# Variational problems on graphs and their continuum limits

#### Dejan Slepčev Carnegie Mellon University

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• Partition the data into meaningful groups.

## Graph-Based Clustering



- Determine a similarity measure between images
- Construct a graph based on the similarity measure.

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- Construct a graph based on the similarity measure.
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• Connect nearby vertices: Edge weights  $W_{i,j}$ .

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#### Graph cut

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- Connect nearby vertices: Edge weights *W<sub>i,j</sub>*
- Graph Cut:  $A \subset V$ .

$$Cut(A, A^c) = \sum_{i \in A} \sum_{j \in A^c} W_{i,j}.$$

• Let  $V = \{X_1, \ldots, X_n\}$  be a point cloud in  $\mathbb{R}^d$ :



- Connect nearby vertices: Edge weights W<sub>i,i</sub>
- Minimize:  $A \subset V$ .

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• Graph Cut:  $A \subset V$ .

$$Cut(A, A^c) = \sum_{i \in A} \sum_{j \in A^c} W_{i,j}$$

• Cheeger Cut: Minimize

$$GC(A) = \frac{Cut(A, A^c)}{\min\{|A|, |A^c|\}}.$$

### **Graph Constructions**

proximity based graphs



• kNN graphs: Connect each vertex with its k nearest neighbors

Task

Minimize

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Algorithm of Bresson, Laurent, Uminsky and von Brecht (2013).

#### *k*-means clustering

Given  $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$  find a set of *k* points  $A = \{a_1, \ldots, a_k\}$  which minimizes

$$\min_{A} \frac{1}{n} \sum_{i=1}^{n} \operatorname{dist}(x_i, A)^2$$

ľ

where dist $(x, A) = \min_{a \in A} |x - a|$ .



## Spectral Clustering

•  $V_n = \{X_1, \ldots, X_n\}$ , similarity matrix W, as before:

$$W_{ij} := rac{1}{arepsilon^{\mathcal{d}}} \, \eta \left( |X_i - X_j| / arepsilon 
ight).$$

The weighted degree of a vertex is  $d_i = \sum_j W_{i,j}$ . • Dirichlet energy of  $u_n : V_n \to \mathbb{R}$  is

$$F(u) = \frac{1}{2} \sum_{i,j} W_{ij} |u_n(X_i) - u_n(X_j)|^2.$$

Associated operator is the (unnormalized) graph laplacian

$$L = D - W$$
,

where  $D = \text{diag}(d_1, \ldots, d_n)$ .

**Input:** Number of clusters k and similarity matrix W.

- Construct the unnormalized graph Laplacian L.
- Compute the eigenvectors  $u_1, \ldots, u_k$  of *L* associated to the *k* smallest eigenvalues of *L*.
- Define the matrix  $U \in \mathbb{R}^{k \times n}$ , where the *i*-th row of *U* is the vector  $u_i$ .
- For i = 1, ..., n, let  $y_i \in \mathbb{R}^k$  be the *i*-th column of *U*.
- Use the *k*-means algorithm to partition the set of points  $\{y_1, \ldots, y_n\}$  into *k* groups, that we denote by  $G_1, \ldots, G_k$ .

**Output:** Clusters  $G_1, \ldots, G_k$ .

# Spectral Clustering: Two moons (easy)



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#### Spectral Clustering: Two moons (easy)



1D embedding:  $x_i \mapsto v_2(x_i)$ 

## Comparison of Clustering Algorithms



(a) k - means

(b) spectral

(c) Cheeger cut

## Comparison of Clustering Algorithms



#### **Ground Truth Assumption**

Assume points  $X_1, X_2, \ldots$ , are drawn i.i.d out of measure  $d\nu = \rho dx$ 



## Consistency of Cheeger cut clustering

**Consistency of clustering** 

Do the minimizers of

$$GC(A) = rac{\sum_{i \in A} \sum_{j \in A^c} W_{i,j}}{\min\{|A|, |A^c|\}}$$

converge as the number of data points  $n \rightarrow \infty$ ?

Can one characterize the limiting object as a minimizer of a continuum functional?



### **Graph Total Variation**

#### Graph total variation

For a function  $u: V \to \mathbb{R}$ 

$$GTV_n(u) = \frac{1}{n^2} \sum_{i,j} W_{i,j} \left| u_i - u_j \right|$$

where  $u_i = u(X_i)$ .

