Subsampling in Large Networks

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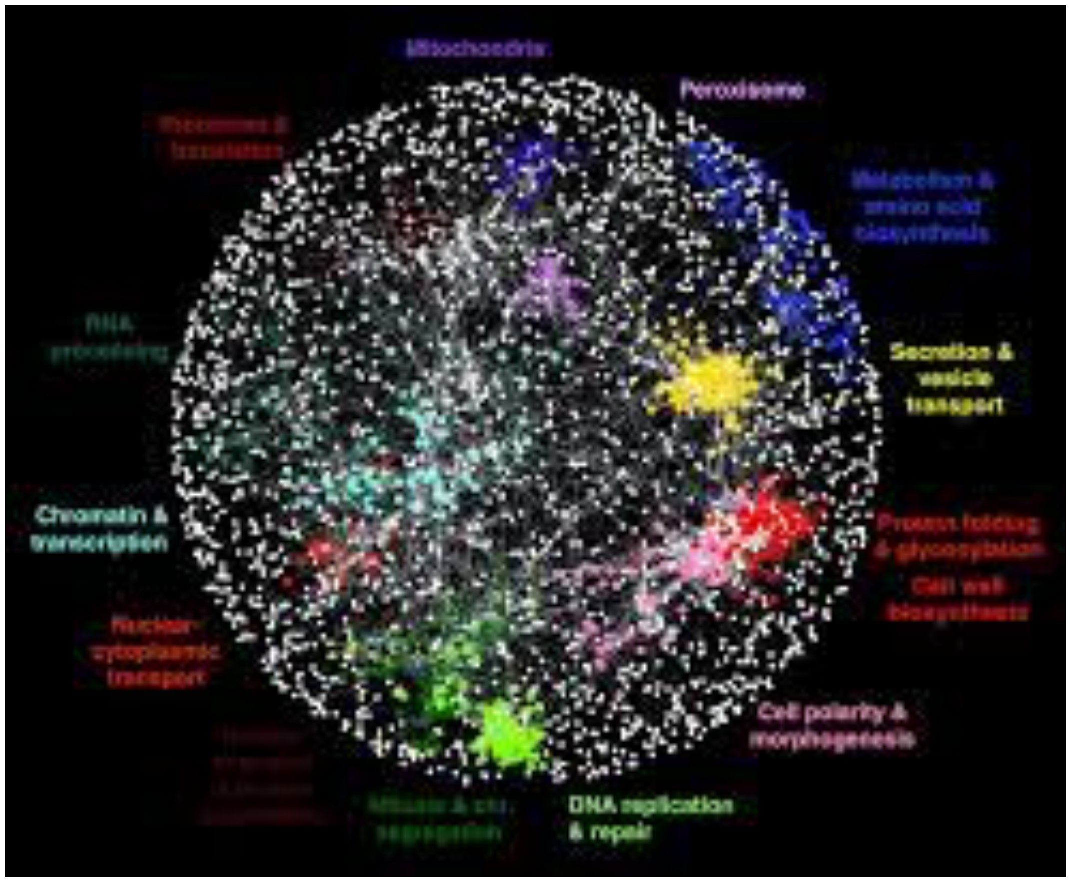
Transaction Networks

Billions of entities (nodes) with at least 100 billions of transactions (edges)

Protein-Protein Interaction Networks



0.5 millions of nodes

Large Networks

- Hard to visualize
- Hard to analyze
- Hard for downstream computation

Subnetwork

- A representation (or a sketch) of the large network
- Subsampling: methods for taking subnetwork from the large network

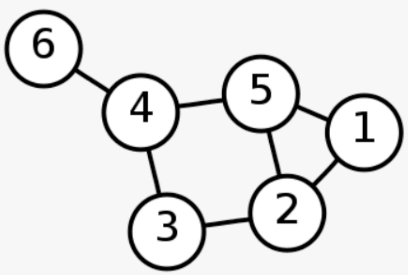
Three Settings

- The original large network is accessible
- The original large network is not accessible
- Something in between

Desirable Properties of Subsampling

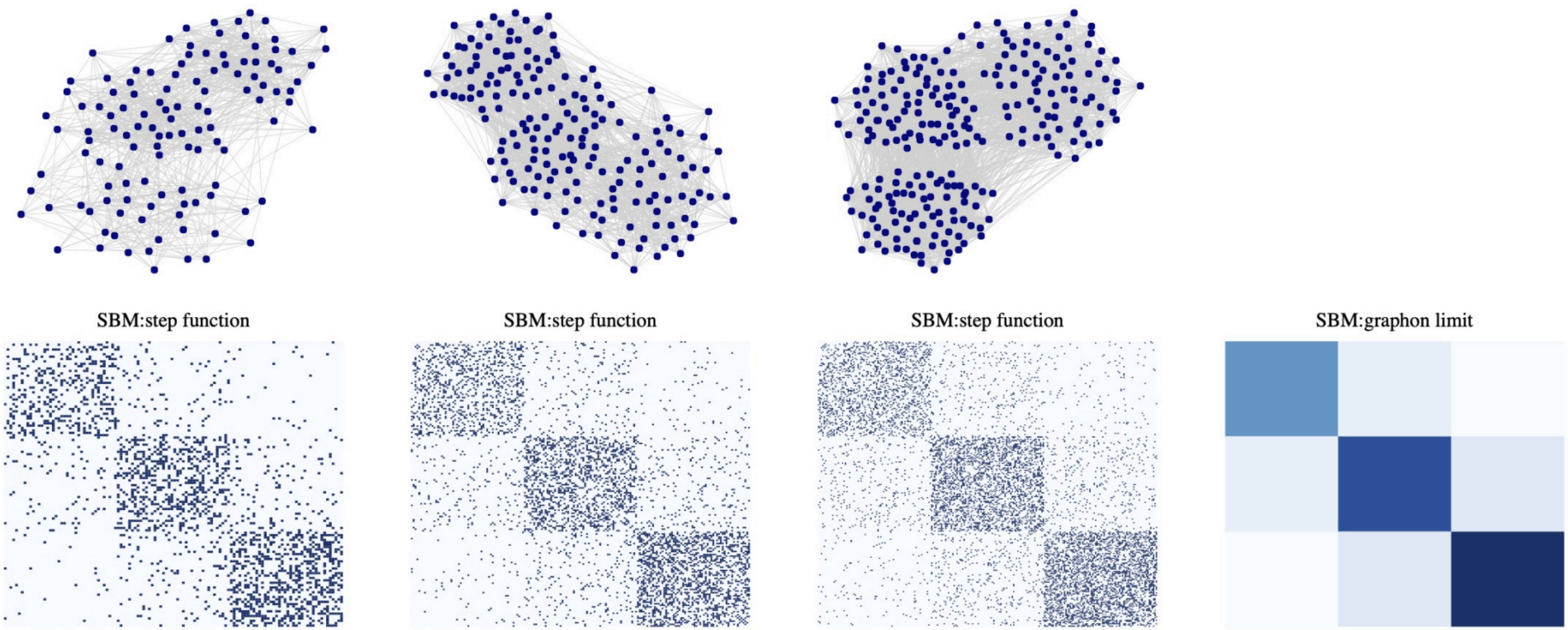
- Local to global: Importance indices of nodes and/or edges are local features with global (whole network) information
- Local computation: The subsampling methods do not need to compute the importance indices of all nodes and/or edges.

