

# From clustering with graph cuts to isoperimetric inequalities: quantitative convergence rates of Cheeger cuts on data clouds

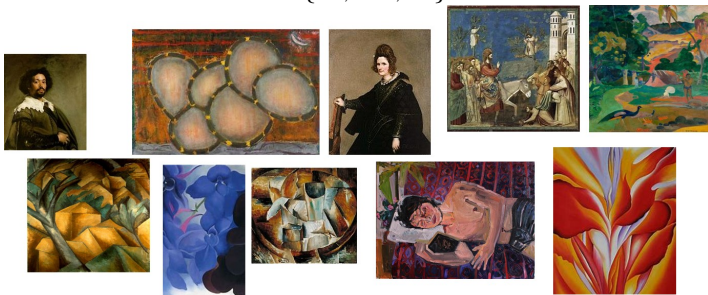
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Joint work with Ryan Murray (NCSU) and Matthew Thorpe (U Manchester)

IPAM High Dimensional Hamilton-Jacobi PDEs Workshop 2  
April 24th 2020

**Goal:** Given a data set  $X = \{x_1, \dots, x_n\}$ :



- Unsupervised learning: Find coarse structure of  $X$  (find meaningful clusters).

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0 0 0 0 0 0 0 0 0 0  
1 1 1 1 1 1 1 1 1 1  
2 2 2 2 2 2 2 2 2 2  
3 3 3 3 3 3 3 3 3 3  
4 4 4 4 4 4 4 4 4 4  
5 5 5 5 5 5 5 5 5 5  
6 6 6 6 6 6 6 6 6 6  
7 7 7 7 7 7 7 7 7 7  
8 8 8 8 8 8 8 8 8 8  
9 9 9 9 9 9 9 9 9 9

- Unsupervised learning: Find coarse structure of  $X$  (find meaningful clusters).

# Graph based learning

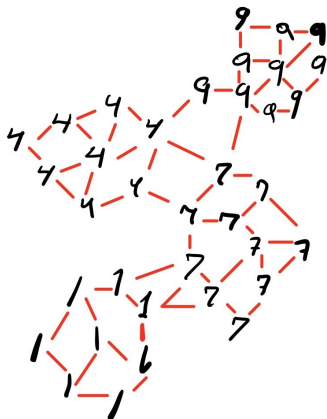
**Goal:** Given a data set  $X = \{x_1, \dots, x_n\}$  and similarity matrix  $\{\omega_{ij}\}_{ij}$ :

0	0	0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	2	2	2	2	2
3	3	3	3	3	3	3	3	3	3
4	4	4	4	4	4	4	4	4	4
5	5	5	5	5	5	5	5	5	5
6	6	6	6	6	6	6	6	6	6
7	7	7	7	7	7	7	7	7	7
8	8	8	8	8	8	8	8	8	8
9	9	9	9	9	9	9	9	9	9

- Find coarse structure of  $X$  (find meaningful clusters).

# Graph based learning

Given  $G = (X, \omega)$ :

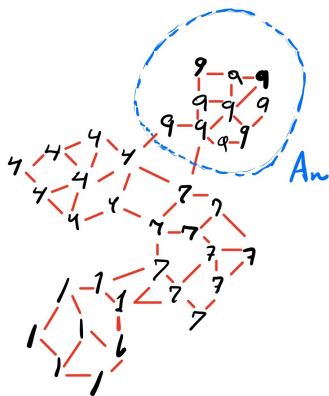


# What can we do with a graph?

Define **graph cut (graph perimeter)** for arbitrary  $A_n \subseteq X$  :

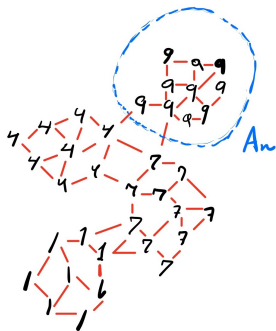
$$Cut(A_n) := \sum_{x_i \in A_n} \sum_{x_j \notin A_n} \omega_{ij} = \sum_{i,j} \omega_{ij} |\mathbb{1}_{A_n}(x_i) - \mathbb{1}_{A_n}(x_j)|$$

# What can we do with a graph?



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Fundamental object that appears in Computer Science and Math (e.g. min cut max flow theorem), but also used for clustering...

