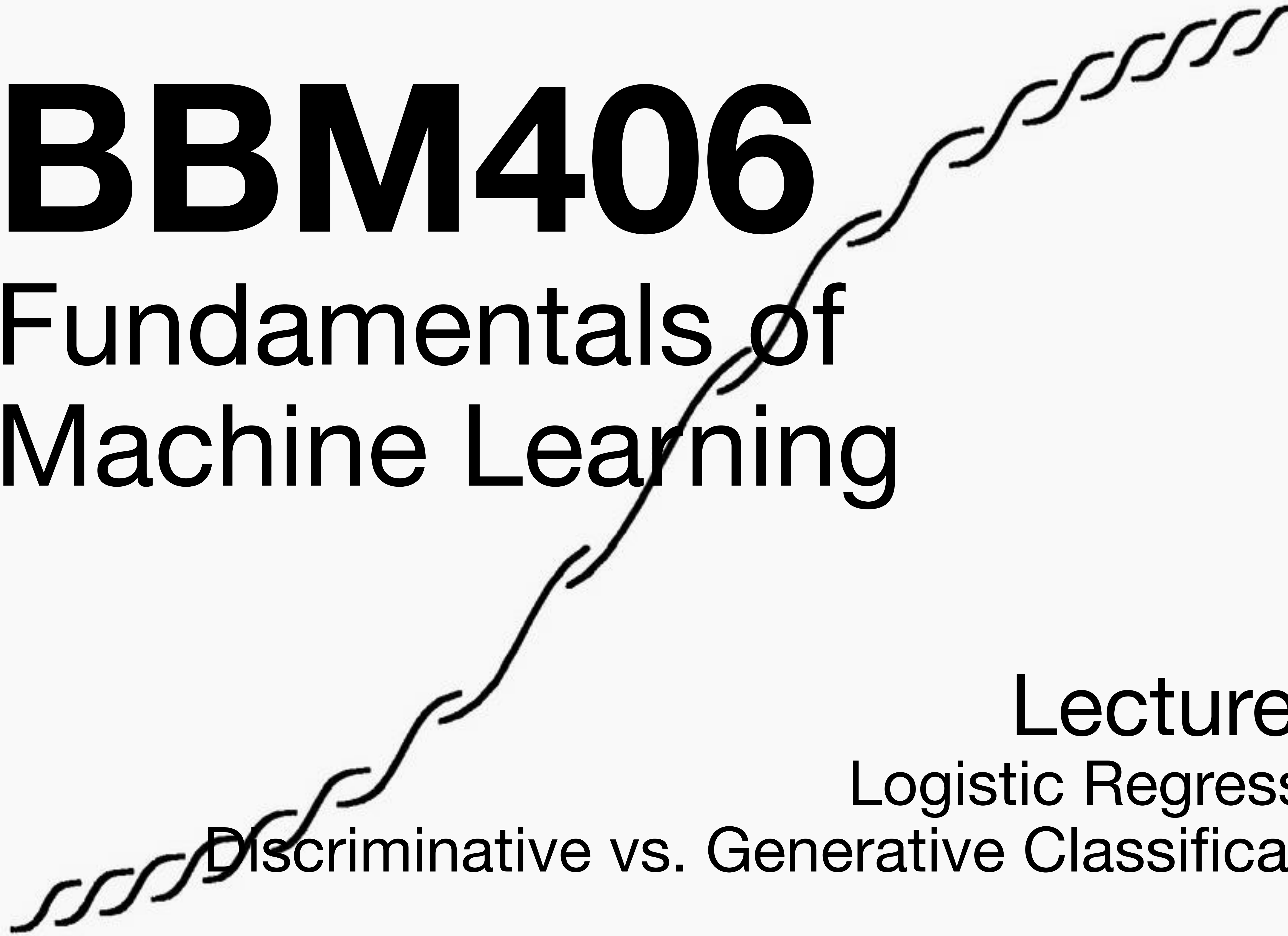
Illustration: Theodore Modis



# BBM406

## Fundamentals of Machine Learning

### Lecture 9:

Logistic Regression
Discriminative vs. Generative Classification

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Aykut Erdem // Hacettepe University // Fall 2019

# **Last time…** Naïve Bayes Classifier

**Given**:

- Class prior $P(Y)$
- $d$ conditionally independent features $X_1,\ldots X_d$ given the class label $Y$
- For each $X_i$ feature, we have the conditional likelihood $P(X_i|Y)$

Naïve Bayes Decision rule:

$$\begin{aligned} f_{NB}(\mathbf{x}) &= \arg\max_y \; P(x_1, \ldots, x_d \mid y) P(y) \\ &= \arg\max_y \prod_{i=1}^{d} P(x_i|y) P(y) \end{aligned}$$

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# **Last time…** Naïve Bayes Algorithm for discrete features

$$f_{NB}(\mathbf{x}) = \arg\max_y \prod_{i=1}^{d} P(x_i|y)P(y)$$ **We need to estimate these probabilities!**

## Estimators

For Class Prior
$$\widehat{P}(y) = \frac{\{\#j : Y^{(j)} = y\}}{n}$$

For Likelihood
$$\frac{\widehat{P}(x_i, y)}{\widehat{P}(y)} = \frac{\{\#j : X_i^{(j)} = x_i, Y^{(j)} = y\}/n}{\{\#j : Y^{(j)} = y\}/n}$$

**NB Prediction for test data:** $X = (x_1, \ldots, x_d)$

$$Y = \arg\max_y \widehat{P}(y) \prod_{i=1}^{d} \frac{\widehat{P}(x_i, y)}{\widehat{P}(y)}$$

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# **Last time...** Text Classification

MEDLINE Article


Brain and Cognition

Syntactic frame and verb bias in aphasia: Plausibility judgments of undergoer-subject sentences

?