Graph and Matrix

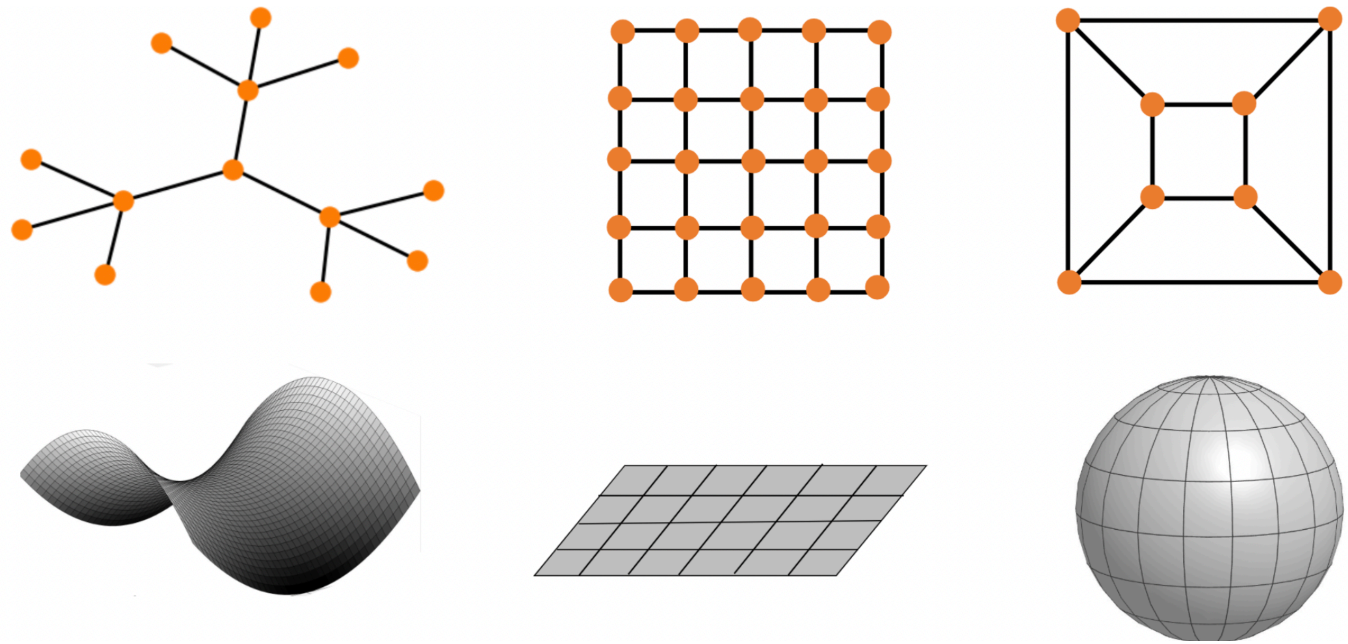
Labelled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

Numerical Linear Algebra

Graphon and Graphex



Manifolds



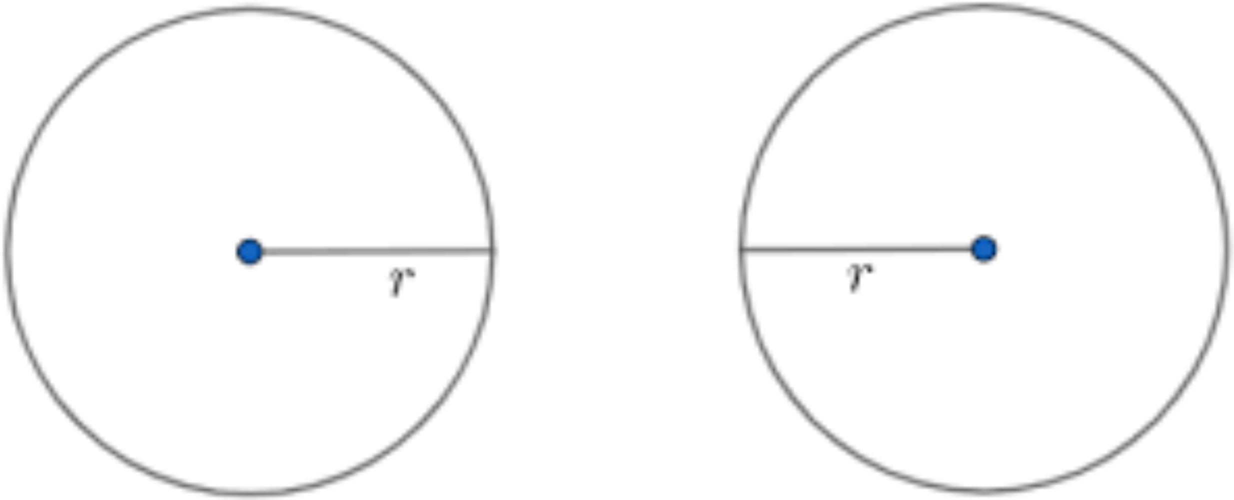
Manifolds

No predetermined coordinates

- The flexibility to choose coordinates arbitrarily
- Ensure that any objects we define globally on a manifold do not depend on a particular choice of coordinates.

