1 Spectral clustering

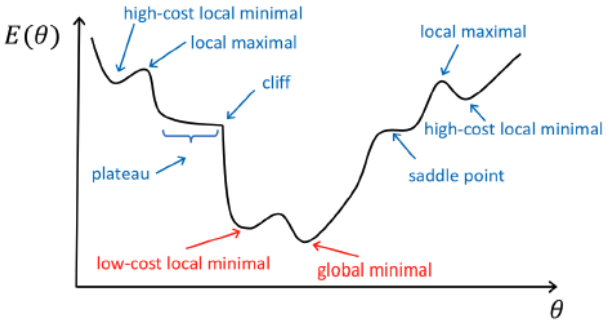
MinCut: $q = \underset{q\in[-1,1]^n}{argmin}\ CutSize; CutSize = \frac{1}{4}\sum_{i,j}(q_i - q_j)^2 w_{i,j}$
Relaxation: 1. relax q to be real number $J = q^T(D-W)q; d_i = \sum_j w_{i,j}, D = [d_i\delta_{i,j}] \rightarrow q^* = argmin q^T(D-W)q, s.t. \sum_k q_k^2 = n.$ The solution is the second minimum eigenvector for $D-W$.
Graph Laplacian: $L = D - W; w = [w_{i,j}], D = [\delta_{i,j}(\sum_j w_{i,j})]$. L is semi-positive definitive matrix ($x^TLx = x^TDx - x^TWx = \sum_{i=1}^n d_i x_i^2 - \sum_{i,j=1}^n w_{i,j} f_i f_j) = 0.5(\sum_{i=1}^n d_i x_i^2 - 2\sum_{i,j=1}^n w_{i,j}x_i x_j + \sum_{j=1}^n d - j x_j^2) = 0.5(\sum_{i,j=1}^n w_{i,j}(f_i - f_j)^2) \geq 0$ and min eigenvalue is 0 (eigenvector is $[1,...,1]^T$. For **Dv**, the value at ith row is $\sum_j w_{i,j}$, which picks the degree of node i from the diagonal degree matrix **D**. For **Av**, the value at ith row is also $\sum_j w_{i,j}$. Therefore, $(\mathbf{D}-\mathbf{A})\mathbf{v} = 0$ is always satisfied and **v** is the eigenvector). Parition based on the eigenvector: $A = \{i | q_i < 0\}$
Spectral clustering: mincut doesn't balance the size of bipartite graph. $Cut(A,B) = \sum_{i\in A; j\in B} w_{i,j}$ and $Vol(A) = \sum_{i\in A}\sum_{j=1}^n w_{i,j}$ Obj1: min inter-cluster connection (min cut(A,B)); Obj2: max intra-cluster connection: max vol(A,A) and vol(B,B). $J = Cut(A,B)(\frac{1}{vol(A)} + \frac{1}{vol(B)})$. Solution: 2nd smallest eigenvector of $(D-W)y = \lambda Dy$

2 Feed forward NN

Why multiple layers: Automatic feature learning; Learn non-linear mapping function. Process: feed forward; compute gradient $\frac{\partial}{\partial\theta}J_\theta$: update parameter: $\theta = \theta - \eta\frac{\partial}{\partial\theta}J_\theta$
BP: error term $\delta_j^{(l)}$ is a function of (1): all $\delta_k^{(l+1)}$ in the layer l+1, if layer l is hidden layer; (2) the overall loss function value, if layer l is the output layer

3 Deep learning

Challenges: optimization is non-convex (find high-quality local optima); generalization: min generalization error (reduce overfitting)



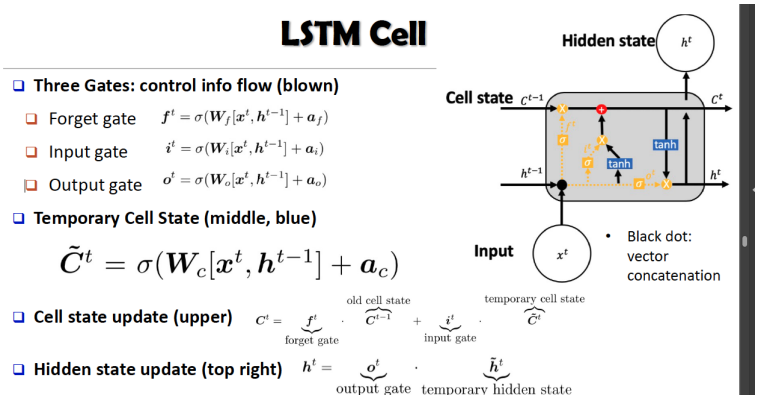
Responsive activation function: saturation of sigmoid: $O = \sigma(I) = \frac{1}{1+exp(-I)}$; derivative: $\frac{\partial O}{\partial I} = O(1-O)$; error: $\delta_j = O_j(1-O_j)(O_j - T_j)$. If O_j is close to 0 or 1, bother derivative and error is close 0 (gradient vanishing).
ReLU: $O = IifI > 0, otherwise0$. No decaying in error, avoid gradient vanishing.
Adaptive learning rate: SGD $\theta_{t+1} = \theta_t - \eta g_t$. Potential problems: slow progress, jump over gradient cliff; oscillation. Strategy: 1. $\eta_t = \frac{1}{t}\eta_0$; 2. $\eta_t = (1-t/T)\eta_0 + t/T\eta_\infty$; 3. AdaGrad: $\eta_t = \frac{1}{\rho + r_i}\eta_0, r_i = \sqrt{\sum_{k=1}^t -1 g_{i,k}^2}$. Intuition: the magnitude of gradient g_t as the indicator of overall progress.
Dropout: to prevent overfitting by randomly dropout of some non-output units. Regularization; Force the model to be more robust to noise, and to learn more generalizable features. VS bagging: each model is trained independently, while the model of current dropout network are updated based on previous dropout network.
Pre-training: the process of initializing the model in a suitable region. Greedy supervised pretraining; pre-set model parameters layer-by-layer in a greedy way; unsupervised pretraining: auto-encoder; hybrid.
Cross-entropy: MSE for regression. CE Loss $-Tlog(O) - (1-T)log(1-O)$; error: $O - T$

