# Topics in Quantitative Finance (FIN 528): Machine Learning for Finance

Jaehyuk Choi

March 23, 2017

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### Quantitative finance courses in PHBS

- Y1-M3: Stochastic Finance by Jaehyuk Choi [required for Qfin MA]
- Y1-M4: Derivative Pricing by Lei (Jack) Sun
- Y2-M1: Applied Stochastic Processes by Jaehyuk CHOI Application, Programming, Course project
- Y2-M3: Topics in Quantitative Finance by Jaehyuk CHOI Machine Learning for Finance (Mon-Thurs 1:30 PM)
- Y2-M3: Numerical Methods and Analysis by Jake ZHAO (Mon-Thurs 3:30 PM)
- Y2-M3: Bayesian Statistics by Qian CHEN (Mon-Thurs 10:30 AM)

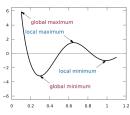
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### AlphaGo vs Humans (LEE Sedol, KE Jie)





We have to think again about joseki / dìngshì (定石/ 定式) . In Go (围棋), a joseki is the studied sequences of moves for which the result is considered balanced for both black and white sides.



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### LEE Sedol afterwards · · ·





- Became more popular and richer
- Perhaps titled as the last human who beat the machine in Go

# ML/AI: Rise of the machines?

#### Probabily not!



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# What and why now?

#### What is ML?

- Prediction based on data (data into knowledge)
- Extended linear/logistic regression
- Pattern recognition

#### Why now?

- Abundant Data (Big Data)
- Faster computer (Graphics Processing Unit: GPU)
- Advances in research: Geoffrey Hinton (Google), Yann LeCun (Facebook).

# Recent applications of ML

- Automated driving system (Google, Apple, etc)
- Suggestion engine (Amazon, Taobao)
- Cancer diagnosis (IBM Watson)
- Digitizing images (Facebook, Google)
- Shopping without checkout (Amazon Go: big data)

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### ML in finance?

#### Prediction

- Asset management / investment
- Trading algorithm (alpha)
- Earnings prediction: e.g., Prediction Valley

#### Cost cut / labor reduction

- Automated accounting / tax
- Automated analyst report
- Chat-bot (trading and sales)
- Data analytics: e.g., Kensho

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#### Softwares to use

#### Python'

- Anaconda (Python distribution + Environment management)
- Python Language Tutorial
- Sci-Kit Learn
- TensorFlow (wrapped by Keras)

#### Github.com

- Distributed version control system
- Clone or fork a repository to create a local copy
- https://github.com/PHBS/2016.M3.TQF-ML (our course)
- https://github.com/rasbt/python-machine-learning-book (PML)

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#### Other resources for ML

- Coursera ML course (CML) by Andrew Ng (Baidu)
- Stanford CS229 Machine Learning: course notes, student projects, etc
- The Elements of Statistical Learning (ESL)
- An Introduction to Statistical Learning (with R) (ISLR)
- Pattern Recognition and Machine Learning by Bishop (Microsoft)

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#### Homework

- Install Anaconda (Ver 4.3 Python 3.6)
- Create GitHub account, join PHBS (organization) and 2016.M3.TQF-ML (team).
- Fork the two repositories (the PML book and our course)
- Watch the first lecture of CML

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#### Notations and conventions: vector and matrix

### General rules (guess from the context)

- Scalar (non-bold): x, y, X, Y
- Vector (lowercase bold):  $\mathbf{x} = (x_i), \mathbf{y} = (y_i)$
- Matrix (uppercase bold):  $\boldsymbol{X} = (X_{ij}), \, \boldsymbol{Y} = (Y_{ij})$
- The (i,j) component of  $X: X_{ij}$
- The *i*-th row vector of  $\boldsymbol{X}$ :  $\boldsymbol{X}_{i*} = (X_{i1}, X_{i2}, \cdots, X_{ip})^T$
- The *j*-th column vector of  $\boldsymbol{X}$ :  $\boldsymbol{X}_{*j} = (X_{1j}, X_{2j}, \cdots, X_{Nj})$

#### Examples

- Dot product:  $\langle x, y \rangle = x^T y$
- Vector norm:  $|x| = \sqrt{x^T x}$
- Matrix multiplication:  ${m Z} = {m X} {m Y} o Z_{ij} = {m X}_{i*} {m Y}_{j*}$

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#### Notation and conventions: variables and observations

