Probabilistic Methods for Classification

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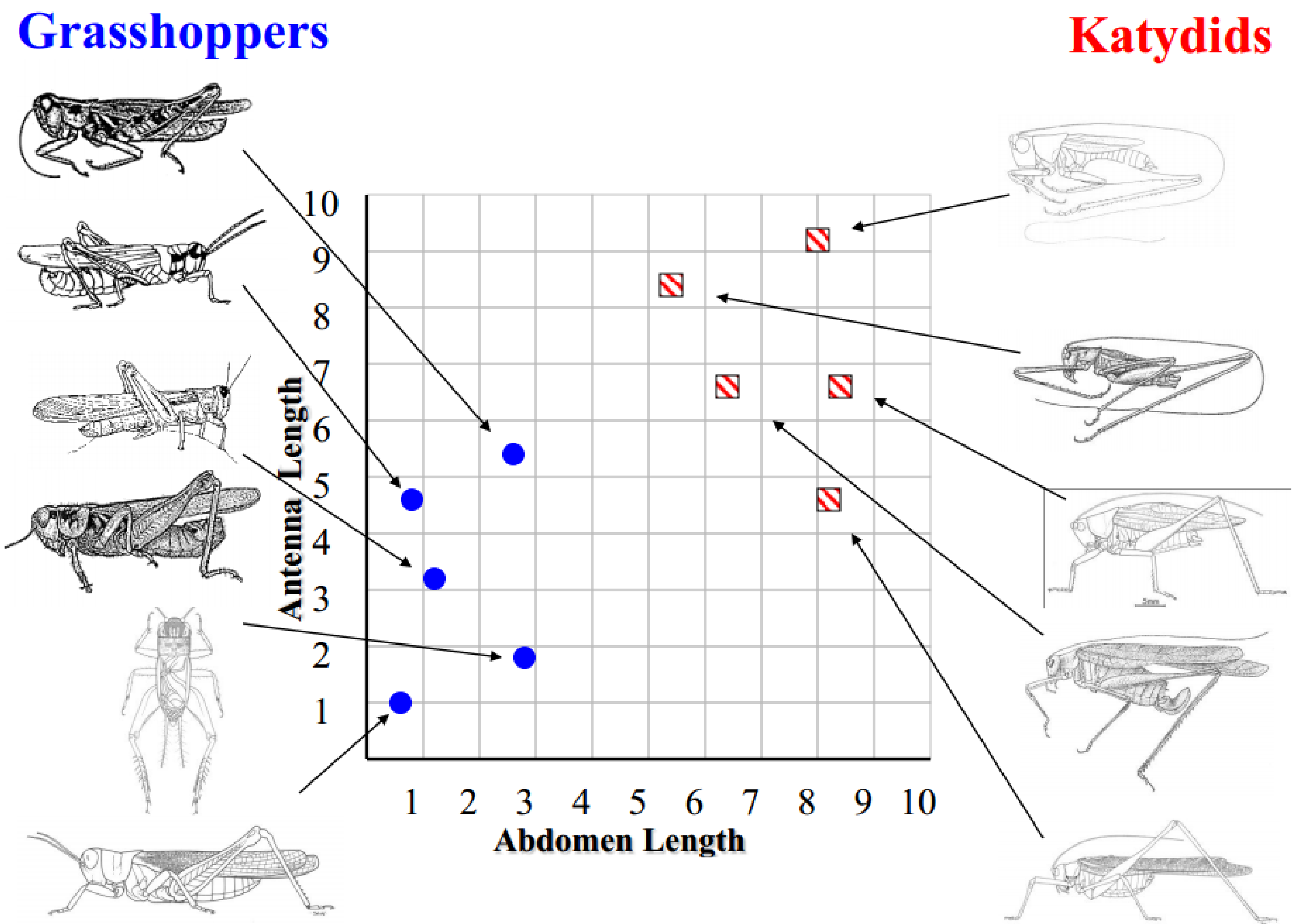
Outline

- Probabilistic methods for supervised learning
- Naive Bayes classifier
- Logistic regression
- Exponential family distributions
- Generalized linear models

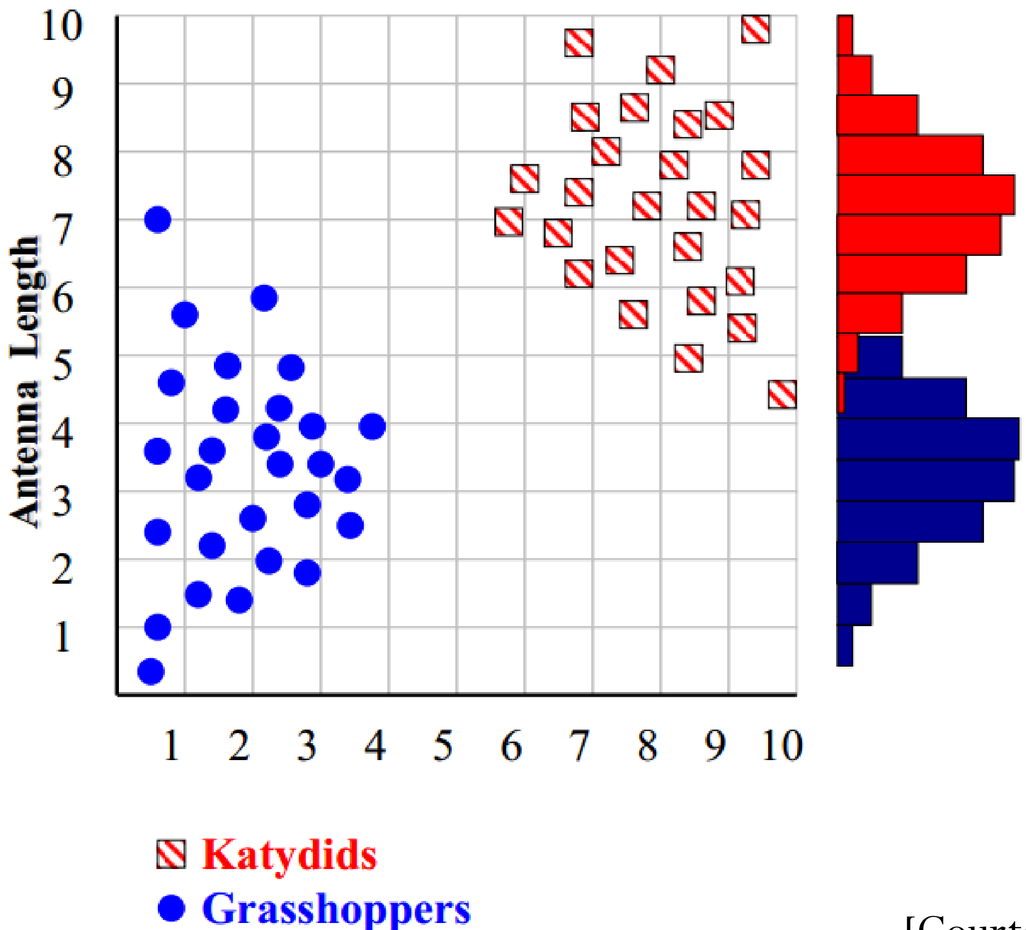
An Intuitive Example



[Courtesy of E. Keogh]

With more data …

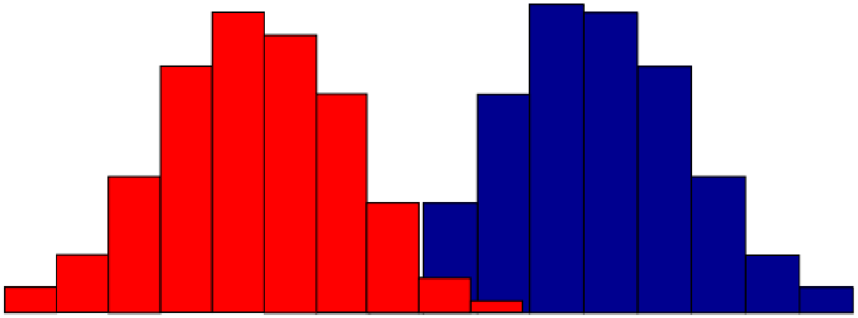
- Build a histogram, e.g., for "Antenna length"



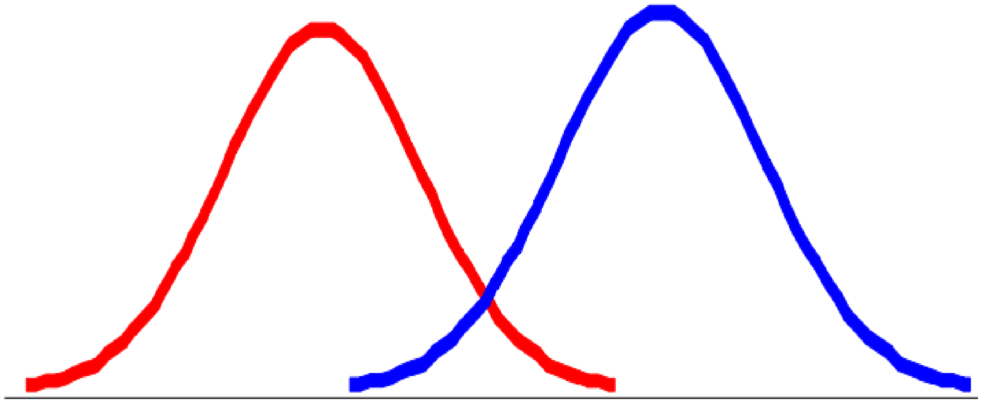
[Courtesy of E. Keogh]

Empirical distribution

- **Histogram** (or empirical distribution)



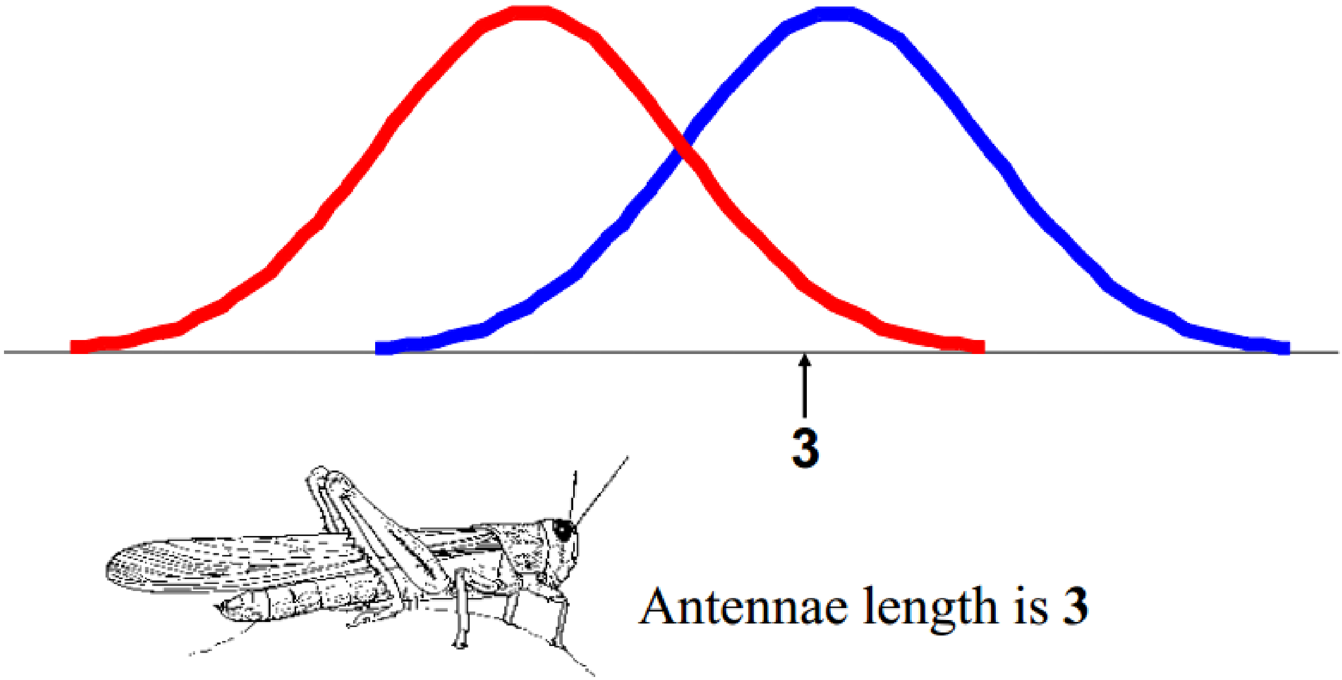
- Smoothing with kernel density estimation (KDE):



[Courtesy of E. Keogh]

Classification?