**MeSH Subject Category Hierarchy**

- Antogonists and Inhibitors
- Blood Supply
- Chemistry
- Drug Therapy
- Embryology
- Epidemiology
- …

How to represent a text document?

slide by Dan Jurafsky

# **Last time…** Bag of words model

Typical additional assumption:

**Position in document doesn't matter**:

P($X_i$=$x_i$|Y=y) = P($X_k$=$x_i$|Y=y)

- "Bag of words" model – order of words on the page ignored
  The document is just a bag of words: i.i.d. words
- Sounds really silly, but often works very well!

$\Rightarrow$ K(50000-1) parameters to estimate

The probability of a document with words $x_1, x_2, \ldots$

$$\prod_{i=1}^{LengthDoc} P(x_i|y) = \prod_{w=1}^{W} P(w|y)^{count_w}$$

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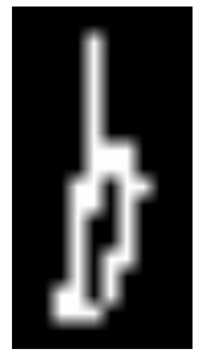
# **Last time…** What if features are continuous?

e.g., character recognition: $X_i$ is intensity at $i^{th}$ pixel

## Gaussian Naïve Bayes (GNB):

$$P(X_i = x \mid Y = y_k) = \frac{1}{\sigma_{ik}\sqrt{2\pi}} \; e^{\frac{-(x-\mu_{ik})^2}{2\sigma_{ik}^2}}$$

**Different mean and variance for each class k and each pixel i.**

Sometimes assume variance

- is independent of Y (i.e., $\sigma_i$),
- or independent of $X_i$ (i.e., $\sigma_k$)
- or both (i.e., $\sigma$)

$$\boxed{\widehat{\mu}_{MLE} = \frac{1}{N}\sum_{j=1}^{N} x_j}$$

$$\boxed{\widehat{\sigma}^2_{unbiased} = \frac{1}{N-1}\sum_{j=1}^{N} (x_j - \widehat{\mu})^2}$$

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# Logistic Regression

# Recap: Naïve Bayes

- NB Assumption: $P(X_1 ... X_d|Y) = \prod_{i=1}^{d} P(X_i|Y)$

- NB Classifier:

$$f_{NB}(x) \;=\; \arg\max_y \prod_{i=1}^{d} P(x_i|y)P(y)$$

- Assume parametric form for $P(X_i|Y)$ and $P(Y)$
  - Estimate parameters using MLE/MAP and plug in

# Gaussian Naïve Bayes (GNB)

- There are several distributions that can lead to a linear boundary.
- As an example, consider Gaussian Naïve Bayes:

$$Y \sim \text{Bernoulli}(\pi)$$

$$P(X_i|Y = y) = \frac{1}{\sqrt{2\pi\sigma_{i,y}^2}}\, e^{\frac{-(X_i - \mu_{i,y})^2}{2\sigma_{i,y}^2}}$$

**Gaussian class conditional densities**

- What if we assume variance is independent of class, i.e. $\sigma_{i,0}^2 = \sigma_{i,1}^2$

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# GNB with equal variance is a Linear Classifier!

$$P(X_i|Y=y) = \frac{1}{\sqrt{2\pi\sigma_i^2}}\, e^{\frac{-(X_i-\mu_{i,y})^2}{2\sigma_i^2}}$$

**Decision boundary:**

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

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# GNB with equal variance is a Linear Classifier!

$$P(X_i|Y=y) = \frac{1}{\sqrt{2\pi\sigma_i^2}}\, e^{\frac{-(X_i-\mu_{i,y})^2}{2\sigma_i^2}}$$

**Decision boundary:**

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

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

# GNB with equal variance is a Linear Classifier!

$$P(X_i|Y=y) = \frac{1}{\sqrt{2\pi\sigma_i^2}}\, e^{\frac{-(X_i-\mu_{i,y})^2}{2\sigma_i^2}}$$

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$$= \underbrace{\log\frac{1-\pi}{\pi} + \sum_i \frac{\mu_{i,1}^2-\mu_{i,0}^2}{2\sigma_i^2}}_{\text{Constant term}} + \underbrace{\sum_i \frac{\mu_{i,0}-\mu_{i,1}}{\sigma_i^2}}_{\text{First-order term}} X_i =: w_0 + \sum_i w_i X_i$$

