times \prod_{d=1}^{D} \theta_d^{+[x_d=1,y=+1]}(1-\theta_d^+)^{[x_d=0,y=+1]}$$ // label +1

$$\ldots \times \prod_{d=1}^{D} \theta_d^{-[x_d=1,y=-1]}(1-\theta_d^-)^{[x_d=0,y=-1]}$$ // label -1

Naive Bayes: parameter estimation

- Given data we can estimate the parameters by maximizing data likelihood
- Similar to the coin toss example the maximum likelihood estimates are:

$$\hat{\theta}_0 = \frac{\sum_n [y_n = +1]}{N}$$

// fraction of the data with label as +1

$$\hat{\theta}_d^+ = \frac{\sum_n [x_{d,n} = 1, y_n = +1]}{\sum_n [y_n = +1]}$$

// fraction of the instances with 1 among +1

$$\hat{\theta}_d^- = \frac{\sum_n [x_{d,n} = 1, y_n = -1]}{\sum_n [y_n = -1]}$$

// fraction of the instances with 1 among -1

- Other cases:
  - Nominal features: Multinomial distribution (like rolling a die)
  - Continuous features: Gaussian distribution

inductive bias

Naive Bayes: prediction

- To make predictions compute the posterior distribution:

$$\hat{y} = \arg\max_y p_\theta(y|\mathbf{x})$$ // Bayes optimal prediction

$$= \arg\max_y \frac{p_\theta(y, \mathbf{x})}{p_\theta(\mathbf{x})}$$ // Bayes rule

$$= \arg\max_y p_\theta(y, \mathbf{x})$$

- For binary labels we can also compute the likelihood ratio:

$$\boxed{\mathrm{LR} = \frac{p_\theta(+1, \mathbf{x})}{p_\theta(-1, \mathbf{x})}}$$

$$\hat{y} = \begin{cases} +1 & \mathrm{LR} \geq 1 \\ -1 & \text{otherwise} \end{cases}$$

- Or the log likelihood ratio:

$$\boxed{\mathrm{LLR} = \log\left(p_\theta(+1, \mathbf{x})\right) - \log\left(p_\theta(-1, \mathbf{x})\right)}$$

$$\hat{y} = \begin{cases} +1 & \mathrm{LLR} \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

Naive Bayes: decision boundary

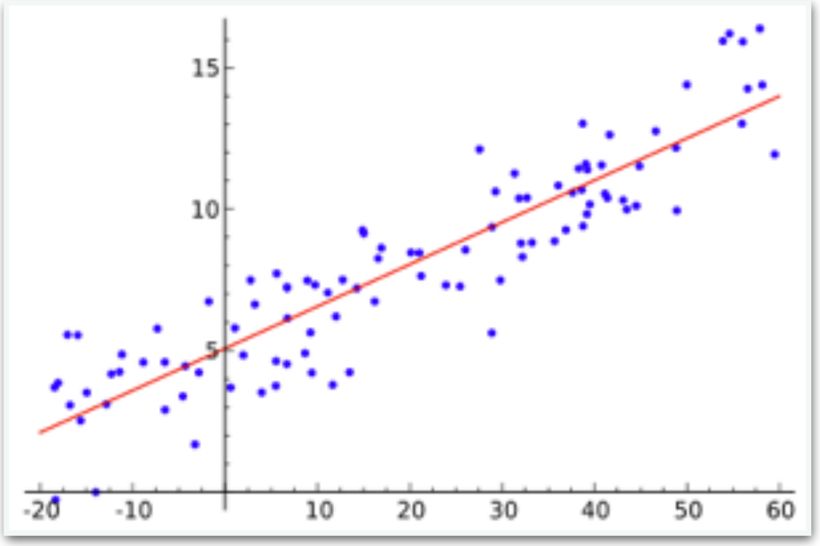
$$
\begin{aligned}
\text{LLR} &= \log\left(p_\theta(+1,\mathbf{x})\right) - \log\left(p_\theta(-1,\mathbf{x})\right) \\
&= \log\left(\theta_0 \prod_{d=1}^{D} \theta_d^{+[x_d=1]}(1-\theta_d^+)^{[x_d=0]}\right) - \log\left((1-\theta_0)\prod_{d=1}^{D} \theta_d^{-[x_d=1]}(1-\theta_d^-)^{[x_d=0]}\right) \\
&= \log\theta_0 - \log(1-\theta_0) + \sum_{d=1}^{D}[x_d=1]\left(\log\theta_d^+ - \log\theta_d^-\right) \\
&\quad \ldots + \sum_{d=1}^{D}[x_d=0]\left(\log(1-\theta_d^+) - \log(1-\theta_d^-)\right) \\
&= \log\left(\frac{\theta_0}{1-\theta_0}\right) + \sum_{d=1}^{D}[x_d=1]\log\left(\frac{\theta_d^+}{\theta_d^-}\right) + \sum_{d=1}^{D}[x_d=0]\log\left(\frac{1-\theta_d^+}{1-\theta_d^-}\right) \\
&= \log\left(\frac{\theta_0}{1-\theta_0}\right) + \sum_{d=1}^{D}x_d\log\left(\frac{\theta_d^+}{\theta_d^-}\right) + \sum_{d=1}^{D}(1-x_d)\log\left(\frac{1-\theta_d^+}{1-\theta_d^-}\right) \\
&= \log\left(\frac{\theta_0}{1-\theta_0}\right) + \sum_{d=1}^{D}x_d\left(\log\left(\frac{\theta_d^+}{\theta_d^-}\right) - \log\left(\frac{1-\theta_d^+}{1-\theta_d^-}\right)\right) + \sum_{d=1}^{D}\log\left(\frac{1-\theta_d^+}{1-\theta_d^-}\right) \\
&= \mathbf{w}^T\mathbf{x} + b
\end{aligned}
$$

Naive bayes classifier has a linear decision boundary!