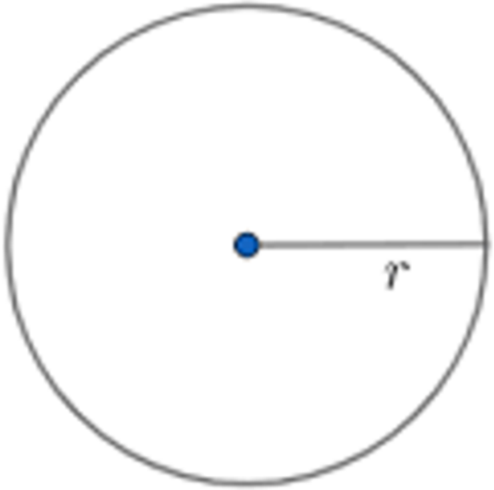
Classification Theorem of Circles

Congruence: same radius *r*



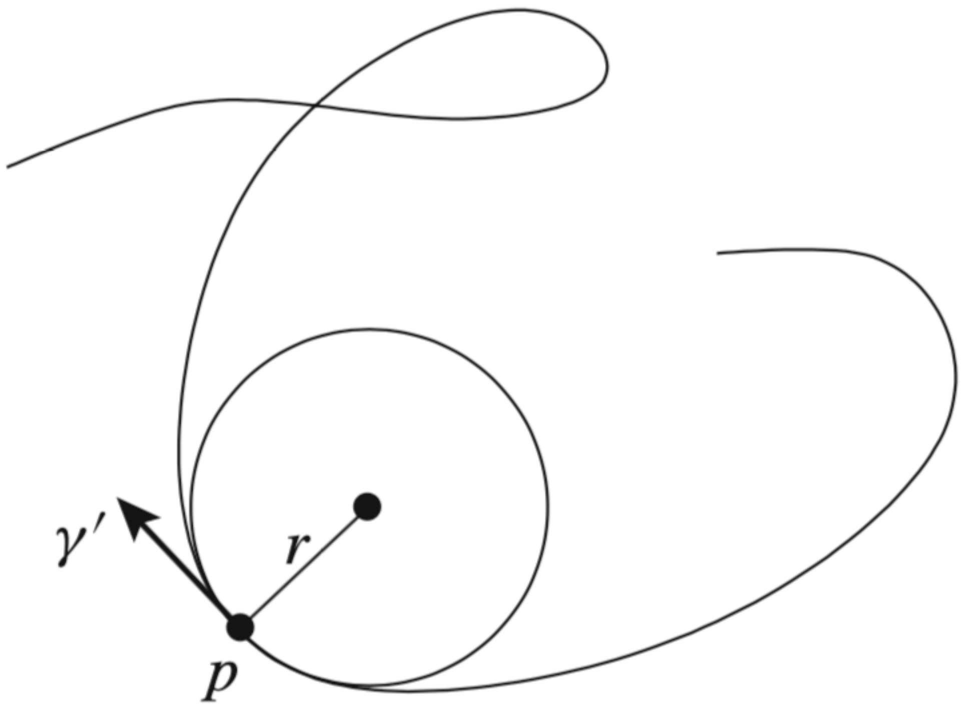
Local-to-Global Theorem of Circles

Circumference: $2\pi r$



Curvature

$$\kappa(t) = |\gamma''(t)|$$

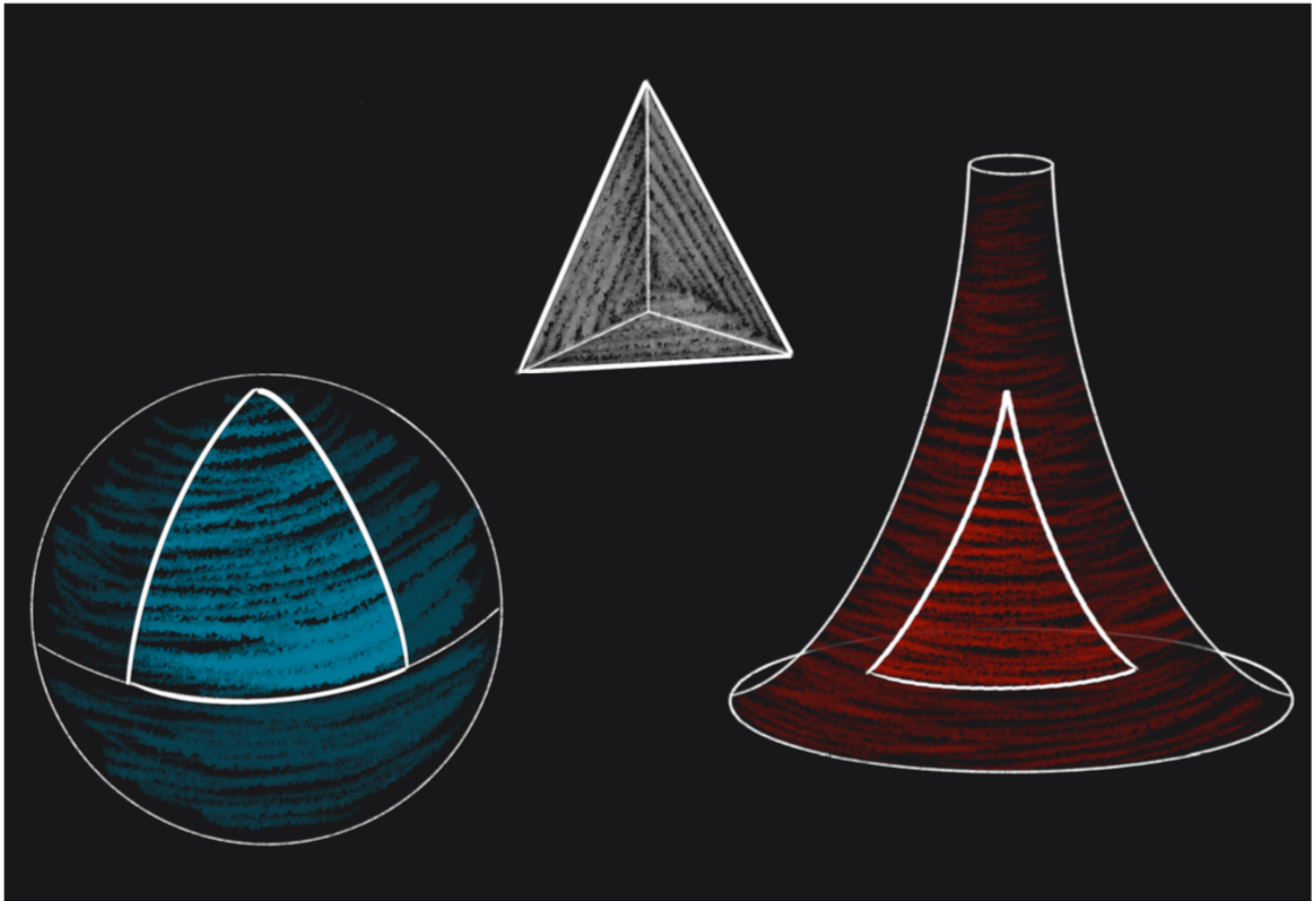


Lee (2018)

Curvature Theorems

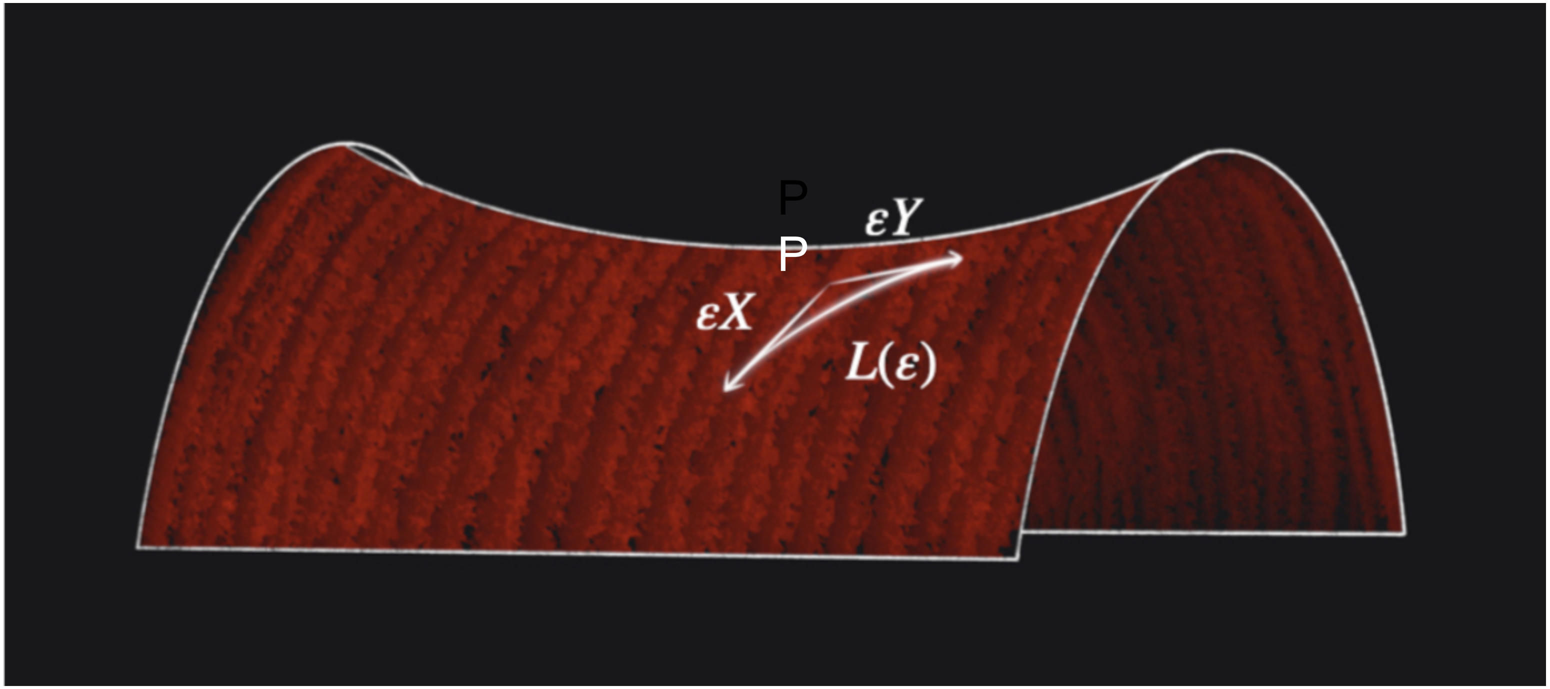
- Classification: Two curves are congruent iff their curvatures are the same.
- Local-to-global: For a simple closed curve, the integration of its curvature is 2π.

