Statistical Machine Learning
Hilary Term 2019

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Slide credits and other course material can be found at:
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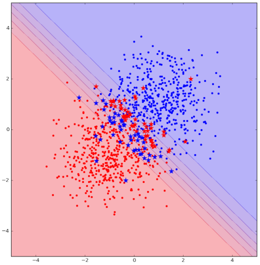
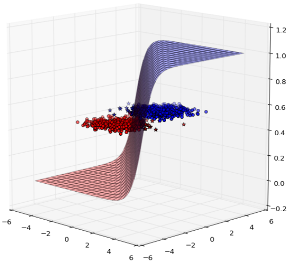
Logistic regression

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

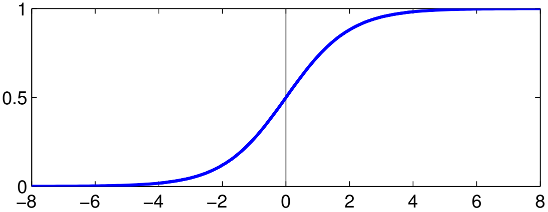
- $a + b^\top x$ models the **log-odds ratio**:

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

- 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

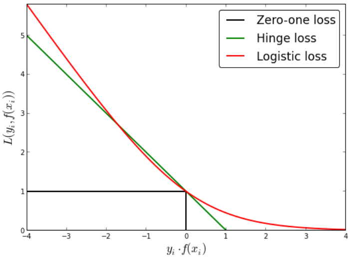
How to learn a and b given a training data set $(x_i, y_i)_{i=1}^n$?

- 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**:

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



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

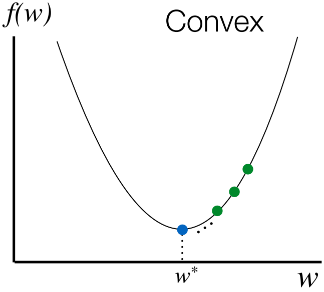
$$\begin{aligned} s(-z) &= 1 - s(z) \\ \nabla_z s(z) &= s(z)s(-z) \\ \nabla_z \log s(z) &= s(-z) \\ \nabla_z^2 \log s(z) &= -s(z)s(-z) \end{aligned}$$

- Differentiate wrt b:

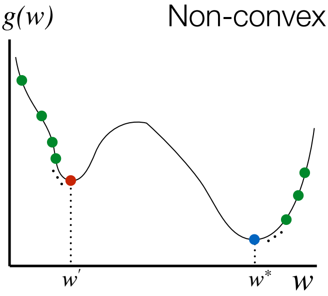
$$\begin{aligned} \nabla_b \widehat{R}_{\text{log}} &= \frac{1}{n}\sum_{i=1}^{n} -s(-y_i x_i^\top b) y_i x_i \\ \nabla_b^2 \widehat{R}_{\text{log}} &= \frac{1}{n}\sum_{i=1}^{n} s(y_i x_i^\top b) s(-y_i x_i^\top b) x_i x_i^\top \succeq 0. \end{aligned}$$

- 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)

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

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

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

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.

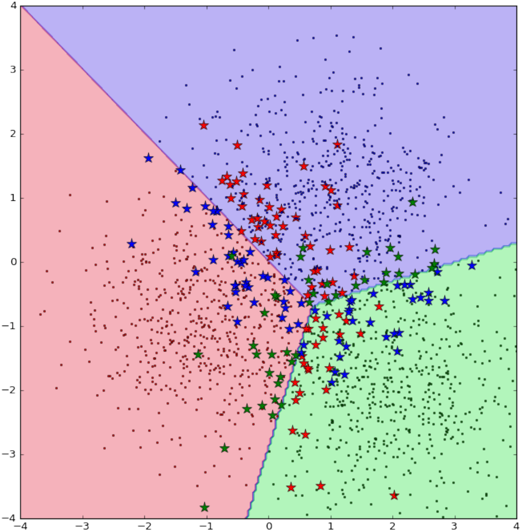
Multi-class logistic regression

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)
```

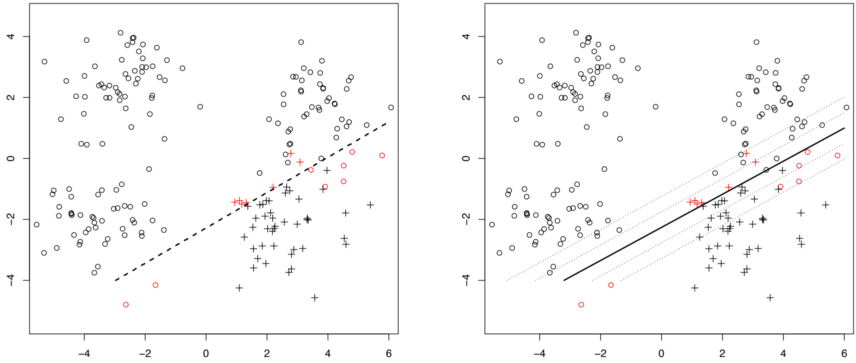
Crab Dataset

