Exponentially smoothed spectral clustering and dynamic stochastic block model

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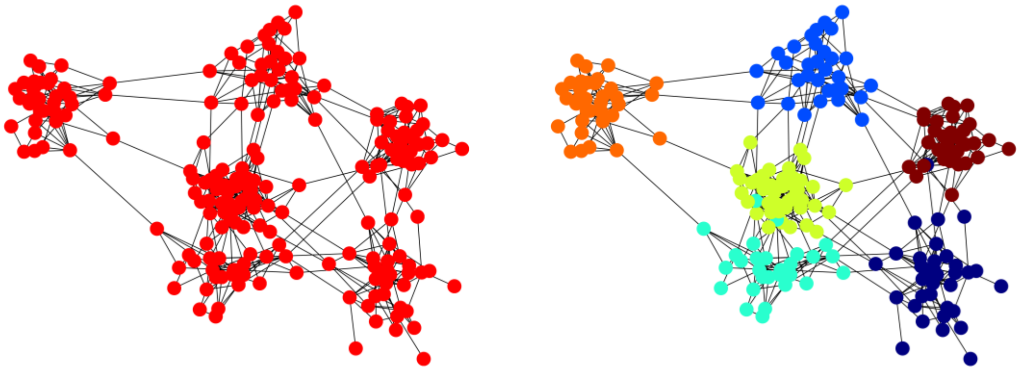
GraphSig May 2019

Spectral Clustering



Cluster the nodes of a graph using its structure.

Application in :

- Social network analysis
- Protein analysis
- etc

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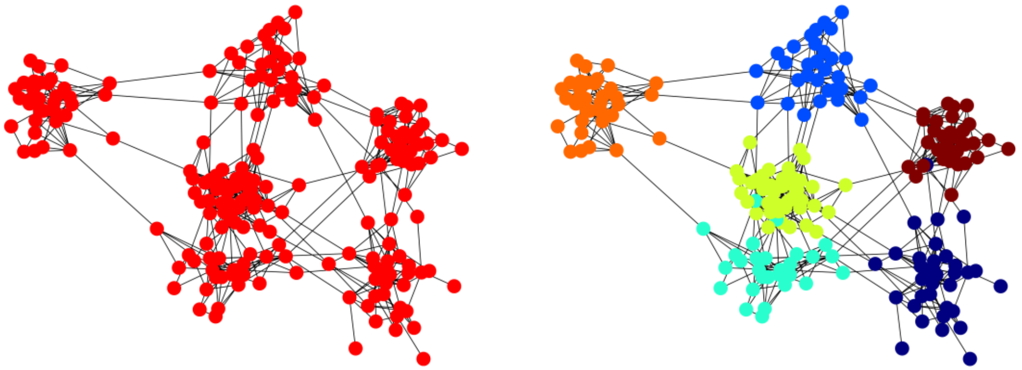

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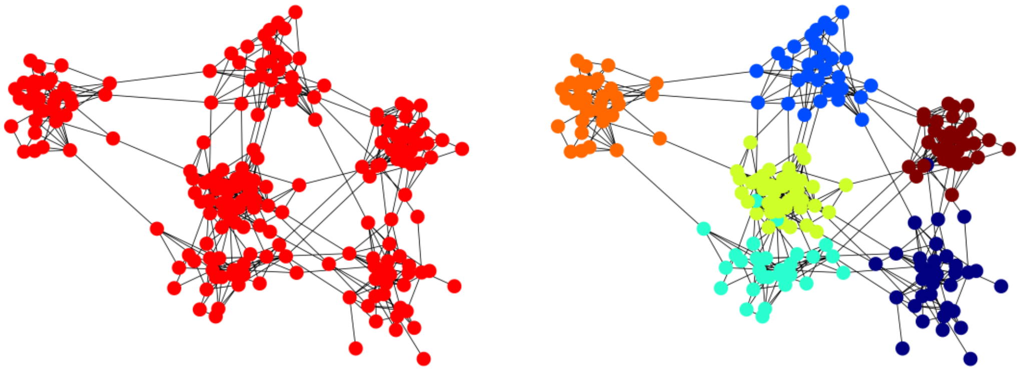

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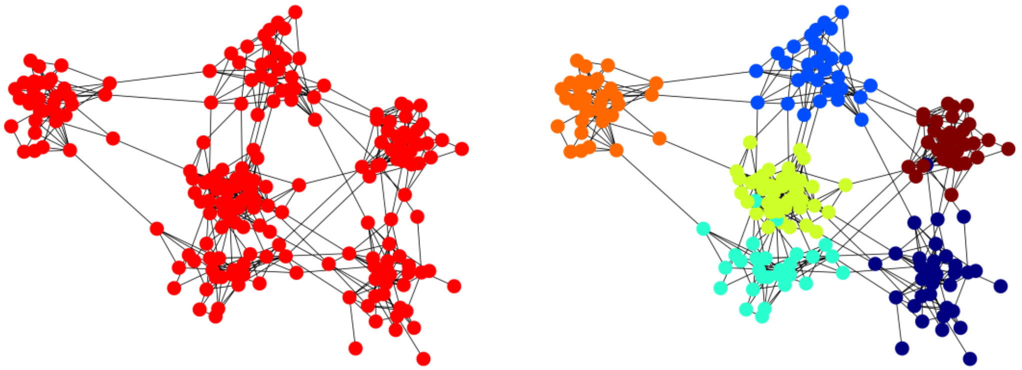

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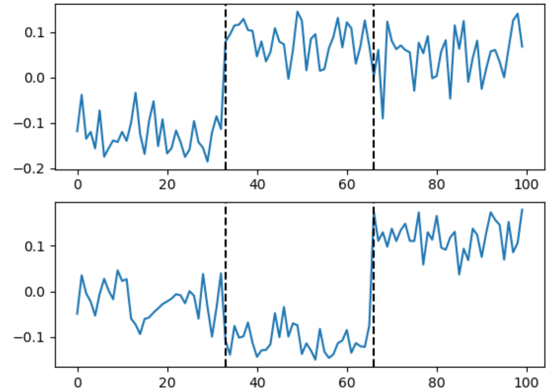
Eigenvectors :



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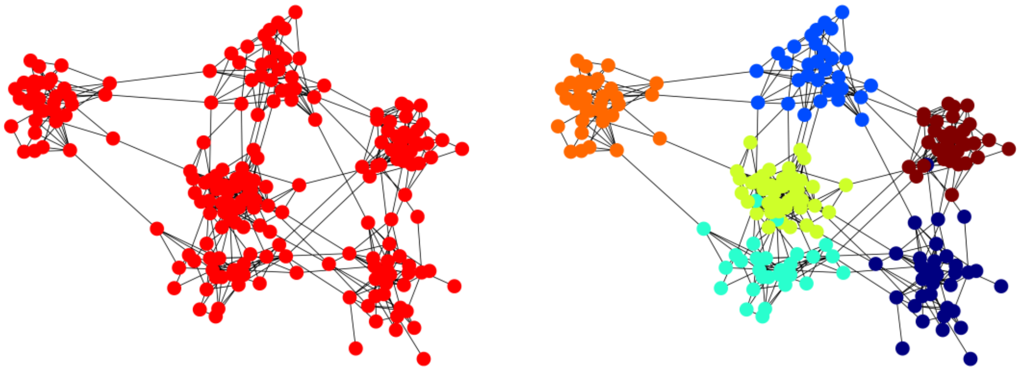

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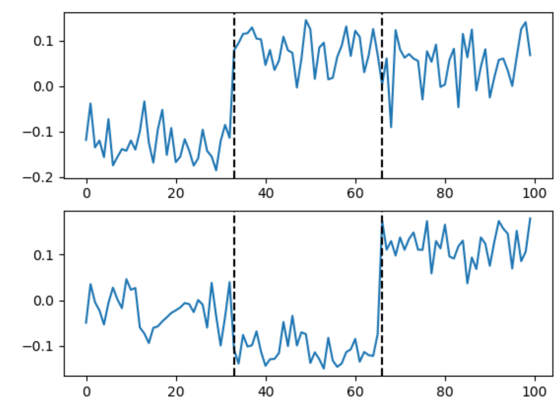