Note that for a set of vertices  $A \subset V$ 

$$GTV_n(\chi_A) = \frac{1}{n^2}Cut(A, A^c)$$

where  $\chi_A$  is the characteristic function of A

$$\chi_{\mathcal{A}}(X_i) = egin{cases} 1 & ext{if } x_i \in \mathcal{A} \ 0 & ext{otherwise}. \end{cases}$$

#### **Relaxed Problem**

$$GTV_n(u) = \frac{1}{n^2}\sum_{i,j}W_{i,j}|u_i - u_j|.$$

Balance term

$$B_n(u) = \frac{1}{n} \min_{c \in \mathbb{R}} \sum_i |u_i - c|$$

$$B_n(\chi_A) = \frac{1}{n} \min\{|A|, |A^c|\}.$$

Relaxed problem

Minimize

$$GC_n(u) = rac{GTV_n(u)}{B_n(u)}$$

#### Theorem

Relaxation is exact: There exists a set of vertices  $A_n$  such that  $u_n = \chi_{A_n}$  minimizes  $GC_n$ .

## Total variation in continuum setting

•  $d\nu = \rho dx$  probability measure, supp $(\nu) = D$ ,  $0 < \lambda \le \rho \le \frac{1}{\lambda}$  on D.

Weighted relative perimeter

$$P(A; D, 
ho^2) = \int_{D \cap \partial A} 
ho^2 dS_{d-1}$$

Weighted TV

Given  $A \subset D$ 

$$TV(u,\rho^2) = \int_D |\nabla u| \rho^2 dx$$



## Total variation in continuum setting

•  $d\nu = \rho dx$  probability measure, supp $(\nu) = D$ ,  $0 < \lambda \le \rho \le \frac{1}{\lambda}$  on D.

#### Weighted relative perimeter

$$\mathcal{P}(\mathcal{A}; \mathcal{D}, \rho^2) = \int_{\mathcal{D}\cap\partial\mathcal{A}} \rho^2 dS_{d-1} = TV(\chi_{\mathcal{A}}, \rho^2)$$

Weighted TV

Given  $A \subset D$ 

$$TV(u, 
ho^2) = \sup\left\{\int_D u \operatorname{div}(\phi) dx : |\phi| \le 
ho^2, \ \phi \in C^\infty_c(D, \mathbb{R}^d)
ight\}$$



# Clustering in continuum setting

- $\nu$  probability measure with compact support supp $(\nu) = D$ .
- $\nu$  has continuous on *D* density  $\rho$  and  $0 < \lambda \le \rho \le \frac{1}{\lambda}$  on *D*.

Weighted TV

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ho^2) = \sup\left\{\int_D u\, {
m div}(\phi) {dx} \; : \; |\phi| \leq 
ho^2 \; , \; \phi \in C^\infty_c(D,\mathbb{R}^d)
ight\}$$

Weighted relative perimeter

Given 
$$A \subset D$$
  $P(A; D, \rho^2) = TV(\chi_A, \rho^2)$ 

Balance term

$$B(A) = \min\{|A|, 1 - |A|\}$$
 where  $|A| = \nu(A)$ .

Weighted Cheeger Cut: Minimize

$$C(A) = \frac{P(A; D, \rho^2)}{B(A)}$$

## Relaxation in continuum setting

- $\nu$  probability measure with compact support supp $(\nu) = D$ .
- $\nu$  has continuous on *D* density  $\rho$  and  $0 < \lambda \le \rho \le \frac{1}{\lambda}$  on *D*.

#### Weighted TV

$$TV(u, \rho^2) = \sup\left\{\int_D u \operatorname{div}(\phi) dx : |\phi| \le \rho^2 \ , \ \phi \in C^\infty_c(D, \mathbb{R}^d)
ight\}$$

**Balance term** 

$$B(u) = \min_{c \in \mathbb{R}} \int_D |u(x) - c|\rho(x)dx$$

Minimize

$$C(u) = \frac{TV(u, \rho^2)}{B(u)}$$

# Clustering in continuum setting

#### Minimize

$$C(u) = \frac{TV(u, \rho^2)}{B(u)}$$



Localizing the kernel as  $n \to \infty$ 

$$\eta_{\varepsilon}(z) = \frac{1}{\varepsilon^{d}} \eta\left(\frac{z}{\varepsilon}\right).$$

