Semi-supervised Learning

Introduction

Labelled data

cat

dog

Unlabeled data

(Image of cats and dogs without labeling)

Introduction

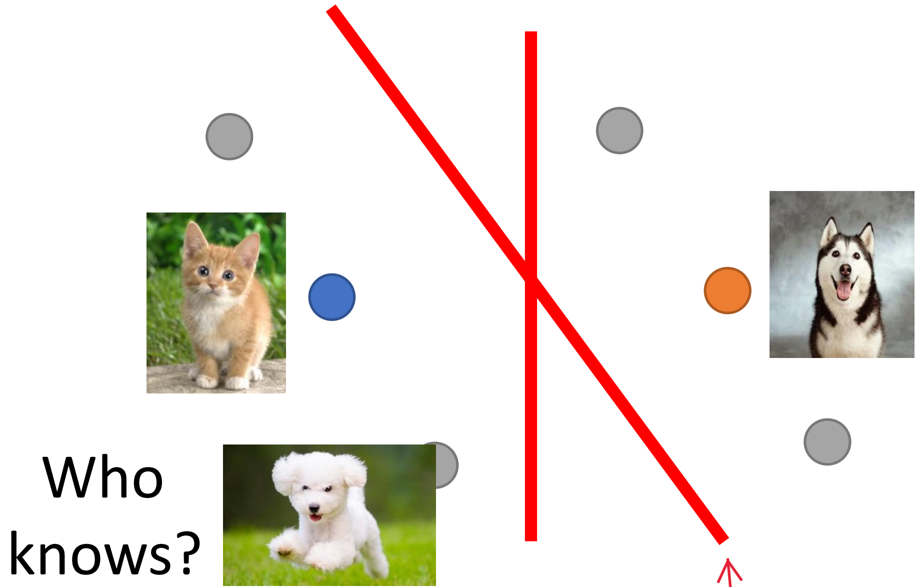
有一大堆的training data　　input - output (配對)

- Supervised learning: $\{(x^r, \hat{y}^r)\}_{r=1}^{R}$
  - E.g. x^r: image, $\hat{y}^r$: class labels

unlabel data，只有input

- Semi-supervised learning: $\{(x^r, \hat{y}^r)\}_{r=1}^{R}$, $\{x^u\}_{u=R}^{R+U}$
  - A set of unlabeled data, usually U >> R 通常希望unlabel的數量>label的數量
  - 1. Transductive learning: unlabeled data is the testing data 用feature
  - 2. Inductive learning: unlabeled data is not the testing data
- Why semi-supervised learning?
  - 不缺data，式缺有label的data
  - Collecting data is easy, but collecting "labelled" data is expensive
  - We do semi-supervised learning in our lives

Why semi-supervised learning helps?



灰色原點

The distribution of the unlabeled data tell us ***something***.

Usually with some assumptions

semi-supervised learning有沒有用取決於假設成立與否

Outline

Semi-supervised Learning for Generative Model

Low-density Separation Assumption

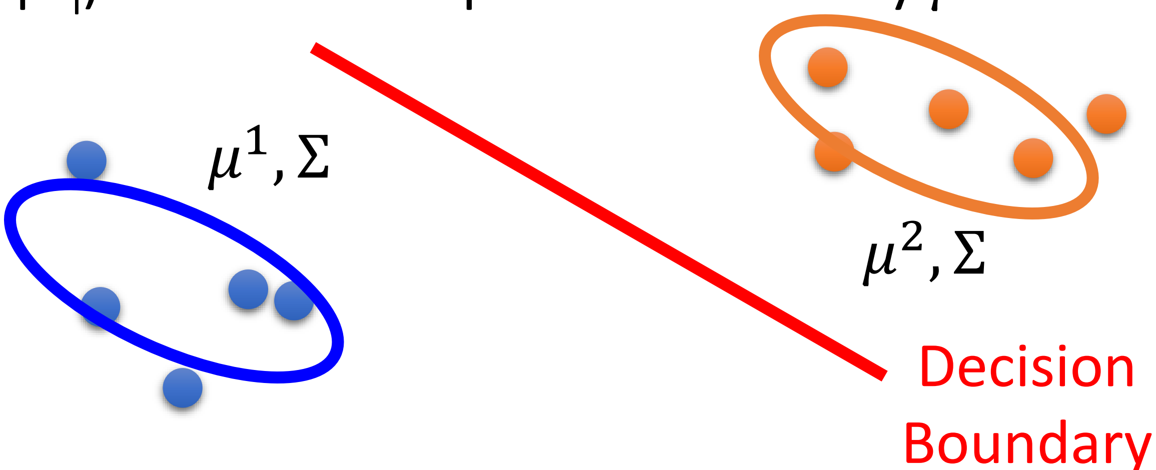
Smoothness Assumption

Better Representation

Semi-supervised Learning for Generative Model

Supervised Generative Model

- Given labelled training examples $x^r \in C_1, C_2$
  - looking for most likely prior probability $P(C_i)$ and class-dependent probability $P(x|C_i)$
  - $P(x|C_i)$ is a Gaussian parameterized by μ^i and Σ

