

Laplacian Eigenmaps for Dimensionality Reduction and Data Representation

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Presentation for CSE291 sp07

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 - The Algorithm
- 2 Explaining The Algorithm
 - The optimization
 - Continuous Manifolds - The Heat Kernel
- 3 Results
 - The Swiss roll
 - Syntactic structure of words

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The problem

In AI, information retrieval and data mining we get Intrinsically Low m -dimensional data lying in high N -dimensional space.

Recovering the initial dimensionality results

- Smaller data sets
 - ▶ Faster computations
 - ▶ Reduce the space needed
- More meaningful representations
- . . . much more

Non Linearity

PCA, MDS and their variations create linear embeddings of the data. For non-linear structures their linear embeddings fail.

IsoMAP, LLE and Laplacian eigenmaps partially solve this problem. The heart of these approaches is some kind of non-linear method

- IsoMAP, Adjacency Graph of "Neighbor nodes"-edges
- LLE, Each node is expressed by a limited number of neighbor nodes
- In Laplacian Eigenmaps, Adjacency Graphs of "Neighbor nodes"-edges

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Step 1. Construct the Graph

We construct the Adjacency Graph A putting (i, j) edges if x_i, x_j are "close"

Close may mean:

- ϵ -neighborhoods $\|x_i - x_j\|^2 < \epsilon$
- n nearest neighbors
- Combination of the above (at most n nearest neighbors with $\|x_i - x_j\|^2 < \epsilon$)

Step 2. Choose the Weights

The edges have weights that can be

- Simple-minded: 1 if connected 0 else
- Heat Kernel: $W_{ij} = e^{-\frac{\|x_i - x_j\|^2}{t}}$

We note that with $t = \infty$ we get the simple-minded approach
The second method includes more information in our model

Step 3. The Laplacian eigenvalues

Let A be the Adjacency matrix and D the degree matrix of the graph
We introduce the Laplacian matrix $L = A - D$ and we solve the generalized eigenvector problem

$$Lf = \lambda Df$$

We sort the eigenvectors according to their eigenvalues
 $0 = \lambda + 0 \leq \lambda_1 \leq \lambda_2 \dots \lambda_{k-1}$ We leave out f_0 and use the first m eigenvectors for embedding in m -dimensional Euclidian space.

$$x_i \rightarrow (f_1(i), \dots, f_m(i))$$

A quick overview

- There are several efficient approximate techniques for finding the nearest neighbors.
- The algorithm consists of a few local computations and one sparse eigenvalue problem.
- It is a member of the IsoMap-LLE family of algorithms.
- As LLE and IsoMap does not give good results for non-convex manifolds.

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Our minimization problem for 1 Dimension

Let $y = (y_1, y_2, \dots, y_n)^T$ be our mapping.

We would like to minimize

$$\sum_{ij} (y_i - y_j)^2 W_{ij}$$

under appropriate constraints

$$\begin{aligned} \sum_{ij} (y_i - y_j)^2 W_{ij} &= \sum_{ij} (y_i^2 + y_j^2 - 2y_i y_j) W_{ij} = \\ \sum_i y_i^2 D_{ii} + \sum_j y_j^2 D_{jj} - 2 \sum_{ij} y_i y_j W_{ij} &= 2y^T L y \end{aligned}$$

So we need to find

$$\operatorname{argmin}_y y^T L y$$

Our Constraints

The constraint

$$y^T D y = 1$$

removes an arbitrary scaling factor in the embedding

$\operatorname{argmin}_y y^T L y, y^T D y = 1$ is exactly the generalized eigenvalue problem

$$L y = \lambda D y$$

The additional constraint $y^T D \mathbf{1} = 0$ the solution $\mathbf{1}$ with $\lambda_0 = 0$

So the final problem is:

$$\operatorname{argmin}_y y^T L y, y^T D y = 1, y^T D \mathbf{1} = 0$$

The general problem for m dimensions is similar and gives exactly the first m smallest eigenvalues.

Sum Up

So each eigenvector is a function from nodes to \mathbb{R} in a way that "close by" points are assigned "close by" values.

The eigenvalue of each eigenfunction gives a measure of how "close by" are the values of close by points

By using the first m eigenfunctions for determining our m -dimensions we have our solution.

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Continuous Manifolds

When we are using continuous spaces the Graph Laplacian becomes the Laplace Beltrami Operator (More on this by Nakul.)

And our optimization problem is finding functions f that map the manifold points to \mathbb{R} , in a way that $\int_{\mathcal{M}} \|\nabla f(x)\|^2$ is minimum. Intuitively minimizing the gradient minimizes the values assigned to close by points.