Consistency of clustering II

Do the minimizers of

$$GC_{n,\varepsilon_n}(u^n) = \frac{1}{n} \frac{\frac{1}{\varepsilon_n} \sum_{i,j} \eta_{\varepsilon_n}(X_i - X_j) |u_i^n - u_j^n}{\min_{c \in \mathbb{R}} \sum_i |u_i^n - c|}$$

converge as the number of data points  $n \to \infty$  to a minimizer of

$$C(u) = \frac{TV(u, \rho^2)}{\min_{c \in \mathbb{R}} \int_D |u(x) - c|\rho(x) dx}$$
?

**Question 1:** For what scaling of  $\varepsilon(n)$  can this hold? **Question 2:** What is the topology for which  $u^n \longrightarrow u$ ?



 $n = 120, \varepsilon = 0.30$ 



 $n = 120, \varepsilon = 0.40$ 



$$n = 500, \varepsilon = 0.14$$

$$n = 500, \varepsilon = 0.2$$

#### Consistency results in statistics/machine learning

- Arias Castro, Pelletier, and Pudlo 2012 partial results on the problem
- Pollard 1981 k -means
- Hartigan 1981 single linkage
- Belkin and Niyogi 2006 Laplacian eigenmaps
- von Luxburg, Belkin, and Bousquet 2004, 2008 spectral embedding

#### What was known

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#### **Calculus of Variations**

Discrete to continuum for functionals on grids: *Braides 2010, Braides and Yip 2012, Chambolle, Giacomini and Lussardi 2012, Gobbino and Mora 2001, Van Gennip and Bertozzi 2014*
## **Γ-Convergence**

$$(Y, d_Y)$$
 - metric space,  $F_n : Y \to [0, \infty]$ 

### Definition

The sequence  $\{F_n\}_{n\in\mathbb{N}}$   $\Gamma$ -converges (w.r.t  $d_Y$ ) to  $F: Y \to [0,\infty]$  if: Liminf inequality: For every  $y \in Y$  and whenever  $y_n \to y$ 

 $\liminf_{n\to\infty}F_n(y_n)\geq F(y),$ 

**Limsup inequality:** For every  $y \in Y$  there exists  $y_n \to y$  such that

 $\limsup_{n\to\infty} F_n(y_n) \leq F(y).$ 

#### Definition (Compactness property)

$$\begin{split} \{F_n\}_{n\in\mathbb{N}} \text{ satisfies the compactness property if} \\ \{y_n\}_{n\in\mathbb{N}} \text{ bounded and} \\ \{F_n(y_n)\}_{n\in\mathbb{N}} \text{ bounded} \end{split} \bigg\} \Longrightarrow \{y_n\}_{n\in\mathbb{N}} \text{ has convergent subsequence} \end{split}$$

### Proposition: Convergence of minimizers

Γ-convergence and Compactness imply: If  $y_n$  is a minimizer of  $F_n$  and  $\{y_n\}_{n \in N}$  is bounded in *Y* then along a subsequence

 $y_n \to y$  as  $n \to \infty$ 

and

y is a minimizer of F.

In particular, if *F* has a unique minimizer, then a sequence  $\{y_n\}_{n \in \mathbb{N}}$  converges to the unique minimizer of *F*.

### Consistency of clustering III

Show that

$$GC_{n,\varepsilon_n}(u^n) = \frac{1}{n} \frac{\frac{1}{\varepsilon_n} \sum_{i,j} \eta_{\varepsilon_n}(X_i - X_j) |u_i^n - u_j^n|}{\min_{c \in \mathbb{R}} \sum_i |u_i^n - c|}$$

**Γ-converge** as the number of data points  $n \to \infty$ , and  $\varepsilon_n \to 0$  at certain rate to

$$F(u) = \frac{\sigma TV(u, \rho^2)}{\min_{c \in \mathbb{R}} \int_D |u(x) - c|\rho(x) dx}$$

and show that compactness property holds.

#### Questions

- For what scaling of  $\varepsilon(n)$  can this hold?
- 2 What is the topology for  $u^n \longrightarrow u$ ?

