# Limits of Spectral Clustering

Presented By: Ashish Shrivastava

University of Maryland, College Park

Oct 04, 2011

Outline

- Introduction/Motivation
- "Goodness" aka Consistenecy
- Theorems
  - Theorem Statements
- Sketch of proof for Theorem 2
  - Step 1
  - Step 2
  - Step 3
  - Step 4
  - Step 5
- Conclusion



- Introduction/Motivation
- 2 "Goodness" aka Consistenecy
- Theorems
  - Theorem Statements
- Sketch of proof for Theorem 2
  - Step 1
  - Step 2
  - Step 3
  - Step 4
  - Step 5
- Conclusion



## Introduction/Motivation

• How to measure the "goodness" of the clustering algorithms?



## Introduction/Motivation

- How to measure the "goodness" of the clustering algorithms?
  - Unnormalized Clustering Algorithm:

$$L_n = D_n - K_n$$

where  $[K_n]_{(i,j)} = s(X_i, X_j)$  and  $D_n$  is a diagonal matrix with  $[D_n]_{(i,i)} = \sum_{j=1}^n s(X_i, X_j)$ .



# Introduction/Motivation

- How to measure the "goodness" of the clustering algorithms?
  - Unnormalized Clustering Algorithm:

$$L_n = D_n - K_n$$

where  $[K_n]_{(i,j)} = s(X_i, X_j)$  and  $D_n$  is a diagonal matrix with  $[D_n]_{(i,i)} = \sum_{i=1}^n s(X_i, X_i)$ .

Normalized Clustering Algorithm

$$L'_n = D_n^{-1/2} L_n D_n^{-1/2}$$



- "Goodness" aka Consistenecy
- - Theorem Statements
- - Step 1
  - Step 2
  - Step 3
  - Step 4
  - Step 5



# "Goodness" aka Consistenecy

Consistenecy:



6 / 21

# "Goodness" aka Consistenecy

- Consistenecy:
  - Well defined partitions given sufficiently many datapoints.



# "Goodness" aka Consistenecy

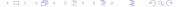
- Consistenecy:
  - Well defined partitions given sufficiently many datapoints.
  - Focus on limit behavior for sample size tending to infitnity (Convergence).

- Introduction/Motivation
- 2 "Goodness" aka Consistenecy
- Theorems
  - Theorem Statements
- Sketch of proof for Theorem 2
  - Step 1
  - Step 2
  - Step 3
  - Step 4
  - Step 5
- Conclusion



### **Theorems**

• Theorem 1: Convergence of normalized spectral clustering.



- Theorem 1: Convergence of normalized spectral clustering.
- Theorem 2: Convergence of unnormalized spectral clustering.

#### Theorems

- Theorem 1: Convergence of normalized spectral clustering.
- Theorem 2: Convergence of unnormalized spectral clustering.
- Theorem 3: Structure of the limit operators.

#### Theorem 1:

Assumptions:

- General assumptions
- first r eigenvalues of the limit operator U' have multiplicity 1.

Claim: The first r eigenvalues of U', and the corresponding eigenvectors converge almost surely.

**Notations:** U' is the limit operator of  $L'_n$  and  $d \in C(\mathcal{X})$  is "degree function" defined later.

#### Theorem 2:

Assumptions:

- General assumptions
- first r eigenvalues of the limit operator U have multiplicity 1, and are not element of range(d)

Claim: The first r eigenvalues of U', and the corresponding eigenvectors converge almost surely.

**Notations:** U is the limit operator of  $L_n$ .



#### Theorem 3:

Let  $\mathcal{X} = \bigcup_{i=1}^k \mathcal{X}_i$  be a partition of the data space. Let  $L_{ii,n}$  be the sub-matrices of  $L_n$ ,  $U_{ii}: \mathcal{C}(\mathcal{X}_i) \to \mathcal{C}(\mathcal{X}_i)$  the restrictions of U corresponding to the set  $\mathcal{X}_i$  and  $\mathcal{X}_i$ , and  $U'_{ii,n}$  and  $U'_{ii}$  the analogous quantities for the normalized case. Then under the general assumptions,  $\frac{1}{n}L_{ii,n}$  converges compactly to  $U_{ij}$  a.s. and  $L'_{ii.n}$  converges compactly to  $U'_{ii}$  a.s.

- - Theorem Statements
- Sketch of proof for Theorem 2
  - Step 1
  - Step 2
  - Step 3
  - Step 4
  - Step 5



• Since dimension of  $L_n$  increases as n increases, an operator  $U_n$  is constructed and its convergence is showed.

$$U_n f(x) := d_n(x) f(x) - \int s(x, y) f(y) dP_n(y)$$

where, 
$$d_n(x) := \int s(x, y) dP_n(y)$$
 and  $f \in C(\mathcal{X})$ .



• Since dimension of  $L_n$  increases as n increases, an operator  $U_n$  is constructed and its convergence is showed.

$$U_n f(x) := d_n(x) f(x) - \int s(x, y) f(y) dP_n(y)$$

where,  $d_n(x) := \int s(x,y) dP_n(y)$  and  $f \in C(\mathcal{X})$ .

