

Mathematics of Data Science

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1 Ranking Methods

1.1 Plurality

Most naive way of ranking candidates by taking the number of first place votes.

1.2 Borda Count

Count the number of times a candidate appears in i th position and apply the following set of weights as follows:

Let n be the total number of candidates. $(n - 1)$ points are given to first place, $(n - k)$ to k -th place, and 0 is given to last place. The tallies are summed and the winner is the candidate with the highest sum.

1.3 Massey Ranking

Assume there are n teams. Let r_i denote the scoring power of a team, where $r_i - r_j = y_{ij}$ for the margin of victory of team i over team j . Solve the following system of equations for r :

$$Xr = y$$

Each row of matrix X is zero except 1 at position i and -1 at position j , y is a list of the head-to-head scores. We can solve this using least squares.

$$\min_r \|Xr - y\|_2^2$$

$$X^T X r = X^T y$$

Denote $M = X^T X r$, $d = X^T y$

$$Mr = d$$

$$\begin{pmatrix} t_1 & -m_{12} & \dots & -m_{1n} \\ -m_{21} & t_2 & \dots & -m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -m_{n1} & -m_{n2} & \dots & t_n \end{pmatrix} * \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{pmatrix}$$

Here, t_i is the total games team i has played, m_{ij} is the number of games team i played against team j , and d_j is the score differential of the team.

It is possible to use this method to rank candidates. In this case, each voters ranking counts as a game (if there are 5 candidates, each candidate plays a total of 4 matches for each voter).

1.4 PageRank Algorithm

Give each page a score x_j that indicates importance. A page votes for another page by having n_j outgoing links, each vote counts as $\frac{x_j}{n_j}$. The problem becomes:

$$x = Ax$$

Where $x = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$ and A is a matrix whose x columns is a vector whose y entry is $\frac{1}{n_j}$ if there is a link from website x to y . If A is not reducible, we can modify the algorithm to be

$$\tilde{A} = \alpha A + \frac{(1 - \alpha)}{n} * 1, 0 < \alpha < 1$$

This algorithm can also be used to rank candidates. Matrix A columns become 0 for a win and $\frac{1}{j_i}$, j_1 represents the number of loses. Replace the undefeated candidate vector of 0^T with $(\frac{1}{n}, \dots, \frac{1}{n})$

2 Linear Regression

2.1 Ordinary Linear Regression

Take m data points x_1, x_2, \dots, x_m , each of which has n features, which gives us x_{ij} . Denote the response variable y_i . Approximate y as a linear function of x.

$$h(x_i) = \sum_k^n w_k x_{ik} + b = w^T x_i + b$$

To do this we minimize the cost function.

$$\min_{w,b} \|X^T w + b1 - \hat{y}\|_2$$

Here, X is a n x m matrix, whose columns are data points. w is a length n vector of weights. b is a scalar. The optimal solution to this is:

$$\tilde{X} \tilde{X}^T \begin{bmatrix} w \\ b \end{bmatrix} = \tilde{X} \hat{y}, \tilde{X} = \begin{bmatrix} X \\ 1^T \end{bmatrix}$$

This equation is the **least squares problem**.

2.2 Polynomial Regression

Approximate y as a polynomial of degree M.

$$h(x_i) = \sum_{a_1+a_2+\dots+a_n \leq M} c_{i_2, i_2, \dots, i_n} x_{i1}^{a_1} x_{i2}^{a_2} \dots x_{in}^{a_n}$$

There are $r = \binom{M+n}{n}$ monomials. We apply these monomials to data X, with m columns (data points) and r rows.

$$\Phi(X) = \begin{bmatrix} h_1(x_1) & \dots & h_r(x_1) \\ h_1(x_2) & \dots & h_r(x_2) \\ \vdots & \vdots & \vdots \\ h_1(x_m) & \dots & h_r(x_m) \end{bmatrix}^T$$

Then our least squares problem becomes:

$$\min_w \|\Phi(X^T)w - \hat{y}\|_2$$

2.3 Ridge Regression

Idea of Ridge Regression is to introduce a little bit of bias to severely decrease the variance of our estimator.

Let $Y \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times d}$, and $y \in \mathbb{R}^d$

Our true model is $Y = B^T X + \epsilon$

We are given n samples: $(x_1, y_1), \dots, (x_n, y_n)$

Recall our estimation of β using ordinary least squares:

$$\hat{\beta} = \min_{\beta} \|Y - X\beta\|_2^2 \rightarrow \hat{\beta} = (X^T X)^{-1} X^T Y$$

Instead of minimizing over \mathbb{R}^d , we can minimize over a constrained set $\beta \in \{\beta : \|\beta\|_2^2 \leq \tau\}$. This can also be written as an unconstrained problem (λ , the tuning parameter, is the dual of τ , also not when $\lambda \rightarrow 0$, $\tau \rightarrow \infty$ we have ordinary least squares):

$$\hat{\beta} = \min_{\beta} \|Y - X\beta\|_2^2 + \lambda \|\beta\|_2^2 \rightarrow \hat{\beta}(\lambda) = (X^T X + \lambda I)^{-1} X^T Y$$

As with least squares we seek coefficients that estimate data well, but add the second term (shrinkage penalty), which becomes small when β_1, \dots, β_j are close to zero, and has the effect of shrinking these estimates towards zero. λ controls the relative impact of these two terms.

$$[\hat{\beta}_r(\lambda)]_j = \frac{\hat{\beta}_j}{1 + \lambda}$$

We can use the expectation of $\hat{\beta}_r$ to calculate the bias and variance.

$$MSE = \|Bias^2(\hat{\beta}_r(\lambda))\|_2^2 + \sum_{j=1}^p Var(\hat{\beta}_r(\lambda)_j) = \frac{p\sigma^2}{(1 + \lambda)^2} + \frac{\lambda^2 \|\beta\|_2^2}{(1 + \lambda)^2}$$

We need to know σ^2 . Hence, use cross-validation to select λ .

2.4 LASSO

Ridge regression has one obvious disadvantage, despite shrinking β_1, \dots, β_p , the final model includes all p predictors.