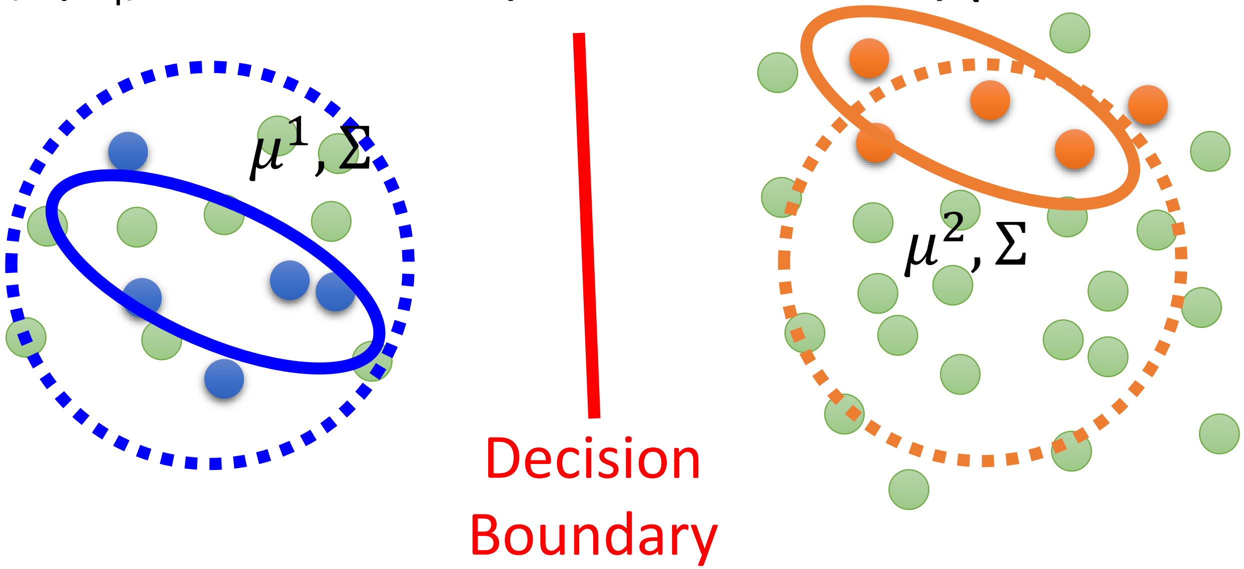


With $P(C_1)$, $P(C_2)$,μ^1,μ^2, Σ

$$P(C_1|x) = \frac{P(x|C_1)P(C_1)}{P(x|C_1)P(C_1) + P(x|C_2)P(C_2)}$$

Semi-supervised Generative Model

- Given labelled training examples $x^r \in C_1, C_2$
  - looking for most likely prior probability $P(C_i)$ and class-dependent probability $P(x|C_i)$
  - $P(x|C_i)$ is a Gaussian parameterized by μ^i and Σ



The unlabeled data x^u help re-estimate $P(C_1)$, $P(C_2)$, μ^1,μ^2, Σ

Semi-supervised Generative Model

The algorithm converges eventually, but the initialization influences the results.

- Initialization: $\theta = \{P(C_1), P(C_2), \mu^1, \mu^2, \Sigma\}$

E

- Step 1: compute the posterior probability of unlabeled data

$$P_\theta(C_1|x^u)$$

Depending on model θ

Back to step 1

M

- Step 2: update model

$$P(C_1) = \frac{N_1 + \sum_{x^u} P(C_1|x^u)}{N}$$

N: total number of examples

N_1: number of examples belonging to C_1

$$\mu^1 = \frac{1}{N_1}\sum_{x^r \in C_1} x^r + \frac{1}{\sum_{x^u} P(C_1|x^u)} \sum_{x^u} P(C_1|x^u) x^u \quad \ldots\ldots$$

Why?

$$\theta = \{P(C_1), P(C_2), \mu^1, \mu^2, \Sigma\}$$

- Maximum likelihood with labelled data

$$logL(\theta) = \sum_{(x^r,\hat{y}^r)} logP_\theta(x^r|\hat{y}^r)$$

- Maximum likelihood with labelled + unlabeled data

$$logL(\theta) = \sum_{(x^r,\hat{y}^r)} logP_\theta(x^r|\hat{y}^r) + \sum_{x^u} logP_\theta(x^u)$$

Solved iteratively

$$\boxed{P_\theta(x^u) = P_\theta(x^u|C_1)P(C_1) + P_\theta(x^u|C_2)P(C_2)}$$

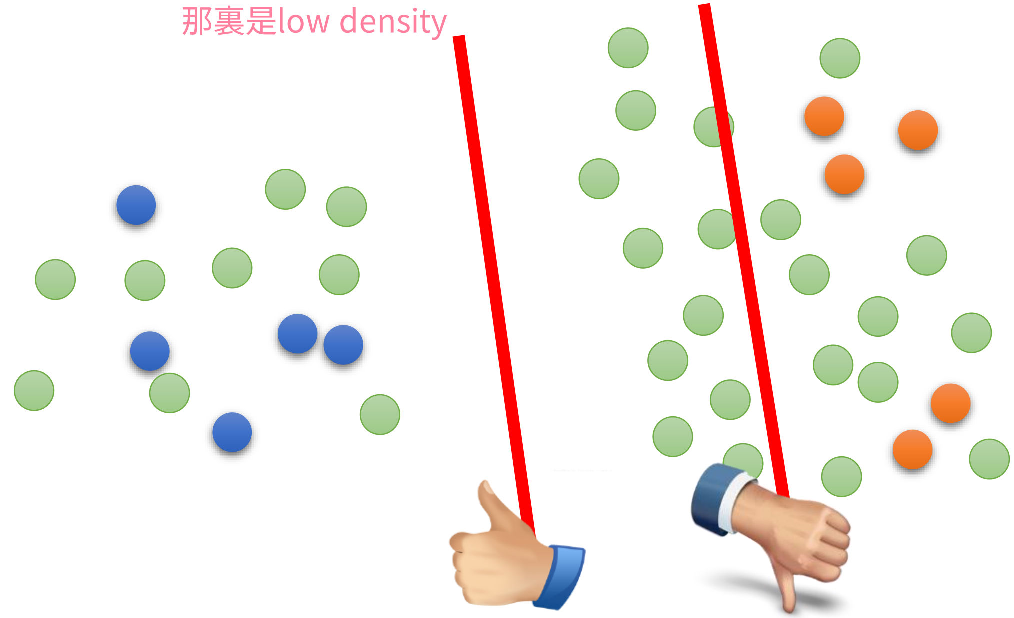
(x^u can come from either C_1 and C_2)

Semi-supervised Learning
Low-density Separation

雖然兩條線的正確率都是100%，但左邊的boundary比較好，因為那裏是low density

非黑即白

"Black-or-white"



Self-training

- Given: labelled data set = $\{(x^r, \hat{y}^r)\}_{r=1}^{R}$, unlabeled data set = $\{x^u\}_{u=1}^{U}$
- Repeat:
  - Train model f^* from labelled data set

回歸不能用self-training

You can use any model here.

Regression?

  - Apply f^* to the unlabeled data set
    - Obtain $\{(x^u, y^u)\}_{u=1}^{U}$

Pseudo-label

  - Remove a set of data from unlabeled data set, and add them into the labeled data set

How to choose the data set remains open

You can also provide a weight to each data.

Self-training

強制一筆data屬於某個class　　根據posterior probability部分屬於class1or2

- Similar to semi-supervised learning for generative model
- Hard label v.s. Soft label

Considering using neural network

θ^* (network parameter) from labelled data

Hard

$x^u \rightarrow \boxed{\theta^*} \rightarrow$ class1 $\begin{bmatrix} 0.7 \\ 0.3 \end{bmatrix}$ class2

Class 1 → New target for x^u is $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

It looks like class 1, then it is class 1.