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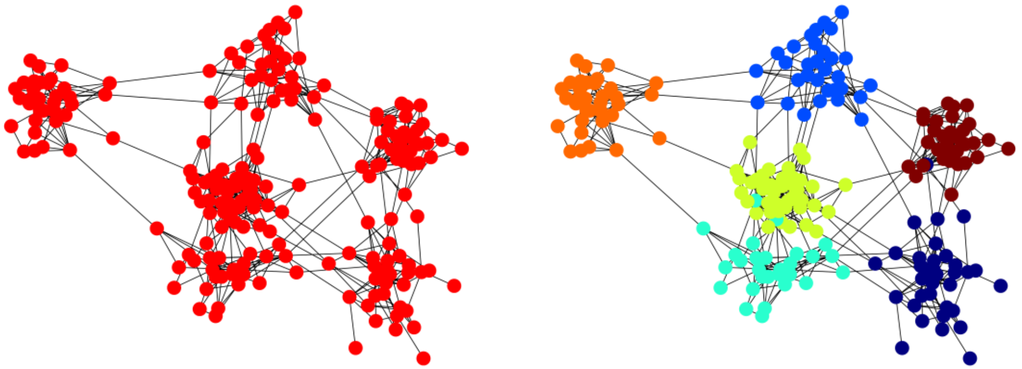

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- Many many (fast) variants…

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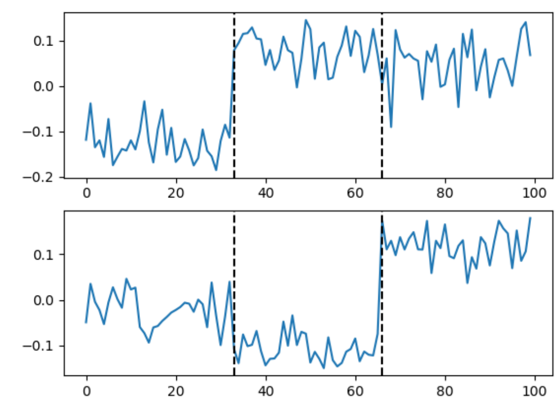
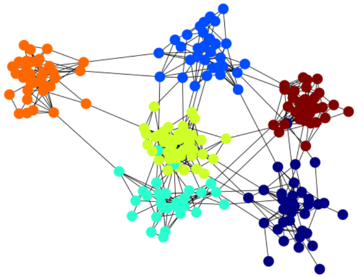


SBM : theoretical analysis

Stochastic Block Model (SBM)

$$\begin{cases} a_{ij} \sim \mathrm{Ber}(B_{k\ell}) \\ \text{when } \Theta_{ik} = 1, \Theta_{j\ell} = 1 \end{cases}$$



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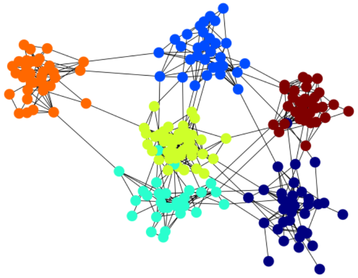

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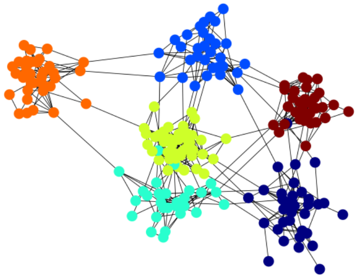

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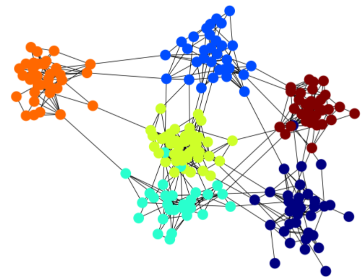

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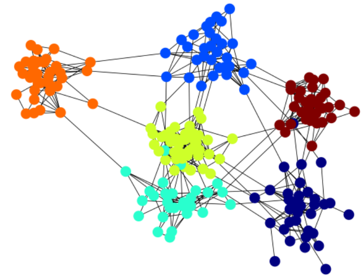

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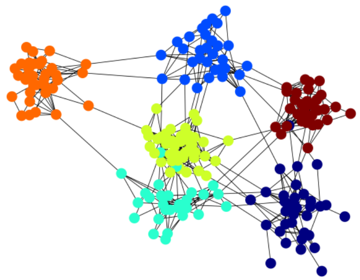

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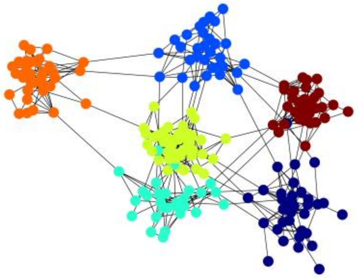

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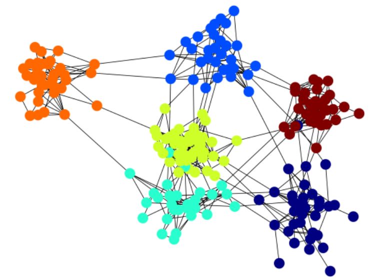

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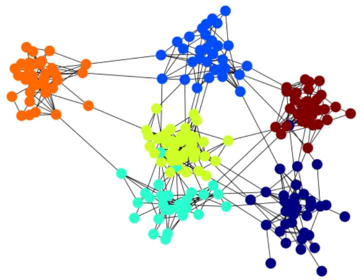

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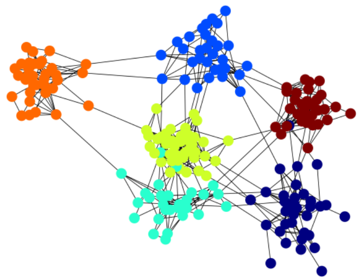

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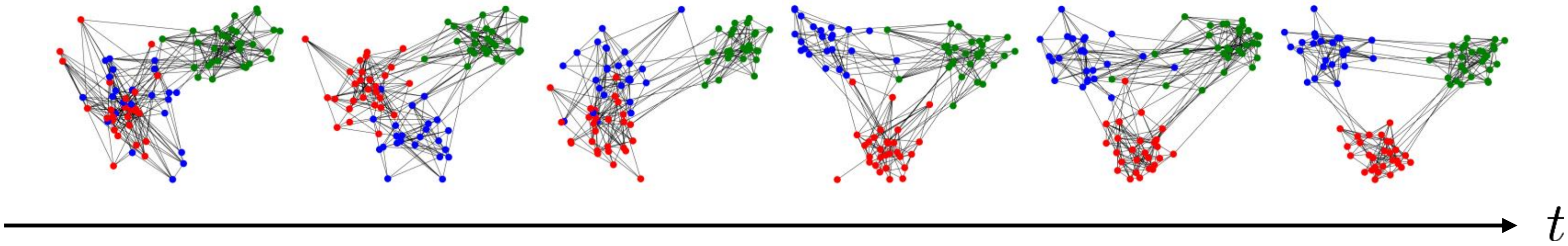
- With proba $1 - n^{-r}$:

$$\boxed{L(\hat{\Theta}, \Theta) \lesssim \frac{K^2}{n\alpha_n}}$$

$$L(\hat{\Theta}, \Theta) = \min_P \|\hat{\Theta}P - \Theta\|_0$$

Dynamic Spectral Clustering



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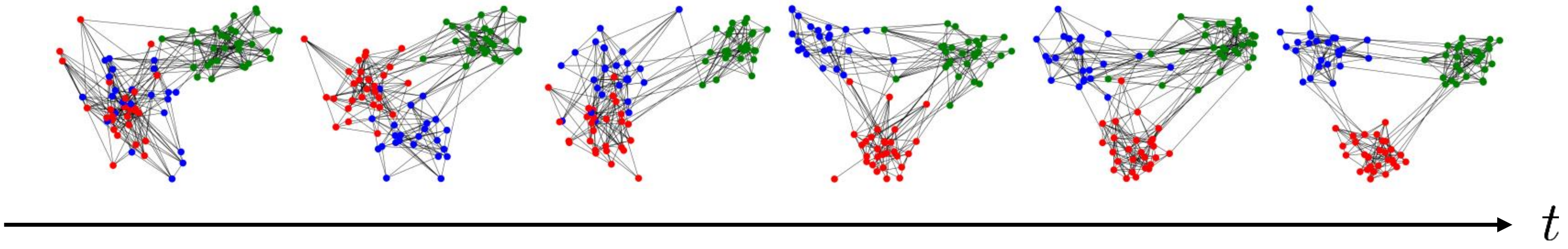