Generative and conditional models

- Generative models:
  - Model the joint distribution p(**x**,y)
  - Use Bayes rule to compute the label posterior
  - Need to make simplifying assumptions (e.g. Naive bayes)
- In most cases we are given **x** and are only interested in the labels y
- Conditional models:
  - Model the distribution p(y | **x**)
  - Saves some modeling effort
  - Can assume a simpler parametrization of the distribution p(y | **x**)
  - Most of ML we did so far directly aimed at predicting y from **x**

Conditional models: regression



- Assume that y has a linear relationship with **x**
- Generative story of the dataset:
  - For i = 1 to N,
    - Compute: $t_n = \mathbf{w}^T\mathbf{x}_n$
    - Compute: $\epsilon_n = N(0, \sigma^2)$
    - Compute: $y_n = t_n + \epsilon_n$
- This can be written as: $y_n \sim N(\mathbf{w}^T\mathbf{x}_n, \sigma^2)$, and

$$p(y_n|\mathbf{x}_n) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y_n - \mathbf{w}^T\mathbf{x}_n)^2}{2\sigma^2}\right)$$

- The log-likelihood of the dataset is:

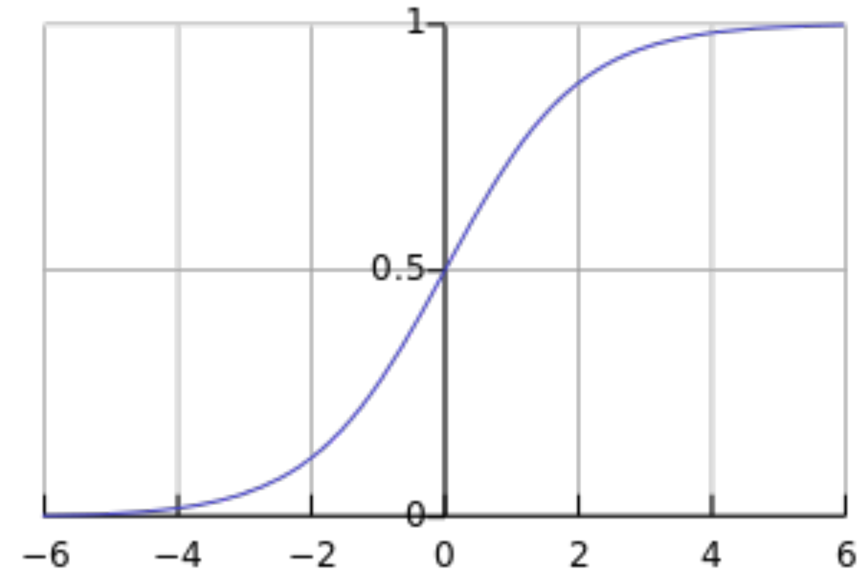
$$\log(\mathcal{D}) = \sum_n -\frac{(y_n - \mathbf{w}^T\mathbf{x}_n)^2}{2\sigma^2} + \text{constants}$$

Maximizing log-likelihood is equivalent to minimizing squared error

Conditional models: classification

- The sigmoid function:

$$\sigma(z) = \frac{1}{1 + \exp[-z]}$$



  - Maps -∞ → 0, ∞ → 1
  - $\sigma(-z) = 1-\sigma(z)$,
  - $d\sigma/dz = \sigma(z)(1-\sigma(z))$

- Generative story of the data:
  - For i = 1 to N,
    - Compute: $t_n = \sigma(\mathbf{w}^T\mathbf{x}_n)$
    - Compute: $z_n = \texttt{Bernoulli}(t_n)$
    - Compute: $y_n = 2z_n - 1$

Conditional models: classification

- The log-likelihood of the dataset is:

$$
\begin{aligned}
\log(\mathcal{D}) &= \sum_n [y_n = +1] \log \sigma(\mathbf{w}^T \mathbf{x}_n) + [y_n = -1] \log(1 - \sigma(\mathbf{w}^T \mathbf{x}_n)) \\
&= \sum_n [y_n = +1] \log \sigma(\mathbf{w}^T \mathbf{x}_n) + [y_n = -1] \log(\sigma(-\mathbf{w}^T \mathbf{x}_n)) \\
&= \sum_n \log \sigma(y_n \mathbf{w}^T \mathbf{x}_n) \\
&= \sum_n - \log(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)) \\
&= \sum_n -\ell^{(\log)}(y_n, \mathbf{w}^T \mathbf{x}_n) \qquad \text{// ignoring constants}
\end{aligned}
$$

Maximizing log-likelihood is equivalent to minimizing logistic loss

This is also called as logistic regression

Regularization with priors

- **Coin toss:** {H,H,H,H} → β = 1
- Maximum likelihood estimation (MLE):

$$\arg\max_{\theta} p(\mathcal{D}|\theta)$$

likelihood

- Maximum a-posteriori estimation (MAP):

prior likelihood

$$\arg\max_{\theta} p(\theta|\mathcal{D}) = \arg\max_{\theta} \frac{p(\theta,\mathcal{D})}{p(\mathcal{D})} = \arg\max_{\theta} p(\theta)p(\mathcal{D}|\theta)$$

$$p(\mathcal{D}) = \int_{\theta} p(\theta,\mathcal{D})d\theta$$

data probability

log-prior log-likelihood

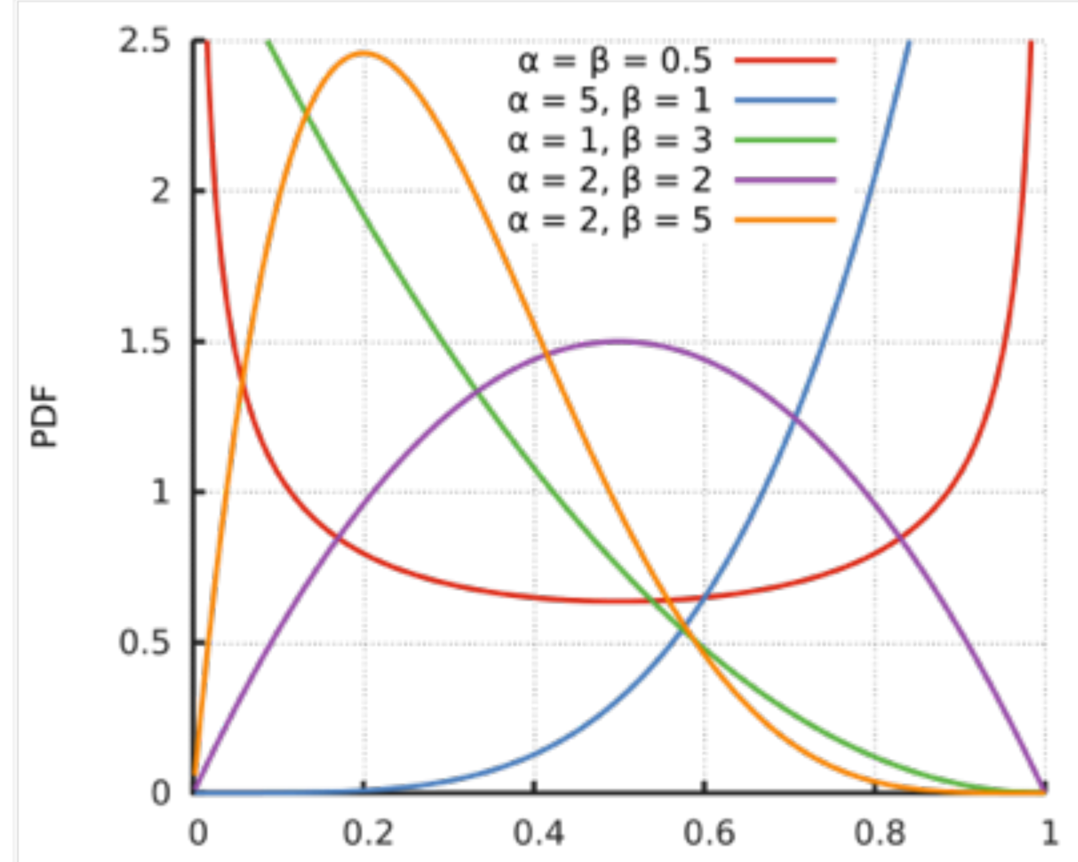
- MAP estimation in log space: $\arg\max_{\theta} \left[\log p(\theta) + \log p(\mathcal{D}|\theta)\right]$