Curvature in High Dimension



Khan (2022)

Sectional Curvature



$$L(\varepsilon) = \varepsilon\|X - Y\| \left(1 - \frac{1}{12}K(X,Y)(1 + \langle X, Y \rangle)\varepsilon^2\right) + O\left(\varepsilon^4\right)$$

K(X, Y) is defined to be the sectional curvature of the tangent plane spanned by X and Y

Ricci Curvature

$$\mathrm{Ric}(X,X) = \frac{1}{2}\frac{(n-1)}{\omega\left(\mathbb{S}^{n-2}\right)}\oint_{\|Y\|=1 \text{ and } X\perp Y} K(X,Y)\,\mathrm{d}\mathbb{S}^{n-2}(Y)$$

$\omega\left(\mathbb{S}^{n-2}\right)$ is the surface area of the $(n-2)$-dimensional sphere.

The Ricci curvature Ric(X,X) is (n − 1) times the average of all of the sectional curvatures of tangent planes containing X.

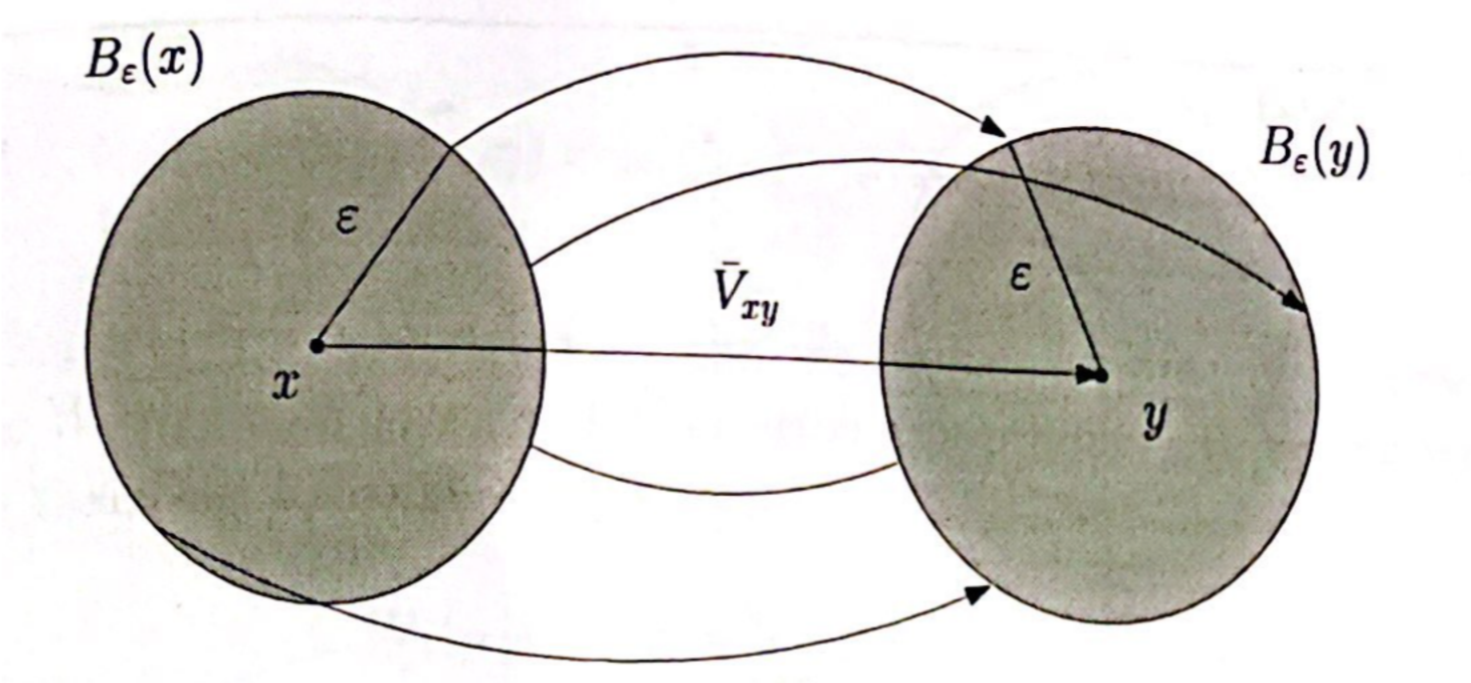
$$\mathrm{Ric}(X,Y) = \frac{1}{2}\left(\mathrm{Ric}(X+Y,X+Y) - \mathrm{Ric}(X,X) - \mathrm{Ric}(Y,Y)\right)$$

Ricci Curvature

- Measuring the degree to which the geometry determined by a given Riemannian metric might differ from that of ordinary Euclidean space

Olivier-Ricci Curvature

Transport ball B(x) to ball B(y).



The average distance is

$$\delta\left[1-\frac{\varepsilon^2}{2(n+2)}\mathrm{Ric}(\bar{\mathbf{v}}_{xy})+O(\varepsilon^3+\varepsilon^2\delta)\right]$$

$$\delta = d(x,y).$$

Olivier-Ricci Curvature

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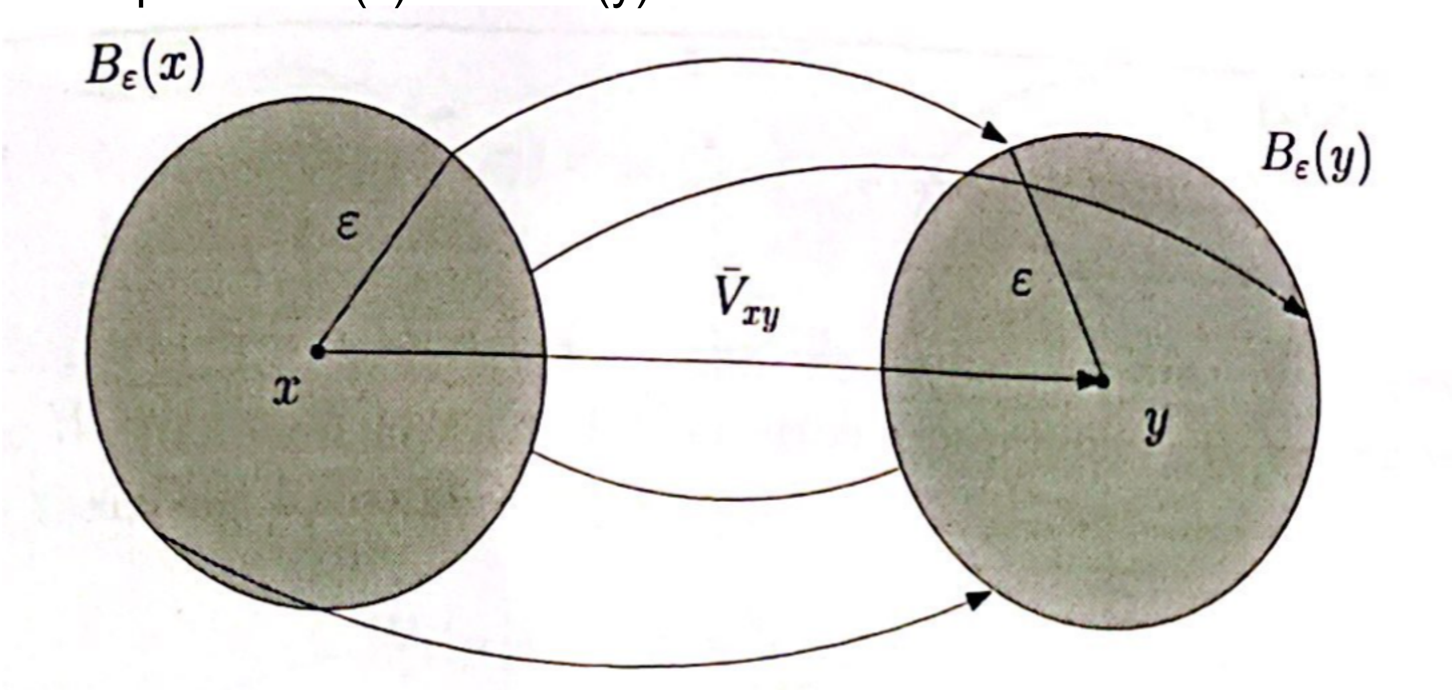

