Machine Learning for Data Mining

Introduction to Semi-supervised Methods

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Outline

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Introduction

Semi-supervised learning

Semi-Supervised Learning (SSL) is halfway between supervised and unsupervised learning. I

Your Data

Some labels are provided, but not for all data

Thus the data set $X = \{x_1, x_2, \ldots, x_N\}$

It can be divided into two parts:

- The points $X_l = \{x_1, x_2, \ldots, x_l\}$ for which labels are provided $Y_l = \{y_1, y_2, \ldots, y_l\}$
- The points $X_u = \{x_{l+1}, x_{l+2}, \ldots, x_u\}$ where the labels are unknown.

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It was proposed in self-learning!!!

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It starts by training on the labeled data only.

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In each step a part of the unlabeled points is labeled according to the current decision function:

$$\text{Given } x_i \rightarrow y_i = f(x_i) \tag{1}$$

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We have several authors proposing this idea for a long time

Scudder (1965), Fralick (1967) and Agrawala (1970).

- An unsatisfactory aspect of self-learning is that the effect of the wrapper depends on the supervised method used inside it.

Closely related

A problem related to SSL was introduced by Vapnik already several decades ago.

Transductive learning (Vapnik and Chervonenkis, 1974)

The idea of transduction is to perform predictions only for the test points.

- This is in contrast to inductive learning, where the goal is to output a prediction function which is defined on the entire space!!!

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Estimating the Fisher linear discriminant rule with unlabeled data was considered.

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Setting

The setting was in the case where each class conditional density is Gaussian with equal covariance matrix.

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The likelihood of the model was calculated using EM... thus the labels (Hidden data) are estimated!!!

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During the 1990's

The SSL became a subject of great interest

Mostly due to applications in natural language problems and text classification.

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A simple question

Is semi-supervised learning meaningful?

This question is about the information that the unlabeled data can provide.

Making possible to say the following

Using enough data semi-supervised learning will be superior than supervised learning

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In a more mathematical formulation

You could say that

1. The knowledge on $p(\boldsymbol{x})$ that one gains through the unlabeled data has to carry information.
2. That is useful in the inference of $p(l_{\boldsymbol{x}}|x)$!!!

Something Notable

If this is not the case, semi-supervised learning will not yield an improvement over supervised learning.

It might even happen

Usage unlabeled data degrades the prediction accuracy by misguiding the inference.

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Assumptions to be made

However, your data must have the four principles

1. The Semi-Supervised Smoothness Assumption.
2. The Cluster Assumption.
3. The Manifold Assumption.
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Supervised Smoothness Assumption

Definition

If two points $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ are close, then the corresponding outputs $f(\boldsymbol{x}_1)$ and $f(\boldsymbol{x}_2)$.

- Where f is the supervised algorithm.
- Strictly speaking, this assumption only refers to continuity rather than smoothness.

Without such assumptions

It would never be possible to generalize from a finite training set to a set of possibly infinitely many unseen test cases.

Remember?

ill-posed problems.

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The Semi-Supervised Smoothness Assumption