Soft

70% Class 1
30% Class 2 → New target for x^u is $\begin{bmatrix} 0.7 \\ 0.3 \end{bmatrix}$

Doesn't work …

因為做一樣的事情

非黑即白太武斷?那接下來這個方法會好一點...(因為機率分布)

Entropy-based Regularization

input

output

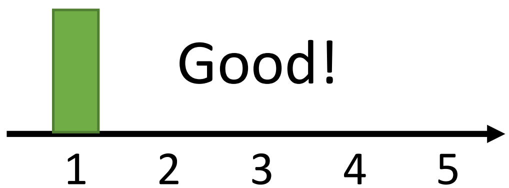
$x^u \rightarrow \boxed{\theta^*} \rightarrow y^u$

Distribution

一定要集中分布

y^u

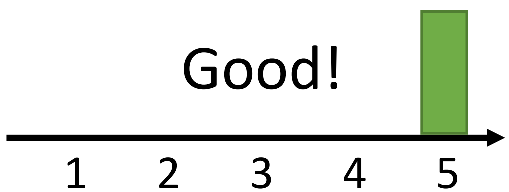
Good!



$E(y^u) = 0$

y^u

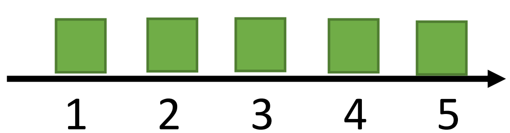
Good!



$E(y^u) = 0$

y^u

Bad!



$$E(y^u) = -ln\left(\frac{1}{5}\right) = ln5$$

算output的分布到底集不集中

Entropy of y^u :
Evaluate how concentrate the distribution y^u is

$$E(y^u) = -\sum_{m=1}^{5} y_m^u ln(y_m^u)$$

As small as possible

$$L = \sum_{x^r} C(y^r, \hat{y}^r)$$

labelled data

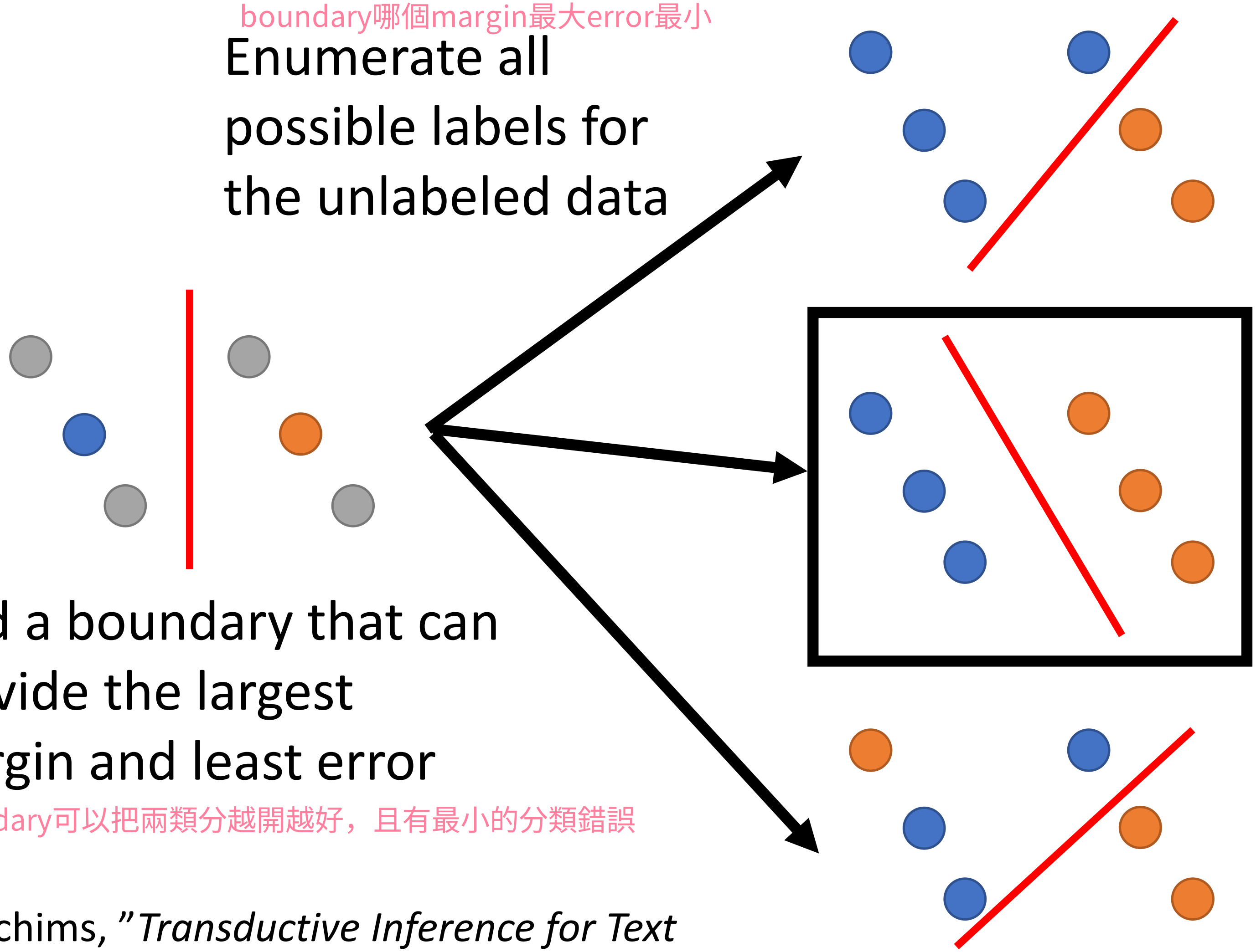
$$+\lambda \sum_{x^u} E(y^u)$$

unlabeled data

Outlook: Semi-supervised SVM

會窮舉所有可能的label，再看這些boundary哪個margin最大error最小

Enumerate all possible labels for the unlabeled data



Find a boundary that can provide the largest margin and least error

boundary可以把兩類分越開越好，且有最小的分類錯誤

Thorsten Joachims, *"Transductive Inference for Text Classification using Support Vector Machines"*, ICML, 1999

Semi-supervised Learning
Smoothness Assumption

近朱者赤，近墨者黑

“You are known by the company you keep”

Smoothness Assumption

- Assumption: "similar" x has the same $\hat{y}$
- More precisely:
  分布不平均
  - x is not uniform.
  - If x^1 and x^2 are close in a high density region, $\hat{y}^1$ and $\hat{y}^2$ are the same.

