DS 4400

Machine Learning and Data Mining I

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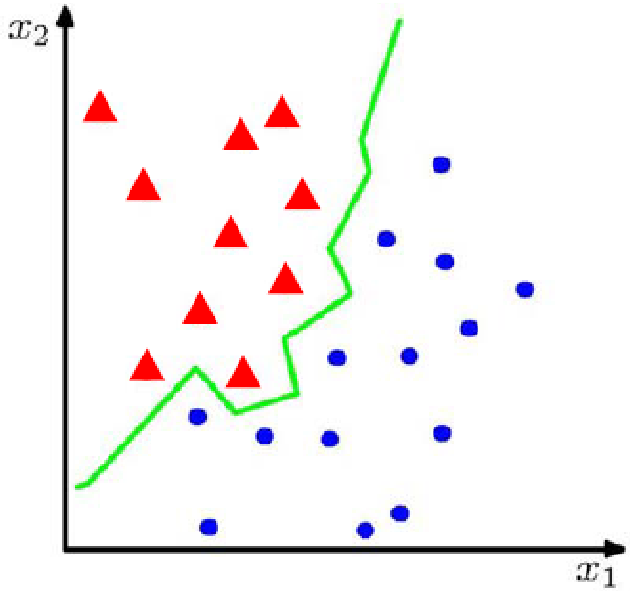
Review

- Metrics for evaluating classification models
  - Accuracy, precision, recall
- Cross-validation should be used to avoid over-fitting
  - K-fold or LOOCV
- Logistic regression
  - Estimates $\Pr[Y = 1|X = x]$ using sigmoid
  - Maximum Likelihood Estimation (MLE) for objective
  - Can use gradient descent for training
  - Very interpretable

Outline

- Logistic regression
  - Gradient descent for logistic regression
- Linear Discriminant Analysis (LDA)
- Lab (logistic regression, LDA, kNN)
- Feature selection
  - Wrapper
  - Filter
  - Embedded methods

Classification



Binary or discrete

- Suppose we are given a training set of N observations

$$\{x^{(1)}, \dots, x^{(n)}\} \text{ and } \{y^{(1)}, \dots, y^{(n)}\}, x^{(i)} \in R^d, y^{(i)} \in \{-1, 1\}$$

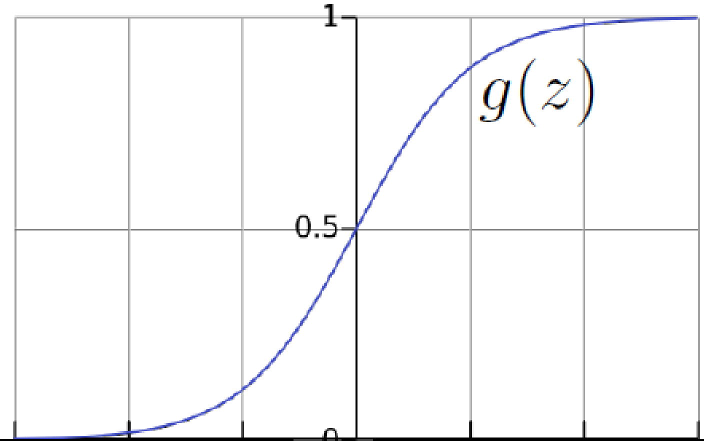
- Classification problem is to estimate f(x) from this data such that

$$f\left(x^{(i)}\right) = y^{(i)}$$

Logistic Regression

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^{\intercal}\boldsymbol{x}\right)$$

$$g(z) = \frac{1}{1+e^{-z}}$$

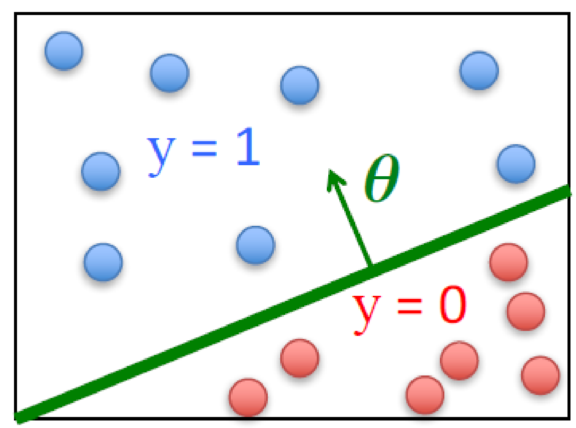


$\boldsymbol{\theta}^{\intercal}\boldsymbol{x}$ should be large negative values for negative instances

$\boldsymbol{\theta}^{\intercal}\boldsymbol{x}$ should be large positive values for positive instances

Probabilistic model $h_{\theta(x)} = \mathrm{P}[y = 1|x; \theta]$

- Predict y = 1 if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq 0.5$
- Predict y = 0 if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$



Logistic Regression is a linear classifier!