Definition

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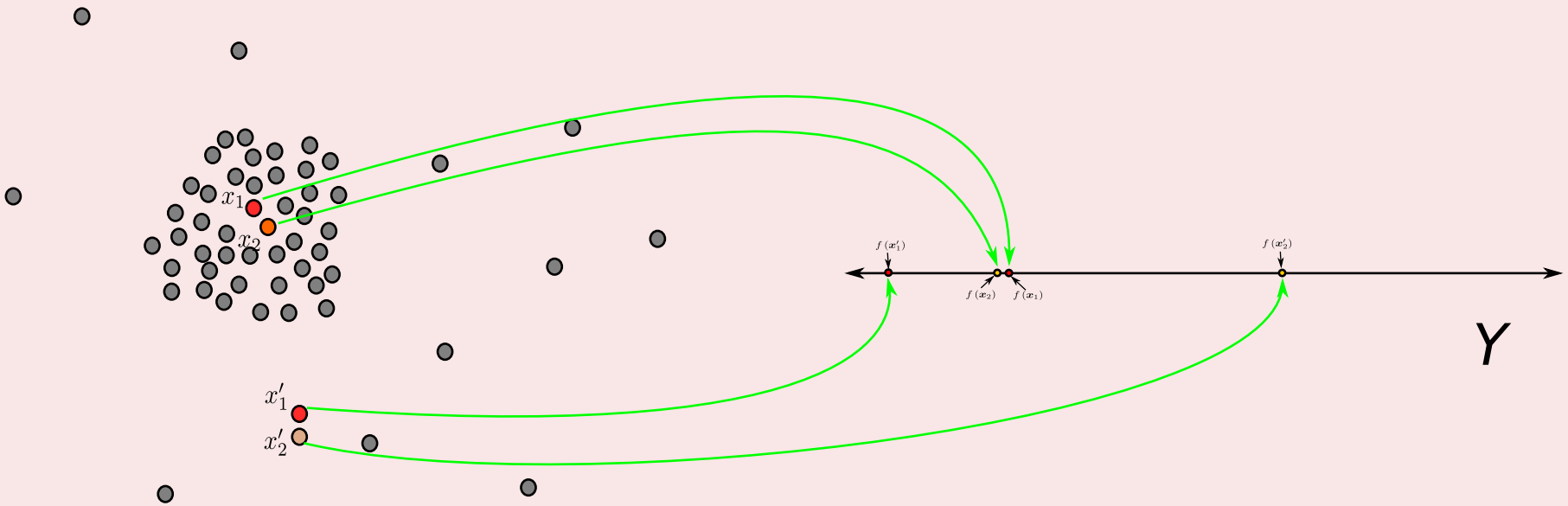

Implications

Given Transitivity

The assumption implies that if two points are linked by a path of high density, then their outputs are likely to be close

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We can use the unlabeled data could help to find the boundary of each cluster more accurately.

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In fact

This is the earliest form of semi-supervised learning.

The Cluster Assumption

Definition

If points are in the same cluster, they are likely to be of the same class.

Remark

This assumption may be considered reasonable on the basis of the sheer existence of classes

It is more

if there is a densely populated continuum of objects, it is unlikely that they could be distinguished into different classes.

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Meaning

Something Notable

It means that, usually, we do not observe objects of two distinct classes in the same cluster.

In addition

Low density separation: The decision boundary should lie in a low-density region.

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Thing about this!!!

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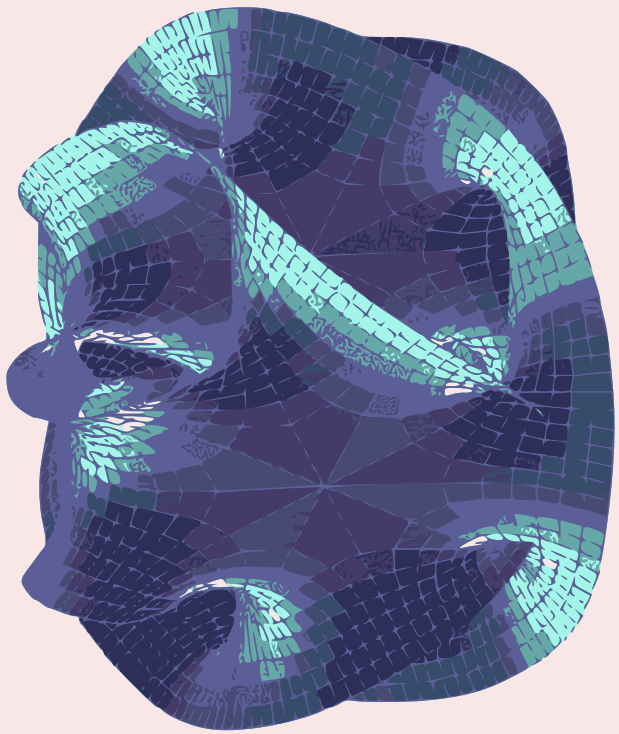

