Probabilistic Methods for Classification

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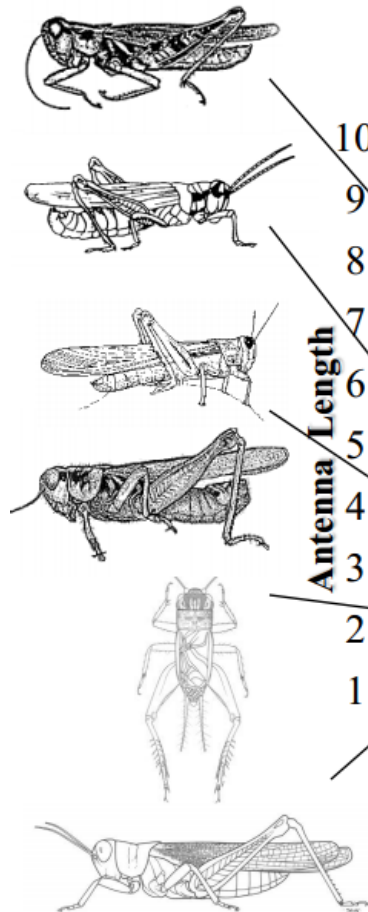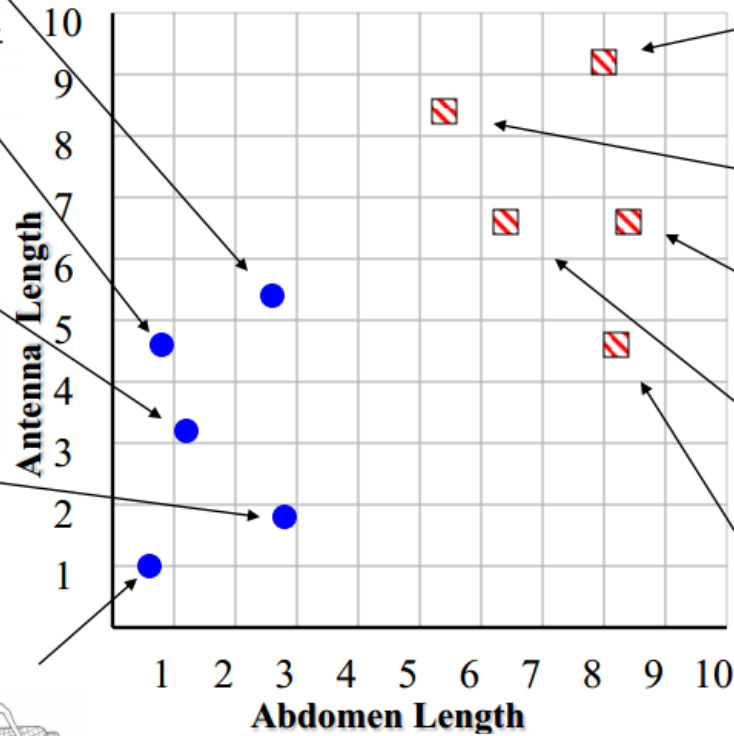
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Outline
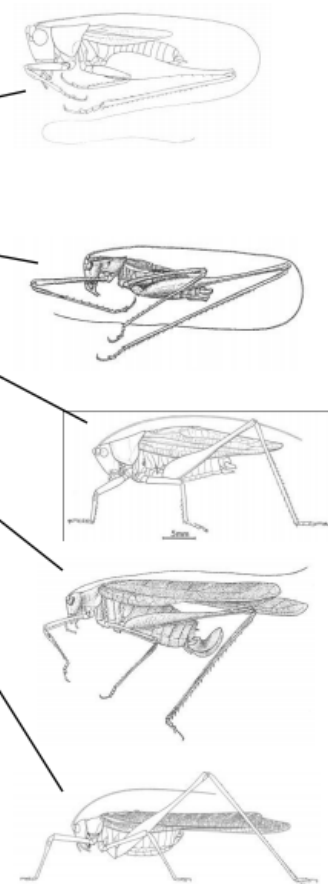
- Probabilistic methods for supervised learning
- Naive Bayes classifier
- Logistic regression
- Exponential family distributions
- Generalized linear models

An Intuitive Example

Grasshoppers

Katydids

[Courtesy of E. Keogh]

With more data …

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

⬛ **Katydids**
⬤ **Grasshoppers**

[Courtesy of E. Keogh]
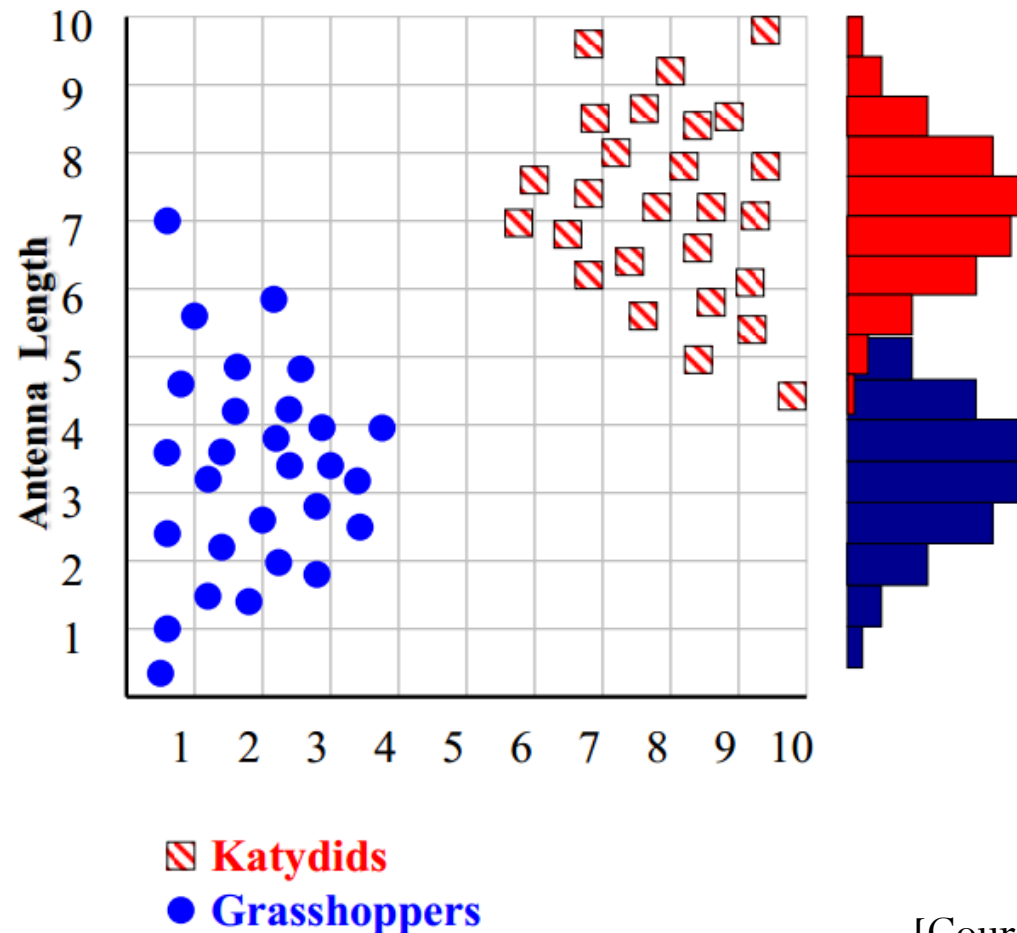
Empirical distribution