- Classify another insect we find. Its antennae are 3 units long
- Is it more probable that the insect is a **Grasshopper** or a **Katydid**?

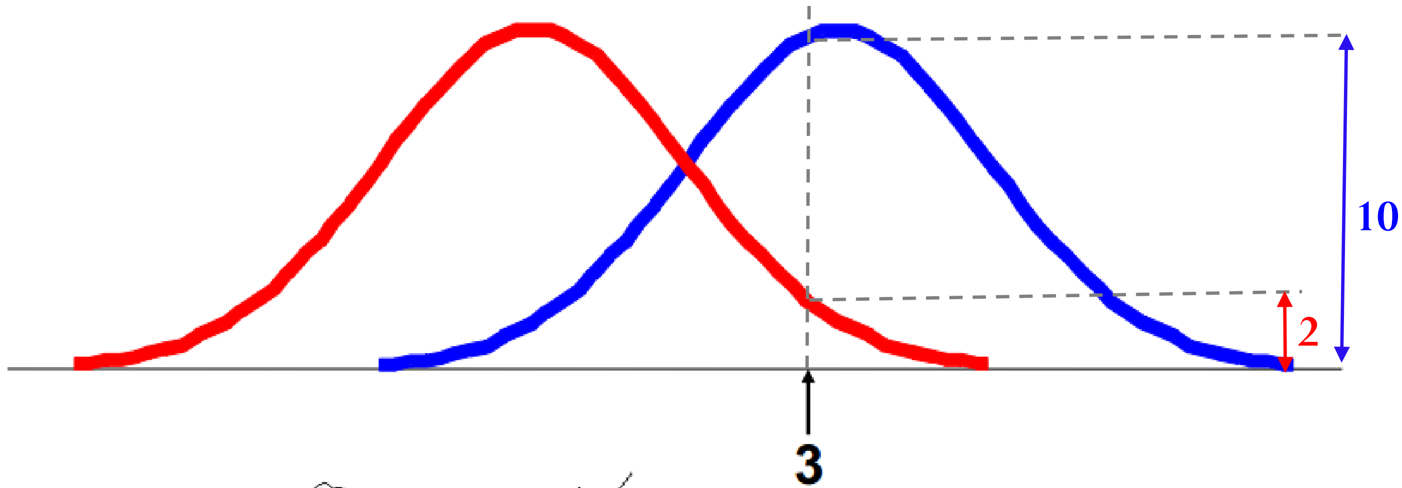


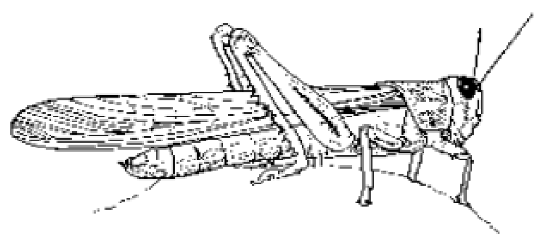
[Courtesy of E. Keogh]

Classification Probability

P(**Grasshopper** | **3**) = 10 / (10 + 2) = 0.833

P(**Katydid** | **3**) = 2 / (10 + 2) = 0.166





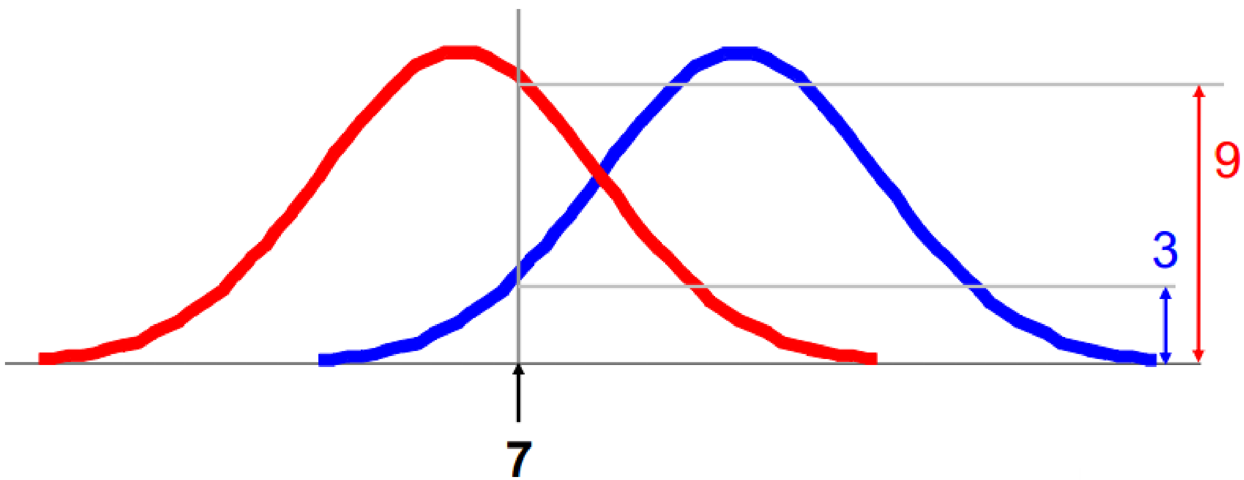
Antennae length is **3**

[Courtesy of E. Keogh]

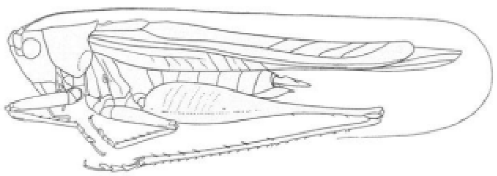
Classification Probability

P(**Grasshopper** | **7**) = 3 / (3 + 9) = 0.250

P(**Katydid** | **7**) = 9 / (3 + 9) = 0.750



Antennae length is **7**

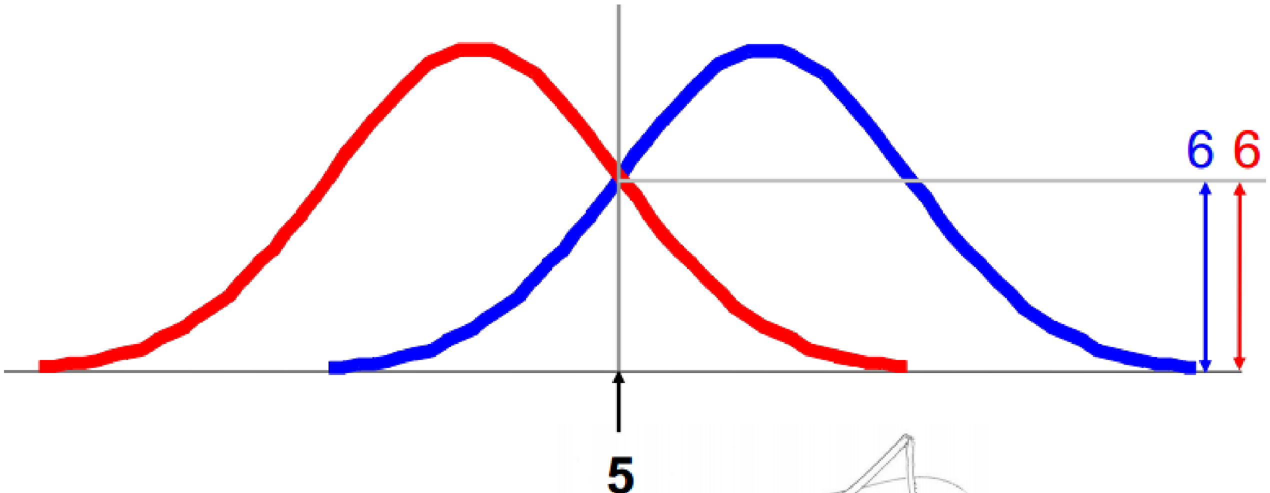


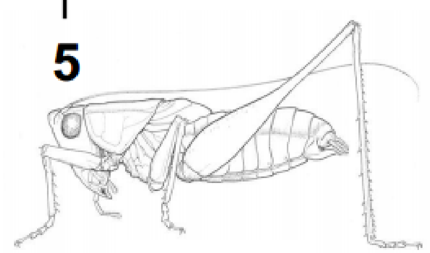
[Courtesy of E. Keogh]

Classification Probability

P(**Grasshopper** | **5**) = 6 / (6 + 6) = 0.500

P(**Katydid** | **5**) = 6 / (6 + 6) = 0.500



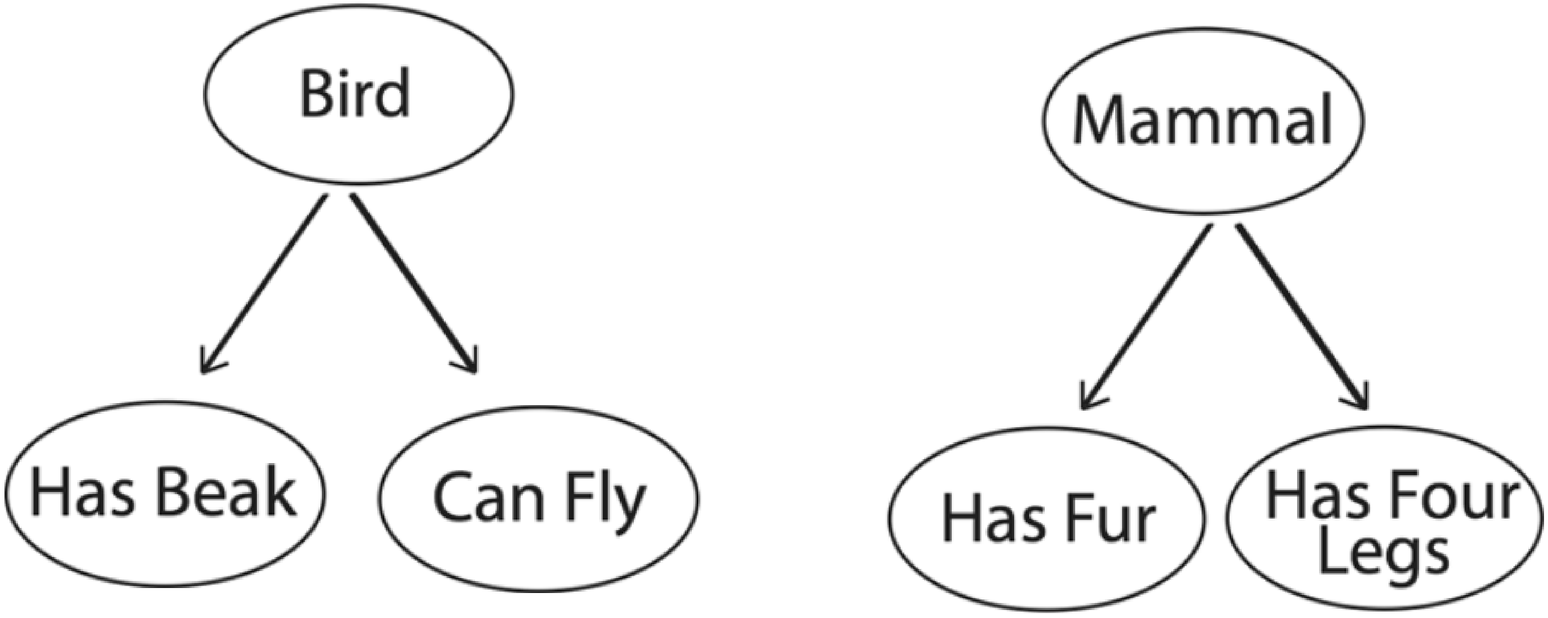


Antennae length is **5**

[Courtesy of E. Keogh]