The **Cheeger** cut problem (an example of **balanced graph cut**):

$$\min_{A_n \subseteq \mathcal{M}_n} \frac{\text{Cut}(A_n)}{\min\{\mu_n(A_n), \mu_n(A_n^c)\}}$$

The **Cheeger** cut problem (an example of **balanced graph cut**):

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Computational complexity: **NP hard**.

First notice that,

$$\sum_{i,j} \omega_{ij} |\mathbb{1}_{A_n}(x_i) - \mathbb{1}_{A_n}(x_j)| = \sum_{i,j} \omega_{ij} |\mathbb{1}_{A_n}(x_i) - \mathbb{1}_{A_n}(x_j)|^2$$

Second, consider problem over all functions  $f : X \rightarrow \mathbb{R}$ :

$$\min_f \frac{\sum_{i,j} \omega_{ij} |f(x_i) - f(x_j)|^2}{\sum_{i=1}^n (f(x_i) - \frac{1}{n} \sum_{j=1}^n f(x_j))^2}$$

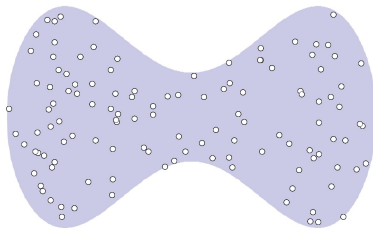
Eigenvalue problem for **graph Laplacian**  $\Delta_n$ :

$$\Delta_n f(x_i) := \sum_{ij} \omega_{ij} (f(x_i) - f(x_j)).$$

**Spectral clustering:** Ng et al (2002), von Luxburg (2007).

# What if the data was already embedded in Euclidean space?

$X := \{x_1, \dots, x_n\} \subseteq \mathcal{M} \subseteq \mathbb{R}^d$  with  $m \ll d$  (**the manifold assumption**).





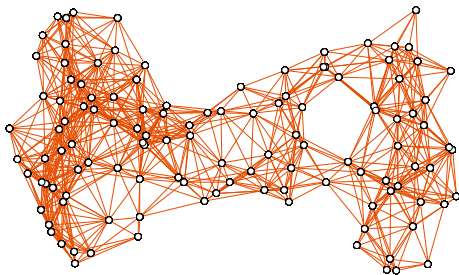
Here

$$\omega_{ij} = \eta\left(\frac{|x_i - x_j|}{\varepsilon}\right), \quad \text{e.g. } \eta(t) := \begin{cases} 1 & \text{if } t \leq 1 \\ 0 & \text{else} \end{cases}$$



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Other families of proximity graphs:  $k$ -NN graphs, self-tuning graphs, graphs based on polar curvature of points (e.g. Chen and Lerman 2007).

What is the behavior of algorithms as  $n \rightarrow \infty$  (and  $\varepsilon \rightarrow 0$ )?



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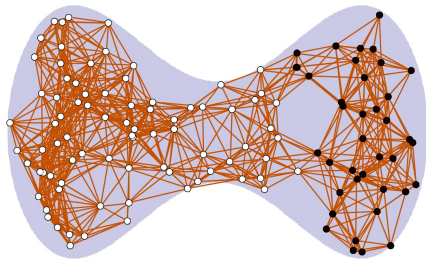


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# Manifold Learning for graph Laplacian:

- Towards a theoretical foundation for Laplacian based methods. Belkin and Niyogi (2005).
- Diffusion maps. Coifman et al (2005).
- From graph to manifold Laplacian: the convergence rate. Singer (2006).
- Consistency of Spectral clustering. von Luxburg, Belkin, and Bousquet (2007).
- ...
- A graph-discretization of the Laplace-Beltrami operator. Burago et al (2014).
- A variational approach to the consistency of spectral clustering. NGT and Slepčev (2015).
- Error estimates for spectral convergence of the graph Laplacian on random geometric graphs towards the Laplace-Beltrami operator. NGT et al (2018).
- Improved spectral convergence rates for graph Laplacians on epsilon and  $k$ -NN graphs. Calder and NGT (2019).

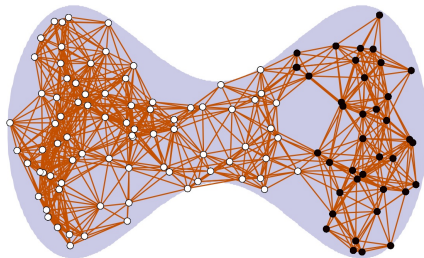
But let's go back to the un-relaxed Cheeger cut problem...



$$A_n^* = \operatorname{argmin}_{A_n \subseteq X} \frac{GTV_{n,\varepsilon}(\mathbb{1}_{A_n})}{\min\{\mu_n(A_n), \mu_n(A_n^c)\}}$$

$$\begin{aligned} GTV_{n,\varepsilon}(\mathbb{1}_{A_n}) &:= \frac{1}{n^2 \varepsilon^{m+1}} \sum_{i,j} \eta\left(\frac{|x_i - x_j|}{\varepsilon}\right) |\mathbb{1}_{A_n}(x_i) - \mathbb{1}_{A_n}(x_j)| \\ &= \frac{1}{n^2 \varepsilon^{m+1}} \operatorname{Cut}(A_n) \end{aligned}$$

# Consistency question

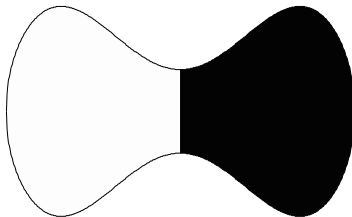
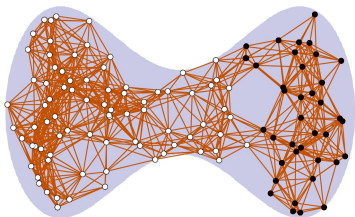


$$A_n^* = \operatorname{argmin}_{A_n \subseteq X} \frac{GTV_{n,\varepsilon}(\mathbb{1}_{A_n})}{\min\{\mu_n(A_n), \mu_n(A_n^c)\}}$$

$X = \{x_1, \dots, x_n\} \sim_{i.i.d.} \mu$  where  $\mu$  is a distribution over manifold  $\mathcal{M}$ . What happens as  $n \rightarrow \infty$  and simultaneously  $\varepsilon \rightarrow 0$ ?

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# What are the difficulties?

$$\min_{A_n \subseteq X} \frac{GTV_{n,\varepsilon}(\mathbb{1}_{A_n})}{\min\{\mu_n(A_n), \mu_n(A_n^c)\}}$$

- 1 Non-linear, non-convex, random variational problem.
- 2 Optimizing over **all** subsets  $A_n$  of  $X$ .

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- 2 Optimizing over **all** subsets  $A_n$  of  $X$ .  
**Arias-Castro et al:** consider  $A_n$ s that are restrictions of "nice" subsets of  $\mathcal{M}$ ; for this family one can bound VC dimension.

# The classical approach from statistical learning

Try to estimate:

$$\sup_{f \in \mathcal{F}} |\mathcal{E}_n(f) - \mathcal{E}(f)|$$

using **capacity measure** of class of functions  $\mathcal{F}$ .