Maximum Likelihood Estimation (MLE)

Given training data $X = \{x^{(1)}, \ldots, x^{(n)}\}$ with labels $\mathrm{Y} = \{y^{(1)}, \ldots, y^{(n)}\}$

What is the likelihood of training data for parameter θ?

Define likelihood function

$$Max_\theta \; L(\theta) = P[Y|X;\theta]$$

Assumption: training points are independent

$$L(\theta) = \prod_{i=1}^{n} P[y^{(i)}|x^{(i)};\theta]$$

MLE for Logistic Regression

$$p(y|x,\theta) = h_\theta(x)^y \left(1 - h_\theta(x)\right)^{1-y}$$

$$\begin{aligned}\boldsymbol{\theta}_{\text{MLE}} &= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(y^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta}) \\ &= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} y^{(i)} \log h_\theta\left(x^{(i)}\right) + (1 - y^{(i)}) \log\left(1 - h_\theta(x)\right)\end{aligned}$$

- Substitute in model, and take negative to yield

Logistic regression objective:

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

$$J(\boldsymbol{\theta}) = -\sum_{i=1}^{n} \left[y^{(i)} \log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1 - y^{(i)}\right) \log\left(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right) \right]$$

Gradient Descent for Logistic Regression

$$J(\boldsymbol{\theta}) = -\sum_{i=1}^{n} \left[y^{(i)} \log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1 - y^{(i)}\right) \log \left(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)\right]$$

$$J(\theta) = -\sum_{i=1}^{n} C_i$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update for j = 0 ... d

Computing Gradients

- Derivative of sigmoid
  - $g(z) = \frac{1}{1+e^{-z}}$; $g'(z) = \frac{e^{-z}}{(1+e^{-z})^2} = g(z)(1 - g(z))$
- Derivative of hypothesis
  - $h_\theta(x) = g(\theta^T x) = g(\theta_j x_j + \sum_{k \neq j} \theta_k x_k)$
  - $\frac{\partial h_\theta(x)}{\partial \theta_j} = \frac{\partial g(\theta^T x)}{\partial \theta_j} x_j = g(\theta^T x)\big(1 - g(\theta^T x)\big) x_j$
- Derivation of C_i
  - $\frac{\partial C_i}{\partial \theta_j} = y^{(i)} \frac{1}{h_\theta(x^i)} \mathrm{g}\big(\theta^T x^{(i)}\big) \left(1 - \mathrm{g}\big(\theta^T x^{(i)}\big)\right) x_j^{(i)}$ -

    $(1 - y^{(i)}) \frac{1}{1 - h_\theta(x^i)} \mathrm{g}\big(\theta^T x^{(i)}\big) \left(1 - \mathrm{g}\big(\theta^T x^{(i)}\big)\right) x_j^{(i)}$

    $= \left(y^{(i)} - h_\theta\big(x^{(i)}\big)\right) x_j^{(i)}$

Gradient Descent for Logistic Regression

$$J(\boldsymbol{\theta}) = -\sum_{i=1}^{n}\left[y^{(i)}\log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1-y^{(i)}\right)\log\left(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)\right]$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for j = 0 ... d)

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)$$

$$\theta_j \leftarrow \theta_j - \alpha \left[\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)x_j^{(i)}\right]$$

Gradient Descent for Logistic Regression

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for j = 0 ... d)

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)$$

$$\theta_j \leftarrow \theta_j - \alpha \left[\sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} \right]$$

This looks IDENTICAL to Linear Regression!