Consistency of graph total variation

Show that

$$GTV_{n,\varepsilon_n}(u^n) = \frac{1}{\varepsilon_n n^2} \sum_{i,j} \eta_{\varepsilon_n}(X_i - X_j) |u_i^n - u_j^n|$$

**Γ-converge** to  $\sigma TV(u, \rho^2)$ , as the number of data points  $n \to \infty$ , and  $\varepsilon_n \to 0$  at certain rate and show that compactness property holds.

### Questions

- For what scaling of  $\varepsilon(n)$  can this hold?
- **2** What is the topology for  $u^n \longrightarrow u$ ?

Consider domain *D* and  $V_n = \{X_1, \ldots, X_n\}$  random i.i.d points.



• How to compare  $u_n : V_n \to \mathbb{R}$  and  $u : D \to \mathbb{R}$  in a way consistent with  $L^1$  topology?

Note that  $u \in L^1(\nu)$  and  $u_n \in L^1(\nu_n)$ , where  $\nu_n = \frac{1}{N} \sum_{i=1}^n \delta_{X_i}$ .

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Consider domain *D* and  $V_n = \{X_1, \ldots, X_n\}$  random i.i.d points.



• How to compare  $u_n \in L^1(\nu_n)$  and  $u \in L^1(D)$  in a way consistent with  $L^1$  topology?

An idea: Divide the domain *D* into *n* sets of the same  $\nu$  measure and to each piece associate a point  $X_i$ . That is, consider a map  $T_n : D \to D$  such that  $T_{\#}\nu = \nu_n$ .



Divide the domain *D* into *n* pieces and to each piece associate a point  $X_i$ . That is, consider a map  $T_n : D \to D$  such that  $T_{n\sharp}\nu = \nu_n$ .



To compare  $u \in L^1(\nu)$  and  $u_n \in L^1(\nu_n)$  we compare  $u_n \circ T_n$  and u in  $L^1(\nu)$ .

### A different partition:



### A different partition:



Consider domain *D* and  $V_n = \{X_1, \ldots, X_n\}$  random i.i.d points.



• Let  $T_n$  be a transportation map from  $\nu$  to  $\nu_n$ 

For 
$$u \in L^1(\nu)$$
 and  $u_n \in L^1(\nu_n)$   
$$d((\nu, u), (\nu_n, u_n)) = \inf_{T_n \notin \nu = \nu_n} \int_D (|u_n(T_n(x)) - u(x)| + |T_n(x) - x|) \rho(x) dx$$

where

$$T_{n\sharp}\nu = \nu_n$$

# TL<sup>1</sup> Space

#### Definition

$$TL^{p} = \{(\nu, f) : \nu \in \mathcal{P}(D), f \in L^{p}(\nu)\}$$
$$d^{p}_{TL^{p}}((\nu, f), (\sigma, g)) = \inf_{\pi \in \Pi(\nu, \sigma)} \int_{D \times D} |y - x|^{p} + |g(y) - f(x))|^{p} d\pi(x, y).$$

where

$$\Pi(\nu,\sigma) = \{\pi \in \mathcal{P}(D \times D) : \pi(A \times D) = \nu(A), \ \pi(D \times A) = \sigma(A)\}.$$

If  $T_{\sharp}\nu = \sigma$  then  $\pi = (I \times T)_{\sharp}\nu \in \Pi(\nu, \sigma)$  and the integral becomes  $\int |T(x) - x|^p + |g(T(x)) - f(x)|^p d\nu(x)$ 

Lemma

 $(TL^{p}, d_{TL^{p}})$  is a metric space.

# *TL*<sup>1</sup> convergence

• 
$$(\nu, f_n) \xrightarrow{TL^p} (\nu, f)$$
 iff  $f_n \xrightarrow{L^1(\nu)} f$ 

- (ν<sub>n</sub>, f<sub>n</sub>) → (ν, f) iff the measures (I × f<sub>n</sub>)<sub>\$</sub>ν<sub>n</sub> weakly converge to (I × f)<sub>\$</sub>ν. That is if graphs, considered as measures converge weakly.
- The space *TL<sup>p</sup>* is not complete. Its completion are the probability measures on the product space *D* × ℝ.

If  $(\nu_n, f_n) \xrightarrow{TL^p} (\nu, f)$  then there exists a sequence of transportation plans  $\nu_n$  such that

(1) 
$$\int_{D\times D} |x-y|^p d\pi_n(x,y) \longrightarrow 0 \text{ as } n \to \infty.$$

We call a sequence of transportation plans  $\pi_n \in \Pi(\nu_n, \nu)$  stagnating if it satisfies (1).