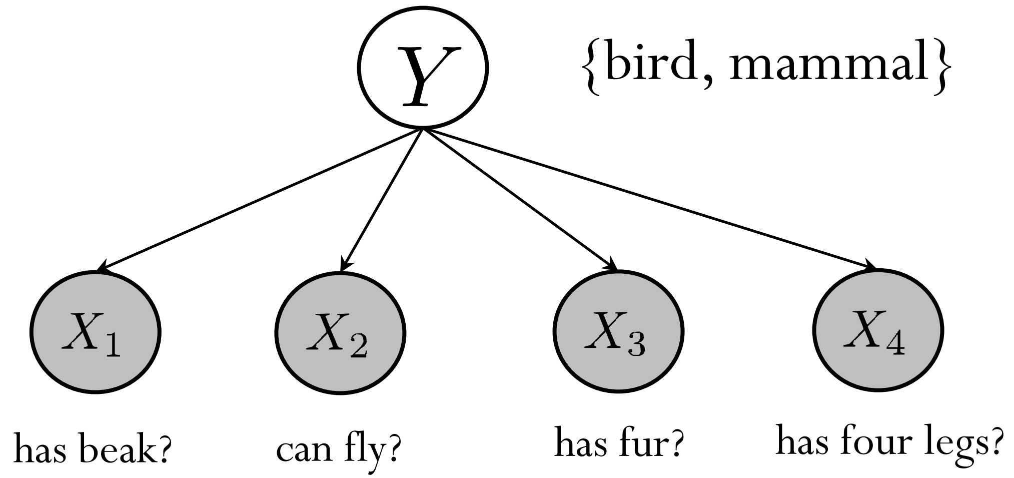
Naïve Bayes Classifier

- The simplest "**category-feature**" generative model:
  - **Category**: "bird", "Mammal"
  - **Features**: "has beak", "can fly" …



Naïve Bayes Classifier

- **A mathematic model**:
  - **Naive Bayes assumption**: features $X_1, \ldots, X_d$ are conditionally independent given the class label Y



A joint distribution:

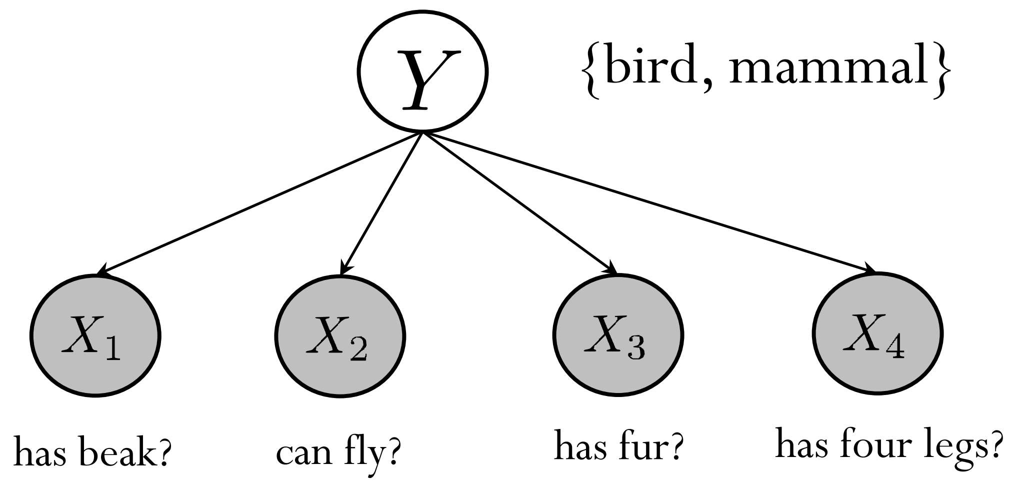
prior

likelihood

$$p(\mathrm{x}, y) = p(y)p(\mathrm{x}|y)$$

Naïve Bayes Classifier

- **A mathematic model**:



Inference via Bayes rule:

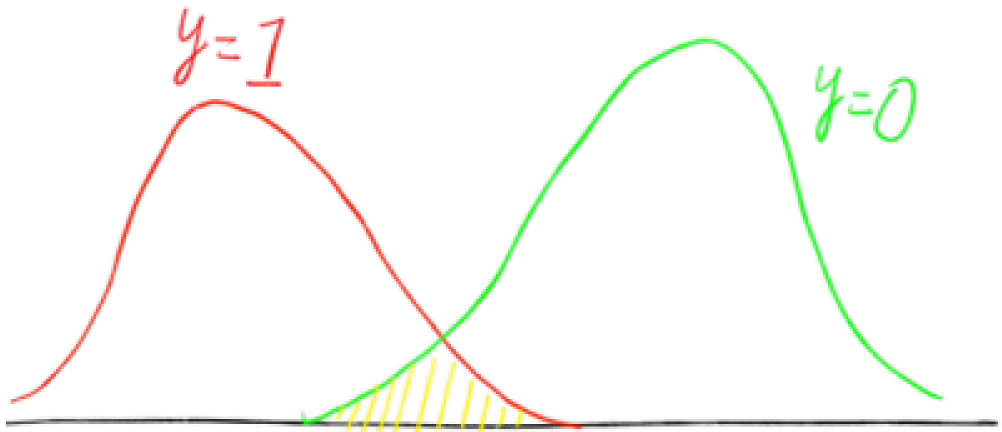
$$p(y|\mathrm{x}) = \frac{p(\mathrm{x}, y)}{p(\mathrm{x})} = \frac{p(y)p(\mathrm{x}|y)}{p(\mathrm{x})}$$

Bayes' decision rule:

$$y^* = \arg\max_{y \in \mathcal{Y}} p(y|\mathrm{x})$$

Bayes Error

- **Theorem**: Bayes classifier is optimal!



$$p(error|\mathbf{x}) = \begin{cases} p(y=1|\mathbf{x}) & \text{if we decide } y=0 \\ p(y=0|\mathbf{x}) & \text{if we decide } y=1 \end{cases}$$

$$p(error) = \int_{-\infty}^{\infty} p(error|\mathbf{x})p(\mathbf{x})d\mathbf{x}$$

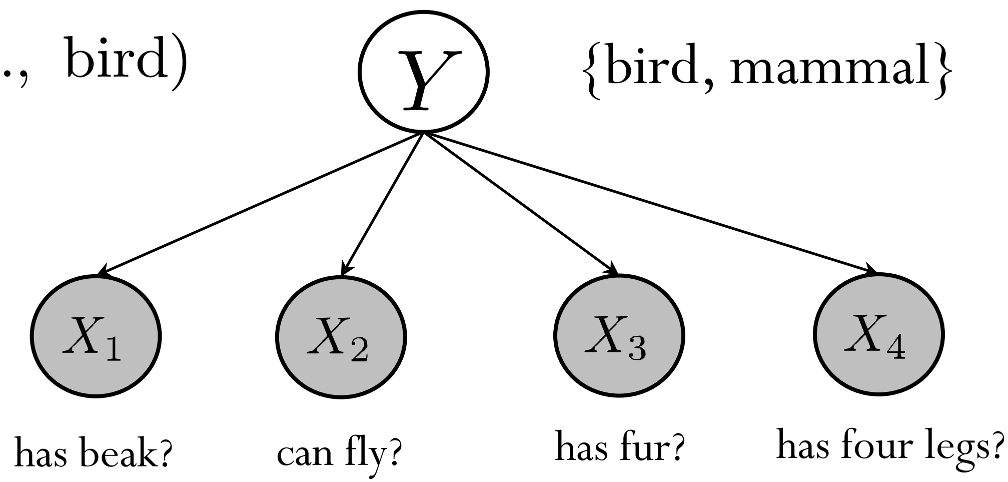
- *However, the true distribution is unknown.*

- *Learning!*
  - *We need to estimate it!*

Naïve Bayes Classifier

- **How to learn model parameters?**
  - Assume X are d binary features, Y has 2 possible labels

$$p(y|\pi) = \begin{cases} \pi & \text{if } y = 1 \ (i.e., \ \text{bird}) \\ 1 - \pi & \text{otherwise} \end{cases}$$



$$p(x_j|y = 0, q) = \begin{cases} q_{0j} & \text{if } x_j = 1 \\ 1 - q_{0j} & \text{otherwise} \end{cases} \qquad p(x_j|y = 1, q) = \begin{cases} q_{1j} & \text{if } x_j = 1 \\ 1 - q_{1j} & \text{otherwise} \end{cases}$$

  - *How many parameters to estimate?*

单选题 1分

设置

Assume X are d binary features, Y has 2 possible labels

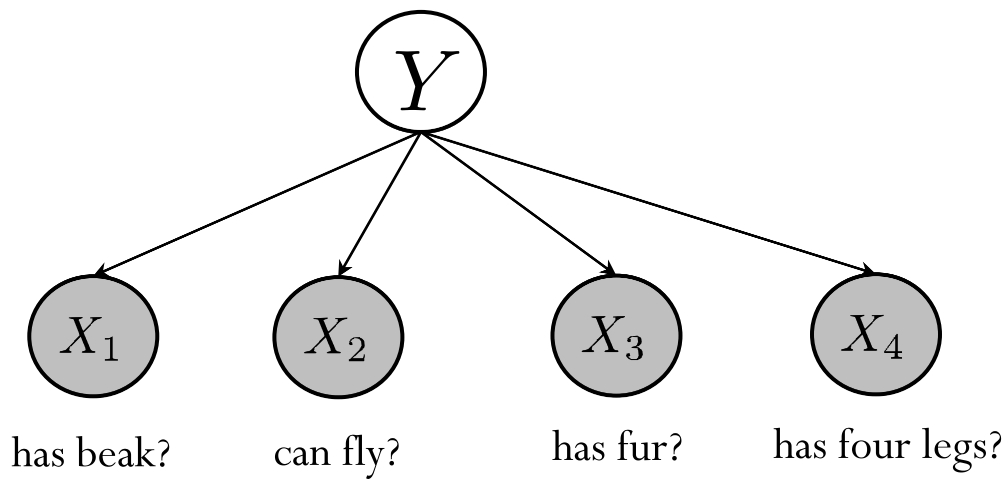
How many parameters to estimate?

A 5

B 9

C 10

D 32



提交

Naïve Bayes Classifier

- **How to learn model parameters?**
  - Assume X are d binary features, Y has 2 possible labels

$$p(y|\pi) = \begin{cases} \pi & \text{if } y = 1 \ (i.e., \ \text{bird}) \\ 1 - \pi & \text{otherwise} \end{cases}$$

$$p(x_j|y=0,q) = \begin{cases} q_{0j} & \text{if } x_j = 1 \\ 1 - q_{0j} & \text{otherwise} \end{cases} \qquad p(x_j|y=1,q) = \begin{cases} q_{1j} & \text{if } x_j = 1 \\ 1 - q_{1j} & \text{otherwise} \end{cases}$$

  - *How many parameters to estimate?*

Naïve Bayes Classifier

- **How to learn model parameters?**
- **A set of training data:**
  - (1, 1, 0, 0; 1)
  - (1, 0, 0, 0; 1)
  - (0, 1, 1, 0; 0)
  - (0, 0, 1, 1; 0)
- **Maximum likelihood estimation** (N: # of training data)

$$p(\{\mathbf{x}_i, y_i | \pi, q\}) = \prod_{i=1}^{N} p(\mathbf{x}_i, y_i | \pi, q)$$

Naïve Bayes Classifier

- **Maximum likelihood estimation** (N: # of training data)

$$(\hat{\pi}, \hat{q}) = \arg\max_{\pi, q} p(\{\mathbf{x}_i, y_i\} | \pi, q)$$

$$(\hat{\pi}, \hat{q}) = \arg\max_{\pi, q} \log p(\{\mathbf{x}_i, y_i\} | \pi, q)$$

- **Results (**count frequency! Exercise?**)**:

$$\hat{\pi} = \frac{N_1}{N} \qquad \hat{q}_{0j} = \frac{N_0^j}{N_0} \qquad \hat{q}_{1j} = \frac{N_1^j}{N_1}$$

$$N_k = \sum_{i=1}^{N} \mathbf{I}(y_i = k) : \ \# \text{ of data in category } k$$

$$N_k^j = \sum_{i=1}^{N} \mathbf{I}(y_i = k,\ x_{ij} = 1) : \ \# \text{ of data in category } k \text{ that has feature } j$$

Naïve Bayes Classifier

- Data scarcity issue (zero-counts problem):

$$\hat{\pi} = \frac{N_1}{N} \qquad \hat{q}_{0j} = \frac{N_0^j}{N_0} \qquad \hat{q}_{1j} = \frac{N_1^j}{N_1}$$