Regularization with priors: coin toss

- Beta distribution as a prior on β

$$\text{Beta}(\beta; a, b) = c\beta^{a-1}(1-\beta)^{b-1}$$

$$\text{Mode} = \frac{a-1}{a+b-2}$$



- Posterior over β given the prior and **H-**many heads and **T-**many tails:

$$p(\beta|\mathcal{D}) \propto p(\beta)p(\mathcal{D}|\beta)$$

$$\propto \beta^{a-1}(1-\beta)^{b-1}\beta^{H}(1-\beta)^{T} = \text{Beta}(a+H, b+T)$$

$$\beta_{\text{MAP}} = \frac{a+H-1}{a+H+b+T-2}$$

$$\beta_{\text{MLE}} = \frac{H}{H+T}$$

Conjugate priors

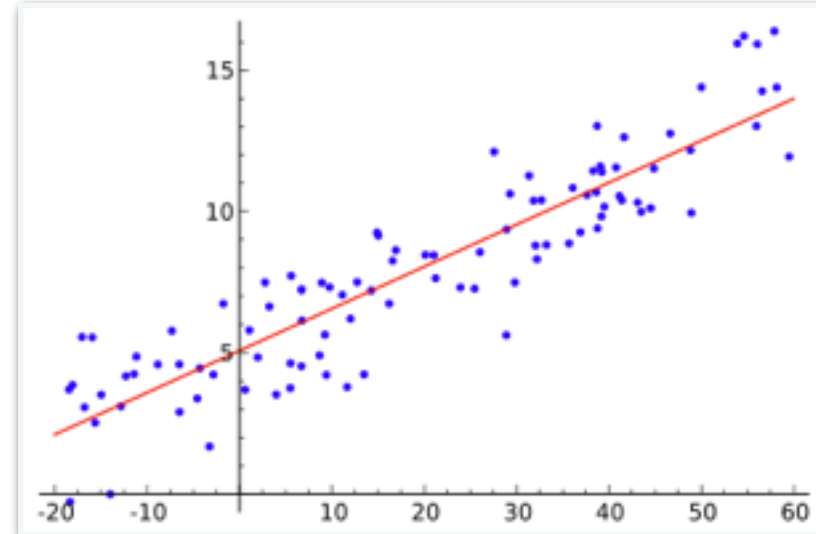
- If the prior and posterior are in the same family, then the prior is conjugate to the likelihood

posterior prior likelihood

$$p(\theta|\mathcal{D}) \propto p(\theta)p(\mathcal{D}|\theta)$$

- Beta is conjugate to Bernoulli
  - Prior: Beta(a, b)   Data: {H, T}   Posterior: Beta(a+H, b+T)
  - Interpretation of the prior: pseudo count of a-1 heads and b-1 tails
- Dirichlet is conjugate to Multinomial
  - Prior: $\text{Dirichlet}(\theta; a_1, a_2, \ldots, a_n) \propto \prod_k \theta_k^{a_k - 1}$
  - Data: $\{k_1, k_2, \ldots, k_n\}$ occurrence of each side
  - Posterior: $\text{Dirichlet}(\theta; a_1 + k_1, a_2 + k_2, \ldots, a_n + k_n)$
  - Interpretation of the prior: pseudo count of a_i -1 for the i^{th} side

Regularization with priors: regression



- Assume that y has a linear relationship with **x**
- Generative story of the dataset:
  - For i = 1 to N,
    - Compute: $t_n = \mathbf{w}^T \mathbf{x}_n$
    - Compute: $\epsilon_n = N(0, \sigma^2)$
    - Compute: $y_n = t_n + \epsilon_n$ $\longrightarrow$ $y_n \sim N(\mathbf{w}^T \mathbf{x}_n, \sigma^2)$
- Assume a Gaussian prior on the weights:

$$p(\mathbf{w}) = N(0_D, \tau^2 \mathbf{I}_D) = c \exp\left(\sum_i -\frac{w_i^2}{2\tau^2}\right)$$

$$c \exp\left(\sum_i -\frac{|w_i|}{b}\right)$$

Laplace prior for l_1

- MAP estimate of **w:**

$$\arg\max_{\mathbf{w}} \sum_i -\frac{w_i^2}{2\tau^2} + \sum_n -\frac{(y_n - \mathbf{w}^T \mathbf{x}_n)^2}{2\sigma^2} + \text{constants}$$

MAP is same as l_2 regularized least-squares regression

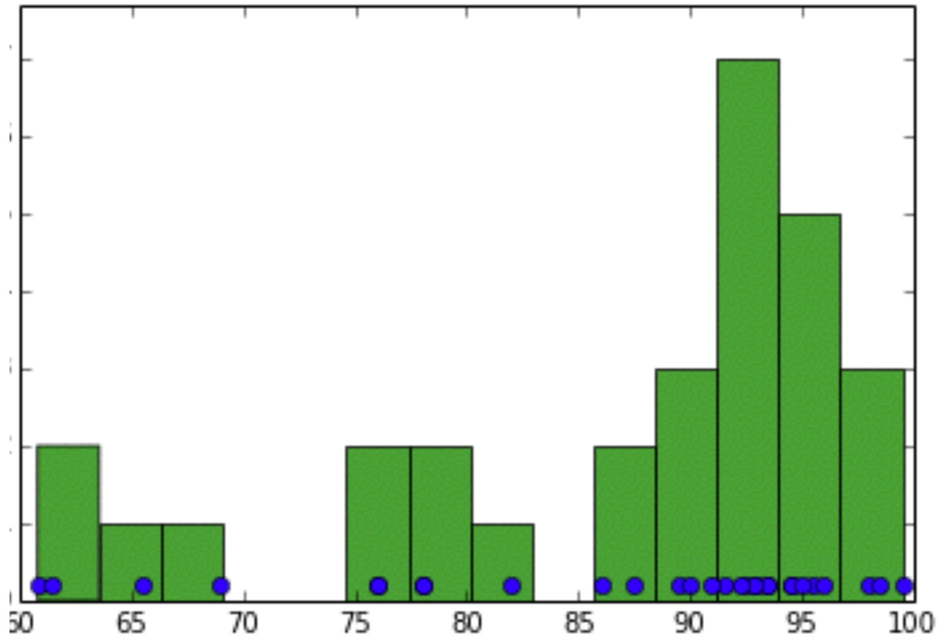
Non-parametric density models

- So far we assumed that the probability distribution was parametric
  - Gaussian distribution, Binomial distribution, etc
  - This allowed us to estimate the data distribution by estimating the parameters of the probability distribution
- However, the data distribution can be complicated
  - For example there might be multiple modes
- Non-parametric density models offer a flexible alternative

