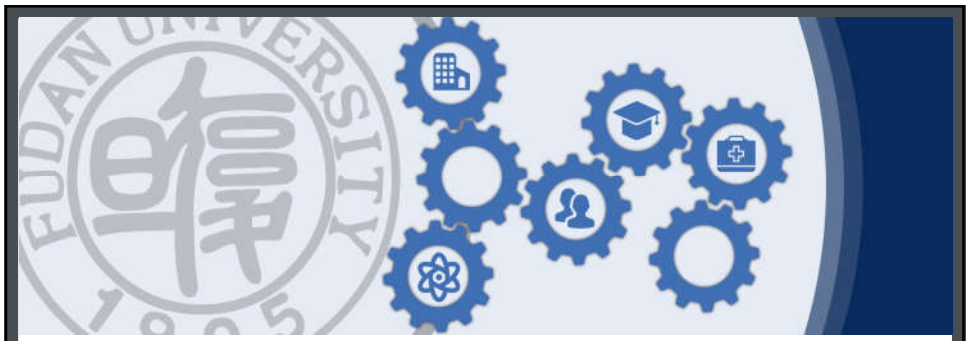

智能系统原理与开发
第06章 统计机器学习

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Deduction & Induction

- 演绎（Deduction）是从知识推导出事实的过程
  ——人定规则（知识），输入事实（数据），得出结论
- 归纳（Induction）是从事实推导出知识的过程
  ——给定事实（数据）与结论，学习规则（知识）

All men are mortal
Socrates is man

Socrates is mortal

Deduction
Always right

My disk has never crashed

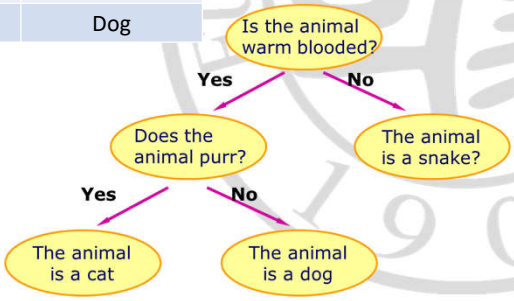
My disk will never crash

Induction
degree of confidence

Decision Tree Revisited

- Can the decision rule be learned automatically?

Feature x_1 (warm blood)	Feature x_2 (can purr)	Label y
No	No	Snake
Yes	Yes	Cat
Yes	No	Dog

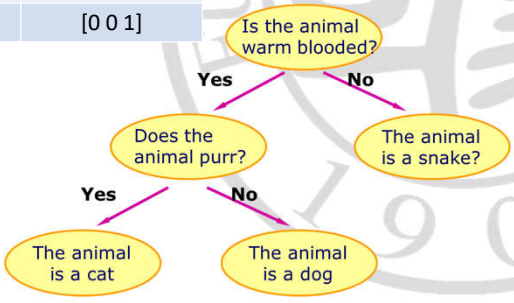


Decision Tree Revisited

- Can we learn a function $f(x) = y$ as a decision rule?

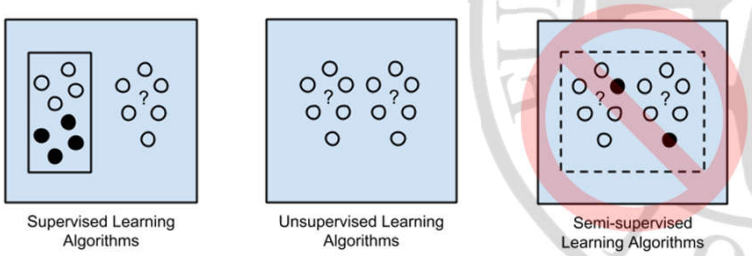
Feature x_1 (warm blood)	Feature x_2 (can purr)	Label y
0	0	[1 0 0]
1	1	[0 1 0]
1	0	[0 0 1]

Snake: $f([0\ 0]) = [1\ 0\ 0]$
Cat: $f([1\ 1]) = [0\ 1\ 0]$
Dog: $f([1\ 0]) = [0\ 0\ 1]$



ML Problems in Intelligent Systems

- There are two commonly seen ML problem settings
  - Supervised learning: Classification, Regression
  - Unsupervised learning: Clustering, Dimensionality Reduction



