This cheatsheet is the summary of content taken from UCSD course:

CSE 258: Web Mining and Recommender System

General Modeling Knowledge

Learning Methods

Supervised Learning aims to directly model the relationship between input and output variables, so that the output variables can be predicted accurately given the input

Unsupervised Learning approaches find patterns, relationships and structure in data, but **are not** optimized to solve a particular predictive task. Most of the Unsupervised Machine Learning Methods are data reconstruction or data encoding algorithms.

Data Encodings

There are three types of features: **real-value feature**, **categorical feature** and **random feature**

Categorical feature is especially tricky to deal with because its possible values are discrete rather than continuous. We cannot simply fit a line across categorical data, in which case sequence doesn't matter.

- Ordinal Data (Temporal Data): Encode it as (1, 2, 3, .. n)
- Unordinal Data: Use **One-Hot Encoding** [0, 1, 0, . . . , 0]

Mathematic Formula for One-Hot Encoding in Regression

$$c = \theta_0 + \theta_1[\text{is male}] + \theta_2[\text{is female}]$$

Model Selection

(Train | Validation | Test) split is important for determining various aspect of a predictive function.

- Training set: used to **optimize the model's parameters** : choose θ
- Test set: used to report how well we expect the model to perform on unseen data: only used **once**

- Validation set: used to **tune** any model parameters that are not directly optimized: choose λ

Theorems

- The training error **increases** as λ increases
- The validation and test error are at least as large as the training error (assuming infinitely large random partitions)
- The validation/test error will usually have a "sweet" spot between under- and over-fitting

Imbalanced Dataset

When implimenting classifiers, sometimes there are far **fewer** positive examples than negative examples we may want to assign additional weight to negative instances.

Definition:

- True Positive (TP): label is true, prediction is true (correct predictions)
- True Negative (TN): label is false, prediction is false
- False Positive (FP): label is false, prediction is true (incorrect predictions)
- False Negative (FN): label is true, prediction is false

Balanced Error Rate:

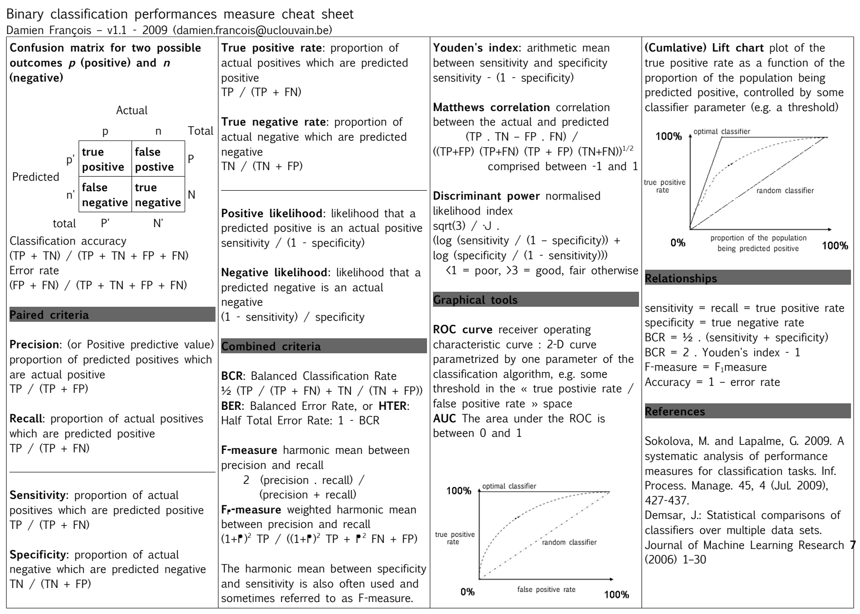
$$\begin{aligned}
\text{BER} &= \frac{1}{2}(\text{FPR} + \text{FNR}) \\
&= \frac{1}{2}(\frac{\text{FP}}{\text{number of Negative labels}} + \frac{\text{FN}}{\text{number of Positive labels}}) \\
&= \frac{1}{2}(\frac{\text{FP}}{\text{TN} + \text{FP}} + \frac{\text{FN}}{\text{FN} + \text{TP}})
\end{aligned}$$