◆ **Histogram** (or empirical distribution)
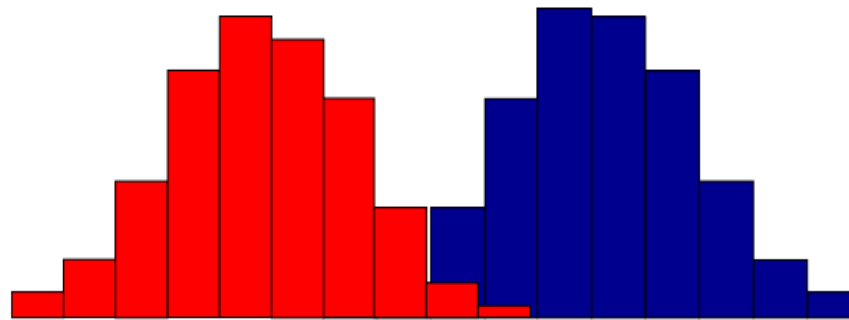
◆ Smooth with kernel density estimation (KDE):
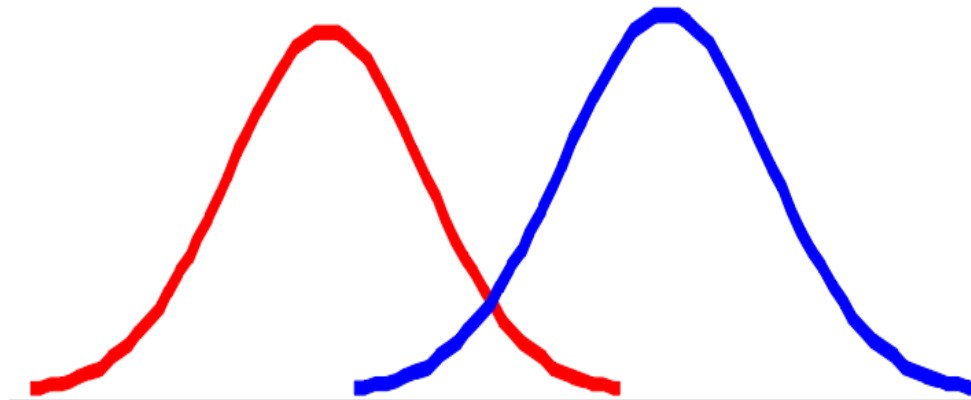
Classification?

- Classify another insect we find. Its antennae are 3 units long

- Is it more probable that the insect is a **Grasshopper** or a **Katydid**?

3

Antennae length is **3**
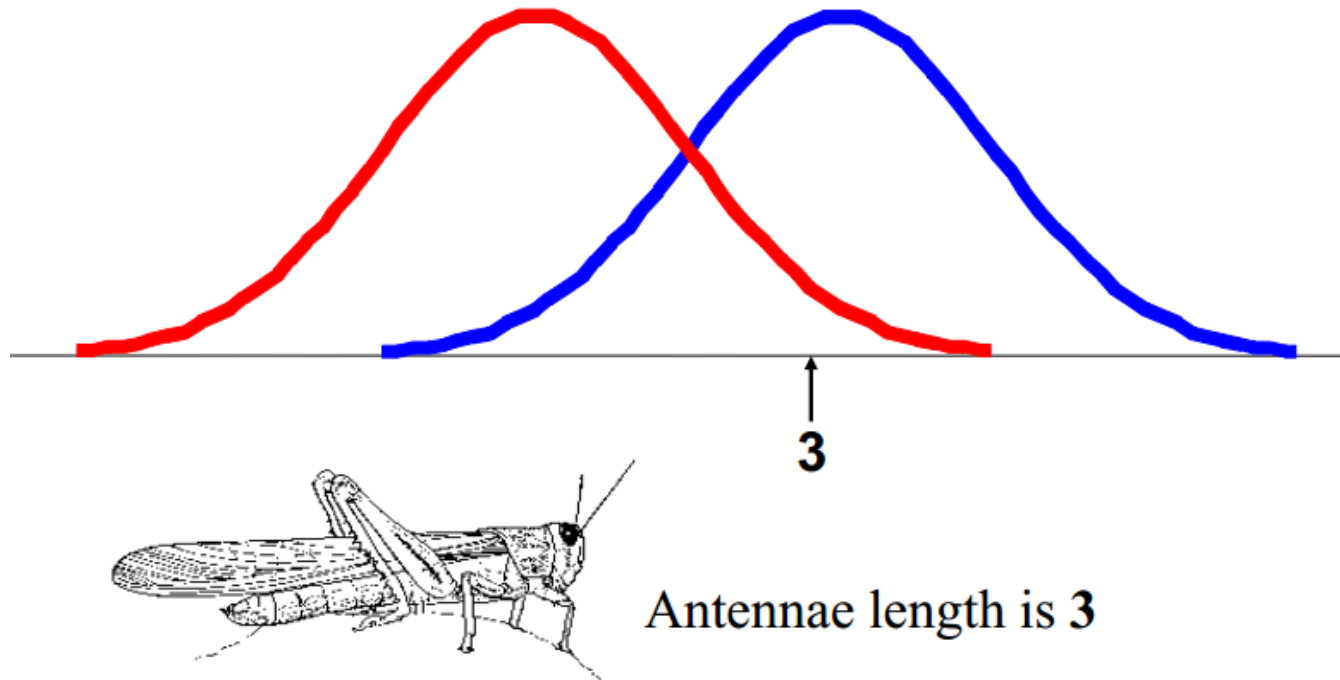
Classification Probability

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

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

10

2

3

Antennae length is **3**

[Courtesy of E. Keogh]

Classification Probability

$$P(\text{Grasshopper} \mid 7) = 3 / (3 + 9) \qquad = 0.250$$

$$P(\text{Katydid} \mid 7) \qquad = 9 / (3 + 9) \qquad = 0.750$$

9

3

7
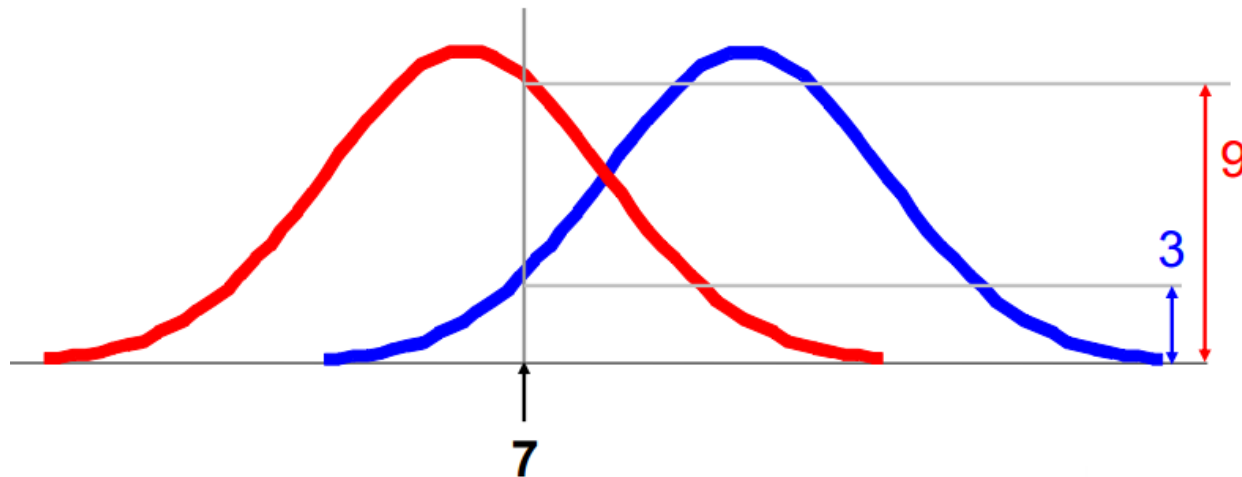
Antennae length is 7
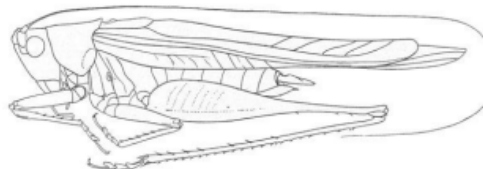
Classification Probability