[1] https://machinelearningmastery.com/a-tour-of-machine-learning-algorithms/

Classification Problem

- Inputs:
  - Instances: $x_1, x_2, \ldots \in X$, where X is feature space
  - Class labels: $y_1, y_2, \ldots \in Y$, where $Y = \{1,2,\ldots,L\}$ is label set
- Classification problem setting:
  - Training data: $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$
  - Test data: $\{(x', ?), (x'', ?), \ldots,\}$
- Objective: Learn a function $f: X \to Y$ on the training data such that $f(x_N) = y_n$ for $n = 1,2,\ldots,N$

$$\min_f \frac{1}{N} \sum_{n=1}^{N} classification\_loss(f(x_n), y_n)$$

Classification Problem

- Supervised learning example: Image classification
  - Instances: $x_1, x_2, \ldots$ are images
  - Class labels: $y_1, y_2, \ldots \in \{dog, cat, snake\}$

$f(\text{🐶}) = \text{"}dog\text{"}$

$f(\text{🐱}) = \text{"}cat\text{"}$

$f(\text{🐍}) = \text{"}snake\text{"}$

Classification Problem

- Application provides the dataset $\{(x_1, y_1), \ldots, (x_N, y_N)\}$
  - Image annotation: x_n pixel image
  - Document categorization: x_n bag-of-words representation
  - User classification: x_n user profile
- $f: X \to Y$ is a selected model for certain applications
  - Nearest Neighbors Classifier
  - Linear Classifier
  - Logistic Regression
  - Support Vector Machine
  - Multilayer Perceptron
  - Decision Tree

Regression Problem

- Inputs:
  - Instances: $x_1, x_2, \ldots \in X$, where X is feature space
  - Targets: $y_1, y_2, \ldots \in Y$, where $Y \subset \mathrm{R}^m$ is target domain
- Regression problem setting:
  - Training data: $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$
  - Test data: $\{(x', ?), (x'', ?), \ldots,\}$
- Objective: Learn a function $f: X \to Y$ on the training data such that $f(x_N) = y_n$ for $n = 1,2, \ldots, N$

$$\min_f \frac{1}{N} \sum_{n=1}^{N} regression\_loss(f(x_n), y_n)$$

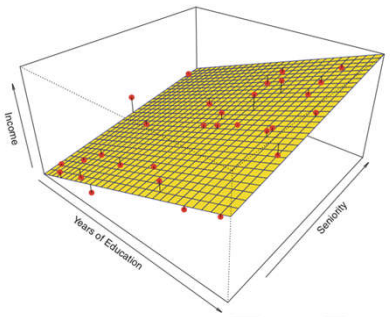
Regression Problem

- Supervised learning example: Income Prediction
  - Instances: $x_1, x_2, \ldots \in Education \times Seniority$
  - Targets: $y_1, y_2, \ldots \in Income$

$$f(12, 3) = 50K$$

$$f(16, 5) = 80K$$

$$f(19, 8) = 200K$$

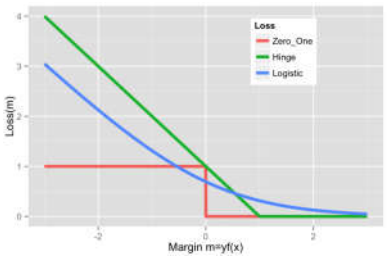


Regression Problem

- Application provides the dataset $\{(x_1, y_1), \dots, (x_N, y_N)\}$
  - Stock trend prediction: x_n variates, y_n index
  - Location prediction: x_n previous locations, y_n new location
  - Rating prediction: x_n user profile, y_n rating
- $f: X \to Y$ is a selected model for certain applications
  - Nearest Neighbors Regression
  - Linear Regression
  - Support Vector Regression
  - Gaussian Process Regression
  - Multi-Layer Perceptron
  - Decision Tree

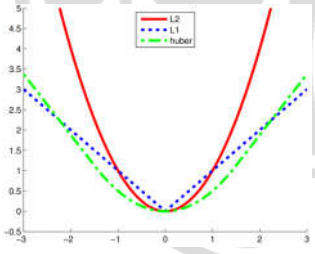
Classification vs Regression

- It seems that classification and regression are similar
- What makes them different? – Loss ※



