Statistical Machine Learning

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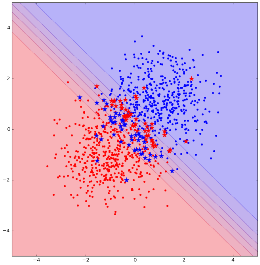
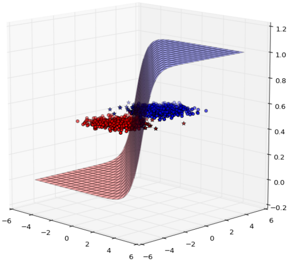
Slide credits and other course material can be found at:
http://www.stats.ox.ac.uk/~palamara/SML_BDI.html

Logistic regression

Review

- In LDA and QDA, we estimate $p(x|y)$, but for classification we are mainly interested in $p(y|x)$
- Why not estimate that directly? Logistic regression[1] is a popular way of doing this.





[1] Despite the name "regression", we are using it for classification!

Linearity of log-odds and logistic function

- $a + b^\top x$ models the **log-odds ratio**:

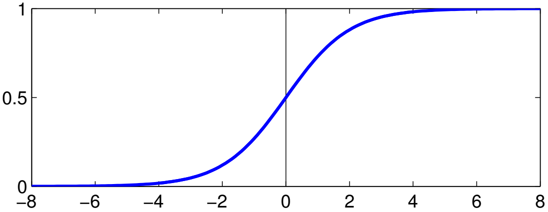
$$\log \frac{p(Y = +1|X = x; a, b)}{p(Y = -1|X = x; a, b)} = a + b^\top x.$$

- Solve explicitly for conditional class probabilities (using $p(Y = +1|X = x; a, b) + p(Y = -1|X = x; a, b) = 1$):

$$p(Y = +1|X = x; a, b) = \frac{1}{1 + \exp(-(a + b^\top x))} =: s(a + b^\top x)$$

$$p(Y = -1|X = x; a, b) = \frac{1}{1 + \exp(+(a + b^\top x))} = s(-a - b^\top x)$$

where $s(z) = 1/(1 + \exp(-z))$ is the **logistic function**.



Fitting the parameters of the hyperplane

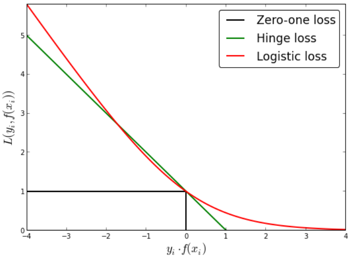
How to learn a and b given a training data set $(x_i, y_i)_{i=1}^n$?

- Consider maximizing the **conditional log likelihood**:

$$\ell(a,b) = \sum_{i=1}^n \log p(y_i|x_i) = \sum_{i=1}^n \log s(y_i(a + b^\top x_i)).$$

- Equivalent to minimizing the empirical risk associated with the **log loss**:

$$\widehat{R}_{\mathrm{log}}(f_{a,b}) = \frac{1}{n}\sum_{i=1}^n -\log s(y_i(a+b^\top x_i)) = \frac{1}{n}\sum_{i=1}^n \log(1+\exp(-y_i(a+b^\top x_i)))$$



Logistic Regression

- Log-loss is differentiable, but it is not possible to find optimal a, b analytically.
- For simplicity, absorb a as an entry in b by appending '1' into x vector, as we did before.
- Objective function:

$$\widehat{R}_{\text{log}} = \frac{1}{n} \sum_{i=1}^{n} -\log s(y_i x_i^\top b)$$

Logistic Function

$$s(-z) = 1 - s(z)$$
$$\nabla_z s(z) = s(z)s(-z)$$
$$\nabla_z \log s(z) = s(-z)$$
$$\nabla_z^2 \log s(z) = -s(z)s(-z)$$

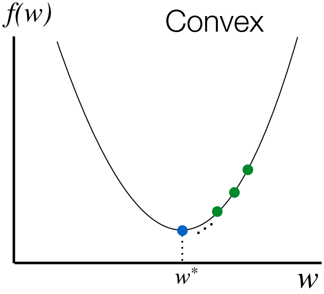
- Differentiate wrt b:

$$\nabla_b \widehat{R}_{\text{log}} = \frac{1}{n} \sum_{i=1}^{n} -s(-y_i x_i^\top b) y_i x_i$$

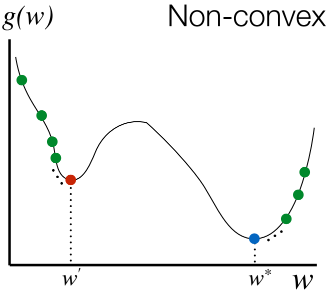
$$\nabla_b^2 \widehat{R}_{\text{log}} = \frac{1}{n} \sum_{i=1}^{n} s(y_i x_i^\top b) s(-y_i x_i^\top b) x_i x_i^\top \succeq 0.$$

- We cannot set $\nabla_b \widehat{R}_{\text{log}} = 0$ and solve: no closed form solution. We'll use numerical methods.