- However, the form of the model is very different:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}}}$$

LDA

- Classify to one of k classes
- Logistic regression computes directly
  - $\mathrm{P}[Y = 1|X = x]$
  - Assume sigmoid function
- LDA uses Bayes Theorem to estimate it
  - $\mathrm{P}[Y = k|X = x] = \frac{\mathrm{P}[X = x|Y = k]\mathrm{P}[Y=k]}{\mathrm{P}[X=x]}$
  - Let $\pi_k = \mathrm{P}[Y = k]$ be the prior probability of class k and $f_k(x) = \mathrm{P}[X = x|Y = k]$

LDA

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

Assume $f_k(x)$ is Gaussian!
Unidimensional case (d=1)

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x - \mu_k)^2\right)$$

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_l)^2\right)}.$$

Assumption: $\sigma_1 = \ldots \sigma_k = \sigma$

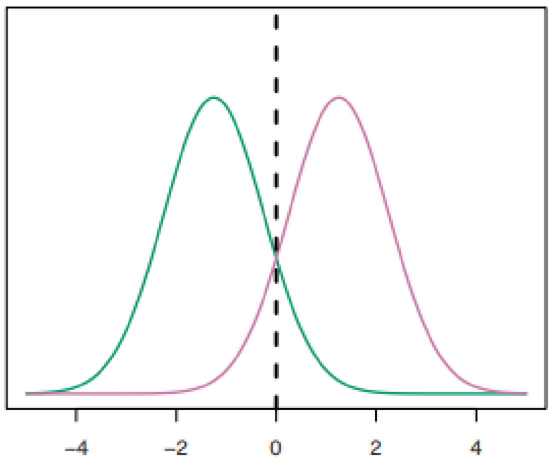
LDA decision boundary

Pick class k to maximize

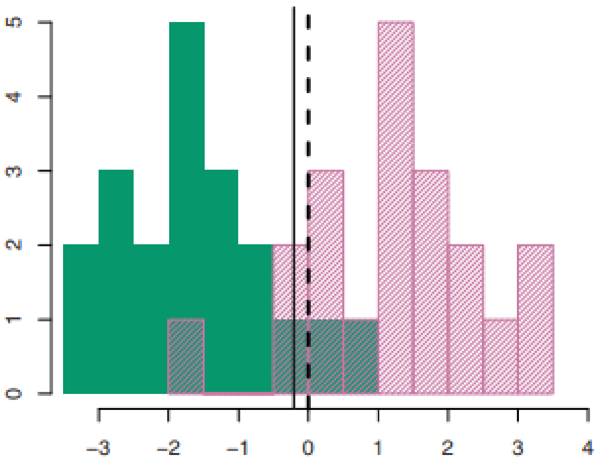
$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

Example: $k = 2, \pi_1 = \pi_2$

Classify as class 1 if $x > \frac{\mu_1 + \mu_2}{2}$



Bayes decision boundary



Estimated decision boundary

LDA in practice

Given training data $\left(x^{(i)}, y^{(i)}\right), i = 1, \dots, n, y^{(i)} \in \{1, \dots, K\}$

1. Estimate mean and variance

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x^{(i)}$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x^{(i)} - \hat{\mu}_k)^2$$

2. Estimate prior

$$\hat{\pi}_k = n_k / n.$$

Given testing point x, predict k that maximizes:

$$\hat{\delta}_k(x) = x \cdot \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)$$

LDA vs Logistic Regression

- Logistic regression computes directly $\Pr[Y = 1|X = x]$ by assuming sigmoid function
  - Uses Maximum Likelihood Estimation
- LDA uses Bayes Theorem to estimate it
  - Estimates mean, co-variance, and prior from training data
  - Assumes Gaussian distribution for $f_k(x) = \Pr[X = x|Y = k]$
- Which one is better?
  - LDA can be sensitive to outliers
  - LDA works well for Gaussian distribution
  - Logistic regression is more complex to solve, but more expressive