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$=W$

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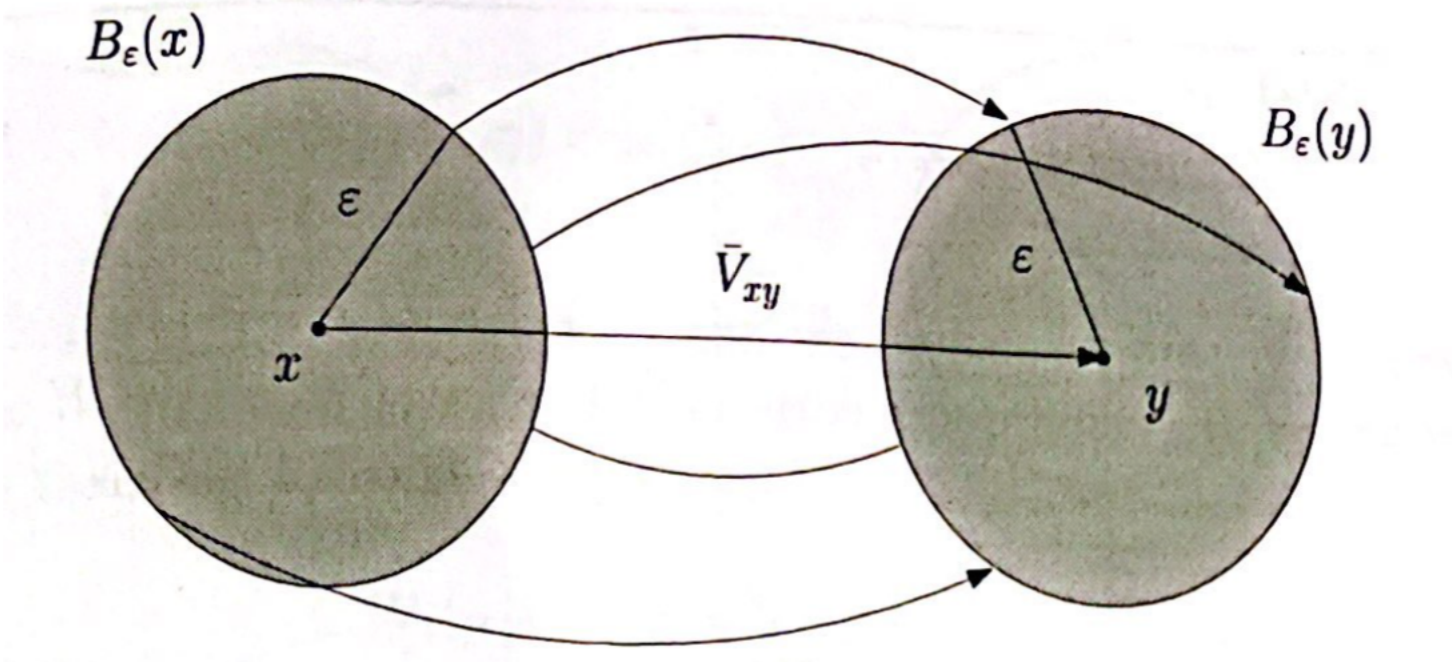

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$$\delta\left[1-\frac{\varepsilon^2}{2(n+2)}\mathrm{Ric}(\bar{\mathbf{v}}_{xy})+O(\varepsilon^3+\varepsilon^2\delta)\right]$$

$$\delta = d(x,y).$$

$=W$

κ

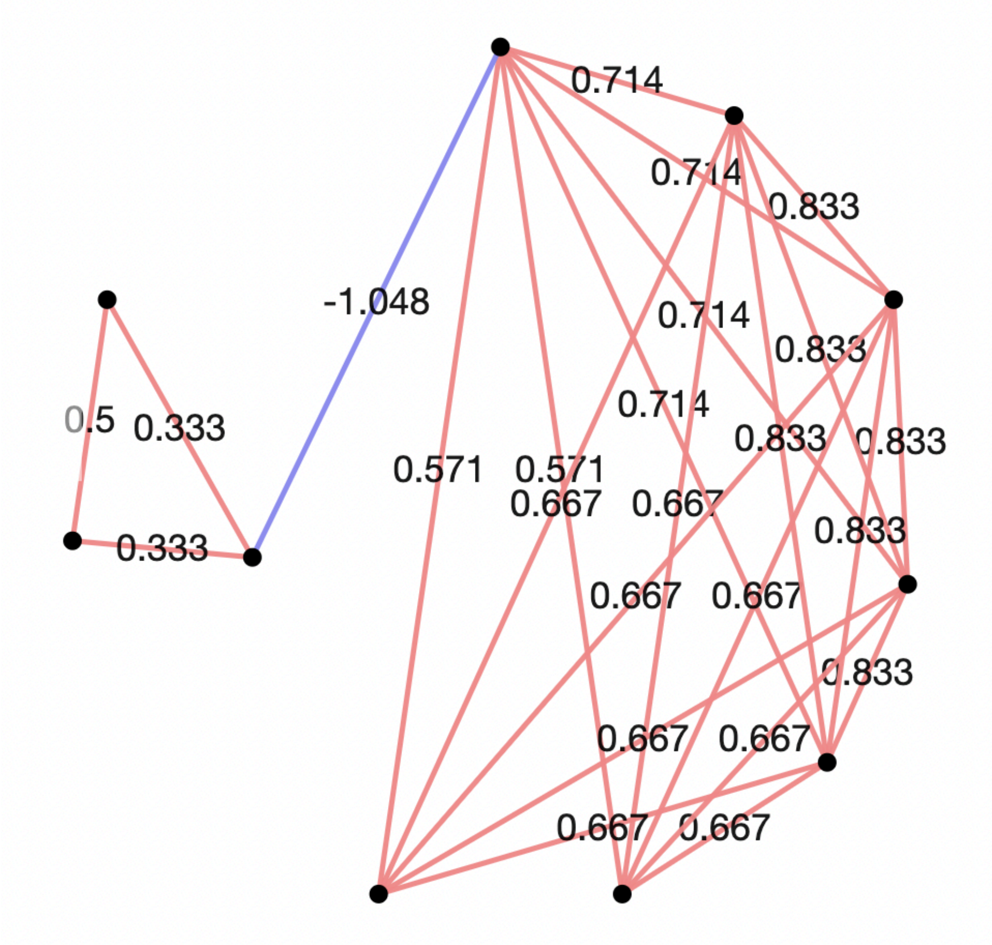
Olivier-Ricci Curvature

$$\kappa(u,v) = 1 - \frac{W(m_u^\alpha, m_v^\alpha)}{d(u,v)} \qquad W(m_u^\alpha, m_v^\alpha) = \inf_{\xi} \sum_{u,v \in V} \xi(u,v) d(u,v)$$

$$m_u^\alpha(x) = \begin{cases} \alpha & \text{if } x = u \\ (1-\alpha)/d_u & \text{if } x \in \delta(u) \\ 0 & \text{otherwise} \end{cases}$$

- Graphs are generated from manifold
- OR curvature on Graphs $\rightarrow$ Ricci curvature on Manifold

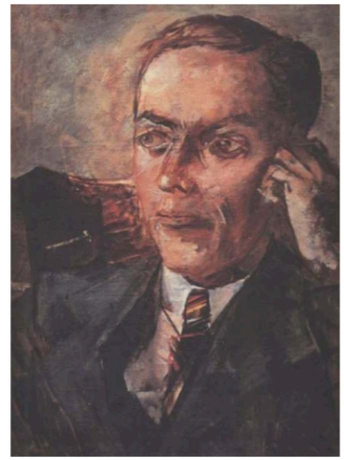
Subsampling in Graphs



Edges with large curvature are within a community;
Edges with small curvature are between communities

Leonid Kantorovich (1912-1986)

Леонид Витальевич Канторович



[Kantorovich 1942]

Journal of Mathematical Sciences, Vol. 133, No. 4, 2006

ON THE TRANSLOCATION OF MASSES

L. V. Kantorovich*

The original paper was published in Dokl. Akad. Nauk SSSR, **37**, No. 7–8, 227–229 (1942).