  - ***How about if some features do not appear?***

- Laplace smoothing (Additive smoothing):

$$\hat{q}_{0j} = \frac{N_0^j + \alpha}{N_0 + 2\alpha}$$

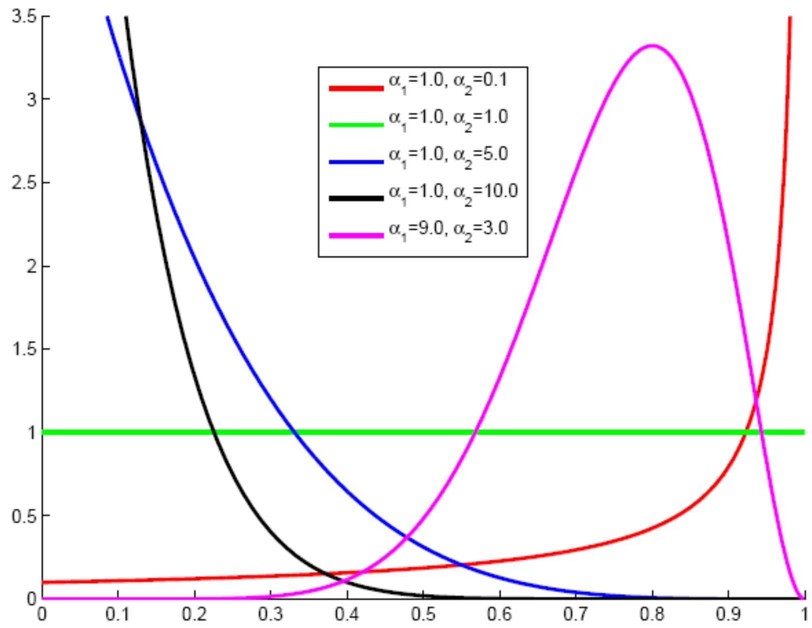
$$\alpha > 0$$

$$\hat{q}_{1j} = \frac{N_1^j + \alpha}{N_1 + 2\alpha}$$

A Bayesian Treatment

- Put a prior on the parameters

$$p_0(q_{0j}|\alpha_1,\alpha_2) = \mathrm{Beta}(\alpha_1,\alpha_2) = \frac{\Gamma(\alpha_1+\alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} q_{0j}^{\alpha_1-1}(1-q_{0j})^{\alpha_2-1}$$



A Bayesian Treatment

- Maximum a Posterior Estimate (MAP):

$$\hat{q} = \arg\max_{q} \log p(q|\{\mathbf{x}_i, y_i\})$$
$$= \arg\max_{q} \log p_0(q) + \log p(\{\mathbf{x}_i, y_i\}|q)$$

- Results (Exercise?):

$$\hat{q}_{0j} = \frac{N_0^j + \alpha_1 - 1}{N_0 + \alpha_1 + \alpha_2 - 2}$$

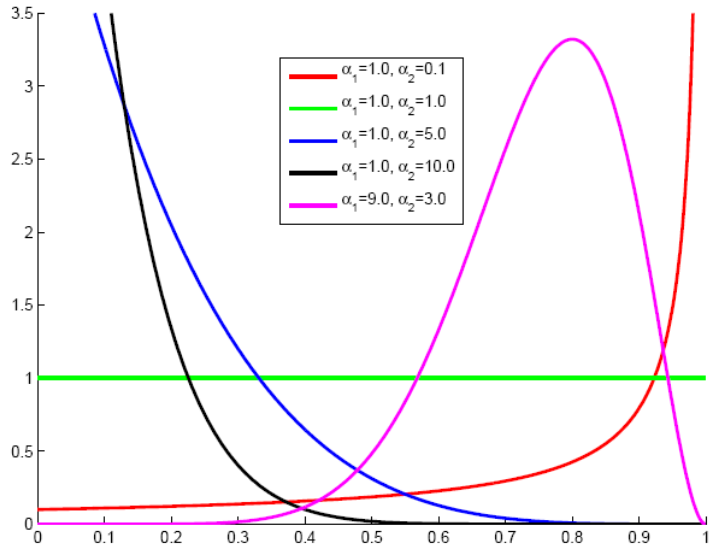
$$\hat{q}_{1j} = \frac{N_1^j + \alpha_1 - 1}{N_1 + \alpha_1 + \alpha_2 - 2}$$

A Bayesian Treatment

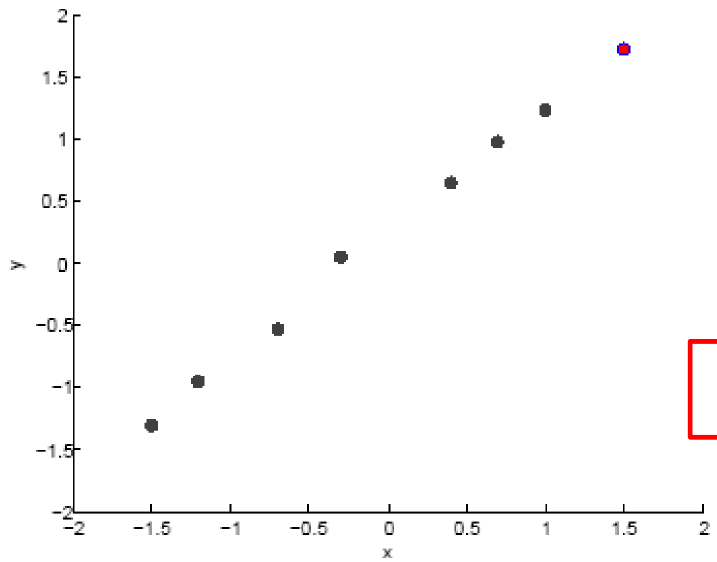
- Maximum a Posterior Estimate (MAP):

$$\hat{q}_{0j} = \frac{N_0^j + \alpha_1 - 1}{N_0 + \alpha_1 + \alpha_2 - 2}$$

- If $\alpha_1 = \alpha_2 = 1$ (non-informative prior), no effect
  - MLE is a special case of Bayesian estimate
- Increase α_1, α_2 , lead to heavier influence from prior



Bayesian Regression



$$\boxed{f : \mathcal{X} \rightarrow \mathcal{Y}}$$

- Goal: learn a function from noisy observed data
  - Linear $\mathcal{F}_{linear} = \{f : \ f = wx + b, \ w, b \in \mathbb{R}\}$
  - Polynomial $\mathcal{F}_{polynomial} = \{f : \ f = \sum_k w_k x^k, \ w_k \in \mathbb{R}\}$
  - …

$$\vdots$$

Bayesian Regression

- Noisy observations

$$y = f(\mathbf{x}) + \epsilon, \text{ where } \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

- Gaussian likelihood function for linear regression $f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i$

$$p(\mathbf{y}|X, \mathbf{w}) = \prod_{i=1}^{N} p(y_i|\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(X^\top \mathbf{w}, \sigma_n^2 I)$$

- Gaussian prior (Conjugate)

$$\mathbf{w} \sim \mathcal{N}(0, \Sigma_d)$$

- Inference with Bayes' rule
  - Posterior $$p(\mathbf{w}|X, \mathbf{y}) = \mathcal{N}(\frac{1}{\sigma_n^2} A^{-1} X \mathbf{y}, A^{-1}), \text{ where } A = \sigma_n^{-2} X X^\top + \Sigma_d^{-1}$$
  - Marginal likelihood
  - Prediction

$$p(\mathbf{y}|X) = \int p(\mathbf{y}|X, \mathbf{w}) p(\mathbf{w}) d\mathbf{w}$$

$$p(f_*|\mathbf{x}_*, X, \mathbf{y}) = \int p(f_*|\mathbf{x}_*, \mathbf{w}) p(\mathbf{w}|X, \mathbf{y}) d\mathbf{w} = \mathcal{N}\left(\frac{1}{\sigma_n^2} \mathbf{x}_*^\top A^{-1} X \mathbf{y}, \mathbf{x}_*^\top A^{-1} \mathbf{x}_*\right)$$

Extensions of NB

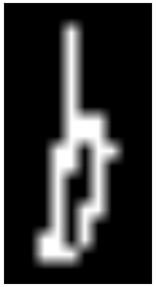
- We covered the case with binary features and binary class labels

- NB is applicable to the cases:
  - Discrete features + discrete class labels
  - Continuous features + discrete class labels
  - …

- More dependency between features can be considered
  - Tree augmented NB
  - …

Gaussian Naive Bayes (GNB)

- E.g.: character recognition: feature X_i is intensity at pixel i:

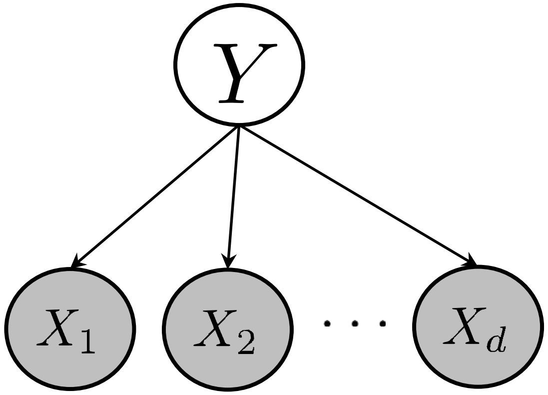


- The generative process is

$$Y \sim \text{Bernoulli}(\pi)$$
$$P(X_i|Y = y) = \mathcal{N}(\mu_{iy}, \sigma_{iy}^2)$$

  - Different mean and variance for each class *k* and each feature *i*

- Sometimes assume variance is:
  - independent of Y (i.e., σ_i)
  - or independent of X (i.e., σ_y)
  - or both (i.e., σ)



Estimating Parameters & Prediction

- MLE estimates

$$\hat{\mu}_{ik} = \frac{1}{\sum_n \mathbb{I}(y_n = k)} \sum_n x_{ni} \mathbb{I}(y_n = k)$$

pixel i in
training image n

$$\hat{\sigma}^2_{ik} = \frac{1}{\sum_n \mathbb{I}(y_n = k)} \sum_n (x_{ni} - \hat{\mu}_{ik})^2 \mathbb{I}(y_n = k)$$

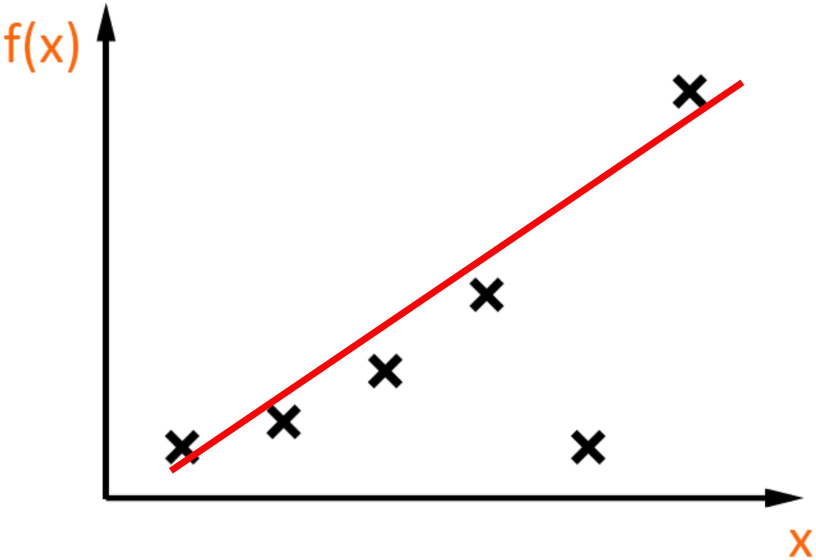
- Prediction:

$$h(\mathbf{x}) = \operatorname*{argmax}_y P(y) \prod_i P(x_i | y)$$

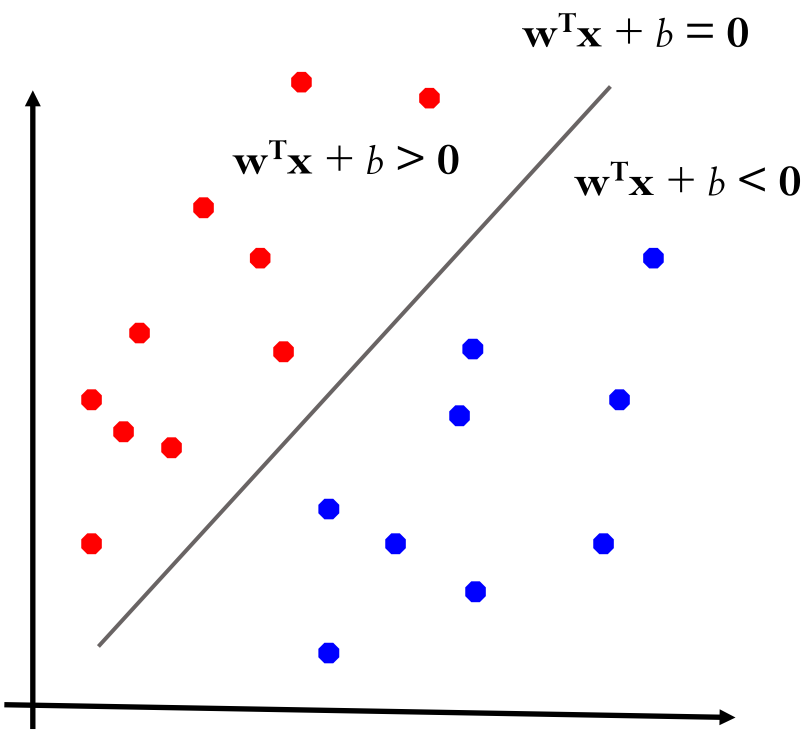
What you need to know about NB classifier

- What's the assumption
- Why we use it
- How do we learn it
- Why is Bayesian estimation (MAP) important

Linear regression and linear classification



Linear fit



Linear decision boundary

What's the decision boundary of NB?