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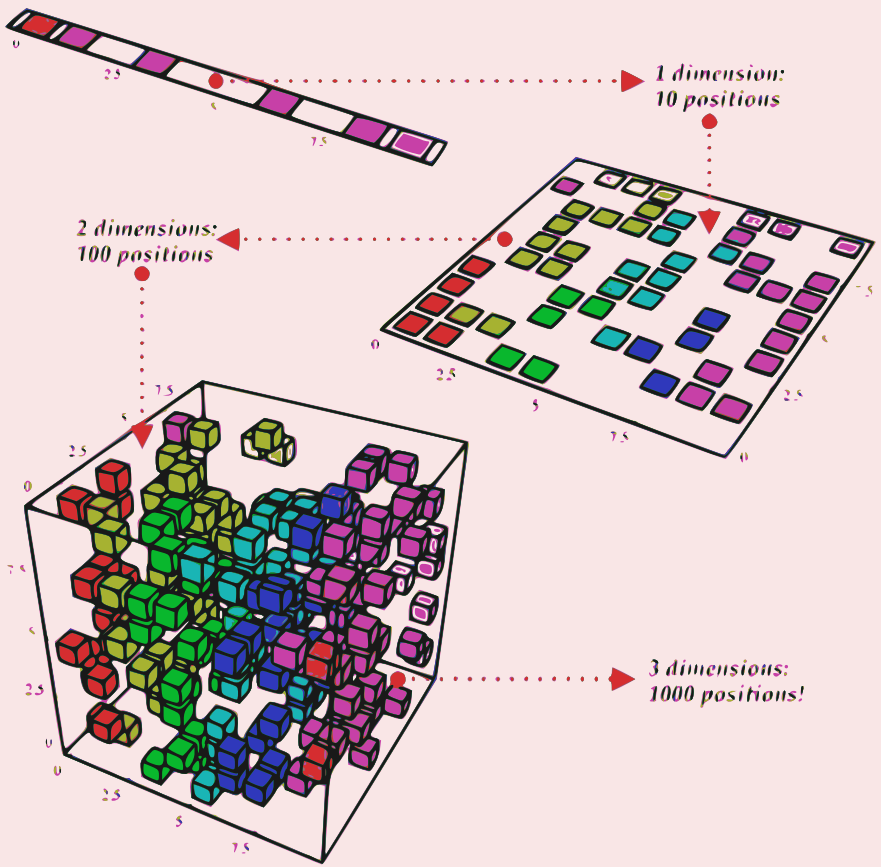

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Facts

First

Working with manifolds can be seen as approximately implementing the semi-supervised smoothness assumption.

- Algorithms use the metric of the manifold for computing geodesic distances.

Second

If we view the manifold as an approximation of the high-density regions.

- The semi-supervised smoothness assumption reduces to the standard smoothness assumption of supervised learning, applied on the manifold.

Third

if the manifold is embedded into the high-dimensional input space in a curved fashion (i.e., it is not just a subspace)

- Geodesic distances differ from those in the input space.

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Vapnik's principle

Definition

High-dimensional estimation problems should attempt to follow the following principle:

- When trying to solve some problem, one should not solve a more difficult problem as an intermediate step.

For example in supervised learning

- Generative models estimate the density of x as an intermediate step.
- Discriminative methods directly estimate the labels.

Given that

Label predictions are only required for a given test set in the transductive setting.

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Therefore

While an inductive method infers a function

$$f : \mathcal{X} \rightarrow \mathcal{Y} \tag{2}$$

Over the entire space to obtain inferences $f(x_i)$ over inputs x_i.

This is different of Transduction

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Transduction VS SSL

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What?

To see why the difference, imagine the following example

Suppose we are given a transductive algorithm which produces a solution superior to an inductive algorithm trained on the same labeled data (Discarding the unlabeled data).

This difference might be due to the following points

- Transduction follows Vapnik's principle more closely than induction does.
- The transductive algorithm takes advantage of the unlabeled data in a way similar to semi-supervised learning algorithms.

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- There is ample evidence for improvements being due to the second of these points.
- It seems that there are no empirical results that selectively support the first point.