LASSO works by replacing ℓ_2 with ℓ_1 . We minimize over a constrained set $\beta \in \{\beta : \|\beta\|_1 \leq S\}$

$$\hat{\beta} = \min_{\beta} \|Y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

$$(\hat{\beta}_L)_j(\lambda) = \text{sign}(\hat{\beta}_j) \left[|\hat{\beta}_j| - \frac{\lambda}{2} \right]_+$$

3 Linear Classification Models

3.1 Bayes Classification Rule

The optimal Bayes classifier rule is given by:

$$f^*(X) = \begin{cases} +1 & \text{if } \eta(X) \geq \frac{1}{2} \\ -1 & \text{otherwise} \end{cases}$$

Where $\eta(X) = \mathbb{P}(Y = 1|X = x) = \frac{\mathbb{P}(X=x|Y=1)\mathbb{P}(Y=1)}{\mathbb{P}(X=x)}$

This can also be written as $f^*(X) = \text{sign}(\log(\frac{\mathbb{P}(Y=1|X)}{\mathbb{P}(Y=-1|X)}))$, which is referred to as the log-odds ratio.

3.2 Discriminative Case

Map $\mathbb{P}(Y = 1|X = x)$ (predict directly using observed values)

3.3 Generative Case

Map $\mathbb{P}(X = x|Y = 1)$ (attempt to model $\mathbb{P}(X = x|Y = 1)$)

3.4 Logistic Regression

Logistic Regression model:

$$\eta(X) = \mathbb{P}(Y = y|X = x) = \frac{1}{1 + e^{-y(x^T \beta)}}$$

Let $p = \mathbb{P}(Y = 1|X)$

$$\log\left(\frac{p}{1-p}\right) = X^T \beta$$

Given a vector of inputs (X, Y) , estimate β

$$\hat{\beta} = \min_{\beta} \sum_{i=1}^n \log(1 + e^{-y_i(\beta^T x_i)})$$

3.5 Discriminate Analysis

Assume $X|Y = y \sim N(\mu_y, \Sigma_y)$, (μ_y, Σ_y) are the mean vector and covariance matrix of $X|Y = y$.
Model $\mathbb{P}(X = x|Y = y)$ as:

$$\mathbb{P}(X = x|Y = y) = (2\pi)^{-d/2} |\Sigma_y|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x - \mu_y)^T \Sigma_y^{-1} (x - \mu_y)\right)$$

Thus, the Bayes optimal classifier becomes:

$$f^*(x) = \text{sign}\left(\log \frac{\Sigma_{-1}}{\Sigma_1} + 2 \log \frac{\mathbb{P}(Y = 1)}{\mathbb{P}(Y = -1)} - (X - \mu_1)^T \Sigma_1^{-1} (X - \mu_1) + (X - \mu_{-1})^T \Sigma_{-1}^{-1} (X - \mu_{-1})\right)$$

The classifier is linear if $\Sigma_1 = \Sigma_{-1} = \Sigma$

$$f^*(x) = \text{sign}\left(2(\mu_1 - \mu_{-1})^T \Sigma^{-1} X + \mu_{-1}^T \Sigma^{-1} \mu_{-1} - \mu_1^T \Sigma^{-1} \mu_1 + 2 \log \frac{\mathbb{P}(Y = 1)}{\mathbb{P}(Y = -1)}\right)$$

3.6 Support Vector Machines

Separable case:

$$\begin{aligned} \min_{\beta} \quad & \beta^T \beta \\ \text{s.t.} \quad & y_i(\beta^T x_i) \geq 1 \end{aligned}$$

Inseparable case (cannot satisfy $y_i(\beta^T x_i) \geq 1$):

$$\min_{\beta} \quad \lambda \beta^T \beta + \sum_{i=1}^n \max(0, 1 - y_i \beta^T x_i), \lambda > 0$$

This can also be represented as a quadratic programming problem. Let $t_i = \max(0, 1 - y_i \beta^T x_i)$, $A = m \times n$ with rows as data points, D be an $m \times m$ diagonal matrix with $D_{ii} = 1$ if $x_i \in P_+$, else -1 , $e = (1, 1, \dots, 1)^T$

$$\begin{aligned} \min_w \quad & \lambda w^T w + e^T t \\ \text{s.t.} \quad & D(Aw + eb) + t \geq e, \\ & t \geq 0 \end{aligned}$$

4 Kth-nearest neighbor

Given a positive integer K and a test observation x_0 , identify the K points in the training data that are closest to x_0 , denoted by N_0 . Model probability of class j as:

$$\mathbb{P}(Y = j | X = x_0) = \frac{1}{K} \sum_{i \in N_0} I(y_i = j)$$

5 Decision Trees

Model data based on decisions. Rectangles can be achieved by making successive binary splits on predictor variables X_1, \dots, X_p . At a given internal node, the label (of the form $X_j < t_k$) indicates the left-hand branch emanating from that split, and the right-hand branch corresponds to $X_j \geq t_k$.

Classification Trees:

Let $(x_i, y_i), i = 1, \dots, n$ be our training data, where $y_i \in 1, \dots, K$, $x_i \in \mathbb{R}^p$. We want m rectangles R_1, \dots, R_m . Each R_j has a class label $c_j \in 1, \dots, K$. Given a new point, the classification is:

$$\hat{f}^{tree}(x) = \sum_{j=1}^m c_j I(x \in R_j) = c_j$$

We can also estimate the probability a label k lies in region R_j

$$\hat{p}_k(R_j) = \frac{1}{n_k} \sum_{x_i \in R_j} I(y_i = k)$$

which finds the proportion of points in the region that are of class k .

Regression Trees:

Just as in classification, the regression function takes the form

$$\hat{f}^{tree}(x) = \sum_{j=1}^m c_j I(x \in R_j) = c_j$$

However, we now just take c_j to be the average response of points in the region:

$$c_j = \frac{1}{n_j} \sum_{x_i \in R_j} y_i$$

5.1 CART Algorithm

1. Start by defining regions

$$R_1 = \{X \in \mathbb{R}^p; X_j \leq s\}, R_2 = \{X \in \mathbb{R}^p; X_j \geq s\}$$

Choose j, s by minimizing the misclassification error:

$$\min_{j,s} ([1 - \hat{p}_{c_1}(R_1)] + [1 - \hat{p}_{c_2}(R_2)])$$

Here c_1 is the most common class in R_1 and c_2 is the most common class in R_2 .