4 CNN

Challenges of MLP: Long training time, slow convergence, local minima. Motivation: Sparse interactions (Units in deeper layers still connect to a wide range of inputs); Parameter sharing (Reduce parameters); Translational equivalence $f(g(x)) = g(f(x))$. CNN layer followed by non-linear activation and pooling. The deeper the better: learn from a larger receptive field.
Pooling: Introduces invariance to local translations; Reduces the number of hidden units in hidden layer

5 RNN

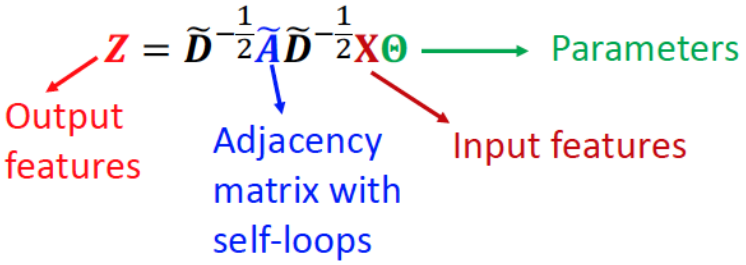
Handle sequence. $h^t = f(Ux^t, Wh^{t-1} + a)$; $\hat{y}^T = g(Vh^T + b)$. Recurrence to capture long-term dependence: same hidden-to-hidden matrix W; same input-to-hidden matrix U, same bias a. VS CNN: localized dependence.
Challenges: long-term dependence. It needs deep RNN, leading to gradient vanishing or exploding. Solution: Gated RNN (LSTM, GRU) or attention mechanism.
LSTM: cell state; accumulate the information from the past; three gate to control info flow (forget; input; output).



Attention: Key Idea of Attention Mechanism: context vectors. Augment hidden state of 2nd RNN with context vectors. Introduce an alignment vector a and use linear weighted sum to obtain context vector.

6 GNN

Challenges: Irregular graph structure (non-Euclidean): Unfixed size of node neighborhoods; Permutation invariance: Node ordering does not matter; Undefined convolution computation
Graph convolution in spectral domain: spectral-based model (GCN): $x *_\theta y \approx \theta(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2})x, \tilde{A} = A + I_n$



A two-layer architecture for node classification: $\tilde{Y} = softmax(\hat{A}\sigma(\hat{A}X\theta_1)\theta_2), \hat{A} = \tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}$
Graph convolution in spatial domain: $x(i) = w_{i,i}x(i)\sum_{j\in(i,k)} w_{i,j}x(j)$, where N is the k-hop neighborhood. key idea: message passing: how to aggregate node representations.

7 Outlier

Global Outliers (=point anomalies); Contextual Outliers (=conditional outliers); Collective Outliers (=group anomaly) Challenge: Difficulty in modeling normality, ambiguity between normal and abnormal. Application-specific outlier detection; noise vs outlier (Noise: unavoidable, less interesting to the users, but make outlier detection more challenge); model interpretability.
Statistical approaches: Assume normal data are generated by a stochastic process Data objects in low density regions are flagged as outlier. Parametric Methods: The normal data objects are generated by a parametric distribution with a finite number of parameters: Single Variable Data: Grubb's test; Multi variable Data: Mahalanobis distance; χ^2-statistics; mixture models Non Parametric Methods: Do not assume a priori statistical model with a finite number of parameters: Outlier Detection by Histogram (Construct histogram data objects outside bins are outliers); Outlier Detection by Kernel Density Estimation (Kernel function: influence of a sample within its neighbor)
Proximity-based approaches: Intuition: objects that are far from others can be regarded as outliers. Assumption: the proximity of an outlier object to its nearest neighbors significantly deviates from the proximity of most other objects to their nearest neighbors
Distance-based outlier detection: Consult the neighborhood of a sample. Outlier: if there are not enough objects in its neighborhood. r: distance threshold; π: fraction threshold. o is a $DB(r,\pi)$ -outlier if $\frac{\|\{o'|dist(o,o') \le r\}\|}{\|D\|} \le \pi$. Equivalent criteria: if $dist(o,o_k) > r$. o_k is the k-nearest neighbor of o; $k = \lceil \pi\|D\| \rceil$