#### General rules

- Generic (or representative) variables (uppercase non-bold): X (input), Y (output), G (classification output)
- The predictions:  $\hat{Y}$ ,  $\hat{G}$
- X (input) may be p-dimensional (features):  $X_j$  ( $j \leq p$ ), row vector
- Y (output) may be K-dimensional (responses):  $Y_k$  ( $k \leq K$ ), row vector.
- The N observations of X or Y is stacked as rows: X ( $N \times p$ ), Y ( $N \times K$ )
- The *i*-th observation set:  $\boldsymbol{X}_{i*}$   $(1 \times p)$
- All observation of *j*-th feature  $X_j$ :  $X_{*j}$  ( $N \times 1$ )
- $X = (X_{*1} \cdots X_{*p})$  (column-wise concatenation)
- ullet The weight vector: eta or  $oldsymbol{w}$  used interchangeably.

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# Simple Linear Regression (Ordinary Least Square)

For scalar predictor (X) and response (Y),

$$Y \approx \beta_0 + \beta_1 X \longrightarrow \hat{\mathbf{y}} = \beta_0 + \beta_1 \mathbf{x}.$$

For N observations  $(x_1, y_1), \dots, (x_N, y_N)$ , the set of  $(\hat{\beta}_0, \hat{\beta}_1)$  to minimize the residual sum of squares (RSS):

$$RSS(\beta) = \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_i)^2 = (\boldsymbol{y} - \beta_0 - \beta_1 \boldsymbol{x})^T (\boldsymbol{y} - \beta_0 - \beta_1 \boldsymbol{x})$$

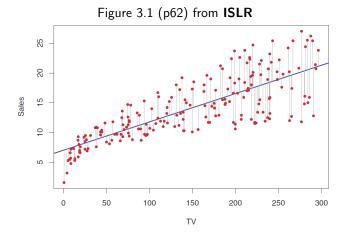
is given as

$$\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{\mathsf{Cov}(X, Y)}{\mathsf{Var}(X)},$$
$$\hat{\beta}_0 = \bar{y} - \beta_1 \bar{x}$$

for  $\bar{x} = \sum x_i/N$  and  $\bar{y} = \sum y_i/N$ .



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### Multi-dimensional Linear Regression

For (p+1)-vector predictor (X) and scalar response (Y),

$$Y \approx X\beta \longrightarrow \hat{\mathbf{y}} = \mathbf{X}\beta,$$

where  $X_0 = 1$  ( $X_{*0} = 1$ ) and  $\beta$  is a (p+1)-column vector.

$$RSS(\beta) = \frac{1}{2} (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$

$$\frac{\partial}{\partial \boldsymbol{\beta}} RSS(\boldsymbol{\beta}) = -\boldsymbol{X}^{T} (\boldsymbol{y} - \boldsymbol{X} \boldsymbol{\beta}) \quad \Rightarrow \quad \hat{\boldsymbol{\beta}} = (\boldsymbol{X}^{T} \boldsymbol{X})^{-1} \boldsymbol{X}^{T} \boldsymbol{y}$$

For (p+1)-vector predictor (X) and K-vector response (Y), the result is similarly given as

$$\hat{\pmb{Y}} = \pmb{X} \pmb{B}$$
 where  $\hat{\pmb{B}} = (\pmb{X}^T \pmb{X})^{-1} \pmb{X}^T \pmb{Y}$ ,

which is the independent regressions on  $Y_j$  ( $Y_{*j}$ ) combined together,

$$\boldsymbol{\hat{B}}_{*j} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{Y}_{*j}$$



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#### Newton's method

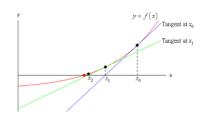
The root x satisfying f(x) = 0 can be found by the following iteration:

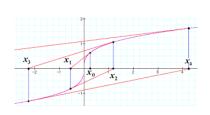
$$x_{n+1} = x_n - \eta \frac{f(x_n)}{f'(x_n)}$$

In multi-dimensional problems, the gradient is used instead of the differentiation:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \eta \frac{f(\mathbf{x}_n) \nabla f(\mathbf{x}_n)}{|\nabla f(\mathbf{x}_n)|^2}$$

Typically we use  $0 < \eta < 1$  to avoid *overshooting*.