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Exploit past data to:

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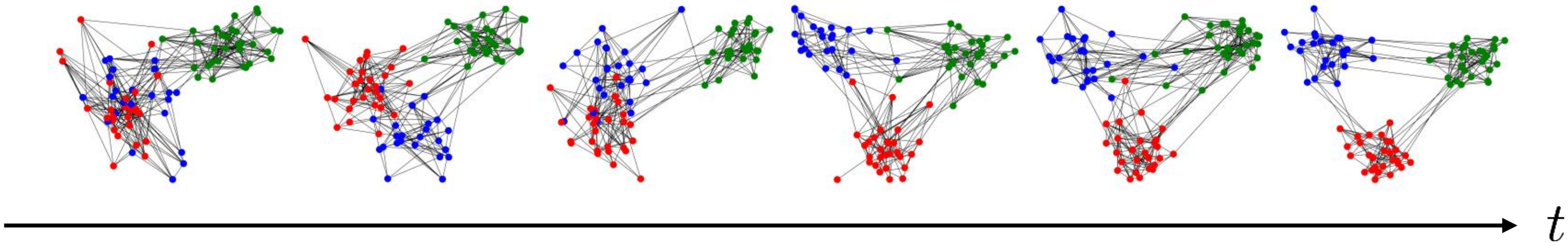

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Exploit past data to:
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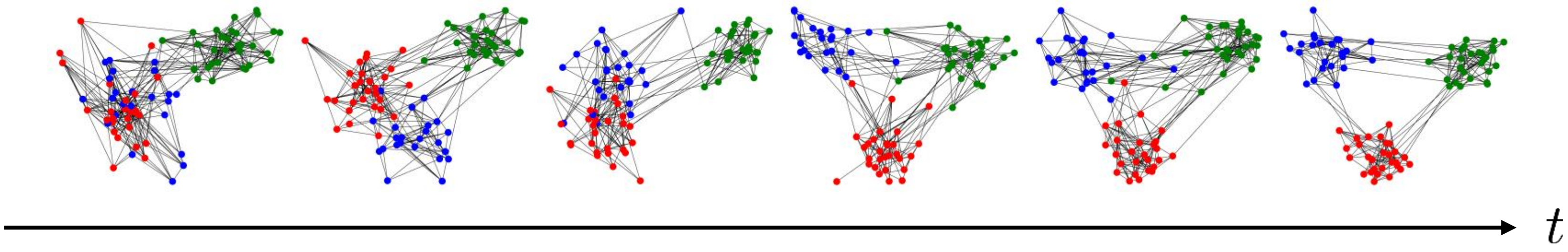

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Exploit past data to:

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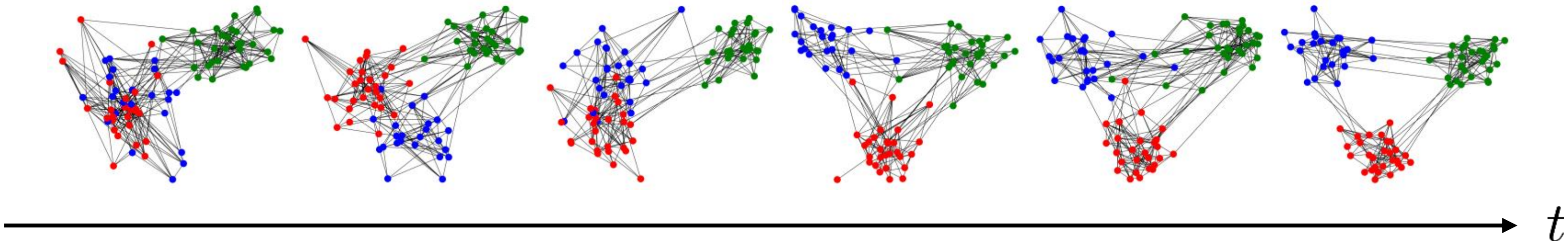

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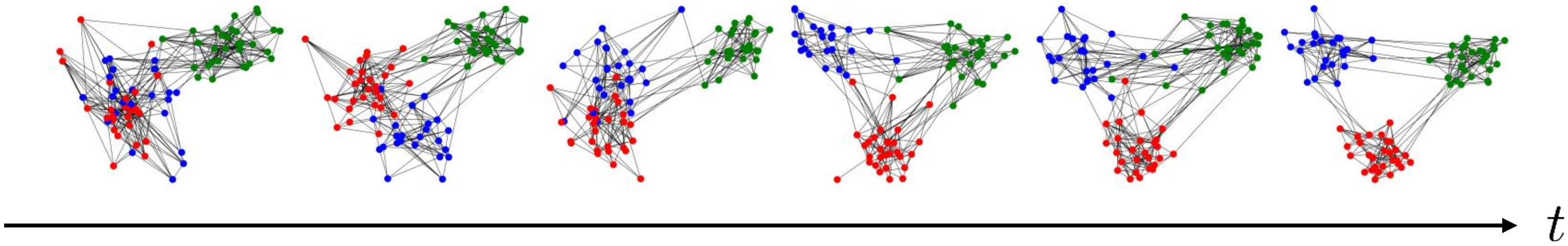

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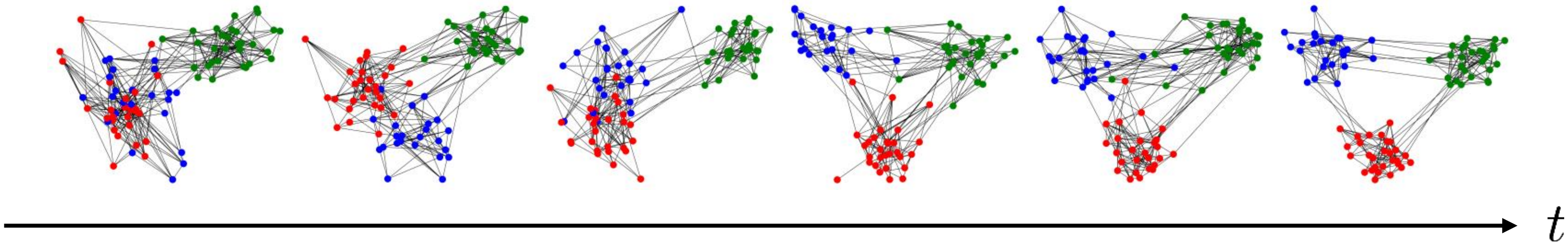

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- Variational…

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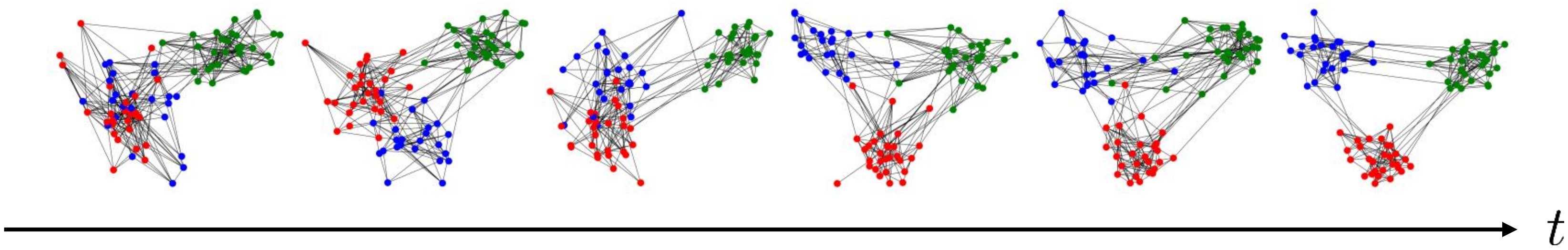