Where Will We Converge?



Any local minimum is a global minimum



Multiple local minima may exist

Least Squares, Ridge Regression and Logistic Regression are all convex!

Convexity

How to determine convexity? $f(x)$ is convex if

$$f^{''}(x) \geq 0$$

Examples:

$$f(x) = x^2, f^{''}(x) = 2 > 0$$

How to determine convexity in this case?

Matrix of second-order derivatives (Hessian)

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 f(\boldsymbol{x})}{\partial {x_1}^2} & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_D} \\ \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_2} & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2^2} & \dots & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_D} \\ \dots & \dots & \dots & \dots \\ \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_D} & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_D} & \dots & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_D^2} \end{pmatrix}$$

How to determine convexity in the multivariate case?

If the Hessian is positive semi-definite $\mathbf{H} \succeq 0$, then f is convex.

A matrix $\mathbf{H}$ is positive semi-definite if and only if, $\forall \boldsymbol{z}$,

$$\boldsymbol{z}^T \mathbf{H} \boldsymbol{z} = \sum_{j,k} H_{j,k} z_j z_k \geq 0$$

Logistic Regression

- Hessian is positive-definite: objective function is **convex** and there is **a single unique global minimum**.
- Many different algorithms can find optimal b, e.g.:
  - Gradient descent:

$$b^{\text{new}} = b + \epsilon \frac{1}{n} \sum_{i=1}^{n} s(-y_i x_i^\top b) y_i x_i$$

  - Stochastic gradient descent:

$$b^{\text{new}} = b + \epsilon_t \frac{1}{|I(t)|} \sum_{i \in I(t)} s(-y_i x_i^\top b) y_i x_i$$

    where $I(t)$ is a subset of the data at iteration t, and $\epsilon_t \to 0$ slowly ($\sum_t \epsilon_t = \infty, \sum_t \epsilon_t^2 < \infty$).
  - Conjugate gradient, LBFGS and other methods from numerical analysis.
  - Newton-Raphson:

$$b^{\text{new}} = b - (\nabla_b^2 \widehat{R}_{\text{log}})^{-1} \nabla_b \widehat{R}_{\text{log}}$$

    This is also called **iterative reweighted least squares**.

Iterative reweighted least squares (IRLS)

- We can write gradient and Hessian in a more compact form. Define $\mu_i = s(x_i^\top b)$, and the diagonal matrix $\mathbf{S}$ with $\mu_i(1-\mu_i)$ on its diagonal. Also define the vector $\mathbf{c}$ where $c_i = \mathbb{1}(y_i = +1)$. Then

$$\begin{aligned}
\nabla_b \widehat{R}_{\text{log}} =& \frac{1}{n}\sum_{i=1}^{n} -s(-y_i x_i^\top b) y_i x_i \\
=& \frac{1}{n}\sum_{i=1}^{n} x_i(\mu_i - c_i) \\
=& \mathbf{X}^\top(\mu - \mathbf{c}) \\
\nabla_b^2 \widehat{R}_{\text{log}} =& \frac{1}{n}\sum_{i=1}^{n} s(y_i x_i^\top b) s(-y_i x_i^\top b) x_i x_i^\top \\
=& \mathbf{X}^\top \mathbf{S}\mathbf{X}
\end{aligned}$$

Iterative reweighted least squares (IRLS)

Let $\mathbf{b}_t$ be the parameters after t "Newton steps".
The gradient and Hessian at step t are given by:

$$\begin{aligned}\mathbf{g}_t &= \mathbf{X}^\mathsf{T}(\boldsymbol{\mu}_t - \mathbf{c}) = -\mathbf{X}^\mathsf{T}(\mathbf{c} - \boldsymbol{\mu}_t) \\ \mathbf{H}_t &= \mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X}\end{aligned}$$

The Newton Update Rule is:

$$\begin{aligned}\mathbf{b}_{t+1} &= \mathbf{b}_t - \mathbf{H}_t^{-1}\mathbf{g}_t \\ &= \mathbf{b}_t + (\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}(\mathbf{c} - \boldsymbol{\mu}_t) \\ &= (\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{S}_t(\mathbf{X}\mathbf{b}_t + \mathbf{S}_t^{-1}(\mathbf{c} - \boldsymbol{\mu}_t)) \\ &= (\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{z}_t\end{aligned}$$