- Is it linear or non-linear?

- There are several distributions that lead to a linear decision boundary, e.g., GNB with equal variance

$$P(X_i|Y=y) = \mathcal{N}(\mu_{iy}, \sigma_i^2)$$

  - Decision boundary (??):

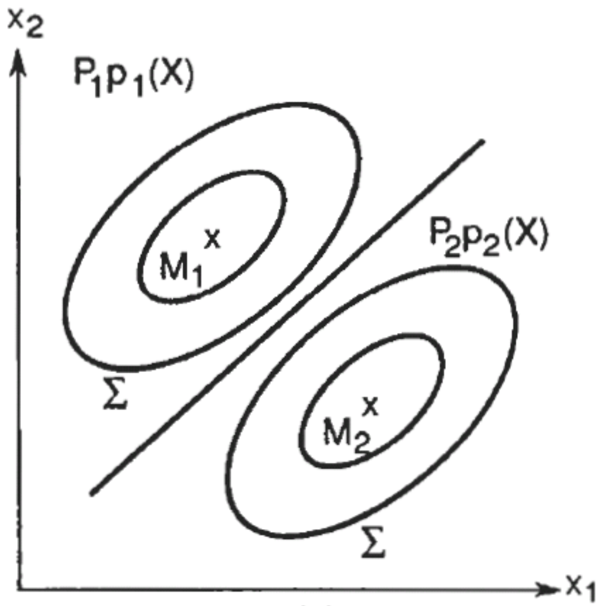
$$\log \frac{\prod_{i=1}^d P(X_i|Y=0)P(Y=0)}{\prod_{i=1}^d P(X_i|Y=1)P(Y=1)} = 0$$

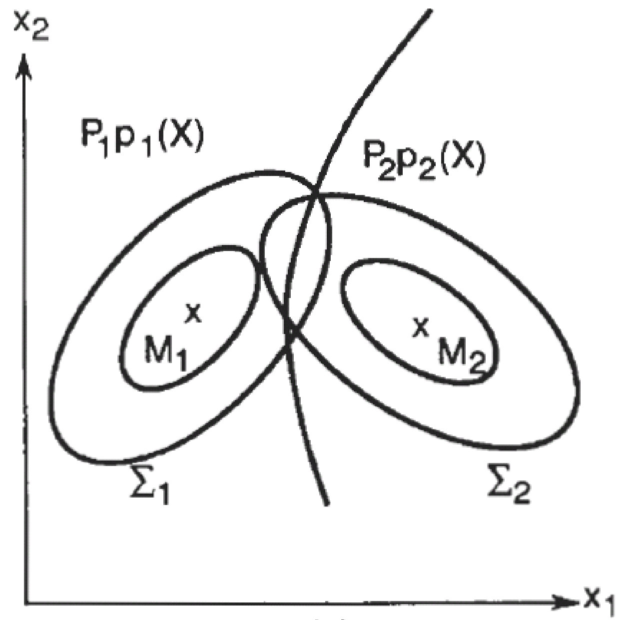
$$\Rightarrow \quad \log \frac{1-\pi}{\pi} + \sum_i \frac{\mu_{i1}^2 - \mu_{i0}^2}{2\sigma_i^2} + \sum_i \frac{\mu_{i0} - \mu_{i1}}{\sigma_i^2} x_i = 0$$

$$\Rightarrow \quad w_0 + \sum_i w_i x_i = 0$$

Gaussian Naive Bayes (GNB)

- Decision boundary (the general multivariate Gaussian case):





$$P_1 = P(Y=0), \quad P_2 = P(Y=1)$$

$$p_1(X) = p(X|Y=0) = \mathcal{N}(M_1, \Sigma_1)$$

$$p_2(X) = p(X|Y=1) = \mathcal{N}(M_2, \Sigma_2)$$

The predictive distribution of GNB

- Understanding the predictive distribution

$$p(y=1|\mathbf{x},\mu,\Sigma,\pi) = \frac{p(y=1,\mathbf{x}|\mu,\Sigma,\pi)}{p(\mathbf{x}|\mu,\Sigma,\pi)}$$

- Under naive Bayes assumption:

$$\begin{aligned}
p(y=1|\mathbf{x},\mu,\Sigma,\pi) &= \frac{1}{1+\frac{p(y=0,\mathbf{x}|\mu,\Sigma,\pi)}{p(y=1,\mathbf{x}|\mu,\Sigma,\pi)}} \\
&= \frac{1}{1+\frac{(1-\pi)\prod_i \mathcal{N}(x_i|\mu_{i0},\sigma_i^2)}{\pi\prod_i \mathcal{N}(x_i|\mu_{i1},\sigma_i^2)}} \\
&= \frac{1}{1+\exp(-\mathbf{w}^\top\mathbf{x}-w_0)}
\end{aligned}$$

- **Note**: For multi-class, the predictive distribution is softmax!

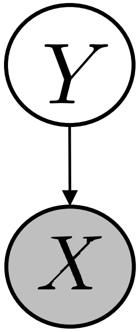
Generative vs. Discriminative Classifiers

- **Generative classifiers** (e.g., Naive Bayes)
  - Assume some functional form for P(X,Y) (or P(Y) and P(X|Y))
  - Estimate parameters of P(X,Y) directly from training data
  - Make prediction

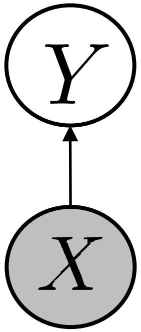
$$\hat{y} = \operatorname*{argmax}_y P(\mathbf{x}, Y = y)$$

  - But, we note that

$$\hat{y} = \operatorname*{argmax}_y P(Y = y|\mathbf{x})$$



- Why not learn P(Y|X) directly? Or, why not learn the decision boundary directly?



- **Discriminative classifiers** (e.g., Logistic regression)
  - Assume some functional form for P(Y|X)
  - Estimate parameters of P(Y|X) directly from training data

Logistic Regression

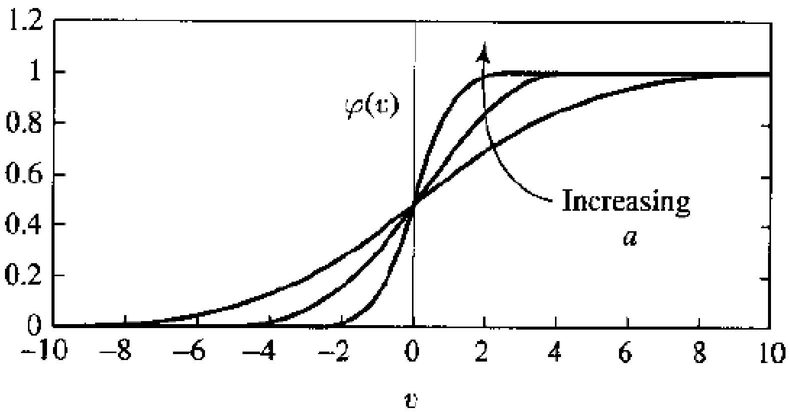
- Recall the predictive distribution of GNB!

- Assume the following functional form for P(Y | X)

$$P(y=1|\mathbf{x}) = \frac{1}{1+\exp(-(w_0+\mathbf{w}^\top \mathbf{x}))}$$

  - Logistic function (or Sigmoid) applied to a linear function of the data (for $\alpha = 1$):

$$\psi_\alpha(v) = \frac{1}{1+\exp(-\alpha v)}$$



$a \to \infty$: step function

use a large α can be good for some neural networks

单选题 1分

设置

What's the decision boundary of logistic regression? (linear or nonlinear?)

$$P(y=1|\mathbf{x}) = \frac{1}{1+\exp(-(w_0+\mathbf{w}^\top\mathbf{x}))}$$

A Linear

B Nolinear

C Don' t know

提交

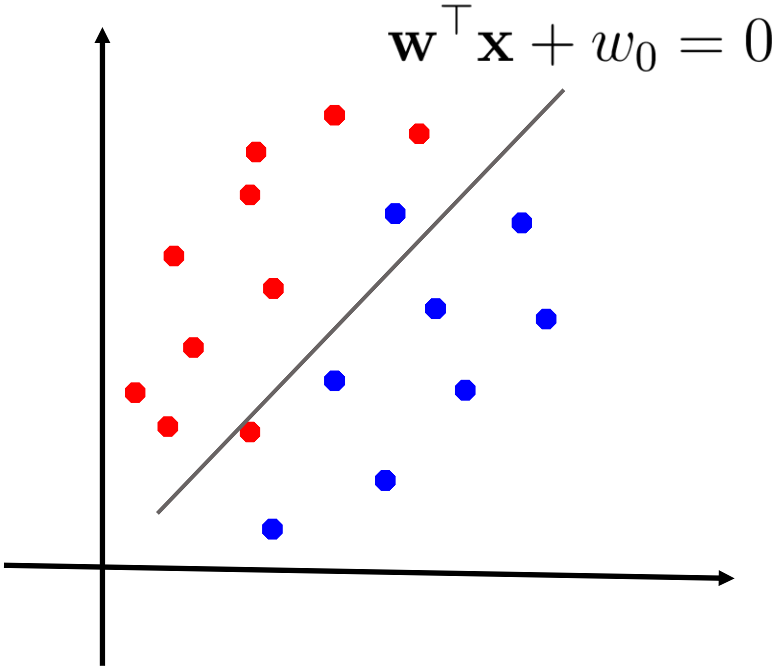
Logistic Regression

- What's the decision boundary of logistic regression? (linear or nonlinear?)

$$P(y=1|\mathbf{x}) = \frac{1}{1+\exp(-(w_0+\mathbf{w}^\top\mathbf{x}))}$$

$$\log\frac{P(Y=1|\mathbf{x})}{P(y=0|\mathbf{x})} = 0$$

$$\mathbf{w}^\top\mathbf{x} + w_0 = 0$$



Logistic regression is a linear classifier!

Representation

- Logistic regression

$$P(y=1|\mathbf{x}) = \frac{1}{1+\exp(-(w_0+\mathbf{w}^\top\mathbf{x}))}$$

- For notation simplicity, we use the augmented vector:

$$\text{input features}: \begin{pmatrix} 1 \\ \mathbf{x} \end{pmatrix} \quad \text{model weights}: \begin{pmatrix} w_0 \\ \mathbf{w} \end{pmatrix}$$

  - Then, we have

$$P(y=1|\mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^\top\mathbf{x})}$$

Multiclass Logistic Regression

- For more than 2 classes, where $y \in \{1, \ldots, K\}$, logistic regression classifier is defined as

$$\forall k < K : \quad P(Y = k|\mathbf{x}) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \mathbf{x})}$$

$$P(Y = K|\mathbf{x}) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \mathbf{x})}$$

  - Well normalized distribution! No weights for class K!

- Is the decision boundary still linear?

单选题 1分

设置

What’ s the decision boundary of multiclass logistic regression?

$$\forall k < K : P(Y = k|\mathbf{x}) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \mathbf{x})}$$

$$P(Y = K|\mathbf{x}) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^\top \mathbf{x})}$$

A Linear

B Piecewise linear

C Smoothly nonlinear

D Don’ t know

提交

Training Logistic Regression

- We consider the binary classification

$$P(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}$$

- Training data $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$

- How to learn the parameters?
- Can we do MLE?

$$\hat{\mathbf{w}}_{MLE} = \operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{N} P(\mathbf{x}_i, y_i|\mathbf{w})$$

  - *No! Don't have a model for P(X) or P(X | Y)*

Maximum Conditional Likelihood Estimate

- We learn the parameters by solving

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmax}} \prod_{i=1}^{N} P(y_i | \mathbf{x}_i, \mathbf{w})$$

- **Discriminative philosophy** – don't waste effort on learning P(X), focus on P(Y | X) – that's all that matters for classification!