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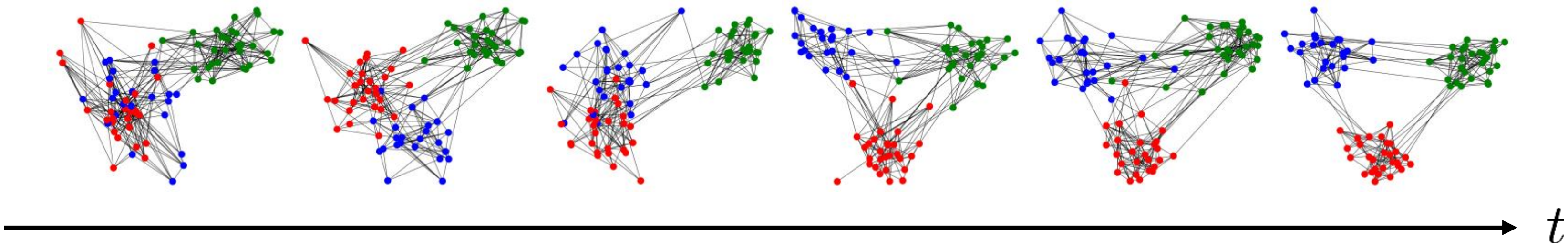

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- Uniform average ? *[Pensky 2017]*

$$\bar{A}_t = \sum_{l=t-w}^{t} A_l$$

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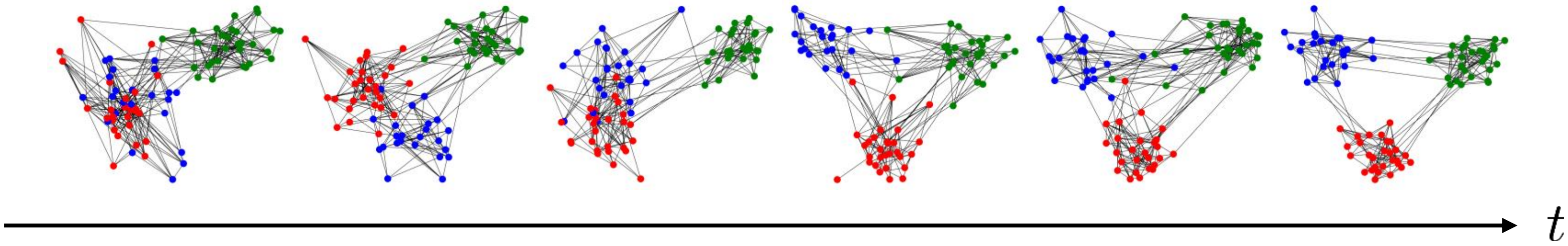

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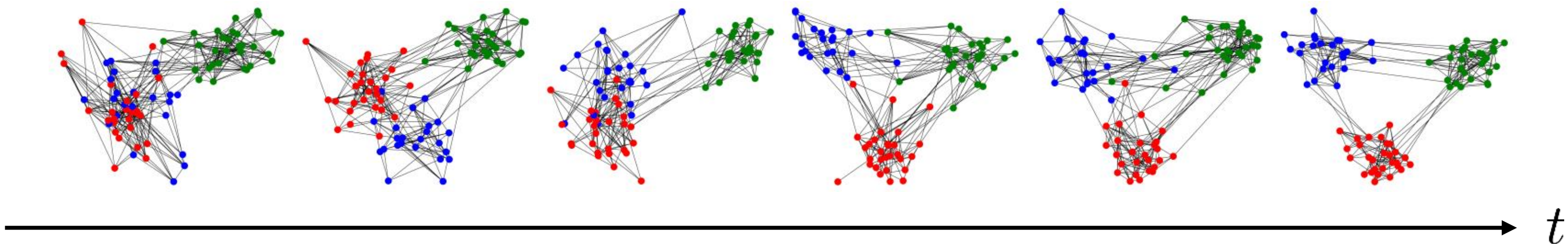
- Here : **Exponential Smoothing** *[Chi 2007, Xu 2010…]*

$$\bar{A}_t = (1-\lambda)\bar{A}_{t-1} + \lambda A_t$$

  - More appropriate for online computing

Dynamic SBM



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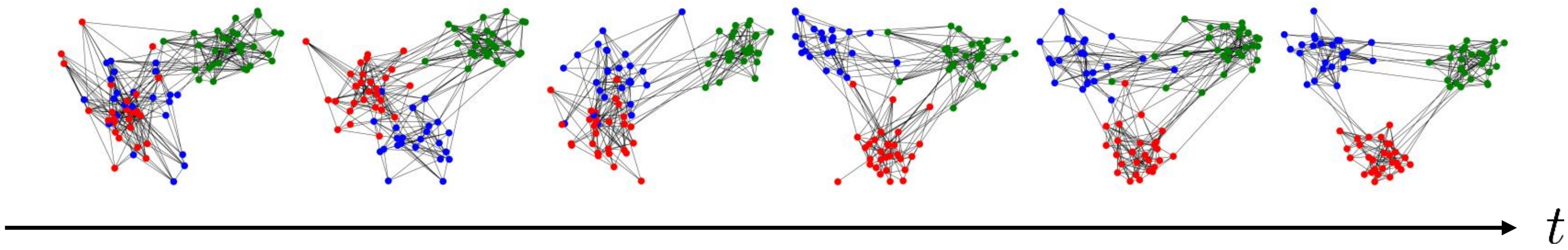

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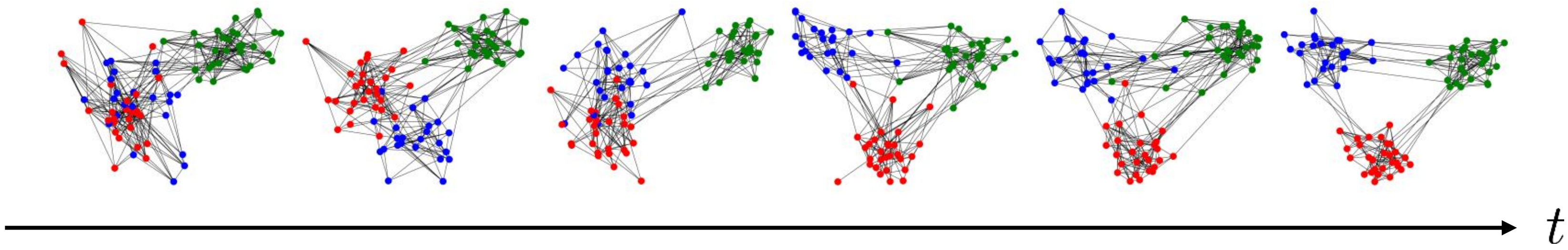

$$\Theta_1 \longrightarrow \Theta_2 \longrightarrow \cdots \longrightarrow \Theta_t$$

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Hidden Markov Model (HMM)

- At each time step, each node change community with proba ε

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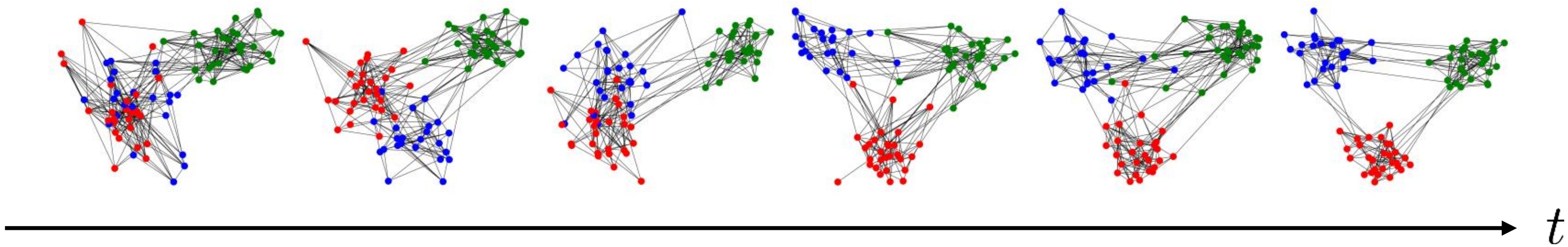