Stagnating sequence:  $\int_{D \times D} |x - y| d\pi_n(x, y) \longrightarrow 0$ 

### TFAE:

$$(\nu_n, f_n) \xrightarrow{TL^p} (\nu, f) \text{ as } n \to \infty.$$

2  $\nu_n \rightarrow \nu$  and **there exists** a stagnating sequence of transportation plans  $\{\pi_n\}_{n \in \mathbb{N}}$  for which

(2) 
$$\int\!\!\!\int_{D\times D} |f(x)-f_n(y)|^p d\pi_n(x,y) \to 0, \text{ as } n \to \infty.$$

3  $\nu_n \rightarrow \nu$  and **for every** stagnating sequence of transportation plans  $\pi_n$ , (2) holds.

Formally  $TL^{p}(D)$  is a fiber bundle over  $\mathcal{P}(D)$ .





$$GTV_{n,\varepsilon_n}(u^n) = \frac{1}{\varepsilon_n n^2} \sum_{i,j} \eta_{\varepsilon_n}(X_i - X_j) |u_i^n - u_j^n|$$

Γ-convergence of Total Variation (García Trillos and S.)

Let  $\{\varepsilon_n\}_{n\in\mathbb{N}}$  be a sequence of positive numbers converging to 0 satisfying

$$\lim_{n \to \infty} \frac{(\log n)^{3/4}}{n^{1/2}} \frac{1}{\varepsilon_n} = 0 \text{ if } d = 2,$$
$$\lim_{n \to \infty} \frac{(\log n)^{1/d}}{n^{1/d}} \frac{1}{\varepsilon_n} = 0 \text{ if } d \ge 3.$$

Then,  $GTV_{n,\varepsilon_n}$   $\Gamma$ -converge to  $\sigma TV(\cdot, \rho^2)$  as  $n \to \infty$  in the  $TL^1$  sense, where  $\sigma$  depends explicitly on  $\eta$ .

### **Γ**-convergence of Perimeter

The conclusions hold when all of the functionals are restricted to characteristic functions of sets. That is, the graph perimeters  $\Gamma$ -converge to the continuum perimeter.

### Compactness

With the same conditions on  $\varepsilon_n$  as before, if

$$\sup_{n\in\mathbb{N}}\|u_n\|_{L^1(D,\nu_n)}<\infty,$$

and

$$\sup_{n\in\mathbb{N}}GTV_{n,\varepsilon_n}(u_n)<\infty,$$

then  $\{u_n\}_{n \in N}$  is  $TL^1$ -precompact.

# Consistency of Cheeger Cuts

Recall:

$$GC_{n,\varepsilon_n}(u^n) = \frac{1}{n} \frac{\frac{1}{\varepsilon_n} \sum_{i,j} \eta_{\varepsilon_n} (X_i - X_j) |u_i^n - u_j^n|}{\min_{c \in \mathbb{R}} \sum_i |u_i^n - c|}$$
$$C(u) = \frac{\sigma TV(u, \rho^2)}{\min_{c \in \mathbb{R}} \int_D |u(x) - c|\rho(x) dx}$$



# Consistency of Cheeger Cuts

Recall:

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$$C(u) = \frac{\sigma TV(u, \rho^2)}{\min_{c \in \mathbb{R}} \int_D |u(x) - c|\rho(x) dx}$$

Consistency of Cheeger Cuts (von Brecht, García Trillos, Laurent, S.) For the same conditions on  $\varepsilon_n$  as before, with probability one:

$$GC_{n,\varepsilon_n} \xrightarrow{\Gamma} C$$
 w.r.t.  $TL^1$  metric.

Moreover, for any sequence of sets  $E_n \subseteq \{X_1, \ldots, X_n\}$  of almost minimizers of the Cheeger energy, every subsequence has a convergent subsequence (in the  $TL^1$  sense ) to a minimizer of the Cheeger energy on the domain D.

• We require

$$\lim_{n \to \infty} \frac{(\log n)^{3/4}}{n^{1/2}} \frac{1}{\varepsilon_n} = 0 \text{ if } d = 2,$$
$$\lim_{n \to \infty} \frac{(\log n)^{1/d}}{n^{1/d}} \frac{1}{\varepsilon_n} = 0 \text{ if } d \ge 3.$$

- Note that for  $d \ge 3$  this means that typical degree  $\gg \log(n)$ .
- Does convergence hold if fewer than log(n) neighbors are connected to?