$$P(\text{Grasshopper} \mid 5) = 6 / (6 + 6) \qquad = 0.500$$

$$P(\text{Katydid} \mid 5) \qquad = 6 / (6 + 6) \qquad = 0.500$$

6 6

5

Antennae length is 5
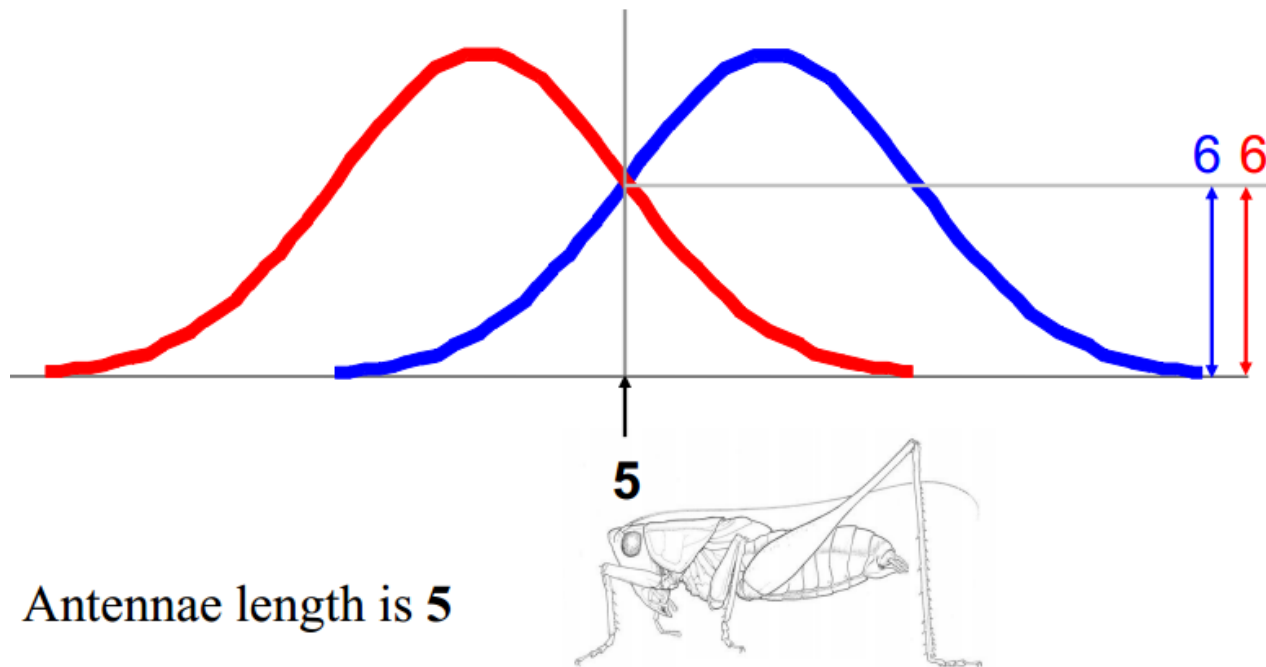
Naïve Bayes Classifier

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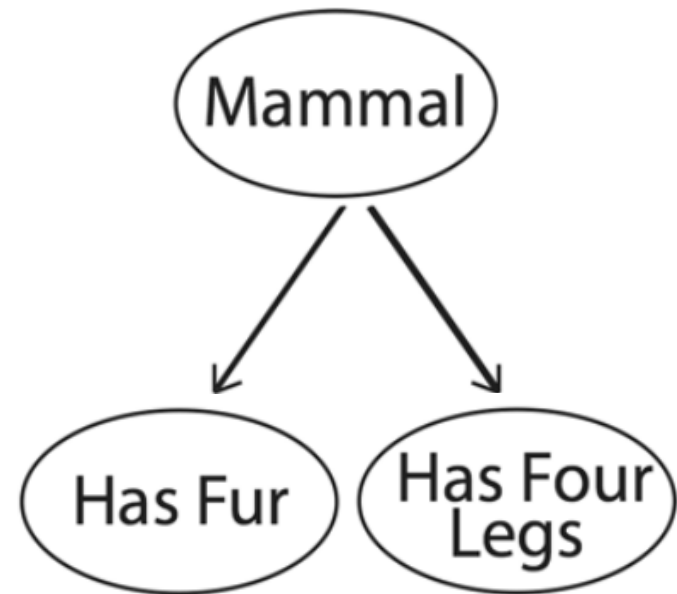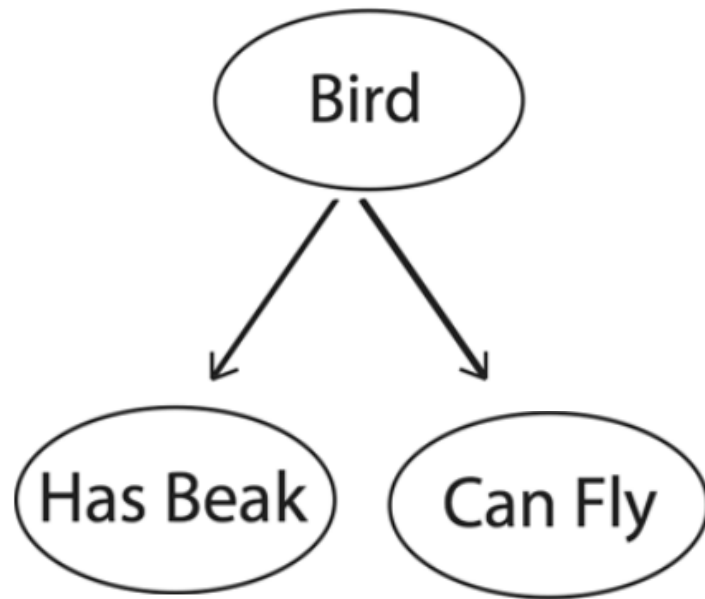
Naïve Bayes Classifier

◆ **A mathematic model**:

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

Y {bird, mammal}

X_1 X_2 X_3 X_4

has beak?   can fly?   has fur?   has four legs?
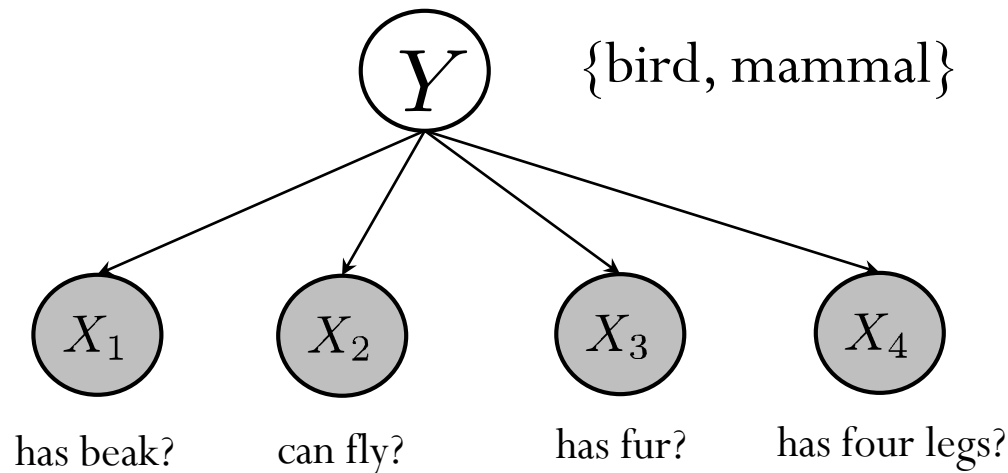
A joint distribution:

prior   likelihood

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

Naïve Bayes Classifier

◆ **A mathematic model**:
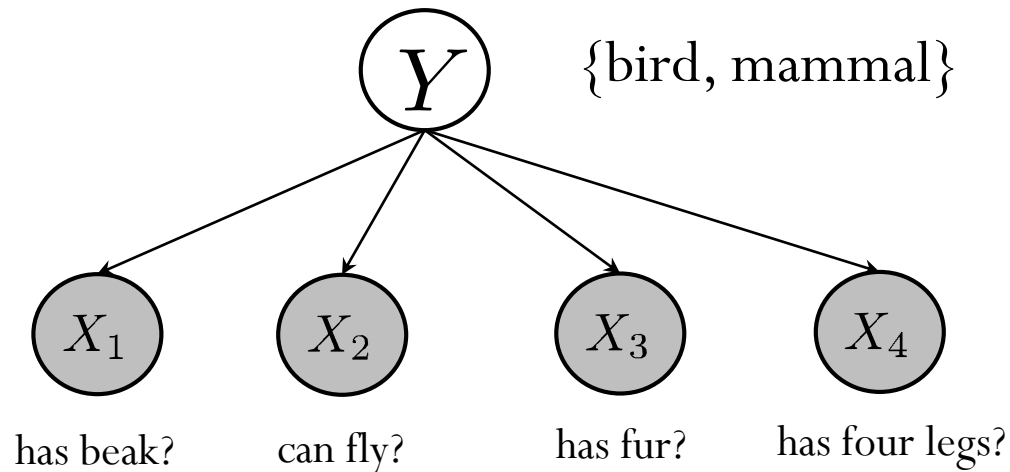
Inference via Bayes rule:

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

Bayes' decision rule:

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

Bayes Error

◆ **Theorem**: Bayes classifier is optimal!
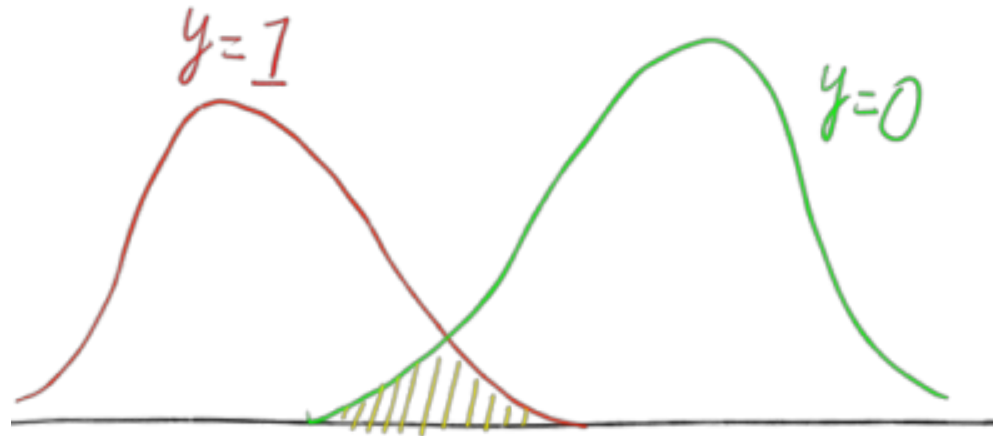
$$p(error|\mathbf{x}) = \begin{cases} p(y = 1|\mathbf{x}) & \text{if we decide } y = 0 \\ p(y = 0|\mathbf{x}) & \text{if we decide } y = 1 \end{cases}$$

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

◆ *However, the true distribution is* *unknown*.