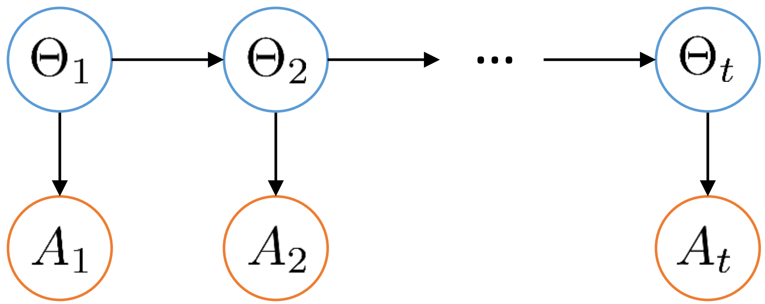

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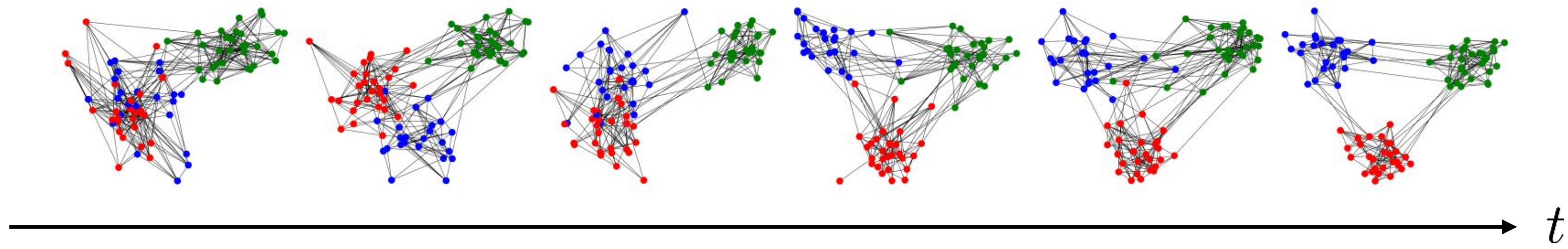

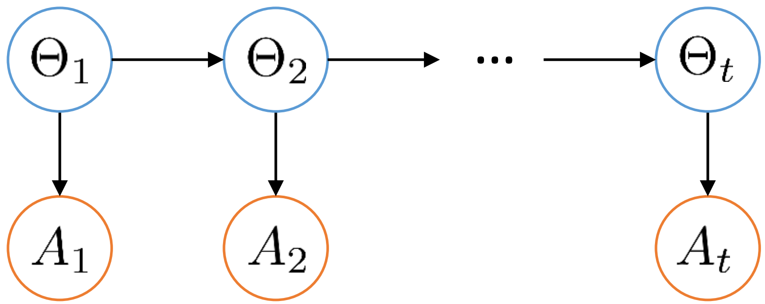

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- To simplify, connectivity matrix does not change

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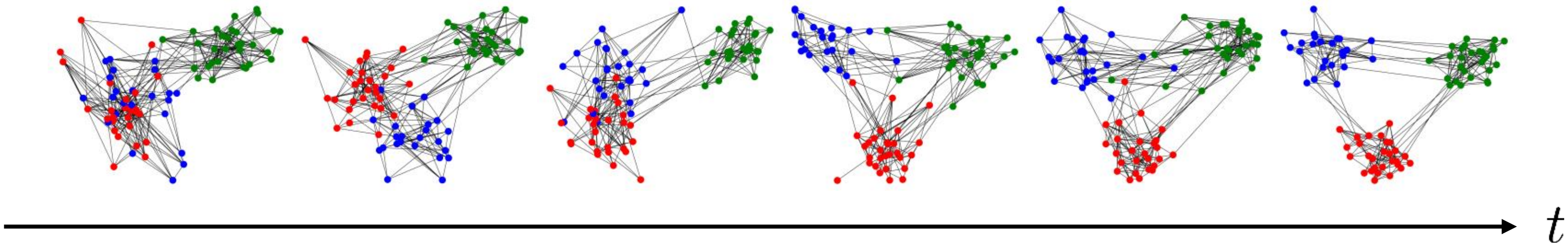

Uniform Average *[Pensky et al. 2017]*

- Uniform smoothing

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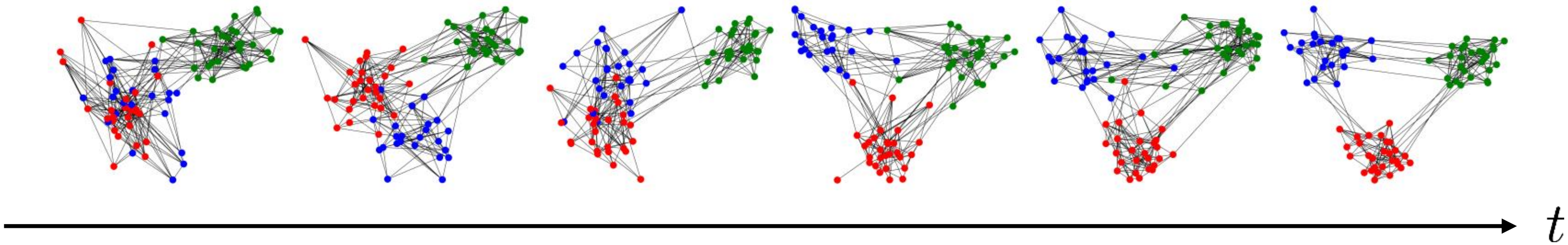

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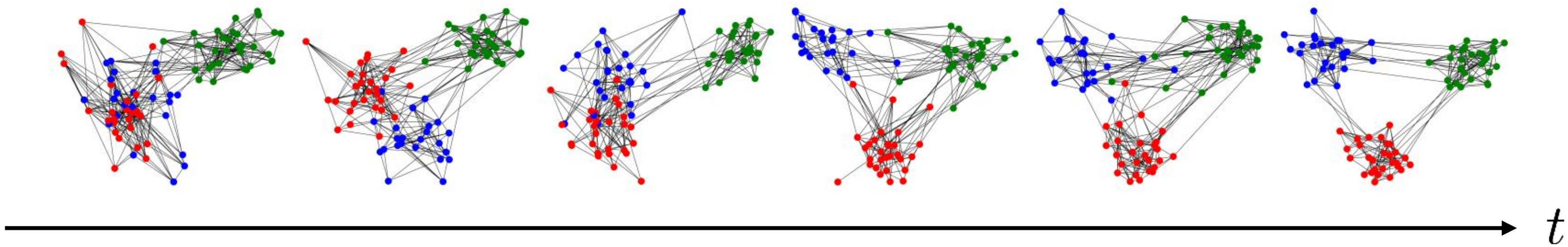

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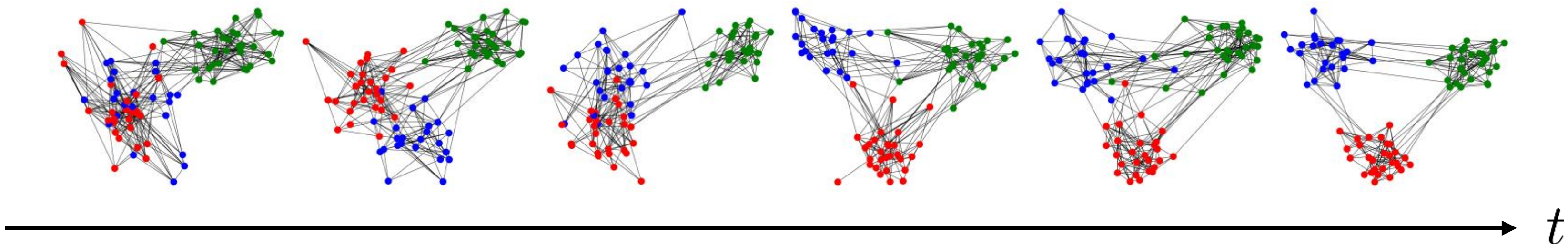

