Linear classification methods

Lecture 2a

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Overview

- Elements of decision theory
- Logistic regression
- Discriminant Analysis models

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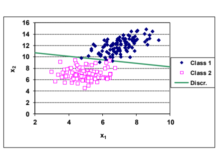
Classification

- Given data $D = \left((X_i, Y_i), i = 1 \ldots N\right)$
  - $Y_i = Y(X_i) = C_j \in \boldsymbol{C}$
  - Class set $\boldsymbol{C} = (C_1, \ldots, C_K)$

Classification problem:

- Decide $\hat{Y}(x)$ that maps **any** x into some class C_K
  - Decision boundary



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Classifiers

- **Deterministic**: decide a rule that directly maps X into $\hat{Y}$
- **Probabilistic:** define a model for $P(Y = C_i|X), i = 1 \ldots K$

Disanvantages of deterministic classifiers:

- Sometimes simple mapping is not enough (risk of cancer)
- Difficult to embed loss-> rerun of optimizer is often needed
- Combining several classifiers into one is more problematic
  - Algorithm A classifies as spam, Algorithm B classifies as not spam → ???
  - P(Spam|A)=0.99, P(Spam|B)=0.45 → better decision can be made

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Bayesian decision theory

- Machine learning models estimate $p(y|x)$ or $p(y|x,\widehat{w})$
- Transform probability into action→ which value to predict?→decision step
  - $p(Y = Spam|x) = 0.83$→do we move the mail to Junk?
  - What is more dangerous: deleting 1 non-spam mail or letting 1 spam mail enter Inbox?
- →**Loss function** or **Loss matrix**

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Loss matrix

- Costs of classifying $Y = C_k$ to C_j:
  - Rows: true, columns: predicted

$$L = \|L_{ij}\|, i = 1, \dots, n, j = 1, \dots, n$$

- Example 1: 0/1-loss

$$L = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

- Example 2: Spam

$$L = \begin{pmatrix} 0 & 100 \\ 1 & 0 \end{pmatrix}$$

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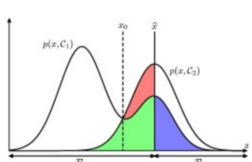
Loss and decision

- Expected loss minimization
  - R_j : classify to C_j

$$EL = \sum_k \sum_j \int_{R_j} L_{kj} p(\boldsymbol{x}, C_k) d\boldsymbol{x}$$

- **Choose such R_j that EL is minimized**
- Two classes



$$EL = \int_{R_1} L_{21} p(x, C_2) dx + \int_{R_2} L_{12} p(x, C_1)\, dx$$

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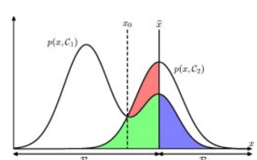
Loss and decision

- Loss minimization

$$\min_{\hat{f}} EL(y, \hat{f}) = \min_{\hat{f}} \int L(y, \hat{f}) p(y, x|w) dxdy$$



When loss is
$$\begin{cases} 1, wrongly\ classified \\ 0, correctly\ classified \end{cases}$$

Classify Y as
$$\hat{Y} = \arg\max_c p(Y = c|X)$$

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Loss and decision

- How to minimize *EL with two classes?*
- Rule:
  - $L_{12}p(x,C_1) > L_{21}p(x,C_2)$ →predict y as C_1
- 0/1 Loss: classify to the class which is more probable!

$$\boxed{\frac{p(C_1|x)}{p(C_2|x)} > \frac{L_{21}}{L_{12}} \rightarrow predict\ y\ as\ C_1}$$

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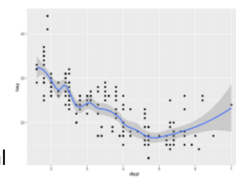
Loss and decision

- Continuous targets: squared loss
  - Given a model $p(x,y)$, minimize

$$EL = \int L\left(y, \hat{Y}(x)\right) p(x,y)dxdy$$



- Using **square loss**, the optimal is posterior mean

$$\hat{Y}(x) = \int yp(y|x)dy$$

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ROC curves

- Binary classification
- The choice of the thershold $\hat{x} = \frac{L_{21}}{L_{12}}$ affects prediction→ what if we don't know the loss? Which classifier is better?
- **Confusion matrix**

		PREDICTED		
T		1	0	Total
R U	1	TP	FN	N_+
E	0	FP	TN	N_-

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ROC curves

- **True Positive Rates** (TPR) = **sensitivity** = **recall**
  - Probability of detection of positives: TPR=1 positives are correctly detected

$$TPR = TP/N_+$$

- **False Positive Rates** (FPR)
  - Probability of false alarm: system alarms (1) when nothing happens (true=0)

$$FPR = FP/N_-$$

- **Specificity**

$$Specificity = 1 - FPR$$

- **Precision**

$$Precision = \frac{TP}{TP + FP}$$

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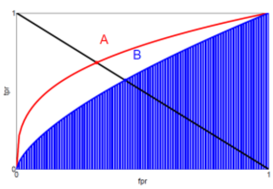
ROC curves

