Ch 12.1, 12.4: Unsupervised Learning & Clustering

Lecture 32 - CMSE 381

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Mon, Apr 14, 2025

Announcements

Last time:

- Convolutional Neural Nets

This lecture:

- Clustering (Just hierarchical clustering)

Announcements:

- No more homework!
- Weds: Project office hours, zoom only!
- Fri Apr 18 : Review - Bring questions!
- Mon Apr 21: Exam
  - Content since 2nd Exam (Ch 7 and on)
  - One page (8.5x11) handwritten cheat sheet
  - Calculator if you want it

21	W	3/19	Polynomial & Step Functions	7.1-7.2		
22	F	3/21	Step Functions; Basis functions; Start Splines	7.2-7.4		
23	M	3/24	Regression Splines	7.4		
24	W	3/26	Decision Trees	8.1	HW #6 Due Wed 3/26	Q7
25	F	3/28	Random Forests	8.2.1, 8.2.2	HW #7 Due Sun 3/30	
26	M	3/31	Maximal Margin Classifier	9.1		
27	W	4/2	SVC	9.2		Q8
28	F	4/4	SVM	9.3, 9.4	HW #8 Due Sun 4/6	
29	M	4/7	Single Layer NN	10.1		
30	W	4/9	Multi Layer NN	10.2		Q9
31	F	4/11	CNN	10.3	HW #9 Due Sun 4/13	
32	M	4/14	Unsupervised learning / clustering	12.1, 12.4		
33	W	4/16	Virtual: Project Office Hours			Q10
	F	4/18	***Review***			
	M	4/21	**Midterm #3**			
	W	4/23				
	F	4/25			**Project Due**	
			No final exam			

Section 1

Unsupervised learning

Supervised vs Unsupervised Learning

Supervised

Unupervised

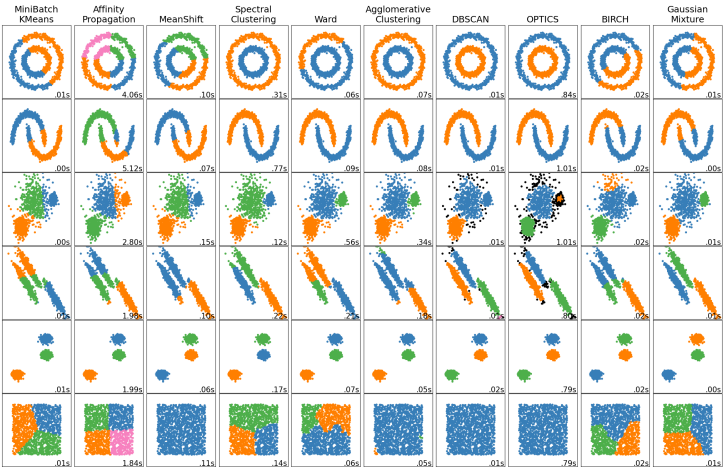
Some examples of unsupervised problems

- Assay gene expression levels in 100 patients with breast cancer, looking for subgroups with similar qualities
- Online shopping: find groups of shoppers with similar browsing and purchase histories and show relevant related products.
- Search engine picking results to show

Section 2

Clustering

Big idea


MiniBatch KMeans
Affinity Propagation
MeanShift
Spectral Clustering
Ward
Agglomerative Clustering
DBSCAN
OPTICS
BIRCH
Gaussian Mixture
.01s
4.06s
.10s
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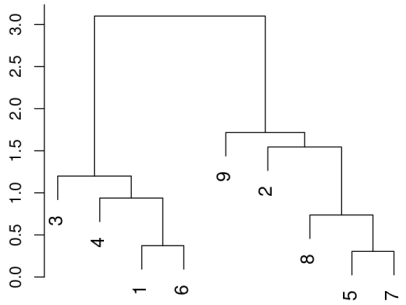
Section 3