Maximum Conditional Likelihood Estimate

$$\hat{\mathbf{w}} = \operatorname*{argmax}_{\mathbf{w}} \prod_{i=1}^{N} P(y_i | \mathbf{x}_i, \mathbf{w})$$

$$P(y = 1 | \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}$$

- We have:

$$\mathcal{L}(\mathbf{w}) = \log \prod_{i=1}^{N} P(y_i | \mathbf{x}_i, \mathbf{w})$$

$$= \sum_i \left[y_i \mathbf{w}^\top \mathbf{x}_i - \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i)) \right]$$

Maximum Conditional Likelihood Estimate

$$\hat{\mathbf{w}} = \operatorname*{argmax}_{\mathbf{w}} \mathcal{L}(\mathbf{w})$$

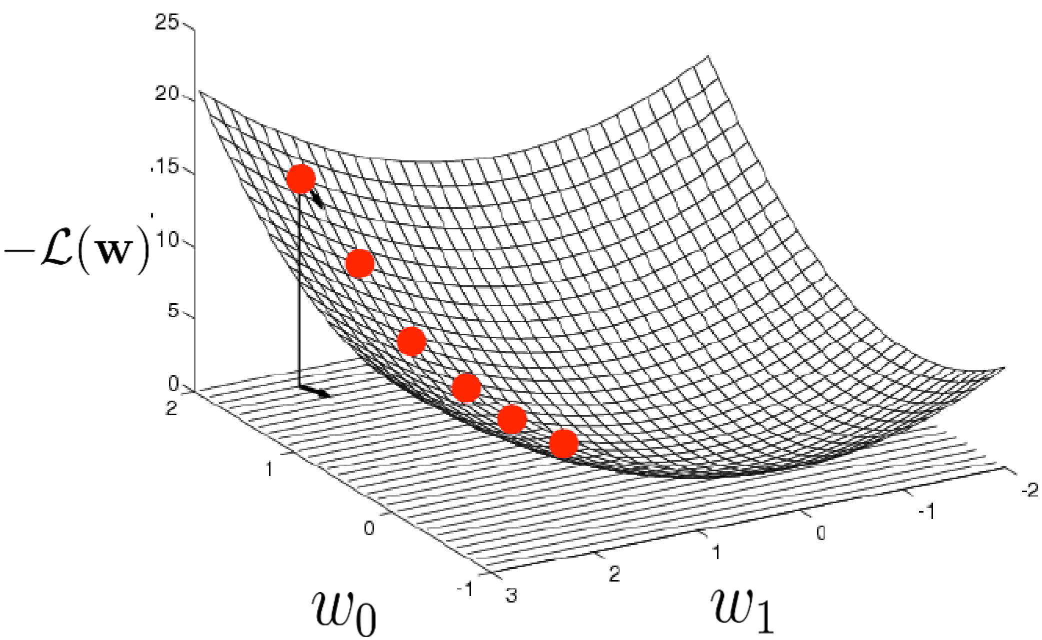
$$\mathcal{L}(\mathbf{w}) = \sum_i \left[y_i \mathbf{w}^\top \mathbf{x}_i - \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i)) \right]$$

- Bad news: no closed-form solution!
- Good news: $\mathcal{L}(\mathbf{w})$ is a concave function of w!
  - Is the original logistic function concave?

Read [S. Boyd, Convex Optimization, Chap. 1] for an introduction to convex optimization.

Optimizing concave/convex function

- Conditional likelihood for logistic regression is concave
- Maximum of a concave function = minimum of a convex function
    - Gradient ascent (concave) / Gradient descent (convex)



Gradient:

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = \begin{pmatrix} \frac{\partial \mathcal{L}(\mathbf{w})}{\partial w_0} \\ \vdots \\ \frac{\partial \mathcal{L}(\mathbf{w})}{\partial w_d} \end{pmatrix}$$

Update rule:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \eta \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w})|_{\mathbf{w}_t}$$

Gradient Ascent for Logistic Regression

- Property of sigmoid function

$$\Rightarrow \nabla_{\nu} \psi = \psi(1-\psi)$$

- Gradient ascent algorithm iteratively does:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \eta \sum_{i=1}^{N} \mathbf{x}_i \left(y_i - \mu_i^t \right)$$

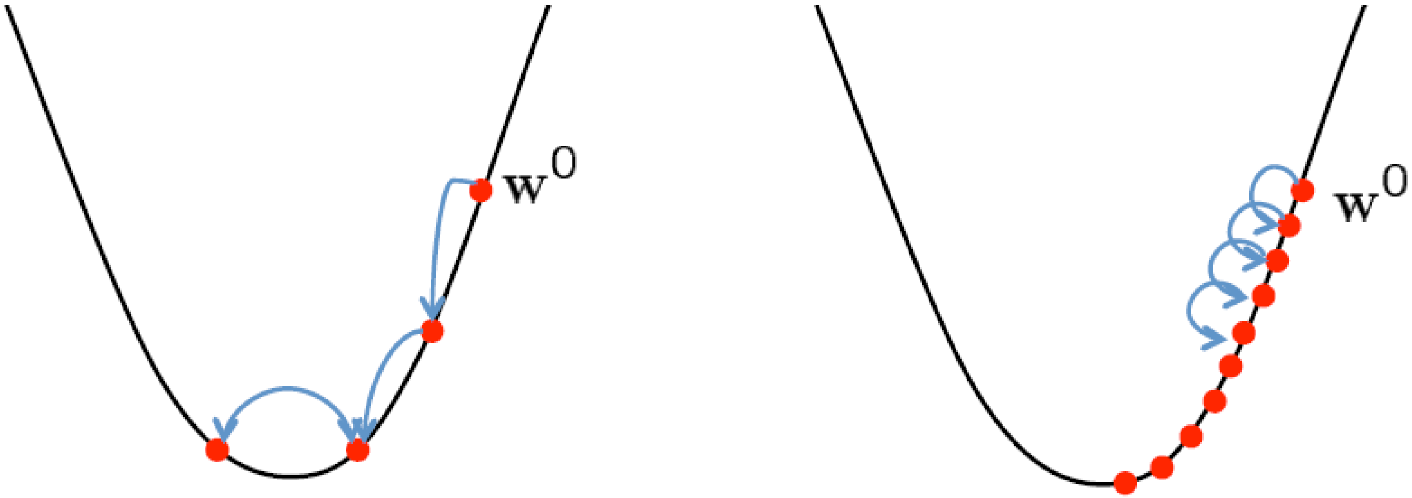
  - where $\mu_i^t = P(y = 1 | \mathbf{x}_i, \mathbf{w}_t)$ is the prediction made by the current model

- Until the change (of objective or gradient) falls below some threshold

Issues

- Gradient descent is the simplest optimization methods, faster convergence can be obtained by using
  - E.g., Newton method, conjugate gradient ascent, IRLS (iterative reweighted least squares)
- The vanilla logistic regression often over-fits; using a regularization can help a lot!

Effects of step-size

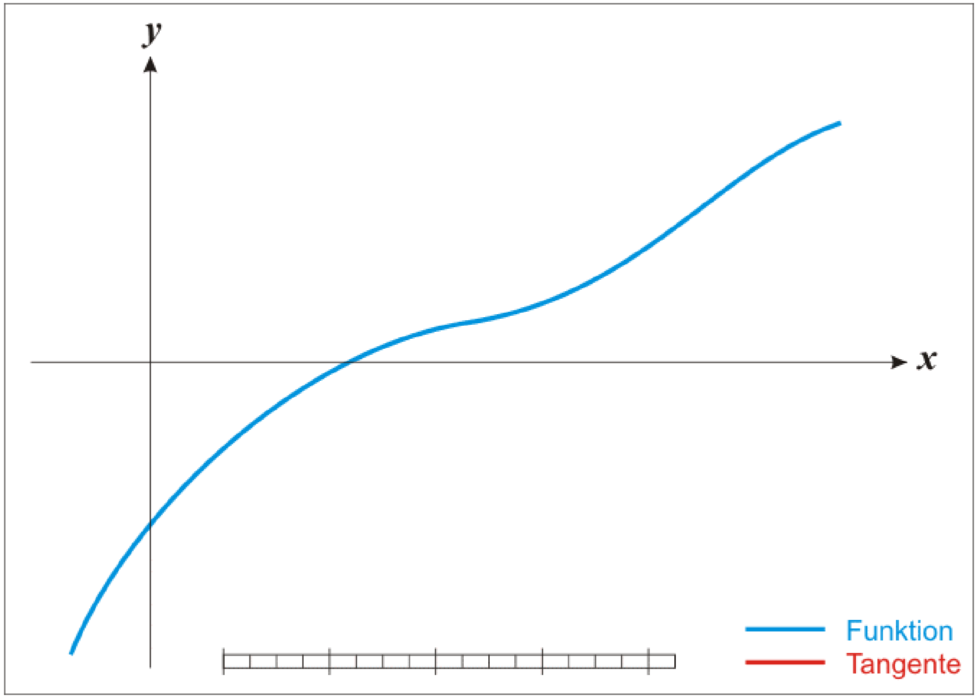


- Large η => fast convergence but larger residual error; Also possible oscillations
- Small η => slow convergence but small residual error

The Newton's Method

- AKA: Newton-Raphson method
- A method that finds the root of: $f(x) = 0$

$$x_{t+1} = x_t - \frac{f(x_t)}{f'(x_t)}$$



For Wikipedia

The Newton's Method

- To maximize the conditional likelihood

$$\mathcal{L}(\mathbf{w}) = \sum_i \left[y_i \mathbf{w}^\top \mathbf{x}_i - \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i)) \right]$$

  - We need to find $\mathbf{w}^*$ such that

$$\nabla \mathcal{L}(\mathbf{w}^*) = 0$$

- So we can perform the following iteration:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - H^{-1} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w})|_{\mathbf{w}_t}$$

  - where *H* is known as the Hessian matrix:

$$H = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w})|_{\mathbf{w}_t}$$

Newton's Method for LR

- The update equation

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - H^{-1} \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w})|_{\mathbf{w}_t}$$

  - where the gradient is:

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w})|_{\mathbf{w}_t} = \sum_i (y_i - \mu_i)\mathbf{x}_i = X(\mathbf{y} - \boldsymbol{\mu})$$

$$\mu_i = \psi(\mathbf{w}_t^\top \mathbf{x}_i)$$

  - The Hessian matrix is:

$$H = \nabla^2_{\mathbf{w}} \mathcal{L}(\mathbf{w})|_{\mathbf{w}_t} = -\sum_i \mu_i(1-\mu_i)\mathbf{x}_i \mathbf{x}_i^\top = -XRX^\top$$

$$\text{where } R_{ii} = \mu_i(1-\mu_i)$$

Iterative reweighted least squares (IRLS)

- In least square estimate of linear regression, we have

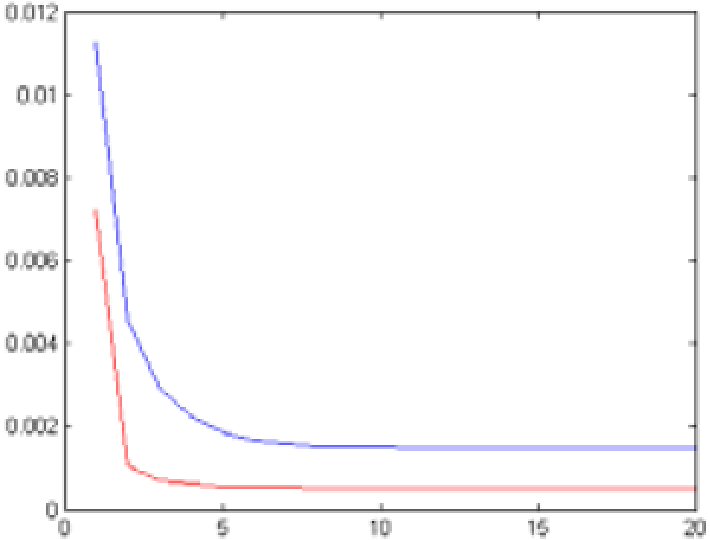
$$\mathbf{w} = (XX^\top)^{-1}X\mathbf{y}$$

- Now, for logistic regression

$$\begin{aligned}
\mathbf{w}_{t+1} &= \mathbf{w}_t - H^{-1}\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}_t) \\
&= \mathbf{w}_t - (XRX^\top)^{-1}X(\boldsymbol{\mu} - \mathbf{y}) \\
&= (XRX^\top)^{-1}\left\{XRX^\top\mathbf{w}_t - X(\boldsymbol{\mu} - \mathbf{y})\right\} \\
&= (XRX^\top)^{-1}XR\mathbf{z}
\end{aligned}$$

$$\boxed{\text{where } \mathbf{z} = X^\top\mathbf{w}_t - R^{-1}(\boldsymbol{\mu} - \mathbf{y})}$$