Lab

```
> library(ISLR)
> fix(Smarket)
```

Data Editor

	Year	Lag1	Lag2	Lag3	Lag4	Lag5	Volume	Today	Direction
1	2001	0.381	-0.192	-2.624	-1.055	5.01	1.1913	0.959	Up
2	2001	0.959	0.381	-0.192	-2.624	-1.055	1.2965	1.032	Up
3	2001	1.032	0.959	0.381	-0.192	-2.624	1.4112	-0.623	Down
4	2001	-0.623	1.032	0.959	0.381	-0.192	1.276	0.614	Up
5	2001	0.614	-0.623	1.032	0.959	0.381	1.2057	0.213	Up
6	2001	0.213	0.614	-0.623	1.032	0.959	1.3491	1.392	Up
7	2001	1.392	0.213	0.614	-0.623	1.032	1.445	-0.403	Down
8	2001	-0.403	1.392	0.213	0.614	-0.623	1.4078	0.027	Up
9	2001	0.027	-0.403	1.392	0.213	0.614	1.164	1.303	Up
10	2001	1.303	0.027	-0.403	1.392	0.213	1.2326	0.287	Up
11	2001	0.287	1.303	0.027	-0.403	1.392	1.309	-0.498	Down
12	2001	-0.498	0.287	1.303	0.027	-0.403	1.258	-0.189	Down
13	2001	-0.189	-0.498	0.287	1.303	0.027	1.098	0.68	Up
14	2001	0.68	-0.189	-0.498	0.287	1.303	1.0531	0.701	Up
15	2001	0.701	0.68	-0.189	-0.498	0.287	1.1498	-0.562	Down

Lab Logistic Regression

Train on data before 2005

```
> train=(Year<2005)
> Smarket.2005=Smarket[!train,]
> dim(Smarket.2005)
[1] 252   9
> Direction.2005=Direction[!train]
> glm.fits=glm(Direction~Lag1+Lag2+Lag3+Lag4+Lag5+Volume,data=Smarket,family=binomial,subset=train)
> summary(glm.fits)

Call:
glm(formula = Direction ~ Lag1 + Lag2 + Lag3 + Lag4 + Lag5 +
    Volume, family = binomial, data = Smarket, subset = train)

Deviance Residuals:
   Min       1Q   Median       3Q      Max
-1.302   -1.190   1.079    1.160    1.350

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.191213   0.333690   0.573    0.567
Lag1        -0.054178   0.051785  -1.046    0.295
Lag2        -0.045805   0.051797  -0.884    0.377
Lag3         0.007200   0.051644   0.139    0.889
Lag4         0.006441   0.051706   0.125    0.901
Lag5        -0.004223   0.051138  -0.083    0.934
Volume      -0.116257   0.239618  -0.485    0.628
```

Lab Logistic Regression

Test on data in 2005

```
>
> glm.probs=predict(glm.fits,Smarket.2005,type="response")
> glm.pred=rep("Down",nrow(Smarket.2005))
> glm.pred[glm.probs>.5]="Up"
> head(Smarket.2005)
     Year   Lag1   Lag2   Lag3   Lag4   Lag5 Volume  Today Direction
999  2005 -0.134  0.008 -0.007  0.715 -0.431 0.7869 -0.812      Down
1000 2005 -0.812 -0.134  0.008 -0.007  0.715 1.5108 -1.167      Down
1001 2005 -1.167 -0.812 -0.134  0.008 -0.007 1.7210 -0.363      Down
1002 2005 -0.363 -1.167 -0.812 -0.134  0.008 1.7389  0.351        Up
1003 2005  0.351 -0.363 -1.167 -0.812 -0.134 1.5691 -0.143      Down
1004 2005 -0.143  0.351 -0.363 -1.167 -0.812 1.4779  0.342        Up
> head(glm.probs)
      999      1000      1001      1002      1003      1004
0.5282195 0.5156688 0.5226521 0.5138543 0.4983345 0.5010912
> head(glm.pred)
[1] "Up"   "Up"   "Up"   "Up"   "Down" "Up"
> table(glm.pred,Direction.2005)
        Direction.2005
glm.pred Down Up
    Down   77 97
    Up     34 44
> mean(glm.pred==Direction.2005)
[1] 0.4801587
```