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- Low-Density Separation
- Graph-Based methods

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Classes are modeled using a distribution $P(\boldsymbol{x}|y)$

For this, we use a family of models parametrized by

$$\{P(\boldsymbol{x}|y,\theta)\} \tag{4}$$

Furthermore

The class of priors $P(y)$ for the labels is model by

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After all we are using a full joint density $P(\boldsymbol{x}, y)$ by
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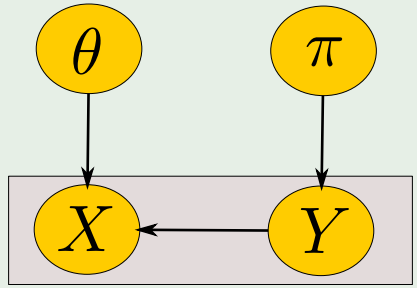
Example

Graphical Model of the Joint Density



Thus for any fixed $\hat{\theta}$ and $\hat{\pi}$, and a labels $y \in \{1, \ldots, M\}$

$$P\left(y|x, \hat{\theta}, \hat{\pi}\right) = \frac{P\left(x|y, \hat{\theta}\right)\hat{\pi}_y}{\sum_{y'=1}^{M} P\left(x|y', \hat{\theta}\right)\hat{\pi}_{y'}} \tag{6}$$

Alternatively

One can obtain the Bayesian predictive distribution $P\left(y|x, D_l\right)$ (D_l the labeled data) by averaging

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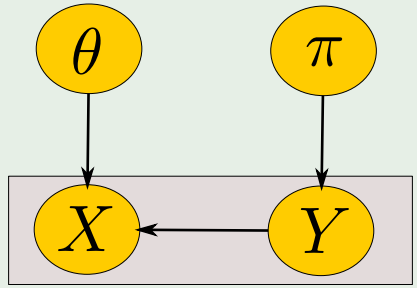

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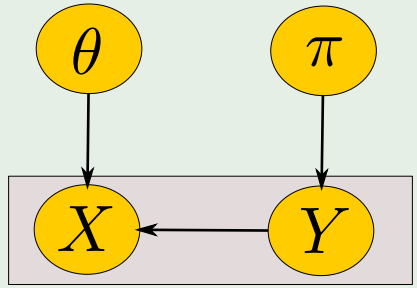

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If labeled and unlabeled data are available

A natural criterion emerges as the joint log likelihood of both D_l and D_u:

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It is an issue of maximum likelihood in the presence of missing data by threating y as a latent variable.

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We can deal with this problem using EM algorithm.

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Some researchers have been quick in hailing this strategy as an obvious solution SSL:

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We want to

To push the decision boundary away from the unlabeled points.

The most common approach

To use a maximum margin algorithm as SVM.

This method is known as

The method of maximizing the margin for unlabeled as well as labeled points is called the Transductive SVM (TSVM).

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Alternatives

Two alternatives to the TSVM are

1. Probability framework.
2. Information theoretic framework.

For example

We can use binary Gaussian process classification

- By introducing a null class that occupies the space between the two regular classes.

Another example

Using Entropy Minimization, it is possible to push the class-conditional probabilities $P(y|x)$ to 0 or 1 at unlabeled and labeled points.

- Given the smoothness assumption, the probability will tend to 0 or 1 in any high-density region.
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Graph-Based Methods

This has been an active area of research in SSL

The common denominator of these methods is that

- The data are represented by the nodes of a graph.
- The edges are the pairwise distance between nodes.
  - Missing edges correspond to infinite distances.

Now

If the distance of two points is computed by minimizing the aggregate path distance over all paths connecting the two points.

- This is an approximation to the geodesic distance of the two points!!!

Then, the graph

It can be argued to build on the manifold assumption.

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They refer to the graph by utilizing the Laplacian Matrix.

Setup

Let be $G = (V, E)$ a graph with real edge weights given by weight function $w : E \to \mathbb{R}$ with:

- $w(e)$ represents the similarity of the incident nodes.
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The weighted adjacency matrix $\boldsymbol{W}$ of graph G is defined by

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Definition

The diagonal matrix $\boldsymbol{D}$ defined by $\boldsymbol{D}_{ii} = \sum_j \boldsymbol{W}_{ij}$ is called the degree matrix of G.

Although there are different ways of defining the Laplacian Matrix

We decided to use the normalized and unormalized versions.

Laplacian Matrix

- Normalized Matrix: $\mathcal{L} = I - D^{-1/2} W D^{-1/2}$.
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2. Transductive Support Vector Machines.

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Outline

A Generative Model for Text

We assume documents are generated by a *mixture of multinomials* model

Each mixture component corresponds to a class.