2. Repeat this for our newly created regions R_1, R_2 .
3. We will get a big tree T_0 . We prune this tree, we collapse some of the leaves into the parent nodes.

Let $|T|$ denote the number of leaves. Define the cost complexity as:

$$C_\alpha(T) = \sum_{j=1}^{|T|} [1 - \hat{p}_{c_j}(R_j)] + \alpha|T|$$

Seek $T \in T_0$ that minimizes $C_\alpha(T)$. Do this by pruning the weakest leaf one at a time.

4. Choose α by using k-fold cross-validation.

For regression trees, use the squared error loss instead of the misclassification error.

5.2 Bagging

Make B decision trees:

$$f^1(x), \dots, f^B(x)$$

$$f_{avg}(x) = \frac{1}{B} \sum_{b=1}^B f^b(x)$$

Training data: $D = (x_1, y_1), \dots, (x_n, y_n)$

$f^b(x)$: pick ' n ' samples from D with replacement

5.3 Random Forests

Same idea as bagging but we attempt to decorrelate the trees. Do so by not considering all the predictors for each split. Typically if there are m predictors we take $p = \sqrt{m}$.

5.4 Adaboost

We have training data $(x_1, y_1), \dots, (x_n, y_n)$

1. Initialize weights $w_1 = \frac{1}{n}, \dots, w_n = \frac{1}{n}$
2. for $b = 1 : B$
 - (a) fit decision tree $\hat{f}^{(b)}$ with weights w_1, \dots, w_n
 - (b) $e_b = \frac{\sum_{i=1}^n w_i 1_{\{y_i \neq \hat{f}^{(b)}\}}}{\sum_{i=1}^n w_i}$
 - (c) $\alpha_b = \frac{1}{2} \log \left[\frac{1 - e_b}{e_b} \right]$
 - (d) Update weights $w_i = w_i \exp \left[-\alpha_b y_i \hat{f}^{(b)}(x_i) \right]$ for all i
3. final model $\hat{f}_{boost}(x) = \text{sign} \left[\sum_{b=1}^B \hat{f}^{(b)}(x) \alpha_b \right]$

6 Splines

6.1 Cubic Spline

A cubic spline with K knots can be modeled as:

$$f(x) = \beta_0 + \beta_1 b_1(x) + \beta_2 b_2(x) + \dots + \beta_{k+3} b_{k+3}(x)$$

6.2 Smoothing Splines

$$\min_g \sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

Here, $\lambda > 0$ is a *tuning parameter*.

7 Additive Models

Let $X \in \mathbb{R}^d$ and $y \in \mathbb{R}$ Our GAM model is:

$$y = \sum_{j=1}^d f_j(x_j)$$

To solve for f_j we have the following problem:

$$\min_{f_1, \dots, f_d} \mathbb{E} \left(y - \sum_{j=1}^d f_j(x_j) \right)^2$$

8 Kernel Methods

The idea of Kernel Methods is your estimates of β is essentially a linear combination of your training samples.

For OLS:

$$\hat{\beta} = X^T (X(X^T X)^{-1} X^T Y) = X^T \alpha$$

Define a Kernel (inner-product kernel): $k(u, v) = u^T v$

Given a new sample \bar{x} , the prediction is:

$$\begin{aligned}\bar{x}^T \sum x_i \alpha_i \\ = \alpha_1 k(\bar{x}, x_1) + \dots + \alpha_n k(\bar{x}, x_n)\end{aligned}$$

You can change the linear kernel to other kernels.

Polynomial Kernel:

$$k(u, v) = (1 + u^T v)^p$$

Gaussian Kernel:

$$k(u, v) = \exp(-\lambda \|u - v\|_2^2)$$

8.1 Kernel Ridge Regression

$$\alpha = (XX^T + \lambda I)^{-1}Y$$

Our prediction is:

$$\sum \alpha_i k(\bar{x}^T, x_i)$$

8.2 Kernel SVM

Let α be the solution given to us by the SVM optimization problem where $\hat{\beta} = \sum \alpha x$

Given a new test sample, the prediction is:

$$\text{sign}(\sum \alpha_i k(\bar{x}^T, x_i))$$

9 Resampling Methods

9.1 K-fold Cross-validation

The validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set. In the validation approach, only a subset of the observations — those that are included in the training set rather than in the validation set — are used to fit the model. This suggests that the validation set error may tend to overestimate the test error for the model fit on the entire data set.

Solution: We randomly divide the training data into K equal sized parts. We leave out part k , then fit the model on the other $k-1$ parts. We do this for $k = 1, \dots, K$, then combine the results.

Denote the K part of the training data as C_1, \dots, C_k , and let each observation have n_k observations. Compute:

$$CV_k = \sum_{k=1}^K \frac{n_k}{n} MSE_k$$

Where $MSE_k = \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$. When $K = n$, we have leave-one out cross-validation.

9.2 Bootstrap

What bootstrap accomplishes:

- quantify the uncertainty associated with a given estimator or statistical learning method
- provide an estimate of the standard error of a coefficient, or a confidence interval for that coefficient.

What bootstrap does:

Bootstrap mimics the process of obtaining new data sets from one single dataset, so we can estimate the variability of our estimate without generating additional samples. We instead obtain distinct data sets by repeatedly sampling observations from the original data set with replacement. Each of these 'bootstrap data sets' is created by sampling with replacement, and is the same size as our original dataset

In notation, suppose we repeat this procedure B times, and produce B different bootstrap data sets Z^{*1}, \dots, Z^{*B} , and the corresponding estimates $\hat{\alpha}^{*1}, \dots, \hat{\alpha}^{*B}$. We can estimate the standard error using the formula:

$$SE_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1} \sum_{r=1}^B (\hat{\alpha}^{*r} - \bar{\hat{\alpha}}^*)^2}$$

where $\bar{\hat{\alpha}}^*$ is the average of $\hat{\alpha}^*$

Classic Bootstrap C.I.: $\hat{\alpha} \pm SE * z_{0.025}$

Bootstrap Percentile C.I. (works better for skewed data): Consider the 2.5th and 97.5th percentile of $\hat{\alpha}^{*1}, \dots, \hat{\alpha}^{*B}$

9.3 Bag of Little Bootstrap

The efficacy of bootstrapping depends on two things: the size of the dataset and the number of resamplings. Both need to be high in order to have accurate bootstrapping results. However, when the size of the dataset becomes too large, in otherwords dealing with "big data", the computational efficiency of performing bootstrap dramatically decreases.