Where $\mathbf{z}_t = \mathbf{X}\mathbf{b}_t + \mathbf{S}_t^{-1}(\mathbf{c} - \boldsymbol{\mu}_t)$. Then $\mathbf{b}_{t+1}$ is a solution of the "weighted least squares" problem:

$$\text{minimise} \quad \sum_{i=1}^{N} S_{t,ii}(z_{t,i} - \mathbf{b}^\mathsf{T}\mathbf{x}_i)^2$$

Linearly separable data

Assume that the data is linearly separable, i.e. there is a scalar α and a vector β such that $y_i(\alpha + \beta^\top x_i) > 0$, $i = 1, \dots, n$. Let $c > 0$. The empirical risk for $a = c\alpha$, $b = c\beta$ is

$$\widehat{R}_{\mathsf{log}}(f_{a,b}) = \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-cy_i(\alpha + \beta^\top x_i)))$$

which can be made arbitrarily close to zero as $c \to \infty$, i.e. soft classification rule becomes $\pm\infty$ (overconfidence) $\to$ overfitting.

Regularization provides a solution to this problem.

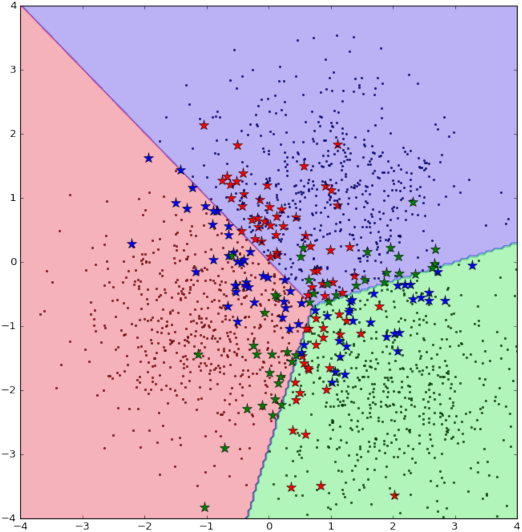
Multi-class logistic regression

The **multi-class/multinomial** logistic regression uses the **softmax** function to model the conditional class probabilities $p\left(Y=k|X=x;\theta\right)$, for K classes $k=1,\ldots,K$, i.e.,

$$p\left(Y=k|X=x;\theta\right)=\frac{\exp\left(w_k^\top x+b_k\right)}{\sum_{\ell=1}^{K}\exp\left(w_\ell^\top x+b_\ell\right)}.$$

Parameters are $\theta=(b,W)$ where $W=(w_{kj})$ is a $K\times p$ matrix of weights and $b\in\mathbb{R}^K$ is a vector of bias terms.

Multi-class logistic regression



Crab Dataset

```
library(MASS)
## load crabs data
data(crabs)
ct <- as.numeric(crabs[,1])-1+2*(as.numeric(crabs[,2])-1)
## project into first two LD
cb.lda <- lda(log(crabs[,4:8]),ct)
cb.ldp <- predict(cb.lda)
x <- cb.ldp$x[,1:2]
y <- as.numeric(ct==0)
eqscplot(x,pch=2*y+1,col=y+1)
```

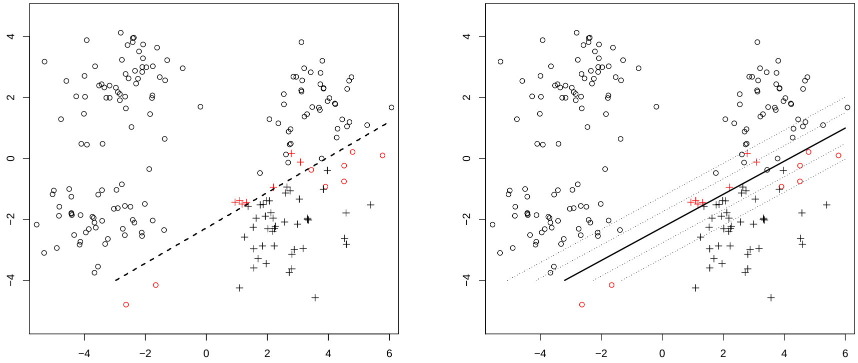
Crab Dataset

```
## visualize decision boundary
gx1 <- seq(-6,6,.02)
gx2 <- seq(-4,4,.02)
gx <- as.matrix(expand.grid(gx1,gx2))
gm <- length(gx1)
gn <- length(gx2)
gdf <- data.frame(LD1=gx[,1],LD2=gx[,2])

lda <- lda(x,y)
y.lda <- predict(lda,x)$class
eqscplot(x,pch=2*y+1,col=2-as.numeric(y==y.lda))
y.lda.grid <- predict(lda,gdf)$class
contour(gx1,gx2,matrix(y.lda.grid,gm,gn),
   levels=c(0.5), add=TRUE,d=FALSE,lty=2,lwd=2)
```