Precision Recall:

$$\text{Precision} = \frac{\text{TP}}{\text{FP} + \text{TP}} = \frac{\text{TP}}{\text{number of label predicted Positive}}$$

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} = \frac{\text{TP}}{\text{number of Positive label}}$$

Reference to Binary Classification Performance Cheat Sheet *Figure 1*



Binary classification performances measure cheat sheet
Damien François – v1.1 - 2009 (damien.francois@uclouvain.be)

Confusion matrix for two possible outcomes *p* (positive) and *n* (negative)

		Actual		
		p	n	Total
Predicted	p'	**true positive**	**false postive**	P
	n'	**false negative**	**true negative**	N
	total	P'	N'	

Classification accuracy
(TP + TN) / (TP + TN + FP + FN)
Error rate
(FP + FN) / (TP + TN + FP + FN)

Paired criteria

Precision: (or Positive predictive value) proportion of predicted positives which are actual positive
TP / (TP + FP)

Recall: proportion of actual positives which are predicted positive
TP / (TP + FN)

Sensitivity: proportion of actual positives which are predicted positive
TP / (TP + FN)

Specificity: proportion of actual negative which are predicted negative
TN / (TN + FP)

True positive rate: proportion of actual positives which are predicted positive
TP / (TP + FN)

True negative rate: proportion of actual negative which are predicted negative
TN / (TN + FP)

Positive likelihood: likelihood that a predicted positive is an actual positive
sensitivity / (1 - specificity)

Negative likelihood: likelihood that a predicted negative is an actual negative
(1 - sensitivity) / specificity

Combined criteria

BCR: Balanced Classification Rate
½ (TP / (TP + FN) + TN / (TN + FP))
BER: Balanced Error Rate, or **HTER**: Half Total Error Rate: 1 - BCR

F-measure harmonic mean between precision and recall
2 (precision . recall) /
(precision + recall)
F_β-measure weighted harmonic mean between precision and recall
$(1+\beta)^2$ TP / ($(1+\beta)^2$ TP + β^2 FN + FP)

The harmonic mean between specificity and sensitivity is also often used and sometimes referred to as F-measure.

Youden's index: arithmetic mean between sensitivity and specificity
sensitivity - (1 - specificity)

Matthews correlation correlation between the actual and predicted
(TP . TN – FP . FN) /
((TP+FP) (TP+FN) (TP + FP) (TN+FN))$^{1/2}$
comprised between -1 and 1

Discriminant power normalised likelihood index
sqrt(3) / ·J .
(log (sensitivity / (1 – specificity)) +
log (specificity / (1 - sensitivity)))
<1 = poor, >3 = good, fair otherwise

Graphical tools

ROC curve receiver operating characteristic curve : 2-D curve parametrized by one parameter of the classification algorithm, e.g. some threshold in the « true postivie rate / false positive rate » space
AUC The area under the ROC is between 0 and 1

(Cumlative) Lift chart plot of the true positive rate as a function of the proportion of the population being predicted positive, controlled by some classifier parameter (e.g. a threshold)

Relationships

sensitivity = recall = true positive rate
specificity = true negative rate
BCR = ½ . (sensitivity + specificity)
BCR = 2 . Youden's index - 1
F-measure = F_1measure
Accuracy = 1 – error rate

References

Sokolova, M. and Lapalme, G. 2009. A systematic analysis of performance measures for classification tasks. Inf. Process. Manage. 45, 4 (Jul. 2009), 427-437.
Demsar, J.: Statistical comparisons of classifiers over multiple data sets. Journal of Machine Learning Research 7 (2006) 1–30

Figure 1: Link to Binary Classification Performances Measure Cheat Sheet

Machine Learning Algorithms

Linear Regression

Formula

$$X\theta = y$$

- X is matrix of features (data)
- θ is unknowns (which features are relevant)
- y is the vector of outputs (labels)

Movitation

If X is a mxn matrix and $m \geq n$ (number of observations $\geq$ number of predictive features), then X is an **inconsistent** matrix. Since X is inconsistent with y not exists in the subspace of X, we need to project y onto the span of θ.