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Try to estimate:

$$\sup_{f \in \mathcal{F}} |\mathcal{E}_n(f) - \mathcal{E}(f)|$$

using **capacity measure** of class of functions  $\mathcal{F}$ . In Arias-Castro:

$$\mathcal{F} = \{\mathbb{1}_A : A \text{ is "nice" enough subset of } \mathcal{M}\}$$

$$\mathcal{E}_n(f) := \frac{GTV_{n,\varepsilon}(\mathbb{1}_{A_n})}{\min\{\mu_n(A_n), \mu_n(A_n^c)\}}, \quad A_n := A \cap X$$

$$\mathcal{E}(f) := \frac{TV_\varepsilon(\mathbb{1}_A)}{\min\{\mu(A), \mu(A^c)\}}.$$

Where  $TV_\varepsilon(f)$  is the **non-local** TV seminorm:

$$TV_\varepsilon(f) := \frac{1}{\varepsilon^{m+1}} \int_{\mathcal{M}} \int_{\mathcal{M}} \eta\left(\frac{|x_i - x_j|}{\varepsilon}\right) |f(x) - f(y)| d\mu(y) d\mu(x)$$

But if we want to analyze the true Cheeger cut problem, this approach can not work.

Need to: "Pass the probabilistic estimates to where they do not harm".

- N. Garcia Trillos, D. Slepcev, J. Von Brecht, T. Laurent, and X. Bresson. *Consistency of cheeger and ratio graph cuts*. JMLR, 17(1):6268-6313, 2016.
- N. Garcia Trillos and D. Slepcev. *Continuum limit of total variation on point clouds*. ARMA, 220(1):193-241, 2016.

# Asymptotic consistency

**Theorem:** Suppose that  $\varepsilon$  scales like:

$$\frac{\log(n)^{p_m}}{n^{1/m}} \ll \varepsilon \ll 1, \quad p_m = \begin{cases} 3/4 & \text{if } m = 2 \\ 1/m & \text{if } m \geq 3 \end{cases}$$

Then, with probability one,

$$\lim_{n \rightarrow \infty} C_{n,\varepsilon} = \sigma_\eta C, \quad \text{and } A_n^* \rightarrow_{TL1} A^*.$$

Where  $C$  and  $A^*$  solve:

$$\min_{A \subseteq \mathcal{M}} \frac{\text{TV}(\mathbb{1}_A)}{\min\{\mu(A), \mu(A^c)\}}$$

and

$$\sigma_\eta := \int_{\mathbb{R}^m} \eta(|z|) |z_1| dz,$$

$$TV(f) = \sup \left\{ \int_{\mathcal{M}} f \operatorname{div}(V) dx : V \in C_c^\infty(\mathcal{M}), \quad |V(x)| \leq 1, \quad \forall x \right\}.$$

$$\operatorname{Per}(A) := TV(\mathbb{1}_A)$$

These expressions reduce to

$$TV(f) = \int_{\mathcal{M}} |\nabla f(x)| dx,$$

for  $f$  **smooth**, and

$$\operatorname{Per}(A) = \int_{\partial A} d\mathcal{H}^{m-1}(x).$$

for  $A$  with **smooth boundary**.

# Asymptotic consistency

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Then, with probability one,

$$\lim_{n \rightarrow \infty} \mathcal{C}_{n,\varepsilon} = \sigma_\eta \mathcal{C}, \quad \text{and } A_n^* \rightarrow_{TL^1} A^*.$$

Where  $\mathcal{C}$  and  $A^*$  solve:

$$\min_{A \subseteq \mathcal{M}} \frac{\text{TV}(\mathbb{1}_A)}{\min\{\mu(A), \mu(A^c)\}}$$

**Remarks:**

- 1 **Proof:** relied on  $\Gamma$ -convergence... and **NO rates of convergence.**
- 2 Penrose and Muller (2018) improved the result for  $m = 2$ .