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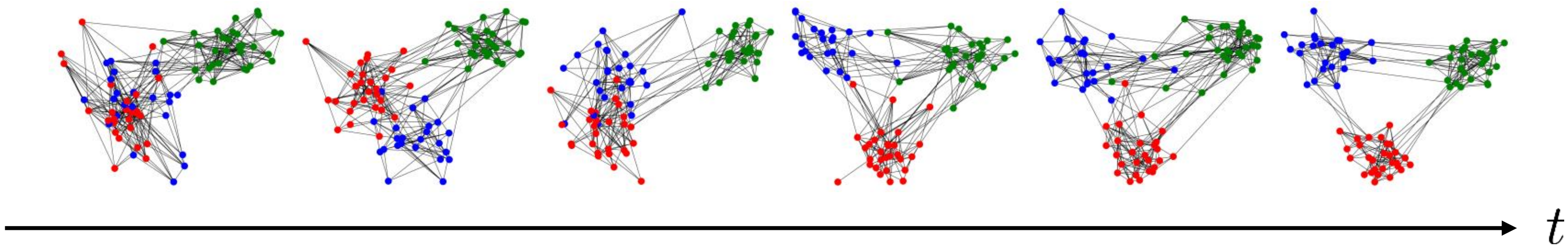

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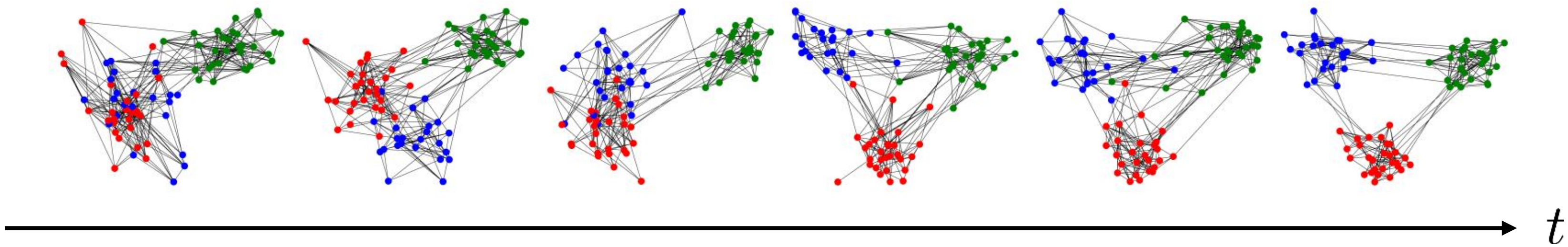

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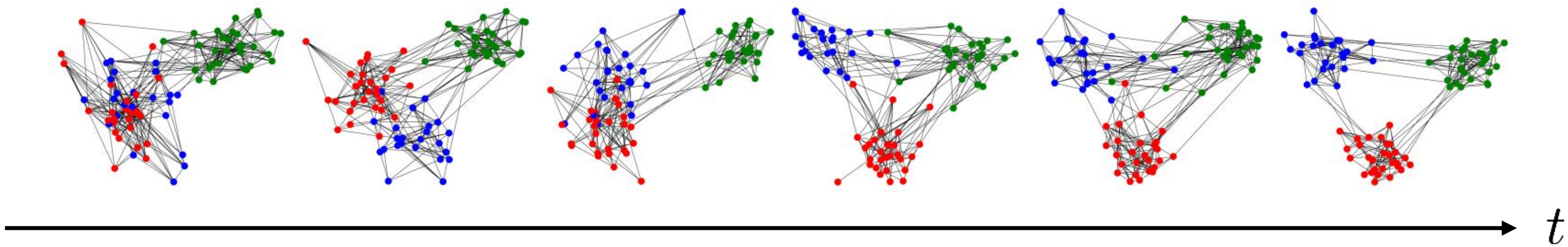

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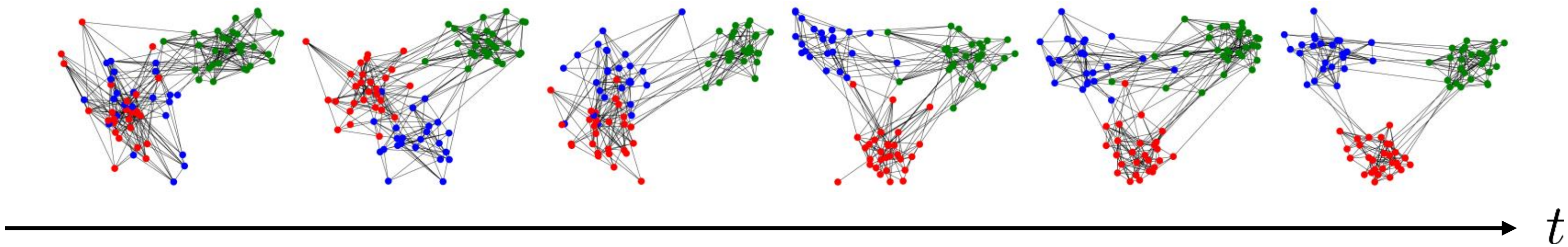

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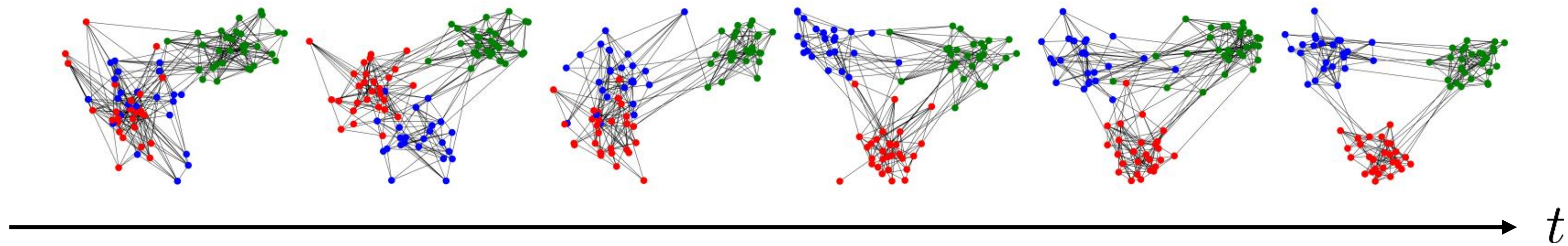

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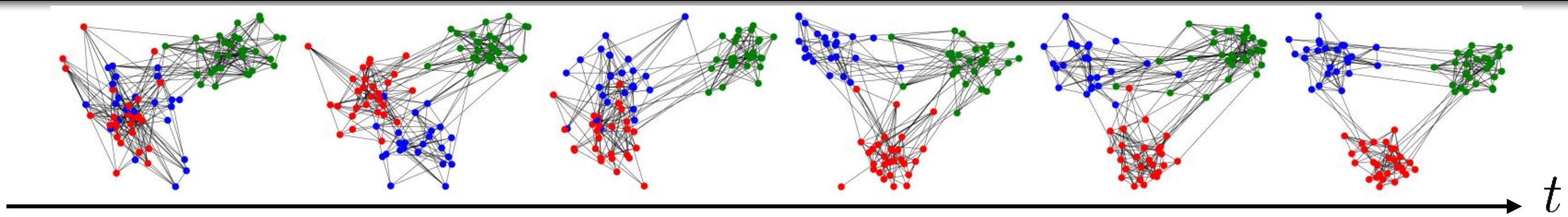
Outline