connected by a high density path

公館 v.s. 台北車站

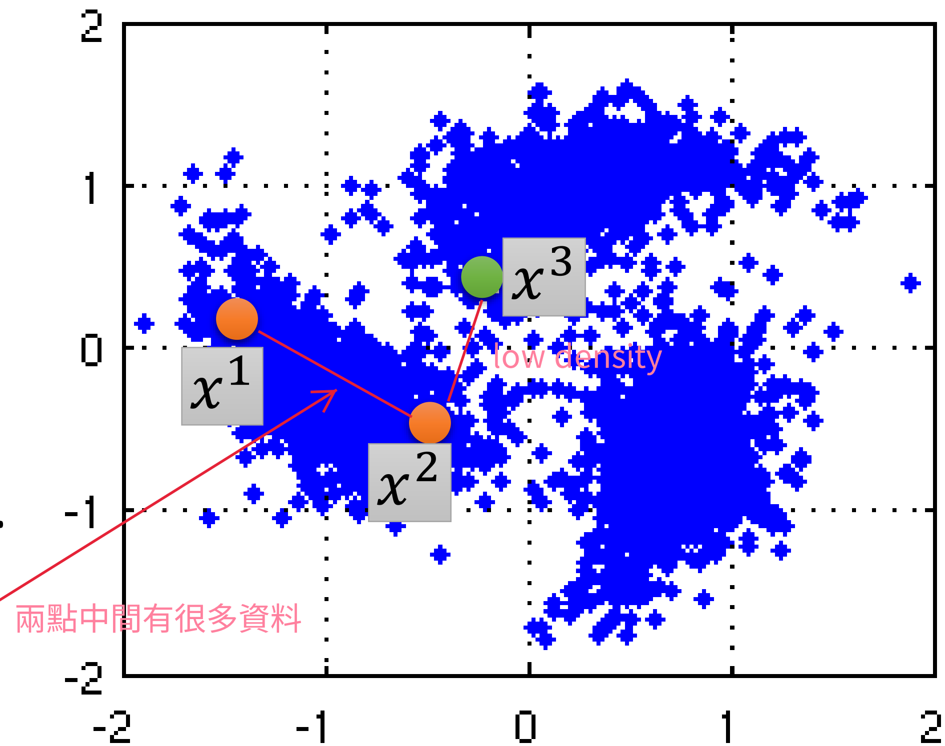
公館 v.s. 科技大樓

Source of image: http://hips.seas.harvard.edu/files/pinwheel.png

Smoothness Assumption

- Assumption: "similar" x has the same $\hat{y}$
- More precisely:
  - x is not uniform.
  - If x^1 and x^2 are close in a high density region, $\hat{y}^1$ and $\hat{y}^2$ are the same.

connected by a high density path

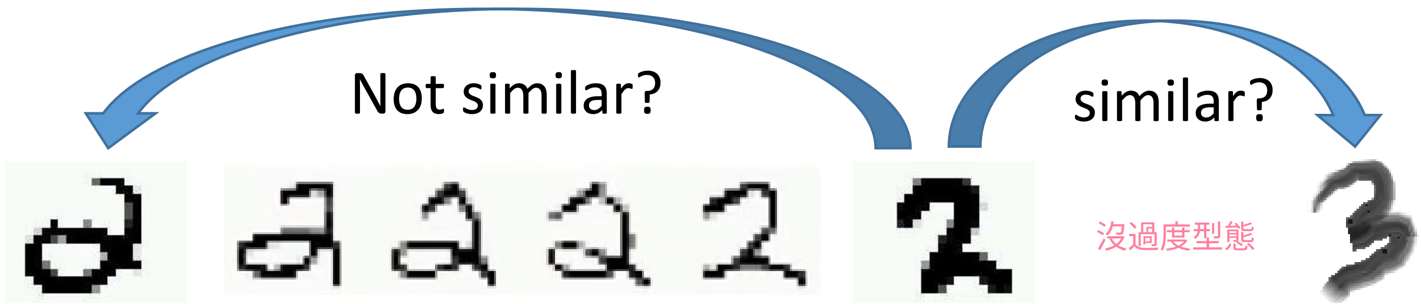


x^1 and x^2 have the same label

x^2 and x^3 have different labels

Source of image: http://hips.seas.harvard.edu/files/pinwheel.png

Smoothness Assumption



“indirectly” similar
with stepping stones

(The example is from the tutorial slides of Xiaojin Zhu.)

Source of image: http://www.moehui.com/5833.html/5/

Smoothness Assumption

- Classify astronomy vs. travel articles

有overlap

	d_1	d_3	d_4	d_2
asteroid	●	●		
bright	●	●		
comet		●		
year				
zodiac				
⋮				
airport				
bike				
camp			●	
yellowstone			●	●
zion				●

(The example is from the tutorial slides of Xiaojin Zhu.)

