深蓝学院
shenlanxueyuan.com

3D Point Clouds
Lecture 4 – Clustering & Model Fitting

主讲人 黎嘉信

Aptiv 自动驾驶
新加坡国立大学 博士
清华大学 本科

1. Clustering - Spectral Clustering
2. Clustering – Mean-Shift and DBSCAN
3. Model Fitting - LSQ
4. Model Fitting – Hough Transform
5. Model Fitting - RANSAC

Lecture 3

K-Means

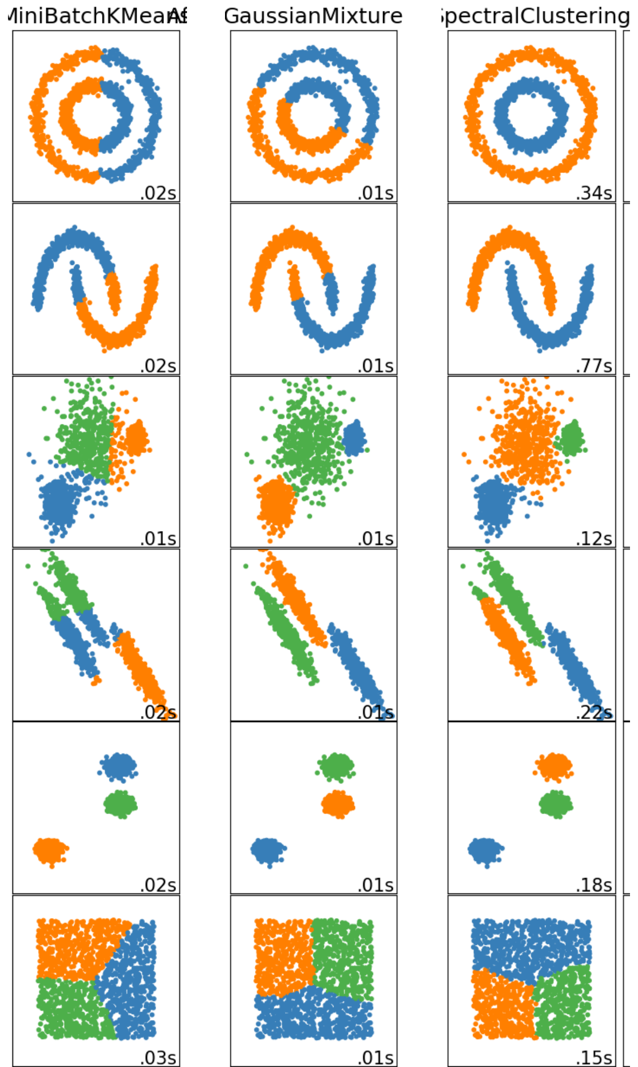
- Euclidean distance
- Hard assignment
- No modeling for a cluster
- Pre-defined cluster number k

GMM

- Euclidean distance
- Probability formulation – soft clustering
- Mean and variance estimation for each cluster
- Pre-defined cluster number k

Spectral Clustering

- Works with connectivity
- Heuristic to determine cluster number k

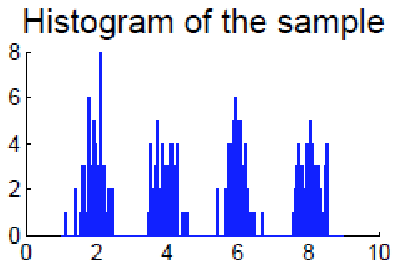


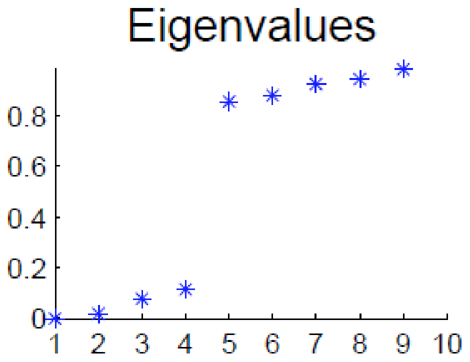
Unnormalized Spectral Clustering

1. Build the graph to get adjacency matrix $W \in \mathbb{R}^{n\times n}$
2. Compute unnormalized Laplacian L
3. Compute the first (smallest) k eigenvectors $v_1, \cdots, v_k$ of L
4. Let $V \in \mathbb{R}^{n\times k}$ be the matrix contraining the vectors $v_1, \cdots, v_k$ as columns
5. For $i = 1, \cdots n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of V
6. Cluster the points $\{y_i \in \mathbb{R}^k\}$ with k-means algorithm into clusters $C_1, \cdots, C_k$
7. The final output clusters are $A_1, \cdots, A_k$ where $A_i = \{j | y_j \in C_i\}$

Spectral Clustering

- Selection of k can be done by eigenvalue analysis
- Most stable clustering is given by the value of k that maximizes the eigen-gap
  - Eigengap is the difference between consecutive eigenvalues
  - $\Delta_k = |\lambda_k - \lambda_{k-1}|$





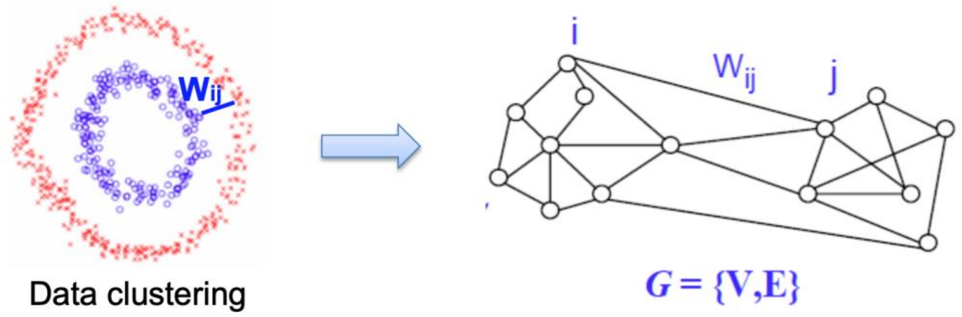
Normalized Spectral Clustering

- Unnormalized Spectral Clustering -> approximated RatioCut

$$\mathrm{RatioCut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{|A_i|}$$

- Normalized Spectral Clustering -> approximated NormalizedCut

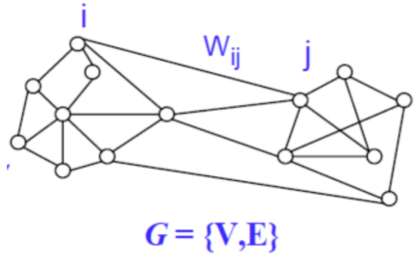
$$\mathrm{Ncut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{\mathrm{vol}(A_i)}$$

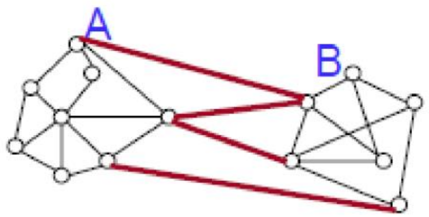


Graph Min-cut

- Min-cut: Partition graph $G = (V, E)$ into two sets A, B, such that the weights of edges connecting A, B is minimum

$$cut(A,B) = \sum_{i \in A, j \in B} w_{ij}$$



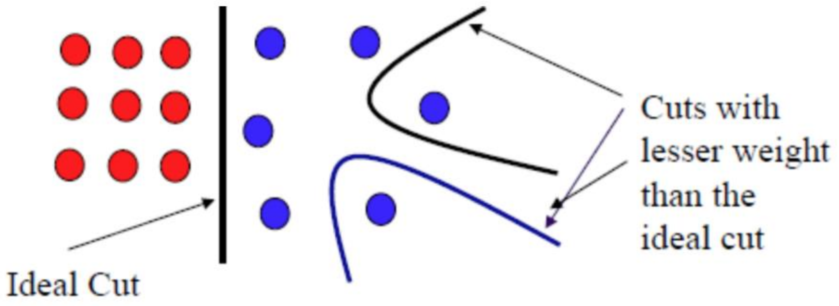


- Min-cut for k partitions. $\bar{A}_i$ is the complement of subset $A_i \subset V$

$$cut(A_1, \cdots, A_k) = \sum_{i=1}^{k} cut(A_i, \overline{A_i})$$

Graph Min-cut

- Naïve min-cut suffers from degenerate results



- Solution:
  - Add constrains that the partition A_i can not be too small

- How to evaluate the size of a partition A_i?

Graph Min-cut – Size of A

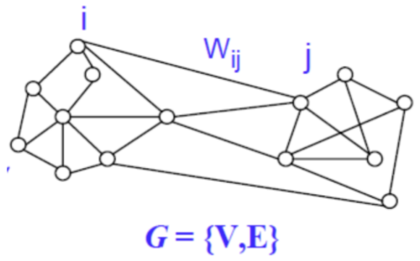
1. Number of vertices in A

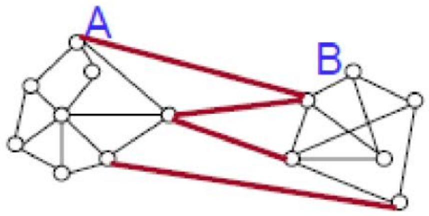
$$|A| := \text{ the number of vertices in } A$$

2. Sum of weights in A

$$\mathrm{vol}(A) := \sum_{i \in A} d_i \qquad d_i = \sum_{j=1}^{n} w_{ij}$$

Weight sum for node i





Spectral Clustering

Unnormalized Spectral Clustering -> approximated RatioCut

- Constrains the cluster have similar size
- Size(A) = |A|

Normalized Spectral Clustering -> approximated NormalizedCut

- Constrains the cluster have similar size
- Size(A) = vol(A)
- Vol(A) is large means nodes are closely connected inside A → A's element is similar.

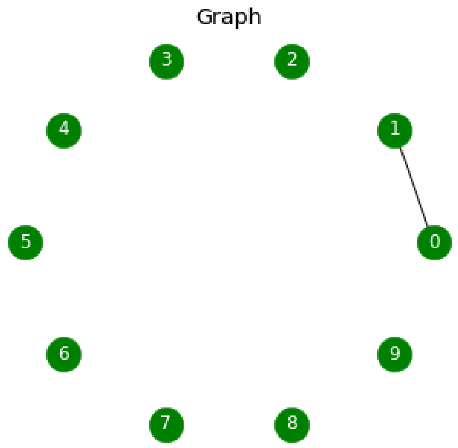
Spectral Clustering – Laplacian Matrix

- Degree matrix D
  - A diagonal matrix with degrees $d_1, \cdots, d_n$ on the diagonal
  - $d_i = \sum_{j=1}^{n} w_{ij}$ is the row sum of adjacency matrix W → "how many edges are connected to node i"
- Unnormalized graph Laplacian matrix $L = D - W$
- Normalized graph Laplacian matrix
  - $L_{sym} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2}$
  - $L_{rw} = D^{-1} L = I - D^{-1} W$

Spectral Clustering

Why do we need Laplacian matrix L?