Blb is a technique that combines the map reduce algorithm with bootstrapping to create a robust and computationally efficient resampling method that is scalable for large amounts of data. First, the dataset is divided into n approximately equal sized subsets. Bootstrapping is then performed on each of these subsets. The results of each subset are then averaged.

10 SVD

Any non-zero real ($m \times n$) matrix A of rank $r > 0$ can be factored as:

$$A = P \Sigma Q^T$$

P ($m \times r$) orthonormal columns

Σ ($r \times r$) diagonal matrix with eigenvalues of A

Q^T ($r \times n$) orthonormal rows

1. Numerical Applications:

Let $\sigma_1 > \dots > \sigma_n$. Define the condition number of the matrix as $\frac{\sigma_1}{\sigma_n}$

An ill-conditioned matrix has a large condition number (Almost Singular, computation of inverse prone to high numeric errors).

2. Image Compression:

For an image matrix, we only need to keep the large σ

3. Low-rank Approximations:

We can choose the first few basis vectors to approximate our matrix.

11 Dimension Reduction

11.1 PCA

Data X_1, \dots, X_n that is p dimensions arranged into a $n \times p$ data matrix \mathbb{X} . The idea is to change the axis to $W = (w_1, \dots, w_p)$, called the principle component loading vectors, to maximize the variance

$$\underbrace{Z}_{(n \times p)} = \underbrace{\mathbb{X}}_{(n \times p)} \underbrace{W}_{(p \times p)},$$

The rows are called the principle component scores. These rows also happen to be uncorrelated. w_i is just the i th eigenvector of the sample covariance matrix ($\mathbb{X}_c^T \mathbb{X}_c$, \mathbb{X}_c is the centered data matrix)

We can do dimension reduction by taking the first w_1, \dots, w_k . Keeping the first k σ will keep $\frac{\sigma_1 + \dots + \sigma_k}{\sigma_1 + \dots + \sigma_p}$ of the variation.

We can also reconstruct the original by finding the approximation of $X_j - \bar{X}_n$ by only using the first k coordinates in the new basis, and then adding back the mean:

$$\hat{X}_j = \bar{X}_n + \sum_{i=1}^k Z_{ji} w_i.$$

11.2 CCA

Two sets of variables $X = \begin{pmatrix} X_1 \\ \vdots \\ X_p \end{pmatrix}$ and $Y = \begin{pmatrix} Y_1 \\ \vdots \\ Y_r \end{pmatrix}$.

Like PCA, we can define U, V as linear combinations of X, Y .

$$U_i = a_{i1}X_1 + \dots + a_{ip}X_p$$

$$V_j = a_{j1}X_1 + \dots + a_{jq}X_q$$

Let:

$$(U_i, V_i)$$

be the i th canonical pair, which are iteratively found using

$$\begin{aligned}
& \max \quad \text{corr}(U_i X, V_i Y) \\
& \text{s.t.} \quad \text{corr}(U_i X, U X) = 0, \\
& \quad \text{corr}(V_i X, V X) = 0
\end{aligned}$$

Similar to PCA, in practice, we just use the sample covariance matrix of X and Y , which we will denote $S_{XX} \in \mathbf{R}^{p \times p}$, $S_{YY} \in \mathbf{R}^{q \times q}$ and the cross sample covariance matrix as $S_{XY} \in \mathbf{R}^{p \times q}$. The solution matrices U, V satisfy:

$$S_{XX}^{-1} S_{XY} S_{YY}^{-1} S_{YX} U = U D^2$$

where $D^2 = \text{diag}(\lambda_1^2, \dots, \lambda_r^2)$, and

$$V = S_{YY}^{-1} S_{YX} U D^{-1}.$$

11.3 Multidimensional Scaling

Let δ_{ij} be dissimilarities between points i and j .

Classical MDS:

$$\min \text{Strain}(Z_1, \dots, Z_n) = \sum_{i=1}^n \sum_{j=1}^n (B_{ij} - \langle Z_i, Z_j \rangle)^2$$

where $B_{ij} = \tilde{\delta}_{ij} - \tilde{\delta}_{i.} - \tilde{\delta}_{.j} + \tilde{\delta}_{..}$, and $\tilde{\delta}_{ij} = -\frac{1}{2}\delta_{ij}^2$.

Metric MDS:

$$\min \text{Stress}(Z_1, \dots, Z_n) = \sum_{i=1}^n \sum_{j=1}^n (\delta_{ij} - \|Z_i - Z_j\|)^2.$$

Non-Metric MDS:

Instead of using the dissimilarities itself, however, one uses a monotonic transformation

$$f(\delta_{ij}), \quad \text{with } f \text{ monotonically increasing,}$$

We estimate f using isotonic regression.

Isotonic Regression:

Find a non-decreasing function $\hat{f}(x_i)$ such that

$$\hat{f} = \min_f \sum_{i=1}^n (Y_i - f(x_i))^2.$$

Algorithm:

Choose an embedding dimension k and an initial embedding $\tilde{X}_1^{(0)}, \dots, \tilde{X}_n^{(0)} \in \mathbb{R}^k$.

FOR $\ell = 0, 1, 2 \dots$ UNTIL CONVERGENCE DO

(I) Find the pairwise distances $d_{ij}^{(\ell)} = \|\tilde{X}_i^{(\ell)} - \tilde{X}_j^{(\ell)}\|$.