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- Note that for  $d \ge 3$  this means that typical degree  $\gg \log(n)$ .
- Does convergence hold if fewer than log(n) neighbors are connected to?

**No.** There exists c > 0 such that  $\varepsilon_n < c \frac{\log(n)^{1/d}}{n^{1/d}}$  then with probability one the random geometric graph is asymptotically disconnected. *Penrose (1999); Gupta and Kumar (1999); Goel,Rai and Krishnamachari (2004).* 

This implies that for large enough *n*, min  $GC_{n,\varepsilon_n} = 0$ . While inf C > 0.

So for  $d \ge 3$  the condition is optimal in terms of scaling.

## Hint about the proof

Assume that  $u_n \xrightarrow{TL^1} u$  as  $n \to \infty$ . There exists  $T_{n\sharp}\nu = \nu_n$  stagnating  $(\int |x - T_n(x)| d\nu(x) \to 0)$ .

$$GTV_{n,\varepsilon_n}(u^n) = \frac{1}{\varepsilon_n} \int_{D \times D} \eta_{\varepsilon_n} (\tilde{x} - \tilde{y}) |u_n(\tilde{x}) - u_n(\tilde{y})| d\nu_n(\tilde{x}) d\nu_n(\tilde{y})$$
$$= \frac{1}{\varepsilon_n} \int_{D \times D} \eta_{\varepsilon_n} (T_n(x) - T_n(y)) |u_n \circ T_n(x) - u_n \circ T_n(y)| \rho(x) \rho(y) dx dy$$

Define 
$$TV_{\varepsilon}(u; \rho) := rac{1}{arepsilon} \int_{D imes D} \eta_{arepsilon}(x-y) |u(x) - u(y)| 
ho(x) 
ho(y) dx dy.$$

- $TV_{\varepsilon} \stackrel{\Gamma}{\longrightarrow} TV(\cdot, \rho^2)$  wrt  $L^1(\nu_0)$  metric. (Alberti-Bellettini, Chambolle-Giacomini-Lussardi, Savin-Valdinocci, Ponce)
- If |T<sub>n</sub>(x) − x| ≪ ε<sub>n</sub> then one may be able to compare GTV<sub>n,ε<sub>n</sub></sub>(u<sup>n</sup>) and TV<sub>ε</sub>(u<sub>n</sub> ∘ T<sub>n</sub>; ρ).

 $\infty-$ transportation distance:

$$d_\infty(\mu,
u) = \inf_{\pi\in\Pi(\mu,
u)} ext{esssup}_\pi\{|x-y| \ : \ x\in X, y\in Y\}$$

- There exists a minimizer  $\pi \in \Pi(\mu, \nu)$ . • If  $\mu = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$  and  $\nu = \frac{1}{n} \sum_{j=1}^{n} \delta_{y_j}$  then  $d_{\infty}(\mu, \nu) = \min_{\sigma-\text{permutation}} \max_{i} |x_i - y_{\sigma(i)}|.$
- If  $\mu$  has density then OT map, *T* exists (Champion, De Pascale, Juutinen 2008) and

$$d_{\infty}(\mu,\nu) = \|T - Id\|_{L^{\infty}(\mu)}.$$

## $\infty$ -OT between a measure and its random sample

Optimal matchings in dimension  $d \ge 3$ : Ajtai-Komlós-Tusnády (1983), Yukich and Shor (1991), Garcia Trillos and S. (2014)



#### Theorem

There are constants c > 0 and C > 0 (only depending on d) such that with probability one we can find a sequence of transportation maps  $\{T_n\}_{n \in \mathbb{N}}$  from  $\nu_0$  to  $\nu_n$  ( $T_{n \#}\nu_0 = \nu_n$ ) and such that:

$$c \leq \liminf_{n \to \infty} \frac{n^{1/d} \| Id - T_n \|_{\infty}}{(\log n)^{1/d}} \leq \limsup_{n \to \infty} \frac{n^{1/d} \| Id - T_n \|_{\infty}}{(\log n)^{1/d}} \leq C.$$