- Its eigenvalues / eigenvectors has some good properties.
  - One 0 eigenvalue → one connected component
  - Corresponding eigenvectors → which node belongs to that connected components



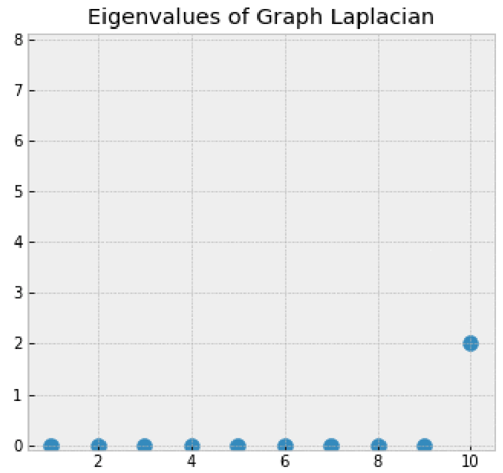
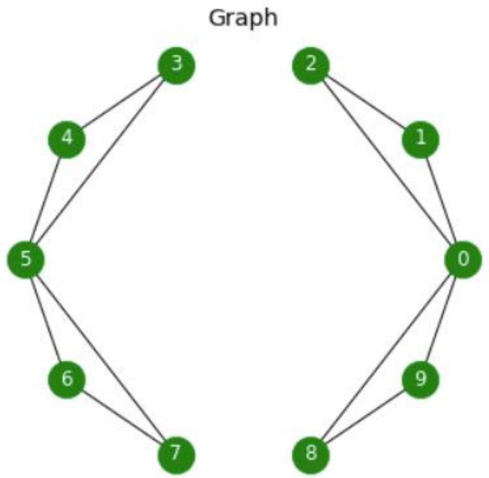


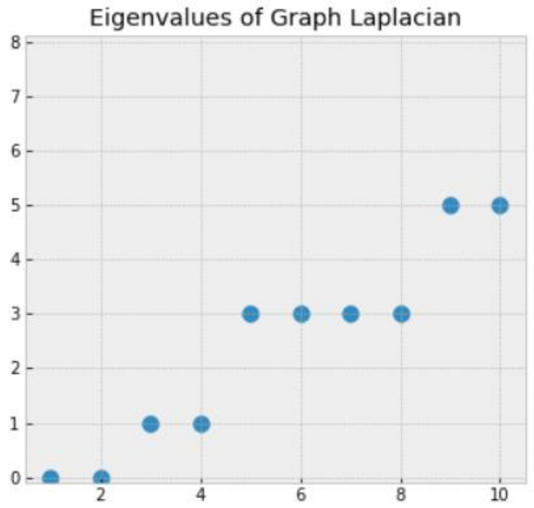
Image source: https://towardsdatascience.com/spectral-clustering-aba2640c0d5b

Spectral Clustering

$$W=\begin{matrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{matrix}$$

- Why do we need Laplacian matrix L?
  - Its eigenvalues / eigenvectors has some good properties.
    - One 0 eigenvalue → one connected component
    - Corresponding eigenvectors → which node belongs to that connected components





$$\begin{array}{|c|c|} \hline 1 & 0 \\ \hline 1 & 0 \\ \hline 1 & 0 \\ \hline 0 & 1 \\ \hline 0 & 1 \\ \hline 0 & 1 \\ \hline 0 & 1 \\ \hline 0 & 1 \\ \hline 1 & 0 \\ \hline 1 & 0 \\ \hline \end{array} = \begin{array}{|c|c|} \hline 1 & 0 \\ \hline 1 & 0 \\ \hline 1 & 0 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 1 \\ \hline 1 & 0 \\ \hline 1 & 0 \\ \hline \end{array}$$

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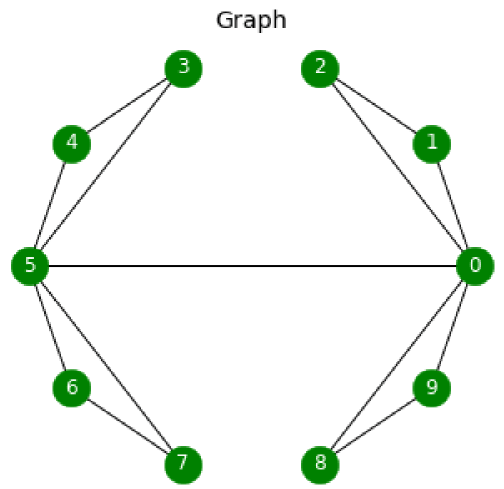
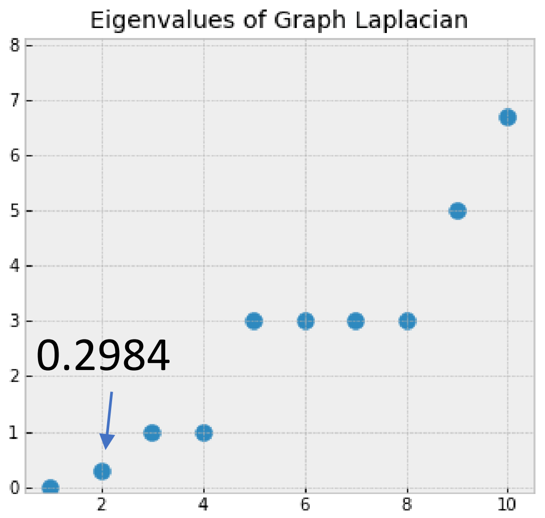
Spectral Clustering

$$W=\begin{matrix} 0 & 1 & 1 & 0 & 0 & \boxed{1} & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ \boxed{1} & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{matrix}$$

Why do we need Laplacian matrix L?

- Its eigenvalues / eigenvectors has some good properties.
  - One 0 eigenvalue → one connected component
  - Corresponding eigenvectors → which node belongs to that connected components





1	0
1	0
1	0
0	**1**
0	**1**
0	**1**
0	**1**
0	**1**
1	0
1	0

1	-0.23
1	-0.33
1	-0.33
1	**0.33**
1	**0.33**
1	**0.23**
1	**0.33**
1	**0.33**
1	-0.33
1	-0.33

Image source: https://towardsdatascience.com/spectral-clustering-aba2640c0d5b

Spectral Clustering – Graph Cut View

- Unnormalized graph Laplacian matrix $L = D - W$

Proposition 1 (Properties of L) *The matrix L satisfies the following properties:*

1. *For every vector $f \in \mathbb{R}^n$ we have*

$$f^T L f = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2$$

2. *L is symmetric and positive semi-definite.*
3. *The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\mathbb{1}$.*
4. *L has n non-negative, real-valued eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$.*

Proposition 1.1

1. For every vector $f \in \mathbb{R}^n$ *we have* $f^T L f = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2$

$$f^T L f = f^T D f - f^T W f$$

Proposition 1.2 & 1.3 & 1.4

2. *L is symmetric and positive semi-definite.*
   - $L = D - W$, D, W are symmetric
   - $f^T L f \geq 0, \ \forall f \in \mathbb{R}^n$

3. *The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\mathbb{1}$.*

$$Lf = (D-W)f = [\cdots, d_i f_i - \sum_{j=1}^{n} w_{ij} f_j, \cdots]^T = 0 \cdot f, \ f = \mathbb{1}$$

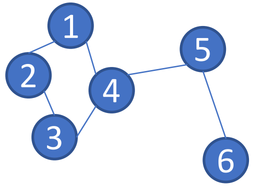
$$\boxed{d_i = \sum_{j=1}^{n} w_{ij}}$$

4. *L has n non-negative, real-valued eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$.*

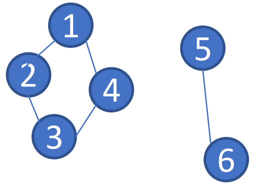
   Direct result of 2 & 3

Spectral Clustering – Graph Cut View

Proposition 2 (Number of connected components) *Let G be an undirected graph with non-negative weights. Then the multiplicity k of the eigenvalue 0 of L equals the number of connected components $A_1, \dots, A_k$ in the graph. The eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbb{1}_{A_1}, \dots, \mathbb{1}_{A_k}$ of those components.*



$$\begin{bmatrix}1\\1\\1\\1\\1\\1\end{bmatrix}$$



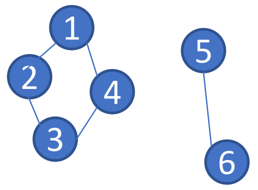
$$\begin{bmatrix}1\\1\\1\\1\\0\\0\end{bmatrix} \quad \begin{bmatrix}0\\0\\0\\0\\1\\1\end{bmatrix}$$

Spectral Clustering

- Wait, the eigenvector of the following graph is NOT constant one?

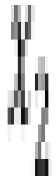
3. The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\mathbb{1}$.

- $Lx = \lambda x$
- $Lx_1 + Lx_2 = \lambda_1 x_1 + \lambda_2 x_2$
- $\lambda_1 = \lambda_2 = 0$
- $L(x_1 + x_2) = \lambda(x_1 + x_2)$



$$\begin{array}{cc} x_1 & x_2 \\ \begin{bmatrix}1\\1\\1\\1\\0\\0\end{bmatrix} & \begin{bmatrix}0\\0\\0\\0\\1\\1\end{bmatrix} \end{array}$$

$x_1 + x_2$



Spectral Clustering – Graph Cut View

Proposition 2 (Number of connected components) *Let G be an undirected graph with non-negative weights. Then the multiplicity k of the eigenvalue 0 of L equals the number of connected components $A_1, \dots, A_k$ in the graph. The eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbb{1}_{A_1}, \dots, \mathbb{1}_{A_k}$ of those components.*

- Consider $k = 1$, i.e., G is a connected graph
- Assume f is eigenvector associated with eigenvalue 0

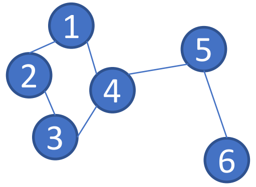
$$f^T L f = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2 = f^T \cdot 0 = 0$$

- $\forall i, j,\ f_i = f_j$ is the only choice to satisfy the above equation.

Spectral Clustering – Graph Cut View

$$f^T L f = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 = f^T \cdot 0 = 0$$

Graph



Connectivity / Similarity matrix

$$\begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$f^T L f = (f_1 - f_2)^2 + (f_2 - f_3)^2 + (f_3 - f_4)^2$$
$$+ (f_4 - f_5)^2 + (f_5 - f_6)^2 = 0$$

$$\Longrightarrow$$

$$f_1 = f_2 = f_f = f_4 = f_5 = f_6$$

That is, the smallest eigenvector is constant vector

Spectral Clustering – Graph Cut View

Proposition 2 (Number of connected components) *Let G be an undirected graph with non-negative weights. Then the multiplicity k of the eigenvalue 0 of L equals the number of connected components $A_1, \dots, A_k$ in the graph. The eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbb{1}_{A_1}, \dots, \mathbb{1}_{A_k}$ of those components.*

- Consider $k \geq 2$, reorganize L into block diagonal matrix on the left
- The spectrum of L is the union of spectrum of L_i. So the 0-eigenvalue eigenvectors of L is shown on the right

$$L = \begin{pmatrix} L_1 & & & \\ & L_2 & & \\ & & \ddots & \\ & & & L_k \end{pmatrix}$$

$$\begin{bmatrix} \mathbb{1}_1 & 0 & \cdots & 0 \\ 0 & \mathbb{1}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \mathbb{1}_k \end{bmatrix}$$

Spectral Clustering – Graph Cut Definition

For two disjoint subsets, $A, B \subset V$

$$\mathrm{cut}(A, B) = \sum_{i \in A, j \in B} w_{ij}.$$

For k disjoint subsets, $A_1, \cdots, A_k$

$$\mathrm{cut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \mathrm{cut}(A_i, \overline{A}_i)$$

- Unnormalized Spectral Clustering -> approximated RatioCut

$$\mathrm{RatioCut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{|A_i|}$$

- Normalized Spectral Clustering -> approximated NormalizedCut

$$\mathrm{Ncut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{\mathrm{vol}(A_i)}$$

Approximated RatioCut for $k = 2$

- The problem is simplified into

$$\min_{A \subset V} \text{RatioCut}(A, \bar{A}) = \min_{A \subset V} \left(\frac{\text{cut}(A, \bar{A})}{|A|} + \frac{\text{cut}(\bar{A}, A)}{|\bar{A}|} \right)$$

- Given a subset $A \subset \text{V}$, construct a vector $f = [f_1, \cdots, f_n]^T \in \mathbb{R}^n$

$$f_i = \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \in \overline{A}. \end{cases}$$

- f determines the results of graph cut, but how to solve f?

$$\begin{cases} v_i \in A & \text{if } f_i \geq 0 \\ v_i \in \overline{A} & \text{if } f_i < 0. \end{cases}$$