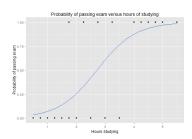
# Logistic Regression (Classification)

- ullet Qualitative (categorical) response (binary dependent variable,  $Y \in \{0,1\}$ )
- Multiple categories: how to give order?
- Linear regression (quantitative) is not proper
- Logistic (sigmoid) function:  $\sigma(logit) = quantile$

$$p = \phi(t) = \frac{e^t}{1 + e^t} = \frac{1}{1 + e^{-t}}$$
 for  $t = X\beta (X_0 = 1)$ 

Logit function (the inverse): log odds

$$\phi^{-1}(p) = \log\left(\frac{p}{1-p}\right) = \log(p) - \log(1-p)$$



### Fitting of logistic regression

#### Likelihood function

- For a given the prediction model, measures the likelihood of a data set.
- The best prediction model/weight is the one that maximizes the likelihood of the dataset.

For a data set  $(\mathbf{X}, \mathbf{y})$  where  $y_i \in \{0, 1\}$ ),

$$L(\beta) = \prod_{i} P(y_i = \hat{y}_i) = \prod_{i:y_i=1} \phi(\mathbf{X}_{i*}\beta) \prod_{i:y_i=0} (1 - \phi(\mathbf{X}_{i*}\beta))$$

$$= \prod_{i} \phi(\mathbf{X}_{i*}\beta)^{y_i} (1 - \phi(\mathbf{X}_{i*}\beta))^{1-y_i}$$

$$\log L(\beta) = \sum_{i} y_i \log \phi(\mathbf{X}_{i*}\beta) + (1 - y_i) \log (1 - \phi(\mathbf{X}_{i*}\beta))$$

The cost function (to minimize) is  $J(\beta) = -\log L(\beta)$ 



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# Updating weights

After some algebra,

$$\mathbf{w} := \mathbf{w} + \Delta \mathbf{w}, \quad \Delta \mathbf{w} = -\eta \nabla J(\mathbf{w})$$
 (1)

$$\frac{\partial J(\boldsymbol{w})}{\partial w_j} = -\sum_i (y_i - \phi(\boldsymbol{X}_{i*}w))X_{ij} = -\boldsymbol{X}_{*j}^T(\boldsymbol{y} - \phi(\boldsymbol{X}w))$$
(2)

or 
$$\nabla J(\mathbf{w}) = -\mathbf{X}^T(\mathbf{y} - \phi(\mathbf{X}\mathbf{w})).$$
 (3)

We get a similar weight updating rule as that of linear regression and Adaline! It gives a basis for Perceptron's updating rule.

### Regularization

We avoid  $\boldsymbol{w}$  being too big.

$$J(\beta) = -\log L(\mathbf{w}) + \frac{\lambda}{2} |\mathbf{w}|^2$$
 (4)

$$J(\beta) = -C \log L(\mathbf{w}) + \frac{1}{2} |\mathbf{w}|^2 \quad (C = \frac{1}{\lambda}, \text{SciKit-Learn})$$
 (5)

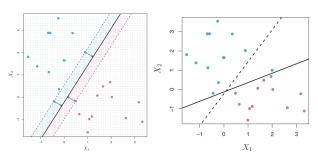
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### Maximal margin classifier

For  $y_i \in \{-1, 1\}$ , maximize the margin of the separating hyperplane M,

$$y_i(w_0 + \sum_{j=1}^p X_{ij}w_j) = y_i(w_0 + \pmb{X}_{i*}\pmb{w}) \geq M > 0$$
 for all  $i$ , with  $|\pmb{w}| = 1$ 

Maximal margin classifier only works for the separable data set and is sensitive to the change in the *support vectors*.



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### Support vector classifier

We make maximal margin classifier flexible: maximize the margin of the separating hyperplane M with  $|\mathbf{w}| = 1$ ,

$$y_i(w_0 + \boldsymbol{X}_{i*}\boldsymbol{w}) \ge M(1 - \epsilon_i) \text{ for all } i, \quad \sum_{i=1}^n \epsilon_i \le C,$$

where  $\epsilon_i > 0$  is slack variable indicating the degree of violation ( $\epsilon_i = 0$ : no violation,  $\varepsilon_i < 1$ : margin violation,  $\varepsilon_i > 1$ : classification violation) and C is a budget for the amount of violations by all observations. Alternatively (in PML), we minimize

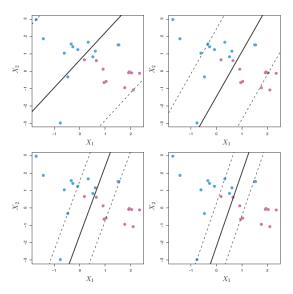
$$\frac{1}{2}|\boldsymbol{w}|^2 + C'\sum_{i=1}^n \xi_i,$$

where  $\{\xi_i \geq 0\}$  satisfies  $y_i(w_0 + \boldsymbol{X}_{i*}\boldsymbol{w}) \geq 1 - \xi_i$  for all i. The model converges to maximal margin classifier if C' is very large, so the role of C' is opposite to that of C in the original formulation.

