## 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

## Plug-in Classification

- Consider the 0-1 loss and the risk:

$$
\mathbb{E}[L(Y, f(X)) \mid X=x]=\sum_{k=1}^{K} L(k, f(x)) \mathbb{P}(Y=k \mid X=x)
$$

The Bayes classifier provides a solution that minimizes the risk:

$$
f_{\text {Bayes }}(x)=\underset{k=1, \ldots, K}{\arg \max } \pi_{k} g_{k}(x)
$$

- We know neither the conditional density $g_{k}$ nor the class probability $\pi_{k}$ !
- The plug-in classifier chooses the class

$$
f(x)=\underset{k=1, \ldots, K}{\arg \max } \widehat{\pi}_{k} \widehat{g}_{k}(x),
$$

- where we plugged in
- estimates $\widehat{\pi}_{k}$ of $\pi_{k}$ and $k=1, \ldots, K$ and
- estimates $\widehat{g}_{k}(x)$ of conditional densities,
- Linear Discriminant Analysis is an example of plug-in classification.


## Summary: Linear Discriminant Analysis

- LDA: a plug-in classifier assuming multivariate normal conditional density $g_{k}(x)=g_{k}\left(x \mid \mu_{k}, \Sigma\right)$ for each class $k$ sharing the same covariance $\Sigma$ :

$$
X \mid Y=k \sim \mathcal{N}\left(\mu_{k}, \Sigma\right)
$$

$$
g_{k}\left(x \mid \mu_{k}, \Sigma\right)=(2 \pi)^{-p / 2}|\Sigma|^{-1 / 2} \exp \left(-\frac{1}{2}\left(x-\mu_{k}\right)^{\top} \Sigma^{-1}\left(x-\mu_{k}\right)\right) .
$$

- LDA minimizes the squared Mahalanobis distance between $x$ and $\widehat{\mu}_{k}$, offset by a term depending on the estimated class proportion $\widehat{\pi}_{k}$ :

$$
\begin{aligned}
f_{\mathrm{LDA}}(x) & =\underset{k \in\{1, \ldots, K\}}{\operatorname{argmax}} \log \widehat{\pi}_{k} g_{k}\left(x \mid \widehat{\mu}_{k}, \widehat{\Sigma}\right) \\
& =\underset{k \in\{1, \ldots, K\}}{\operatorname{argmax}} \underbrace{\left(\log \widehat{\pi}_{k}-\frac{1}{2} \widehat{\mu}_{k}^{\top} \widehat{\Sigma}^{-1} \widehat{\mu}_{k}\right)+\left(\widehat{\Sigma}^{-1} \widehat{\mu}_{k}\right)^{\top} x}_{\text {terms depending on } k \text { linear in } x} \\
& =\underset{k \in\{1, \ldots, K\}}{\operatorname{argmin}} \frac{1}{2} \underbrace{\left(x-\widehat{\mu}_{k}\right)^{\top} \widehat{\Sigma}^{-1}\left(x-\widehat{\mu}_{k}\right)}_{\text {squared Mahalanobis distance }}-\log \widehat{\pi}_{k} .
\end{aligned}
$$

## LDA projections



Figure by R. Gutierrez-Osuna

## LDA vs PCA projections




LDA separates the groups better.

## Fisherfaces



Eigenfaces vs. Fisherfaces, Belhumeur et al. 1997

## Conditional densities with different covariances

Given training data with $K$ classes, assume a parametric form for conditional density $g_{k}(x)$, where for each class

$$
X \mid Y=k \sim \mathcal{N}\left(\mu_{k}, \Sigma_{k}\right)
$$

i.e., instead of assuming that every class has a different mean $\mu_{k}$ with the same covariance matrix $\Sigma$ (LDA), we now allow each class to have its own covariance matrix.
Considering $\log \pi_{k} g_{k}(x)$ as before,