Smoothness Assumption

- Classify astronomy vs. travel articles

沒有overlap

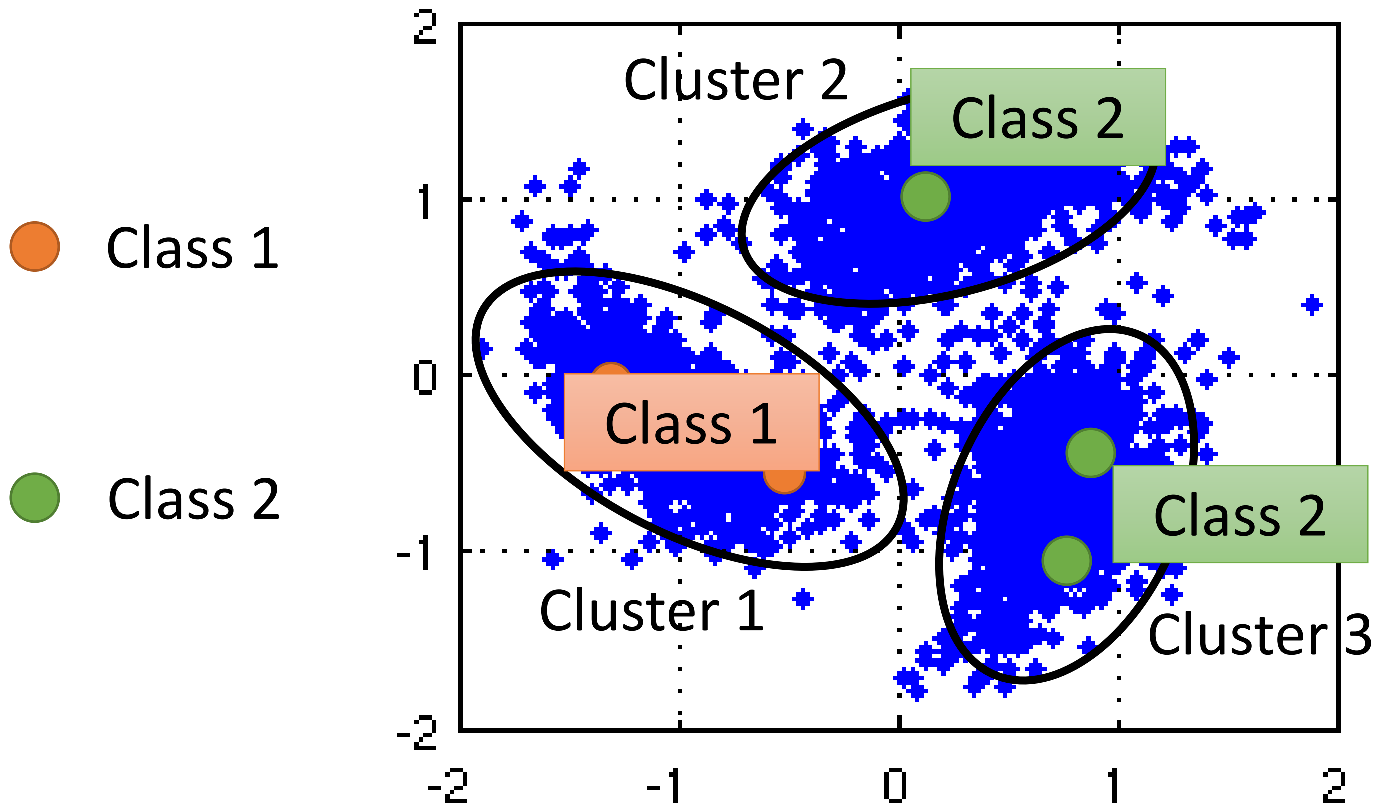
	d_1	d_3	d_4	d_2
asteroid	●			
bright	●			
comet				
year				
zodiac		●		
⋮				
airport			●	
bike			●	
camp				
yellowstone				●
zion				●

但如果蒐集很多unlabel data…

	d_1	d_5	d_6	d_7	d_3				
asteroid	●								
bright	●	●							
comet		●	●						
year			●	●					
zodiac				●	●				
⋮									
airport						●			
bike						●	●		
camp							●	●	
yellowstone								●	●
zion									●

(The example is from the tutorial slides of Xiaojin Zhu.)

Cluster and then Label



Using all the data to learn a classifier as usual

Graph-based Approach

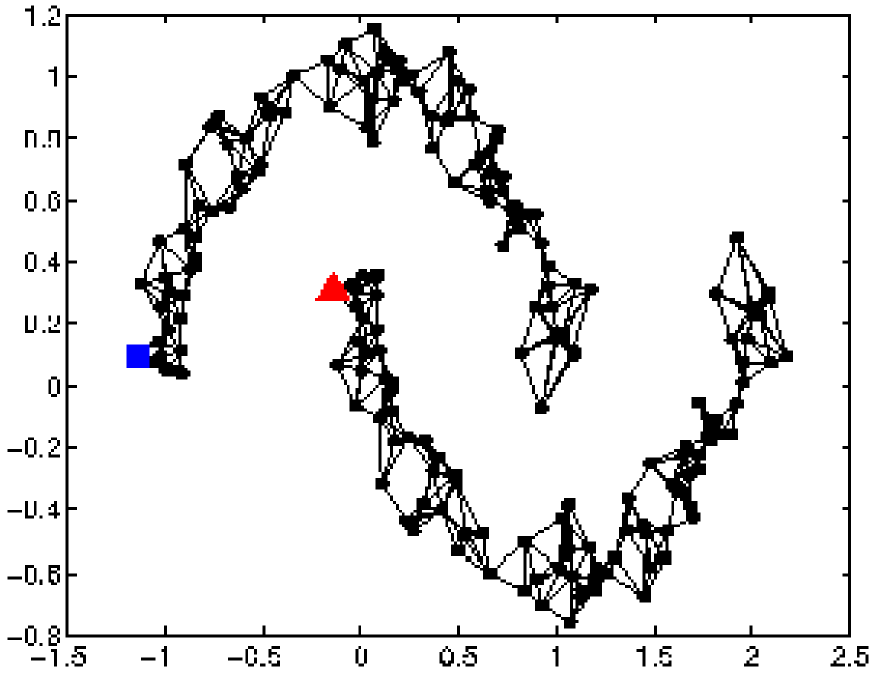
- How to know x^1 and x^2 are connected by a high density path

Represented the data points as a ***graph***

Graph representation is nature sometimes.

E.g. Hyperlink of webpages, citation of papers

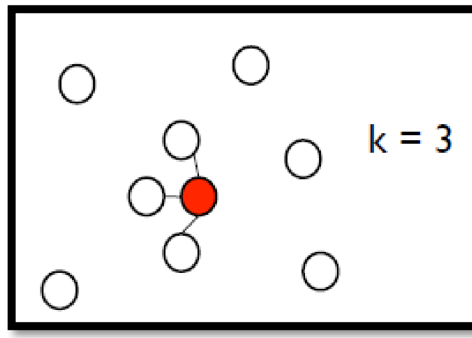
Sometimes you have to construct the graph yourself.