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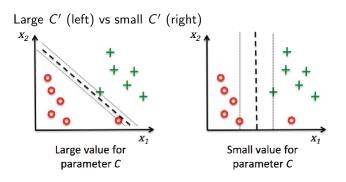
### Support vector classifier: role of *C*



The value of  ${\it C}$  decreasing from the largest value on top left.

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# Support vector classifier: role of C'





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# Support vector machines (SVM)

How can we deal with non-linear decision boundary?

#### Enlarging feature space

Including high-order terms,  $1, X_j, \dots, X_j^2, \dots, X_i X_j, \dots$ , can be helpful, but the computation becomes very heavy.

#### Kernel

Instead we introduce kernel function, as a generalization of dot product in hyperplane:

- Linear:  $K(X_{i*}, X_{i'*}) = X_{i*} X_{i'*}^T$
- Polynomial:  $K(X_{i*}, X_{i'*}) = (1 + X_{i*} X_{i'*}^T)^d$
- Radial basis:  $K(\boldsymbol{X}_{i*}, \boldsymbol{X}_{i'*}) = \exp(-\gamma |\boldsymbol{X}_{i*} \boldsymbol{X}_{i'*}|^2)$

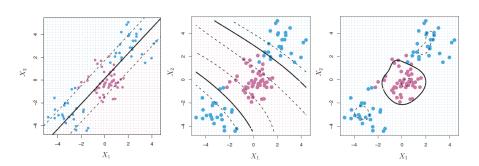
Kernel  $K(\boldsymbol{X}_{i*}, \boldsymbol{X}_{i'*})$  can be understood as a *distance* between two observations:  $\boldsymbol{X}_{i*}$  and  $\boldsymbol{X}_{i'*}$  are similar if the kernel value is high (low) whereas they are different if low (high).

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### SVM: non-linear decision boundary

SVM classification with linear kernel (left) polynomial kernel of degree 3 (middle) and radial basis kernel (right)



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# K Nearest Neighbor (KNN)

If  $N_K(x)$  is the set of the K nearest neighbors around x,

Regression: 
$$\hat{y} = f(x) = \frac{1}{K} \sum_{x_i \in N_K(x)} y_i$$

Classifier:  $\hat{y} = \text{majority of } \{y_i\} \text{ for } x_i \in N_K(x)$ 

$$\mathsf{Prob}(y=j|x) = \frac{1}{K} \sum_{x_i \in N_K(x)} I(y_i = j)$$

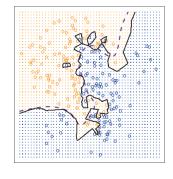
- Parametric vs Non-parametric model
- Learning step is not required, but KNN is intensive in both computation and storage (*memorize* training data set for prediction)

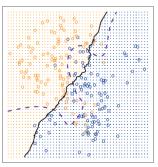
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# KNN: Classfier example

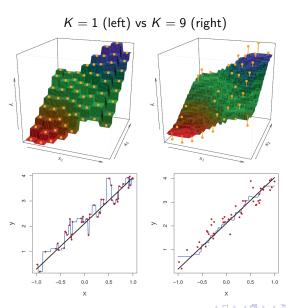
KNN: K=1

KNN: K=100

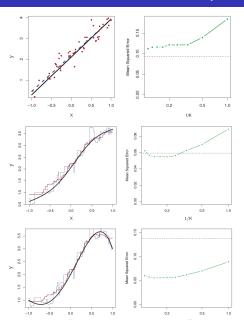




# KNN: Regression example



### KNN: Parametric vs Non-parametric

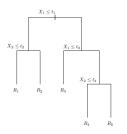


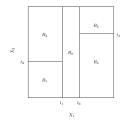
Non-parametric regression works better as the true function deviates from the basis function (linear function in this example).