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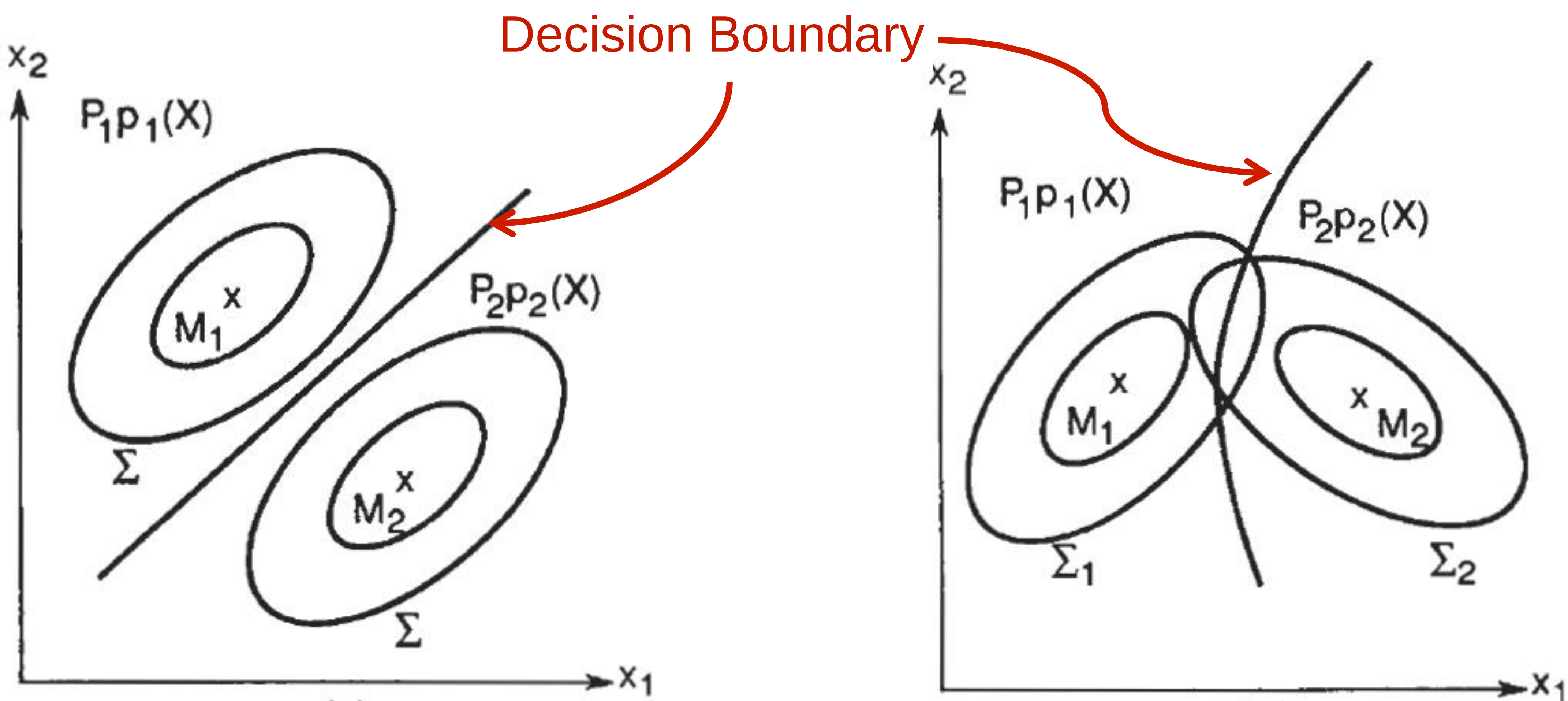
# Gaussian Naive Bayes (GNB)




$$\begin{aligned} X &= (x_1, x_2) \\ P_1 &= P(Y=0) \\ P_2 &= P(Y=1) \\ p_1(X) &= p(X|Y=0) \sim \mathcal{N}(M_1, \Sigma_1) \\ p_2(X) &= p(X|Y=1) \sim \mathcal{N}(M_2, \Sigma_2) \end{aligned}$$

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# Generative vs. Discriminative Classifiers

- Generative classifiers (e.g. Naïve Bayes)
  - Assume some functional form for P(X,Y) (or P(X|Y) and P(Y))
  - Estimate parameters of P(X|Y), P(Y) directly from training data
- But arg max_Y P(X|Y) P(Y) = arg max_Y P(Y|X)
- Why not learn P(Y|X) directly? Or better yet, why not learn the decision boundary directly?
- Discriminative classifiers (e.g. Logistic Regression)
  - Assume some functional form for P(Y|X) or for the decision boundary
  - Estimate parameters of P(Y|X) directly from training data