The Multinomial Distribution

Definition

$(u_1, u_2, ..., u_k)$ is said to b follow a multinomial distribution with parameters $(\mathfrak{N}, p_1, p_2, ..., p_k)$.

$$p\left(x_1, x_2, ..., x_k | \mathfrak{N}, p_1, p_2, ..., p_k\right) = \frac{\mathfrak{N}!}{x_1! x_2! \cdots x_k!} p_1^{x_1} p_2^{x_2} \cdots p_k^{x_k} \tag{11}$$

Under the following conditions

- Number of trials $\mathfrak{N} > 0$.
- $x_i \in \{0, 1, 2, ..., \mathfrak{N}\}$.
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Second

Then, we pick up the biased $|\mathfrak{X}|$-sided die that corresponds to the chosen class.

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We roll this die $|x_i|$ times, and count how many times each word occurs.

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We roll this die $|\boldsymbol{x}_i|$ times, and count how many times each word occurs.

- These word counts form the generated document.

Model

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We roll a biased M-sided die to determine the class of our document.

Second

Then, we pick up the biased $|\mathfrak{X}|$-sided die that corresponds to the chosen class.

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We roll this die $|\boldsymbol{x}_i|$ times, and count how many times each word occurs.

- These word counts form the generated document.

Formally

Every document

It is generated according to a probability distribution with parameter θ.

The probability distribution for the documents

It consists of a mixture of components $c_j \in \{1, 2, ..., M\}$.

Thus

A document x_i is created by first selecting a mixture component according to the mixture weights (Class probability), $P(c_j|\theta)$.

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Next

We can use this mixture component

This selected mixture component to to generate a document according to its own parameters, with distribution $P(\boldsymbol{x}_i|c_j,\theta)$

Thus the likelihood to see a particular document $\boldsymbol{x}_i$ is

$$P(\boldsymbol{x}_i|\theta) = \sum_{j\in\{1,2,\ldots,M\}} P(c_j|\theta)\,P(\boldsymbol{x}_i|c_j,\theta) \tag{12}$$

Each document has a class label

We assume a one-to-one correspondence between mixture model components and classes.

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We use c_j to indicate the jth mixture component as well the jth class.

Not only that

The class label for a particular document x_i is written y_i.

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If document x_i was generated by mixture component c_j we say $y_i = c_j$.

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A document, $\boldsymbol{x}_i$, is a vector of word counts

Thus, we write x_{it} to be the number of times word w_t occurs in document $\boldsymbol{x}_i$.

Length of the Document

When a document is to be generated by a particular mixture component the document length is chosen independently of the component.

$$|\boldsymbol{x}_i| = \sum_{t=1}^{|\mathbf{x}|} x_{it} \tag{13}$$

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The selected mixture component is used to generate a document of the specified length, by drawing from its multinomial distribution

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The probability of a document given a mixture component in terms of its constituent features

$$P(\boldsymbol{x}_i|c_j,\theta) \propto P(|\boldsymbol{x}_i|) \prod_{w_t \in \mathfrak{X}} P(w_t|c_j,\theta)^{x_{it}} \tag{14}$$

Under the standard naive assumption

The words of a document are conditionally independent of the other words in the same document, given the class label.

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The parameters of an individual mixture component define a multinomial distribution over words.

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The collection of word probabilities

Each written $\theta_{w_t|c_j}$ such that $\theta_{w_t|c_j} \equiv P(w_t|c_j, \theta)$ where $t \in \{1, 2, ..., |\mathfrak{X}|\}$ and $\sum_t P(w_t|c_j, \theta) = 1$.

In addition

Since we assume that for all classes, document length is identically distributed, it does not need to be parameterized for classification.

What else we need?

We only need the mixture weights (Class probabilities), $\theta_{c_j} \equiv P(c_j|\theta)$.

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Thus

The complete collection of model parameters, θ, defines a set of multinomials and class probabilities

$$\theta = \left\{ \theta_{w_t|c_j} | w_t \in \mathfrak{X}, c_j \in \{1, ..., M\}, \theta_{c_j} : c_j \in \{1, ..., M\} \right\} \tag{15}$$

Thus, we get

$$P(x_i|\theta) = P(|x_i|) \sum_{j \in \{1,2,...,M\}} P(c_j|\theta) \prod_{w_t \in \mathfrak{X}} P(w_t|c_j, \theta)^{n_{it}} \tag{16}$$

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Outline

Now

Given the generative model

We need to estimate the values $\hat{\theta}$.