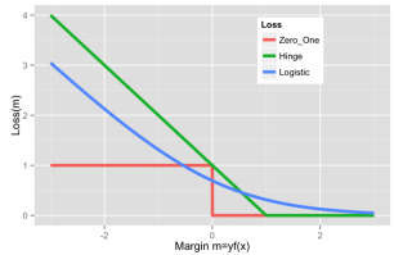
$$\min_f \frac{1}{N} \sum_{n=1}^{N} classification\_loss(f(x_n), y_n)$$

$$\min_f \frac{1}{N} \sum_{n=1}^{N} regression\_loss(f(x_n), y_n)$$



Classification Loss

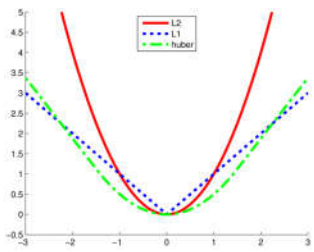
- Zero-One Loss: $l_{0-1}(f(x_n), y_n) = 1(y_n f(x_n) \leq 0)$
- Hinge Loss: $l_{hinge}(f(x_n), y_n) = \max(1 - y_n f(x_n), 0)$
- Logistic Loss: $l_{logistic}(f(x_n), y_n) = \ln(1 + exp(-y_n f(x_n)))$



$$\min_f \frac{1}{N} \sum_{n=1}^{N} classification\_loss(f(x_n), y_n)$$

Regression Loss

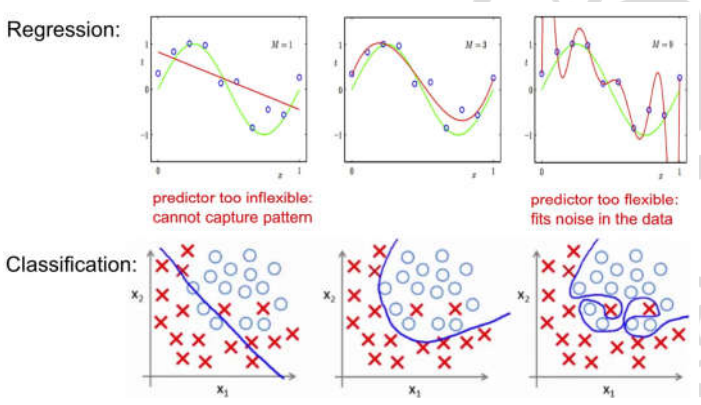
- Quadratic Loss ($L2$-Loss): $l_{L2}(f(x_n), y_n) = \left(y_n - f(x_n)\right)^2$
- Absolute Loss ($L1$-Loss): $l_{L1}(f(x_n), y_n) = |y_n - f(x_n)|$
- Huber Loss: $l_{Huber}(f(x_n), y_n) = \begin{cases} \left(y_n - f(x_n)\right)^2, & |y_n - f(x_n)| \leq \delta \\ |y_n - f(x_n)|, & |y_n - f(x_n)| > \delta \end{cases}$



$$\min_f \frac{1}{N} \sum_{n=1}^{N} regression\_loss(f(x_n), y_n)$$

Generalization

- Generalization error is a measure of how accurately a model is able to predict outcome values for previously unseen data ※



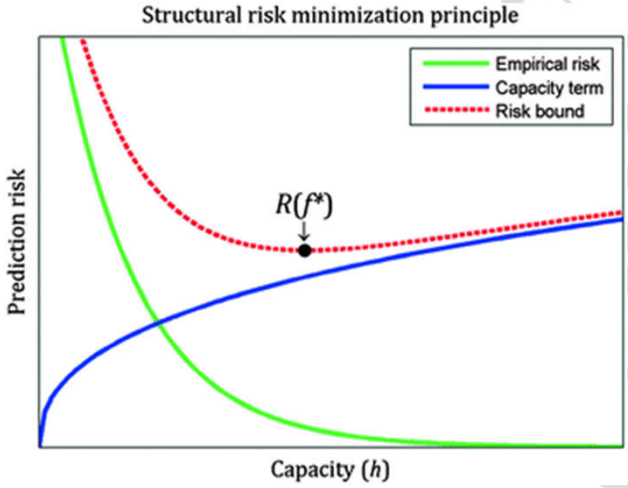
Regularization

- In ML, regularization is a process of introducing additional information in order to prevent overfitting
- Regularized Empirical Risk Minimization:

$$\min_f \frac{1}{N}\sum_{n=1}^{N} loss(f(x_n), y_n) + \lambda R(f)$$

- Some explanations for regularization
  - Solve ill-posed (underdetermined) problem
  - Impose Occam's razor on the solution
  - Impose certain prior distributions on model parameters