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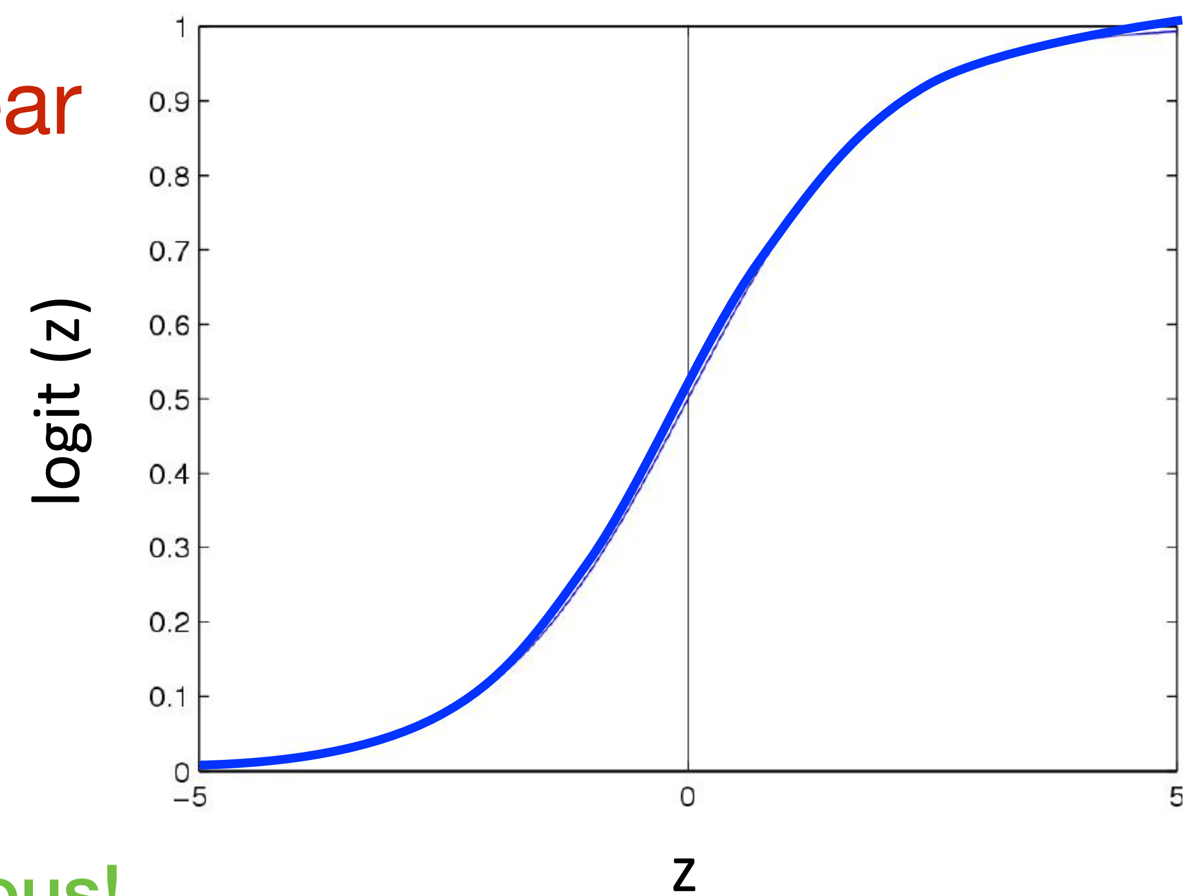
# Logistic Regression

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_i w_i X_i)}$$

Logistic function applied to linear function of the data

Logistic function (or Sigmoid): $\frac{1}{1+exp(-z)}$




Features can be discrete or continuous!

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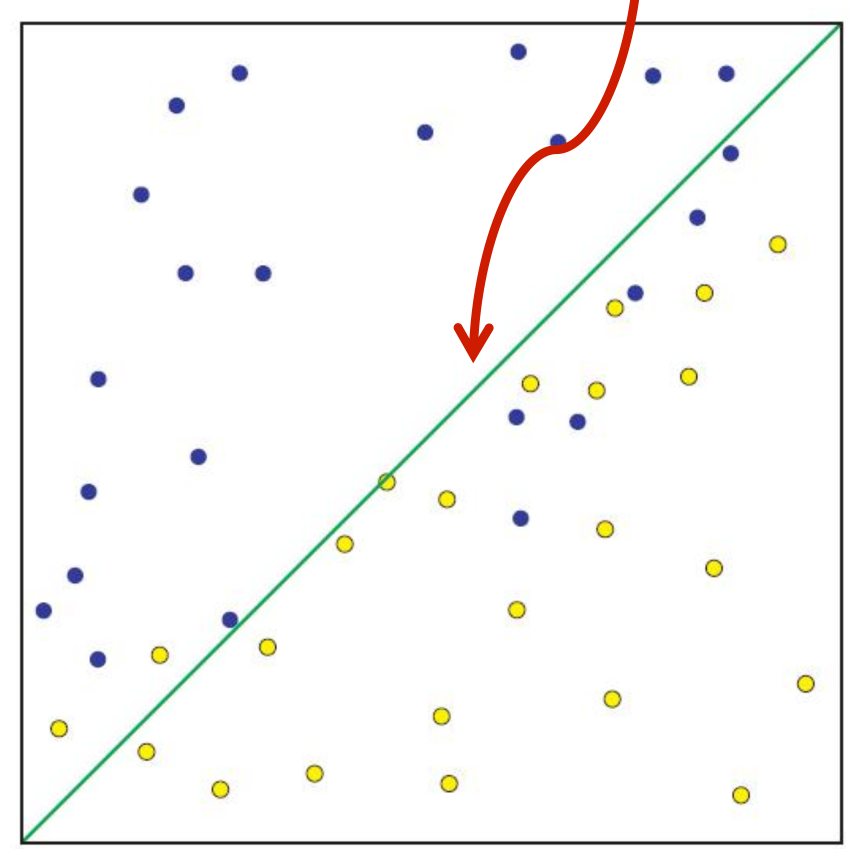
# Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_i w_i X_i)}$$

$$w_0 + \sum_i w_i X_i = 0$$

Decision boundary:



$$P(Y=0|X) \overset{0}{\underset{1}{\gtrless}} P(Y=1|X)$$

$$w_0 + \sum_i w_i X_i \overset{0}{\underset{1}{\gtrless}} 0$$

**(Linear Decision Boundary)**

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# Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow P(Y = 0|X) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow \frac{P(Y = 0|X)}{P(Y = 1|X)} = \exp(w_0 + \sum_i w_i X_i) \quad \overset{0}{\underset{1}{\gtrless}} \quad 1$$

$$\Rightarrow \boxed{w_0 + \sum_i w_i X_i \quad \overset{0}{\underset{1}{\gtrless}} \quad 0}$$