Heat Kernels

Continuous manifolds give the idea for the Heat Kernel

That is assigning weights $W_{ij} = e^{-\frac{\|x_i - x_j\|^2}{t}}$

The heat function is a solution for the Laplace Beltrami Operator, and as a result by assigning the weights according to it we get better approximation of the "ideal" infinite points case.

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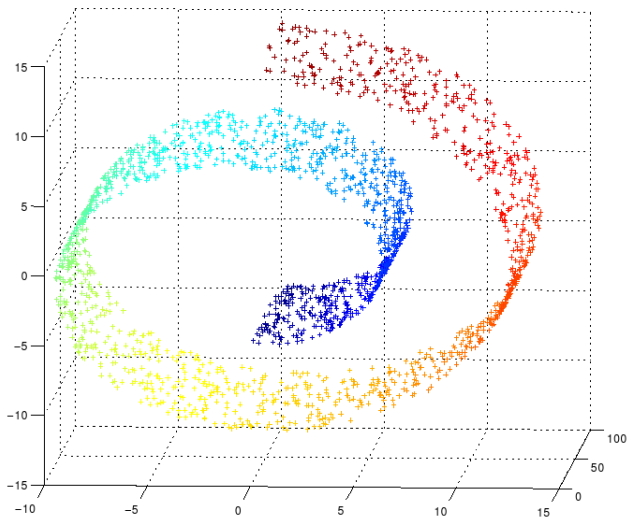
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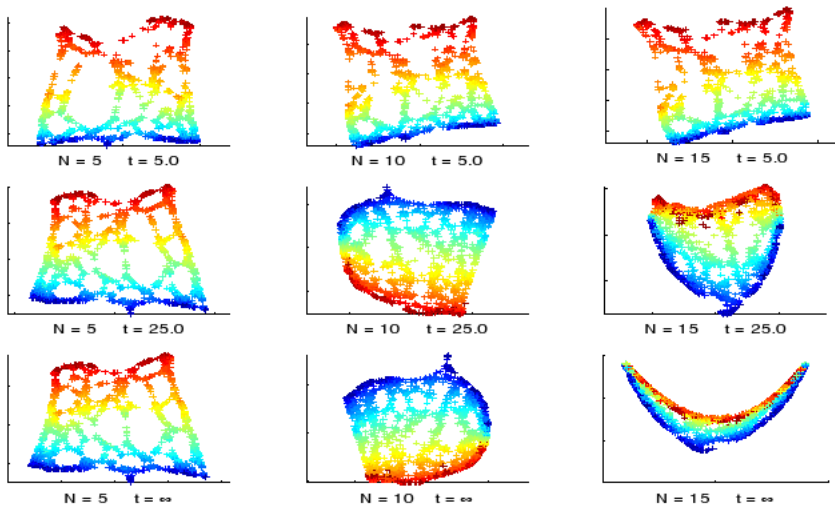
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One more Swiss roll!



Unfolding the Swiss roll - the parameters t, N



- N =number of nearest neighbors, t the heat kernel parameter

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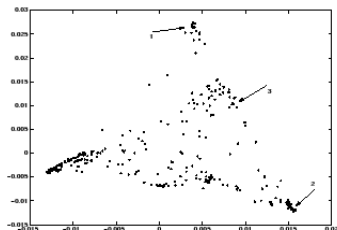
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Understanding syntactic structure of words

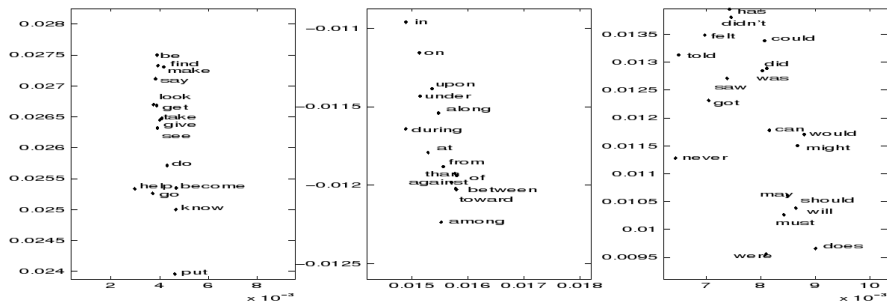
Input:

- 300 most frequent words of Brown corpus
- Information about the frequency of its left and right neighbors (600 Dimensional space.)

The algorithm run with $N = 14$, $t = \infty$



Understanding syntactic structure of Words



- Three parts of the output. We can see verbs, prepositions, and auxiliary and modal verbs are grouped.

Discussion

- Laplacian Eigenvalues is a part of the Isomap LLE family
- They actually prove that LLE minimizes approximately the same value
- Many times we need to skip eigenvectors, as eigenvectors with bigger eigenvalues give better results. However variations for doing so exist.
- Although all these algorithms give good results for convex non-linear structures, they do not give much better results in other cases.