$$
\begin{aligned}
\log \pi_{k} g_{k}(x)= & \text { const }+\log \left(\pi_{k}\right)-\frac{1}{2}\left(\log \left|\Sigma_{k}\right|+\left(x-\mu_{k}\right)^{T} \Sigma_{k}^{-1}\left(x-\mu_{k}\right)\right) \\
= & \text { const }+\log \left(\pi_{k}\right)-\frac{1}{2}\left(\log \left|\Sigma_{k}\right|+\mu_{k}^{T} \Sigma_{k}^{-1} \mu_{k}\right) \\
& \quad+\mu_{k}^{T} \Sigma_{k}^{-1} x-\frac{1}{2} x^{T} \Sigma_{k}^{-1} x \\
= & a_{k}+b_{k}^{T} x+x^{T} c_{k} x
\end{aligned}
$$

A quadratic discriminant function instead of linear.

## Quadratic decision boundaries

Again, by considering that we choose class $k$ over $k^{\prime}$,

$$
\begin{gathered}
a_{k}+b_{k}^{T} x+x^{T} c_{k} x-\left(a_{k^{\prime}}+b_{k^{\prime}}^{T} x+x^{T} c_{k^{\prime}} x\right) \\
=a_{\star}+b_{\star}^{T} x+x^{T} c_{\star} x>0
\end{gathered}
$$

we see that the decision boundaries of the Bayes Classifier are quadratic surfaces.

- The plug-in Bayes Classifer under these assumptions is known as the Quadratic Discriminant Analysis (QDA) Classifier.


## QDA

LDA classifier:

$$
f_{\mathrm{LDA}}(x)=\underset{k \in\{1, \ldots, K\}}{\arg \min }\left\{\left(x-\widehat{\mu}_{k}\right)^{T} \widehat{\Sigma}^{-1}\left(x-\widehat{\mu}_{k}\right)-2 \log \left(\widehat{\pi}_{k}\right)\right\}
$$

QDA classifier:

$$
f_{\mathrm{QDA}}(x)=\underset{k \in\{1, \ldots, K\}}{\arg \min }\left\{\left(x-\widehat{\mu}_{k}\right)^{T} \widehat{\Sigma}_{k}^{-1}\left(x-\widehat{\mu}_{k}\right)-2 \log \left(\widehat{\pi}_{k}\right)+\log \left(\left|\widehat{\Sigma}_{k}\right|\right)\right\}
$$

for each point $x \in \mathcal{X}$ where the plug-in estimate $\widehat{\mu}_{k}$ is as before and $\widehat{\Sigma}_{k}$ is (in contrast to LDA) estimated for each class $k=1, \ldots, K$ separately:

$$
\widehat{\Sigma}_{k}=\frac{1}{n_{k}} \sum_{j: y_{j}=k}\left(x_{j}-\widehat{\mu}_{k}\right)\left(x_{j}-\widehat{\mu}_{k}\right)^{T} .
$$

## Computing and plotting the QDA boundaries.

```
##fit QDA
iris.qda <- qda(x=iris.data,grouping=ct)
##create a grid for our plotting surface
x <- seq(-6,6,0.02)
y <- seq(-4,4,0.02)
z <- as.matrix(expand.grid(x,y),0)
m <- length(x)
n <- length(y)
iris.qdp <- predict(iris.qda,z) $class
contour(x,y,matrix(iris.qdp,m,n),
    levels=c(1.5,2.5), add=TRUE, d=FALSE, lty=2)
```


## Iris example: QDA boundaries



## Iris example: QDA boundaries



## LDA or QDA?

- Having seen both LDA and QDA in action, it is natural to ask which is the "better" classifier.
- If the covariances of different classes are very distinct, QDA will probably have an advantage over LDA.
- Parametric models are only ever approximations to the real world, allowing more flexible decision boundaries (QDA) may seem like a good idea. However, there is a price to pay in terms of increased variance and potential overfitting.


## Regularized Discriminant Analysis

In the case where data is scarce, to fit

- LDA, need to estimate $K \times p+p \times p$ parameters
- QDA, need to estimate $K \times p+K \times p \times p$ parameters.