# Convergence rates for Cheeger constants $\mathcal{C}_{n,\varepsilon}$

# Upper bound: $\mathcal{C}_{n,\varepsilon} \lesssim \sigma_\eta \mathcal{C}$

Fix  $f := \mathbb{1}_{A^*}$ . Concentration inequalities to estimate:

$$\mathbb{P}(|GTV_{n,\varepsilon}(f) - \mathbb{E}(GTV_{n,\varepsilon}(f))| \geq t).$$

Also,

$$\mathbb{E}(GTV_{n,\varepsilon}(f)) = TV_\varepsilon(f)$$

and

$$\sigma_\eta TV(\mathbb{1}_{A^*}) \gtrsim TV_\varepsilon(\mathbb{1}_{A^*}) = GTV_{n,\varepsilon}(\mathbb{1}_{A^*}) + (TV_\varepsilon(\mathbb{1}_{A^*}) - GTV_{n,\varepsilon}(\mathbb{1}_{A^*})).$$

# Upper bound: $\mathcal{C}_{n,\varepsilon} \lesssim \sigma_\eta \mathcal{C}$

Combine:

$$GTV_{n,\varepsilon}(\mathbf{1}_{A^*}) \leq \sigma_\eta TV(\mathbf{1}_{A^*}) + error_{n,\varepsilon}$$

with

$$|\mu_n(A^*) - \mu(A^*)| \leq error_{n,\varepsilon}$$

to conclude:

$$\begin{aligned} \mathcal{C}_{n,\varepsilon} &\leq \frac{GTV_{n,\varepsilon}(\mathbf{1}_{A^*})}{\min\{\mu_n(A^*), \mu_n(A^{*c})\}} \leq \frac{\sigma_\eta TV(\mathbf{1}_{A^*})}{\min\{\mu(A^*), \mu(A^{*c})\}} + error_{n,\varepsilon} \\ &= \sigma_\eta \mathcal{C} + error_{n,\varepsilon} \end{aligned}$$

**Proposition:**[NGT, Murray, Thorpe 20'] As long as

$\left(\frac{\log(n)}{n}\right)^{1/m} \ll \varepsilon \ll 1$ , w.v.h.p. **for all**  $A_n \subset X$  there is  $A \subset \mathcal{M}$  such that:

- 1  $\mu_n(A_n \triangle A) \leq GTV_{n,\varepsilon}(\mathbb{1}_{A_n}) \cdot error_{n,\varepsilon}$ .
- 2  $\sigma_\eta TV(\mathbb{1}_A) \leq (1 + error_{n,\varepsilon}) GTV_{n,\varepsilon}(\mathbb{1}_{A_n})$ .

Pass the probabilistic estimates to where they do not harm...  
(typically involves a "good" interpolation map)

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- 2  $TV(\sigma_\eta \mathbb{1}_A) \leq (1 + error_{n,\varepsilon}) GTV_{n,\varepsilon}(\mathbb{1}_{A_n})$ .

Take  $A_n := A_n^*$  and proceed as in the upper bound to get:

$$\sigma_\eta \mathcal{C} \leq \mathcal{C}_{n,\varepsilon} + error_{n,\varepsilon}.$$

# A collection of (deterministic) inequalities

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$$\sigma_\eta TV(f) \leq (1 + C\varepsilon^2)TV_\varepsilon(f) + C\|f\|_{C^2(\mathcal{M})}\varepsilon.$$

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- ④ For all  $0 < h \leq a$  small enough, for all  $f \in L^1(\mathcal{M})$

$$\|f - \Lambda_a f\|_{L^1(\mathcal{M})} \leq CaTV_h(f).$$

# A collection of inequalities

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- 2 If  $f \in C^2(\mathcal{M})$  then,

$$\sigma_\eta TV(f) \leq (1 + C\varepsilon^2)TV_\varepsilon(f) + C\|f\|_{C^2(\mathcal{M})}\varepsilon.$$