Note in *Figure 2*, $v - (v \cdot n)n$ is the **residual** vector which is **orthogonal** to vector n.

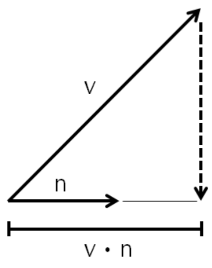


Figure 2: projection of v onto the dimension n

Optimization

Find θ such that $||X\theta - y||_2^2$ is minimized. The reason we use the residual norm of 2 is for convenient differentiation of the function.

$$\begin{aligned}||X\theta - y||_2^2 &= (X\theta - y)^T(X\theta - y)\\ &= \theta^T X^T X\theta - y^T X\theta - \theta^T X^T y + y^T y\end{aligned}$$

Because $y^T X$ is scalar, which implies $y^T X\theta = (y^T X\theta)^T = \theta^T X^T y$

$$||X\theta - y||_2^2 = \theta^T X^T X\theta - 2y^T X\theta + y^T y$$

Differentiate the cost function:

$$\frac{\partial}{\partial_\theta} f = 2X^T X\theta - 2y^T X = 0$$

$$X^T X\theta = y^T X$$
$$\theta = (X^T X)^{-1} y^T X$$

MSE Mean-squared error (Numeric Explanation)

$$\frac{1}{N}||y - X\theta||_2^2 = \frac{1}{N}\sum_{i=1}^{N}(y_i - X_i \cdot \theta)^2$$

Motivation behind MSE is the assumption that label (truth) = prediction+error, where error is distributed with a normal distribution of $N(0, \sigma)$. This results in the prediction function as:

$$P_\theta(y|X, \theta) = \prod_i \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{-(y_i - x_i \cdot \theta)^2}{2\sigma^2}}$$

$$\begin{aligned}\max_\theta P_\theta(y|X,\theta) &= \max_\theta \prod_i e^{-(y_i - x_i\cdot\theta)^2} \\ &= \min_\theta \sum_i (y_i - x_i\cdot\theta)^2\end{aligned}$$

Coefficient of determination (R^2 statistic): Regression Diagnostics

FVU, fraction of variance unexplained. If $\text{FVU}(f) = 1$, f is **trivial** predictor. If $\text{FVU}(f) = 0$, f is **perfect** predictor.

$$\text{FVU}(f) = \frac{\text{MSE}(f)}{\text{Var}(y)}$$

If $R^2 = 0$, f is **trivial** predictor. If $R^2 = 1$, f is **perfect** predictor.

$$R^2 = 1 - \text{FVU}(f) = 1 - \frac{\text{MSE}(f)}{\text{Var}(y)}$$

Regularization

Regularization is the process of penalizing model complexity during training.

Naive Bayes

Naive Bayes is a classification algorithms that assumes that features are **conditionally independent** given the label.

$$(\text{feature}_i, \text{feature}_j|\text{label}) = (\text{feature}_i|\text{label})(\text{feature}_j|\text{label})$$

Using Bayes Theorem:

$$p(\text{label}|\text{features}) = \frac{p(\text{label})\prod_i p(\text{feature}_i|\text{label})}{p(\text{features})}$$

Assume label is binary result, and the probability of **not label** is represented as $p(\text{-label}|\text{features})$

$$\frac{p(\text{label}|\text{features})}{p(\text{-label}|\text{features})} = \frac{p(\text{label})\prod_i p(\text{features}_i|\text{label})}{p(\text{-label})\prod_i p(\text{features}_i|\text{-label})}$$

Advantages

- Easiest to implement, most efficient to "train"
- If we have a process that generates feature that are independent given the label, it's a very sensible idea

Disadvantage of Naive Bayes

Because both features encode essentially the same information when calculating p(label|features) and p(-label|features), we will end up **double-counting** their effect.

