# Multiscale Analysis of Dynamic Graphs

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## Random walks on graphs and data

Given a weighted graph (G, E, W): vertices represent data points, edges connect  $x_i, x_j$  with weight  $W_{ij} := W(x_i, x_j)$ , when positive (or above a threshold). Let  $D_{ii} = \sum_j W_{ij}$  and

$$\underbrace{P = D^{-1}W}_{\text{random walk}}, \quad \underbrace{T = D^{-\frac{1}{2}}WD^{-\frac{1}{2}}}_{symm. "random walk"}, \quad \underbrace{L = I - T}_{norm.Laplacian}, \quad \underbrace{H = e^{-tL}}_{Heat \ kernel}$$

Let  $1 = \lambda_0 \ge \lambda_1 \ge \ldots$  and  $\varphi_i$  the eigenval.'s and eigenvec.'s of T. We shall consider the map  $G \ni x \mapsto (\varphi_1(x), \ldots, \varphi_m(x)) \in \mathbb{R}^m$ .

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We may construct weighted graphs from data: given

. Data  $X = \{x_i\}_{i=1}^n \subset \mathbb{R}^D$ .

. Local similarities via a kernel function  $W(x_i, x_j) \ge 0$ .

Simplest example:  $W_{\sigma}(x_i, x_j) = e^{-||x_i - x_j||^2/\sigma}$ .

#### Dynamic Graphs

J. Lee, MM, Thesis, 2010, *Proc. SampTA*, 2011

Given: time series of graphs  $G_t$ . Objective: to analyze this time series. Desiderata:

- . Sensitive to large and small significative changes in the network, and to their location.
- . Should capture both topological and quantitative geometric changes.
- . Should yield measures of change: want to do analysis, statistics...
- . Robust to "noisy" perturbations of the network.

We are used to performing similar tasks on real-valued time series, how do we extend similar tools to a "space of graphs"? How can we quantify change? How do we construct multiple resolutions on graphs?

#### Multiscale Graphs - Toy Model

The graphs we start with will have a strong multiscale structure. They are constructed as follows: we start with a dictionary  $\mathcal{D}$  of graphs, including for example complete graphs, trees, paths, loops, etc... Then:

- (i) Pick J graph flavors  $F_1, \ldots, F_J$ , from  $\mathcal{D}$ , i.e. on flavor per scale
- (ii) Let the graph at the coarsest scale be of flavor  $G_1$ , with edges with weight  $O(2^1)$
- (iii) For j = 2, ..., J, replace each vertex of  $G_{j-1}$  with a graph  $G_j$  of flavor  $F_j$ and edges of weight  $O(2^j)$ .





### Multiscale Graphs - Toy Model

The generalizations below are *trivially* handled by the algorithms that follow, that do not depend on the symmetries above. For example different models used at different locations at different scales.

What matters is that the random walk has multiple time scales.

Intuitively: there is clear definition of scales, and what it means to "look at the graph at a certain scale".



## Dynamic Graphs - Toy Model

We consider a small set of "elementary moves", including:

- (i) adding or removing a vertex
- (ii) adding or removing an edge
- (iii) changing an edge weight

The scale of the change is important.



## Multiscale analysis of Dynamic Graphs

Our construction consists of 3 steps:

- . Construct multiscale partitions of  $G_t$
- . Map  $G_t$  to a feature vector whose coordinates are operators, more specifically versions of  $P^t$  compressed on the multiscale partitions
- . Compare  $G_{t+1}$  and  $G_t$  based on the feature vectors constructed above: these are now vectors of operators, and we know how to compare operators.

## Algorithm: Multiscale Partitions

Recursive cuts lead to a multiscale partition

we one such at each time snapshot



Clusters at each scale

## Algorithm: Multiscale Partitions

> Total number of edges in cluster

Alternative: instead on N-cut use a conductance based criterion and local partitioning methods (D. Spielman, F. Chung, ...). This has stronger theoretical guarantees, and a good option for very large graphs.

## Algorithm: Multiscale Partitions

Algorithm for constructing partitions. What is a good partition? Ncut should be small:  $1 \stackrel{k}{\longrightarrow} W(C^i (C^i)^c) \stackrel{\text{Cluster}}{\longrightarrow} Cluster$ 

$$Ncut(C^{1},...,C^{k}) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(C^{i},(C^{i})^{c})}{vol(C^{i})}$$

Total number of edges in cluster

where  $W(A, B) = \sum_{x \in A, y \in B} W(x, y)$  and  $vol(A) = \sum_{x \in A} \sum_{y} W(x, y)$ . NP-Hard to minimize, approximation algorithms exist [Arora]. Oftentimes relaxed to spectral clustering on  $P = D^{-1}W$ : compute top k + 1 eigenvectors of  $P: \varphi_1, \ldots, \varphi_{k+1}$ , embed the graph in Euclidean space by  $x \mapsto (\varphi_i(x))_{i=1}^{k+1}$ , and perform k-means in this space.

At any time t, we perform the above recursively, with k = 2, obtaining a multiscale family of partitions  $\{C_{j,t}\}$  organized in a binary tree.