Lab LDA

```
> library(MASS)
> lda.fit=lda(Direction~Lag1+Lag2,data=Smarket,subset=train)
> lda.fit
Call:
lda(Direction ~ Lag1 + Lag2, data = Smarket, subset = train)

Prior probabilities of groups:
    Down       Up
0.491984 0.508016

Group means:
            Lag1        Lag2
Down  0.04279022  0.03389409
Up   -0.03954635 -0.03132544

Coefficients of linear discriminants:
            LD1
Lag1 -0.6420190
Lag2 -0.5135293
> lda.pred=predict(lda.fit, Smarket.2005)
> lda.class=lda.pred$class
> table(lda.class,Direction.2005)
         Direction.2005
lda.class Down  Up
     Down   35  35
     Up     76 106
> mean(lda.class==Direction.2005)
[1] 0.5595238
```

Lab kNN

```
>
> library(class)
> train.X=cbind(Lag1,Lag2)[train,]
> test.X=cbind(Lag1,Lag2)[!train,]
> train.Direction=Direction[train]
> set.seed(1)
> knn.pred=knn(train.X,test.X,train.Direction,k=1)
> table(knn.pred,Direction.2005)
        Direction.2005
knn.pred Down Up
    Down   43 58
    Up     68 83
> mean(knn.pred==Direction.2005)
[1] 0.5
> knn.pred=knn(train.X,test.X,train.Direction,k=3)
> table(knn.pred,Direction.2005)
        Direction.2005
knn.pred Down Up
    Down   48 54
    Up     63 87
> mean(knn.pred==Direction.2005)
[1] 0.5357143
> knn.pred=knn(train.X,test.X,train.Direction,k=7)
> table(knn.pred,Direction.2005)
        Direction.2005
knn.pred Down Up
    Down   41 65
    Up     70 76
> mean(knn.pred==Direction.2005)
[1] 0.4642857
```

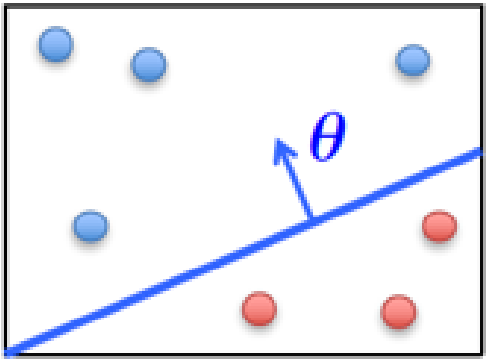
Linear models

- Perceptron

$$h(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{\theta}^\intercal \boldsymbol{x})$$

- Logistic regression

$$\boxed{h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\intercal \boldsymbol{x}}}}$$



- LDA

$$Max_k \;\; \delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

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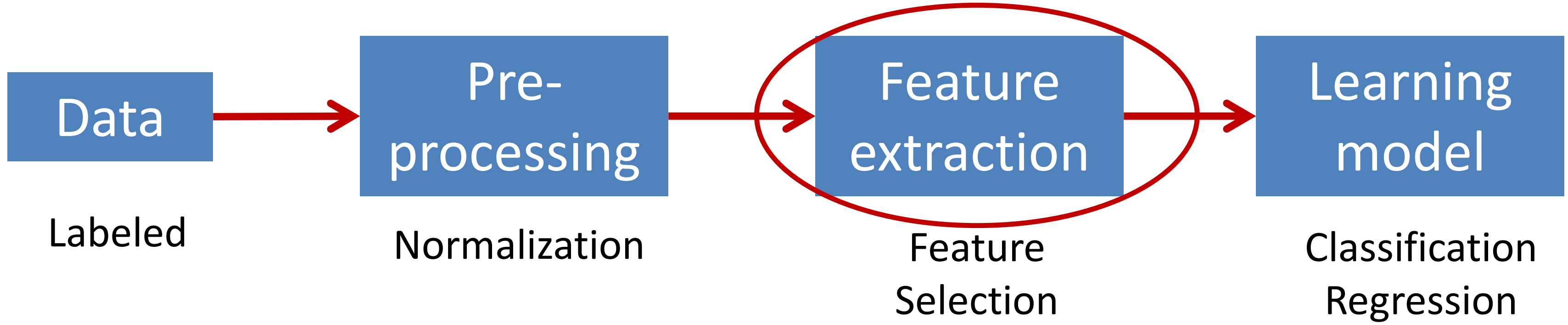
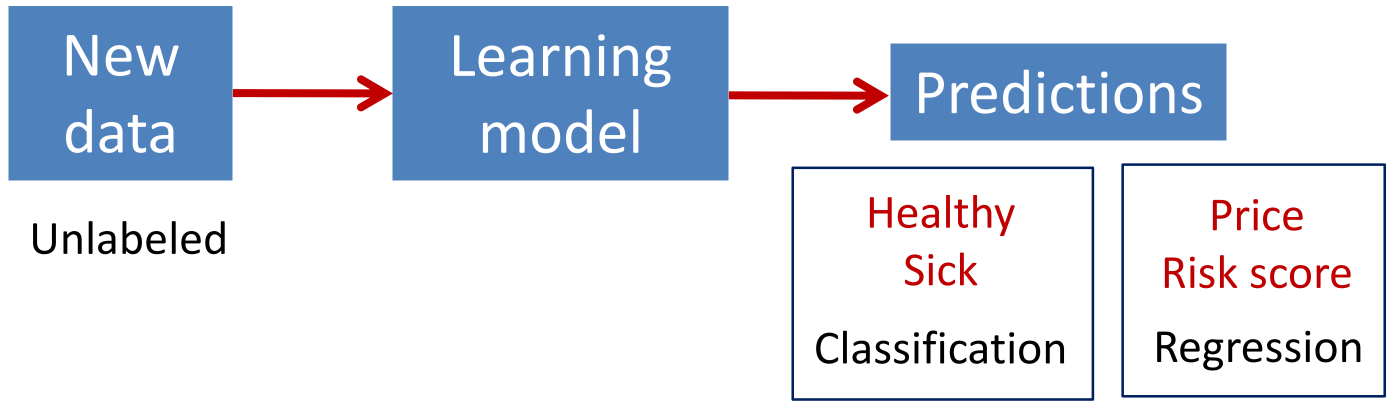
  - Wrapper
  - Filter
  - Embedded methods