Approximated RatioCut for $k = 2$

- Apply Proposition 1.1

$$
\begin{aligned}
f^T L f &= \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2 \\
&= \frac{1}{2}\sum_{i\in A, j\in \overline{A}} w_{ij}\left(\sqrt{\frac{|\overline{A}|}{|A|}} + \sqrt{\frac{|A|}{|\overline{A}|}}\right)^2 + \frac{1}{2}\sum_{i\in \overline{A}, j\in A} w_{ij}\left(-\sqrt{\frac{|\overline{A}|}{|A|}} - \sqrt{\frac{|A|}{|\overline{A}|}}\right)^2 \\
&= \operatorname{cut}(A, \overline{A})\left(\frac{|\overline{A}|}{|A|} + \frac{|A|}{|\overline{A}|} + 2\right) \\
&= \operatorname{cut}(A, \overline{A})\left(\frac{|A| + |\overline{A}|}{|A|} + \frac{|A| + |\overline{A}|}{|\overline{A}|}\right) \\
&= |V| \cdot \operatorname{RatioCut}(A, \overline{A}).
\end{aligned}
$$

$$
f_i = \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \in \overline{A}. \end{cases}
$$

$$
\operatorname{cut}(A, B) = \sum_{i\in A, j\in B} w_{ij}
$$

$$
\operatorname{RatioCut}(A, \bar{A}) = \frac{\operatorname{cut}(A, \bar{A})}{|A|} + \frac{\operatorname{cut}(\bar{A}, A)}{|\bar{A}|}
$$

Approximated RatioCut for $k = 2$

- In addition, f is orthogonal to constant vector $\mathbb{1}$

$$\sum_{i=1}^{n} f_i = \sum_{i \in A} \sqrt{\frac{|\overline{A}|}{|A|}} - \sum_{i \in \overline{A}} \sqrt{\frac{|A|}{|\overline{A}|}} = |A| \sqrt{\frac{|\overline{A}|}{|A|}} - |\overline{A}| \sqrt{\frac{|A|}{|\overline{A}|}} = 0.$$

- $\|f\| = \sqrt{n}$

$$\|f\|^2 = \sum_{i=1}^{n} f_i^2 = |A| \frac{|\overline{A}|}{|A|} + |\overline{A}| \frac{|A|}{|\overline{A}|} = |\overline{A}| + |A| = n.$$

Approximated RatioCut for $k = 2$

- Now the problem is converted to:

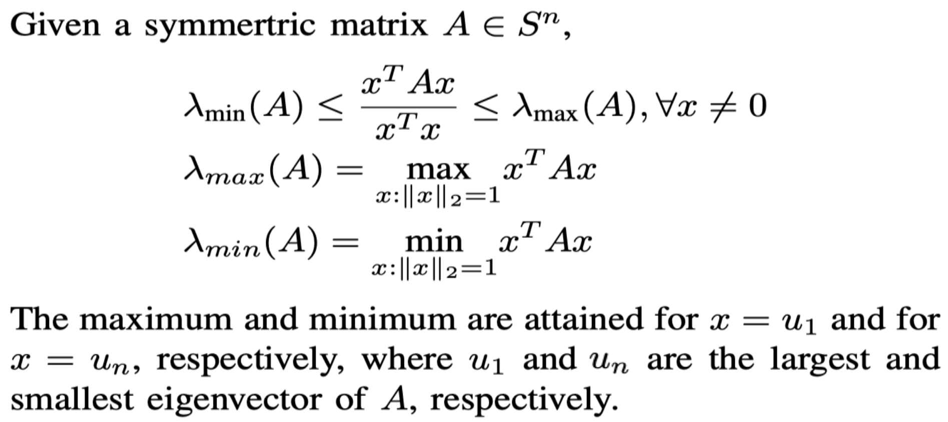
$$\min_{A \subset V} f^T L f, \;\; s.t., \; f \perp \mathbb{1}, \|f\| = \sqrt{n}, \qquad f_i = \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \in \overline{A}. \end{cases}$$

- Approximation by dropping the last condition:

$$\min_{A \subset V} f^T L f, \;\; s.t., \; f \perp \mathbb{1}, \|f\| = \sqrt{n}$$

Approximated RatioCut for $k = 2$

- We are solving $\min_{A \subset V} f^T L f,\ s.t.,\ f \perp \mathbb{1}, \|f\| = \sqrt{n}$
- L is symmetric and Positive Semi-Definite
- Recall the Rayleigh Quotients



Given a symmertric matrix $A \in S^n$,

$$\lambda_{\min}(A) \leq \frac{x^T A x}{x^T x} \leq \lambda_{\max}(A), \forall x \neq 0$$
$$\lambda_{max}(A) = \max_{x:\|x\|_2=1} x^T A x$$
$$\lambda_{min}(A) = \min_{x:\|x\|_2=1} x^T A x$$

The maximum and minimum are attained for $x = u_1$ and for $x = u_n$, respectively, where u_1 and u_n are the largest and smallest eigenvector of A, respectively.

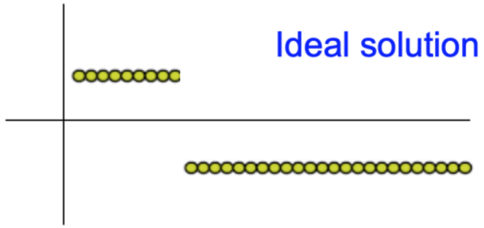
Approximated RatioCut for $k = 2$

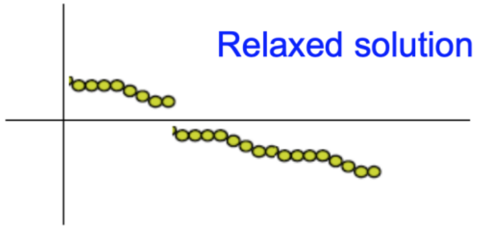
- f is the second eigenvector of L

- How can we get clusters?

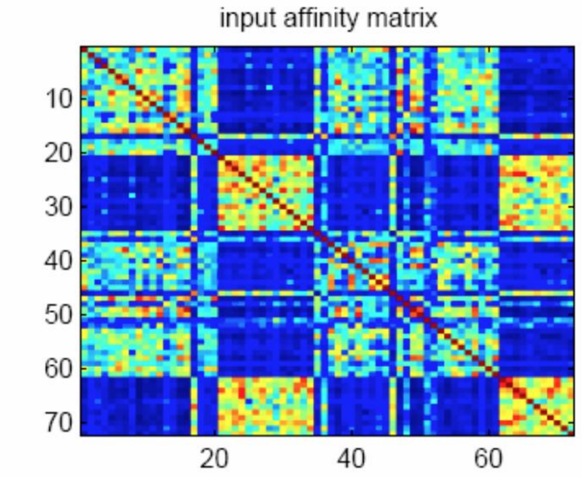
$$\cancel{\begin{cases} v_i \in A & \text{if } f_i \geq 0 \\ v_i \in \overline{A} & \text{if } f_i < 0. \end{cases}}$$

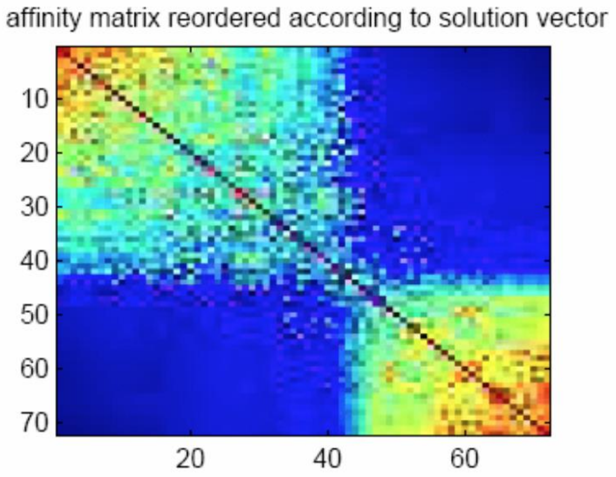
$$\boxed{f_i = \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \in \overline{A}. \end{cases}}$$

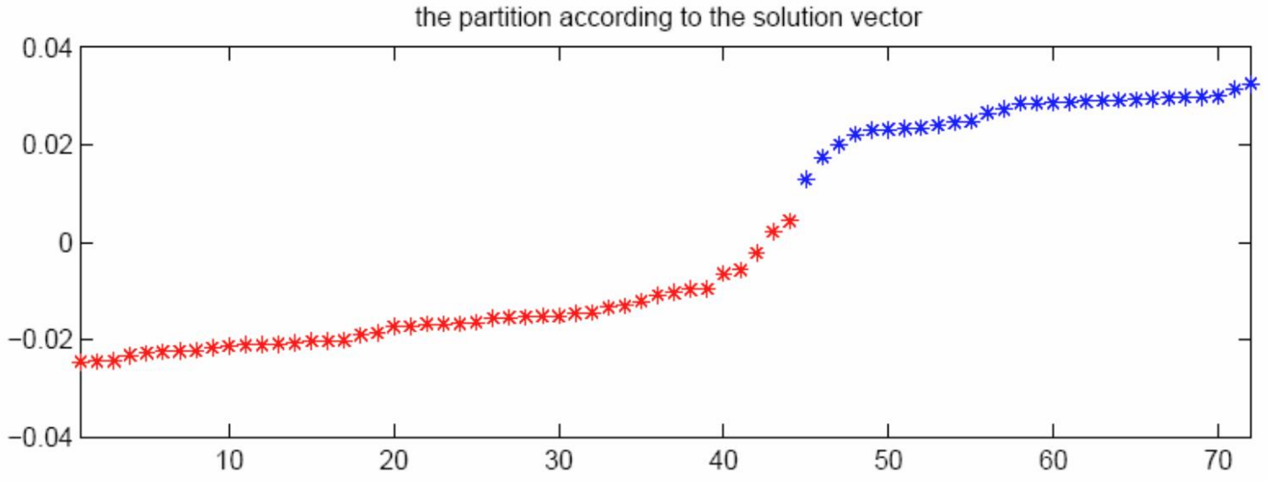




- Run k-means on f.
  - In practice, run k-means on the first two eigenvectors
  - First eigenvector is graph connectivity, which helps as well


input affinity matrix
10
20
30
40
50
60
70
20
40
60


affinity matrix reordered according to solution vector
10
20
30
40
50
60
70
20
40
60

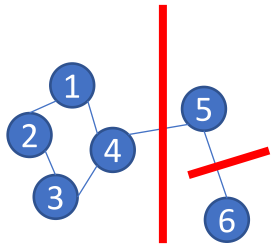

the partition according to the solution vector
0.04
0.02
0
−0.02
−0.04
10
20
30
40
50
60
70

Approximated RatioCut for $k \geq 2$

- Construction the indication matrix $H \in \mathbb{R}^{n \times k}$, where,

$$h_{i,j} = \begin{cases} 1/\sqrt{|A_i|} & \text{if } i \in A_j \\ 0 & \text{otherwise.} \end{cases}$$

- A vertex belongs one cluster only → H has orthonormal columns $H^T H = I$



$$H = \begin{bmatrix} \frac{1}{\sqrt{4}} & 0 & 0 \\ \frac{1}{\sqrt{4}} & 0 & 0 \\ \frac{1}{\sqrt{4}} & 0 & 0 \\ \frac{1}{\sqrt{4}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1}} \end{bmatrix}$$

Approximated RatioCut for $k \geq 2$

- Construction the indication matrix $H \in \mathbb{R}^{n\times k}$, where,

$$h_{i,j} = \begin{cases} 1/\sqrt{|A_i|} & \text{if } i \in A_j \\ 0 & \text{otherwise.} \end{cases}$$

- A vertex belongs one cluster only → H has orthonormal columns $H^T H = I$
- Denote the row vector as $h_i \in \mathbb{R}^k, i = 1, \cdots, n$
- Following similar calculations as $k = 2$, we have,

$$h_i^T L h_i = \frac{\text{cut}(|A_i|, |\bar{A}_i|)}{|A_i|}, \; h_i^T L h_i = (H^T L H)_{ii}$$

Approximated RatioCut for $k \geq 2$

- Recall the definition of RatioCut, we have

$$\begin{aligned}\text{RatioCut}(A_1, \cdots, A_k) &= \sum_{i=1}^{k} \frac{\text{cut}(A_i, \bar{A}_i)}{|A_i|} \\ &= \sum_{i=1}^{k} h_i^T L h_i = \sum_{i=1}^{k} (H^T L H)_{ii} = \text{Tr}(H^T L H)\end{aligned}$$