Crab Dataset

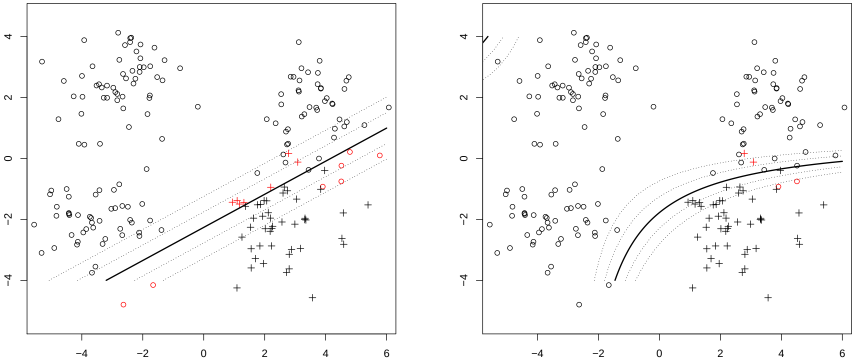
```
## logistic regression
xdf <- data.frame(x)
logreg <- glm(y ~ LD1 + LD2, data=xdf, family=binomial)
y.lr <- predict(logreg,type="response")
eqscplot(x,pch=2*y+1,col=2-as.numeric(y==(y.lr>.5)))
y.lr.grid <- predict(logreg,newdata=gdf,type="response")
contour(gx1,gx2,matrix(y.lr.grid,gm,gn),
   levels=c(.1,.25,.75,.9), add=TRUE,d=FALSE,lty=3,lwd=1)
contour(gx1,gx2,matrix(y.lr.grid,gm,gn),
   levels=c(.5), add=TRUE,d=FALSE,lty=1,lwd=2)

## logistic regression with quadratic interactions
logreg <- glm(y ~ (LD1 + LD2)^2, data=xdf, family=binomial)
y.lr <- predict(logreg,type="response")
eqscplot(x,pch=2*y+1,col=2-as.numeric(y==(y.lr>.5)))
y.lr.grid <- predict(logreg,newdata=gdf,type="response")
contour(gx1,gx2,matrix(y.lr.grid,gm,gn),
   levels=c(.1,.25,.75,.9), add=TRUE,d=FALSE,lty=3,lwd=1)
contour(gx1,gx2,matrix(y.lr.grid,gm,gn),
   levels=c(.5), add=TRUE,d=FALSE,lty=1,lwd=2)
```

Crab Dataset : Blue Female vs. rest



Comparing LDA and logistic regression.

Crab Dataset



Comparing logistic regression with and without quadratic interactions.

Logistic regression Python demo

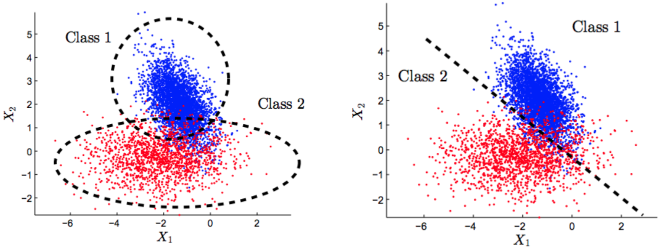
Single-class: https://github.com/vkanade/mlmt2017/blob/master/lecture11/Logistic%20Regression.ipynb

Multi-class: https://github.com/vkanade/mlmt2017/blob/master/lecture11/Multiclass%20Logistic%20Regression.ipynb

Generative vs. Discriminative

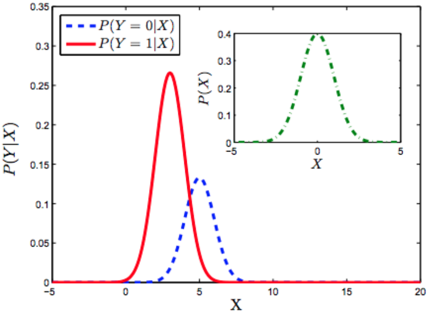
Generative vs Discriminative Learning

- Machine learning: learn a (random) function that maps a variable X (feature) to a variable Y (class) using a (labeled) dataset $\mathcal{D} = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$.
  - Generative Approach: learn $P(Y, X) = P(Y|X)\,P(X)$.
  - Discriminative Approach: learn $P(Y|X)$.