Alternative: instead on N-cut use a conductance based criterion and local partitioning methods (D. Spielman, F. Chung, ...). This has stronger theoretical guarantees, and a good option for very large graphs.

## Algorithm: Multiscale Dynamics

For every t and every scale j, compress  $P_t^{\tau}$ : it is a matrix of size  $|C_{j,t}| \times |C_{j,t}|$ :

 $\tau$ -step r.w. on  $G_t$  compressed at scale j

 $(P_{t,j,\tau})_{il} := \sum_{x \in C_{j,t}^{i}} \frac{1}{C_{j,t}^{i}} \sum_{y \in C_{j,t}^{l}} P^{\tau}(x,y)$ probability mass transported from a starting point in  $C_{j,t}^{i}$  to some point in  $C_{j,t}^{l}$ 

t indexes time

i, l index clusters at scale j

j indexes scale in the partition tree

> au refers to internal averaging time

#### Algorithm: Multiscale compression

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$$(P_{t,j,\tau})_{il} = \sum_{x \in C_{j,t}^i} \frac{1}{C_{j,t}^i} \sum_{y \in C_{j,t}^l} P^{\tau}(x,y)$$

for i, l varying in the index of the sets in the partition  $C_{j,t}$ .

In fact we can do much more, since we can localize this changes, at every scale, and across scales, and develop a full multiscale ("wavelet-like") time series analysis for graphs.

#### Algorithm: Multiscale compression

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for i, l varying in the index of the sets in the partition  $C_{j,t}$ .

At this point we can measure variations in  $P_{t,j,\tau}$  as a function of t, for the scale j and "internal time scale"  $\tau$ , for example by measuring  $||P_{t,j,\tau} - P_{t+1,j,\tau}||_F$ .

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A time series of 51 graphs was constructed with a single vertex and edge noise added after each graph. The initial graph has 3 layers, and 60 nodes. The edge weights on the scales from finest to coarsest are 64, 8, and 1. The initial partitions are fed to the algorithm and we update the partitions using the aforementioned online algorithm. At each step, a new vertex with 3 edges is introduced.











#### Simulated "attacks"

Network of political blogs, 1400 nodes and 19000 edges. We simulate two attacks: a DDOS attack at time 4, when one random vertex is connected to 100 random vertices, till time 6, and then a wormhole attack at time 8, when the two farthest vertices are connected by a heavy edge.



L. A. Adamic and N. Glance, "The political blogosphere and the 2004 US Election", in Proceedings of the WWW-2005 Workshop on the Weblogging Ecosystem (2005)

#### A much finer version

Joint with P. Balachandran and J. Mattingly

- . We consider continuous time, and one scale only. Let  $C_1, \ldots, C_k$  be clusters, constructed according to a conductance criterion, so that a r.w. started in  $C_i$  almost mixes inside  $C_i$  before significant mass leaks to  $C_i^c$ .
- . Compressing the clusters. Let  $\partial^- C_i$  and  $\partial^+ C_i$  be the entry and exit points of  $C_i$ : we encode the probability of first leaving  $C_i$  through  $y \in \partial C_i^+$  having entered at  $x \in \partial C_i^-$ , and approximate (in TV-distance) the distribution of the corresponding first exit time  $\tau_{y|x}$ .
- . Homogenized process. It state space is  $\partial^- C_i \cup \partial^+ C_i$ , and the transitions are as follows: at  $x \in \partial^- C_i$  toss a coin to pick be the exit point  $y \in \partial^+ C_i$ , and drawing a corresponding first exit time  $\tau_{y|x}$ . Then use the edges and transition times on the original graphs to move from  $y \in \partial^+ C_i$  to  $y \in \partial^- C_l$ .
- . Some properties. The homogenized process is semi-Markov (Markov at jump times), with a time-dependent transition kernel  $\overline{P}_t(x, y)$ . Then in a suitable, strong sense (TV distance),  $\overline{P}_t(x, y)$  is close to  $P_t(x, y)$ .
- . The above may be implemented by efficient algorithms.

#### A few notes

. Processes on a graph are the focus, not the graph itself

- . We replaced a graph by a process on it (e.g. the random walk), and then studied that process at multiple scales. If the graph changes in time, we have a family of processes.
- . Eigenfunctions capture large scale/long time dynamics, but expect interesting graphs to have rich multiscale spatial/temporal scales.
- . Functions on graphs are also important, e.g. in machine learning.
- . Spectral graph theory, multiscale analysis, stochastic processes all play fundamental roles.
- . The construction of the processes from data is domain dependent, informed by physical/statistical/geometric models.
- . We know how to construct multiscale basis functions (with fast transforms) on graphs; these may be used to compress processes such as the r.w.

## Open problems & future dir.'s

Too many!

- . Efficient and good local clustering algorithms.
- . Properties of eigenfunctions of Laplacian/r.w. on graphs.
- . Notions of (multiscale?) geometric stability and its relationships with stability of eigenfunctions, clusters, r.w.'s...
- . How to study more general processes where diffusion is not the main component?

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#### THANK YOU!



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