- Now the problem is transformed into

$$\min_{A_1, \cdots, A_k} \text{Tr}(H^T L H) \text{ s.t., } H^T H = I, \quad h_{i,j} = \begin{cases} 1/\sqrt{|A_i|} & \text{if } i \in A_j \\ 0 & \text{otherwise.} \end{cases}$$

Approximated RatioCut for $k \geq 2$

- Approximation by dropping our H construction,

$$\min_{A_1, \cdots, A_k} \mathrm{Tr}(H^T L H) \text{ s.t., } H^T H = I$$

- A more general form of Rayleigh Quotients, gives the solution:
  - H contains the first k eigenvectors of L as columns
- Apply k-means on the rows of H because of the approximation

$$\xcancel{h_{i,j} = \begin{cases} 1/\sqrt{|A_i|} & \text{if } i \in A_j \\ 0 & \text{otherwise.} \end{cases}}$$

Normalized Spectral Clustering

- The derivation is similar
- The goal is Normalized Cut on the graph

- Unnormalized Spectral Clustering -> approximated RatioCut

$$\mathrm{RatioCut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{|A_i|}$$

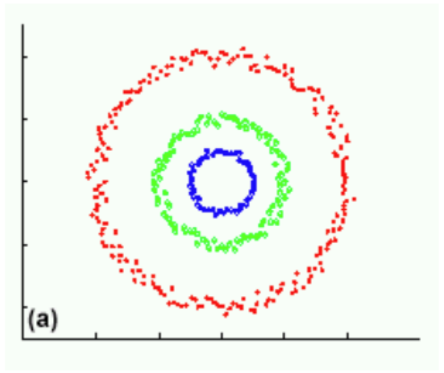
- Normalized Spectral Clustering -> approximated NormalizedCut

$$\mathrm{Ncut}(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{\mathrm{cut}(A_i, \overline{A}_i)}{\mathrm{vol}(A_i)}$$

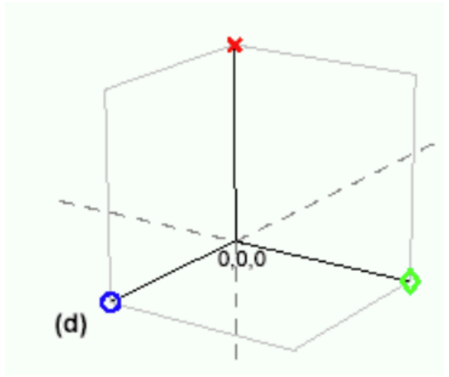
Intuition of Spectral Cluster

1. RatioCut or NormalizedCut
    - Cut the graph into disjoint subsets with minimum cutting weights
    - The size of the each subset should not be too small
2. Dimension Reduction
    - Project the n-dimension data into lower dimension space (spectral/eigenvector domain)

Original data



Projected data

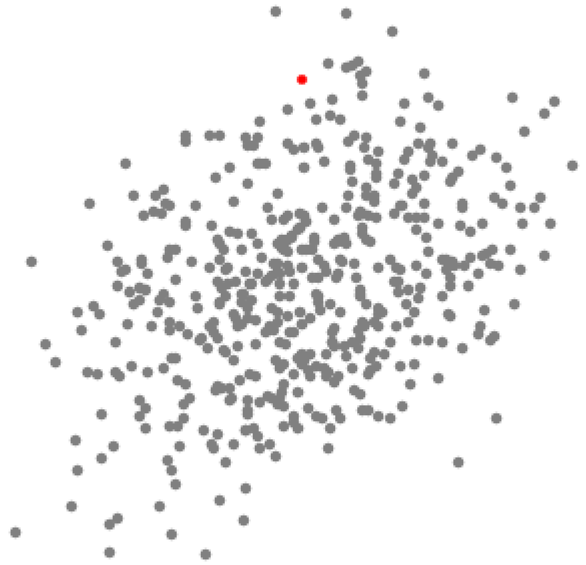


Spectral Clustering - Summary

- Complexity: $O(n^3)$
  - This is the complexity of eigen decomposition
  - K-means complexity is $O(n^2)$
- Advantage
  - No assumption on cluster shape
  - Works with similarity, including Euclidean, connectivity
  - Works with any dimensional data
  - Able to estimate the number of clusters
- Disadvantage
  - Computational expensive
    - Can be alleviated using sparse similarity matrix and sparse eigen solver

Mean Shift

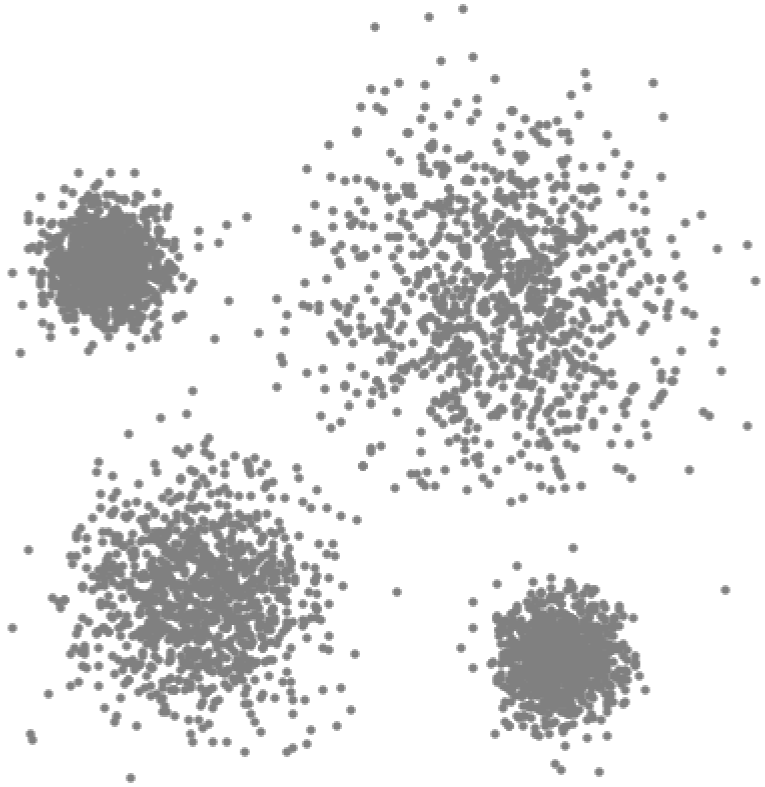
- Sliding windows hill climbing
  - “Hill” is density



Mean Shift

1. Randomly select a circle with radius r
2. Move the circle to the center of the points inside
3. Repeat step-2 until it doesn't move
4. Repeat step-1,2,3. Remove overlapping circles
   - If circles overlap, select the one with most points
5. Determine clusters by finding the nearest circle center (similar to k-means)

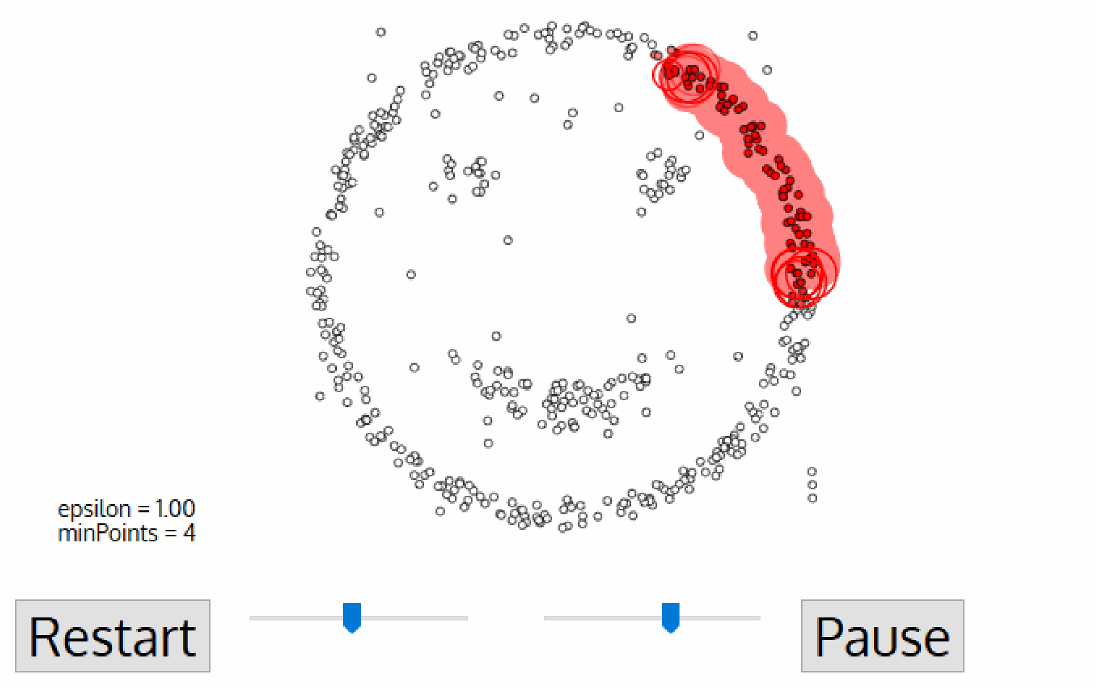
Parameters: radius r



Mean Shift – Summary

- Complexity $O(T \cdot n \cdot log(n))$
  - T is number of centers
  - $n \cdot \log(n)$ is the complexity of radius based neighbor search, given 2D/3D data with kd-tree/octree
- Advantage
  - Automatically determines cluster numbers
  - Single parameter
  - Robust to outliers
- Disadvantage
  - Hill climbing easily falls in local minima
  - Depends on initialization
  - Assumes clusters are in ellipse shape
  - Mainly works in Euclidean space
  - Doesn’t scale with high dimensional data

Density-Based Spatial Clustering of Applications with Noise (DBSCAN)


epsilon = 1.00
minPoints = 4

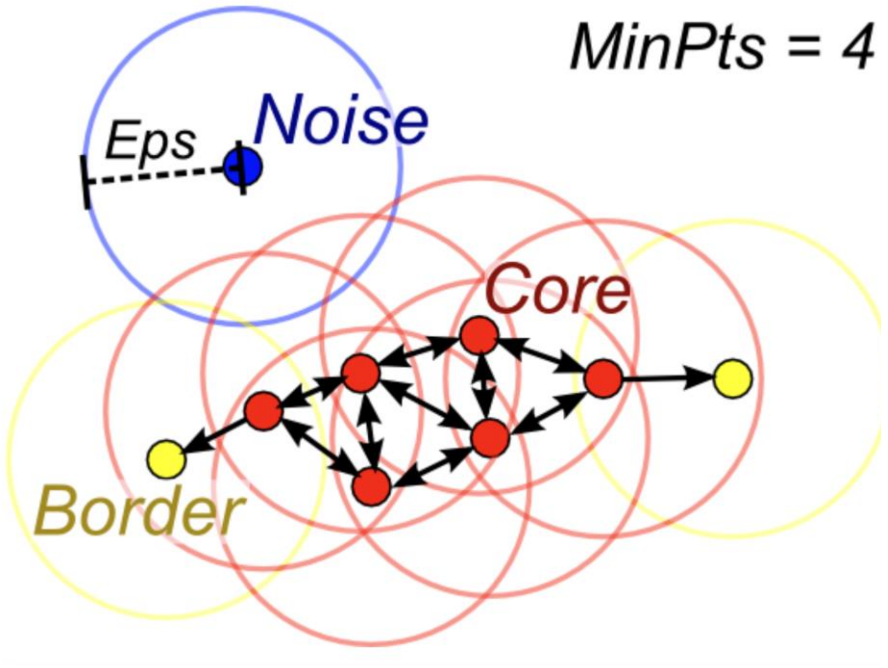
DBSCAN

Preparation: all points labeled as unvisited

Parameters: distance r, $\min\_\text{samples}$

1. Randomly select a unvisited point p, find its neighborhood within r
2. Number of points within $r \geq \min\_samples$?
    - Yes. p is a *core point*, Create a cluster C, go to step 3, mark p as *visited*.
    - No. Mark p as *noise* and *visited*.
3. Go through points within its r-neighborhood, label it as C
    - If it is a *core point*, set it as the "new p", repeat step-3
4. Remove cluster C from the database, go to step-1
5. Terminate when all points are visited.