Logistic Regression

Logistic regression is essentially a linear regression being mapped into a [0, 1] dimension space using a **Sigmoid** function. The classifier form is:

$$y_i = \begin{cases} 1 & \text{if } X_i \cdot \theta > 0 \\ 0 & \text{otherwise} \end{cases}$$

Motivation

With y_i is either 0 or 1, we need to have a linear regression that separate the $P(Y = 0)$ as far away as possible from $P(Y = 1)$, which is to maximize the total probability of $P(Y = 0|X, \theta)$ in addition to the total probability of $P(Y = 1|X, \theta)$. Note there is **no double counting** as it occurs in Naive Bayes.

$$\text{argmax}_\theta = \prod_{y_i=1} P_\theta(y|X) \prod_{y_i=0} (1 - P_\theta(y|X)) \quad = \prod_{y_i=1} \sigma(X_i\theta) \prod_{y_i=0} (1 - \sigma(X_i\theta))$$

Sigmoid Function

$$\sigma(t) = \frac{1}{1 + e^{-t}}$$

Optimization

- Take logarithm
- Subtract regularizer
- Compute gradient
- Solve using gradient ascent

$$L_\theta(y|X) = \prod_{y_i=1} p_\theta(y_i|X_i) \prod_{y_i=0} (1 - p_\theta(y_i|X_i))$$

Take the logarithm of the original Loss function for computational convenience:

$$\begin{aligned}
l_\theta(y|X) &= \sum_{y_i=1} \log \sigma(X_i\theta) + \sum_{y_i=0} \log(1 - \sigma(X_i\theta)) - \lambda||\theta||_2^2 \\
&= \sum_{y_i=1} \log(\frac{1}{1+e^{-X_i\theta}}) + \sum_{y_i=0} \log(\frac{e^{-X_i\theta}}{1+e^{-X_i\theta}}) - \lambda||\theta||_2^2 \\
&= \sum_{y_i=1} -\log(1+e^{-X_i\theta}) + \sum_{y_i=0} -\log(1+e^{-X_i\theta}) + \sum_{y_i=0} -X_i\theta - \lambda||\theta||_2^2 \\
&= \sum_{y_i} -\log(1+e^{-X_i\theta}) + \sum_{y_i=0} -X_i\theta - \lambda||\theta||_2^2
\end{aligned}$$

Taking the Differentiation of the loss function:

$$\begin{aligned}
\frac{\partial l}{\partial \theta_k} &= \sum_i \frac{x_{ik}e^{-X_i\theta}}{1+e^{-X_i\theta}} + \sum_{y_i=0} -x_{ik} - 2\lambda\theta_k \\
&= \sum_i x_{ik}(1 - \sigma(X_i\theta)) - \sum_{y_i=0} x_{ik} - 2\lambda\theta_k
\end{aligned}$$

Perform Gradient Descent:

$$\theta_k := \theta_k - \alpha \frac{d}{d\theta_k} l(\theta)$$

Generalization

We can generalize logistic regression for **binary** classification into **multiclass** classification by training a binary predictor for each class. In the event that **multiclass** predictions are inconsistent, choose the one with the highest confidence.

Advantages

Fixes the “double counting” problem present in naive Bayes

Disadvantages

- Logistic regressors **don't** optimize the **number of "mistakes"**. It is simply trying to separate the difference between the general label groups $Y = 0$ and $Y = 1$.
- No special attention is paid to the "difficult" instances (which can be inconsistent in classifying edge cases laying on top of the boundary) - every instance influence the model
- "easy" instances that has high confidence can affect the model in a bad way
- The model is more expensive to train compared to naive bayes

