Statistical Machine Learning

Pier Francesco Palamara
Department of Statistics
University of Oxford

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:

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

The Bayes classifier provides a solution that minimizes the risk:

$$f_{\mathsf{Bayes}}(x) = \underset{k=1,\ldots,K}{\operatorname{arg}} \max_{k} \pi_k g_k(x).$$

- We know neither the conditional density g_k nor the class probability $\pi_k!$
- The plug-in classifier chooses the class

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

- where we plugged in
 - estimates $\widehat{\pi}_k$ of π_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 $g_k(x) = g_k(x|\mu_k, \Sigma)$ for each class k sharing the same covariance Σ :

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma),$$

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

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

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

LDA projections

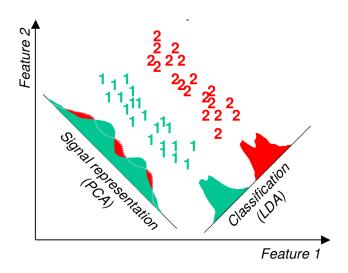
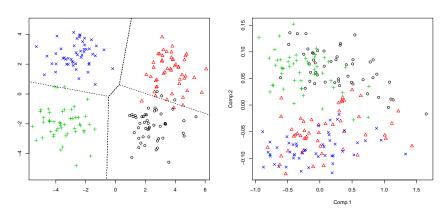


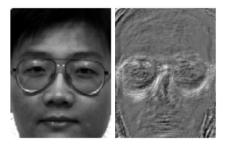
Figure by R. Gutierrez-Osuna

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

$$X|Y=k \sim \mathcal{N}(\mu_k, \Sigma_k),$$

i.e., instead of assuming that every class has a different mean μ_k with the **same** covariance matrix Σ (LDA), we now allow each class to have its own covariance matrix.

Considering $\log \pi_k g_k(x)$ as before,

$$\log \pi_k g_k(x) = \cosh + \log(\pi_k) - \frac{1}{2} \left(\log |\Sigma_k| + (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) \right)$$

$$= \cosh + \log(\pi_k) - \frac{1}{2} \left(\log |\Sigma_k| + \mu_k^T \Sigma_k^{-1} \mu_k \right)$$

$$+ \mu_k^T \Sigma_k^{-1} x - \frac{1}{2} x^T \Sigma_k^{-1} x$$

$$= a_k + b_k^T x + x^T c_k x.$$

A quadratic discriminant function instead of linear.

Quadratic decision boundaries

Again, by considering that we choose class k over k',

$$a_k + b_k^T x + x^T c_k x - (a_{k'} + b_{k'}^T x + x^T c_{k'} x)$$

= $a_{\star} + b_{\star}^T x + x^T c_{\star} x > 0$

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:

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

QDA classifier:

$$f_{\mathsf{QDA}}(x) = \mathop{\arg\min}_{k \in \{1, \dots, K\}} \left\{ (x - \widehat{\mu}_k)^T \widehat{\underline{\Sigma}}_{\pmb{k}}^{-1} (x - \widehat{\mu}_k) - 2\log(\widehat{\pi}_k) + \log(|\widehat{\underline{\Sigma}}_{\pmb{k}}|) \right\}$$

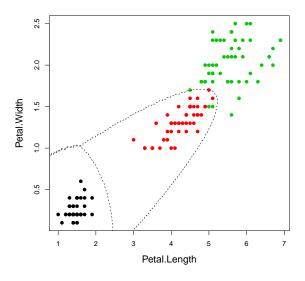
for each point $x \in \mathcal{X}$ where the plug-in estimate $\widehat{\mu}_k$ is as before and $\widehat{\Sigma}_k$ is (in contrast to LDA) estimated for each class $k = 1, \ldots, K$ separately:

$$\widehat{\Sigma}_{k} = \frac{1}{n_k} \sum_{j: y_j = k} (x_j - \widehat{\mu}_k) (x_j - \widehat{\mu}_k)^T.$$

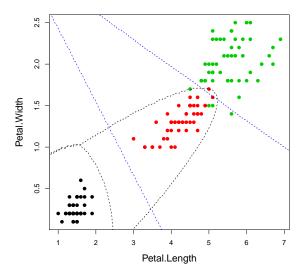
Computing and plotting the QDA boundaries.

##fit ODA

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 Σ . Though QDA allows more flexible decision boundaries, the estimates of the K covariance matrices Σ_k are more variable.

RDA combines the strengths of both classifiers by regularizing each covariance matrix Σ_k in QDA to the single one Σ in LDA

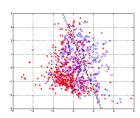
$$\Sigma_k(\alpha) = \alpha \Sigma_k + (1 - \alpha) \Sigma$$
 for some $\alpha \in [0, 1]$.

This introduces a new parameter α 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|y), but for classification we are mainly interested in p(y|x)
- Why not estimate that directly? Logistic regression¹ is a popular way of doing this.