DBSCAN



Red: Core points. point number within circle ≥ 4

Yellow: Border points. Still part of the cluster because it is within r of a core point, but does not meet the min_points criteria

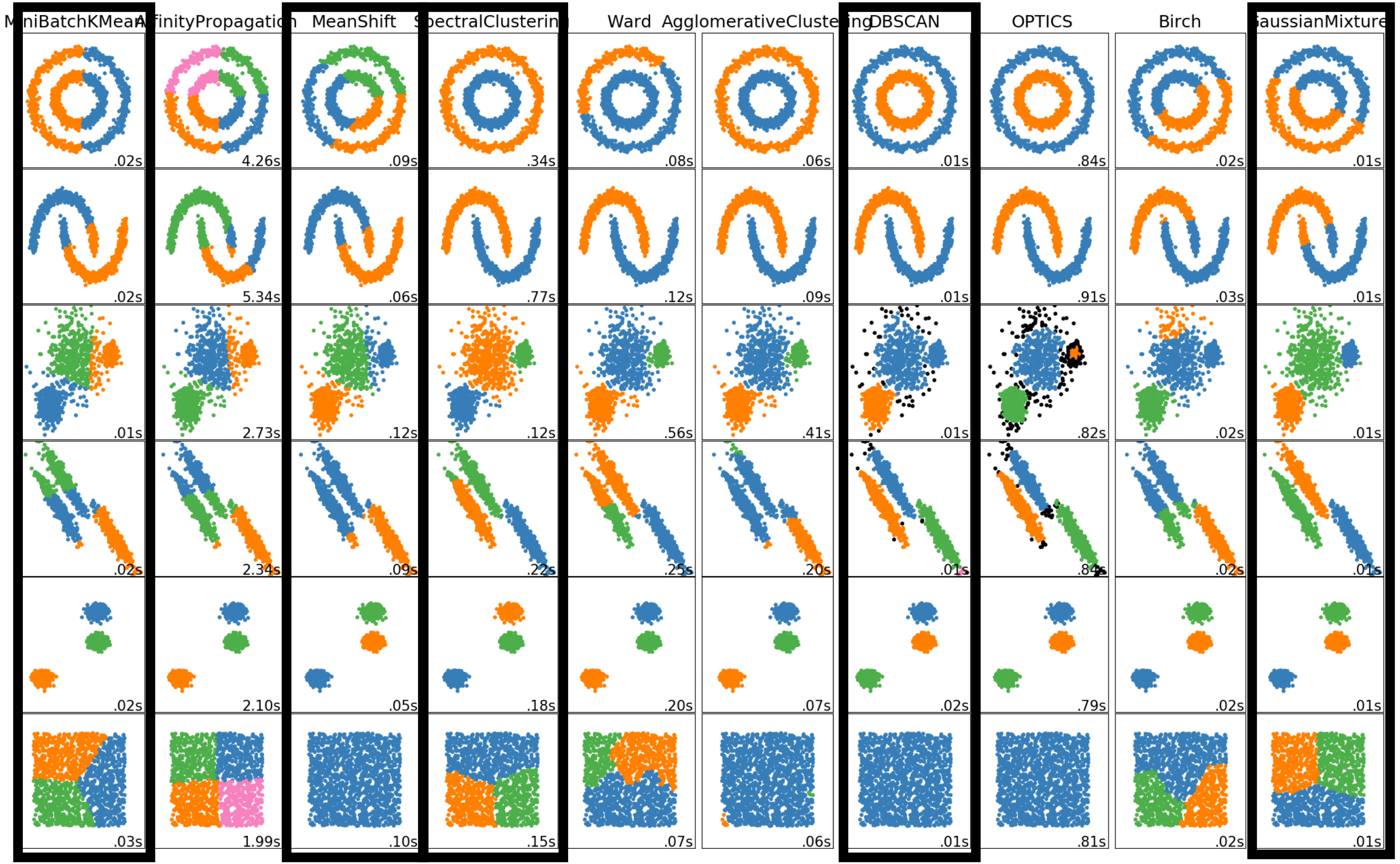
Blue: Noise point. Not assigned to a cluster.

DBSCAN – Summary

- Complexity $O(n \cdot \log(n))$
  - Radius NN search for each point
- Advantage
  - No assumption on cluster shape
  - Automatically determines cluster numbers
  - Robust to outliers
- Disadvantage
  - Doesn’t work well with varying density
    - DBSCAN assume high density clusters are separated by some low density points
  - Mainly works in Euclidean space
  - Doesn’t scale with high dimensional data

Clustering - Summary

	K-Means	GMM	Spectral	Mean Shift	DBSCAN
Metric	Euclidean	Euclidean	Similarity	Density /Euclidean	Density /Euclidean
# of clusters	Pre-defined	Pre-defined	Heuristic	Automatic	Automatic
Robustness to outlier	Bad	Medium	Good	Good	Good
High dimension data	Medium	Medium	Good	Bad	Bad
Complexity	$O(t \cdot k \cdot n \cdot d)$ t: iteration k: # of clusters n: # of data d: dimension	$O(t \cdot k \cdot n \cdot d)$ t: iteration k: # of clusters n: # of data d: dimension	$O(n^3)$ n: # of data	$O(Tnlog(n))$ n: # of data T: # of centers	$O(n \cdot \log(n))$ n: # of data

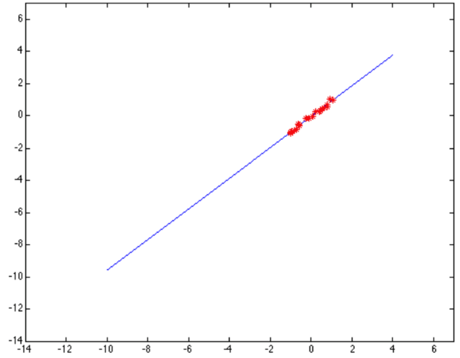

MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
AgglomerativeClustering
DBSCAN
OPTICS
Birch
GaussianMixture
.02s
4.26s
.09s
.34s
.08s
.06s
.01s
.84s
.02s
.01s
.02s
5.34s
.06s
.77s
.12s
.09s
.01s
.91s
.03s
.01s
.01s
2.73s
.12s
.12s
.56s
.41s
.01s
.82s
.02s
.01s
.02s
2.34s
.09s
.22s
.25s
.20s
.01s
.84s
.02s
.01s
.02s
2.10s
.05s
.18s
.20s
.07s
.02s
.79s
.02s
.01s
.03s
1.99s
.10s
.15s
.07s
.06s
.01s
.81s
.02s
.01s

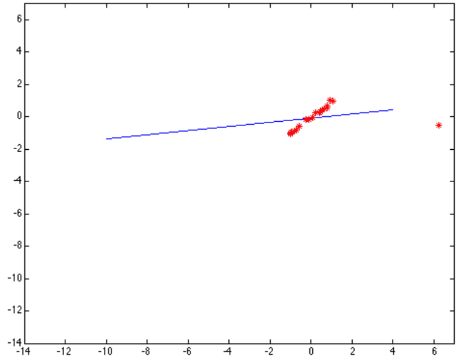
Model Fitting

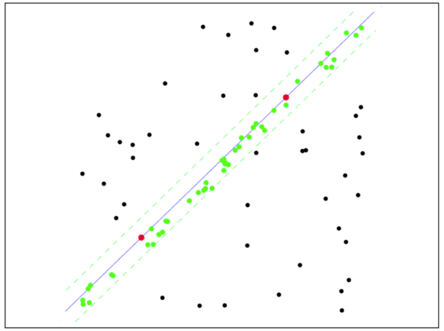
- Take line fitting as example
- Approaches:
  - Least Square
  - Hough Transform
  - Random Sample Consensus (RANSAC)

Model Fitting

- If we know the inlier points
  - Least Square
- What if there is small amount of outliers?
  - Robust Least Square, e.g., robust loss function
  - Hough Transform
  - RANSAC
- What if there are lots of outliers / more than one models in data?
  - Hough Transform
  - RANSAC



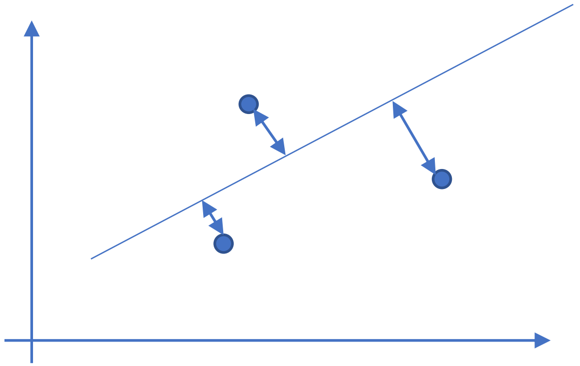




Least Square Fitting

- Given a set of points $\{p_1, \cdots p_n\}$, fine a line that fit the point set best.
- Consider 2-dimension, $p_i \in \mathbb{R}^2$, line model is $ax + by + c = 0$
- Definition of “fit” – minimize the perpendicular distance

$$E = \sum_{i=1}^{n} (ax_i + by_i + c)^2$$



Least Square Fitting

- Re-organize the problem into standard least-square optimization (sometimes called homogeneous equations):

$$\hat{\mathbf{x}} = [\hat{a}, \hat{b}, \hat{c}]^T = \min_{\mathbf{x}} \|A\mathbf{x}\|_2^2, \text{ s.t. } \|\mathbf{x}\|_2 = 1$$

$$A = \begin{bmatrix} x_1 & y_1 & 1 \\ \vdots & \vdots & \vdots \\ x_n & y_n & 1 \end{bmatrix}, \mathbf{x} = [a, b, c]^T$$

- The solution is obvious: $[a, b, c]^T$ is the eigenvector of the smallest eigenvalues of A
  - Given A is full column rank, i.e., $n \geq 3$

Least Square Fitting

- Many model fitting problem can be formulated as least square (LSQ) optimization problem.
- Linear LSQ problem $A\mathrm{x} = 0$

$$\hat{\mathbf{x}} = \min_{\mathbf{x}} \|A\mathbf{x}\|_2^2, \text{s.t.}, \|\mathbf{x}\|_2 = 1\ , A \in \mathbb{R}^{n\times m},\ \mathbf{x} \in \mathbb{R}^m$$

  - Solution given by eigenvector of the smallest eigenvalue of A

- Linear LSQ problem $A\mathrm{x} = \mathrm{b}$:

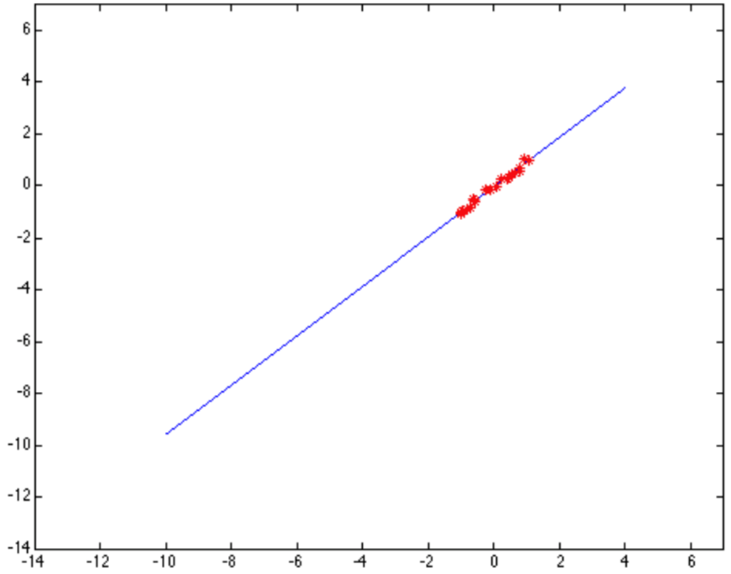
$$\hat{\mathbf{x}} = \min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|_2^2,\ A \in \mathbb{R}^{n\times m},\ \mathbf{x} \in \mathbb{R}^m,\ \mathbf{b} \in \mathbb{R}^n$$

  - In the case that $n \geq m$, the solution is given by $\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}$