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# Logistic Regression for more than 2 classes

- Logistic regression in more general case, where $Y \in \{y_1,\ldots,y_K\}$

for k<K

$$P(Y=y_k|X) = \frac{\exp(w_{k0} + \sum_{i=1}^{d} w_{ki}X_i)}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{d} w_{ji}X_i)}$$

for k=K (normalization, so no weights for this class)

$$P(Y=y_K|X) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{d} w_{ji}X_i)}$$

# Training Logistic Regression

We'll focus on binary classification:

$$P(Y=0|\mathbf{X},\mathbf{w}) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

$$P(Y=1|\mathbf{X},\mathbf{w}) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

**How to learn the parameters $w_0$, $w_1$, …, $w_d$?**

Training Data $\{(X^{(j)}, Y^{(j)})\}_{j=1}^{n}$ $\quad X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)})$

Maximum Likelihood Estimates

$$\widehat{\mathbf{w}}_{MLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P(X^{(j)}, Y^{(j)} \mid \mathbf{w})$$

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# Training Logistic Regression

We'll focus on binary classification:

$$P(Y=0|\mathbf{X},\mathbf{w}) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

$$P(Y=1|\mathbf{X},\mathbf{w}) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

**How to learn the parameters $w_0$, $w_1$, …, $w_d$?**

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Maximum Likelihood Estimates

$$\widehat{\mathbf{w}}_{MLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P(X^{(j)}, Y^{(j)} \mid \mathbf{w})$$

**But there is a problem…**

Don't have a model for P(X) or P(X|Y) — only for P(Y|X)

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# Training Logistic Regression

**How to learn the parameters $w_0, w_1, \ldots, w_d$?**

Training Data $\{(X^{(j)}, Y^{(j)})\}_{j=1}^{n}$ $\quad X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)})$

Maximum (Conditional) Likelihood Estimates

$$\widehat{\mathbf{w}}_{MCLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P(Y^{(j)} \mid X^{(j)}, \mathbf{w})$$

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

# Expressing Conditional log Likelihood

$$l(W) = \sum_l Y^l \ln P(Y^l = 1|X^l, W) + (1 - Y^l) \ln P(Y^l = 0|X^l, W)$$

$$P(Y = 0|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

$$P(Y = 1|X) = \frac{\exp(w_0 + \sum_{i=1}^n w_i X_i)}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

$Y$ can take only values 0 or 1, so only one of the two terms in the expression will be non-zero for any given $Y^l$

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# Expressing Conditional log Likelihood

$$l(W) \;=\; \sum_l Y^l \ln P(Y^l = 1|X^l, W) + (1 - Y^l) \ln P(Y^l = 0|X^l, W)$$

# Expressing Conditional log Likelihood

$$P(Y=0|X) = \frac{1}{1+\exp(w_0+\sum_{i=1}^n w_i X_i)}$$

$$P(Y=1|X) = \frac{\exp(w_0+\sum_{i=1}^n w_i X_i)}{1+\exp(w_0+\sum_{i=1}^n w_i X_i)}$$

$$\begin{aligned} l(W) &= \sum_l Y^l \ln P(Y^l=1|X^l,W) + (1-Y^l)\ln P(Y^l=0|X^l,W) \\ &= \sum_l Y^l \ln \frac{P(Y^l=1|X^l,W)}{P(Y^l=0|X^l,W)} + \ln P(Y^l=0|X^l,W) \end{aligned}$$

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# Expressing Conditional log Likelihood

$$P(Y=0|X) = \frac{1}{1+\exp(w_0+\sum_{i=1}^n w_i X_i)}$$

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$$\begin{aligned} l(W) &= \sum_l Y^l \ln P(Y^l=1|X^l,W) + (1-Y^l)\ln P(Y^l=0|X^l,W) \\ &= \sum_l Y^l \ln \frac{P(Y^l=1|X^l,W)}{P(Y^l=0|X^l,W)} + \ln P(Y^l=0|X^l,W) \\ &= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1+\exp(w_0+\sum_i^n w_i X_i^l)) \end{aligned}$$

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# Maximizing Conditional log Likelihood

$$\max_{\mathbf{w}} \; l(\mathbf{w}) \equiv \ln \prod_j P(y^j|\mathbf{x}^j, \mathbf{w})$$

$$= \sum_j y^j (w_0 + \sum_i^d w_i x_i^j) - \ln(1 + exp(w_0 + \sum_i^d w_i x_i^j))$$