(II) Find the isotonic regression $\hat{d}_{ij}^{(\ell)} = \hat{f}^{(\ell)}(\delta_{ij})$

(III) Find the new embedding $\tilde{X}_1^{(\ell+1)}, \dots, \tilde{X}_n^{(\ell+1)}$ by minimizing $\text{Stress}(Z_1, \dots, Z_n)$ by using $\hat{f}^{(\ell)}(\delta_{ij})$

(IV) Set $\ell = \ell + 1$

11.4 Locally Linear Embedding

LLE algorithm:

1. Approximate X_j as a linear combination of its neighbors by finding a weight matrix $W = (w_{ij})_{ij=1,\dots,n}$ by doing:

$$\min_W \sum_{i=1}^n \left\| X_i - \sum_{j \in N(i)} w_{ij} X_j \right\|^2,$$

where $N(j)$ denotes the set of the k -nearest neighbors, and $\sum_{j \in N(i)} w_{ij} = 1$ for all $i = 1, \dots, n$ and $w_{ij} = 0$ for $j \notin N(j)$.

2. Fix $W = (w_{ij})$. Find $Y_1^*, \dots, Y_n^* \in \mathbb{R}^{d'}$ with $d' \leq d$ through:

$$\min_Y \sum_{i=1}^n \left\| Y_i - \sum_{j \in N(i)} w_{ij} Y_j \right\|^2.$$

11.5 Isomap

1. construct a weighted k -NN graph
2. Approximate geodesic distances $d_M(X_i, X_j)$ by finding the length of the shortest path connecting X_i and X_j in the k -NN graph.
3. Apply classical MDS on the resulting pairwise distance matrix

12 Clustering

12.1 K-Means

Set of points $X = (x_1, \dots, x_n)$, want to group our data into K clusters $c = c_1, \dots, c_k$. K-means finds a partition so that the squared error between the mean of a cluster and the points in the cluster is minimized. Let u_i be the mean of cluster c_i . Define the following:

$$J(c_k) = \sum_{x_j \in c_i} \|x_i - u_i\|^2$$

$$J(c) = \sum J(c_i)$$

1. Select initial partition with K -clusters. Do steps 2 and 3 until clusters stabilize
2. Generate new partition by assigning each point to its closest cluster center
3. Compute new cluster centers

K-means as an optimization problem:

$$\min_C \sum_{i=1}^k \sum_x \in c_i \|x_i - u_i\|^2$$

Can solve this using branch-and-bound.

12.2 K-medoids

PAM algorithm.

1. select k points as the medoids
2. Associate each point to the closest medoid
3. Within each medoid, find the best cost change. If the swap of the best medoid and point does not decrease the cost, the algorithm terminates.

As an optimization problem:

$$\begin{aligned} \min \quad & \sum_{i,j} x_{i,j} p(i,j) \\ \text{s.t.} \quad & \sum_j y_j \leq K, \\ & \sum_j x_{i,j} = 1, \\ & x_{i,j} \leq y_j, \\ & x_{i,j}, y_j \in \{0, 1\} \end{aligned}$$

12.3 Hierarchical Clustering

agglomerative hierarchical clustering (bottom-up) - iteratively combine clusters to larger clusters greedily.

divisive hierarchical clustering (top-down) - break down clusters into smaller clusters.

agglomerative hierarchical clustering algorithm (the more popular one):

1. assign each data point to its own cluster
2. Combine the closest clusters successively
3. Determine which level is optimal

How do we define two clusters as being close?

1. Choose a distance measure:

- Euclidean distance: $d = \sqrt{\sum_{j=1}^d (x_j - y_j)^2}$
- squared Euclidean distance: $d = \sum_{j=1}^d (x_j - y_j)^2$
- maximum distance: $d = \max_{j=1,\dots,d} |x_j - y_j|$
- Manhattan distance: $d = \sum_{j=1}^d |x_j - y_j|$

2. Measure dissimilarities between clusters:

- single linkage: based on the nearest neighbor
- complete linkage: based on the furthest neighbor
- average linkage: based on the average of the clusters

12.4 Mean Shift Clustering

KDE is a non-parametric way to estimate the density function. The shape of the estimated density function is:

$$\hat{f}_{n,h}(x) = \frac{1}{nh} \sum_{j=1}^n K\left(\frac{x - x_i}{h}\right)$$

where K is a kernel, $h > 0$ is the bandwidth. Note: this method suffers from the curse of dimensionality, and is not recommended for high degree data (Notice for high dimensions, h would have to be very large in order to have a decent number of points in a certain area).

The Mean Shift Algorithm is based off the Kernel Density Estimator. Instead of constructing an estimate of the density function, we seek to draw each of the data points in our set to the nearest peak.

Mean shift algorithm: let ϕ be a kernel function, c tuning parameter

1. choose starting point $x^{(0)}$
2. from $j = 0$ to convergence, find weights and weighted mean:

$$w_k(x^{(j)}) = \frac{\phi(c||X_k - x^{(j)}||^2)}{\sum_{k=1}^n \phi(c||X - x^{(j)}||^2)}$$

$$\bar{X}_{x^{(j)}} = \sum_{k=1}^n w_k(x^{(j)})X_k$$

$$\text{set } x^{(j+1)} = \bar{X}_{x^{(j)}}$$

Mean shift clustering algorithm:

1. Apply the mean shift algorithm to all n points. This gives n paths, $(X_i, x^{(N_i)})$
2. group all points with the same $x^{(N_i)}$

12.5 DBSCAN

The DBSCAN Algorithm:

1. Generate an epsilon neighborhood for each point, then count the number of points that lie within a point's neighborhood. Let any point that has more than a certain user determined points be considered a core point.
2. Find the connected components of the core points, by connecting all core points that fall with each others neighborhoods.
3. Assign non-core points that fall within a cluster's neighborhood, otherwise assign point to noise.

12.6 Spectral clustering

Given data points x_1, \dots, x_n and similarities $w(x_i, x_j)$, construct similarity graph: $G(V, E, W)$

V: vertices (data points)

E: edge if similarity > 0

W: edge weights (similarities)

Typical Similarity Graphs:

- K-nearest Neighbor Graphs - Create edge between two vertex if vertex v_i is among the k th nearest neighbors of v_j .
- Fully Connected Graph - Create edge between all vertexes in the

Algorithm using the normalized laplacian:

Normalized Laplacian:

$$L' = I - D^{-1}W$$

where D is a diagonal matrix of d_i , where $d_i = \sum_{j:(i,j) \in E} w_{ij}$

Algorithm:

1. Input: Similarity matrix W , k clusters
2. Build similarity graph
3. compute largest k eigenvectors of matrix L'
4. Build matrix $V \in \mathbb{R}^{n \times k}$ with eigenvectors as columns
5. interpret rows of V as new data points $Z_i \in \mathbb{R}^k$
6. cluster the points Z_i using k-means in \mathbb{R}^k

12.7 Silhouette Score

Silhouette score is used to evaluate clustering results.