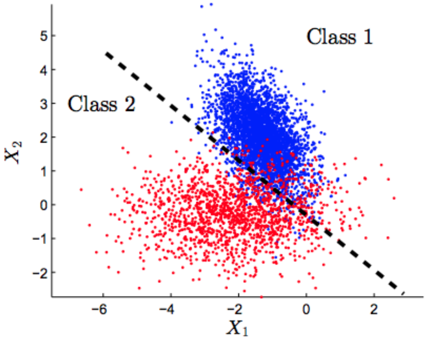
Generative Learning

- **Generative Approach**: Finds a probabilistic model (a joint distribution $P(Y, X)$) that explicitly models the distribution of both the features and the corresponding labels (classes).
- Example techniques: LDA, QDA, Naive Bayes (coming soon), Hidden Markov Models, etc.



Discriminative Learning

- **Discriminative Approach**: Finds a good fit for $P(Y|X)$ without explicitly modeling the generative process.
- Example techniques: linear regression, logistic regression, K-nearest neighbors (coming soon), SVMs, perceptrons, etc.
- Example problem: 2 classes, separate the classes.



Generative vs Discriminative Learning

- **Generative Approach**: Finds parameters that explain all data.

$$\widehat{\theta} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(x_i, y_i | \theta)$$

  - Makes use of all the data.
  - Flexible framework, can incorporate many tasks (e.g. classification, regression, semi-supervised learning, survival analysis, generating new data samples similar to the existing dataset, etc).
  - Stronger modeling assumptions, which may not be realistic (Gaussianity, independence of features).

- **Discriminative Approach**: Finds parameters that help to predict only relevant data.

$$\widehat{\theta} = \underset{\theta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} L(y_i, f_\theta(x_i)) \quad \text{or} \quad \widehat{\theta} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(y_i | x_i, \theta)$$

  - Weaker modeling assumptions (thus often fewer violated assumptions and better calibration of probabilities).
  - Learns to perform better on the given tasks.
  - Less immune to overfitting.
  - Easier to work with preprocessed data $\phi(x)$.

Naïve Bayes

Naïve Bayes: overview

- Naïve Bayes: another **plug-in** classifier with a simple **generative** model - it assumes all measured variables/features are independent given the label.
- Easy to mix and match different types of features, handle missing data.
- Often used with categorical data, e.g. text document classification.
  - A basic standard model for text classification consists of considering a pre-specified dictionary of p words and summarizing each document i by a binary vector x_i ("bag-of-words"):

$$x_i^{(j)} = \begin{cases} 1 & \text{if word } j \text{ is present in document} \\ 0 & \text{otherwise.} \end{cases}$$

    where the presence of the word j is the j-th feature/dimension.

Toy Example

Predict voter preference in US elections

Voted in 2012?	Annual Income	State	Candidate Choice
Y	50K	OK	Clinton
N	173K	CA	Clinton
Y	80K	NJ	Trump
Y	150K	WA	Clinton
N	25K	WV	Johnson
Y	85K	IL	Clinton
⋮	⋮	⋮	⋮
Y	1050K	NY	Trump
N	35K	CA	Trump
N	**100K**	**NY**	**?**

Naïve Bayes Classifier (NBC)

- In order to fit a generative model, we'll express the joint distribution as
$$p(\boldsymbol{x}, y \mid \boldsymbol{\theta}, \boldsymbol{\pi}) = p(y \mid \boldsymbol{\pi}) \cdot p(\boldsymbol{x} \mid y, \boldsymbol{\theta})$$
- To model $p(y \mid \boldsymbol{\pi})$, we'll use parameters π_c such that $\sum_c \pi_c = 1$
$$p(y = c \mid \boldsymbol{\pi}) = \pi_c$$
- For class-conditional densities, for class $c = 1, \ldots, C$, we will have a model:
$$p(\boldsymbol{x} \mid y = c, \boldsymbol{\theta}_c)$$
- We assume that the features are conditionally independent given the class label
$$p(\boldsymbol{x} \mid y = c, \boldsymbol{\theta}_c) = \prod_{j=1}^{D} p(x_j \mid y = c, \boldsymbol{\theta}_{jc})$$
- Clearly, the independence assumption is "naïve" and never satisfied. But model fitting becomes very very easy.
- Although the generative model is clearly inadequate, it actually works quite well. Goal is predicting class, not modelling the data!