**Bad news:** no closed-form solution to maximize $l(\mathbf{w})$

**Good news:** $l(\mathbf{w})$ is concave function of w! concave functions easy to optimize (unique maximum)

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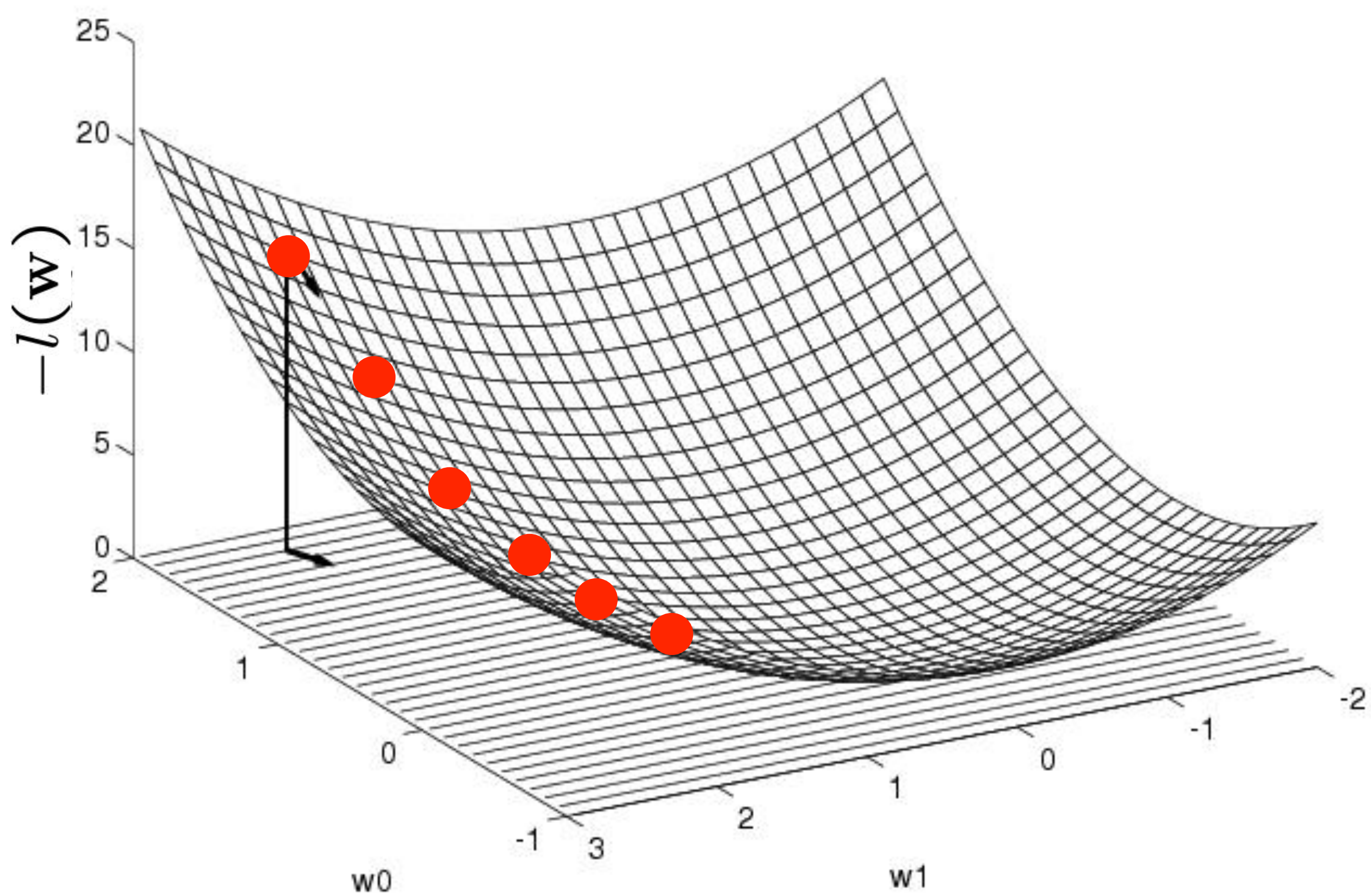
# Optimizing concave/convex functions

- Conditional likelihood for Logistic Regression is concave
- Maximum of a concave function = minimum of a convex function

**Gradient Ascent (concave)/ Gradient Descent (convex)**




**Gradient:**

$$\nabla_{\mathbf{w}} l(\mathbf{w}) = [\frac{\partial l(\mathbf{w})}{\partial w_0}, \ldots, \frac{\partial l(\mathbf{w})}{\partial w_n}]'$$

**Update rule:**

Learning rate, η>0

$$\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \frac{\partial l(\mathbf{w})}{\partial w_i}\Big|_t$$

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# Gradient Ascent for Logistic Regression

Gradient ascent algorithm: iterate until change < ε

$$w_0^{(t+1)} \leftarrow w_0^{(t)} + \eta \sum_j [y^j - \widehat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})]$$

For i-1,…,d,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \underbrace{\widehat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})]}_{\text{Predict what current weight thinks label Y should be}}$$

repeat

- Gradient ascent is simplest of optimization approaches
  – e.g. Newton method, Conjugate gradient ascent, IRLS (see Bishop 4.3.3)