Density estimation using histograms

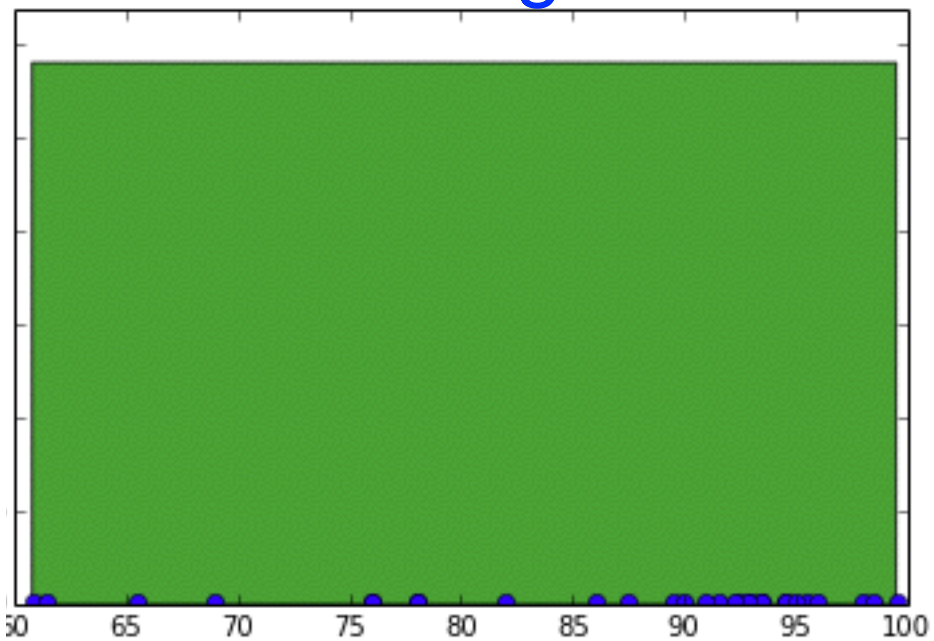
- This is the simplest example of a non-parametric density model