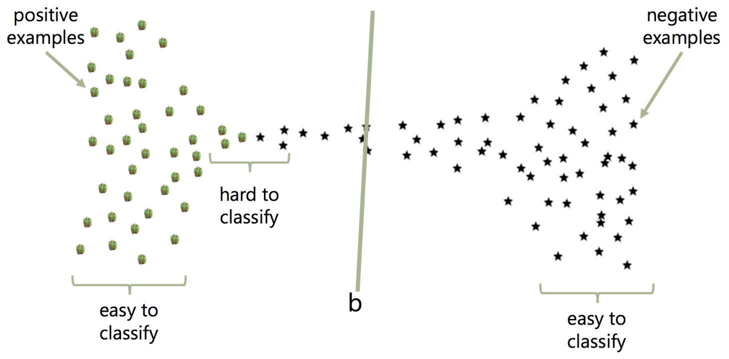


Figure 3: logistic regression for classification

Support Vector Machine

Motivation

The intuition behind Support Vector Machines (SVMs) is to train a classifier that focuses on the **difficult** examples by minimizing the **misclassification error**. Our classifier form is:

$$y_i = \begin{cases} 1 & \text{if } X_i \cdot \theta - \alpha > 0 \\ -1 & \text{otherwise} \end{cases}$$

We want to minimize the number of misclassifications:

$$\text{argmin}_\theta \sum_i \delta(y_i(X_i \cdot \theta - \alpha) \geq 0)$$

Support Vector

Because $\theta x - \alpha = 0$ is a hyperplane and θ is underdeterminated, there are many solutions to θ. In this case, we need regularization to enforce the best solution of θ. Here we will choose the classifier that maximizes the distance to the nearest point.

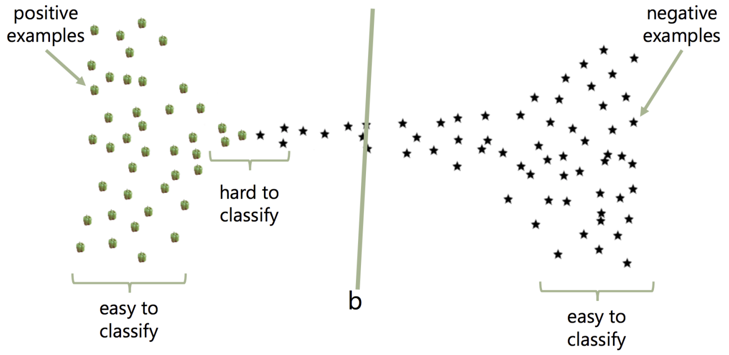


Figure 4: support vector machines use support vector to determin theta

Distance from Point to Line

Suppose we are trying to calculate the distance between a line to a point.

$$\text{line} : ax + by + c = 0$$
$$\text{point} : x_0, y_0$$

Then the distance from the line to the point is:

$$d(\text{line}, \text{point}) = \frac{|ax_0 + by_0 + c|}{\sqrt{a^2 + b^2}}$$

Apply the same principle to the classifier, for all x_i, the distance between x_i to $\theta X - \alpha = 0$ should be greater or equal to the distance from support vector $\theta X - \alpha = 1$ or $\theta X - \alpha = -1$ to $\theta X - \alpha = 0$

$$\frac{(\theta X_i - \alpha)y_i}{||\theta||_2} \geq \frac{1}{||\theta||_2}$$

Optimization

Because the distance between the center regression line and the two support vectors is $\frac{1}{||\theta||}$ and we want to maximize the distance $\frac{2}{||\theta||}$, for mathematic convenience, we can solve the same problem by minimize $\frac{1}{2}||\theta||_2^2$.

$$\text{argmin}_{(\theta,\alpha)}\frac{1}{2}||\theta||_2^2 \quad \text{s.t.}\forall_i y_i(\theta \cdot X_i - \alpha) \geq 1$$

This is known as a **quadratic program** (QP) and can be solved using **standard** techniques.