## $\infty$ -OT between a measure and its random sample

Optimal matchings in dimension  $\mathbf{d} = \mathbf{2}$ : Leighton and Shor (1986), new proof by Talagrand (2005), Garcia Trillos and S. (2014)



#### Theorem

There are constants c > 0 and C > 0 such that with probability one we can find a sequence of transportation maps  $\{T_n\}_{n \in \mathbb{N}}$  from  $\nu_0$  to  $\nu_n$   $(T_{n\#}\nu_0 = \nu_n)$  and such that:

(3) 
$$c \leq \liminf_{n \to \infty} \frac{n^{1/2} \| Id - T_n \|_{\infty}}{(\log n)^{3/4}} \leq \limsup_{n \to \infty} \frac{n^{1/2} \| Id - T_n \|_{\infty}}{(\log n)^{3/4}} \leq C.$$

## **Spectral Clustering**

•  $V_n = \{X_1, \ldots, X_n\}$ , similarity matrix W, as before:

$$W_{ij} := rac{1}{arepsilon^d} \eta\left(rac{|X_i - X_j|}{arepsilon}
ight).$$

The weighted degree of a vertex is  $d_i = \sum_j W_{i,j}$ .

• Dirichlet energy of  $u_n: V_n \to \mathbb{R}$  is

$$F(u) = \frac{1}{2} \sum_{i,j} W_{ij} |u_n(X_i) - u_n(X_j)|^2.$$

- Associated operator is the graph laplacian L = D W, where  $D = \text{diag}(d_1, \ldots, d_n)$ .
- To partition the point cloud into two clusters, consider the eigenvector corresponding to second eigenvalue:

$$u_n := \arg\min\left\{\sum_{i,j} W_{ij}|u(X_i) - u(X_j)|^2 : \sum_i u(X_i) = 0, \|u\|_2 = 1\right\}$$

## Consistency of Spectral Clustering

von Luxburg, Belkin, Bousquet '08, Belkin-Nyogi '07, Ting, Huang, Jordan '10, Singer, Wu '13, Burago, Ivanov, Kurylev '14, Shi, Sun '15

$$u_n := \arg\min\left\{\sum_{i,j} W_{ij}|u(X_i) - u(X_j)|^2 : \sum_i u(X_i) = 0, \|u\|_2 = 1\right\}$$

• Suppose  $X_1, \ldots, X_n, \ldots$  are i.i.d samples of a distribution with density  $\rho$ . Then, for  $\varepsilon_n \to 0$  as before

$$u_n \xrightarrow{TL^1} u$$

where *u* is eigenfunction, corresponding to second eigenvalue, of

$$-\frac{\operatorname{div}(\rho^2 \nabla u)}{\rho} = \lambda_2 u \quad \text{in } D$$
$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial D.$$

## Consistency of Spectral Clustering II

$$u_n^k = \arg\min\left\{\sum_{i,j} W_{ij}|u(X_i) - u(X_j)|^2 : \sum_i u(X_i)u_n^m(X_i) = 0 \; (\forall m < k), \|u\|_2 = 1\right\}$$

• Suppose  $X_1, \ldots, X_n, \ldots$  are i.i.d samples of a distribution with density  $\rho$ . Then, for  $\varepsilon_n \to 0$  as before

$$u_n^k \xrightarrow{TL^1} u^k$$

where  $u^k$  is eigenfunction, corresponding to k-th eigenvalue, of

$$-\frac{1}{\rho}\operatorname{div}(\rho^2 \nabla u^k) = \lambda_k u^k \quad \text{in } D$$
$$\frac{\partial u^k}{\partial n} = 0 \quad \text{on } \partial D.$$

## Consistency of spectral clustering

**Input:** Number of clusters *k* and similarity matrix *W*.

- Construct the unnormalized graph Laplacian L.
- Compute the eigenvectors u<sub>1</sub>,..., u<sub>k</sub> of L associated to the k smallest (nonzero) eigenvalues of L.
- Define the matrix  $U \in \mathbb{R}^{k \times n}$ , where the *i*-th row of U is the vector  $u_i$ .
- For i = 1, ..., n, let  $y_i \in \mathbb{R}^k$  be the *i*-th column of *U*.
- Use the *k*-means algorithm to partition the set of points  $\{y_1, \ldots, y_n\}$  into *k* groups, that we denote by  $G_1, \ldots, G_k$ .