Supervised Learning

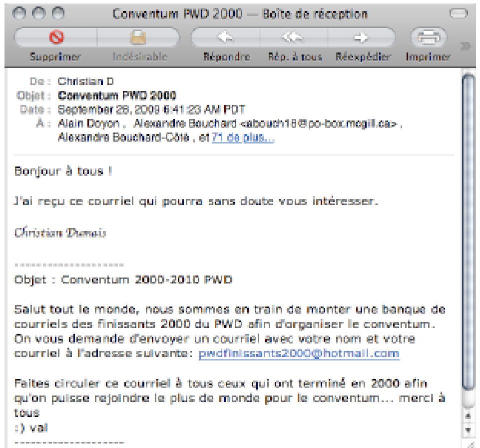
Training



Testing



Example: Email Classification



Conventum PWD 2000 — Boîte de réception

Supprimer Indésirable Répondre Rép. à tous Réexpédier Imprimer

De : Christian D
Objet : Conventum PWD 2000
Date : September 28, 2009 6:41:23 AM PDT
À : Alain Doyon , Alexandre Bouchard <abouch18@po-box.mcgill.ca> , Alexandre Bouchard-Côté , et 71 de plus...

Bonjour à tous !

J'ai reçu ce courriel qui pourra sans doute vous intéresser.

Christian Dumais

Objet : Conventum 2000-2010 PWD

Salut tout le monde, nous sommes en train de monter une banque de courriels des finissants 2000 du PWD afin d'organiser le conventum. On vous demande d'envoyer un courriel avec votre nom et votre courriel à l'adresse suivante: pwdfinissants2000@hotmail.com

Faites circuler ce courriel à tous ceux qui ont terminé en 2000 afin qu'on puisse rejoindre le plus de monde pour le conventum.... merci à tous
:) val

PERSONAL

- Input: a email message
- Output: is the email...
  - spam,
  - work-related,
  - personal, ...