Hierarchical Clustering

Dendrogram


0.0
0.5
1.0
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3
4
1
6
9
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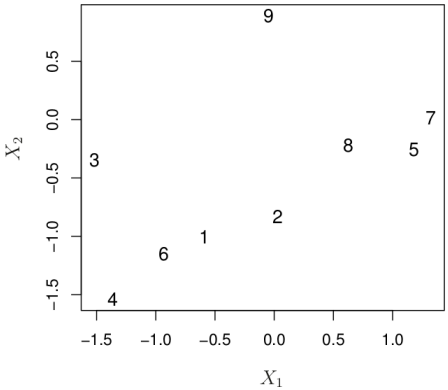
8
5
7


9
7
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0.5
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−0.5
−1.0
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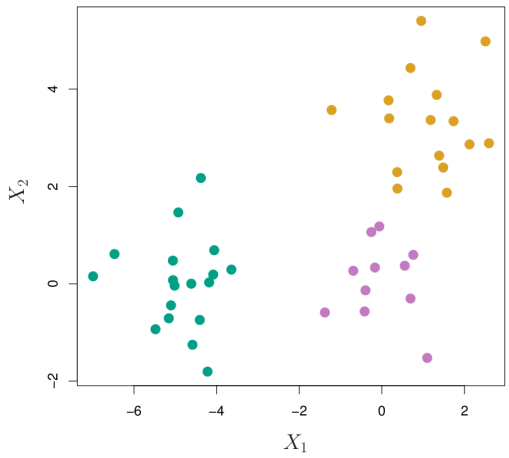
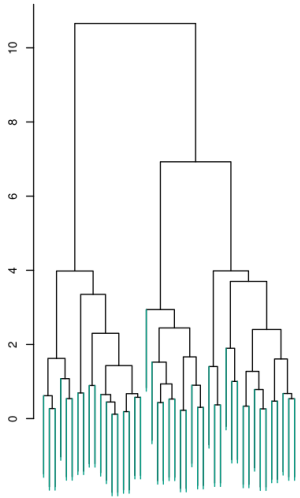
−0.5
0.0
0.5
1.0
X_2
X_1

A bigger example

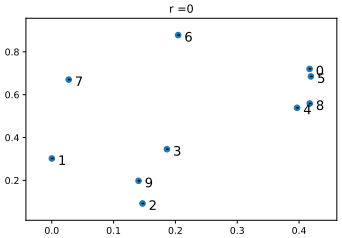


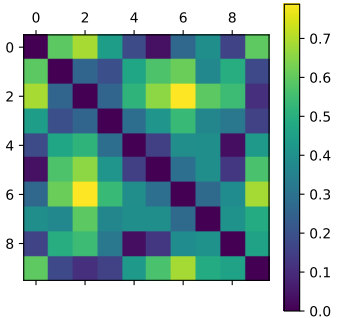


Single linkage

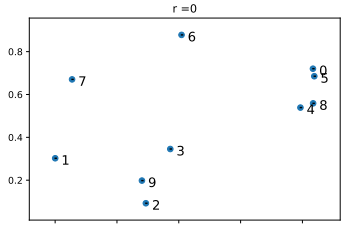
Distance between cluster A and cluster B:
Smallest distance between the points

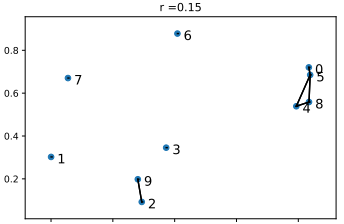
$$L(A, B) = \min_{a \in A, b \in B} \|a - b\|$$