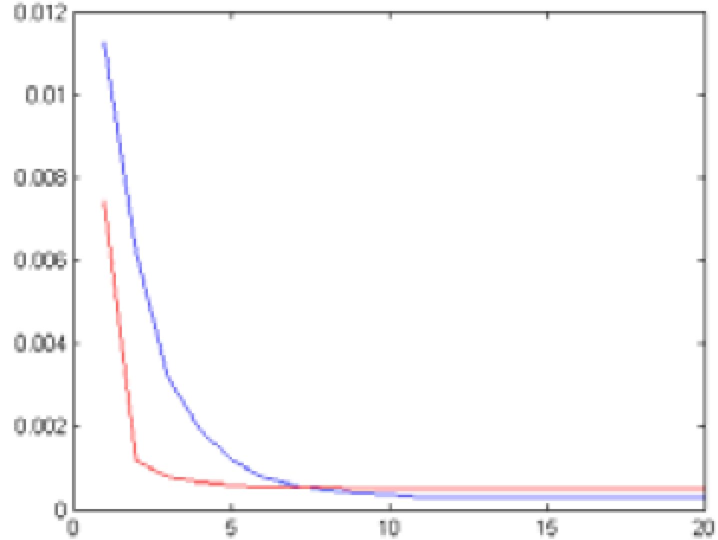
Convergence curves



rec.autos

vs.

rec.sports.baseball



comp.windows.x

vs.

rec.motorcycles

- Legend: X-axis: Iteration #;Y-axis: classification error
- In each figure, red for **IRLS** and blue for **gradient descent**

LR: Practical Issues

- IRLS takes $O(N + d^3)$ per iteration, where N is # training points and d is feature dimension, but converges in fewer iterations

- Quasi-Newton methods, that approximate the Hessian, work faster

- Conjugate gradient takes $O(Nd)$ per iteration, and usually works best in practice

- Stochastic gradient descent can also be used if N is large c.f. perceptron rule

Gaussian NB vs. Logistic Regression

GNB Gaussian parameters	VS	LR Regression parameters

- Representation equivalence
  - But only in some special case! (GNB with class independent variances)
- What's the differences?
  - LR makes no assumption about P(X|Y) in learning
  - They optimize different functions, obtain different solutions

Generative vs. Discriminative

- Given infinite data (asymptotically)
  - (1) If conditional independence assumption holds, discriminative and generative NB perform similar

$$\epsilon_{\mathrm{Dis},\infty} \sim \epsilon_{\mathrm{Gen},\infty}$$

  - (2) If conditional independence assumption does NOT hold, discriminative outperform generative NB

$$\epsilon_{\mathrm{Dis},\infty} < \epsilon_{\mathrm{Gen},\infty}$$

[Ng & Jordan, NIPS 2001]

Generative vs. Discriminative

- Given finite data (N data points, d features)

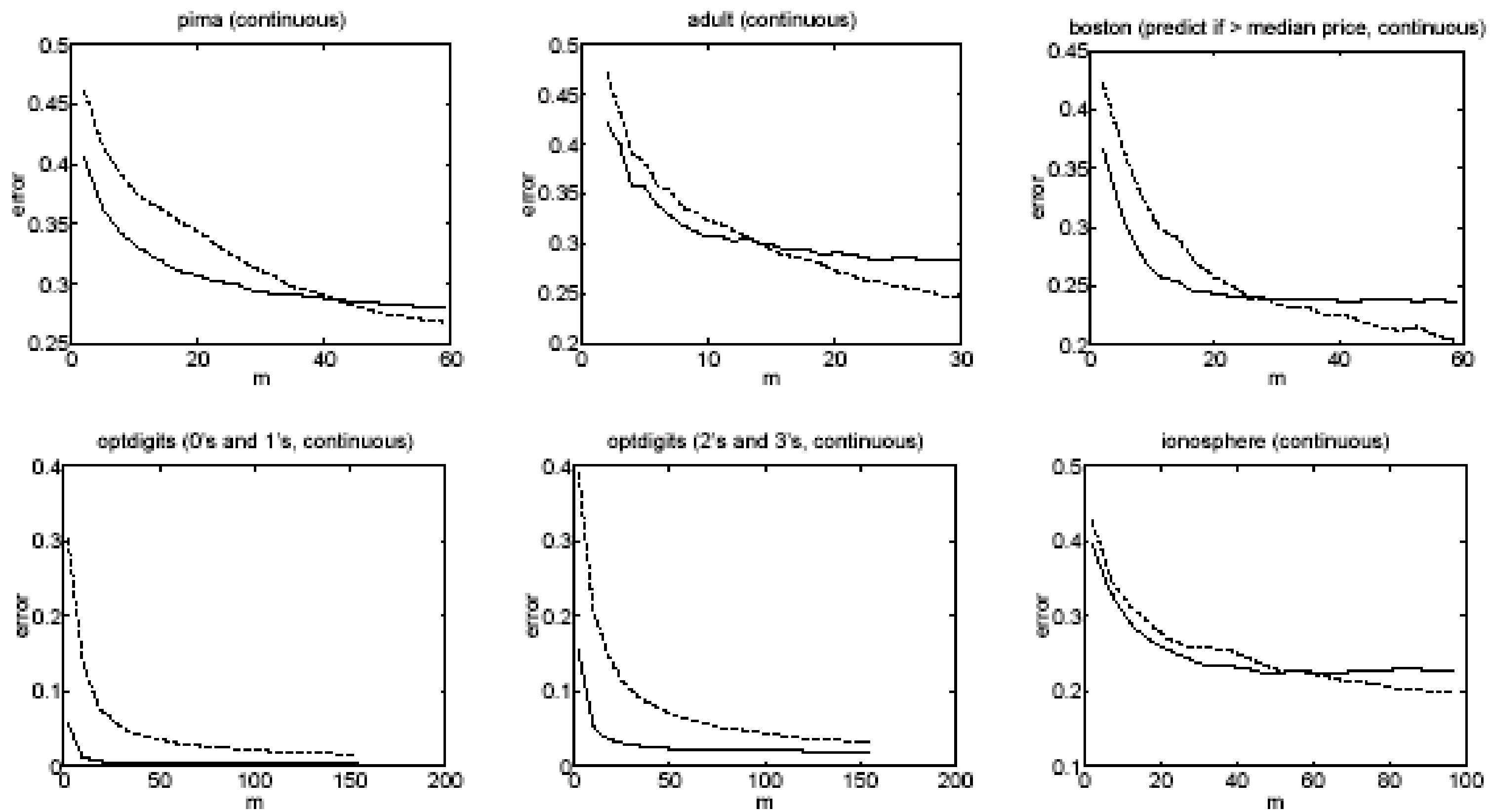
$$\epsilon_{\mathrm{Dis},n} \leq \epsilon_{\mathrm{Dis},\infty} + O\left(\sqrt{\frac{d}{N}}\right)$$

$$\epsilon_{\mathrm{Gen},n} \leq \epsilon_{\mathrm{Gen},\infty} + O\left(\sqrt{\frac{\log d}{N}}\right)$$

  - Naive Bayes (generative) requires $N = O(\log d)$ to converge to its asymptotic error, whereas logistic regression (discriminative) requires $N = O(d)$.
- Why?
  - "Independent class conditional densities" – parameter estimates are not coupled, each parameter is learnt independently, not jointly, from training data

Experimental Comparison

- UCI Machine Learning Repository 15 datasets, 8 continuous features, 7 discrete features



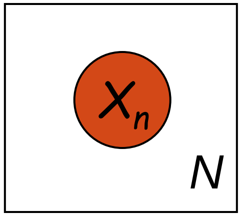
Naive Bayes ------ Logistic Regression

What you need to know

- LR is a linear classifier
  - Decision boundary is a hyperplane
- LR is learnt by maximizing conditional likelihood
  - No closed-form solution
  - Concave! Global optimum by gradient ascent methods
- GNB with class-independent variances representationally equivalent to LR
  - Solutions differ because of objective (loss) functions
- In general, NB and LR make different assumptions
  - NB: features independent given class, assumption on $P(X|Y)$
  - LR: functional form of $P(Y|X)$, no assumption on $P(X|Y)$
- Convergence rates:
  - GNB (usually) needs less data
  - LR (usually) gets to better solutions in the limit

Exponential family

- For a numeric random variable X



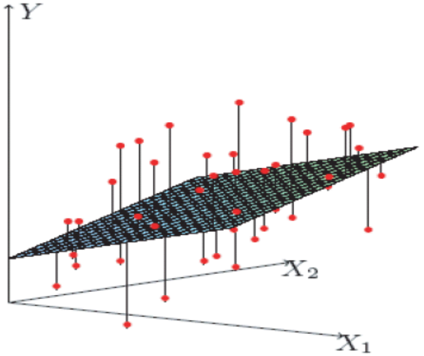
$$
\begin{aligned}
p(\mathbf{x}|\boldsymbol{\eta}) &= h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\top T(\mathbf{x}) - A(\boldsymbol{\eta})\right) \\
&= \frac{1}{Z(\boldsymbol{\eta})} h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\top T(\mathbf{x})\right)
\end{aligned}
$$

is an **exponential family distribution** with natural (canonical) parameter η

- Function $T(x)$ is a *sufficient statistic*.
- Function $A(\eta) = \log Z(\eta)$ is the log normalizer.
- Examples: Bernoulli, multinomial, Gaussian, Poisson, gamma,...

Recall Linear Regression

- Let us assume that the target variable and the inputs are related by the equation:



$$y_i = \boldsymbol{\theta}^\top \mathbf{x}_i + \epsilon_i$$

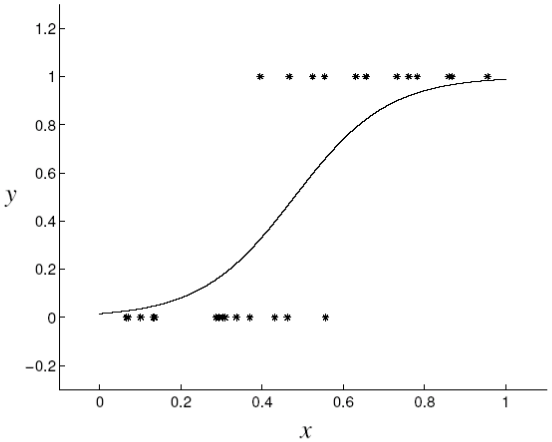
where ε is an error term of unmodeled effects or random noise

- Now assume that ε follows a Gaussian $N(0,\sigma)$, then we have:

$$p(y_i|\mathbf{x}_i, \boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \boldsymbol{\theta}^\top \mathbf{x}_i)^2}{2\sigma^2}\right)$$

Recall: Logistic Regression (sigmoid classifier)

- The condition distribution: a Bernoulli



$$p(y|\mathbf{x}) = \mu(\mathbf{x})^y(1-\mu(\mathbf{x}))^{1-y}$$

where μ is a logistic function

$$\mu(\mathbf{x}) = \frac{1}{1+e^{-\boldsymbol{\theta}^\top \mathbf{x}}}$$

- We can use the brute-force gradient method as in LR

- But we can also apply generic laws by observing the $p(y|x)$ is an exponential family function, more specifically, a generalized linear model!