- **ROC**=Receiver operating characteristics
- Use various thresholds, measure TPR and FPR
- Same FPR, higher TPR→ better classifier
- Best classifier = greatest Area Under Curve (**AUC**)



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Types of supervised models

- **Generative models**: model $p(X|Y,w)$and $p(Y|w)$
  - Example: k-NN classification

$$p(X=x|Y=C_i,K)=\frac{K_i}{N_iV}, p(C_i|K)=\frac{N_i}{N}$$

From Bayes Theorem,

$$p(Y=C_i|x,K)=\frac{K_i}{K}$$

- **Discriminative models**: model $p(Y|X,w)$, X constant
  - Example: logistic regression
  - $p(Y=1|\boldsymbol{w},\boldsymbol{x})=\frac{1}{1+e^{-\boldsymbol{w}^T\boldsymbol{x}}}$

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Generative vs Discriminative

- Generative can be used to generate new data
- Generative normally easier to fit (check Logistic vs K-NN)
- Generative: each class estimated separately→ do not need to retrain when a new class added
- Discriminative models: can replace X with $\phi(X)$ (preprocessing), method will still work
  - Not generative, distribution will change
- Generative: often make too strong assumptions about $p(X|Y,w)$ → bad performance

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Logistic regression

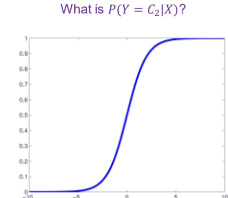
- Discriminative model
- Model for binary output
  - $C=\{C_1=1, C_2=0\}$
    $p(Y=C_1|X)=sigm(\boldsymbol{w}^T\boldsymbol{x})$

$$sigm(a)=\frac{1}{1+e^{-a}}$$

- Alternatively
  $Y \sim Bernoulli(sigm(a)), a=\boldsymbol{w}^T\boldsymbol{x}$

$$sigm(a)=\frac{1}{1+e^{-a}}$$

What is $P(Y=C_2|X)$?



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Logistic regression

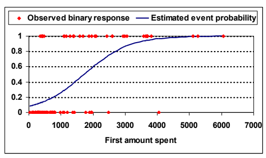
- Logistic model- yet another form

$$ln\frac{p(Y=1|X=x)}{P(Y=0|X=x)} = ln\frac{p(Y=1|X=x)}{1-P(Y=1|X=x)} = logit(p(Y=1|X=x)) = \boldsymbol{w}^T\boldsymbol{x}$$

The log of the odds is linear in *x*

- Here $logit(t) = \ln\left(\frac{t}{1-t}\right)$
- Note $p(Y|X)$ is connected to $\boldsymbol{w}^T\boldsymbol{x}$ via logit link

Example: Probability to buy more than once as function of First Amount Spend



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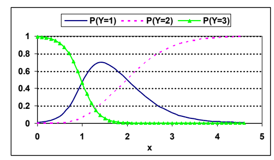
Logistic regression

- When Y is categorical,

$$p(Y=C_i|x) = \frac{e^{\boldsymbol{w}_i^T\boldsymbol{x}}}{\sum_{j=1}^{K} e^{\boldsymbol{w}_j^T\boldsymbol{x}}} = softmax(\boldsymbol{w}_i^T\boldsymbol{x})$$

- Alternatively

$$Y \sim Multinoulli\left(softmax(\boldsymbol{w}_1^T\boldsymbol{x}), \ldots softmax(\boldsymbol{w}_K^T\boldsymbol{x})\right)$$



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Logistic regression

Fitting logistic regression

- In binary case,

$$\log P(D|w) = \sum_{i=1}^{N} y_i \log(sigm(w^T x_i)) + (1-y_i)\log(1-sigm(w^T x_i))$$

  - Can not be maximized analytically, but unique maximizer exists
- To maximize loglikelihood, optimization used
  - Newton's method traditionally used (Iterative Reweighted Least Squares)
  - Steepest descent,Quasi-newton methods…

Estimation:

For new x, estimate $p(y) = [p_1, \ldots p_C]$ and classify as arg $\max_i p_i$

Decision boundaries of logistic regression are linear

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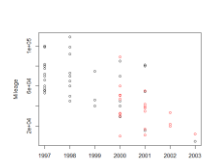
Logistic regression