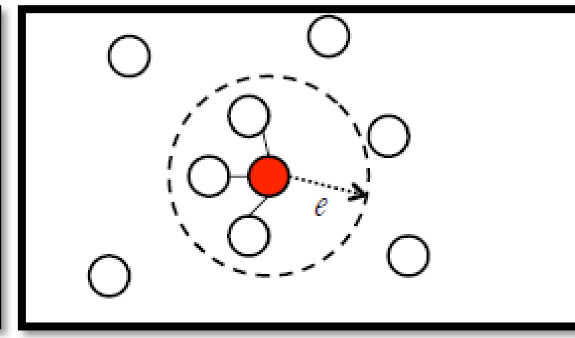


Graph-based Approach - Graph Construction

The images are from the tutorial slides of Amarnag Subramanya and Partha Pratim Talukdar

- Define the similarity $s(x^i, x^j)$ between x^i and x^j
- Add edge:
  - K Nearest Neighbor
  - *e*-Neighborhood

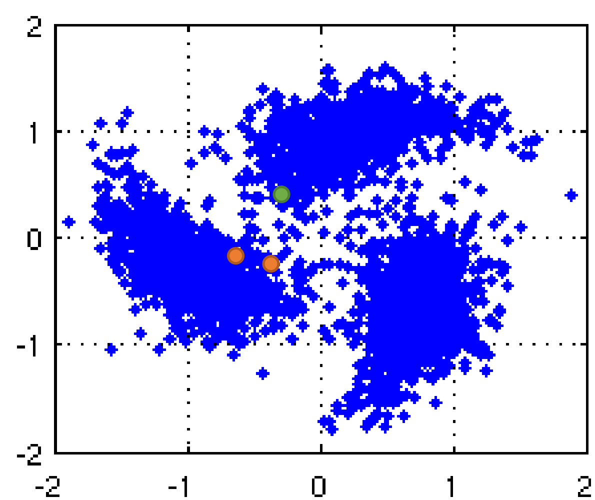




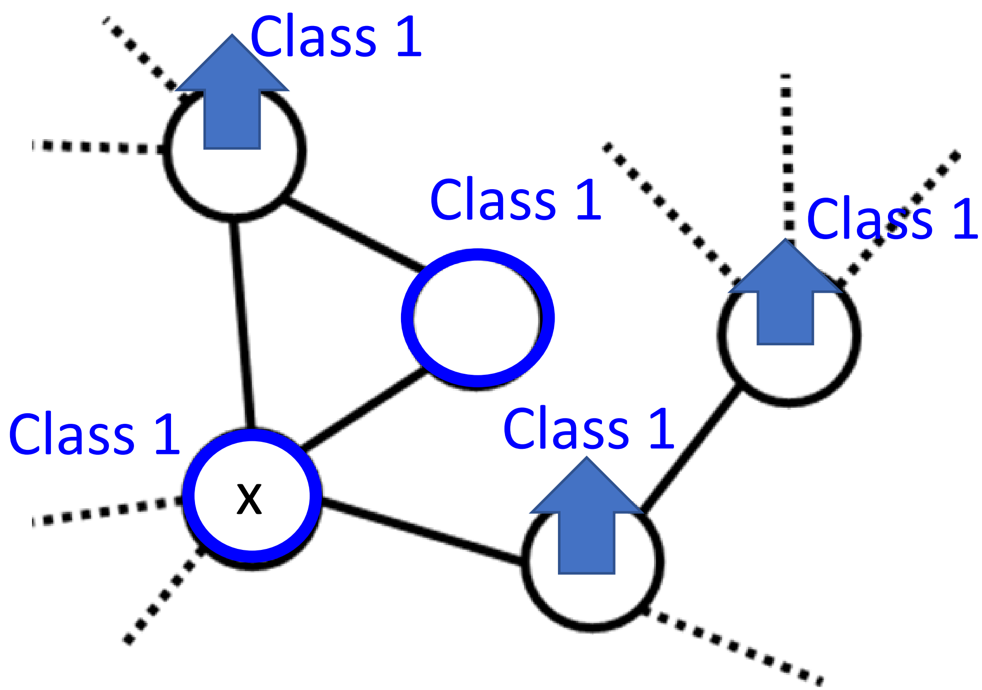
- Edge weight is proportional to s(x^i, x^j)

Gaussian Radial Basis Function:

$$s(x^i, x^j) = exp\left(-\gamma\left\|x^i - x^j\right\|^2\right)$$

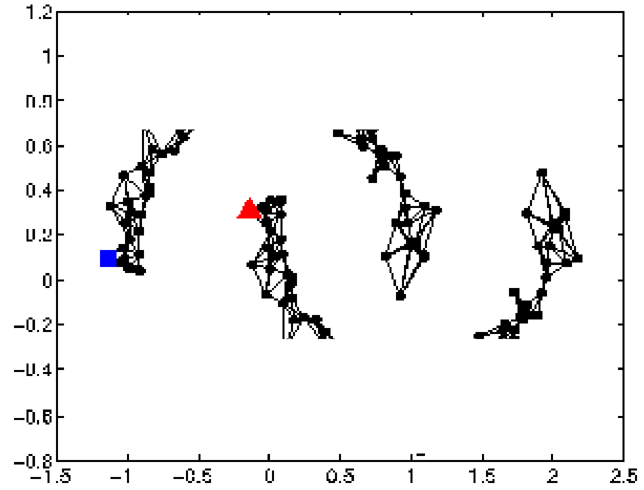


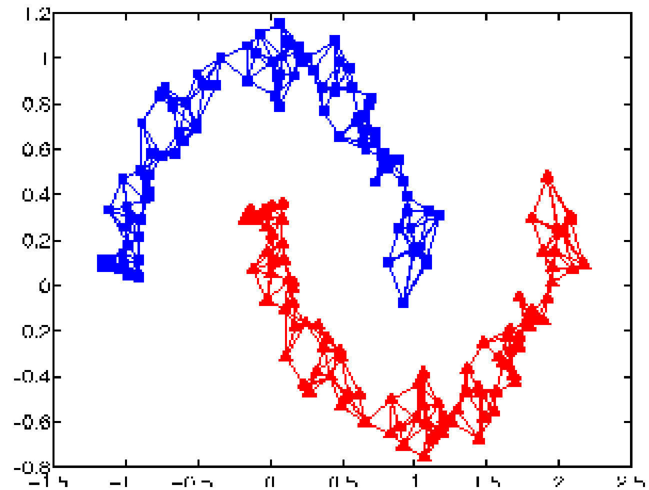
Graph-based Approach



The labelled data influence their neighbors.