For Naive Bayes

We can use MAP to find the $\arg\max_\theta P(\theta|X, Y)$ by using the likelihood of the data and a prior.

We know that the commonly used conjugate prior distribution for multinomial distributions is the Dirichlet Prior

$$P\left(\theta_{w_t|c_j}|\alpha\right) \propto \prod_{w_t \in \mathfrak{X}} P(w_t|c_j)^{\alpha_t - 1} \tag{17}$$

Where α_t are constants greater than zero.

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The Dirichlet Distribution

Let $\Theta = \{\theta_1, \theta_2, ..., \theta_m\}$

We write:

$$\Theta \sim Dirichlet\left(\alpha_1, \alpha_2, ..., \alpha_m\right) \tag{18}$$

The pmf looks like

$$P\left(\theta_1, \theta_2, ..., \theta_m\right) = \frac{\Gamma\left(\sum_k \alpha_k\right)}{\prod_k \Gamma\left(\alpha_k\right)} \prod_{k=1}^{m} \theta_k^{\alpha_k - 1} \tag{19}$$

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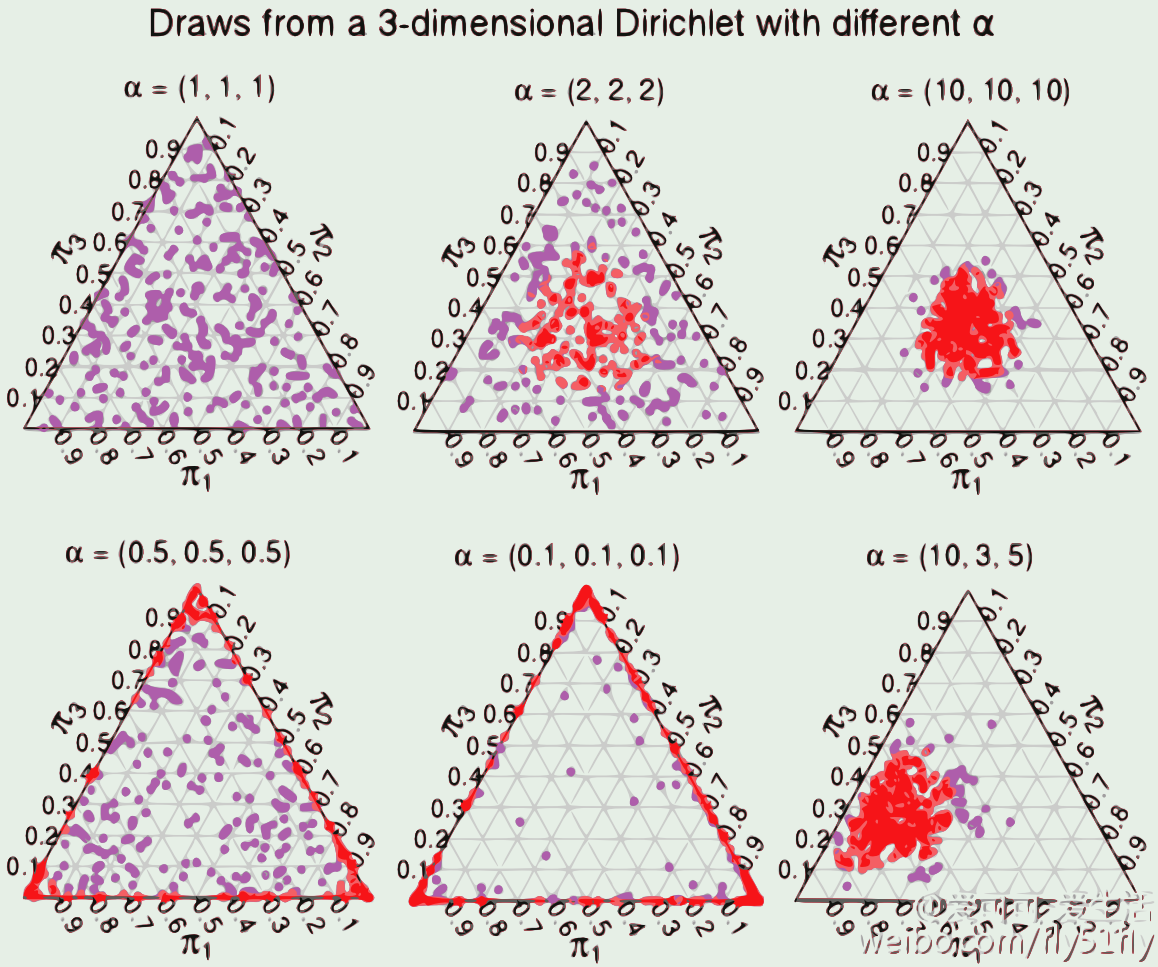
Examples