Using LDA allows us to better estimate the covariance matrix $\Sigma$. Though QDA allows more flexible decision boundaries, the estimates of the $K$ covariance matrices $\Sigma_{k}$ are more variable.
RDA combines the strengths of both classifiers by regularizing each covariance matrix $\Sigma_{k}$ in QDA to the single one $\Sigma$ in LDA

$$
\Sigma_{k}(\alpha)=\alpha \Sigma_{k}+(1-\alpha) \Sigma \quad \text { for some } \alpha \in[0,1] .
$$

This introduces a new parameter $\alpha$ and allows for a continuum of models between LDA and QDA to be used. Can be selected by Cross-Validation for example.

## Logistic regression

## Review

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


[^0]
## Logistic regression

- One of the most popular methods for classification
- Linear model on the probabilities
- Dates back to work on population growth curves by Verhulst [1838, 1845, 1847]
- Statistical use for classification dates to Cox [1960s]
- Independently discovered as the perceptron in machine learning [Rosenblatt 1957]
- Main example of "discriminative" as opposed to "generative" learning
- Naïve approach to classification: we could do linear regression assigning specific values to each class. Logistic regression refines this idea and provides a more suitable model.


## Logistic regression

- Statistical perspective: consider $\mathcal{Y}=\{0,1\}$. Generalised linear model with Bernoulli likelihood and logit link:

$$
Y \mid X=x, a, b \sim \operatorname{Bernoulli}\left(s\left(a+b^{\top} x\right)\right)
$$

$$
s\left(a+b^{\top} x\right)=\frac{1}{1+\exp \left(-\left(a+b^{\top} x\right)\right)}
$$



- ML perspective: a discriminative classifier. Consider binary classification with $\mathcal{Y}=\{+1,-1\}$. Logistic regression uses a parametric model on the conditional $Y \mid X$, not the joint distribution of $(X, Y)$ :

$$
p(Y=y \mid X=x ; a, b)=\frac{1}{1+\exp \left(-y\left(a+b^{\top} x\right)\right)}
$$

## Prediction Using Logistic Regression




## Hard vs Soft classification rules

- Consider using LDA for binary classification with $\mathcal{Y}=\{+1,-1\}$.

Predictions are based on linear decision boundary:

$$
\begin{aligned}
\widehat{y}_{\mathrm{LDA}}(x) & =\operatorname{sign}\left\{\log \widehat{\pi}_{+1} g_{+1}\left(x \mid \widehat{\mu}_{+1}, \widehat{\Sigma}\right)-\log \widehat{\pi}_{-1} g_{-1}\left(x \mid \widehat{\mu}_{-1}, \widehat{\Sigma}\right)\right\} \\
& =\operatorname{sign}\left\{a+b^{\top} x\right\}
\end{aligned}
$$

for $a$ and $b$ depending on fitted parameters $\widehat{\theta}=\left(\widehat{\pi}_{+1}, \widehat{\pi}_{-1}, \widehat{\mu}_{+1}, \widehat{\mu}_{-1}, \Sigma\right)$.

- Quantity $a+b^{\top} x$ can be viewed as a soft classification rule. Indeed, it is modelling the difference between the log-discriminant functions, or equivalently, the log-odds ratio:

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

- $f(x)=a+b^{\top} x$ corresponds to the "confidence of predictions" and loss can be measured as a function of this confidence:
- exponential loss: $L(y, f(x))=e^{-y f(x)}$,
- log-loss: $L(y, f(x))=\log \left(1+e^{-y f(x)}\right)$,
- hinge loss: $L(y, f(x))=\max \{1-y f(x), 0\}$.