$p(x)$

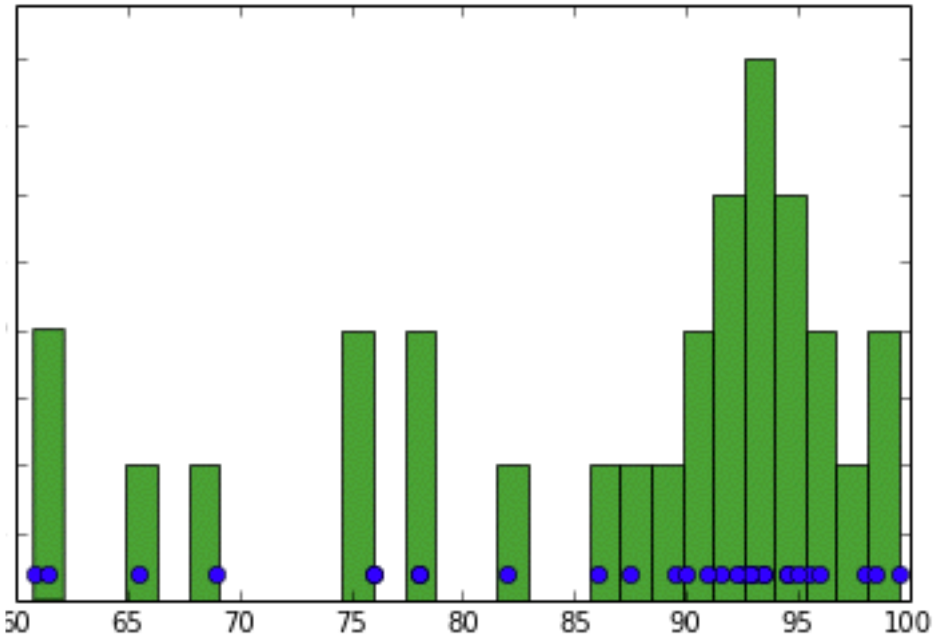


- The bin size is a hyperparameter of the model

too large

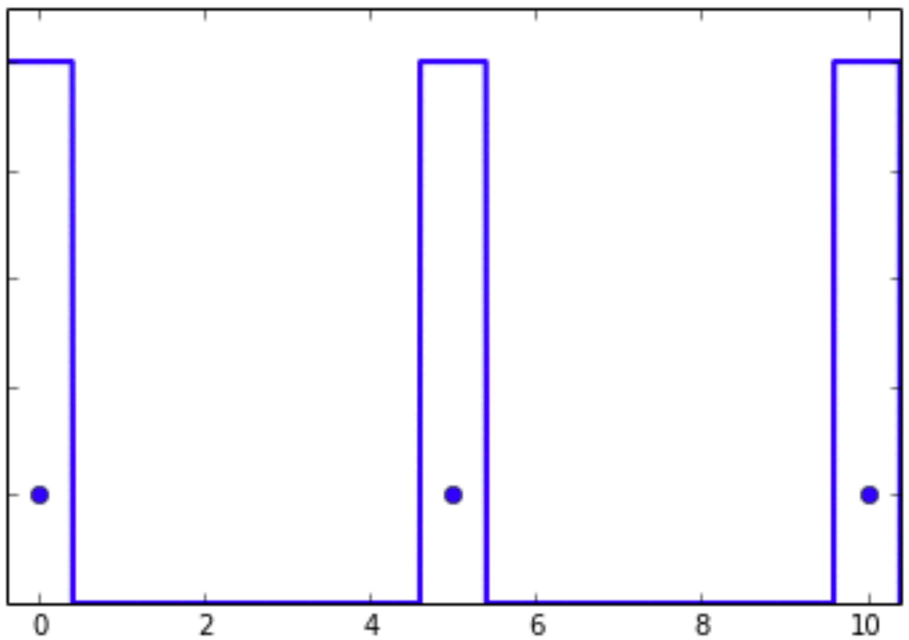


too small



Kernel density estimation

- Histograms are sums of delta functions centered at each point



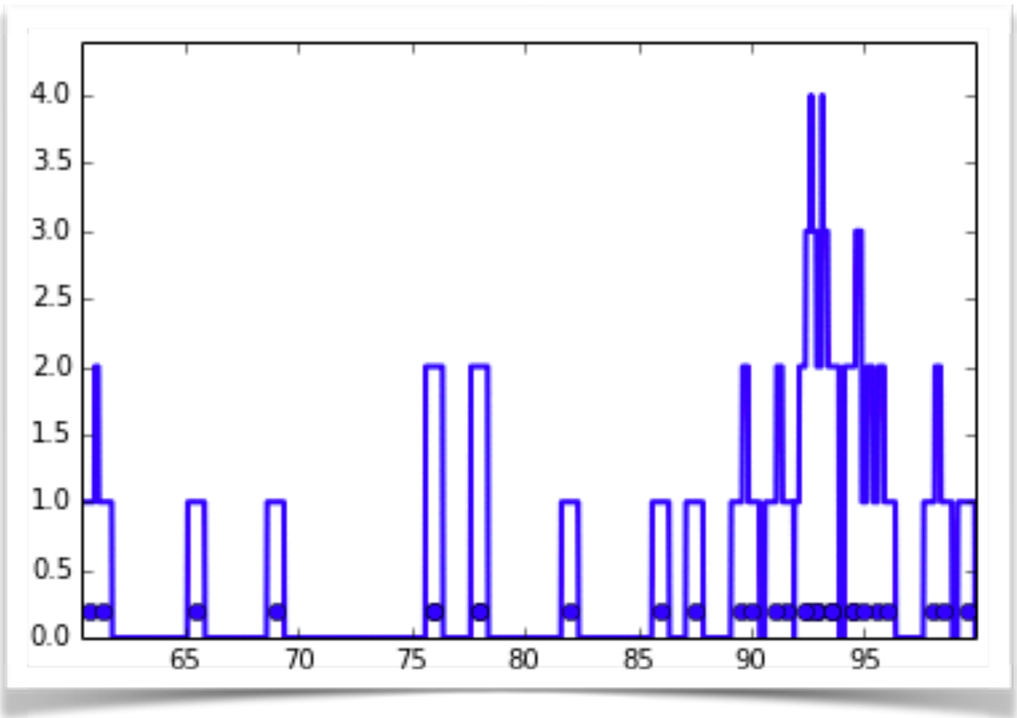
$$p(x) = \frac{1}{N}\sum_{i=1}^{N} K(x - x_i)$$

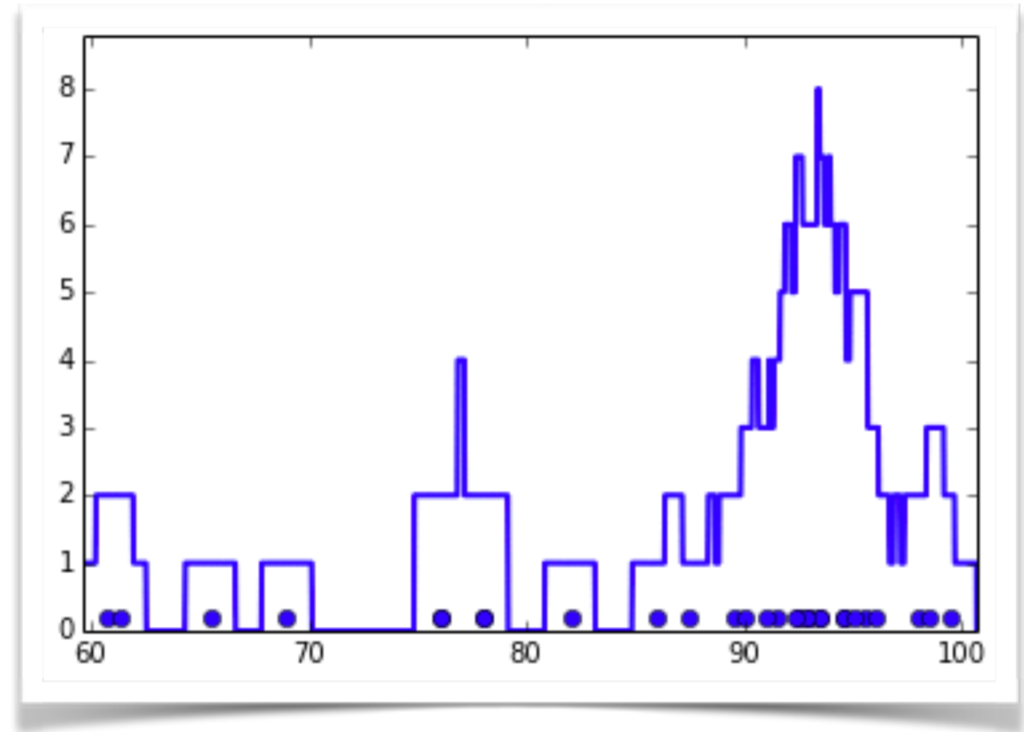
$$K(x - x_i) = \begin{cases} \frac{1}{b} & |x - x_i| \le \frac{b}{2} \\ 0 & \text{otherwise} \end{cases}$$

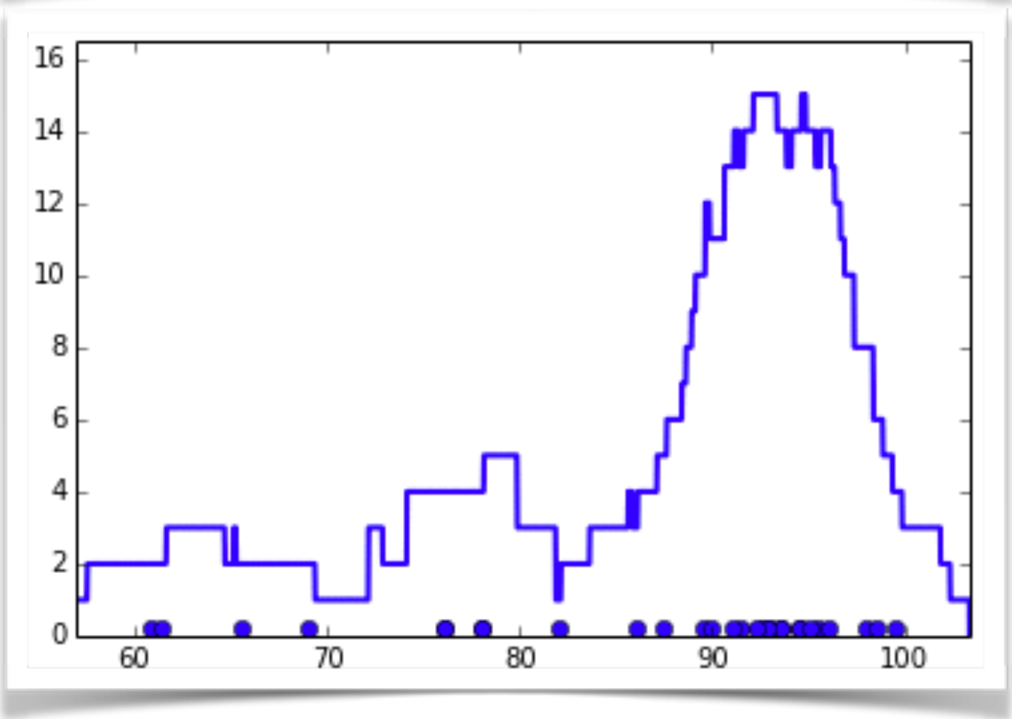
- The hyperparameter *b* controls the width of the delta function
- The function *K* is called the kernel function
- These density estimators are also called as Parzen window estimators
- Set hyperparameters by cross-validation
  - MLE estimate is b=0. This is clearly wrong (overfitting)