Let $d(X_i, X_j)$ be a distance measure between two points, and let C_k denote clusters. Find the average dissimilarity of all points in a cluster by:

$$a(i) = \frac{1}{|C_k| - 1} \sum_{j \in C_k} d(X_i, X_j)$$

Also define the average dissimilarity of a point outside of a cluster to all points within the cluster by:

$$d(i, C_{k'}) = \frac{1}{|C_{k'}|} \sum_{j \in C_{k'}} d(X_i, X_j) = \text{average dissimilarity of } X_i \text{ to all points in } C_{k'}.$$

Denote the smallest one of these by $b(i)$

The silhouette score is defined by:

$$s(i) = \begin{cases} 1 - \frac{a(i)}{b(i)} & \text{for } a(i) < b(i) \\ 0 & \text{for } a(i) = b(i) \\ \frac{b(i)}{a(i)} - 1 & \text{for } a(i) > b(i) \end{cases}.$$

13 Feed Forward Neural Networks

13.1 Architecture

Let m be the number of neurons in the input layer. Weight from i -th node to j -th node is denoted by w_{ij} . We have the value that enters node i in the first hidden layer is:

$$L(X) = w_{1i}x_1 + w_{2i}x_2 + \dots + w_{mi}x_m + b$$

At the node there is an activation function, which determines if node is used or not.

$$\phi(L(X))$$

Activation functions

1. Relu: $ReLU(x) = \max(0, x)$
2. Logistic Sigmoid: $\phi(x) = \frac{e^x}{e^x + 1}$
3. Hyperbolic tangent function: $\phi(x) = \tanh\left(\frac{x}{2}\right) = \frac{e^x - 1}{e^x + 1}$

13.2 Learning

Let training data set $x^{(1)}, x^{(2)}, \dots, x^{(N)}$ contain N points with m features. Labels y_1, \dots, y_N .

Take $X_1^{(1)}$. This becomes the first layer $V_0 = (x_1^{(1)}, \dots, x_m^{(1)})$. K -th layer outputs $V_k = ReLu(A_k V_{k-1} + b_k)$, A_k is $N_{k-1} \times N_k$.

Compare the final layer to the target value using a loss function. Adjust the weights to minimize the error. This becomes an optimization problem, which we should solve using Stochastic Gradient Descent (See section 17.3). Common loss functions used:

1. Square Loss: $L(w) = \frac{1}{N} \sum_{i=1}^N (F(w, x_i) - y_i)^2$
2. Hinge Loss: $L(w) = \frac{1}{N} \sum_{i=1}^N \max\{0, 1 - y_i F(w, x_i)\}, y_i = -1, 1$
3. Cross-Entropy Loss: $L(w) = -\frac{1}{N} \sum_{i=1}^N [y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)], y_i = 0, 1, \hat{y}_i = \frac{1}{1 + e^{w^T x_i}}$

14 Convolutional Neural Network

14.1 Architecture

Convolution Layer:

The convolution of an image x with a kernel k is:

$$(x * k)_{ij} = \sum_{pq} x_{i+p, j+q} k_{p,q}$$

Let the input matrix be of size I , P the amount of zero padding, and S the stride (number of pixels moved after each operation). The output size of the convolution layer is

$$O = \frac{I - F + P_{start} + P_{end}}{S} + 1$$

Suppose we have K filters.

Input: $I \times I \times C$, Output: $O \times O \times K$

Pooling Layer:

Downsizing operation, can take the max or average

Input: $I \times I \times C$, Output: $O \times O \times C$

Fully Connected Layer:

Operates on a flattened input where each input is connected to all neurons. If present, FC layers are usually found towards the end of CNN architectures and can be used to optimize objectives such as class scores.

14.2 YOLO

1. Divide input image into a $G \times G$ grid
2. For each grid cell, run a CNN that predicts y from the following form:

$$y = [\underbrace{p_c, b_x, b_y, b_h, b_w, c_1, c_2, \dots, c_p}_{\text{repeated } k \text{ times}}, \dots]^T \in \mathbb{R}^{G \times G \times k \times (5+p)}$$

p_c is the probability of detecting an object, b_x, b_y, b_h, b_w (center, height, width) are the properties of the detected box, c_1, \dots, c_p is a one-hot representation of which of the p classes were detected, and k is the number of boxes.

3. Run non-max suppression algorithm.

14.3 R-CNN

Region with Convolutional Neural Networks (R-CNN) is an object detection algorithm that first segments the image to find potential relevant bounding boxes and then run the detection algorithm to find most probable objects in those bounding boxes.

15 Recurrent Neural Network

15.1 Architecture

Let $a^{<t>}$ be the activation at time t , $x^{<t>}$ be the input at time t , and $y^{<t>}$ be the output at time t . At each timestep t , the activation $a^{<t>}$ and output $y^{<t>}$ are:

$$a^{<t>} = g_1(W_{aa}a^{<t-1>} + W_{ax}x^{<t>} + b_a)$$

$$y^{<t>} = g_2(W_{ya}a^{<t>} + b_y)$$

15.2 Learning

The loss function is defined as: $L(\hat{y}, y) = \sum_{t=1}^{T_y} L(\hat{y}^{<t>}, y^{<t>})$

Backpropagate:

$$\frac{dL}{dW} = \sum_{t=1}^{T_y} \frac{dL}{dW}$$

15.3 Handling Long-term Dependencies

Multiplicative nature of the gradient causes a phenomenon known as vanishing/exploding gradient, as a small gradient will be exponentially smaller and large gradient exponentially bigger.

To handle exponential gradients, gradient clipping (capping the maximum gradient size) is employed.