◆ *We need to estimate it!*

Naïve Bayes Classifier

◆ **How to learn model parameters?**

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

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

Y {bird, mammal}

X_1 X_2 X_3 X_4

has beak?   can fly?   has fur?   has four legs?
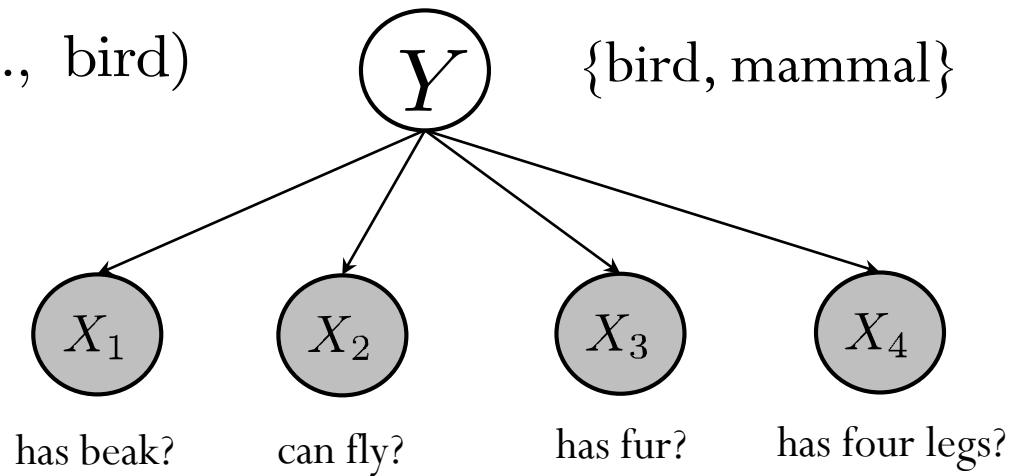
$$p(x_j|y = 0, q) = \begin{cases} q_{0j} & \text{if } x_j = 1 \\ 1 - q_{0j} & \text{otherwise} \end{cases} \qquad p(x_j|y = 1, q) = \begin{cases} q_{1j} & \text{if } x_j = 1 \\ 1 - q_{1j} & \text{otherwise} \end{cases}$$

  ❑ *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

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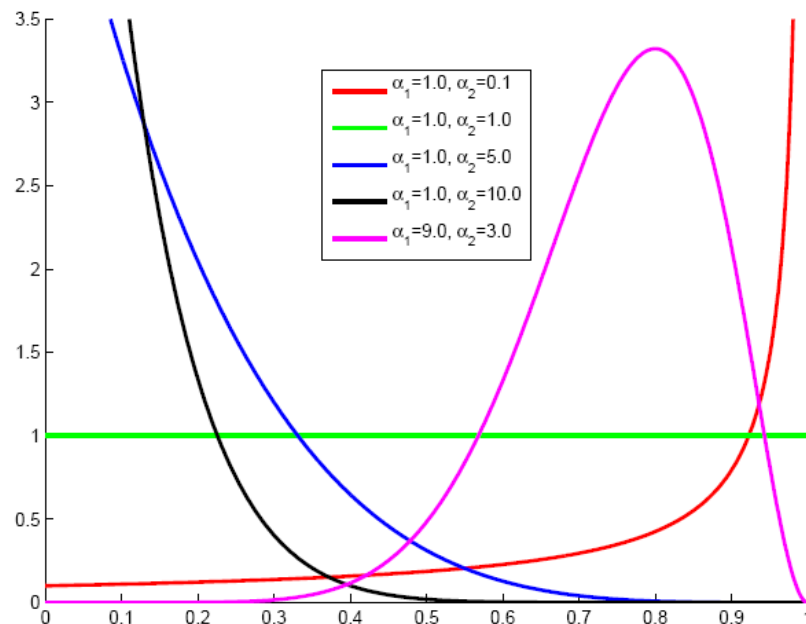
A Bayesian Treatment

◈ 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
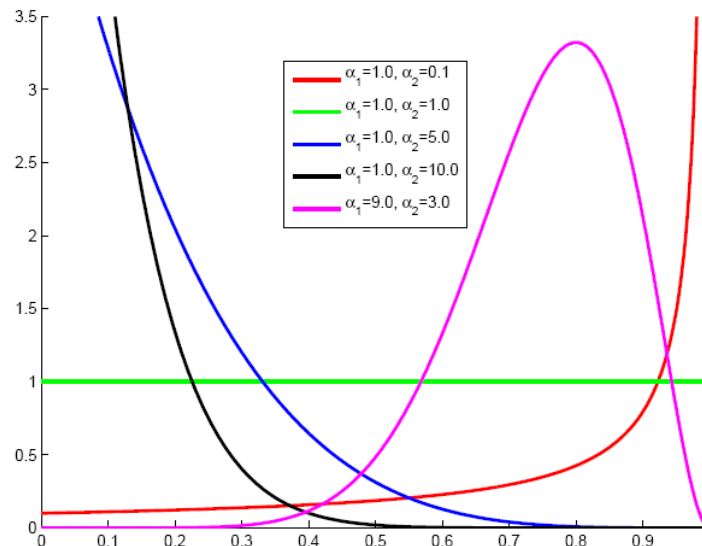
Bayesian Regression
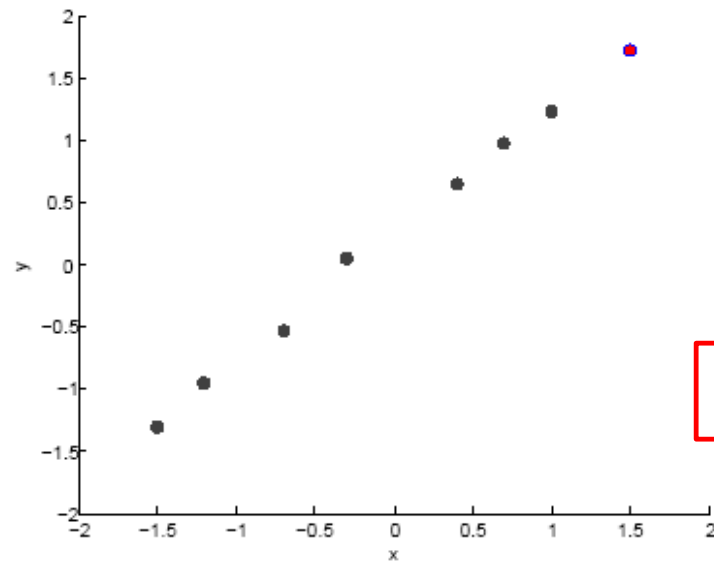
$$f : \ \mathcal{X} \to \mathcal{Y}$$

◆ 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
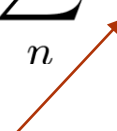
◆ Sometimes assume variance is:

    ❑ independent of Y (i.e., σ_i)

    ❑ or independent of X (i.e., σ_y)