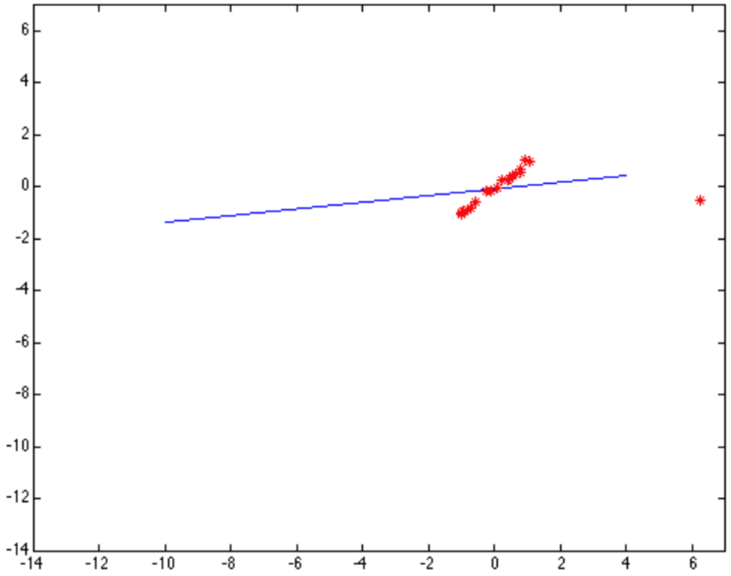
- Linear LSQ problem $A\mathrm{x} = \mathrm{b}$, s.t., $C\mathrm{x} = 0$

Limitations of LSQ

- Sensitive to Outlier



LSQ with No Outlier

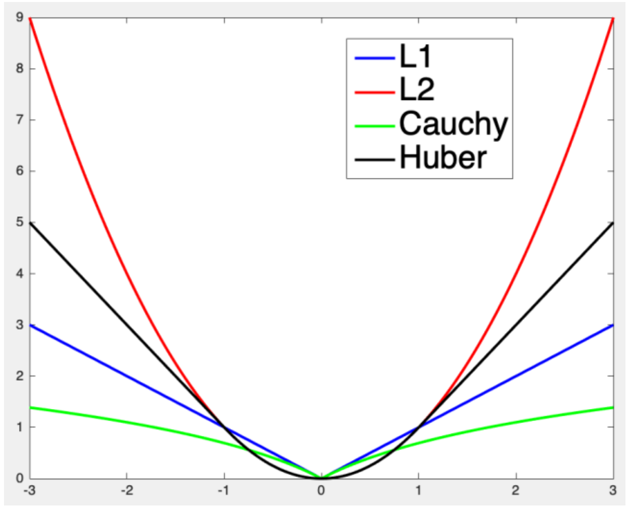


LSQ with One Outlier

Loss functions

Typical loss functions

- L1. $\rho = |s|$
- L2. $\rho = s^2$
- Cauchy. $\rho = \log(1 + |s|)$
- Huber. $\rho = \begin{cases} s^2, & |s| < \delta \\ 2\delta(|s| - \frac{1}{2}\delta), & otherwise \end{cases}$
- etc.



Robust loss functions like Huber, Cauchy reduce the effect of outliers

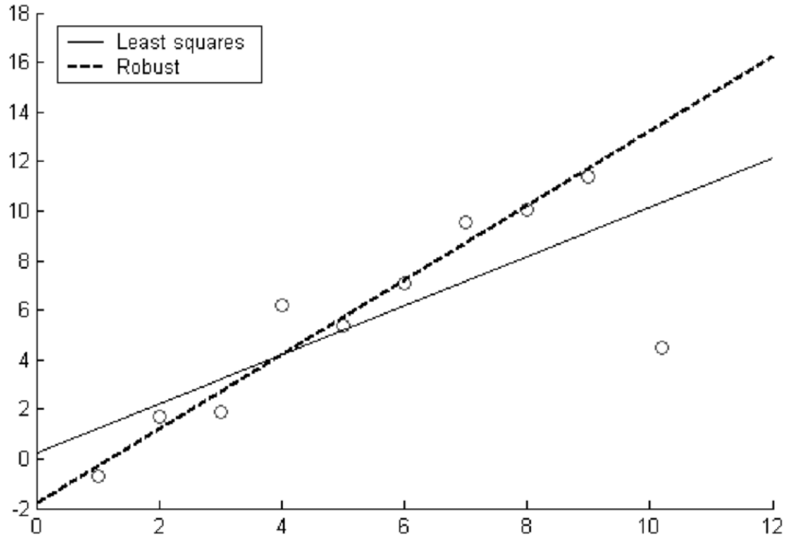
However, the problem becomes *non-linear*!

Non-Linear LSQ

- A general formulation of LSQ

$$\hat{\mathbf{x}} = \min_{\mathbf{x}} \|f(\mathbf{x})\|^2$$

- Function f is the non-linear function
  - e.g., coupling the robust loss function with linear LSQ
- Optimization methods
  - Gradient descent
  - Gauss-Newton
  - Levenberg-Marquardt



Model Fitting

- Least Square / Robust Least Square
  - No outlier / few outlier
  - Simple and fast
- What if:
  - Lots of outliers
  - More than one models in the data, e.g., more than one line.
- Hough Transform
- Random Sample Consensus (RANSAC)

Hough Transform

- Discretize parameter spaces into bins
- For each data point, vote the bins that can generate this data point
- Find the bins with most votes

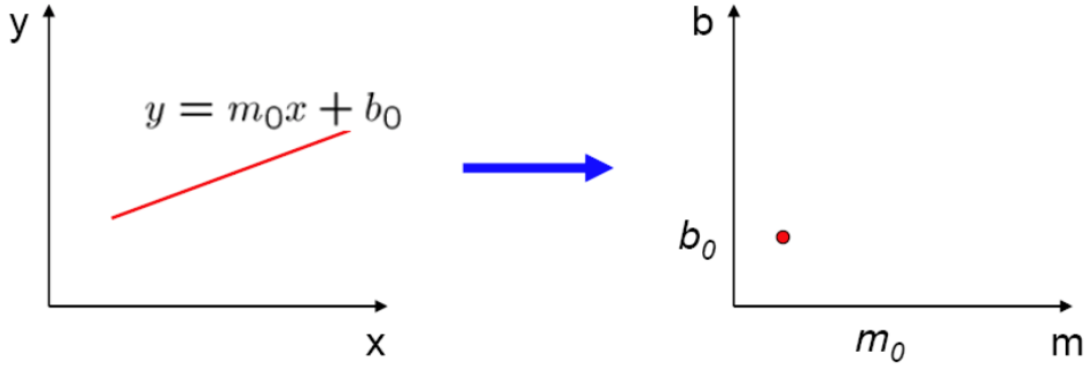
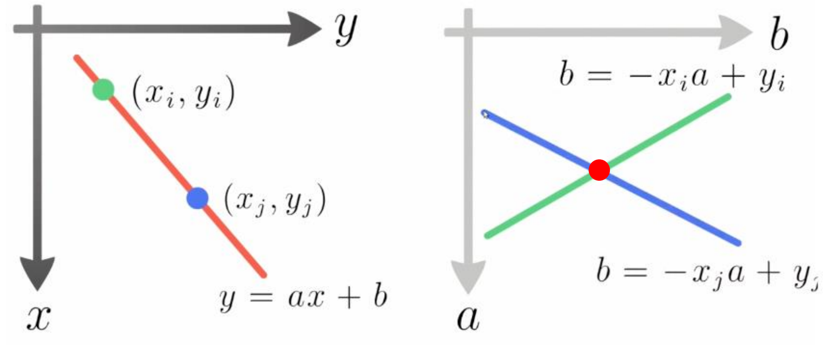


Image space

Line parameter space

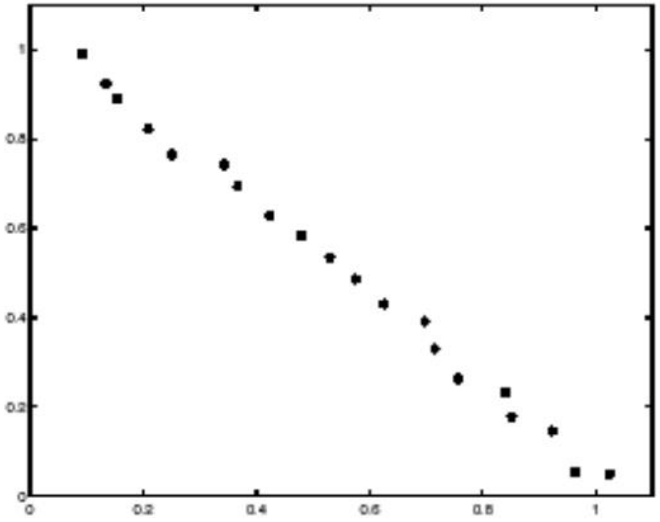
Hough Transform

- A point in the Euclidean space → A line in the parameter space
- Select the bin with most votes

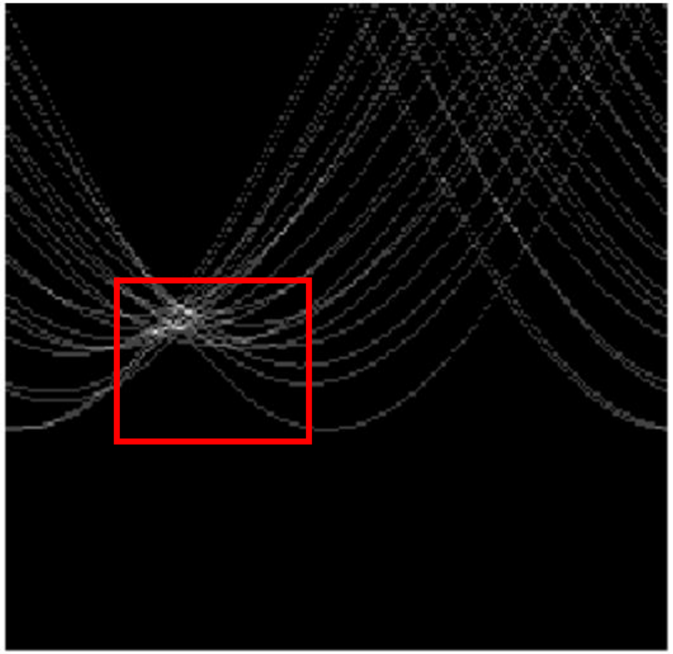


Hough Transform – Effect of Noise

Blurred peak
– in accurate parameter estimation



features



votes

Hough Transform

- Model parameterization. E.g., for a line
  - $y = ax + b$ is non-uniform, can’t represent vertical lines (a is infinity)
  - $xcos\theta + ysin\theta = r$ is a better model with parameters $\{\theta, r\}$
- Selection of resolution
  - Tradeoff between speed and precision
- Apply smoothing at the parameter space before searching for the highest vote
  - E.g., Gaussian smooth
  - Reduce the effect of noise