To handle vanishing gradients, gates (characterized as: $\Gamma = \sigma(Wx^{<t>} + Ua^{<t-1>} + b)$) are employed:

- Update gate Γ_u : How much past should matter now? (GRU/LSTM)
- Relevance gate Γ_r : Drop previous information? (GRU/LSTM)
- Forget Γ_f : Erase a cell or not? (LSTM)
- Output gate Γ_o : How much to reveal of a cell? (LSTM)

15.4 GRU Architect

Inputs: Previous outputs: $a^{<t-1>}, c^{<t-1>}$, new input: $x^{<t>}$

Hidden Unit: $\tilde{c}^{<t>} = \tanh(W_c[\Gamma_r * a^{<t-1>}, x^{<t>}] + b_c)$

Outputs: $c^{<t>} = \Gamma_u * \tilde{c}^{<t>} + (1 - \Gamma_u) * c^{<t-1>}$, $a^{<t>} = c^{<t>}$

15.5 LSTM Architect

Inputs: Previous outputs: $a^{<t-1>}, c^{<t-1>}$, new input: $x^{<t>}$

Hidden Unit: $\tilde{c}^{<t>} = \tanh(W_c[\Gamma_r * a^{<t-1>}, x^{<t>}] + b_c)$

Outputs: $c^{<t>} = \Gamma_u * \tilde{c}^{<t>} + \Gamma_f * c^{<t-1>}$, $a^{<t>} = \Gamma_o * c^{<t>}$

16 Optimization

16.1 Convex Optimization Problem

Takes the form:

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \leq 0, i = 1, \dots, m, \\ & a_i^T x = b_i, i = 1, \dots, p \end{aligned}$$

f_0, \dots, f_m are convex functions (constraints create a convex set/ $f_i(\lambda x + (1 - \lambda)y) \leq \lambda f_i(x) + (1 - \lambda)f_i(y)$, $\forall x, y \in \mathbb{R}^n, \lambda \in [0, 1]$ /any straight line between any two points in the set is contained inside the set.

Lagrangian: $L(x, \lambda, v) = f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{i=1}^p v_i h_i(x)$

16.2 Gradient Descent

1. start with x_0 inside domain
2. At k-th iteration, if $\|\nabla f(x_k)\| \geq \epsilon$, continue. Else we find our optimum.
3. choose $v_k = -\nabla f(x_k)$
4. Give step size $a_k > 0$ /choose $\alpha_k = \min_{\alpha} f(x_k - \alpha \nabla f(x_k))$
5. iterate $x_{k+1} = x_k + \alpha_k v_k$

16.3 Stochastic Gradient Descent

Optimization problem takes the form $\min_w L(X) = \frac{1}{N} \sum_{i=1}^N f_i(w)$, N is large. Assume it is too costly to compute this using normal gradient descent. Instead, choose B as a subset of the indices of N . Instead of $w_{k+1} = w_k - \eta \frac{1}{N} \sum_{i=1}^N \nabla f_i(w_k)$, we calculate:

$$w_{k+1} = w_k - \eta_k \frac{1}{|B|} \sum_{i \in B} \nabla f_i(w_k)$$

To ensure convergence of Stochastic Gradient Descent, a decreasing η must be used. A constant η will converge for normal Gradient Descent.

16.4 KKT

KKT Conditions:

- primal constraints: $f_i(x) \leq 0, i = 1, \dots, m, h_i(x) = 0, i = 1, \dots, p$
- dual constraints: $\lambda \geq 0$
- complementary slackness: $\lambda_i f_i(x) = 0, i = 1, \dots, m$
- gradient of Lagrangian wrt x vanishes: $\nabla f_0(x) + \sum_{i=1}^m \lambda_i \nabla f_i(x) + \sum_{i=1}^p v_i \nabla h_i(x) = 0$

KKT for convex problems

If $\tilde{x}, \tilde{\lambda}, \tilde{v}$ satisfy the KKT conditions for a convex problem, they are optimal.

KKT for NLP (no convexity assumed)

Can only guarantee local optimum for NLP. The mentioned KKT conditions are now the first order KKT conditions. Also need to check for second-order condition:

$$s^T \nabla_{xx}^2 L(\bar{x}, \bar{\lambda}, \bar{v}) s \geq 0$$

If $\bar{x}, \bar{\lambda}, \bar{v}$ satisfy both the first and second order conditions, \bar{X} is a local minimum (Strict if 2nd order condition is strict)

16.5 Branch and Bound

This algorithm is used to solve IP problems. If you solve the LP relaxation of a pure IP and obtain a solution in which all variables are integers, then the optimal solution to the LP relaxation is also the optimal solution to the IP.

1. (Fathoming/Bounding)
2. (Branching)

17 Network Flow

17.1 LP form

Nodes: the sources, destinations, and intermediate points. Denote $1 \dots n$.

Arcs: the transportation links connecting nodes are termed arcs. Denote $i - j$ meaning from node i to node j .

Define x_{ij} as number of units moved from node i to j using arc $i-j$. Our optimization problem becomes:

$$\begin{aligned}
\min \quad & z = \sum_{i,j} c_{ij} x_{ij} \\
\text{s.t.} \quad & \sum_j x_{ij} - \sum_k x_{ki} = b_i, i = 1, \dots, n \text{ (flow balance),} \\
& l_{ij} \leq x_{ij} \leq u_{ij}, \text{ (flow capacities)}
\end{aligned}$$

17.2 Transportation Problem

Want to move units from sources to destinations with no intermediate.