Bag-of-Words

- Input: x (email-valued)
- Feature vector:

Indicator or Kronecker delta function

$$f(\boldsymbol{x}) = \begin{bmatrix} f_1(\boldsymbol{x}) \\ f_2(\boldsymbol{x}) \\ \vdots \\ f_n(\boldsymbol{x}) \end{bmatrix}, \quad \text{e.g. } f_1(\boldsymbol{x}) = \begin{cases} 1 & \text{if the email contain Boston} \\ 0 & \text{otherwise} \end{cases}$$

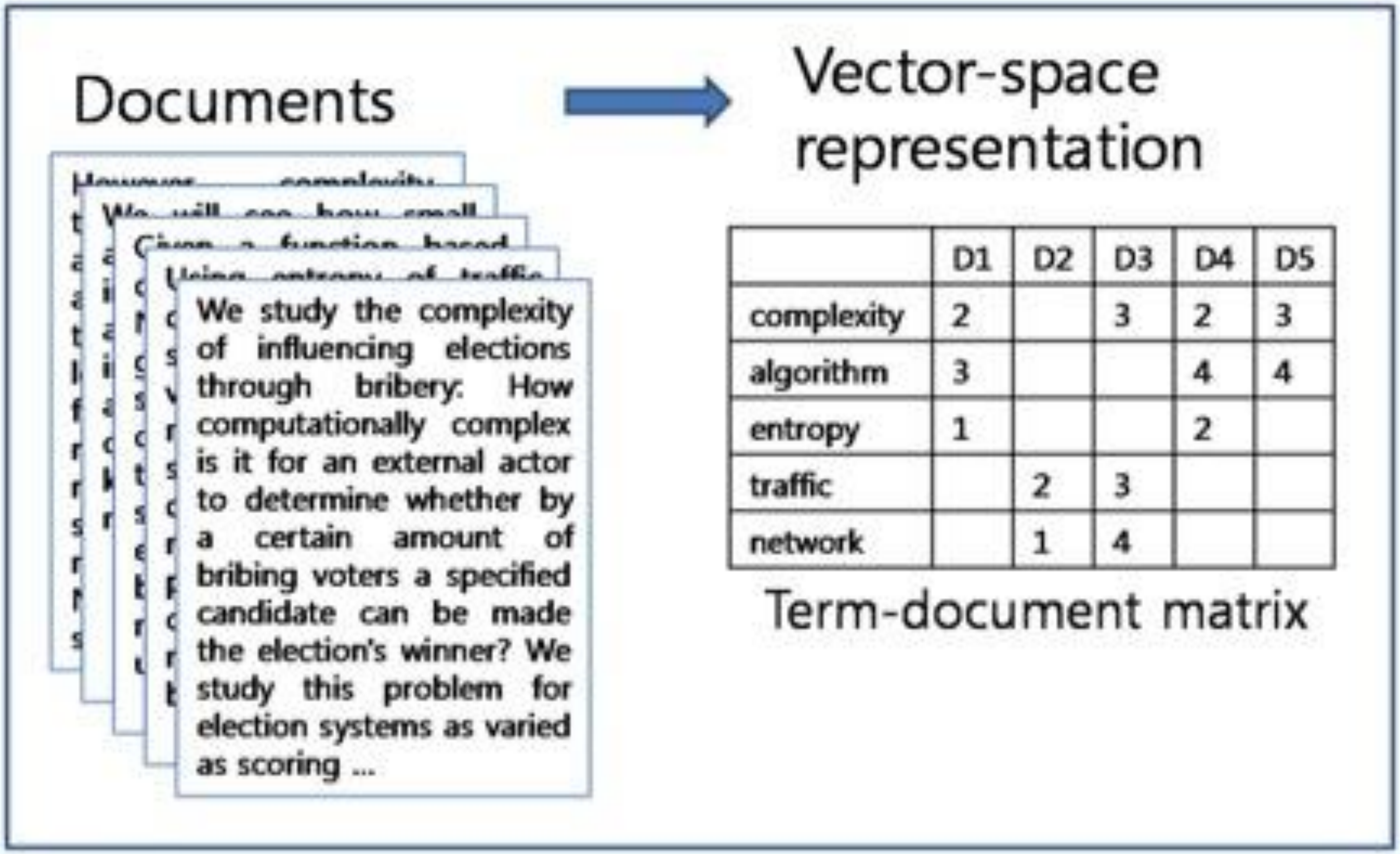
- Learn one weight vector for each class:

$$w_y \in \mathbb{R}^n, \quad y \in \{\text{SPAM,WORK,PERS}\}$$

Could also use frequency

- $f_i(x)$ is the number of times word i appears in x

Representation



- Large number of words in dictionary (>50,000)
- Very sparse representation (many features set at 0)