- 3 (Monotonicity) For all  $0 < h \leq a$  small enough, for all  $f \in L^1(\mathcal{M})$

$$TV_a(f) \leq CTV_h(f).$$

- 4 For every  $a > 0$  small enough and every  $0 < h \leq a$

- 5 For all  $0 < h \leq a$  small enough, for all  $f \in L^1(\mathcal{M})$

$$\|f - \Lambda_a f\|_{L^1(\mathcal{M})} \leq CaTV_h(f).$$

- 6 (Convolution decreases energy) For all  $0 < h \leq a$  small enough, for all  $f \in L^1(\mathcal{M})$

$$TV_h(\Lambda_a f) \leq (1 + Ca)TV_h(f).$$

Bottom line:

For all  $f \in L^1(\mathcal{M}) \cap L^\infty(\mathcal{M})$ :

①  $\|\Lambda_a f - f\| \leq a TV_\varepsilon(f)$

②  $\sigma_\eta TV(\Lambda_a f) \leq TV_\varepsilon(f)$

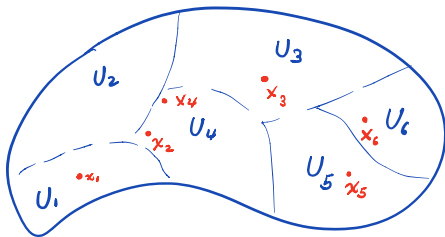
To complete the proof of the proposition we only need to relate  $GTV_{n,\varepsilon}(\mathbb{1}_{A_n^*})$  with  $TV_\varepsilon(f)$  for some conveniently chosen  $f$  (here is where the probabilistic estimate enters).

$$f := \mathbb{1}_{A_n} \circ T_n$$

Here:  $T_n : \mathcal{M} \rightarrow X$  satisfies  $T_{\#}\mu = \mu_n$  and is such that

$$\|T_n - Id\|_{\infty}$$

is as small as possible:



$$U_i = T_n^{-1}(\{x_i\}), \text{ and } \mu(U_i) = 1/n$$

For any such a map we get deterministically:

$$TV_\varepsilon(\mathbb{1}_{A_n} \circ T_n) \lesssim \left(1 + C \frac{\|T_n - Id\|_\infty}{\varepsilon}\right) GTV_{n,\varepsilon}(\mathbb{1}_{A_n}).$$

The probabilistic estimate is used to quantify how good  $T_n$  can be...

**Theorem:**(NGT, Murray, Thorpe 20') As long as  $\left(\frac{\log(n)}{n}\right)^{1/m} \ll \varepsilon \ll 1$ , w.v.h.p.,

$$|\mathcal{C}_{n,\varepsilon} - \sigma_\eta \mathcal{C}| \leq C \left( \frac{\log(n)^{1/m}}{n^{1/m\varepsilon}} + \sqrt[3]{\varepsilon} \right).$$

# What about convergence of **minimizers?**

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... Finding the right notion of convexity

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... Finding the right notion of convexity: a detour into  
isoperimetric inequalities.

# A classical problem

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# A classical problem with rich history

**Q:** (in dimension 2): Find a closed plane curve of a given perimeter that encloses the greatest area. **A:** The circle!

- The greeks.
- J. Steiner (1830's)
- St. Venant (1850's)
- Rayleigh (1870's)
- Poincare (1900's)
- Faber-Krahn (1920's)
- Cartan-Hadamard conjecture.
- Szego-Polya (1930's and 1940's)
- $\vdots$

## Isoperimetric function:

$$\mathbb{I}(v) := \inf_E \{\text{Per}(E) : |E| = v\}.$$

## Isoperimetric inequality in $\mathbb{R}^m$ :

$$C_m |E|^{(m-1)/m} \leq \text{Per}(E).$$

Inequality is equality if and only if  $E$  is a ball.