Soft Margin

If the data is not completely separable or there is a better classification by sacrificing several misclassifications, we can use **soft margin SVM** to treat this issue. By introducing ξ, we are able to penalize points that end up on the wrong side of the support vectors.

$$\text{argmin}_{\theta,\alpha,\xi_i>0}\frac{1}{2}||\theta||_2^2 + \sum_i \xi_i \quad \text{s.t.}\forall_i y_i(\theta \cdot X_i - \alpha) \geq 1 - \xi_i$$

Advantages

Non-probabilistic: optimizes the classification error rather than the likelihood

Disadvantages

More expensive to train compared to logistic regression and naive bayes

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Principle Component Analysis

Motivation

- Denoise the data that is dense in certine dimensions and sparse in other dimension. (Dimensionality Reduction)

Assume $X \in R^{M\times N}$, $\varphi \in R^{M\times M}$, and φ is basis function such that when X is rotated ($Y = \varphi X$)

- $\varphi_i \cdot \varphi_i = 1$, $\varphi_i^{-1} = \varphi_i^T$
- $\varphi_i \cdot \varphi_j = 0$ if $i \neq j$
- Dimension with highest variance is y_0
- Dimension with 2^{nd} highest variance is y_1, etc.

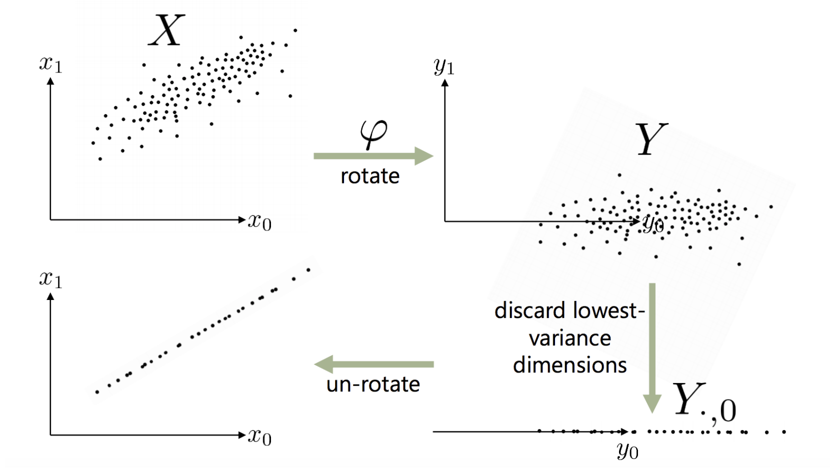

Figure 5: rotate data points across different dimensional space

For a single data point: $y = \varphi x$ $x = \varphi^{-1} y = \varphi^T y$

$$\begin{aligned} x &= \varphi_1 y_1 + \varphi_2 y_2 + \cdots + \varphi_M y_M \\ &= \sum_{j=1}^{M} \varphi_j y_j \end{aligned}$$

Discarding the additional dimension (K+1 to N) by setting y_j where $K + 1 \leq j < N$ to a constant b_j (**Data Reconstruction**)

$$x \simeq \sum_{j=1}^{K} \varphi_j y_j + \sum_{j=K+1}^{M} \varphi_j b_j$$

Optimization

minimize **MSE** to get the "best" overall reconstruction.

$$\begin{aligned} \min_{\varphi,b} \frac{1}{N} \sum_y || \sum_{j=1}^{K} \varphi_j y_j + \sum_{j=K+1}^{M} \varphi_j b_j - \varphi^T y||_2^2 &= \frac{1}{N} \sum_y || \sum_{j=K+1}^{M} \varphi_j (b_j - y_j)||_2^2 \\ &= \frac{1}{N} \sum_y \sum_{i=K+1}^{M} \sum_{j=K+1}^{M} (y_i - b_i)^T \varphi_i^T \varphi_j (y_j - b_j) \\ &= \frac{1}{N} \sum_y \sum_{j=K+1}^{M} (y_j - b_j)^2 \end{aligned}$$

Set $b_j = \bar{y}_j$ as the average of j^{th} dimension:

$$\min_{\varphi} \frac{1}{N} \sum_{y} \sum_{j=K+1}^{M} (y_j - \bar{y}_j)^2$$

(subject to φ **orthonormal**)