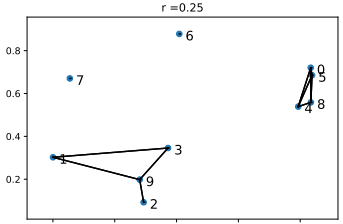


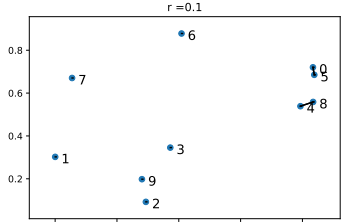


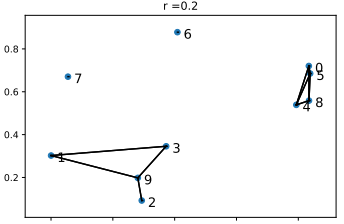
Building the dendrogram

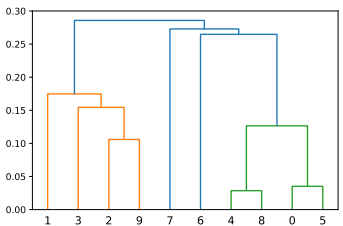




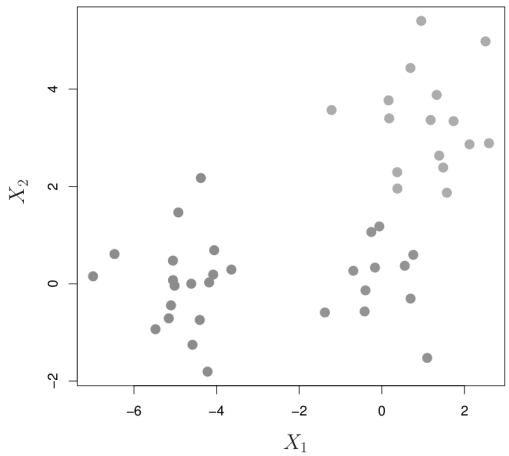


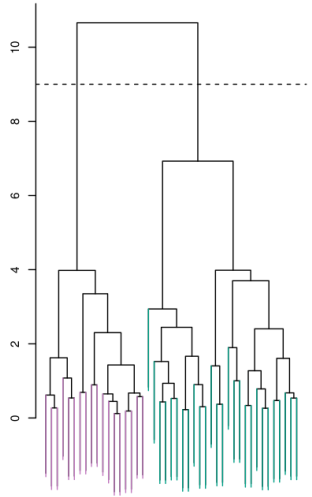




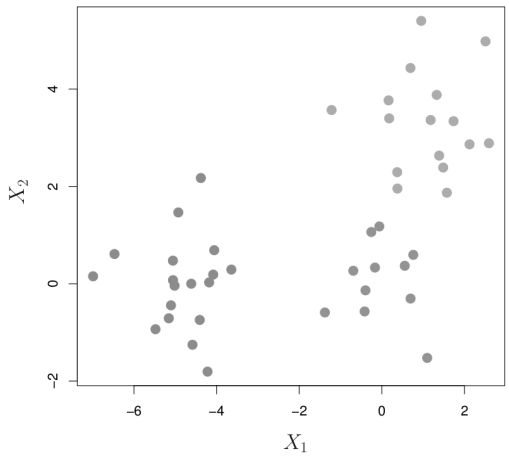


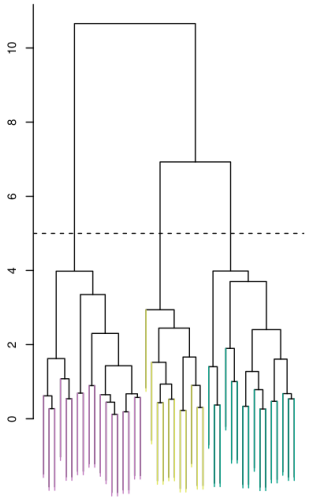
How to get clusters



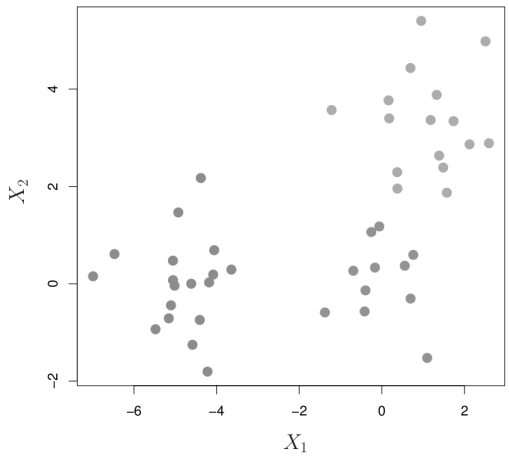


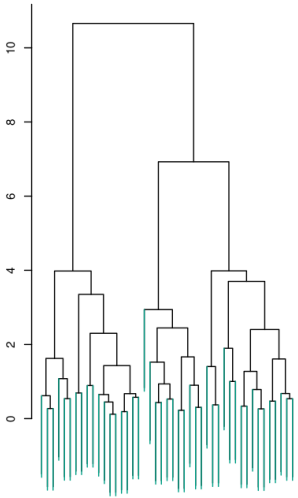
How to get different clusters





Can get any number of clusters

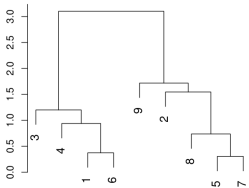




Linkage

Linkage	*Description*