Naïve Bayes Classifier (NBC)

In our example,

$$p(y = \text{clinton} \mid \boldsymbol{\pi}) = \pi_{\text{clinton}}$$
$$p(y = \text{trump} \mid \boldsymbol{\pi}) = \pi_{\text{trump}}$$
$$p(y = \text{johnson} \mid \boldsymbol{\pi}) = \pi_{\text{johnson}}$$

Given that a voter supports Trump

$$p(\boldsymbol{x} \mid y = \text{trump}, \boldsymbol{\theta}_{\text{trump}})$$

models the distribution over $\boldsymbol{x}$ given $y = \text{trump}$ and $\boldsymbol{\theta}_{\text{trump}}$

Similarly, we have $p(\boldsymbol{x} \mid y = \text{clinton}, \boldsymbol{\theta}_{\text{clinton}})$ and $p(\boldsymbol{x} \mid y = \text{johnson}, \boldsymbol{\theta}_{\text{johnson}})$

We need to pick “model” for $p(\boldsymbol{x} \mid y = c, \boldsymbol{\theta}_c)$

Estimate the parameters π_c, $\boldsymbol{\theta}_c$ for $c = 1, \ldots, C$

Naïve Bayes Classifier (NBC)

Real-Valued Features

- x_j is real-valued annual income
- Example: Use a Gaussian model, so $\boldsymbol{\theta}_{jc} = (\mu_{jc}, \sigma^2_{jc})$
- Can use other distributions, age is probably not Gaussian!

Categorical Features

- x_j is categorical with values in $\{1, \ldots, K\}$
- Use the **multinoulli** distribution, i.e. $x_j = i$ with probability $\mu_{jc,i}$

$$\sum_{i=1}^{K} \mu_{jc,i} = 1$$

- The special case when $x_j \in \{0, 1\}$, use a single parameter $\theta_{jc} \in [0, 1]$

Naïve Bayes Classifier (NBC)

- Assume that all the features are binary, i.e. every $x_j \in \{0, 1\}$
- (In this case, the log-discriminant function of each class assumes the form $a_c + b_c^\top x$ for class c. Verify this.)
- If we have C classes, overall we have only $O(CD)$ parameters, θ_{jc} for each $j = 1, \ldots, D$ and $c = 1, \ldots, C$

- Without the conditional independence assumption
    - We have to assign a probability for each of the 2^D combination
    - Thus, we have $O(C \cdot 2^D)$ parameters!
    - The 'naïve' assumption breaks the *curse of dimensionality* and avoids overfitting!

Maximum Likelihood for the NBC

- Let us suppose we have data $\langle (\boldsymbol{x}_i, y_i) \rangle_{i=1}^{N}$ i.i.d. from some joint distribution $p(\boldsymbol{x}, y)$
- The probability for a single datapoint is given by:

$$p(\boldsymbol{x}_i, y_i | \boldsymbol{\theta}, \boldsymbol{\pi}) = p(y_i | \boldsymbol{\pi}) \cdot p(\boldsymbol{x}_i | \boldsymbol{\theta}, y_i) = \prod_{c=1}^{C} \pi_c^{\mathbb{I}(y_i = c)} \cdot \prod_{c=1}^{C} \prod_{j=1}^{D} p(x_{ij} | \boldsymbol{\theta}_{jc})^{\mathbb{I}(y_i = c)}$$

- Let N_c be the number of datapoints with $y_i = c$, so that $\sum_{c=1}^{C} N_c = N$
- We write the log-likelihood of the data, assuming points are i.i.d.:

$$\log p(\mathcal{D} \mid \boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{c=1}^{C} N_c \log \pi_c + \sum_{c=1}^{C} \sum_{j=1}^{D} \sum_{i : y_i = c} \log p(x_{ij} \mid \boldsymbol{\theta}_{jc})$$

- The log-likelihood is easily separated into sums involving different parameters!

Maximum Likelihood for the NBC

- We have the log-likelihood for the NBC

$$\log p(\mathcal{D} \mid \boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{c=1}^{C} N_c \log \pi_c + \sum_{c=1}^{C} \sum_{j=1}^{D} \sum_{i:y_i=c} \log p(x_{ij} \mid \boldsymbol{\theta}_{jc})$$

- We can use maximum likelihood to estimate the parameters (we have done this before). For instance, let's estimate $\boldsymbol{\pi}$. We have the following optimization problem:

$$\text{maximize} \quad \sum_{c=1}^{C} N_c \log \pi_c$$

$$\text{subject to :} \quad \sum_{c=1}^{C} \pi_c = 1$$

- This constrained optimization problem can be solved using Lagrange multipliers

$$\Lambda(\boldsymbol{\pi}, \lambda) = \sum_{c=1}^{C} N_c \log \pi_c + \lambda \left(\sum_{c=1}^{C} \pi_c - 1 \right)$$

Maximum Likelihood for the NBC

We can write the Lagrangean form:

$$\Lambda(\boldsymbol{\pi}, \lambda) = \sum_{c=1}^{C} N_c \log \pi_c + \lambda \left(\sum_{c=1}^{C} \pi_c - 1 \right)$$