## Linearity of log-odds and logistic function

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

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

- Solve explicitly for conditional class probabilities (using

$$
\begin{aligned}
p(Y=+1 \mid X=x ; a, b)+p(Y & =-1 \mid X=x ; a, b)=1): \\
p(Y=+1 \mid X=x ; a, b) & =\frac{1}{1+\exp \left(-\left(a+b^{\top} x\right)\right)}=: s\left(a+b^{\top} x\right) \\
p(Y=-1 \mid X=x ; a, b) & =\frac{1}{1+\exp \left(+\left(a+b^{\top} x\right)\right)}=s\left(-a-b^{\top} x\right)
\end{aligned}
$$

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 $\left(x_{i}, y_{i}\right)_{i=1}^{n}$ ?

- Consider maximizing the conditional log likelihood for $\mathcal{Y}=\{+1,-1\}$ :

$$
p\left(Y=y_{i} \mid X=x_{i} ; a, b\right)=p\left(y_{i} \mid x_{i}\right)=\left\{\begin{array}{lll}
s\left(a+b^{\top} x_{i}\right) & \text { if } \quad Y=+1 \\
1-s\left(a+b^{\top} x_{i}\right) & \text { if } \quad Y=-1
\end{array}\right.
$$

- Noting that $1-s(z)=s(-z)$, we can write the log-likelihood using the compact expression:

$$
\log p\left(y_{i} \mid x_{i}\right)=\log s\left(y_{i}\left(a+b^{\top} x_{i}\right)\right)
$$

- And the log-likelihood over the whole i.i.d. data set is:

$$
\ell(a, b)=\sum_{i=1}^{n} \log p\left(y_{i} \mid x_{i}\right)=\sum_{i=1}^{n} \log s\left(y_{i}\left(a+b^{\top} x_{i}\right)\right)
$$

## Fitting the parameters of the hyperplane

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$$
\ell(a, b)=\sum_{i=1}^{n} \log p\left(y_{i} \mid x_{i}\right)=\sum_{i=1}^{n} \log s\left(y_{i}\left(a+b^{\top} x_{i}\right)\right) .
$$

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

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



## Could we use the 0-1 loss?

- With the 0-1 loss, the risk becomes:

$$
\widehat{R}\left(f_{a, b}\right)=\frac{1}{n} \sum_{i=1}^{n} \operatorname{step}\left(-y_{i}\left(a+b^{\top} x_{i}\right)\right)
$$

- But what is the gradient? ...



## 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:

$$
\widehat{R}_{\log }=\frac{1}{n} \sum_{i=1}^{n}-\log s\left(y_{i} x_{i}^{\top} b\right)
$$

## 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 $b$ :

$$
\begin{aligned}
& \nabla_{b} \widehat{R}_{\log }=\frac{1}{n} \sum_{i=1}^{n}-s\left(-y_{i} x_{i}^{\top} b\right) y_{i} x_{i} \\
& \nabla_{b}^{2} \widehat{R}_{\log }=\frac{1}{n} \sum_{i=1}^{n} s\left(y_{i} x_{i}^{\top} b\right) s\left(-y_{i} x_{i}^{\top} b\right) x_{i} x_{i}^{\top} \succeq 0 .
\end{aligned}
$$

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


## Gradient Descent

Start at a random point Repeat

Determine a descent direction
Choose a step size Update
Until stopping criterion is satisfied


## 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

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

Examples:

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

How to determine convexity in this case?
Matrix of second-order derivatives (Hessian)

$$
\mathbf{H}=\left(\begin{array}{llll}
\frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{1}{ }^{2}} & \frac{\partial^{2} f(\boldsymbol{x})}{\partial x^{2} \partial x_{2}} & \ldots & \frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{1} \partial x_{D}} \\
\frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{1} \partial x_{2}} & \frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{2}^{2}} & \ldots & \frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{2} \partial x_{D}} \\
\ldots & \cdots & \ldots & \ldots \\
\frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{1} \partial x_{D}} & \frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{2} \partial x_{D}} & \ldots & \frac{\partial^{2} f(\boldsymbol{x})}{\partial x_{D}^{2}}
\end{array}\right)
$$