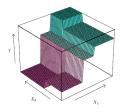
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#### **Decision Tree**

- Regression/classification is made on a series of conditions on input variables
- Final conclusion on each terminal node or leaf of the (upside down) tree.
- The predictor space is broken down to boxes
- Regression: the average value is assigned to each box
- Classification: the majority class is assigned to each box







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### **Growing Tree**

We want to minimize the error in each leaf. For a given leaf of tree, t, Regression Error:

$$RSS(t) = \sum_{i \in t} (y_i - \hat{y}_t)^2$$

Classification Error (measure of impurity):

- Gini index:  $I_G(t) = \sum_{k=1}^K p(k|t) (1 p(k|t)) = 1 \sum_{k=1}^K p^2(k|t)$
- (Cross-)Entropy:  $I_H(t) = -\sum_{i=1}^K p(k|t) \log_2 p(k|t)$
- Classification Error:  $I_E(t) = 1 \max_{1 \le k \le K} p(k|t)$
- $I_G(t) = I_H(t) = I_E(t) = 0$  if the composition is pure, i.e., p(k|t) = 1 for some k. Otherwise > 0.
- $\bullet$   $I_E$  is less sensitive for branching options, so not recommended for growing tree.

Ideally, we can grow tree such that each leaf contains one sample point, but it is over-fitting. Thus we need to regularize the number of leaves or the maximum level of branching.

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### **Growing Tree**

We decide the binary split condition (and feature) in such a way that maximize the information gain (or increase purity):

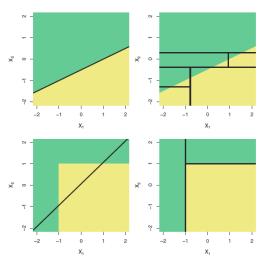
$$\mathsf{IG}(D_P) = I(D_P) - \frac{N_L}{N_p}I(D_L) - \frac{N_R}{N_P}I(D_R)$$

where  $D_P$ ,  $D_L$  and  $D_R$  are the parent, left and right data set and N is the number of the samples in the corresponding sets.

$$I(D) = \sum_{t \in D} I(t)$$
 where  $I = I_E, I_H$  or  $I_G$ 

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#### Tree vs Linear model



Two classification problems (top vs bottom) approached by linear model (left) and decision tree (right) Linear model outperforms decision tree on the top problem, whereas

#### **Decision Tree**

#### Pros

- Intuitive and easy to explain. (Even easier than linear regression)
- Closely mirror human decision making
- Can be displayed graphically and easily interpreted by non-experts

#### Cons

- Prediction is less accurate than other ML methods
- Model variance is high-variant (sensitive to input samples)
  - $\longrightarrow$  Bagging, Random Forests, Boosting

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# Bagging, Random Forest, etc (Ensemble Learning, Ch 7)

Build an ensemble of different classifiers/regressors: the result is interpreted as majority vote/average.

$$\hat{f}_{E}(X) = \mathsf{Avg}_{e \in E}\{\hat{f}_{e}(X)\} \quad \text{or} \quad \hat{f}_{E}(X) = \mathsf{Majority}_{e \in E}\{\hat{f}_{e}(X)\}$$

### Bagging

- Build different trees out of subsets (bags) of training set.
- Increase prediction accuracy and reduce model variance

### Random Forest (RF)

- Build different trees out of subsets of training set.
- At each split, randomly select  $m \ (\approx \sqrt{p})$  out of p features.
- By random selection of features, RF reduces the correlation between the trained trees.

Both bagging and RF can be applied to any ML methods.

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# Data Pre-processing (Ch 4)

## Handling missing data

- Remove the sample
- Fill in NaN with the mean of the average of the feature

#### Normalization

$$X'_{ij} = \frac{X_{ij} - \min(\boldsymbol{X}_{*j})}{\max(\boldsymbol{X}_{*j}) - \min(\boldsymbol{X}_{*j})}$$

### Standardization

$$X'_{ij} = \frac{X_{ij} - E(\boldsymbol{X}_{*j})}{\sigma(\boldsymbol{X}_{*j})}$$

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## Regularization L-1 vs L-2

Give a penalty for complexity or over-fitting. The cost function to minimize:

$$J(\mathbf{w}) = J_0(\mathbf{w}) + \lambda R(\mathbf{w}) \quad (= C J_0(\mathbf{w}) + R(\mathbf{w})),$$

where  $J_0(\mathbf{w})$  is the un-regularized cost function, e.g., log-maximum likelihood (logistic) or RSS/SEE (linear).