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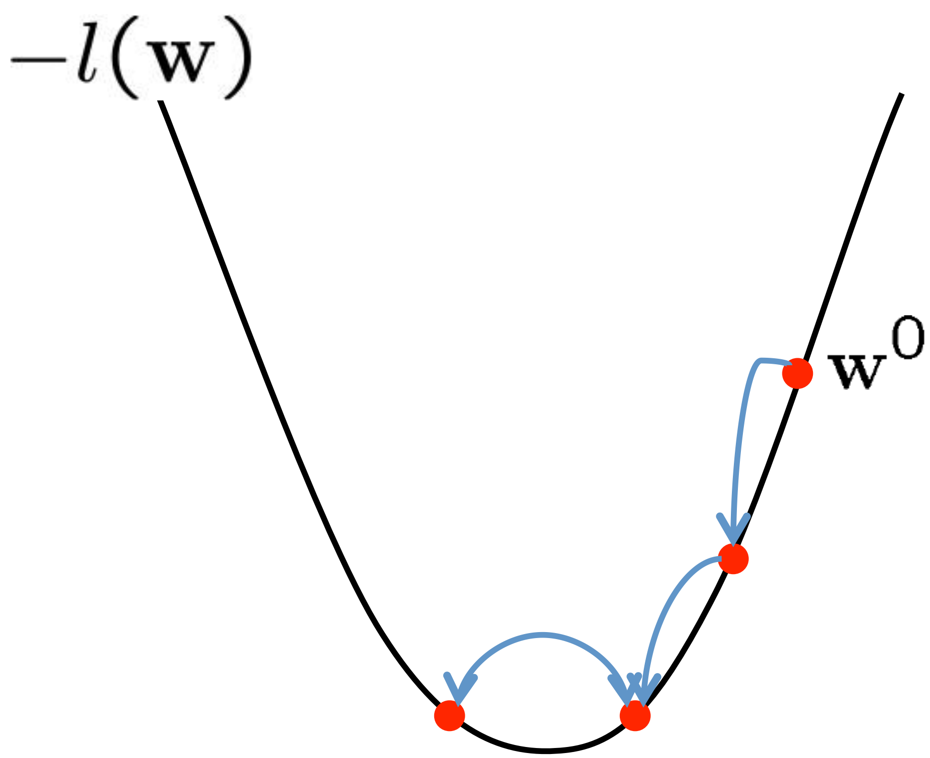
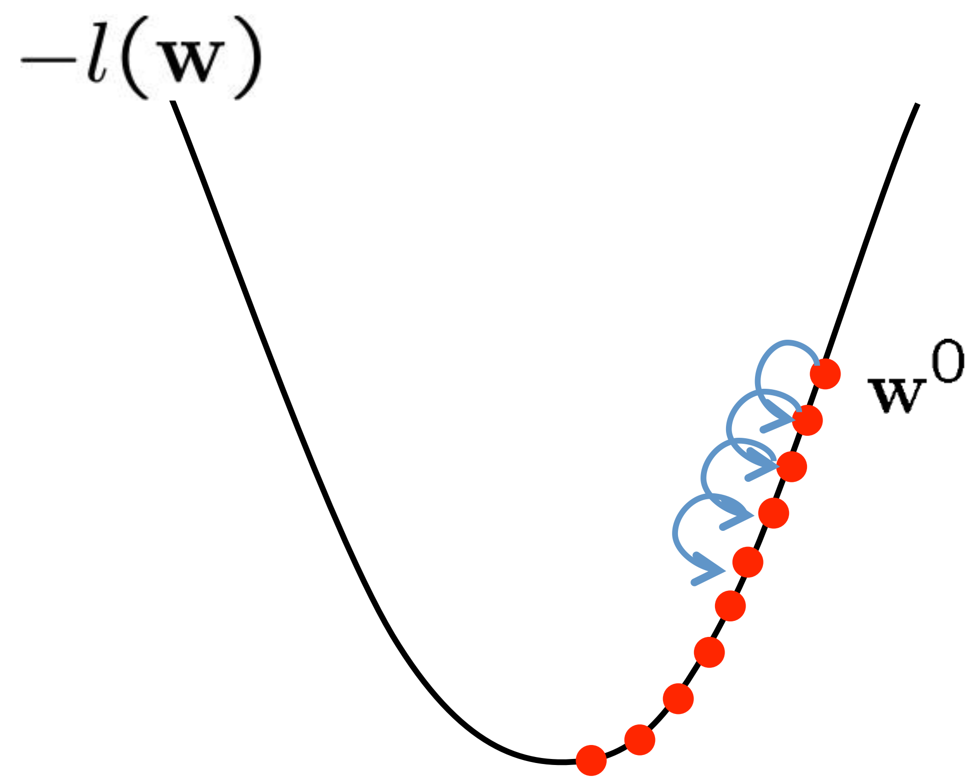
# Effect of step-size $\eta$




Large η → Fast convergence but larger residual error
Also possible oscillations

Small η → Slow convergence but small residual error

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# Naïve Bayes vs. Logistic Regression

**Set of Gaussian Naïve Bayes parameters (feature variance independent of class label)** ⟺ **Set of Logistic Regression parameters**

- Representation equivalence
  - **But only in a special case!!!** (GNB with class-independent variances)
- But what's the difference???

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# Naïve Bayes vs. Logistic Regression

**Set of Gaussian Naïve Bayes parameters (feature variance independent of class label)**

**Set of Logistic Regression parameters**

- Representation equivalence
  - **But only in a special case!!!** (GNB with class-independent variances)
- But what's the difference???
- **LR makes no assumption about** P(**X**|Y) **in learning!!!**
- Loss function!!!
  - Optimize different functions! Obtain different solutions

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# Naïve Bayes vs. Logistic Regression

Consider Y Boolean, $X_i$ continuous $X=<X_1 \ldots X_d>$

Number of parameters:

- NB: 4d+1 $\pi, (\mu_{1,y}, \mu_{2,y}, \ldots, \mu_{d,y}), (\sigma^2_{1,y}, \sigma^2_{2,y}, \ldots, \sigma^2_{d,y})$ y=0,1
- LR: d+1 $w_0, w_1, \ldots, w_d$

Estimation method:

- NB parameter estimates are uncoupled
- LR parameter estimates are coupled

# Generative vs. Discriminative

[Ng & Jordan, NIPS 2001]

Given **infinite data** (asymptotically),

If conditional independence assumption holds,
Discriminative and generative NB perform similar.