    ❑ or both (i.e., σ)
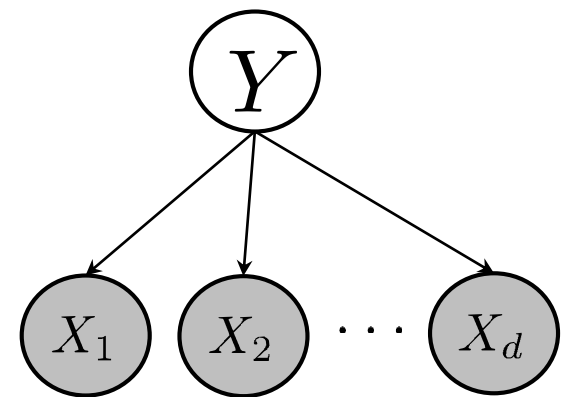
Estimating Parameters & Prediction

◆ 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

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

◆ Prediction:

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

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

f(x)

x

Linear fit

$$\mathbf{w^Tx} + b = 0$$

$$\mathbf{w^Tx} + b > 0$$

$$\mathbf{w^Tx} + b < 0$$
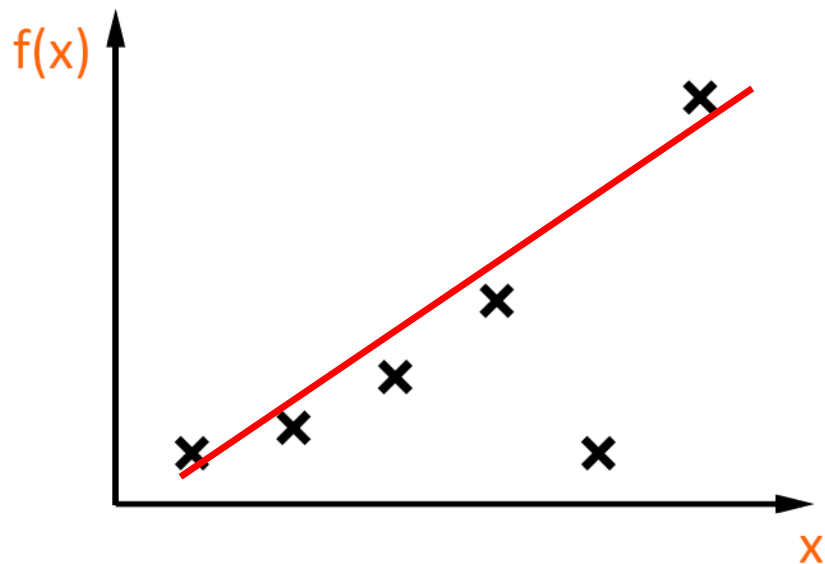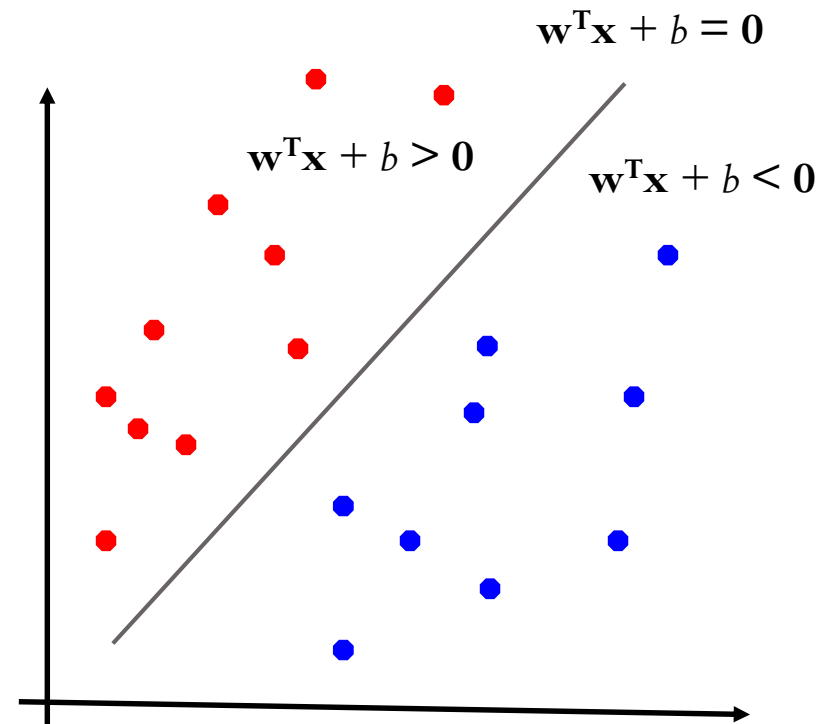
Linear decision boundary

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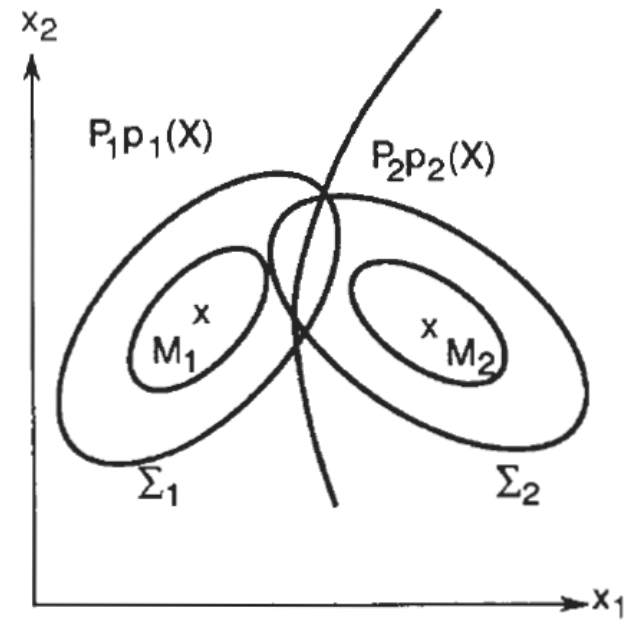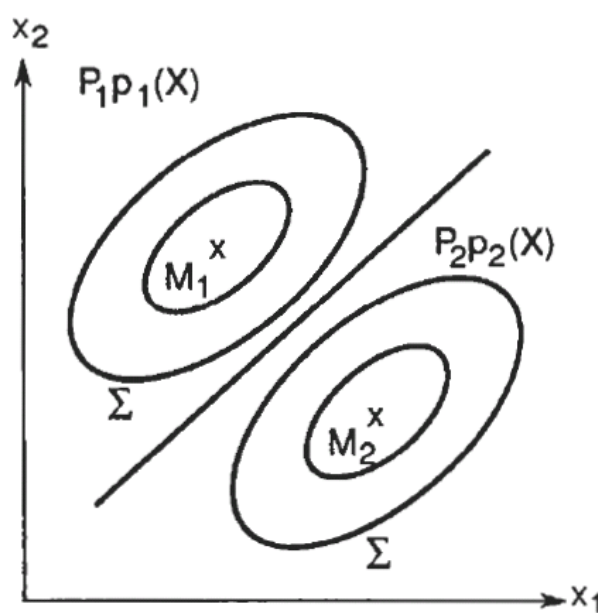
$$P_1 = P(Y = 0), \quad P_2 = P(Y = 1)$$

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

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

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:

$$p(y = 1|\mathbf{x}, \mu, \Sigma, \pi) = \frac{1}{1 + \frac{p(y=0, \mathbf{x}|\mu, \Sigma, \pi)}{p(y=1, \mathbf{x}|\mu, \Sigma, \pi)}}$$

$$= \frac{1}{1 + \frac{(1-\pi) \prod_i \mathcal{N}(x_i|\mu_{i0}, \sigma_i^2)}{\pi \prod_i \mathcal{N}(x_i|\mu_{i1}, \sigma_i^2)}}$$

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

◆ **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

$$\hat{y} = \underset{y}{\arg\max}\, P(\mathbf{x}, Y = y)$$

   ❑ But, we note that

$$\hat{y} = \underset{y}{\arg\max}\, P(Y = y | \mathbf{x})$$
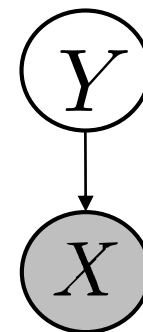
◈ Why not learn P(Y|X) directly? Or, why not learn the decision boundary directly?