**Q:** Quantitative version? i.e. If  $|E| = v$  and  $\text{Per}(E) - \mathbb{I}(v) < \delta$ , can we say how close is  $E$  from a minimizer?

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- Bernstein (1905)
- Bonnesen (1924)
- Fuglede (1989)
- Hall (1992)
- $\vdots$

Theorem (Fusco, Maggi, Pratelli 2008)

There exist constants  $C, \delta > 0$  such that for any  $|E| = |B^*|$  and  $|E \ominus B^*| < \delta$  one has

$$\text{Per}(E) - \text{Per}(B^*) \geq C\alpha(E)^2.$$

Here,  $\alpha$  is the **Fraenkel asymmetry**:

$$\alpha(E) = \inf_{B^*} \{|E \ominus B^*| : |B^*| = |E|, \text{Per}(B^*) = \mathbb{I}(|E|)\}.$$

Also: Figalli, Maggi, Pratelli (2010) using ideas from OT.

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Their proof does not exhibit a “right notion of convexity”, and instead relies on symmetrization arguments. However, the proof of **Cicalese and Leonardi 12'** does, and allows for extension to manifolds...

## Theorem (Chodosh, Engelstein, Spolaor 19')

Suppose that a mass-constrained perimeter minimizer  $E^* \subset \mathcal{M}$  has **smooth** boundary  $\partial E^*$ . Furthermore, suppose that either  $E^*$  is a **strict** perimeter minimizer, or that it is **integrable**. Then there exists constants  $C, \delta > 0$  such that for any  $|E| = |E^*|$  and  $|E \ominus E^*| < \delta$  one has

$$\text{Per}(E) - \text{Per}(E^*) \geq C\alpha(E)^2. \quad (1)$$

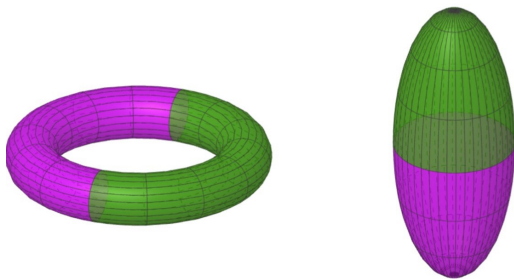
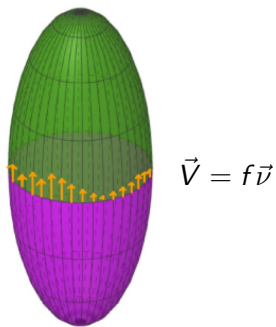


Figure: **Integrable** and **strict** minimizers

# The "right" notion of convexity:



$$D^2 \text{Per}(E^*)[f, f] \geq C \|f\|_{W^{1,2}(\partial E^*)}^2$$

# Convergence of Cheeger cuts

**Theorem:**(NGT, Murray, Thorpe 20') Assume:

- The function  $v \mapsto \frac{\mathbb{I}(v)}{\min\{v, |\mathcal{M}| - v\}}$  is locally strongly convex at its minimizers (denote this set by  $\mathcal{V}^*$ ).
- Minimizers of isoperimetric problem for  $v \in \mathcal{V}^*$  are smooth and either **integrable** or **strict**.

Then, as long as  $\left(\frac{\log(n)}{n}\right)^{1/m} \ll \varepsilon \ll 1$ , w.v.h.p., for every minimizer  $A_n^*$  of graph Cheeger cut problem there exists  $A^*$  solution to the continuum Cheeger cut problem satisfying:

$$\|\mathbb{1}_{A_n^*} - \mathbb{1}_{A^*}\|_{L^1} \leq C \left( \frac{\log(n)^{1/m}}{n^{1/m}\varepsilon} + \sqrt[3]{\varepsilon} \right)^{1/8}.$$

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*From graph cuts to isoperimetric inequalities: Convergence rates of Cheeger cuts on data clouds (2020)*

<https://arxiv.org/abs/2004.09304>

Thank you for your attention!