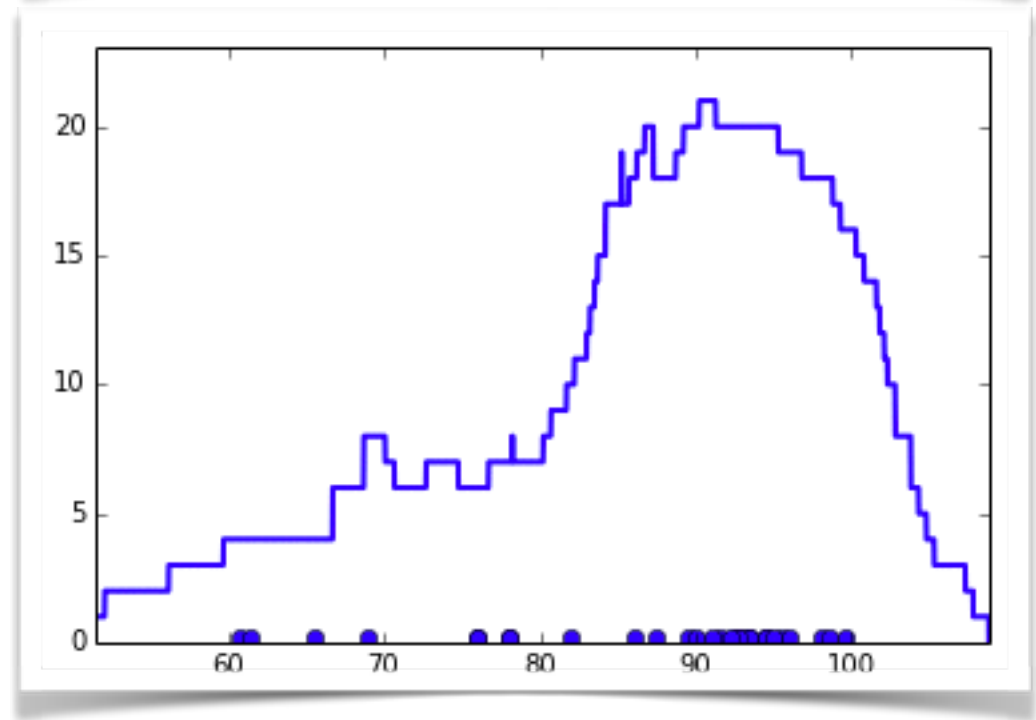
Kernel density estimation: example

Rectangle kernel $K(x - x_i) = \begin{cases} \frac{1}{b} & |x - x_i| \leq \frac{b}{2} \\ 0 & \text{otherwise} \end{cases}$