Similarily, the limit operator is defined as below:

$$Uf(x) := d(x)f(x) - \int s(x,y)f(y)dP(y)$$

where,  $d(x) := \int s(x, y) dP(y)$ 



# Relations between $\sigma(\frac{1}{n}L_n)$ and $\sigma(U_n)$

• The spectrum of  $U_n$  consists of  $range(d_n)$ , plus some isolated eigenvalues with finite multiplicity. The same holds for U and range(d).



# Relations between $\sigma(\frac{1}{n}L_n)$ and $\sigma(U_n)$

- The spectrum of  $U_n$  consists of  $range(d_n)$ , plus some isolated eigenvalues with finite multiplicity. The same holds for U and range(d).
- If  $f \in C(\mathcal{X})$  is an eigenfunction of  $U_n$  with arbitrary eigenvalue  $\lambda$ , then the vector  $v \in \mathbb{R}$  with  $v_i = f(X_i)$  is an eigenvector of the matrix  $\frac{1}{n}L_n$  with eigenvalue  $\lambda$ .

# Relations between $\sigma(\frac{1}{n}L_n)$ and $\sigma(U_n)$

- The spectrum of  $U_n$  consists of  $range(d_n)$ , plus some isolated eigenvalues with finite multiplicity. The same holds for U and range(d).
- If  $f \in C(\mathcal{X})$  is an eigenfunction of  $U_n$  with arbitrary eigenvalue  $\lambda$ , then the vector  $v \in \mathbb{R}$  with  $v_i = f(X_i)$  is an eigenvector of the matrix  $\frac{1}{n}L_n$  with eigenvalue  $\lambda$ .
- If v is an eigenvector of the matrix  $\frac{1}{n}L_n$  with eigenvalue  $\lambda \not\in range(d_n)$ , then the function  $f(x) = \frac{1}{n} (\sum_{i} s(x, X_i) v_i) / (d_n(x) - \lambda)$  is the unique eigenfunction of  $U_n$  with eigen value  $\lambda$  satisfying  $f(X_i) = v_i$ .



## Compact Convergence of $U_n$ to U a.s.

#### Compact convergence:

A sequence of operator  $S_n$  converges compactly to S if it converges pointwise and if for every sequence  $(x_n)_n$  in unit ball B, the sequence  $(S - S_n)x_n$  is relatively compact.

15 / 21

### Compact convergence:

A sequence of operator  $S_n$  converges compactly to S if it converges pointwise and if for every sequence  $(x_n)_n$  in unit ball B, the sequence  $(S-S_n)x_n$  is relatively compact.

$$\sup_{x \in \mathcal{X}} |\int s(x,y) dP_n(y) - \int s(x,y) dP(y)| \to 0$$
 almost surely

#### Compact convergence:

A sequence of operator  $S_n$  converges compactly to S if it converges pointwise and if for every sequence  $(x_n)_n$  in unit ball B, the sequence  $(S - S_n)x_n$  is relatively compact.

•

$$\sup_{x \in \mathcal{X}} |\int s(x,y) dP_n(y) - \int s(x,y) dP(y)| \to 0$$
 almost surely

Remembner.

$$U_n f(x) := d_n(x) f(x) - \int s(x, y) f(y) dP_n(y)$$



# Convergence of eigenfunctions of $U_n$ to those of U

#### Perturbation theory says,

- Compact convergence of operators implies the convergence of isolated eigenvalues.
- Corresponding eigen vectors converge upto a change of sign (if multiplicity is 1).
- For multiplicity larger than 1, but finite, corresponding eigenspaces converge.



# Convergence of unnormalized spectral clustering

The above 4 steps imply:

if  $\lambda$  denotes the j-th eigenvalue of of U with eigenfunction  $f \in C(\mathcal{X})$  and  $\lambda_n$  the j-th eigenvalue of  $\frac{1}{n}L_n$  with eigenvector  $v_n=(v_{n,1},\ldots,v_{n,n})'$ , then there exists a sequence of signs  $a_i \in \{-1, +1\}$  such that  $\sup_{i=1,\ldots,n} |a_i v_{n,i} - f(X_i)| \to 0$  a.s.

- Introduction/Motivation
- 2 "Goodness" aka Consistenecy
- Theorems
  - Theorem Statements
- Sketch of proof for Theorem 2
  - Step 1
  - Step 2
  - Step 3
  - Step 4
  - Step 5
- Conclusion



## Conclusion

- Normalized spectral clustering always converges to a limit partitions of the whole data space.
- Convergence of unnormalized spectral clustering can be guaranteed under strong additional assumption that the first eigenvalues of the Laplacian do not fall inside the range of the degree function.
- Consistency results are a basic sanity check for behavior of statistical learning algorithms. Algorithms that do not converge, can not be expected to exhibit reliable results on finite samples.

### References



Ulrike Von Luxburg, Oliver Bousquet and Mikhail Belkin. Limits of Spectral Clustering.

NIPS. 2004.



Ulrike Von Luxburg, Oliver Bousquet and Mikhail Belkin.

On the Convergence of Spectral Clustering on Random Samples: The Normalized Case.

COLT, 2004.