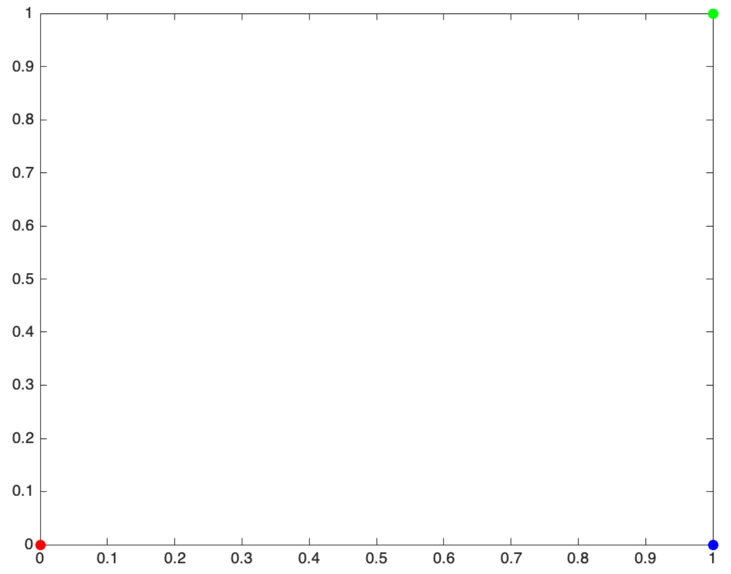
Hough Transform – Extension for Circles

- The circle model with parameters $\{a, b, r\}$

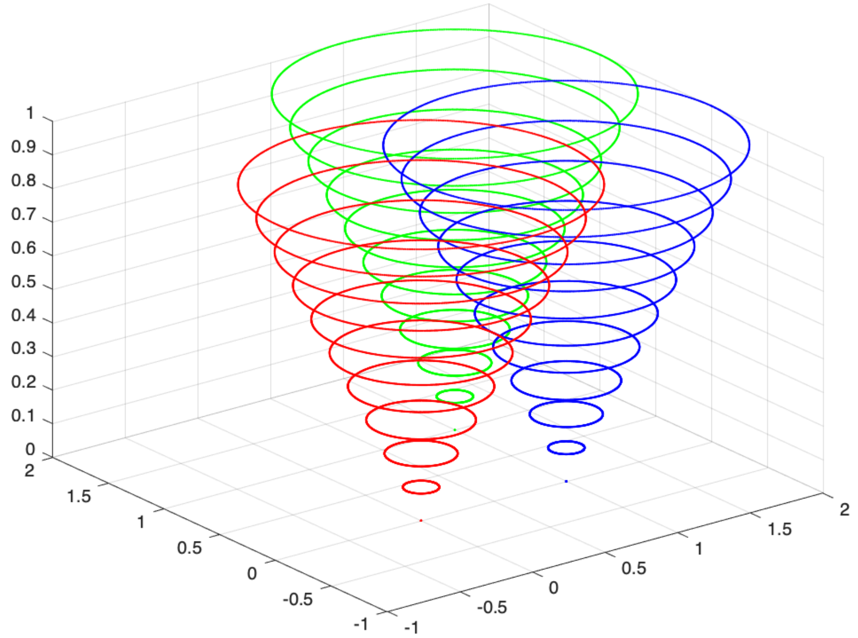
$$(x-a)^2 + (y-b)^2 = r^2$$

- Each point (x, y) fills a set of parameter bins for $\{a, b, r\}$ that fulfills the above function.
- How to find those bins?
  - Fix $r = r_i$
  - Uniformly sample a set of $\{\theta_1, \cdots \theta_k\}$
  - Each θ_j generates a set of $\{a, b\}$
    - $a = x - r_i \cos \theta_j$
    - $b = y - r_i \sin \theta_j$

Hough Transform – Extension for Circles



3 points in Euclidean space: [0, 0], [1,1], [1, 0]



Each point corresponds to a ”cone” in Hough space

Hough Transform – Summary

Advantage

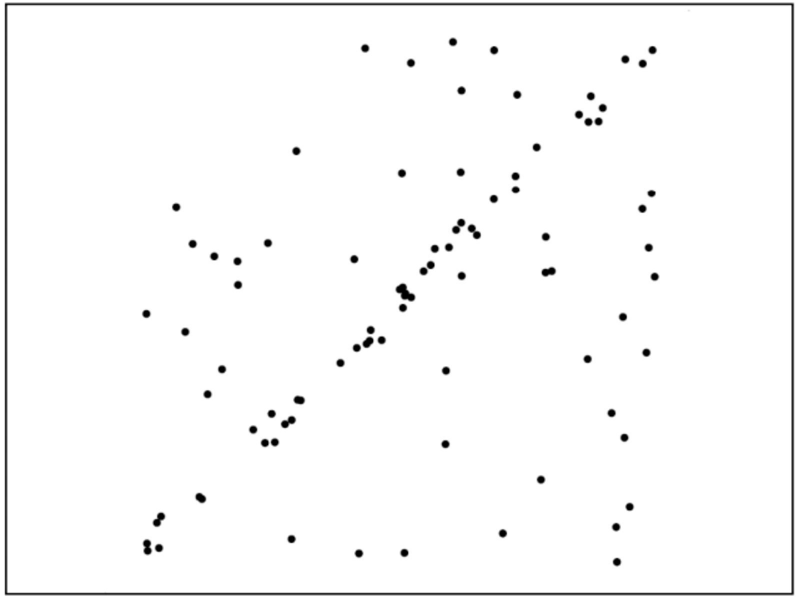
- Robust to noise
- Robust to missing points of the shape
- Can be extended to lots of models

Disadvantage

- Doesn’t scale well with complicated models
  - Usually works for models with less than 3 unknown parameters

RANSAC

- Simple and works well in practice
- Works well with complicated models



RANSAC – Line Fitting

1. Randomly select a sample (minimal subset of points required to solve the model)

$$p_0 = (x_0, y_0), p_1 = (x_1, y_1)$$

2. Solve the line model

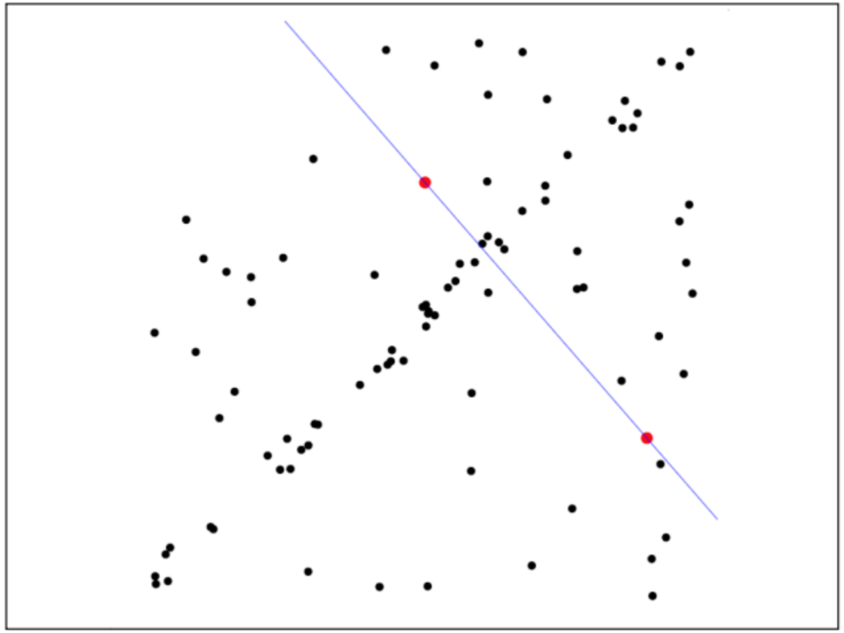
$$x = x_0 + at$$
$$y = y_0 + bt$$

where,

$$p_0 = [x_0, y_0]^T, n = [a, b]^T$$

$$\Delta x = x_1 - x_0, \Delta y = y_1 - y_0$$

$$\Delta x = at, \Delta y = bt \rightarrow \frac{\Delta x}{\Delta y} = \frac{a}{b}$$



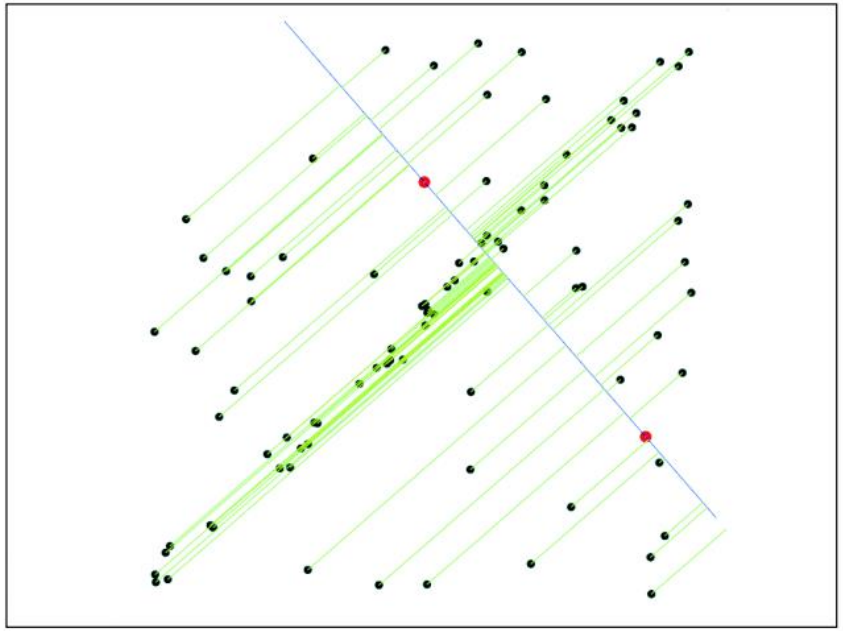
RANSAC – Line Fitting

1. Randomly select a minimal subset of points required to solve the model

2. Solve the model

3. Compute error function for each point $p_i = (x_i, y_i)$

$$d_i = \frac{n^T(\mathrm{p_i} - \mathrm{p_0})}{\|n\|_2}$$



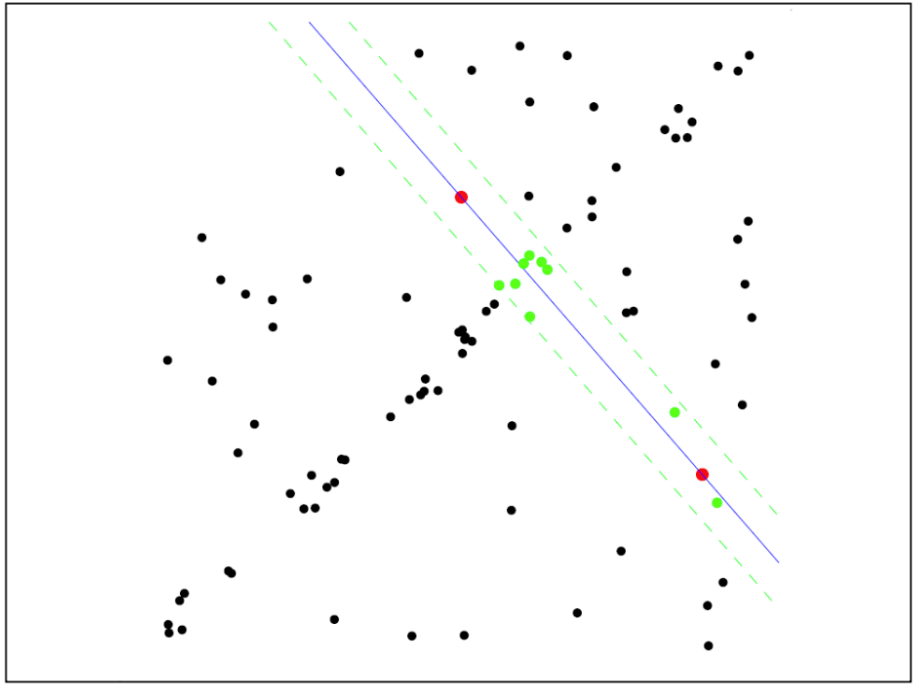
RANSAC – Line Fitting

1. Randomly select a minimal subset of points required to solve the model

2. Solve the model

3. Compute error function for each point $p_i = (x_i, y_i)$

4. Count the points consistent with the model, $d_i < \tau$ (inlier)



RANSAC – Line Fitting

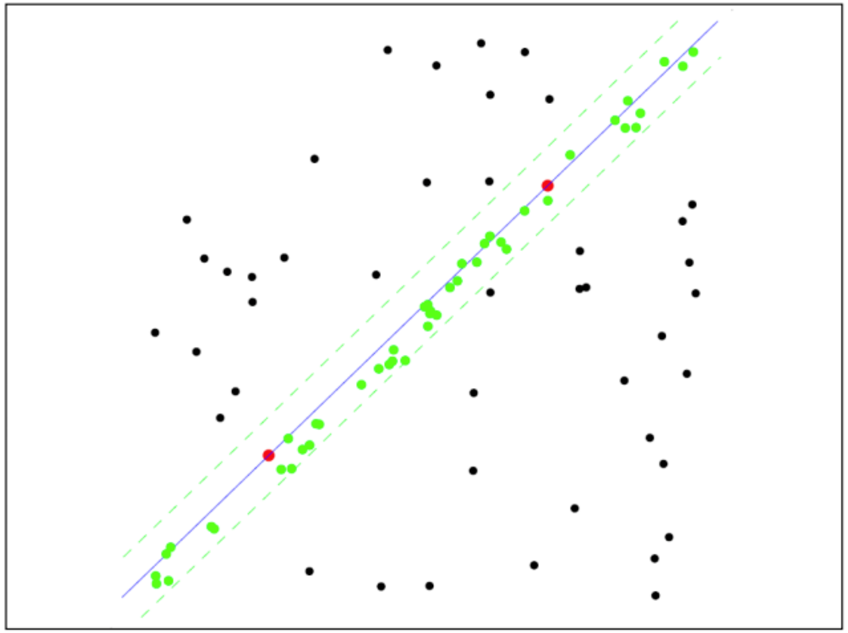
1. Randomly select a minimal subset of points required to solve the model