Example: Multivariate Gaussian Distribution

- For a continuous vector random variable $\mathbf{x} \in \mathbb{R}^d$:

$$p(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

Moment parameter

$$= \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2}\mathrm{tr}(\Sigma^{-1}\mathbf{x}\mathbf{x}^\top) + \boldsymbol{\mu}^\top\Sigma^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}^\top\Sigma^{-1}\boldsymbol{\mu} - \log|\Sigma|\right)$$

- Exponential family representation

Natural parameter

$$\boldsymbol{\eta} = \left[\Sigma^{-1}\boldsymbol{\mu}; -\frac{1}{2}\mathrm{vec}(\Sigma^{-1})\right] = [\boldsymbol{\eta}_1; \mathrm{vec}(\boldsymbol{\eta}_2)], \ \boldsymbol{\eta}_1 = \Sigma^{-1}\boldsymbol{\mu} \text{ and } \boldsymbol{\eta}_2 = -\frac{1}{2}\Sigma^{-1}$$

$$T(\mathbf{x}) = [\mathbf{x}; \mathrm{vec}(\mathbf{x}\mathbf{x}^\top)]$$

$$A(\boldsymbol{\eta}) = \frac{1}{2}\boldsymbol{\mu}^\top\Sigma^{-1}\boldsymbol{\mu} + \log|\Sigma| = -\frac{1}{2}\mathrm{tr}(\boldsymbol{\eta}_2\boldsymbol{\eta}_1\boldsymbol{\eta}_1^\top) - \frac{1}{2}\log(-2|\boldsymbol{\eta}_2|)$$

$$h(\mathbf{x}) = (2\pi)^{-d/2}$$

  - Note: a d-dimensional Gaussian is a $(d+d^2)$ -parameter distribution with a $(d+d^2)$-element vector of sufficient statistics (but because of symmetry and positivity, parameters are constrained and have lower degree of freedom)

Example: Multinomial distribution

- For a binary vector random variable $\mathbf{x} \sim \text{multi}(\mathbf{x}|\pi)$:

$$p(\mathbf{x}|\pi) = \prod_{i=1}^{d} \pi_i^{x_i} = \exp\left(\sum_i x_i \ln \pi_i\right)$$
$$= \exp\left(\sum_{i=1}^{d-1} x_i \ln \pi_i + \left(1 - \sum_{i=1}^{d-1} x_i\right) \ln\left(1 - \sum_{i=1}^{d-1} \pi_i\right)\right)$$
$$= \exp\left(\sum_{i=1}^{d-1} x_i \ln \frac{\pi_i}{1 - \sum_{i=1}^{d-1} \pi_i} + \ln\left(1 - \sum_{i=1}^{d-1} \pi_i\right)\right)$$

- Exponential family representation

$$\boldsymbol{\eta} = [\ln(\pi_i/\pi_d); 0]$$

$$T(\mathbf{x}) = \mathbf{x}$$

$$A(\boldsymbol{\eta}) = -\ln\left(1 - \sum_{i=1}^{d-1} \pi_i\right) = \ln\left(\sum_{i=1}^{d} e^{\boldsymbol{\eta}_i}\right)$$

$$h(\mathbf{x}) = 1$$

Why exponential family?

- Moment generating property (proof?)

$$\nabla_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \nabla_{\boldsymbol{\eta}} \log Z(\boldsymbol{\eta}) = \cdots = \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\eta})}[T(\mathbf{x})]$$

$$\nabla^2_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \cdots = \mathrm{Var}[T(\mathbf{x})]$$

Moment estimation

- We can easily compute moments of any exponential family distribution by taking the derivatives of the log normalizer $A(\eta)$.
- The q^{th} derivative gives the q^{th} centered moment.

$$\nabla_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \text{mean}$$

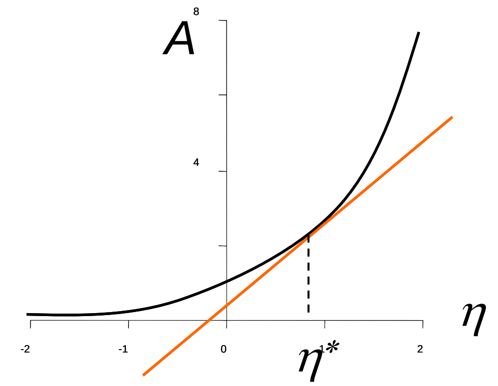
$$\nabla^2_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \text{variance}$$

$$\vdots$$

Moment vs canonical parameters

- The moment parameter μ can be derived from the natural (canonical) parameter

$$\nabla_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\eta})}[T(\mathbf{x})] \triangleq \boldsymbol{\mu}$$



- $A(\eta)$ is convex since

$$\nabla^2_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \mathrm{Var}[T(\mathbf{x})] > 0$$

- Hence we can invert the relationship and infer the canonical parameter from the moment parameter (1-to-1):

$$\boldsymbol{\eta} \triangleq \psi(\boldsymbol{\mu})$$

  - A distribution in the exponential family can be parameterized not only by η – the canonical parameterization, but also by μ – the moment parameterization.

IID Sampling for Exponential Family

- For exponential family distribution, we can obtain the sufficient statistics by inspection once represented in the standard form

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x}) \exp(\boldsymbol{\eta}^\top T(\mathbf{x}) - A(\boldsymbol{\eta}))$$

  - Sufficient statistics: $T(\mathbf{x})$

- For IID sampling, the joint distribution is also an exponential family

$$\begin{aligned} p(D|\boldsymbol{\eta}) &= \prod h(\mathbf{x}_i) \exp\left(\boldsymbol{\eta}^\top T(\mathbf{x}_i) - A(\boldsymbol{\eta})\right) \\ &= \left(\prod_i h(\mathbf{x}_i)\right) \exp\left(\boldsymbol{\eta}^\top \sum_i T(\mathbf{x}_i) - NA(\boldsymbol{\eta})\right) \end{aligned}$$

  - Sufficient statistics: $\sum_i T(\mathbf{x}_i)$

MLE for Exponential Family

- For *iid* data, the log-likelihood is

$$\mathcal{L}(\boldsymbol{\eta}; D) = \sum_n \log h(\mathbf{x}_n) + \left(\boldsymbol{\eta}^\top \sum_n T(\mathbf{x}_n)\right) - NA(\boldsymbol{\eta})$$

- Take derivatives and set to zero:

$$\nabla_{\boldsymbol{\eta}} \mathcal{L}(\boldsymbol{\eta}; D) = \sum_n T(\mathbf{x}_n) - N \nabla_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = 0$$

$$\nabla_{\boldsymbol{\eta}} A(\boldsymbol{\eta}) = \frac{1}{N} \sum_n T(\mathbf{x}_n)$$

$$\hat{\boldsymbol{\mu}}_{MLE} = \frac{1}{N} \sum_n T(\mathbf{x}_n)$$

Only involve sufficient stiatistics!

- This amounts to **moment matching**.
- We can infer the canonical parameters using $\hat{\boldsymbol{\eta}}_{MLE} = \psi(\hat{\boldsymbol{\mu}}_{MLE})$

Examples

- Gaussian:

$$\boldsymbol{\eta} = \left[\Sigma^{-1}\boldsymbol{\mu}; -\frac{1}{2}\mathrm{vec}(\Sigma^{-1})\right]$$

$$T(\mathbf{x}) = [\mathbf{x}; \mathrm{vec}(\mathbf{x}\mathbf{x}^\top)] \qquad \Rightarrow \hat{\boldsymbol{\mu}}_{MLE} = \frac{1}{N}\sum_n T_1(\mathbf{x}_n) = \frac{1}{N}\sum_n \mathbf{x}_n$$

$$A(\boldsymbol{\eta}) = \frac{1}{2}\boldsymbol{\mu}^\top\Sigma^{-1}\boldsymbol{\mu} + \log|\Sigma|$$

$$h(\mathbf{x}) = (2\pi)^{-d/2}$$

- Multinomial:

$$\boldsymbol{\eta} = [\ln(\pi_i/\pi_d); 0]$$

$$T(\mathbf{x}) = \mathbf{x}$$

$$A(\boldsymbol{\eta}) = -\ln\left(1 - \sum_{i=1}^{d-1}\pi_i\right) \qquad \Rightarrow \hat{\boldsymbol{\mu}}_{MLE} = \frac{1}{N}\sum_n \mathbf{x}_n$$

$$h(\mathbf{x}) = 1$$

- Poisson:

$$\eta = \log\lambda$$

$$T(x) = x$$

$$A(\eta) = \lambda = e^\eta \qquad \Rightarrow \hat{\mu}_{MLE} = \frac{1}{N}\sum_n x_n$$

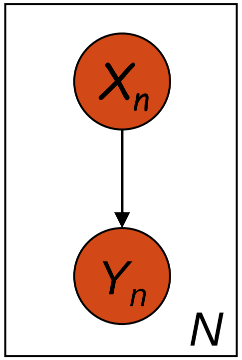
$$h(x) = \frac{1}{x!}$$

Generalized Linear Models (GLIMs)

- The graphical model
  - Linear regression
  - Discriminative linear classification
  - Commonality:

    model $$\mathbb{E}_p[y] = \mu = f(\boldsymbol{\theta}^\top \mathbf{x})$$

    - What is $p()$? the cond. dist. of Y.
    - What is $f()$? the response function.



- GLIM
  - The observed input $\boldsymbol{x}$ is assumed to enter into the model via a linear combination of its elements $\xi = \theta^T x$
  - The conditional mean μ is represented as a function $\boldsymbol{f}(\xi)$ of ξ, where f is known as the response function
  - The observed output $\boldsymbol{y}$ is assumed to be characterized by an exponential family distribution with conditional mean μ.

GLIM, cont.

$$\begin{tikzcd} \theta \arrow[dr] & & & & \\ & \xi \arrow[r, "f"] & \mu \arrow[r, "\psi"] \arrow[rr, bend left, "EXP"] & \eta \arrow[r, "EXP"] & y \\ x \arrow[ur] & & & & \end{tikzcd}$$

$$p(y|\eta) = h(y)\exp\left\{\eta^T(x)y - A(\eta)\right\}$$

$$\Rightarrow p(y|\eta,\phi) = h(y,\phi)\exp\left\{\tfrac{1}{\phi}\left(\eta^T(x)y - A(\eta)\right)\right\}$$

- The choice of exp family is constrained by the nature of the data y
  - Example: y is a continuous vector → multivariate Gaussian
    y is a class label → Bernoulli or multinomial
- The choice of the response function
  - Following some mild constrains, e.g., [0,1]. Positivity …
  - Canonical response function:
    - In this case $\theta^T x$ directly corresponds to canonical parameter η.

$$f = \psi^{-1}(\cdot)$$

MLE for GLIMs

- Log-likelihood

$$\mathcal{L}(\boldsymbol{\theta}; D) = \sum_n \log h(y_n) + \sum_n (\eta_n y_n - A(\eta_n))$$

where $\eta_n = \psi(\mu_n), \; \mu_n = f(\xi_n)$ and $\xi_n = \boldsymbol{\theta}^\top \mathbf{x}_n$

- Derivative of Log-likelihood

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \sum_n \left(y_n \nabla_{\boldsymbol{\theta}} \eta_n - \frac{dA(\eta_n)}{d\eta_n} \nabla_{\boldsymbol{\theta}} \eta_n \right)$$

$$= \sum_n (y_n - \mu_n) \nabla_{\boldsymbol{\theta}} \eta_n$$

This is a fixed point function because μ is a function of θ

MLE for GLIMs with canonical response

- Log-likelihood

$$\mathcal{L}(\boldsymbol{\theta}; D) = \sum_n \log h(y_n) + \sum_n \left(\boldsymbol{\theta}^\top \mathbf{x}_n y_n - A(\eta_n)\right)$$

- Derivative of Log-likelihood

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}} \mathcal{L} &= \sum_n \left(\mathbf{x}_n y_n - \frac{dA(\eta_n)}{d\eta_n} \nabla_{\boldsymbol{\theta}} \eta_n\right) \\
&= \sum_n (y_n - \mu_n)\mathbf{x}_n \\
&= X(\mathbf{y} - \boldsymbol{\mu})
\end{aligned}$$

This is a fixed point function because μ is a function of θ

- Online learning for canonical GLIMs
  - Stochastic gradient ascent = least mean squares (LMS) algorithm:

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \rho(y_n - \mu_n^t)\mathbf{x}_n$$

where $\mu_n^t = f(\boldsymbol{\theta}_t^\top \mathbf{x}_n)$ and ρ is a step size

MLE for GLIMs with canonical response

- Log-likelihood

$$\mathcal{L}(\boldsymbol{\theta}; D) = \sum_n \log h(y_n) + \sum_n \left(\boldsymbol{\theta}^\top \mathbf{x}_n y_n - A(\eta_n)\right)$$

- Derivative of Log-likelihood

$$\begin{aligned} \nabla_{\boldsymbol{\theta}} \mathcal{L} &= \sum_n \left(\mathbf{x}_n y_n - \frac{dA(\eta_n)}{d\eta_n} \nabla_{\boldsymbol{\theta}} \eta_n \right) \\ &= \sum_n (y_n - \mu_n) \mathbf{x}_n \\ &= X(\mathbf{y} - \boldsymbol{\mu}) \end{aligned}$$

This is a fixed point function because μ is a function of θ

- Batch learning applies
  - E.g., the Newton's method leads to an Iteratively Reweighted Least Square (IRLS) algorithm

What you need to know

- Exponential family distribution
- Moment estimation
- Generalized linear models
- Parameter estimation of GLIMs