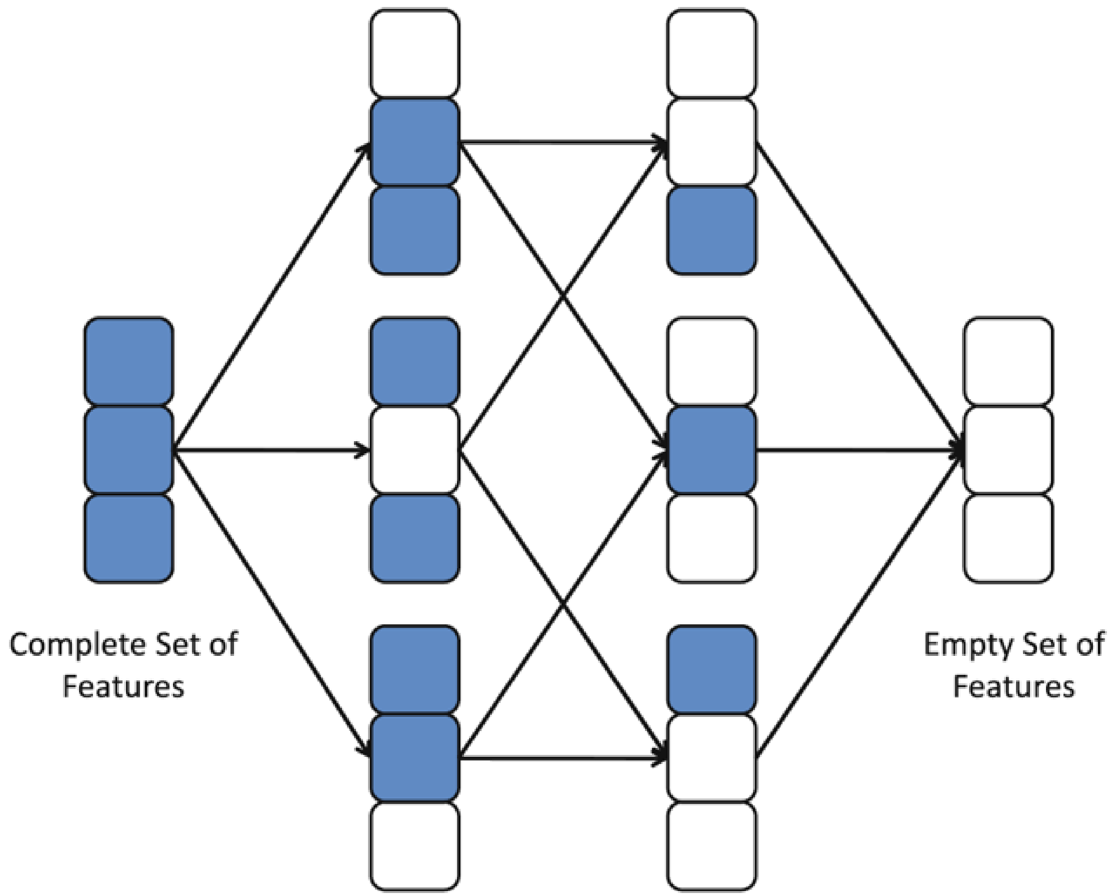
Feature selection

- *Feature Selection*
  - Process for choosing an optimal subset of features according to a certain criteria

- Why we need Feature Selection:
  1. To improve performance (in terms of speed, predictive power, simplicity of the model).
  2. To visualize the data for model selection.
  3. To reduce dimensionality and remove noise.

Feature Search Space

Search Space:



Exponentially large!

Methods for Feature Selection

- Wrappers
  - Select subset of features that gives best prediction accuracy (using cross-validation)
  - Model-specific
- Filters
  - Compute some statistical metrics (correlation coefficient, mutual information)
  - Select features with statistics higher than threshold
- Embedded methods
  - Feature selection done as part of training
  - Example: Regularization (Lasso, L1 regularization)

Feature Engineering

- Feature engineering is crucial to getting good results
- Strategy: overshoot and regularize
  - Define as many features as you can
  - Use regularization for models that support it
  - Use other feature selection methods (e.g., filters) otherwise
- Do cross-validation to evaluate selected features on multiple runs
- When feature selection is frozen, evaluate on test set

Acknowledgements

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  - David Sontag
- Thanks!