Propagate through the graph





Graph-based Approach

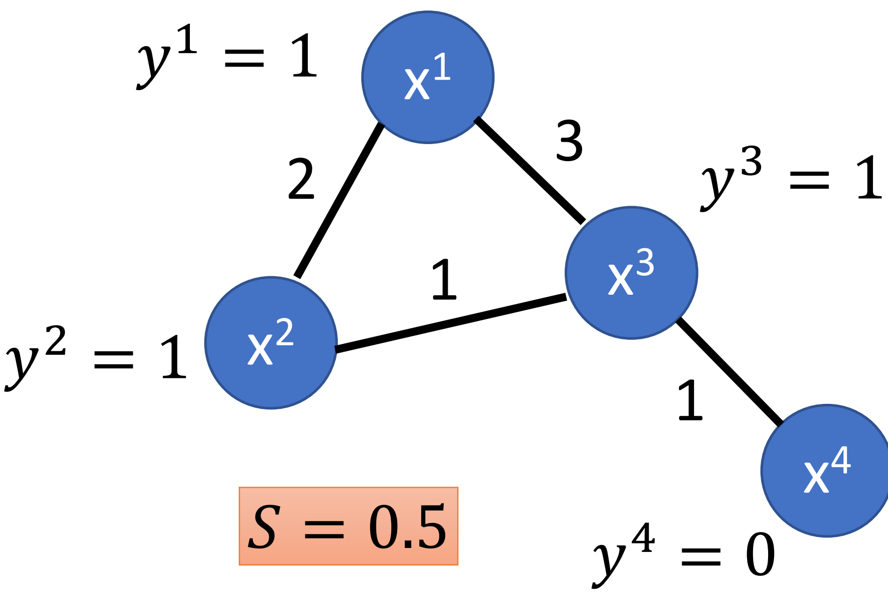
- Define the smoothness of the labels on the graph

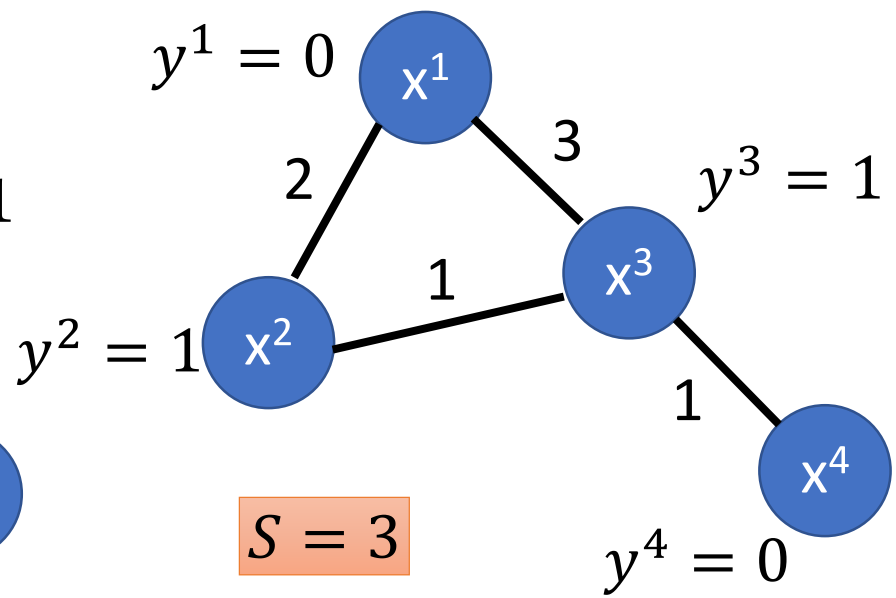
值越小越好

$$S = \frac{1}{2}\sum_{i,j} w_{i,j}\left(y^i - y^j\right)^2$$

Smaller means smoother

For all data (no matter labelled or not)

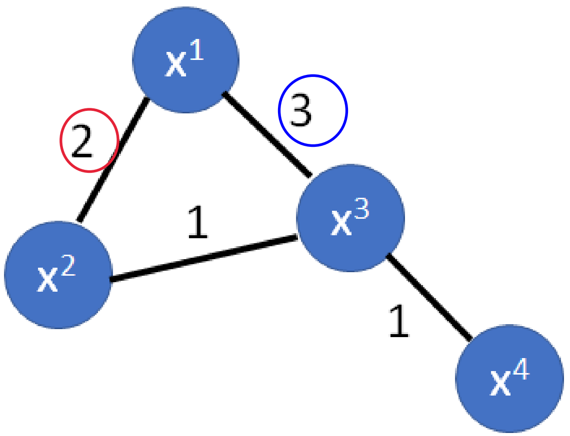




Graph-based Approach

- Define the smoothness of the labels on the graph

$$S = \frac{1}{2}\sum_{i,j} w_{i,j}\left(y^i - y^j\right)^2 = \boldsymbol{y}^T L \boldsymbol{y}$$



y: (R+U)-dim vector

$$\boldsymbol{y} = \left[\cdots y^i \cdots y^j \cdots\right]^{\boldsymbol{T}}$$

L: (R+U) x (R+U) matrix

Graph Laplacian

$$L = D - W$$

$$W = \begin{bmatrix} 0 & 2 & 3 & 0 \\ 2 & 0 & 1 & 0 \\ 3 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad D = \begin{array}{c} \begin{array}{cccc} 2+3 & & & \end{array} \\ \begin{bmatrix} 5 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

Graph-based Approach

- Define the smoothness of the labels on the graph

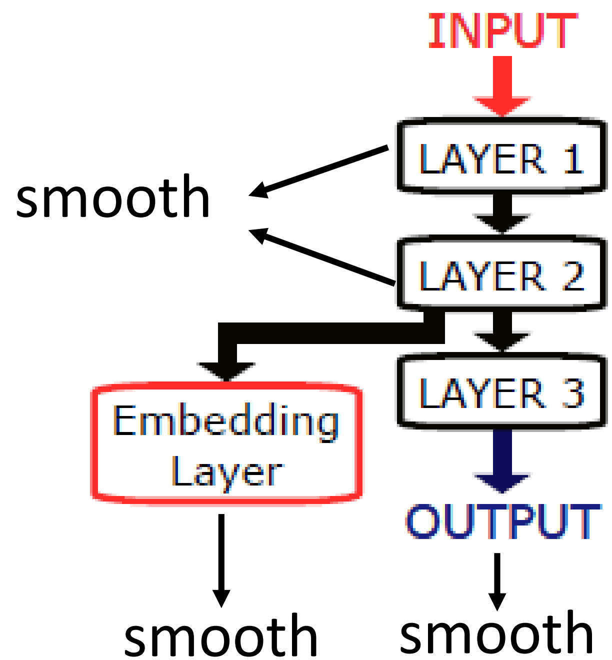
$$S = \frac{1}{2}\sum_{i,j} w_{i,j}\left(y^i - y^j\right)^2 = \boldsymbol{y}^T L \boldsymbol{y}$$