Structural Risk Minimization



Objective Function

- General form of objective function for supervised learning

$$\min_{f} \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{loss}(\boldsymbol{f}(\boldsymbol{x_n}), \boldsymbol{y_n}) + \boldsymbol{\lambda R(f)}$$

- Different combinations of $f(\cdot)$, $loss(\cdot)$, and $R(\cdot)$ will result different machine learning models

- Ordinary Linear Model: Ridge Regression
  - Linear model: $f(x_n) = w^\top x_n$
  - Quadratic loss: $loss(f(x_n), y_n) = (y_n - w^\top x_n)^2$
  - $L2$-norm regularization: $R(f) = ||w||^2$

$$\min_{w} \frac{1}{N}\sum_{n=1}^{N} (y_n - w^\top x_n)^2 + \lambda ||w||^2$$

Ridge Regression

- Ridge Regression
  - Linear model: $f(x_n) = w^\top x_n$
  - Quadratic loss: $loss(f(x_n), y_n) = (y_n - w^\top x_n)^2$
  - $L2$-norm regularization: $R(f) = ||w||^2$

$$\min_w \frac{1}{N}\sum_{n=1}^{N}(y_n - w^\top x_n)^2 + \lambda||w||^2$$

← Convex Optimization (quadratic programming)

$$\Rightarrow \min_w (Y - Xw)^\top (Y - Xw) + \lambda w^\top w$$

  - Let $J(w) = (Y - Xw)^\top (Y - Xw) + \lambda w^\top w$ ※

$$\frac{\partial J(w)}{\partial w} = -2X^\top (Y - Xw) + 2\lambda w = 0$$

$$w = (X^\top X + I\lambda)^{-1} X^\top Y$$

Logistic Regression

- Logistic Regression
  - Linear model: $f(x_n) = w^\top x_n$
  - Logistic loss: $loss(f(x_n), y_n) = -y_n \ln(\sigma_n) - (1 - y_n)\ln(1 - \sigma_n)$, where $\sigma_n = \frac{1}{1+\exp(-w^\top x_n)}$ and $y_n \in \{0,1\}$
  - $L2$-norm regularization: $R(f) = ||w||^2$

$$\min_w \frac{1}{N}\sum_{n=1}^{N} \mathbf{-y_n \ln(\sigma_n) - (1 - y_n)\ln(1 - \sigma_n) + \lambda||w||^2}$$

  - Let $J(w) = -\frac{1}{N}\sum_{n=1}^{N}(y_n \ln(\sigma_n) - (1 - y_n)\ln(1 - \sigma_n)) + \lambda||w||^2$

$$\frac{\partial J(w)}{\partial w} = \frac{1}{N}\sum_{n=1}^{N} -y_n(1 - \sigma_n)x_n + (1 - y_n)\sigma_n x_n + 2\lambda w$$

$$= \frac{1}{N}\sum_{n=1}^{N} x_n(\sigma_n - y_n) + 2\lambda w$$

Maximum Likelihood Estimation

- In statistics, Maximum Likelihood Estimation (MLE) is a method of estimating the parameters of a statistical model, given observations $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- MLE attempts to find the parameter values that maximize the likelihood function ※

$$\max_{\theta \in \Theta} p(D|\theta) \Rightarrow \max_{\theta \in \Theta} \prod_{n=1}^{N} p(x_n, y_n|\theta) \Rightarrow \min_{\theta \in \Theta} \frac{1}{N} \sum_{n=1}^{N} -\log p(x_n, y_n|\theta)$$

  - $p(x_n, y_n|\theta)$ is Gaussian distribution ➔ Quadratic loss
  - $p(x_n, y_n|\theta)$ is Laplacian distribution ➔ Absolute loss
  - $p(x_n, y_n|\theta)$ is Logistic function ➔ Logistic loss

Maximum *a posteriori*

- In Bayesian statistics, Maximum *a posteriori* (MAP) is an estimate of an unknown quantity, that equals the mode of the posterior distribution.
- MAP estimation can be seen as a regularization of MLE.