Let a_i be the number of units available at source i ($i = 1, \dots, m$)

Let b_j be the number of units required at destination j ($j = 1, \dots, n$)

Let c_{ij} Per-unit transportation cost from source i to destination j

Assume total units available = total units required ($\sum a_i = \sum b_i$). Let x_{ij} be the number of units moved from source i to destination j . Problem becomes:

$$\begin{aligned}
\min \quad & \sum_i \sum_j c_{ij} x_{ij} \\
\text{s.t.} \quad & \sum_j x_{ij} = a_i, \\
& \sum_i -x_{ij} = -b_j, \\
& x_{ij} \geq 0
\end{aligned}$$

- c1: units from source i should equal units available at source i
- c2: units shipped to destination j should equal the requirements of destination j

17.3 Assignment Problem

Assign n objects to n places depending on performance of object i to place j denoted c_{ij} . Define $x_{ij} = 1$ if i is assignment to j , 0 otherwise.

$$\begin{aligned}
\min \quad & \sum_i \sum_j c_{ij} x_{ij} \\
\text{s.t.} \quad & \sum_j x_{ij} = 1, \\
& \sum_i -x_{ij} = -1, \\
& x_{ij} = 0, 1
\end{aligned}$$

- c1: i is assigned to only one j
- c2: j has only one i assigned to it

17.4 Max Flow Problem

Send as much material from node s (source) to node t (sink). Let u_{ij} be the capacity for arc i - j . Let v denote material sent from s to t . Let s_{ij} represent flow from node i to j over arc i - j .

$$\begin{aligned} \max \quad & v \\ \text{s.t.} \quad & \sum_j x_{ij} - \sum_k x_{ki} = v, i = s, \\ & \sum_j x_{ij} - \sum_k x_{ki} = -v, i = t, \\ & \sum_j x_{ij} - \sum_k x_{ki} = 0, \text{ for other nodes,} \\ & 0 \leq x_{ij} \leq u_{ij} \end{aligned}$$

Alternate formulation: Introduce arc x_{ts} , has unlimited capacity.

$$\begin{aligned} \max \quad & x_{ts} \\ \text{s.t.} \quad & \sum_j x_{ij} - \sum_j x_{kj} = 0, i = 1, 2, \dots, n \end{aligned}$$

17.5 Shortest Path Problem

Given network with distance c_{ij} , find path from source to sink that has the shortest total distance.

$$\begin{aligned} \min \quad & \sum_j \sum_j c_{ij} x_{ij} \\ \text{s.t.} \quad & \sum_j x_{ij} - \sum_k x_{ki} = 1, i = s, \\ & \sum_j x_{ij} - \sum_k x_{ki} = -1, i = t, \\ & \sum_j x_{ij} - \sum_k x_{ki} = 0, \text{ for other nodes,} \\ & x_{ij} \geq 0 \end{aligned}$$

18 Integer Programming

18.1 Capitol Budgeting

Given projects p_1, \dots, p_n , over t years, with expenditures e_{ij} (expenditure for i th year j th project), with available funds each year f_1, \dots, f_n which gives returns r_1, \dots, r_n .

$$x_j = \begin{cases} 1 & \text{if project } j \text{ is selected} \\ 0 & \text{if project } j \text{ is not selected} \end{cases}$$

$$\begin{aligned}
\max \quad & z = \sum_n p_j x_j \\
\text{s.t.} \quad & \sum_n x_j e_{ij} = f_i, i = 1, \dots, t, \\
& x_j = 0, 1
\end{aligned}$$

18.2 Set-Covering Problem

Select minimal amount of points to cover set. Here, $j = 1, \dots, n$

$$x_j = \begin{cases} 1 & \text{if node } j \text{ is chosen} \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned}
\min \quad & z = \sum_n x_j \\
\text{s.t.} \quad & x_i + x_k \geq 0 \text{ if there exists arc from } i \text{ to } k, \\
& x_j = 0, 1
\end{aligned}$$

18.3 Fixes-Charge Problem

Request services from n companies, each who charge a flat fee and a variable fee. Let x_1, \dots, x_n be the units/time of each company. Define $y_j = 1$ if $x_j > 0$ and 0 if $x_j = 0$, $j = 1, \dots, n$. Let M be the total units demanded.

$$\begin{aligned}
\min \quad & z = \sum_n x_j y_j \\
\text{s.t.} \quad & \sum_n x_j = M, \\
& x_j \leq M y_j, j = 1, \dots, n, \\
& x_j \geq 0, y_j = 0, 1
\end{aligned}$$

18.4 Either-Or Constraint

Either $f(x_1, \dots, x_n) \leq 0$ or $g(x_1, \dots, x_n) \leq 0$, set constraints as:

$$\begin{aligned}
& f(x_1, \dots, x_n) \leq M y \\
& g(x_1, \dots, x_n) \leq M(1 - y) \\
& y = 0, 1, \quad M \text{ Large}
\end{aligned}$$

18.5 If-then Constraint

If $f(x_1, \dots, x_n) > 0$ is satisfied, then constraint $g(x_1, \dots, x_n) \geq 0$ must be satisfied, while if $f(x_1, \dots, x_n) > 0$ is not satisfied, then $g(x_1, \dots, x_n) \geq 0$ may not have to be satisfied. Set constraints as:

$$\begin{aligned}
& f(x_1, \dots, x_n) \leq M(1 - y) - \epsilon \\
& -g(x_1, \dots, x_n) \leq M y \\
& y = 0, 1
\end{aligned}$$

18.6 Traveling Salesperson Problem

A salesperson visits cities $1, 2, \dots, n$ in some order and ends up at the city where he started. c_{ij} is the cost of going from i to j .

Consider the undirected case $(i, j) = (j, i)$. Let the graph be denoted by $K_n = (V, E)$. Let U denote any proper subset of nodes.

$$\begin{aligned} \min \quad & z = \sum_{ij} c_{ij} x_{ij} \\ \text{s.t.} \quad & \sum_{j: (i,j) \in E} x_{ij} = 2, i = 1, \dots, n, \\ & \sum_{i \in U, j \in \bar{U}} x_{ij} \geq 2, \\ & x_{ij} = 0, 1 \end{aligned}$$

Consider the directed case. $x_{ij} = 1$ if there is a path from i to j , otherwise 0.

$$\begin{aligned} \min \quad & z = \sum_{ij} c_{ij} x_{ij} \\ \text{s.t.} \quad & \sum_{j: j \neq i} x_{ij} = 1, i = 1, \dots, n, \\ & \sum_{i: i \neq j} x_{ij} = 1, j = 1, \dots, n, \\ & \sum_{i \in S, j \in \bar{S}, i \neq j} x_{ij} \leq |S| - 1 \text{ for all vertex subset } S \text{ with } 3 \leq |S| \leq n - 3, \\ & x_{ij} = 0, 1 \end{aligned}$$

18.7 Solving IP problems

See section 16.5: Branch and Bound