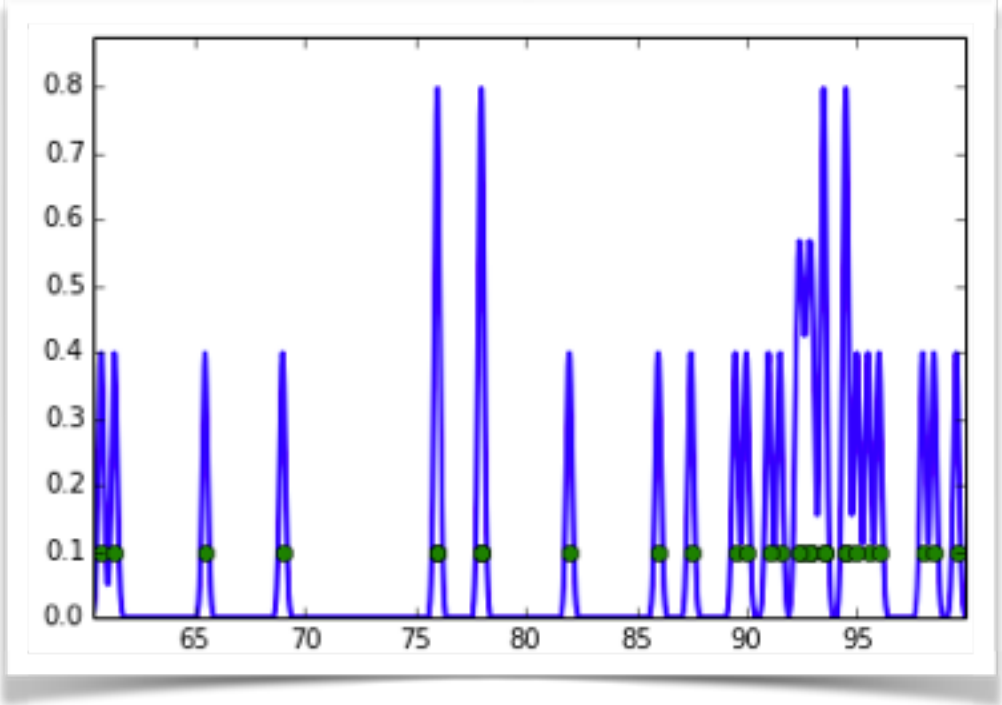


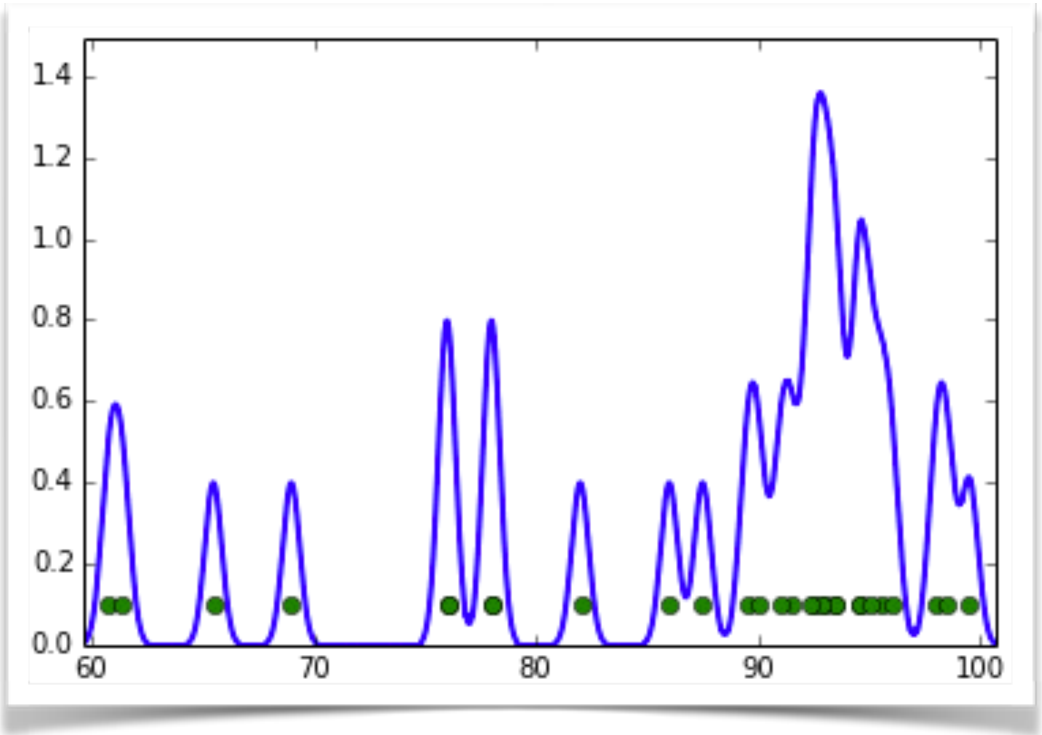


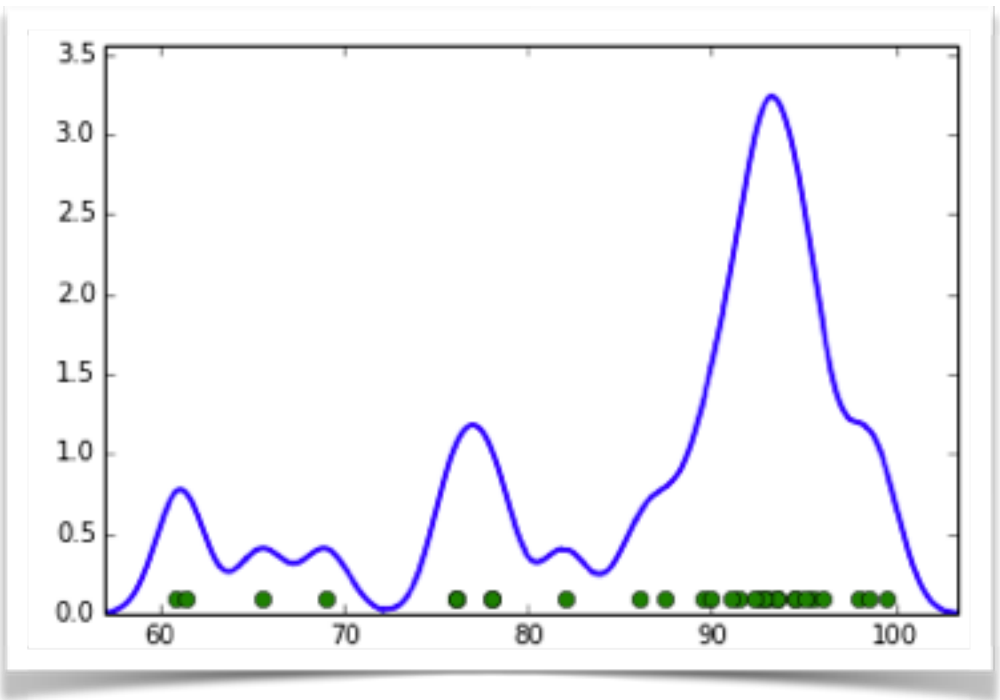


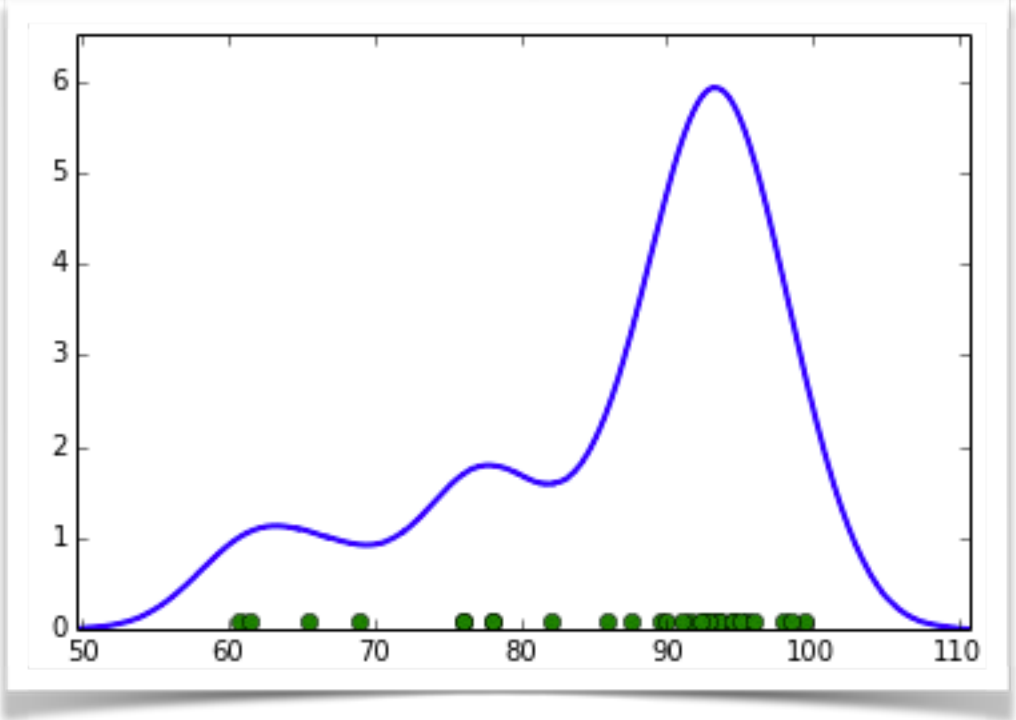
Kernel density estimation: example

Gaussian kernel $$K(x - x_i) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - x_i)^2}{2\sigma^2}\right)$$