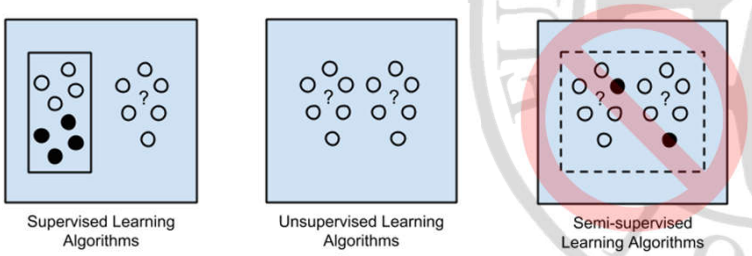
$$\arg\max_{\theta \in \Theta} p(\theta|D) = \arg\max_{\theta \in \Theta} \frac{p(D|\theta)p(\theta)}{\int_{\theta'} p(D|\theta')p(\theta')d\theta'} = \arg\max_{\theta \in \Theta} p(D|\theta)p(\theta)$$

$$\max_{\theta \in \Theta} p(D|\theta)p(\theta) \Rightarrow \max_{\theta \in \Theta} \prod_{n=1}^{N} p(x_n, y_n|\theta)p(\theta)$$
$$\Rightarrow \min_{\theta \in \Theta} \frac{1}{N} \sum_{n=1}^{N} -\log p(x_n, y_n|\theta) - \log p(\theta)$$

- Compare to $\min_f \frac{1}{N} \sum_{n=1}^{N} loss(f(x_n), y_n) + \lambda R(f)$ ※

ML Problems in Intelligent Systems

- There are two commonly seen ML problem settings
  - Supervised learning: Classification, Regression
  - Unsupervised learning: Clustering, Dimensionality Reduction



[1] https://machinelearningmastery.com/a-tour-of-machine-learning-algorithms/

Clustering Problem

- Instances: $x_1, x_2, \ldots \in X$, where X is feature space
- Objective: Input instances $x_1, x_2, \ldots \in X$ and output corresponding cluster indicators $z_1, z_2, \ldots \in \{0,1\}^K$ for each instance, satisfying certain optimization criteria

$$\min_{\{z\},\{\theta\}} \frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} z_{n,k} \mathit{clustering\_loss}(x_n, \theta_k)$$

  - θ_k denotes the parameter set of the k-th cluster
  - $z_{n,k} \in \{0,1\}$ denotes whether the n-th instance belongs to the k-th cluster
  - Goal: Find values of θ_k and $z_{n,k}$ to minimize the objective

K-Means Clustering

- Minimize $J = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{n,k}\,||x_n - \mu_k||^2$ in terms of the mean of the cluster μ_k and the cluster indicator $z_{n,k}$
- Given $\{\mu_1, \dots, \mu_K\}$ fixed, since J is a linear function of $z_{n,k}$, this optimization can be easily obtained by

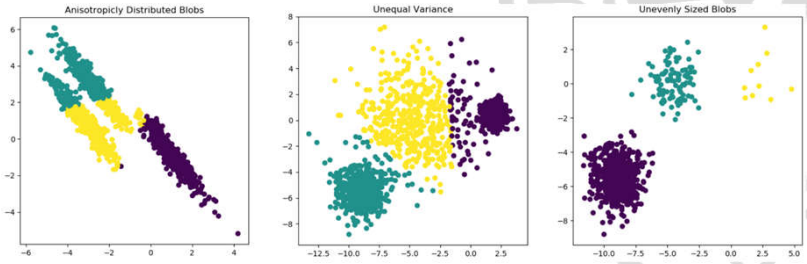
$$z_{n,k} = \begin{cases} 1, & \text{if } k = \arg\min_j ||x_n - \mu_j||^2 \\ 0, & \text{otherwise} \end{cases}$$

- Given $\{z_{1,1}, \dots, z_{N,K}\}$ fixed, J is a quadratic function of μ_k, it can be minimized by setting its derivative w.r.t. μ_k to zero

$$2\sum_{n=1}^{N} z_{n,k}\,(x_n - \mu_k) = 0 \Rightarrow \mu_k = \frac{\sum_{n=1}^{N} z_{n,k}\,x_n}{\sum_{n=1}^{N} z_{n,k}}$$

Assumptions of K-Means

- Assumptions (sometimes limitations) in K-Means
  - Isotropically distributed
  - Distributed with equal variances
  - Clusters are evenly sized



Gaussian Mixture Model (GMM)