**Output:** Clusters  $G_1, \ldots, G_k$ .

**Theorem.** Let  $G_1^n, \ldots, G_k^n$  be the clusters above. Let  $\nu_i^n = \nu_n \sqcup_{G_i^n}$  (the restriction of empirical measure to clusters) for  $i = 1, \ldots, k$ . Then  $(\nu_1^n, \ldots, \nu_k^n)$  is precompact with respect to weak convergence of measures and converges along a subsequence to  $(\nu_1, \ldots, \nu_k) = (\nu_{\sqcup G_1}, \ldots, \nu_{\sqcup G_k})$  where  $G_1, \ldots, G_k$  is a continuum spectral clustering of  $\nu$ .

## Normalized Graph Laplacian

• As before: 
$$W_{ij} := \frac{1}{\varepsilon^d} \eta\left(\frac{|X_i - X_j|}{\varepsilon}\right), \ d_i = \sum_j W_{i,j} = \sum_j \eta_{\varepsilon}(|X_i - X - j|).$$

• Dirichlet energy of  $u_n: V_n \to \mathbb{R}$  is

$$F(u) = rac{1}{2}\sum_{i,j}W_{ij}\left(rac{u_n(X_i)}{\sqrt{d_i}} - rac{u_n(X_j)}{\sqrt{d_j}}
ight)^2$$

- Associated operator is the normalized graph laplacian  $D^{-1/2}LD^{-1/2} = I D^{-1/2}WD^{-1/2}$ , where  $D = \text{diag}(d_1, \dots, d_n)$ .
- To partition the point cloud into two clusters, consider the eigenvector corresponding to second eigenvalue:

$$u_n := \arg\min\left\{\sum_{i,j} W_{ij} \left| \frac{u_n(X_i)}{\sqrt{d_i}} - \frac{u_n(X_j)}{\sqrt{d_j}} \right|^2 : \sum_i u(X_i) = 0, \|u\|_2 = 1 \right\}$$

## Consistency of Normalized Graph Laplacian

$$u_n^k = \arg\min\left\{\sum_{i,j} \left| \frac{u_n(X_i)}{\sqrt{d_i}} - \frac{u_n(X_j)}{\sqrt{d_j}} \right|^2 : \sum_i u(X_i)u_n^m(X_i) = 0 \; (\forall m < k), \|u\|_2 = 1 \right\}$$

• Suppose  $X_1, \ldots, X_n, \ldots$  are i.i.d samples of a distribution with density  $\rho$ . Then, for  $\varepsilon_n \to 0$  as before

$$u_n^k \xrightarrow{TL^1} u^k$$

where  $u^k$  is eigenfunction, corresponding to k-th eigenvalue, of

$$-\frac{1}{\rho^{3/2}}\nabla\cdot\left(\rho^{2}\nabla\left(\frac{u^{k}}{\sqrt{\rho}}\right)\right) = \lambda_{k}u^{k} \quad \text{in } D$$
$$\frac{\partial(u^{k}/\sqrt{\rho})}{\partial n} = 0 \quad \text{on } \partial D.$$

- Jointly with Hein, Garciá Trillos, and Gerlach
  - Consistency of graph cuts and spectral clustering on manifolds
  - Error estimates for consistency of convex functionals (like the Dirichlet functional)
- Mumford–Shah functional on graphs
- Finding better ways to approximate the functionals
## Theorem

Let  $D \subset \mathbb{R}^d$  be a bounded, connected, open set with Lipschitz boundary. Let  $\nu_1, \nu_2$  be measures on D of the same total mass:  $\nu_1(D) = \nu_2(D)$ . Assume the measures are absolutely continuous with respect to Lebesgue measure and let  $\rho_1$  and  $\rho_2$  be their densities. Furthermore assume that for some  $\lambda > 1$ , for all  $x \in D$ 

(4) 
$$\frac{1}{\lambda} \leq \rho_i(x) \leq \lambda$$
 for  $i = 1, 2$ .

Then, there exists a constant  $C(\lambda, D)$  depending only on  $\lambda$  and D such that for all  $\nu_1$ ,  $\nu_2$  as above

$$d_{\infty}(\nu_1,\nu_2) \leq C(\lambda,D) \|\rho_1 - \rho_2\|_{L^{\infty}(D)}.$$