We assume that R is a compact metric space, though some of the definitions and results given below can be formulated for more general spaces.

Let $\Phi(e)$ be a mass distribution, i.e., a set function such that: (1) it is defined for Borel sets, (2) it is nonnegative: $\Phi(e) \geq 0$, (3) it is absolutely additive: if $e = e_1 + e_2 + \cdots$; $e_i \cap e_k = 0$ $(i \neq k)$, then $\Phi(e) = \Phi(e_1) + \Phi(e_2) + \cdots$. Let $\Phi'(e')$ be another mass distribution such that $\Phi(R) = \Phi'(R)$. By definition, a translocation of masses is a function $\Psi(e, e')$ defined for pairs of (B)-sets $e, e' \in R$ such that: (1) it is nonnegative and absolutely additive with respect to each of its arguments, (2) $\Psi(e, R) = \Phi(e)$, $\Psi(R, e') = \Phi'(e')$.

Let $r(x, y)$ be a known continuous nonnegative function representing the work required to move a unit mass from x to y.

We define the work required for the translocation of two given mass distributions as

$$W(\Psi, \Phi, \Phi') = \int_R \int_R r(x, x') \Psi(de, de') = \lim_{\lambda \to 0} \sum_{i,k} r(x_i, x'_k) \Psi(e_i, e'_k),$$

where e_i are disjoint and $\sum_1^n e_i = R$, e'_k are disjoint and $\sum_1^m e'_k = R$, $x_i \in e_i$, $x'_k \in e'_k$, and λ is the largest of the numbers $\operatorname{diam} e_i$ $(i = 1, 2, \ldots, n)$ and $\operatorname{diam} e'_k$ $(k = 1, 2, \ldots, m)$.

Clearly, this integral does exist.