- K-Means is hard-membership clustering technique
  - $z_{n,k} \in \{0,1\}$: Each instance can or cannot belong to a cluster
  - $\sum_{k=1}^{K} z_{n,k} = 1$: Each instance can belong to only one cluster
- Is there a soft-membership clustering technique?
  - $z_{n,k} \in \{0,1\}$ ➔ $\gamma(z_{n,k}) \in [0,1]$
  - $\sum_{k=1}^{K} \gamma(z_{n,k}) = 1$ still holds
- Gaussian Mixture Model

$$p(x_n) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mu_k, \Sigma_k)$$

  - Anisotropically distributed
  - Distributed with different variances
  - Clusters are variously sized

Maximum Likelihood of GMM

- Given $\{x_1, \dots, x_N\}$ and we wish to model these instances using a GMM. The log likelihood function is

$$\ln p(X|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k) \right\}$$

- Set the derivatives of $\ln p(X|\pi, \mu, \Sigma)$ w.r.t. the means μ_k of the Gaussian components to zero

$$-\sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}(x_n|\mu_{k'}, \Sigma_{k'})} \Sigma_k (x_n - \mu_k) = 0$$

$$\gamma(z_{n,k}) = p(z_{n,k} = 1|x_n) = \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}(x_n|\mu_{k'}, \Sigma_{k'})}$$

$$-\sum_{n=1}^{N} \gamma(z_{n,k}) \Sigma_k (x_n - \mu_k) = 0 \Rightarrow \mu_k = \frac{\sum_{n=1}^{N} \gamma(z_{n,k})\, x_n}{\sum_{n=1}^{N} \gamma(z_{n,k})}$$

Maximum Likelihood of GMM

- Set the derivatives of $\ln p(X|\pi,\mu,\Sigma)$ w.r.t. the covariance matrix Σ_k of the Gaussian components to zero

$$\Sigma_k = \frac{\sum_{n=1}^{N}\gamma(z_{n,k})(x_n-\mu_k)(x_n-\mu_k)^{\mathsf{T}}}{\sum_{n=1}^{N}\gamma(z_{n,k})}$$

- Set the derivatives of $\ln p(X|\pi,\mu,\Sigma)$ w.r.t. the mixing coefficients π_k subject to $\sum_{k=1}^{K}\pi_k = 1$

$$\pi_k = \frac{\sum_{n=1}^{N}\gamma(z_{n,k})}{N}$$

- In the MLE of (π_k,μ_k,Σ_k) we assume $\gamma(z_{n,k})$ is given, which however is also conditioned on (π_k,μ_k,Σ_k)

Expectation-Maximization (EM) Algorithm for GMM

- Initialize (π_k,μ_k,Σ_k) and evaluate $\ln p(X|\pi,\mu,\Sigma)$
- **E-Step**: Evaluate $\gamma(z_{n,k})$ using the current (π_k,μ_k,Σ_k)

$$\gamma(z_{n,k}) = \frac{\pi_k\mathcal{N}(x_n|\mu_k,\Sigma_k)}{\sum_{k'=1}^{K}\pi_{k'}\mathcal{N}(x_n|\mu_{k'},\Sigma_{k'})}$$

- **M-Step**. Estimate (π_k,μ_k,Σ_k) using the current $\gamma(z_{n,k})$

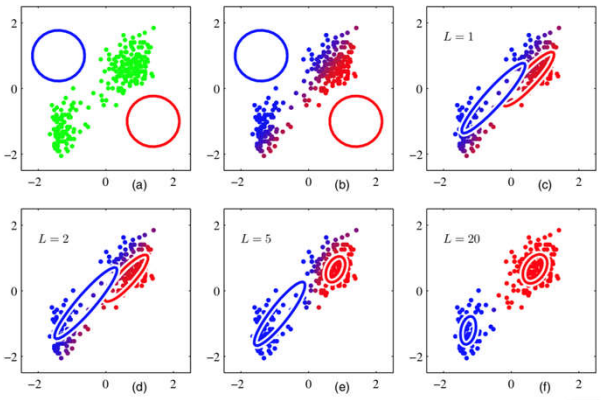
$$\pi_k = \frac{\sum_{n=1}^{N}\gamma(z_{n,k})}{N} \qquad \mu_k = \frac{\sum_{n=1}^{N}\gamma(z_{n,k})\,x_n}{\sum_{n=1}^{N}\gamma(z_{n,k})}$$

$$\Sigma_k = \frac{\sum_{n=1}^{N}\gamma(z_{n,k})(x_n-\mu_k)(x_n-\mu_k)^{\mathsf{T}}}{\sum_{n=1}^{N}\gamma(z_{n,k})}$$