◈ **Discriminative classifiers** (e.g., Logistic regression)

   ❑ Assume some functional form for P(Y|X)

   ❑ Estimate parameters of P(Y|X) directly from training data
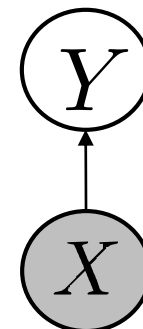
Logistic Regression

◆ 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
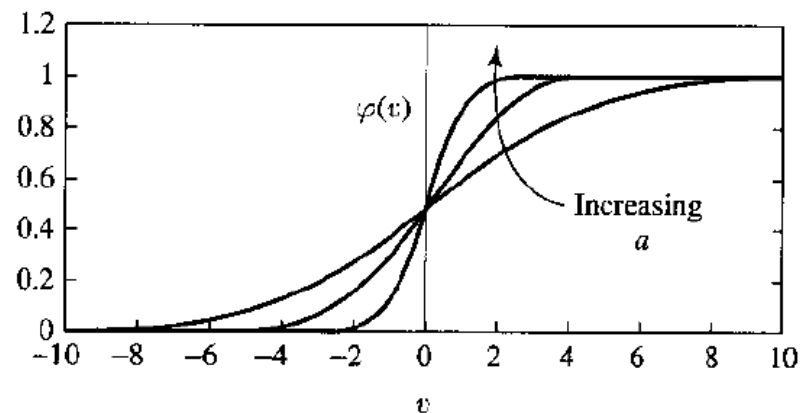
use a large α can be good for some neural networks

Logistic Regression

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

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

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

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

$$\mathbf{w}^\top \mathbf{x} + w_0 = 0$$
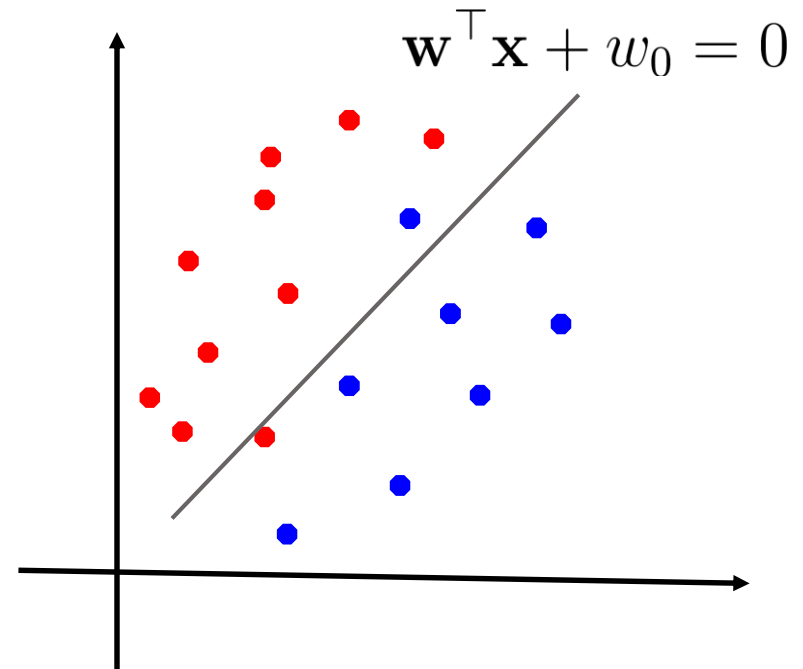
Logistic regression is a linear classifier!

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?

Training Logistic Regression

◆ We consider the binary classification

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

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

◆ How to learn the parameters?

◆ Can we do MLE?

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

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

◆ Can we do large-margin learning?

Maximum Conditional Likelihood Estimate

◆ We learn the parameters by solving

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

◆ **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

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

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

◆ 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

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmax}} \, \mathcal{L}(\mathbf{w})$$

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

◈ 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)
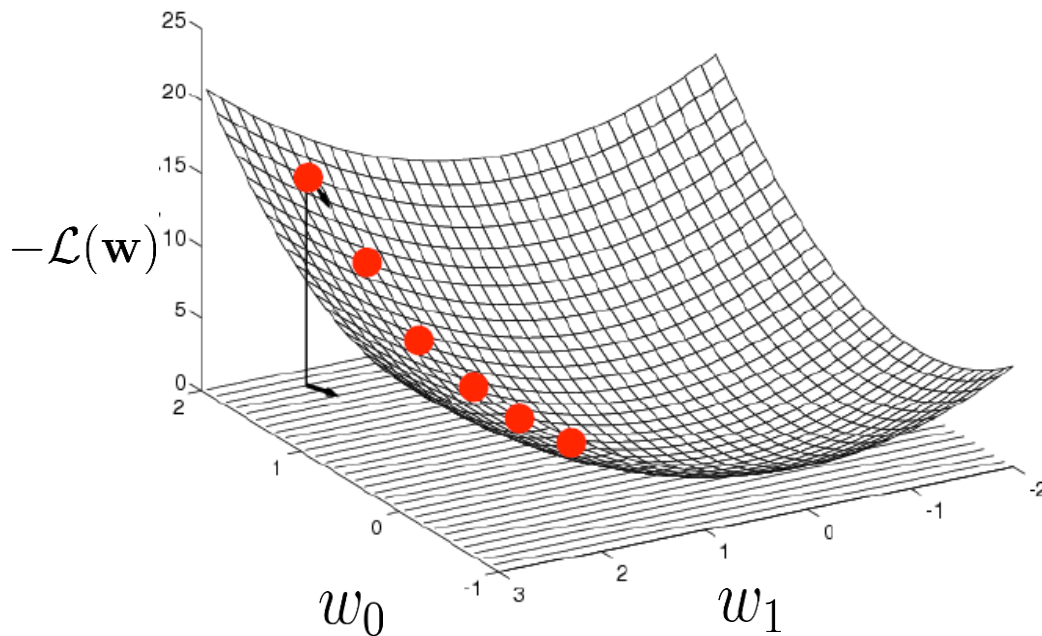
Gradient:

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

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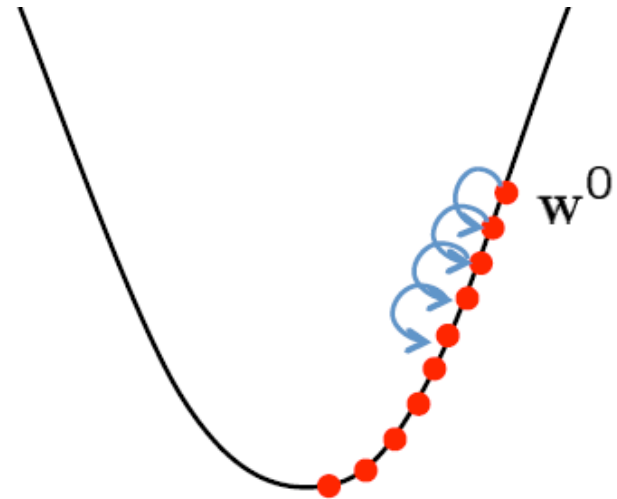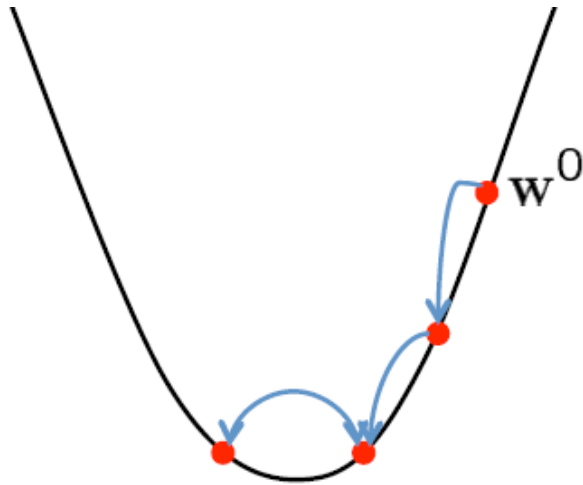
- ◈ Large η => fast convergence but larger residual error; Also possible oscillations
- ◈ Small η => slow convergence but small residual error