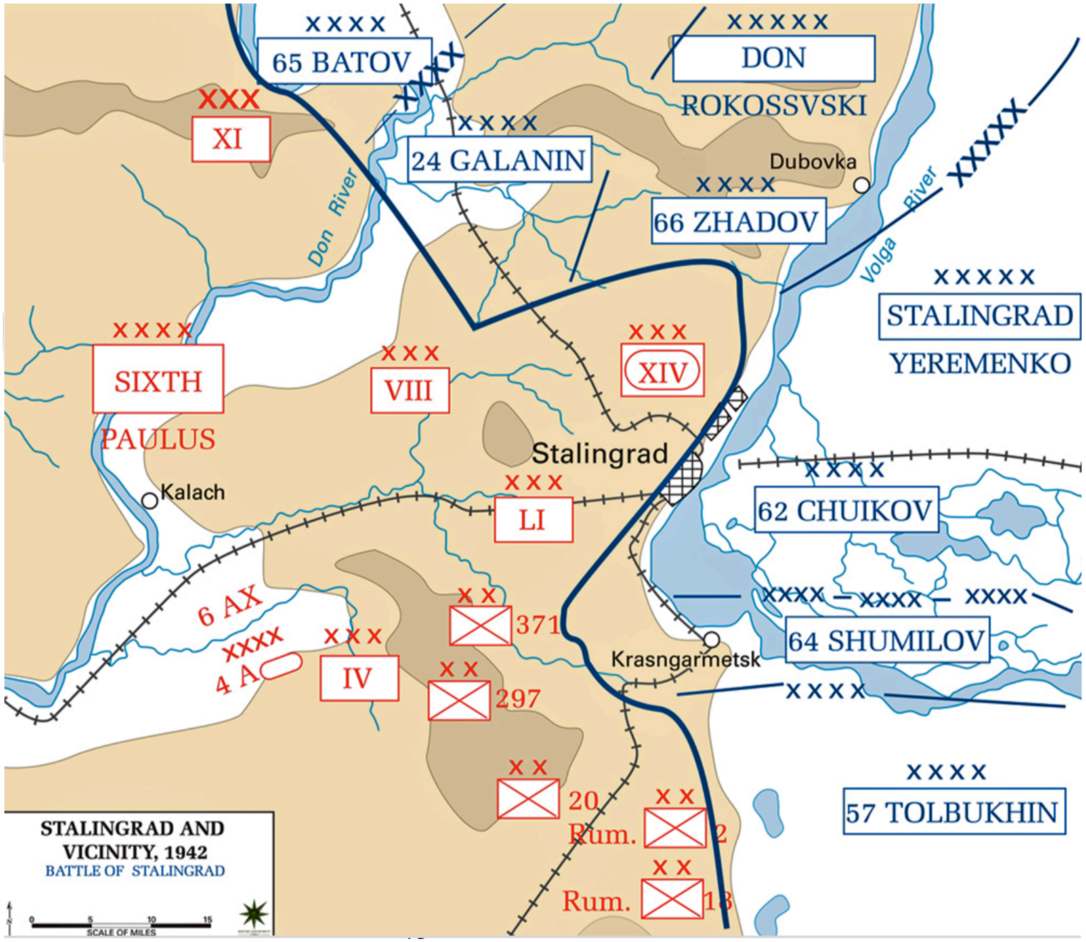
We call the quantity

$$W(\Phi, \Phi') = \inf_{\Psi} W(\Psi, \Phi, \Phi')$$

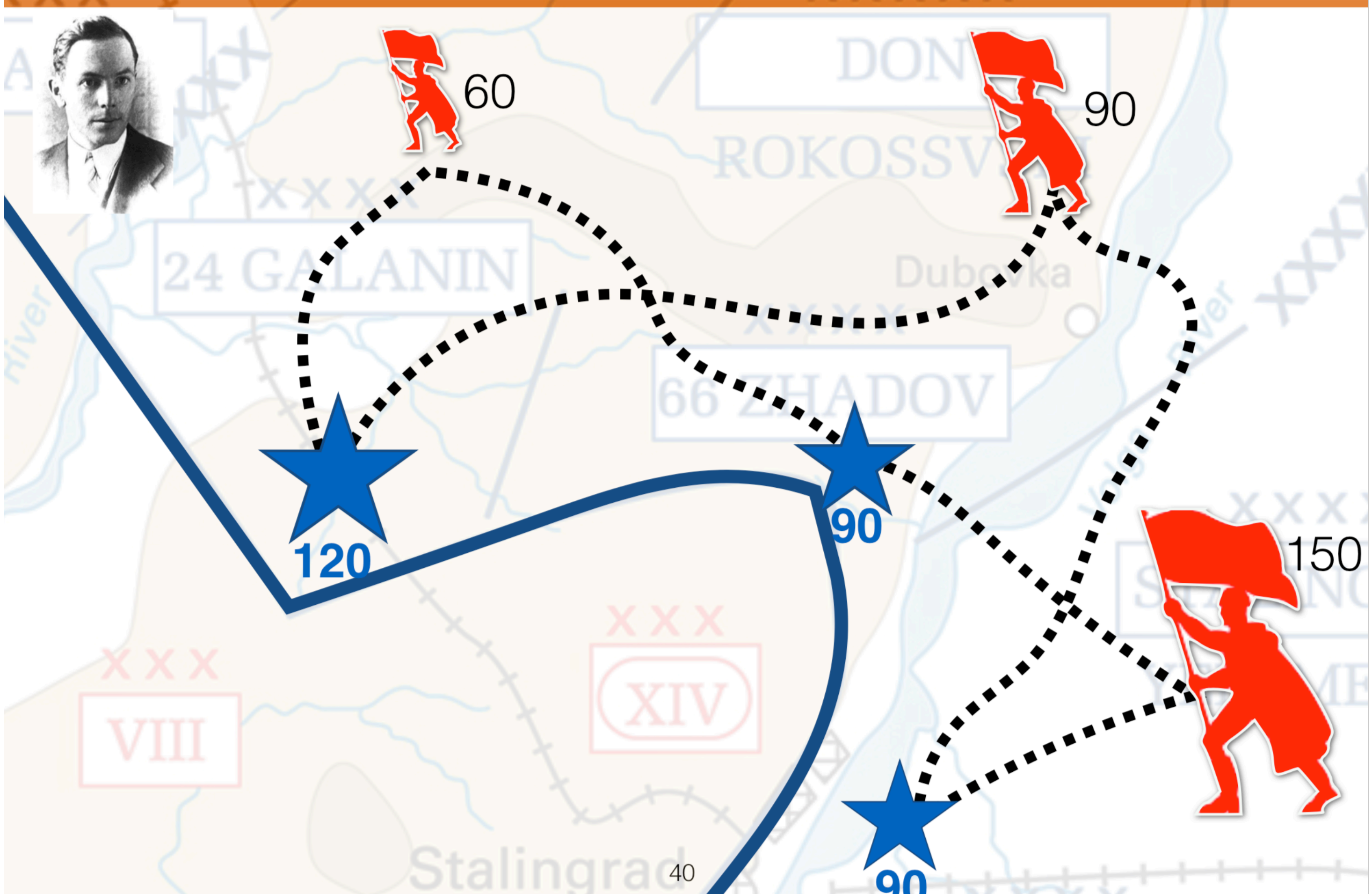
the minimal translocation work. Since the set of all functions $\{\Psi\}$ is compact, there exists a function Ψ_0 realizing this minimun, so that

$$W(\Phi, \Phi') = W(\Psi_0, \Phi, \Phi'),$$

Kantorovich Problem



Kantorovich Problem



Kantorovich Problem

Transportation matrix

60	?	?	?
90	?	?	?
150	?	?	?
	120	90	90

Distance matrix

1	d_{1A}	d_{1B}	d_{1C}
2	d_{2A}	d_{2B}	d_{2C}
3	d_{3A}	d_{3B}	d_{3C}
	A	B	C

Kantorovich Problem

Transportation matrix

$$\begin{array}{c|c|c|c|}
 \hline a_1 & p_{1\mathrm{A}} & p_{1\mathrm{B}} & p_{1\mathrm{C}} \\
 \hline a_2 & p_{2\mathrm{A}} & p_{2\mathrm{B}} & p_{2\mathrm{C}} \\
 \hline a_3 & p_{3\mathrm{A}} & p_{3\mathrm{B}} & p_{3\mathrm{C}} \\
 \hline \multicolumn{1}{c}{} & \multicolumn{1}{c}{b_{\mathrm{A}}} & \multicolumn{1}{c}{b_{\mathrm{B}}} & \multicolumn{1}{c}{b_{\mathrm{C}}}
\end{array}$$

Distance matrix

$$\begin{array}{c|c|c|c|}
 \hline 1 & d_{1\mathrm{A}} & d_{1\mathrm{B}} & d_{1\mathrm{C}} \\
 \hline 2 & d_{2\mathrm{A}} & d_{2\mathrm{B}} & d_{2\mathrm{C}} \\
 \hline 3 & d_{3\mathrm{A}} & d_{3\mathrm{B}} & d_{3\mathrm{C}} \\
 \hline \multicolumn{1}{c}{} & \multicolumn{1}{c}{\mathrm{A}} & \multicolumn{1}{c}{\mathrm{B}} & \multicolumn{1}{c}{\mathrm{C}}
\end{array}$$

Constraints

$$\forall i \in \{1,2,3\}, \quad \sum_{j \in \{\mathrm{A},\mathrm{B},\mathrm{C}\}} p_{ij} = a_i$$

$$\forall j \in \{\mathrm{A},\mathrm{B},\mathrm{C}\}, \quad \sum_{i \in \{1,2,3\}} p_{ij} = b_j$$

$$p_{ij} \geq 0$$

Cost function

$$C(\boldsymbol{P}) = \sum_{j \in \{\mathrm{A},\mathrm{B},\mathrm{C}\}} \sum_{i \in \{1,2,3\}} p_{ij} d_{ij}$$

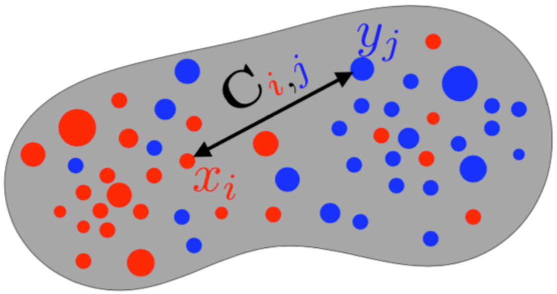
Problem

$$\min_{\text{all valid } \boldsymbol{P}} C(\boldsymbol{P})$$

Kantorovitch's Formulation

Input distributions

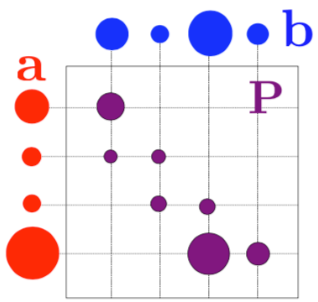
$\alpha = \sum_{i=1}^{n} \mathbf{a}_i \delta_{x_i} \quad \beta = \sum_{j=1}^{m} \mathbf{b}_j \delta_{y_j}$



Points $(x_i)_i$, $(y_j)_j$

Weights $\mathbf{a}_i \geqslant 0$, $\mathbf{b}_j \geqslant 0$.

$\sum_{i=1}^{n} \mathbf{a}_i = \sum_{j=1}^{m} \mathbf{b}_j = 1$

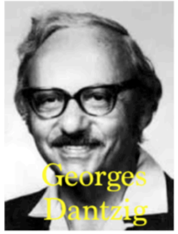


Couplings:

$\mathbf{U}(\mathbf{a},\mathbf{b}) \overset{\text{def.}}{=} \left\{\mathbf{P} \in \mathbb{R}_+^{n\times m} \; ; \; \mathbf{P}\mathbb{1}_m = \mathbf{a}, \mathbf{P}^\top \mathbb{1}_n = \mathbf{b}\right\}$