2. Solve the model

3. Compute error function for each point $p_i = (x_i, y_i)$

4. Count the points consistent with the model, $d_i < \tau$

5. Repeat step 1-4 for N iterations, choose the model with most inlier points



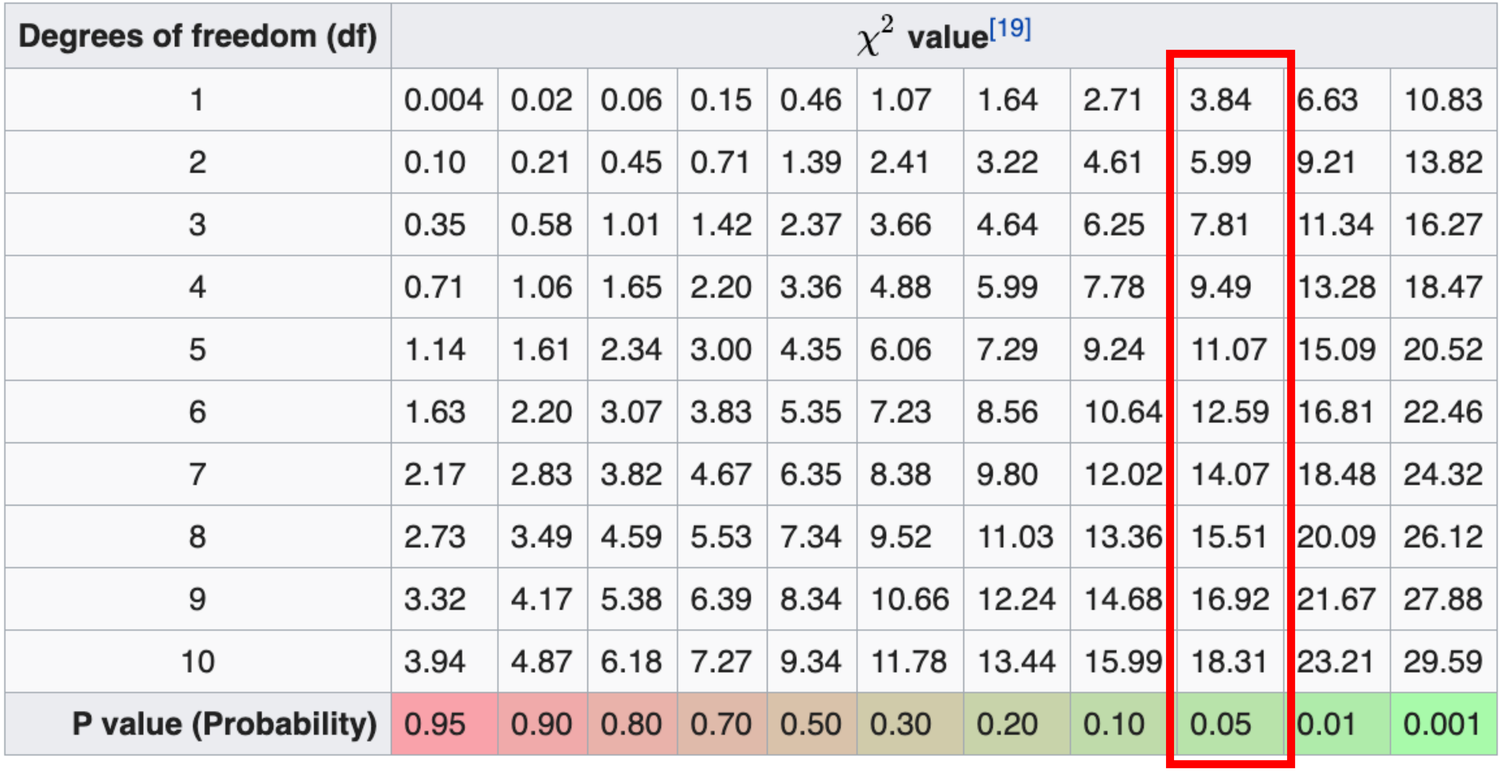
RANSAC – Line Fitting

- Distance threshold τ
  - Usually chosen empirically
  - Chi-square distribution χ^2
- Number of iterations N
  - Choose N so that with probability p, as least one random sample is free from outliers, e.g., $p = 0.99$

RANSAC – Threshold τ by χ^2

- Assume the error between data point and model is Gaussian distribution $d \sim \mathcal{N}(0, \sigma^2)$
- χ^2 distribution – sum of squares of k independent standard normal distribution. Assume 95% confidence that the point is an inlier
  - 1DoF χ_1^2 for 2D/3D line fitting or 3D plane fitting. The error is perpendicular distance
    - $\tau = \sqrt{3.84\sigma^2}$
  - 2DoF χ_2^2 for 2D point distance, because the distance is $\Delta x^2 + \Delta y^2$
    - $\tau = \sqrt{5.99\sigma^2}$
  - 3DoF χ_3^2 for 3D point distance, because the distance is $\Delta x^2 + \Delta y^2 + \Delta z^2$
    - $\tau = \sqrt{7.81\sigma^2}$

RANSAC – Threshold τ by χ^2



Degrees of freedom (df)	χ^2 value[19]										
1	0.004	0.02	0.06	0.15	0.46	1.07	1.64	2.71	3.84	6.63	10.83
2	0.10	0.21	0.45	0.71	1.39	2.41	3.22	4.61	5.99	9.21	13.82
3	0.35	0.58	1.01	1.42	2.37	3.66	4.64	6.25	7.81	11.34	16.27
4	0.71	1.06	1.65	2.20	3.36	4.88	5.99	7.78	9.49	13.28	18.47
5	1.14	1.61	2.34	3.00	4.35	6.06	7.29	9.24	11.07	15.09	20.52
6	1.63	2.20	3.07	3.83	5.35	7.23	8.56	10.64	12.59	16.81	22.46
7	2.17	2.83	3.82	4.67	6.35	8.38	9.80	12.02	14.07	18.48	24.32
8	2.73	3.49	4.59	5.53	7.34	9.52	11.03	13.36	15.51	20.09	26.12
9	3.32	4.17	5.38	6.39	8.34	10.66	12.24	14.68	16.92	21.67	27.88
10	3.94	4.87	6.18	7.27	9.34	11.78	13.44	15.99	18.31	23.21	29.59
P value (Probability)	0.95	0.90	0.80	0.70	0.50	0.30	0.20	0.10	0.05	0.01	0.001

https://en.wikipedia.org/wiki/Chi-squared_distribution

RANSAC – Number of Iterations N

- e: outlier ratio (probability that a point is an outlier)
- s: number of points in a sample (e.g., in line fitting a sample contains 2 points)
- N: sample number N (number of RANSAC iteration)
- p: confidence we get at least a good sample that is free from outliers

$$\Big(1-\underbrace{(1-e)^s}_{\text{Probability of choosing s inliers in a row}}\Big)^N = 1-p$$

$$\Big(\underbrace{1-(1-e)^s}_{\text{Probability that one or more points are outliers}}\Big)^N = 1-p$$

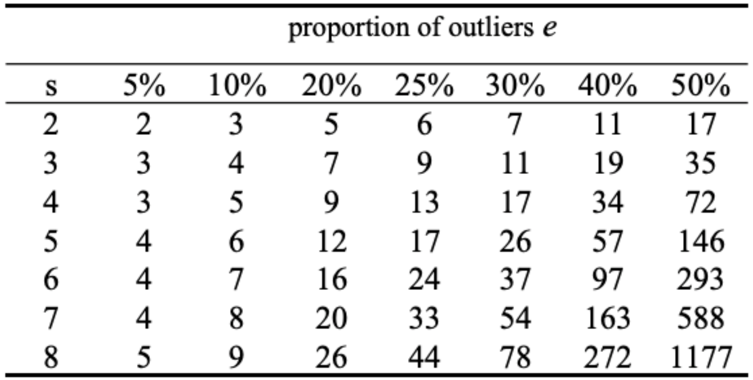
$$\underbrace{\Big(1-(1-e)^s\Big)^N}_{\text{Probability that N samples are contaminated}} = 1-p$$

RANSAC – Number of Iterations N

- Iteration number N is given by

$$N = \frac{log(1-p)}{log(1-(1-e)^s)}$$

- Table for $p = 0.99$



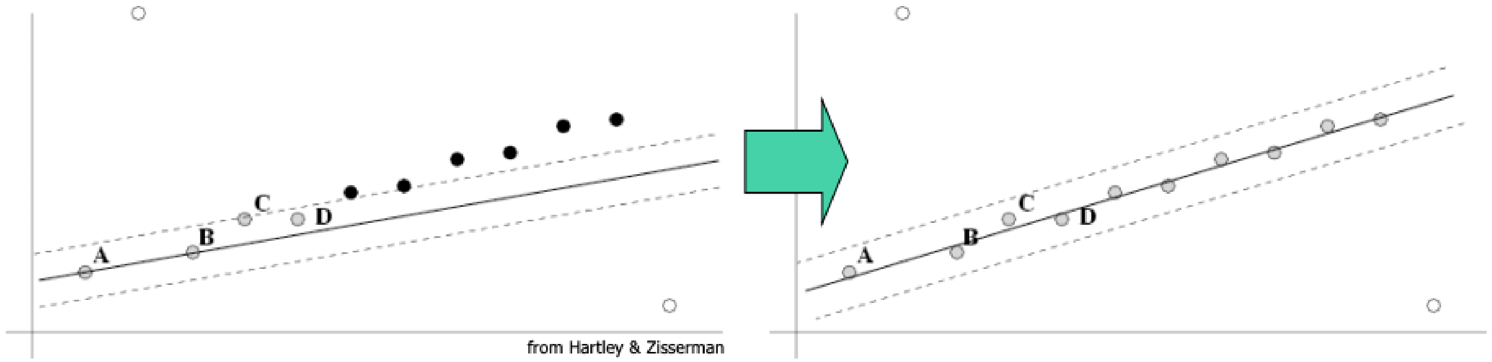
	proportion of outliers e						
s	5%	10%	20%	25%	30%	40%	50%
2	2	3	5	6	7	11	17
3	3	4	7	9	11	19	35
4	3	5	9	13	17	34	72
5	4	6	12	17	26	57	146
6	4	7	16	24	37	97	293
7	4	8	20	33	54	163	588
8	5	9	26	44	78	272	1177

RANSAC - Practical Tricks

- Don’t need to perform N samples/iterations
  - Terminate when the inlier ratio reach the expected inlier ratio

$$T = (1 - e) \cdot total\_num\_of\_data\_points$$

- Run LSQ to refine the model after selecting the final model and inlier points



RANSAC - Summary

Advantages

- Simple and general
- Usually works well in practice, even with low inlier ratio like 10%

Disadvantages

- Need to determine the inlier threshold τ
- Need large number of samples when inlier ratio is low

Homework

Object detection pipeline for lidar

- Use KITTI 3D object detection dataset, select 3 point clouds, do the followings.
- Step 1. Remove the ground from the lidar points. Visualize ground as blue.
    - Any method you want – LSQ, Hough, RANSAC
- Step 2. Clustering over the remaining points. Visualize the clusters with random colors.
    - Any method you want
- Step 3. Classification over the clusters
    - Homework of Lecture 5
- Step 4. Report the detection precision-recall for three categories: vehicle, pedestrian, cyclist
    - Homework of Lecture 5