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
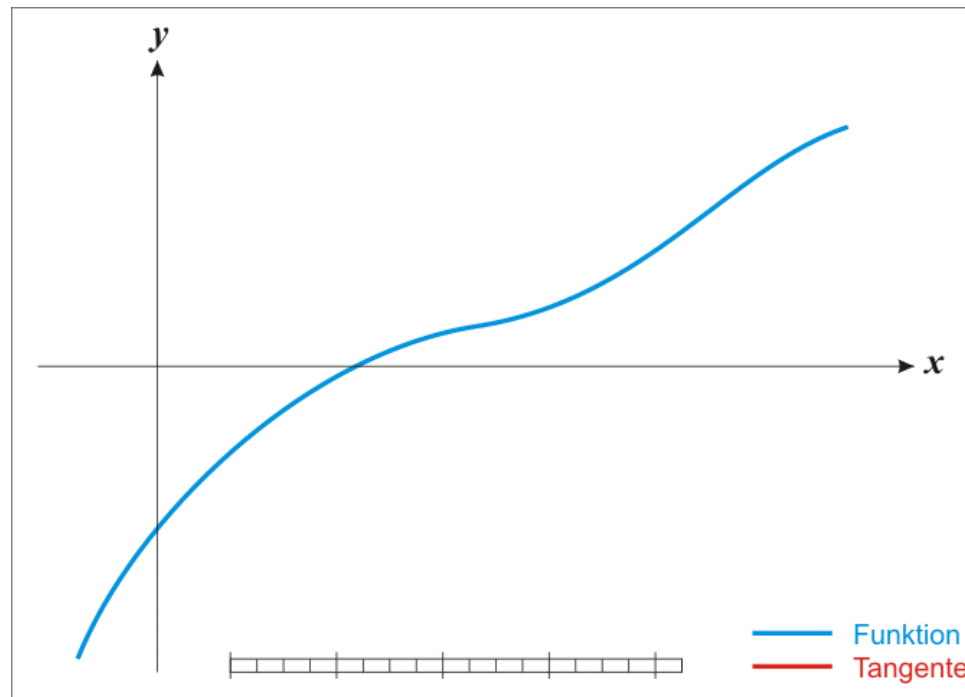
The Newton's Method

◈ 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:

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

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:

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

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

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

$$= \mathbf{w}_t - (XRX^\top)^{-1}X(\boldsymbol{\mu} - \mathbf{y})$$

$$= (XRX^\top)^{-1}\left\{XRX^\top\mathbf{w}_t - X(\boldsymbol{\mu} - \mathbf{y})\right\}$$

$$= (XRX^\top)^{-1}XR\mathbf{z}$$

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

Convergence curves
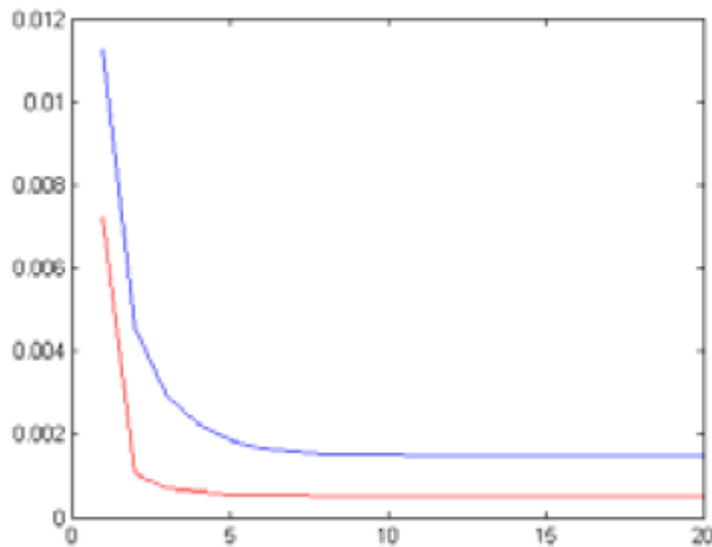
rec.autos
vs.
rec.sports.baseball
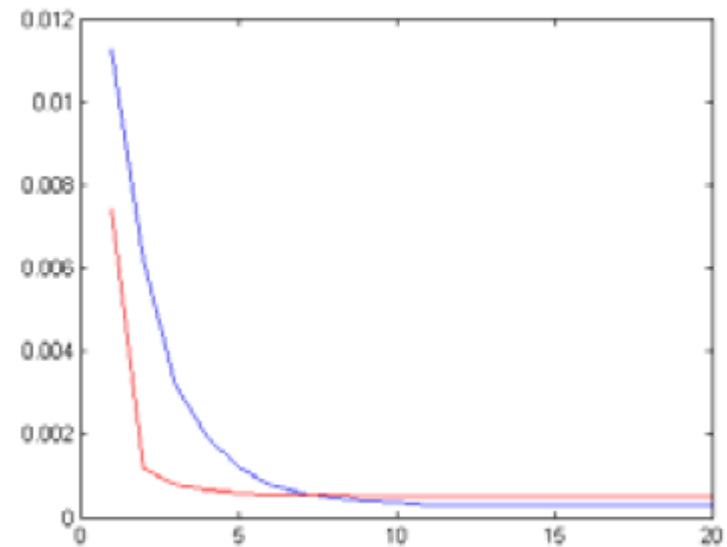
comp.windows.x
vs.
rec.motorcycles

- 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
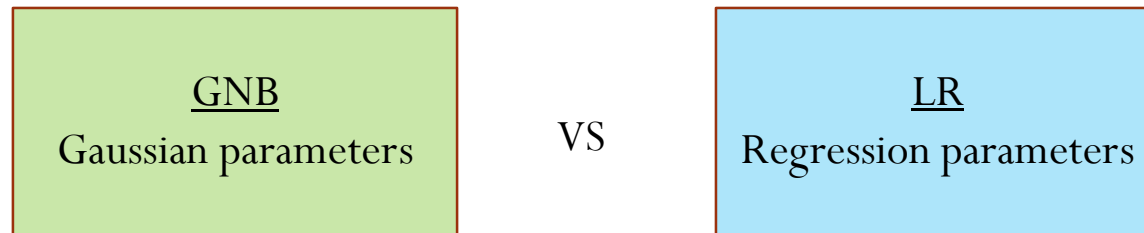
◆ Representation equivalence

- ❑ 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

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

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

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

Generative vs. Discriminative

◆ Given finite data (*N* data points, d features)

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

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

❑ 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 ------
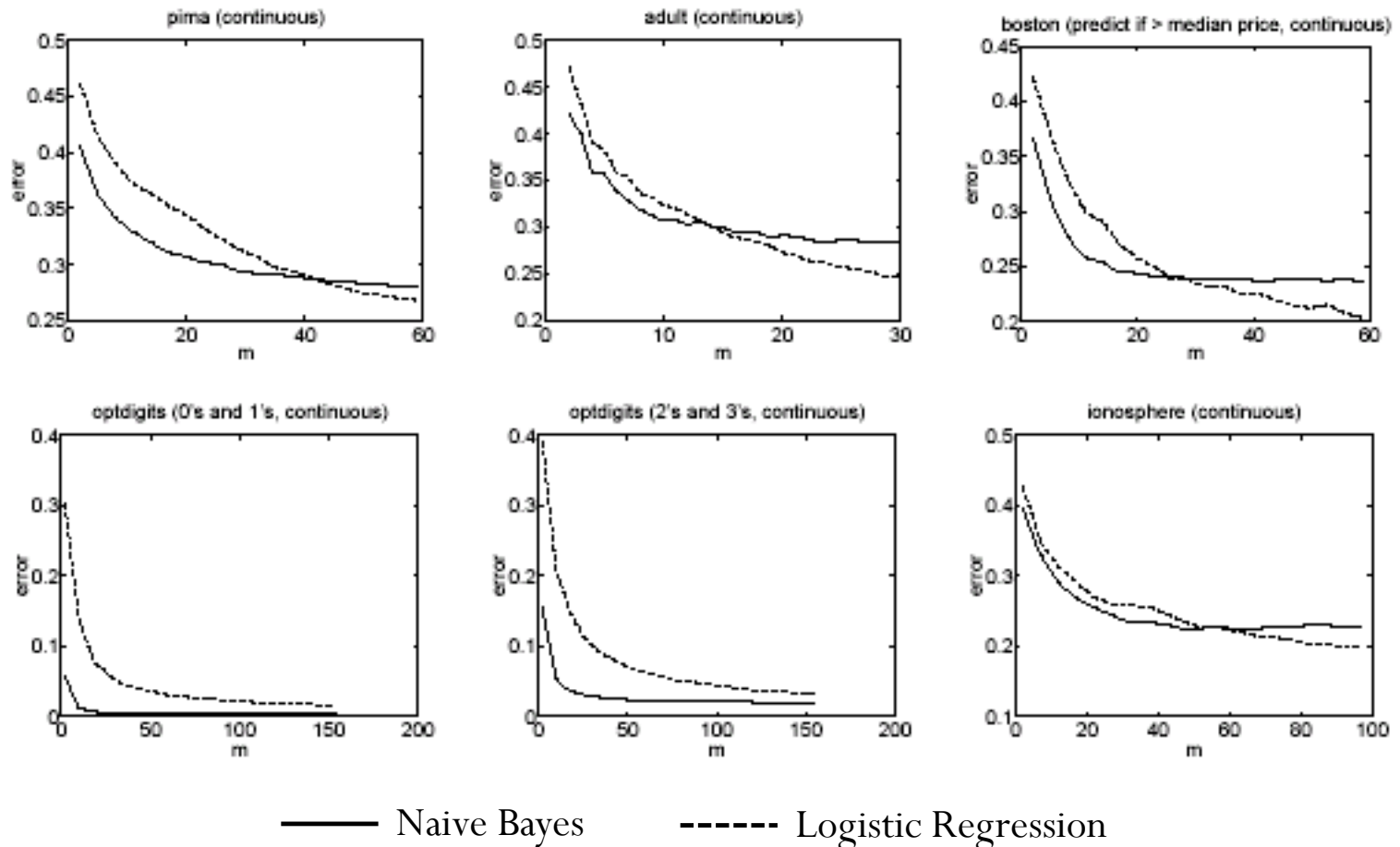
What you need to know