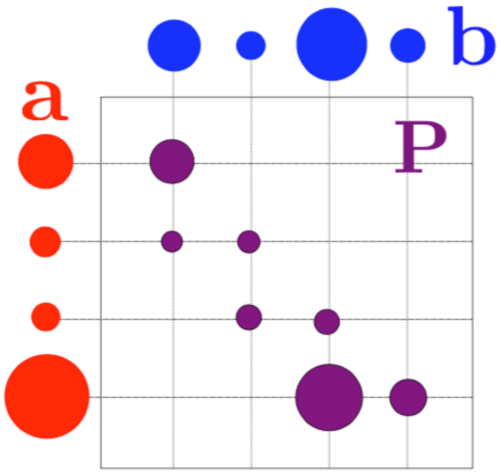
[Kantorovich 1942]

$$\min \left\{ \sum_{i,j} \mathbf{C}_{i,j}\mathbf{P}_{i,j} \; ; \; \mathbf{P} \in \mathbf{U}(\mathbf{a},\mathbf{b}) \right\}$$

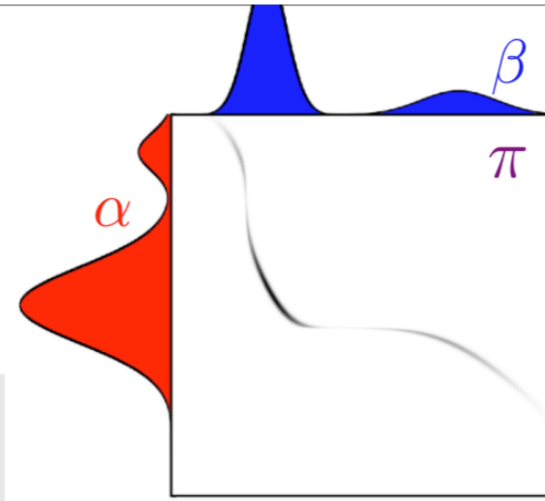


$\rightarrow$ Linear program, simplex $O(n^3 \log(n))$.

Wasserstein Distance



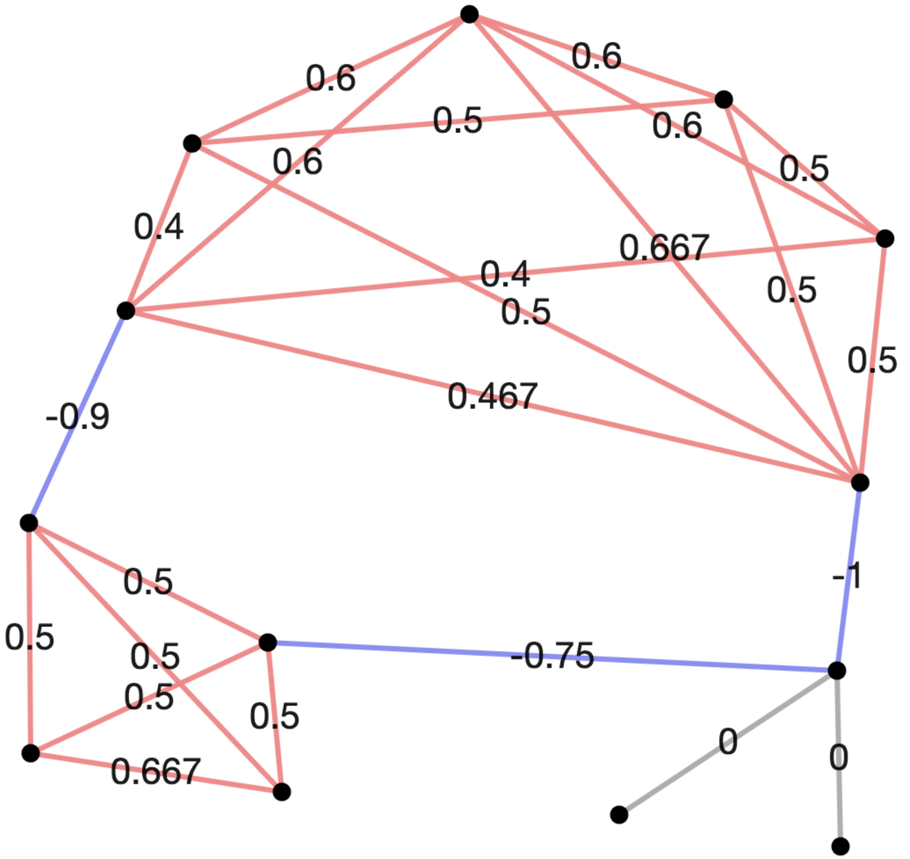
$$\pi = \sum_{i,j} \mathbf{P}_{i,j} \delta_{x_i, y_j}$$



$$c(x,y) = d(x,y)^p$$

$$\mathrm{W}_p(\alpha,\beta)^p \overset{\text{def.}}{=} \min_{\pi \in \mathcal{M}_+^1(\mathcal{X}^2)} \left\{ \int_{\mathcal{X}^2} d(x,y)^p \mathrm{d}\pi(x,y) \; ; \; \pi_1 = \alpha, \pi_2 = \beta \right\}$$

Subsampling in Graphs



Edges with large curvature are within a community;
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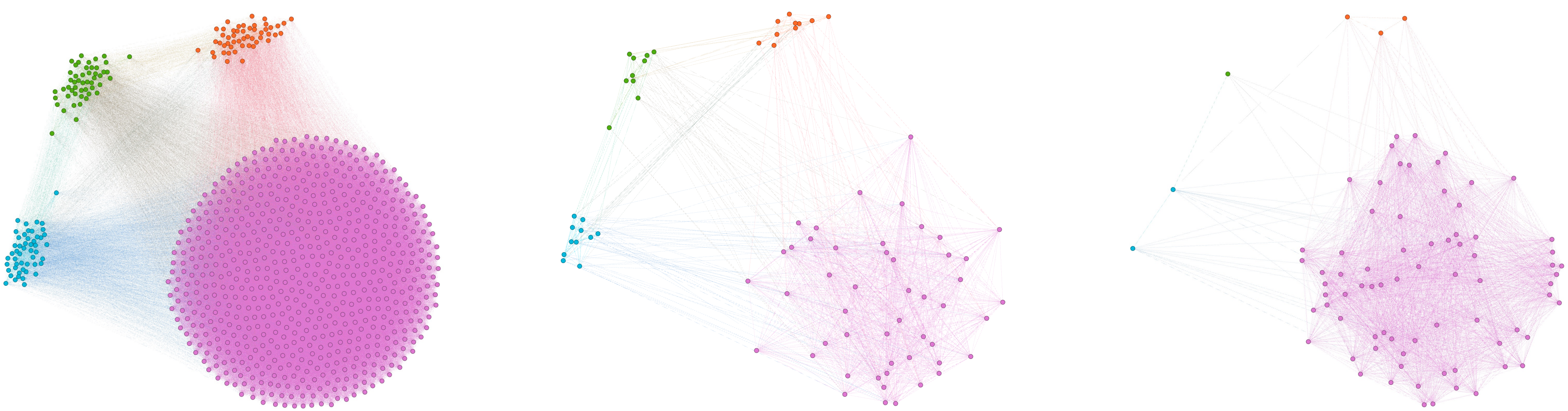
OR Curvature Gradient-based Subsampling

$$\left(x^{(i+1)}, y^{(i+1)}\right) = \text{argmax}_{(x,y)\in\Delta\left(\left(x^{(i)},y^{(i)}\right)\right)}\left|\kappa(x,y) - \kappa\left(x^{(i+1)}, y^{(i+1)}\right)\right|$$



Experiment Results

Dataset	Prop.	ORG-sub	MHRW	CSE	FFS	Snowball	RW	MDRW
Polbooks (T: 1.88 s)	10%	**0.00 (T: 0.10 s)**	1.20	0.62	2.68	0.48	0.33	0.00
Polblogs (T: 48.6 s)	5%	**0.00 (T: 0.23 s)**	1.87	0.90	2.00	0.43	1.03	0.30
PubMed (T: NA)	2%	**0.00 (T: 4.42 s)**	0.30	0.80	0.40	0.20	1.20	1.80

Acknowledgement

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