```
## 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

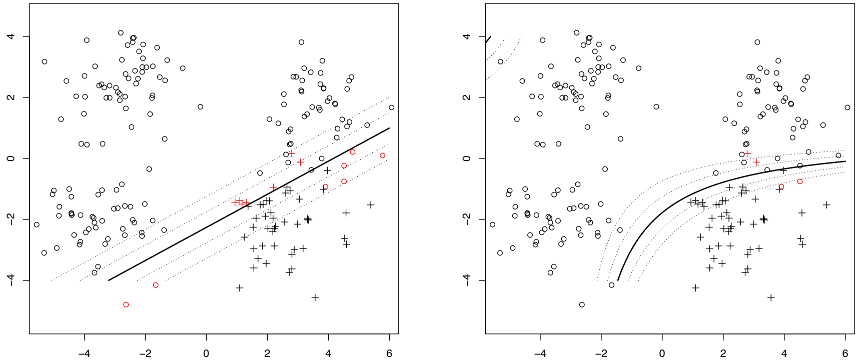
```
## logistic regression
xdf <- data.frame(x)
logreg <- glm(y ~ LD1 + LD2, data=xdf, family=binomial)
y.lr <- predict(logreg,type="response")
eqscplot(x,pch=2*y+1,col=2-as.numeric(y==(y.lr>.5)))
y.lr.grid <- predict(logreg,newdata=gdf,type="response")
contour(gx1,gx2,matrix(y.lr.grid,gm,gn),
   levels=c(.1,.25,.75,.9),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

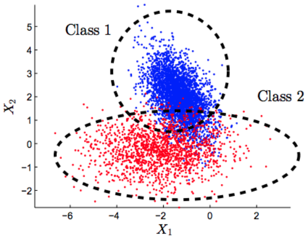
Single-class: https://github.com/vkanade/mlmt2017/blob/master/lecture11/Logistic%20Regression.ipynb

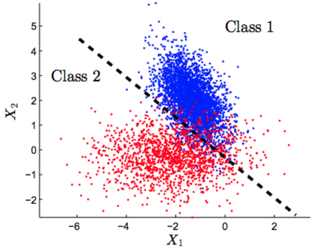
Multi-class: https://github.com/vkanade/mlmt2017/blob/master/lecture11/Multiclass%20Logistic%20Regression.ipynb

Generative vs. Discriminative

Generative vs Discriminative Learning

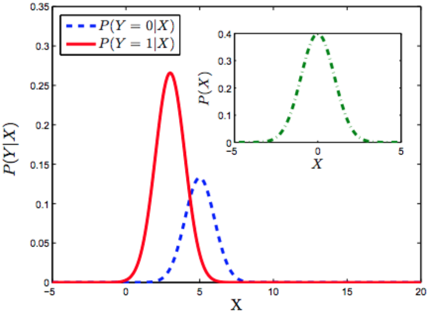
- Machine learning: learn a (random) function that maps a variable X (feature) to a variable Y (class) using a (labeled) dataset $\mathcal{D} = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$.
  - Generative Approach: learn $P(Y, X) = P(Y|X)\,P(X)$.
  - Discriminative Approach: learn $P(Y|X)$.





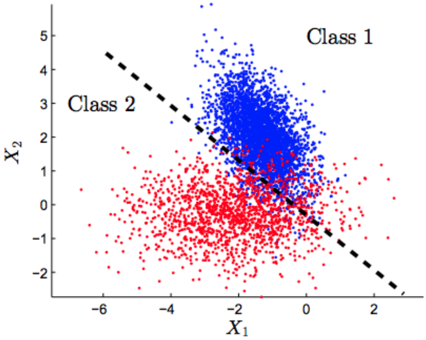
Generative Learning

- **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.

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

  - 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.

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

  - 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 $c = 1, \dots, C$, 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!