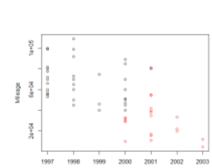
- In R, use glm() with family="binomial"
  - Predicted probabilities: predict(fit,newdata, type="response")

Example Equipment=f(Year, mileage)

Original data



Classified data



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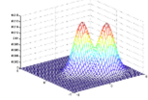
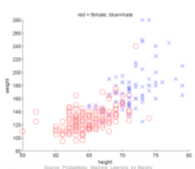
Quadratic discriminant analysis

- Generative classifier
- Main assumptions:
  - $\boldsymbol{x}$ is now **random** as well as y

$$p(\boldsymbol{x}|y = C_i, \theta) = N(\boldsymbol{x}|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$



Unknown parameters $\boldsymbol{\theta} = \{\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\}$



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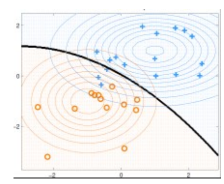
Quadratic discriminant analysis

- If parameters are estimated, classify:

$$\hat{y}(\boldsymbol{x}) = \arg\max_c p(y = c|\boldsymbol{x}, \theta)$$



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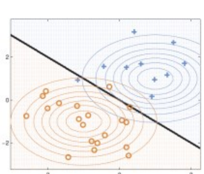
Linear discriminant analysis (LDA)

- Assumtion $\Sigma_i = \Sigma, i = 1, \dots K$
- Then $p(y = c_i|x) = softmax(w_i^T x + w_{0i})$ →exactly the same form as the logistic regression
  - $w_{0i} = -\frac{1}{2}\boldsymbol{\mu}_i^T \Sigma^{-1} \boldsymbol{\mu}_i + \log \pi_i$
  - $w_i = \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_i$



- Decision boundaries are linear
  - **Discriminant function**:

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k$$

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Linear discriminant analysis (LDA)

- Difference LDA vs logistic regression??
  - Coefficients will be estimated differently! (models are different)
- How to estimate coefficients
  - find MLE.

$$\hat{\mu}_c = \frac{1}{N_c} \sum_{i:y_i=c} \mathbf{x}_i, \quad \hat{\Sigma}_c = \frac{1}{N_c} \sum_{i:y_i=c} (\mathbf{x}_i - \hat{\mu}_c)(\mathbf{x}_i - \hat{\mu}_c)^T$$

$$\hat{\Sigma} = \frac{1}{N} \sum_{c=1}^{k} N_c \hat{\Sigma}_c$$

  - Sample mean and sample covariance are MLE!
  - If class priors are parameters (**proportional priors**),

$$\hat{\pi}_c = \frac{N_c}{N}$$

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LDA and QDA: code

- Syntax in R, library **MASS**

lda(formula, data, ..., subset, na.action)
- Prior – class probabiliies
- Subset – indices, if training data should be used

qda(formula, data, ..., subset, na.action)

predict(..)

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LDA: output

```
resLDA=lda(Equipment~Mileage+Year, data=mydata)
 print(resLDA)
```

```
> print(resLDA)
Call:
lda(Equipment ~ Mileage + Year, data = mydata)

Prior probabilities of groups:
        0         1 
0.6440678 0.3559322 

Group means:
   Mileage     Year
0 63539.21 1998.447
1 36857.62 2000.762

Coefficients of linear discriminants:
                  LD1
Mileage -1.500069e-05
Year     5.745893e-01
```


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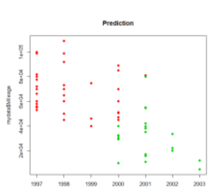
LDA: output

- Misclassified items

```
plot(mydata$Year, mydata$Mileage,
col=as.numeric(Pred$class)+1, pch=21,
bg=as.numeric(Pred$class)+1,
main="Prediction")
```

```
> table(Pred$class, mydata$Equipment)
   
     0  1
  0 31  6
  1  7 15
```



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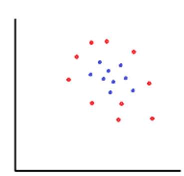
LDA versus Logistic regression

- Generative classifiers are easier to fit, discriminative involve numeric optimization
- LDA and Logistic have same model form but are fit differently
- LDA has stronger assumptions than Logistic, some other generative classifiers lead also to logistic expression
- New class in the data?
  - Logistic: fit model again
  - LDA: estimate new parameters from the new data
- Logistic and LDA: complex data fits badly unless interactions are included



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LDA versus Logistic regression

- LDA (and other generative classifiers) handle missing data easier
- Standardization and generated inputs:
  - Not a problem for Logistic
  - May affect the performance of the LDA in a complex way
- Outliers affect $\Sigma \rightarrow$ LDA is not robust to gross outliers
- LDA is often a good classification method even if the assumption of normality and common covariance matrix are not satisfied.