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

If conditional independence assumption does NOT holds,
Discriminative outperforms generative NB.

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

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# Generative vs. Discriminative

[Ng & Jordan, NIPS 2001]

Given **finite data** (n data points, d features),

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

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

Naïve 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 not coupled – each parameter is learnt independently, not jointly, from training data.

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# Naïve Bayes vs. Logistic Regression

**<u>Verdict</u>**

Both learn a linear decision boundary.
Naïve Bayes makes more restrictive assumptions and has higher asymptotic error,
BUT
converges faster to its less accurate asymptotic error.

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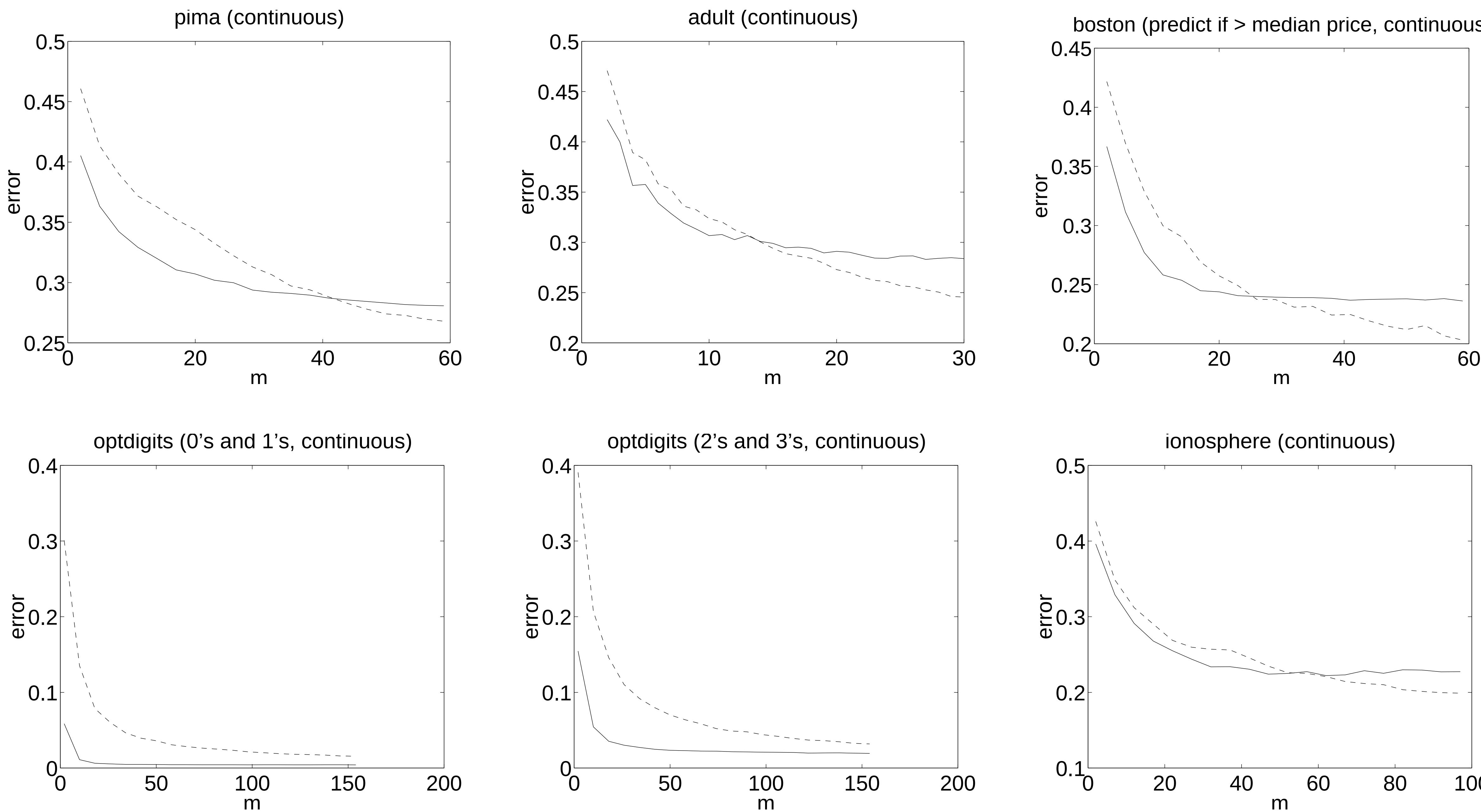
# Experimental Comparison (Ng-Jordan'01)

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




More in the paper...

—— Naïve Bayes ----- Logistic Regression

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# What you should know

- LR is a linear classifier
  - decision rule is a hyperplane
- LR optimized by maximizing conditional likelihood
  - no closed-form solution
  - concave ! global optimum with gradient ascent
- Gaussian Naïve Bayes with class-independent variances representationally equivalent to LR
  - Solution differs because of objective (loss) function
- In general, NB and LR make different assumptions
  - NB: Features independent given class! assumption on $P(\mathbf{X}|Y)$
  - LR: Functional form of $P(Y|\mathbf{X})$, no assumption on $P(\mathbf{X}|Y)$
- Convergence rates
  - GNB (usually) needs less data
  - LR (usually) gets to better solutions in the limit

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