1. Main result
2. Choosing the forgetting factor
3. Experiments
4. Conclusion *(Bonus : GNN ?)*

Result



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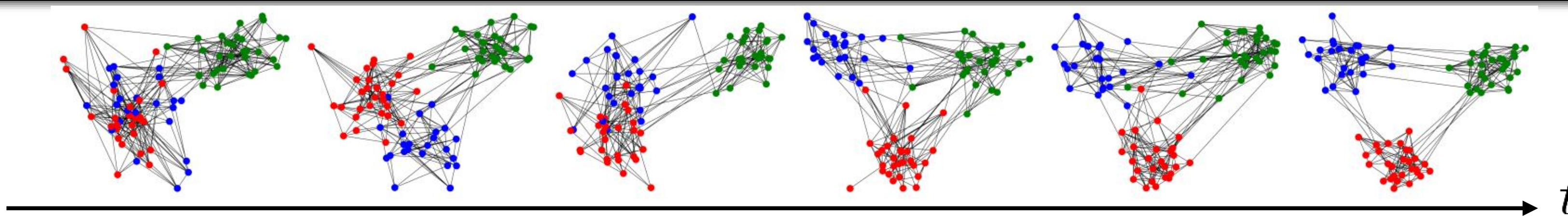

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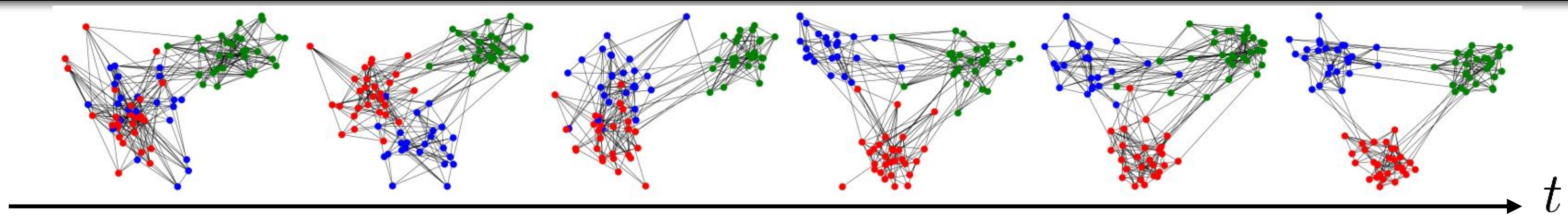

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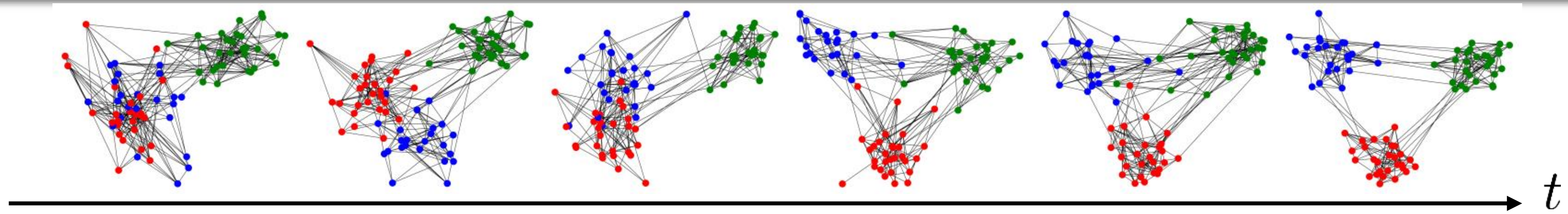

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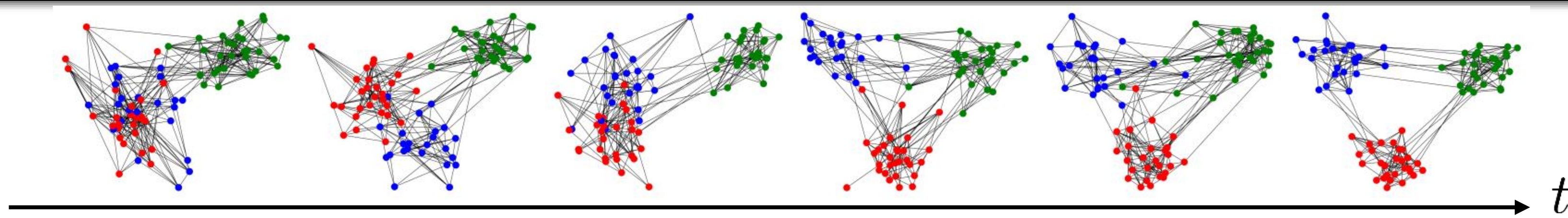

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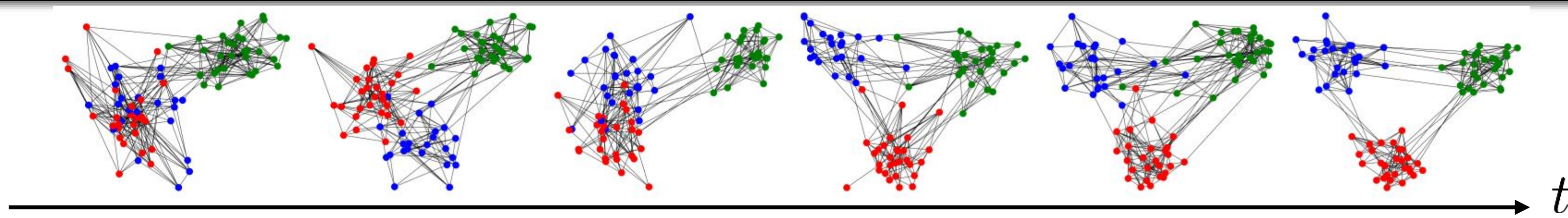

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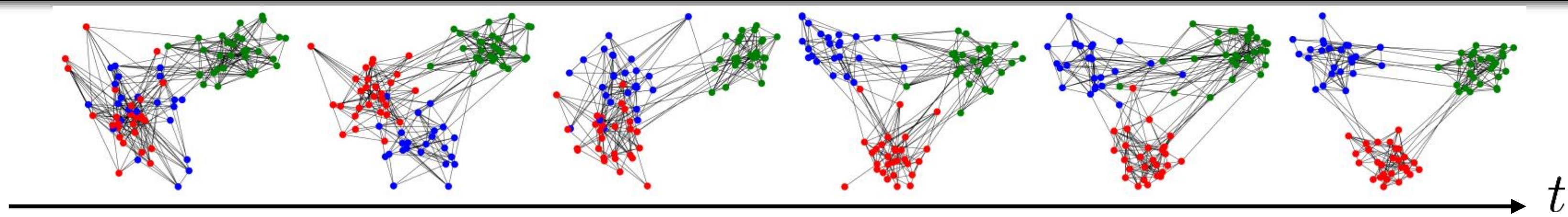

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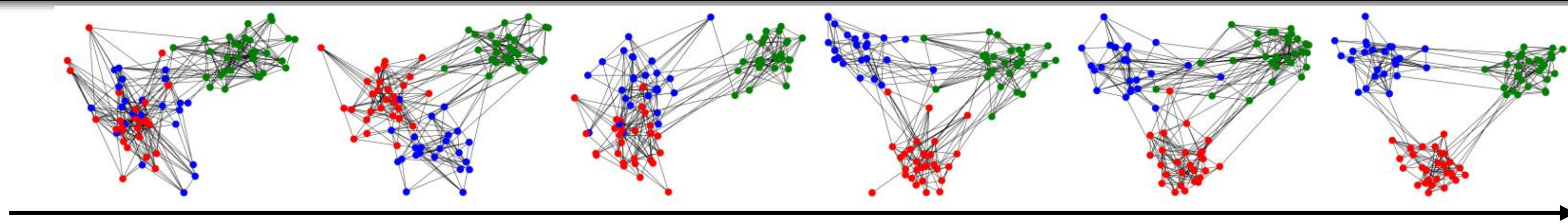