We can write the partial derivatives and set them to 0:

$$\frac{\partial \Lambda(\boldsymbol{\pi}, \lambda)}{\partial \pi_c} = \frac{N_c}{\pi_c} + \lambda = 0; \qquad \frac{\partial \Lambda(\boldsymbol{\pi}, \lambda)}{\partial \lambda} = \sum_{c=1}^{C} \pi_c - 1 = 0$$

The solution is obtained by setting

$$\frac{N_c}{\pi_c} + \lambda = 0 \quad \rightarrow \quad \pi_c = -\frac{N_c}{\lambda}$$

As well as using the second condition,

$$\sum_{c=1}^{C} \pi_c - 1 = \left(\sum_{c=1}^{C} -\frac{N_c}{\lambda} \right) - 1 = 0 \quad \rightarrow \quad \lambda = -\sum_{c=1}^{C} N_c = -N$$

Thus, we get the estimates,

$$\pi_c = \frac{N_c}{N}$$

Maximum Likelihood for the NBC

- We have the log-likelihood for the NBC

$$\log p(\mathcal{D} \mid \boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{c=1}^{C} N_c \log \pi_c + \sum_{c=1}^{C} \sum_{j=1}^{D} \sum_{i:y_i=c} \log p(x_{ij} \mid \boldsymbol{\theta}_{jc})$$

- We obtained the estimates, $\pi_c = \frac{N_c}{N}$
- We can estimate $\boldsymbol{\theta}_{jc}$ by taking a similar approach
- To estimate $\boldsymbol{\theta}_{jc}$ we only need to use the j^{th} feature of examples with $y_i = c$
- Estimates depend on the model, e.g. Gaussian, Bernoulli, Multinoulli, etc.
- Fitting NBC is very very fast!

NBC: Handling Missing Data

Let's recall our example about trying to predict voter preferences

Voted in 2012?	Annual Income	State	Candidate Choice
Y	50K	OK	Clinton
N	173K	CA	Clinton
Y	80K	NJ	Trump
Y	150K	WA	Clinton
N	25K	WV	Johnson
Y	85K	IL	Clinton
⋮	⋮	⋮	⋮
Y	1050K	NY	Trump
N	35K	CA	Trump
?	**100K**	**NY**	**?**

Suppose a voter does not reveal whether or not they voted in 2012

For now, let's assume we had no missing entries during training

NBC: Handling Missing Data

The prediction rule in a generative model is

$$p(y = c \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{\theta}) = \frac{p(y = c \mid \boldsymbol{\theta}) \cdot p(\boldsymbol{x}_{\text{new}} \mid y = c, \boldsymbol{\theta})}{\sum_{c'=1}^{C} p(y = c' | \boldsymbol{\theta}) p(\boldsymbol{x}_{\text{new}} \mid y = c', \boldsymbol{\theta})}$$

Let us suppose our datapoint is $\boldsymbol{x}_{\text{new}} = (?, x_2, \ldots, x_D)$, e.g. $(?, \text{100K}, \text{NY})$

$$p(y = c \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{\theta}) = \frac{\pi_c \cdot \prod_{j=1}^{D} p(x_j \mid y = c, \boldsymbol{\theta}_{cj})}{\sum_{c'=1}^{C} p(y = c' | \boldsymbol{\theta}) \prod_{j=1}^{D} p(x_j \mid y = c', \boldsymbol{\theta}_{jc})}$$

Since x_1 is missing, we can marginalize it out,

$$p(y = c \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{\theta}) = \frac{\pi_c \cdot \prod_{j=2}^{D} p(x_j \mid y = c, \boldsymbol{\theta}_{cj})}{\sum_{c'=1}^{C} p(y = c' | \boldsymbol{\theta}) \prod_{j=2}^{D} p(x_j \mid y = c', \boldsymbol{\theta}_{jc})}$$

This can be done for other generative models, but marginalization requires summation/integration

NBC: Handling Missing Data

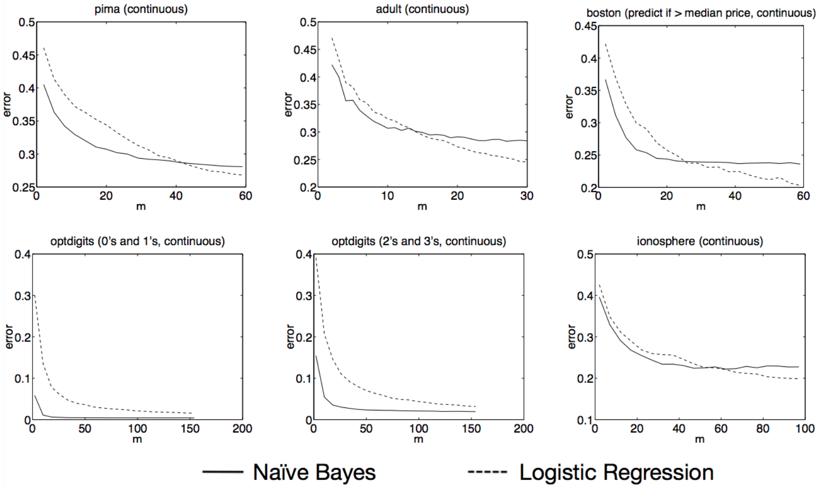
For Naïve Bayes Classifiers, training with missing entries is quite easy