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *largest* of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *smallest* of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *average* of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable *inversions*.

Example with complete linkage



Distance between cluster A and cluster B:
Largest distance between the points

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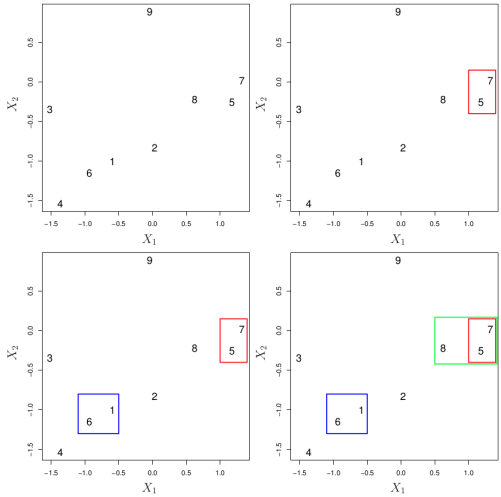
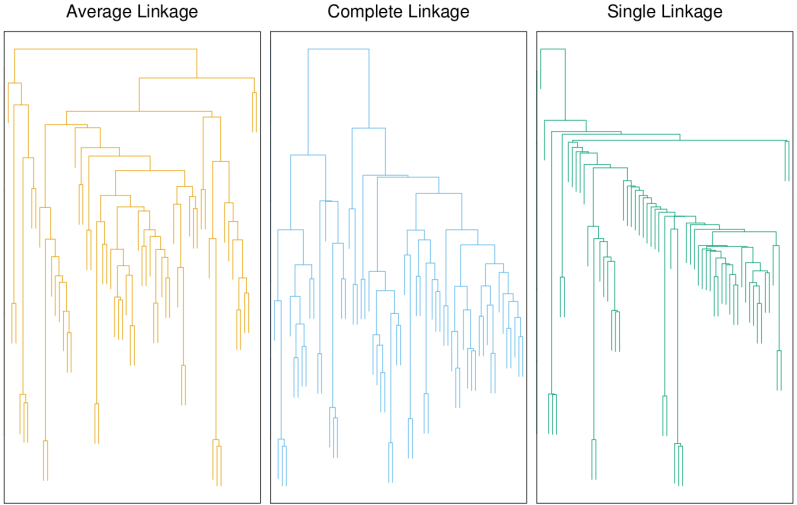


Examples of different linkage



Dependence on dissimilarity measure

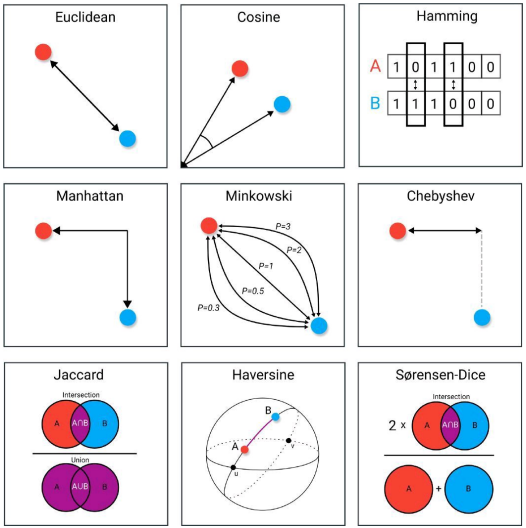


Photo Credit Link

Coding

Next time

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