Expand in terms of X

$$\min \frac{1}{N} \sum_{j=K+1}^{M} \varphi_j (X - \bar{X})(X - \bar{X})^T \varphi_j^T$$

Regularization

We want to minimize **MSE** with subject to the constrain ($\varphi_i \cdot \varphi_i = 1 \ \forall i, i \geq N$)

Apply Lagrange Multipliers

$$\min \frac{1}{N} \sum_{j=K+1}^{M} \varphi_j Cov(X) \varphi_j^T - \lambda(\varphi_j \cdot \varphi_j - 1)$$

Solve

$$\frac{\partial}{\partial \varphi_j} \sum_{j=K+1}^{M} \varphi_j Cov(X) \varphi_j^T - \lambda(\varphi_j \cdot \varphi_j - 1) = 0$$

$$Cov(X) \varphi_j^T = \lambda_j \varphi_j^T$$

$$A \varphi^T = \lambda \varphi^T$$

- This expression can only be satistifed if φ_j and λ_j are an **eigenvectors/eigenvalues** of the covariance matrix
- So to minimize the original expression we'd discard φ_j's corresponding to the smallest eigenvalues

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Graph Algorithms

Graph algorithms are often used for data clustering and community detection purposes. The algorithms require not only individual data points (vertices) but their connections to each other (edges). Different from common clustering algorithms (**group set of points based on features**), graph algorithms **group set of points based on their connectivity**.

There are several types of community detection problems:

- **Disjoint** communities (i.e., groups of friends who don't know each other) e.g. my American friends and my Australian friends
- **Overlapping** communities (i.e., groups with some intersection) e.g. my friends and my girlfriend's friends
- **Nested** communities (i.e., one group within another) e.g. my UCSD friends and my CSE friends

Minimal Cut

A **minimal cut** splits a network into two partitions such that the number of edges crossed by the cut is minimal. Thus, minimal cut algorithm aims to minimize its cut cost

Ratio Cut

$$\text{Ratio Cut}(C) = \frac{1}{|C|} \sum_{c \in C} \frac{\text{cut}(c, \bar{c})}{|c|}$$

where the variables are:

- C: the proposed sets of communities
- $|C|$: the number of proposed sets of communities
- c: a single individual set of community
- $\text{cut}(c, \bar{c})$: # of edges that separates c from the rest of the network

Normalized Cut

Rather counting all nodes equally in a community, we should give additional weight to the "influential", or high-degree nodes.

$$\text{Normalized Cut}(C) = \frac{1}{|C|} \sum_{c \in C} \frac{\text{cut}(c, \bar{c})}{\sum \text{degrees in } c}$$

where the additional variables are:

- $\sum$ degrees in c: summation of # of edges for all vertices in group set c

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Clique Percolation

Clique percolation is one such algorithm, that discovers communities based on their "cliqueishness"

The algorithm steps are:

- Given a clique size K
- Initialize every K-clique as its own community
- While (two communities I and J have a $(K-1)$-clique in common):
- `Merge $I$ and $J$ into a single community`

Network Modularity

Null model: Edges are equally likely between any pair of nodes, regardless of community structure. ("Erdos-Renyi random model")

For a full modular network, the algorithm tend to choose communities that **minimize** connectivity among different network modules and **maximize** connectivity within individual network module. Thus, the algorithm aims to maximize the function:

$$Q = \sum_{k=1}^{k} (e_{kk} - a_k^2)$$

where the variables are:

- $e_{kk} = \frac{\text{\# of edges w/ both endpoints in the community}}{\text{\# edges}}$
- $a_k = \frac{\text{\# of edge endpoints in the community}}{\text{\# edges}}$

The complexity of this algorithm is **NP Hard**, and we can only approximate the solution using greedy algorithm. One algorithmic example shown in homework 4 is to initially split the network into n groups and move one random node at a time from one module to another to maximize the total network modularity.

Recommender Systems

Similarity Metrics

Jaccard