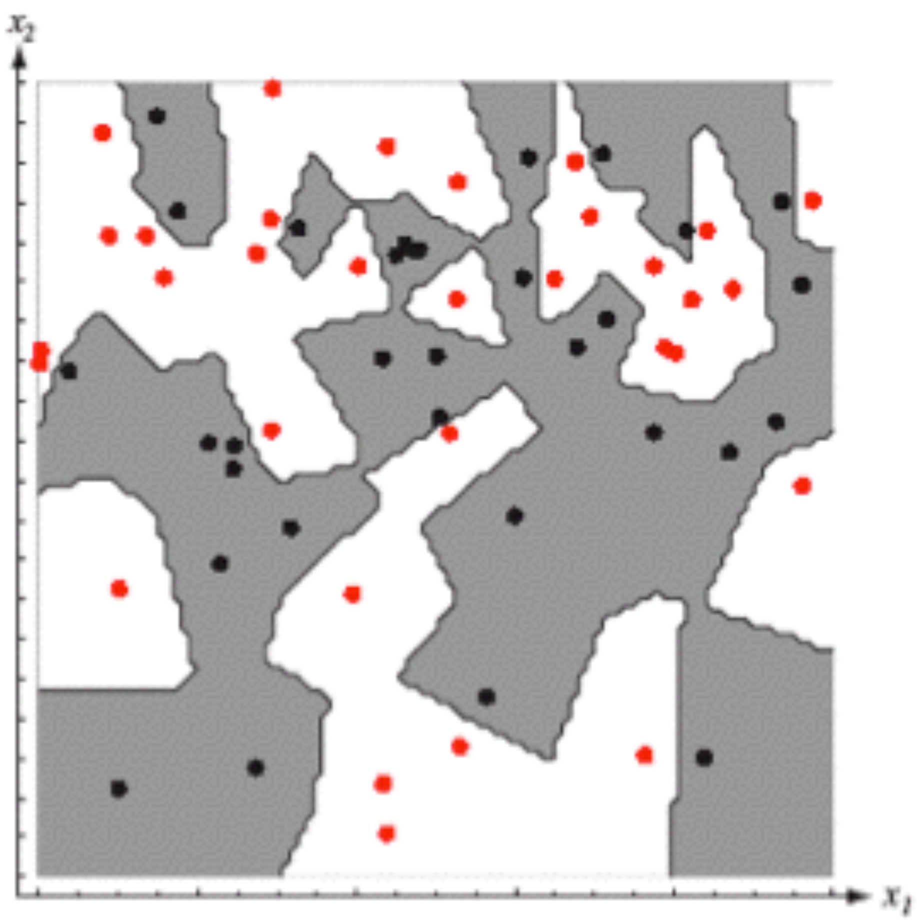




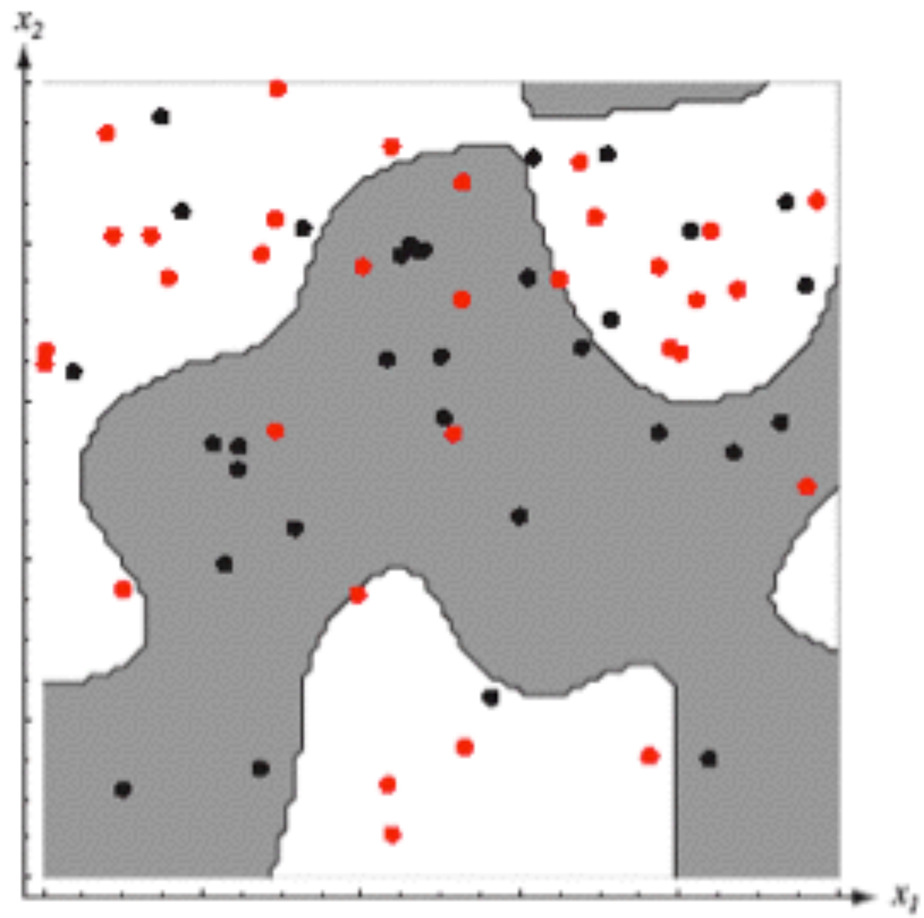


Kernel density classifier

- Estimate p(**x** | +1) and p(**x** | -1) separately
- Compute likelihood ratio: p(+1)p(**x** |+1) / p(-1)p(**x** |-1)
  - Predict class +1 if LR > 1



small width



large width

- kNN classifier is a Kernel density classifier with kernel width = distance to the k^{th} nearest neighbor

Figure from Duda et al.

Summary

- Probabilistic modeling views learning as statistical inference
- Two ways to estimate parameters of the distribution
  - Maximum likelihood: maximize $p(\mathcal{D}|\theta)$
  - Maximum a-posteriori: maximize $p(\theta|\mathcal{D})$
- Two kinds of data models
  - Generative: $p(y, \mathbf{x})$
    - Example: Naive bayes, Kernel density
  - Conditional: $p(y \mid \mathbf{x})$
    - Example: Linear and logistic regression
- Two kinds of probability models
  - Parametric: Gaussian, Bernoulli, etc
    - Learning by MLE and MAP
  - Non-parametric: kernel density estimators
    - Learning by cross validation

Slides credit

- Figure of the logistic and linear regression are from Wikipedia
- Figure of the beta distribution is from Wikipedia
- Figures for kernel density estimation are from http://www.mglerner.com/blog/?p=28 (the page has an interactive demo)
- Parzen window figure: "Pattern Classification", Duda, Hart & Stork
- Some slides are based on the CIML book by Hal Daume III