- 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

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

$$= \frac{1}{Z(\boldsymbol{\eta})} h(\mathbf{x}) \exp\left(\boldsymbol{\eta}^\top T(\mathbf{x})\right)$$
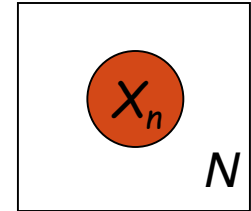
is an **exponential family distribution** with natural (canonical) parameter η

◆ 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:

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

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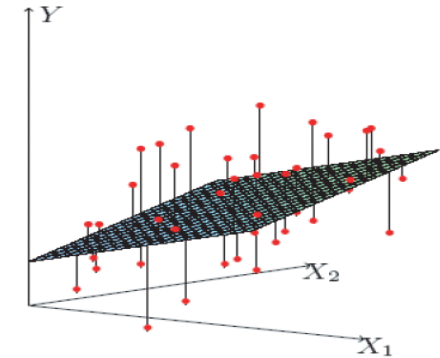
where ε is an error term of unmodeled effects or random noise

◆ 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

$$\mu(\mathbf{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \mathbf{x}}}$$
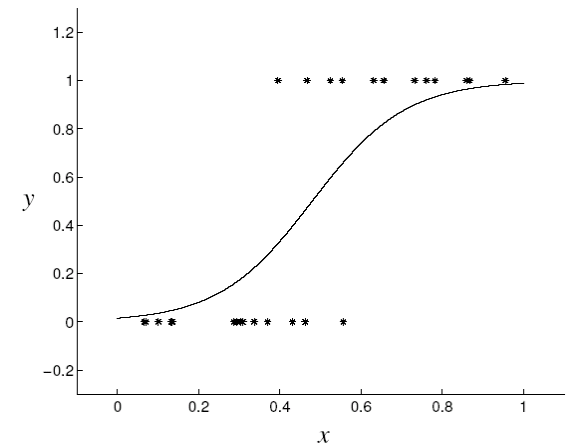
◆ We can use the brute-force gradient method as in LR

◆ 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

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

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

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

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

  ▫ 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 归一化trick

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

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

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

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

Why exponential family?

◆ Moment generating property (proof?)

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

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

Moment estimation

◆ We can easily compute moments of any exponential family distribution by taking the derivatives of the log normalizer $A(\eta)$.

◆ The qth derivative gives the qth centered moment.

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

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

$$\vdots$$

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

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

◆ 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.
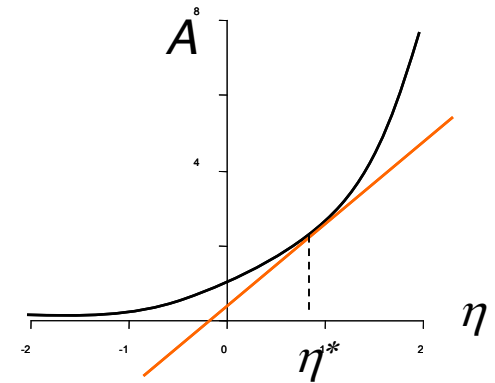
IID Sampling for Exponential Family

◆ 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

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

$$= \left(\prod_i h(\mathbf{x}_i)\right) \exp\left(\boldsymbol{\eta}^\top \sum_i T(\mathbf{x}_i) - NA(\boldsymbol{\eta})\right)$$
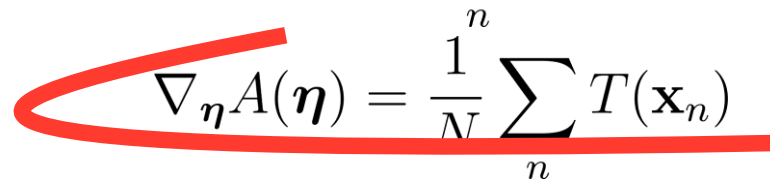
❑ Sufficient statistics:

$$\sum_i T(\mathbf{x}_i)$$

MLE for Exponential Family

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

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

◆ Take derivatives and set to zero:

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

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

$$\hat{\boldsymbol{\mu}}_{MLE} = \frac{1}{N} \sum_n T(\mathbf{x}_n) \qquad \text{\textcolor{blue}{\textbf{Only involve sufficient stiatistics!}}}$$

◆ This amounts to **moment matching**.

◆ We can infer the canonical parameters using $\hat{\boldsymbol{\eta}}_{MLE} = \psi(\hat{\boldsymbol{\mu}}_{MLE})$

Examples

◆ Gaussian: $\quad \boldsymbol{\eta} = \left[\Sigma^{-1}\boldsymbol{\mu}; -\frac{1}{2}\text{vec}(\Sigma^{-1})\right]$

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

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

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

◆ 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: $\quad \eta = \log\lambda$

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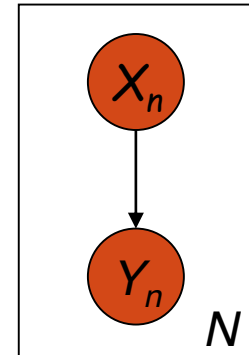$$h(x) = \frac{1}{x!}$$

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

GLIM, cont.

$$\theta$$

$$x \longrightarrow \xi \xrightarrow{f} \mu \xrightarrow{\psi} \eta \xrightarrow{EXP} y$$

EXP (arrow from μ to y)

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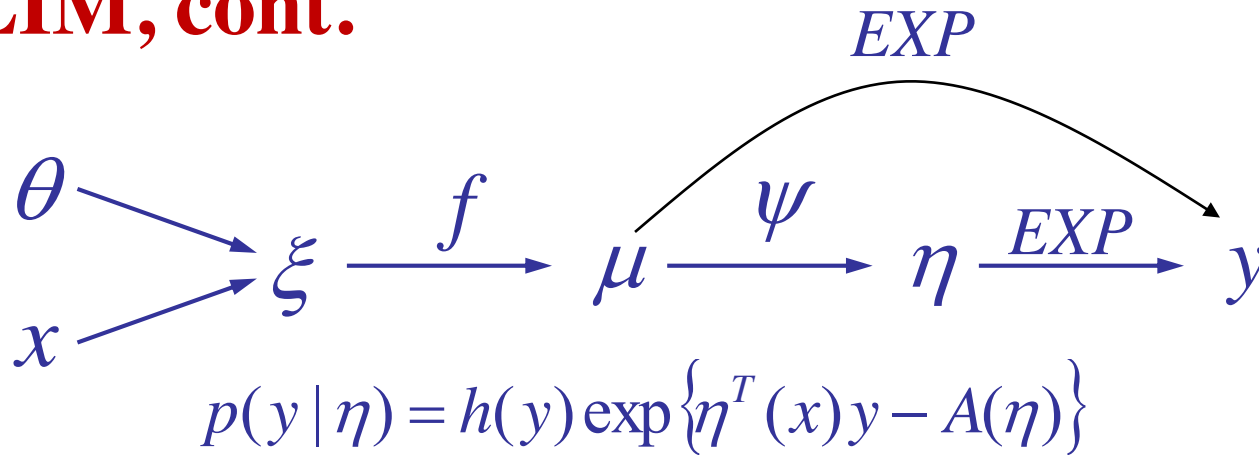
$$\Rightarrow p(y \mid \eta, \phi) = h(y, \phi) \exp\left\{\tfrac{1}{\phi}\left(\eta^T(x)y - A(\eta)\right)\right\}$$

- 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

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

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

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

$$= \sum_n (y_n - \mu_n) \mathbf{x}_n$$

$$= X(\mathbf{y} - \boldsymbol{\mu})$$

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

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

$$= \sum_n (y_n - \mu_n)\mathbf{x}_n$$

$$= X(\mathbf{y} - \boldsymbol{\mu})$$

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