## L-2 Regularization

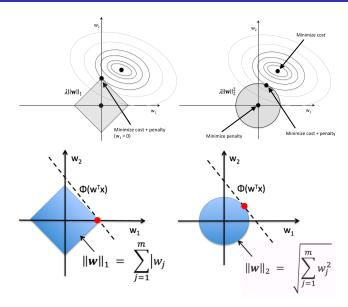
- $R(\mathbf{w}) = ||\mathbf{w}||_2^2 = \sum_i w_i^2$
- *N*-sphere boundary (e.g., circle or sphere). Easy to solve the minimum.

### L-1 Regularization

- $R(\mathbf{w}) = ||\mathbf{w}||_1 = \sum_j |w_j|$
- 'Diamond' boundary: leads to sparse vector (many zero components)
- Effectively works as feature selection



# Regularization L-1 vs L-2

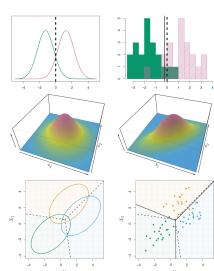


## Feature selection

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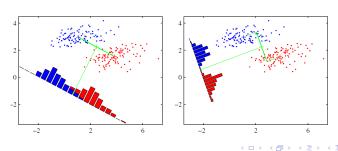
# Linear Discriminant Analysis (LDA) as a classifier

- Assume the samples in each class follow normal (Gaussian) distribution.
- Estimate mean  $\hat{\mu}_k$  and variance  $\hat{\Sigma}_k$  of class k:
- Obtain multi-variate normal PDF:  $f_k(\mathbf{x}) = n(\mathbf{x}|\hat{\boldsymbol{\mu}}_k, \hat{\boldsymbol{\Sigma}}_k) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\mathbf{x}^2}{2\sigma^2}}$
- LDA if  $\Sigma_W = \sum_{k=1}^K \Sigma_k$  (within covariance) is used for all  $\Sigma_k$ .
- QDA if  $\Sigma_k$  is estimated for each class k
- A test sample x is classified to the class k for which  $f_k(x)$  is largest.



## LDA as a dimensionality reduction

- ullet Given the LDA assumptions, which direction  $oldsymbol{w}$  best separates the feature?
- ullet  $oldsymbol{w}pprox oldsymbol{\mu}_2-oldsymbol{\mu}_1$  ? Probably not the best
- Want to minimize  $J(\boldsymbol{w})=\frac{(\mu_2-\mu_1)^2}{\sigma_1^2+\sigma_2^2}$ , where  $(\mu_1,\,\sigma_1^2)$  and  $(\mu_2,\,\sigma_2^2)$  are mean variance of the samples (1-D) projected on  $\boldsymbol{w}$ .
- The best directions  $\mathbf{w}$  are the first eigenvectors of  $\Sigma_W^{-1}\Sigma_B$ , where  $\Sigma_W$  and  $\Sigma_B$  are within and between covariance matrices.
- The transformation z = xW is the extracted factors with the best separability, which can be used for other ML methods.



## Bias-Variance Trade-Off

Given a ML method, we want to minimize the mean squared error (MSE) on **test** data set (test error rate).

$$E(y - \hat{f}(x))^2 = \operatorname{Bias}(\hat{f}(x))^2 + \operatorname{Var}(\hat{f}(x)) + \operatorname{Var}(\varepsilon)$$

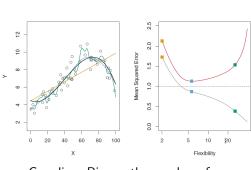
### Bias

- Error from  $\hat{f}$  not correctly representing the true f.
- A model has **high bias** when  $\hat{f}$  overly simply f (e.g. linear regression on non-linear data), the parameters are too few.

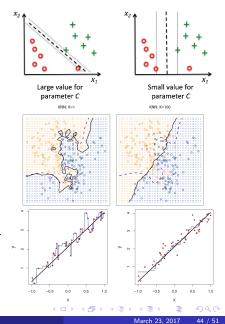
#### Variance

- Error from variability or sensitivity (vs consistency) of the trained model  $\hat{f}$  against the selection of training dataset.
- A model has **high variance** when there are too many parameters (over-fitting), e.g. KNN with K=1, high-order polynomial regression, SVM with large C, logistic regression with large C (or small  $\lambda$ ), decision tree with many leaves, etc.