- Evaluate $\ln p(X|\pi,\mu,\Sigma)$ and check the convergence

EM Algorithm for GMM

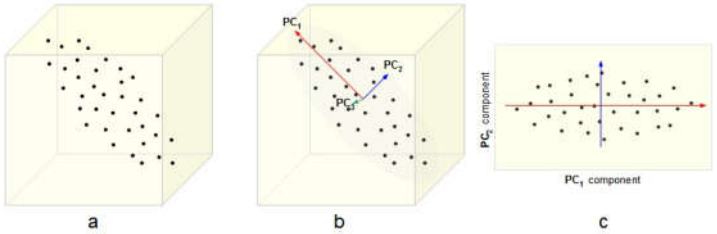
- Illustration of EM iterations for fitting a GMM



[1] Bishop, Pattern Recognition and Machine Learning, page 437.

Principal Component Analysis

- Given $\{x_1, \ldots, x_N\} \in R^D$, PCA is to project the data on to a space that maximizes the variance of the projected data
  - Noise filtering
  - Dimensionality reduction
  - Data visualization
  - Data compression
  - etc.



Principal Component Analysis

- Suppose the first principal component is u_1, then each data point is projected onto a one-dimensional space $u_1^\top x_n$
- The variance of the projected data is given by

$$\frac{1}{N}\sum_{n=1}^{N}\left(u_1^\top x_n - u_1^\top \bar{x}\right)^2 = u_1^\top \left(\frac{1}{N}\sum_{n=1}^{N}(x_n-\bar{x})(x_n-\bar{x})^\top\right)u_1 = u_1^\top \Sigma u_1$$

- Maximize $u_1^\top \Sigma u_1$ w.r.t. u_1 subject to $u_1^\top u_1 = 1$

$$\max_{u_1} u_1^\top \Sigma u_1 + \lambda_1(1 - u_1^\top u_1) \Rightarrow \Sigma u_1 = \lambda_1 u_1$$

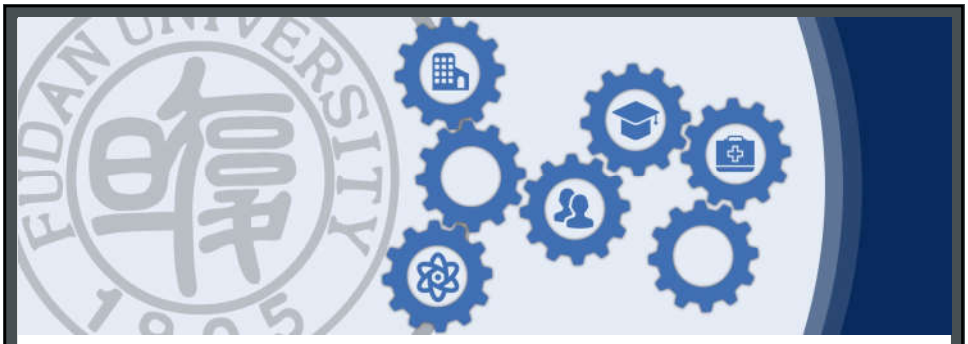
- $\Sigma u_1 = \lambda_1 u_1$ indicates u_1 is an eigenvector of Σ and this can be solved using eigendecomposition.

Dimensionality Reduction

- In statistics and machine learning, dimensionality reduction is to reduce the number of random variables by obtaining a set of principal variables.
  - Principal Component Analysis (PCA)
  - Canonical Correlation Analysis (CCA)
  - Nonnegative Matrix Factorization (NMF)
  - Autoencoder
  - Learning to Hash
  - Random Projection
  - Locality-Sensitive Hashing (LSH)
  - etc.

Model Selection

- A common problem in machine learning is to select a hyper-parameter which usually determines the structure (or complexity) of the model
  - Number of components in a GMM
  - Number of latent dimensions in matrix factorization
  - Hyper-parameters in neural networks
  - Hyper-parameters in kernel methods
  - Hyper-parameters in Bayesian methods
  - etc.
- Criteria for model selection
  - Cross-validation – most frequently used
  - Information theory based criteria (AIC, BIC, MDL, etc.)
  - Bayesian nonparametric methods



Thanks

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