Dirichlet distributions under different $\alpha's$



In addition

Dirichlet distributions have two parameters

- The scale or concentration $\sigma = \sum_t \alpha_t$.
- The base measure $(\alpha'_1, ..., \alpha'_k)$ with $\alpha'_t = \frac{\alpha_t}{\sigma}$.

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We can set all $\alpha_t = 1$

This prior favors the uniform distribution.

Thus

The parameter estimation formulas that result from maximization with the data and our prior are the familiar smoothed ratios of empirical counts.

We have that

$$\hat{\theta}_{w_t|c_j} = P\left(w_t|c_j, \hat{\theta}\right) = \frac{1 + \sum_{x_i \in X} \delta_{ij} x_{it}}{|\mathfrak{X}| + \sum_{s=1}^{|\mathfrak{X}|} \sum_{x_i \in X} \delta_{ij} x_{is}} \tag{20}$$

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Now

Given estimates of these parameters calculated from labeled training documents.

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Final Document classification

Finally

If our task is to classify document $\boldsymbol{x}_i$ in some class, we take $\arg\max_j P\left(y_i = c_j | \boldsymbol{x}_i, \hat{\theta}\right)$ as such a a class.

Outline

What to do?

In the semi-supervised setting with labeled and unlabeled data

We still like to find the MAP parameter estimates.

Given that there is no labeled data

We do not have labeled data, thus the closed-form equations from the previous section are not applicable

For this, we can use the EM technique

The EM technique as applied to the case of labeled and unlabeled data with naive Bayes yields a straightforward algorithm.

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EM Process

First

A naive Bayes classifier is built in the standard supervised fashion from the limited amount of labeled training data.

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Then, we perform classification of the unlabeled data with the naive Bayes model.

- For this, we use the probabilities associated with each class.

Third

We rebuild a new naive Bayes classifier using all the data, labeled and unlabeled, using the estimated class probabilities as true class label.

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Until it converges to a stable classifier and set of labels for the data.

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EM Algorithm

Basic EM algorithm for semi-supervised learning of a text classifier

Input: Collections X_l of labeled documents and X_u of unlabeled documents.

1. Build an initial naive Bayes classifier, with $\hat{\theta}$, from the labeled documents.
2. Use MAP to find an estimation $\hat{\theta} = \arg\max_{\theta} P(X_l|\theta) P(\theta)$.
3. loop while $l(\theta|X, Y)$ improves (The Log probability of all data and prior)
4. (E step) Use the current parameter, $\hat{\theta}$, to estimate component membership
5. of each unlabeled data i.e. $P\left(c_j|x_i, \hat{\theta}\right)$.
6. (M step) Re-estimate the parameter, $\hat{\theta}$, given the estimated component
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The Log Probability of all Data and Prior

We have that

$$l(\theta|X,Y) = \log(P(\theta)) + \sum_{\boldsymbol{x}_i \in X_u} \log\left[\sum_{j\in\{1,\ldots,M\}} P(c_j|\theta)\, P(\boldsymbol{x}_i|c_j,\theta)\right] + \ldots$$

$$\sum_{\boldsymbol{x}_i \in X_l} \log\left[P(y_i = c_j|\theta)\, P(\boldsymbol{x}_i|y_i = c_j,\theta)\right]$$