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

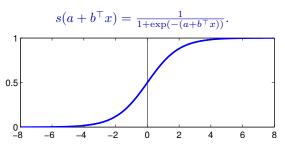
Logistic regression

- 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:

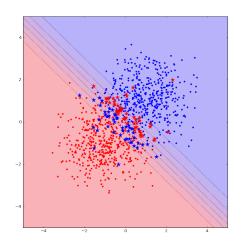
$$Y|X = x, a, b \sim \mathsf{Bernoulli}\left(s(a + b^{\top}x)\right)$$

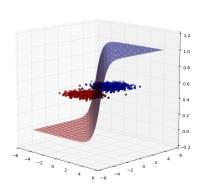


• ML perspective: a **discriminative classifier**. Consider binary classification with $\mathcal{Y} = \{+1, -1\}$. Logistic regression uses a parametric model on the conditional Y|X, not the joint distribution of (X,Y):

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

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:

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

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

• 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**:

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

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

Linearity of log-odds and logistic function

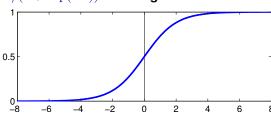
• $a + b^{T}x$ models the **log-odds ratio**:

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

• 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** for $\mathcal{Y} = \{+1, -1\}$:

$$p(Y=y_i|X=x_i;a,b) = p(y_i|x_i) = \left\{ \begin{array}{ll} s(a+b^\top x_i) & \text{if} \quad Y=+1 \\ 1-s(a+b^\top x_i) & \text{if} \quad Y=-1 \end{array} \right.$$

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

$$\log p(y_i|x_i) = \log s(y_i(a+b^{\top}x_i)).$$

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

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

Fitting the parameters of the hyperplane

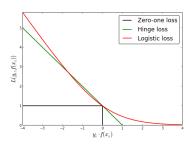
How to learn a and b given a training data set $(x_i, y_i)_{i=1}^n$?

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:

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



Could we use the 0-1 loss?

With the 0-1 loss, the risk becomes:

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

• 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:

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

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:

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

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

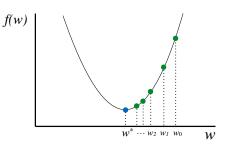
Gradient Descent

Start at a random point

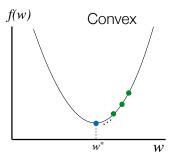
Repeat

Determine a descent direction Choose a step size Update

Until stopping criterion is satisfied



Where Will We Converge?



g(w) Non-convex

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

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

Examples:

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

How to determine convexity in this case?

Matrix of second-order derivatives (Hessian)

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

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 **H** is positive semi-definite if and only if, $\forall z$,

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

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:

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

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:

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

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 **S** with $\mu_i(1-\mu_i)$ on its diagonal. Also define the vector **c** where $c_i = \mathbb{1}(y_i = +1)$. Then

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

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:

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

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:

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

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

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

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.

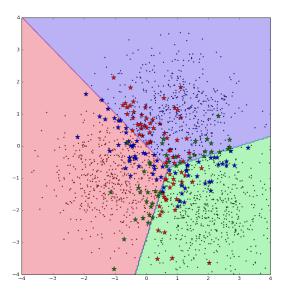
Multi-class logistic regression

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

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

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

Multi-class logistic regression

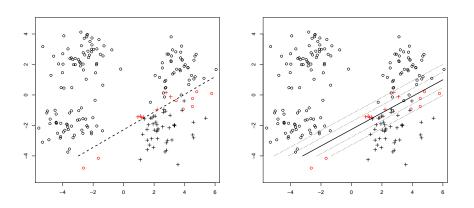


```
library(MASS)
## load crabs data
data(crabs)
ct <- as.numeric(crabs[,1])-1+2*(as.numeric(crabs[,2])-1)
## project into first two LD
cb.lda <- lda(log(crabs[,4:8]),ct)
cb.ldp <- predict(cb.lda)
x <- cb.ldp$x[,1:2]
y <- as.numeric(ct==0)
eqscplot(x,pch=2*y+1,col=y+1)</pre>
```

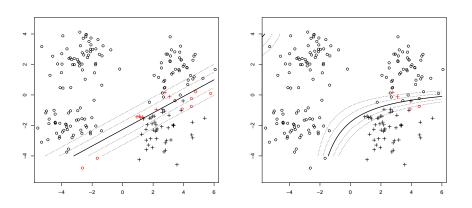
visualize decision boundary

```
## logistic regression
xdf <- data.frame(x)
logreg <- glm(y ~ LD1 + LD2, data=xdf, family=binomial)
y.lr <- predict(logreg, type="response")</pre>
egscplot (x, pch=2*y+1, col=2-as.numeric(y==(v.lr>.5)))
y.lr.grid <- predict(logreg, newdata=gdf, type="response")</pre>
contour (qx1, qx2, matrix (y.lr.qrid, qm, qn),
   levels=c(.1,.25,.75,.9), add=TRUE,d=FALSE,ltv=3,lwd=1)
contour(gx1,gx2,matrix(v.lr.grid,gm,gn),
   levels=c(.5), add=TRUE,d=FALSE,ltv=1,lwd=2)
## logistic regression with quadratic interactions
logreg <- glm(y ~ (LD1 + LD2)^2, data=xdf, family=binomial)
y.lr <- predict(logreg, type="response")</pre>
egscplot(x,pch=2*v+1,col=2-as.numeric(v==(v.lr>.5)))
v.lr.grid <- predict(logreg,newdata=gdf,type="response")</pre>
contour (qx1, qx2, matrix (y.lr.qrid, qm, qn),
   levels=c(.1,.25,.75,.9), add=TRUE,d=FALSE,ltv=3,lwd=1)
contour(gx1,gx2,matrix(y.lr.grid,gm,gn),
   levels=c(.5), add=TRUE,d=FALSE,ltv=1,lwd=2)
```

Crab Dataset: Blue Female vs. rest



Comparing LDA and logistic regression.



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
```