## Bias-Variance Trade-Off

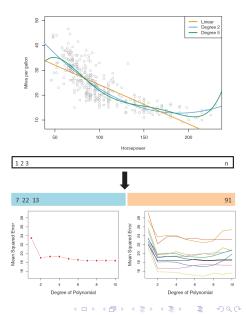


- Grey line: Bias vs the number of parameters
- Red line: MSE measured with the true f (black line).



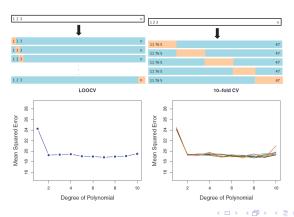
# Cross-Validation(CV): Validation Set (Hold-out set)

- Divide observations into a training set and a validation (hold-out) set.
- Fit model on the training set and measure error on the validation set.
- Error rate is highly variable (sensitive to division)
- Error rate tends to over-estimate the true test error rate as the model is trained on fewer observations.



# Cross-Validation: Leave-One-Out (LOOCV) and k-Fold CV

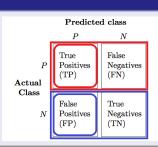
- LOOCV: train model with one sample left out and measure the error on the sample. Error is close to the true test rate but computation is heavy (train n times).
- k-fold CV: divide the samples into k (typically 5 or 10) folds. Train model on k-1 **training** folds and measure error on the remaining **test** fold.



### **Evaluation Metrics**

#### Confusion Matrix

- Error rate:  $ERR = \frac{FP + FN}{FP + FN + TP + TN}$
- True Positive rate:  $TPR = \frac{TP}{TP+FN}$
- False Positive rate:  $FPR = \frac{FP}{FP+TN}$
- Precision(PRE), Recall(REC), F1-Score(F1), · · · .



### Credit card default example

• ERR = 
$$\frac{23+252}{10,000}$$
 = 2.75%

• FPR = 
$$\frac{23}{9.667}$$
 = 0.2%

• 
$$1 - \text{TPR} = \frac{252}{333} = 75.7\%$$

		True default status		
		No	Yes	Total
Predicted	No	9,644	252	9,896
$default\ status$	Yes	23	81	104
	Total	9,667	333	10,000

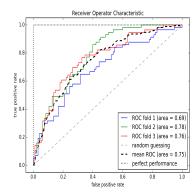
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# Receiver Operator Characteristic (ROC) Curve

 Graph of (FPR, TPR) for varying classification threshold of the binary classification.



- Area Under Curve (AUC) give an overall accuracy of a classifier, summarizing over all possible threshold
- The diagonal line is from random-guessing: ROC AUC = 0.5. A model with lower AUC than 0.5 is worthless.
- A perfect classifier ( $\Gamma$ -shaped lines): ROC AUC = 1.0.



# Unsupervised Learning

No response variable (y) associated to feature variable (X), thus no prediction.

### Goals

- Find interesting things about the observations *X*.
- How to visualize the data?
- How to subgroup (cluster) the observations?

### Challenges

ullet No clear answer  $\longrightarrow$  no clear way to measure performance

Jaehyuk Choi TQF: ML March 23, 2017

## K-mean Clustering

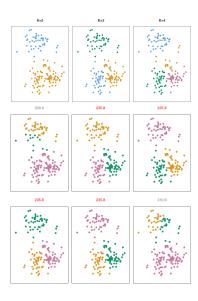
- Assign each observation X<sub>i\*</sub> in to (predetermined) K clusters
- Find  $\mu_k$  and the clusters  $C_k$  which minimize the L2 norm to  $\mu_k$ ,

$$\mathsf{SSE} = \sum_k \sum_{i \in \mathcal{C}_k} |\boldsymbol{X}_{i*} - \boldsymbol{\mu}_k|^2,$$

where  $\mu_k$  is the center of the k-th cluster  $C_k$ .

#### Drawback:

- The number of clusters K has to be manually selected.
- Difficult to solve. The results are sensitive to initial guess.



# K-mean Clustering Iteration

- Given  $\mu_k$ , we assign  $X_{i*}$  to the nearest center.
- Given the cluster C<sub>k</sub>, the center should be the mean,

$$\mu_k = \frac{1}{|C_k|} \sum_{i \in C_k} \boldsymbol{X}_{i*}.$$

## Iteration Step

- Randomly pick K centers (or randomly assign samples to  $C_k$ ).
- Repeat (1) and (2) until  $\{C_k\}$  no-longer changes or the maximum iteration is reached.