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:

$$
b^{\text {new }}=b+\epsilon \frac{1}{n} \sum_{i=1}^{n} s\left(-y_{i} x_{i}^{\top} b\right) y_{i} x_{i}
$$

- Stochastic gradient descent:

$$
b^{\text {new }}=b+\epsilon_{t} \frac{1}{|I(t)|} \sum_{i \in I(t)} s\left(-y_{i} x_{i}^{\top} b\right) y_{i} x_{i}
$$

where $I(t)$ is a subset of the data at iteration $t$, and $\epsilon_{t} \rightarrow 0$ slowly

$$
\left(\sum_{t} \epsilon_{t}=\infty, \sum_{t} \epsilon_{t}^{2}<\infty\right)
$$

- Conjugate gradient, LBFGS and other methods from numerical analysis.
- Newton-Raphson:

$$
b^{\text {new }}=b-\left(\nabla_{b}^{2} \widehat{R}_{\mathrm{log}}\right)^{-1} \nabla_{b} \widehat{R}_{\mathrm{log}}
$$

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 $\mu_{i}=s\left(x_{i}^{\top} b\right)$, and the diagonal matrix $\mathbf{S}$ with $\mu_{i}\left(1-\mu_{i}\right)$ on its diagonal. Also define the vector $\mathbf{c}$ where $c_{i}=\mathbb{1}\left(y_{i}=+1\right)$. Then

$$
\begin{aligned}
\nabla_{b} \widehat{R}_{\log }= & \frac{1}{n} \sum_{i=1}^{n}-s\left(-y_{i} x_{i}^{\top} b\right) y_{i} x_{i} \\
& =\frac{1}{n} \sum_{i=1}^{n} x_{i}\left(\mu_{i}-c_{i}\right) \\
& =\mathbf{X}^{\top}(\mu-\mathbf{c}) \\
\nabla_{b}^{2} \widehat{R}_{\log }= & \frac{1}{n} \sum_{i=1}^{n} s\left(y_{i} x_{i}^{\top} b\right) s\left(-y_{i} x_{i}^{\top} b\right) x_{i} x_{i}^{\top} \\
& =\mathbf{X}^{\top} \mathbf{S X}
\end{aligned}
$$

## 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:

$$
\begin{aligned}
\mathbf{g}_{t} & =\mathbf{X}^{\top}\left(\boldsymbol{\mu}_{t}-\mathbf{c}\right)=-\mathbf{X}^{\top}\left(\mathbf{c}-\boldsymbol{\mu}_{t}\right) \\
\mathbf{H}_{t} & =\mathbf{X}^{\top} \mathbf{S}_{t} \mathbf{X}
\end{aligned}
$$

The Newton Update Rule is:

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

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

$$
\operatorname{minimise} \sum_{i=1}^{N} S_{t, i i}\left(z_{t, i}-\mathbf{b}^{\top} \mathbf{x}_{i}\right)^{2}
$$

## Linearly separable data

Assume that the data is linearly separable, i.e. there is a scalar $\alpha$ and a vector $\beta$ such that $y_{i}\left(\alpha+\beta^{\top} x_{i}\right)>0, i=1, \ldots, n$. Let $c>0$. The empirical risk for $a=c \alpha, b=c \beta$ is

$$
\widehat{R}_{\log }\left(f_{a, b}\right)=\frac{1}{n} \sum_{i=1}^{n} \log \left(1+\exp \left(-c y_{i}\left(\alpha+\beta^{\top} x_{i}\right)\right)\right)
$$

which can be made arbitrarily close to zero as $c \rightarrow \infty$, i.e. soft classification rule becomes $\pm \infty$ (overconfidence) $\rightarrow$ 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 $p(Y=k \mid X=x ; \theta)$, for $K$ classes $k=1, \ldots, K$, i.e.,

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

Parameters are $\theta=(b, W)$ where $W=\left(w_{k j}\right)$ 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,\operatorname{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


[^0]:    ${ }^{1}$ Despite the name "regression", we are using it for classification!