Depending on model parameters

$$L = \sum_{x^r} C\left(y^r, \hat{y}^r\right) \boxed{+\lambda S}$$

As a regularization term

J. Weston, F. Ratle, and R. Collobert, “Deep learning via semi-supervised embedding,” ICML, 2008



Semi-supervised Learning
Better Representation

去蕪存菁，化繁為簡

Looking for Better Representation

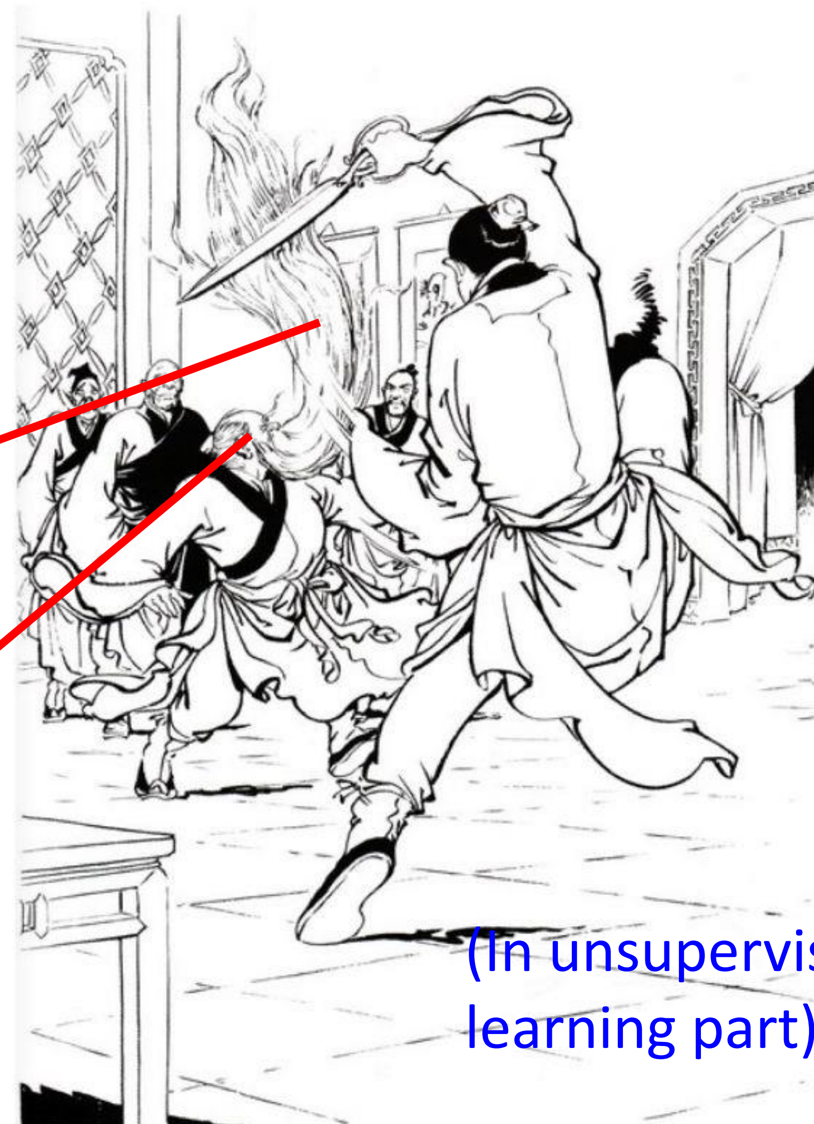
- Find a better (simpler) representations from the unlabeled data

鬍子

Original representation

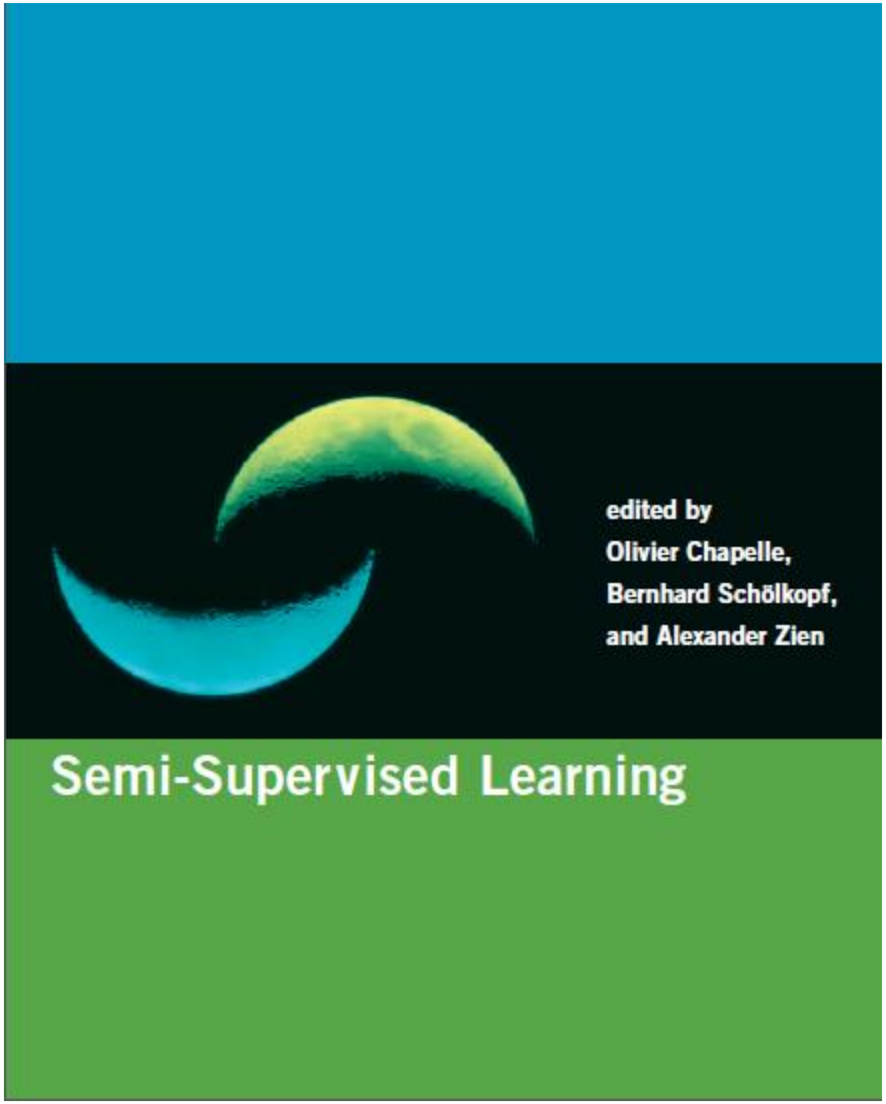
頭

Better representation



(In unsupervised learning part)

Reference



http://olivier.chapelle.cc/ssl-book/

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