Voted in 2012?	Annual Income	State	Candidate Choice
?	50K	OK	Clinton
N	173K	CA	Clinton
?	80K	NJ	Trump
Y	150K	WA	Clinton
N	25K	WV	Johnson
Y	85K	?	Clinton
⋮	⋮	⋮	⋮
Y	1050K	NY	Trump
N	35K	CA	Trump
?	**100K**	**NY**	**?**

Let's say for Clinton voters, 103 had voted in 2012, 54 had not, and 25, didn't answer

You can simply set $\theta = \frac{103}{157}$ as the probability that a voter had voted in 2012, conditioned on being a Clinton supporter

Naïve Bayes vs Logistic regression



"On Discriminative vs. Generative Classifiers: A comparison of logistic regression and naive Bayes" by A. Ng and M. Jordan, NIPS 2001. m represents training dataset size.

Naïve Bayes vs Logistic regression

- For infinite data
  - If generative model is correct (independence assumption holds)

$$Error_{LR,\infty} \sim Error_{NB,\infty}$$

  - If generative model is inaccurate (independence assumption does not hold)

$$Error_{LR,\infty} < Error_{NB,\infty}$$

- For finite data (e.g. n points, d features), NB will require less training to converge to its (possibly asymptotically higher) error

$$Error_{LR,n} \leq Error_{LR,\infty} + O\left(\sqrt{\frac{d}{n}}\right)$$

$$Error_{NB,n} \leq Error_{NB,\infty} + O\left(\sqrt{\frac{\log d}{n}}\right)$$

Preventing numerical underflow (not examinable)

- Generative classifiers often require multiplying a large number of small quantities, leading to **numerical underflow**.

$$\log p(y=c|\boldsymbol{x}) = \log\left[\frac{p(y=c)p(\boldsymbol{x}|y=c)}{\sum_{c'} p(y=c')p(\boldsymbol{x}|y=c')}\right]$$
$$= b_c - \log\left[\sum_{c'=1}^{C} e^{b_{c'}}\right]$$
$$b_c \triangleq \log p(\boldsymbol{x}|y=c) + \log p(y=c)$$

- The terms $e^{b_{c'}}$ are extremely small (e.g. in Naive Bayes), but we cannot sum in the log domain to evaluate $\log\sum_{c'} e^{b_{c'}}$.
- Idea: factor out the largest term[2]. For example:

$$\log(e^{-120}+e^{-121}) = \log(e^{-120}(e^{0}+e^{-1})) = \log(e^{0}+e^{-1}) - 120.$$

- In general, having defined $B = \max_c b_c$:

$$\log\sum_c e^{b_c} = \log\left[\left(\sum_c e^{b_c - B}\right)e^{B}\right] = \left[\log\left(\sum_c e^{b_c - B}\right)\right] + B$$

[2] Also see Murphy 3.5.3.

Naïve Bayes code example: Titanic data I

Predicting Titatinc survival from passenger data using Naïve Bayes[3]:

```
#Install the package
install.packages("e1071")
#Loading the library
library(e1071)
?naiveBayes #The documentation also uses Titanic data
#Next load the Titanic dataset
data("Titanic")
#Save into a data frame and view it
Titanic_df=as.data.frame(Titanic)
#Creating data from table
#This will repeat each combination equal to the frequency
repeating_sequence=rep.int(seq_len(nrow(Titanic_df)),
    Titanic_df$Freq)

#Create the dataset by row repetition created
Titanic_dataset=Titanic_df[repeating_sequence,]
```

Naïve Bayes code example: Titanic data II

```
#We no longer need the frequency, drop the feature
Titanic_dataset$Freq=NULL

#Fitting the Naive Bayes model
Naive_Bayes_Model=naiveBayes(Survived ~.,
    data=Titanic_dataset)
#What does the model say? Print the model summary
Naive_Bayes_Model

#Prediction on the dataset
NB_Predictions=predict(Naive_Bayes_Model,Titanic_dataset)
#Confusion matrix to check accuracy
table(NB_Predictions,Titanic_dataset$Survived)
```

[3] code from https://r-posts.com/understanding-naive-bayes-classifier-using-r/