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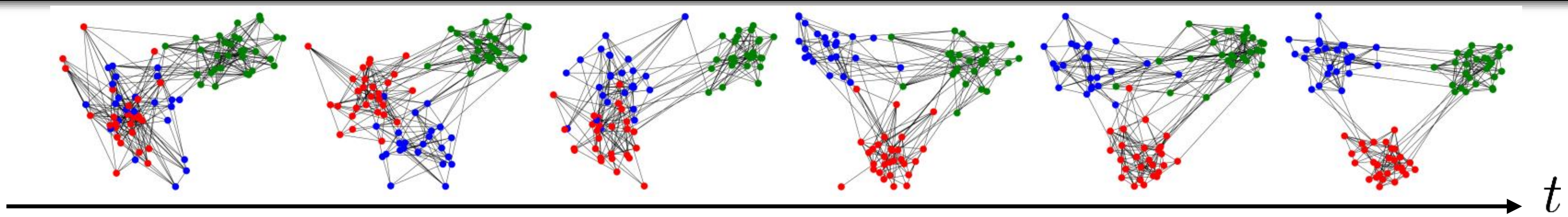

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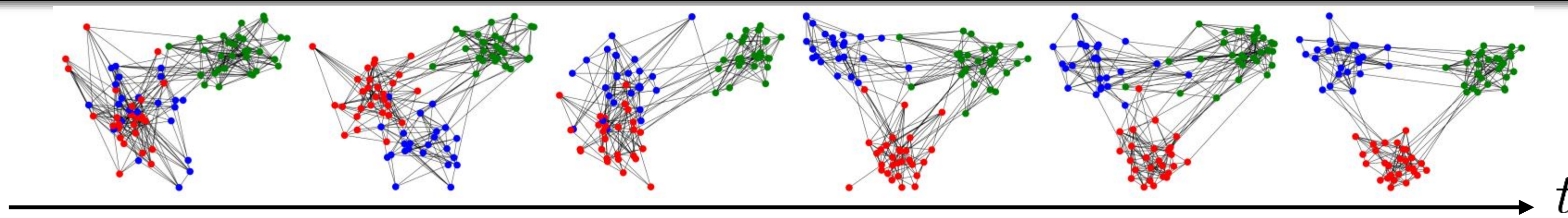

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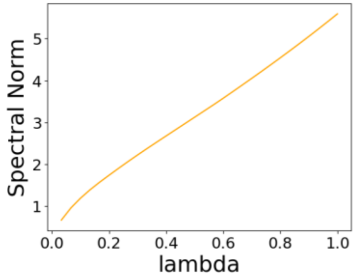

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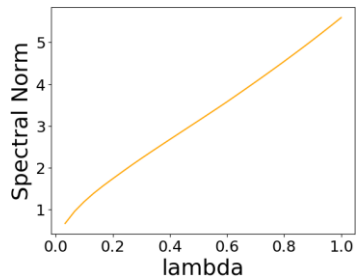

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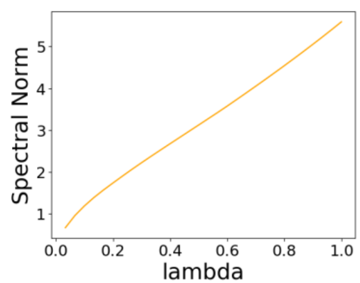

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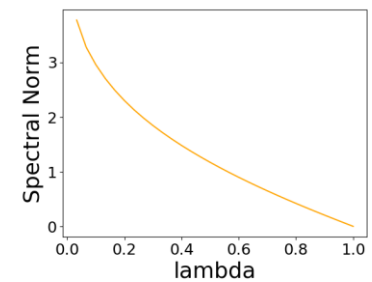

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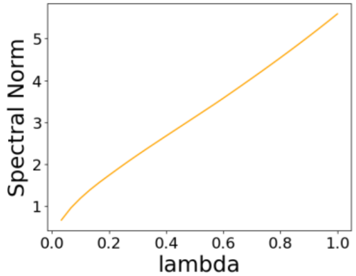

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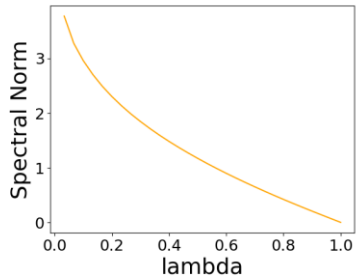
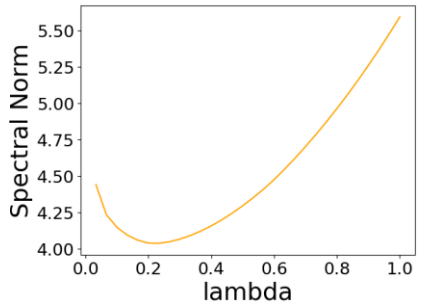


$$\boxed{\lambda^\star = \arg\min(\delta_1(\lambda) + \delta_2(\lambda)) = C_2 C_1^{-1}\sqrt{n\alpha_n\varepsilon}}$$



Sketch of proof (3)

Lei's concentration inequality for (sum of) Bernoulli matrices

$\mathcal{G}$

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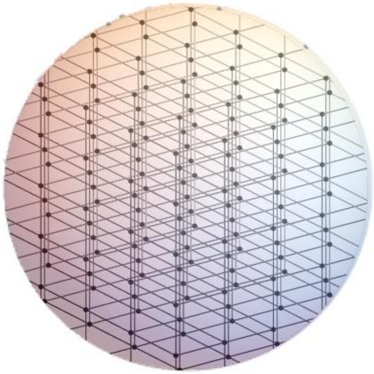

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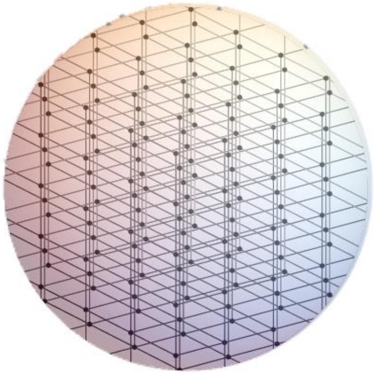

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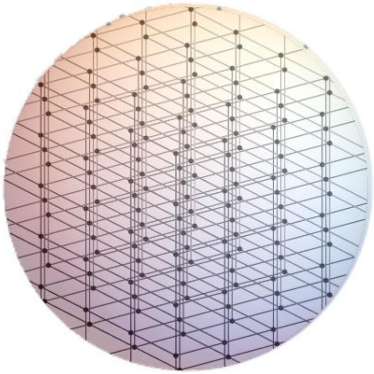

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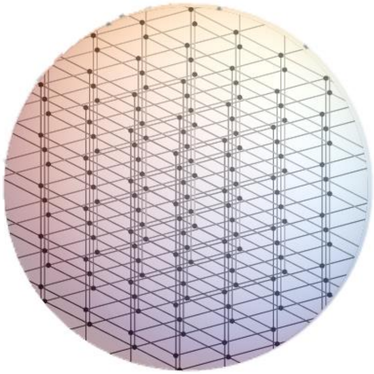

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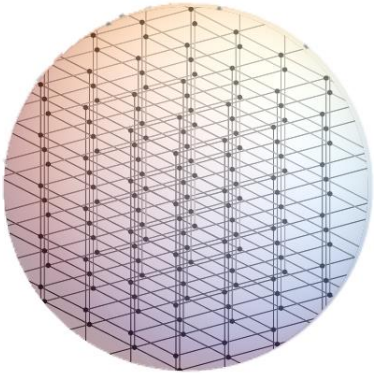

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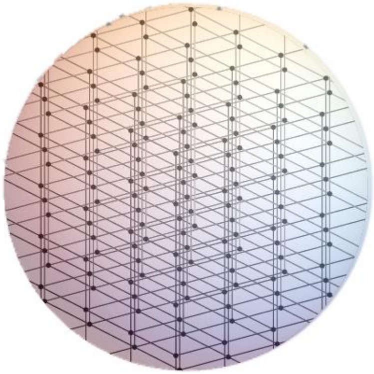

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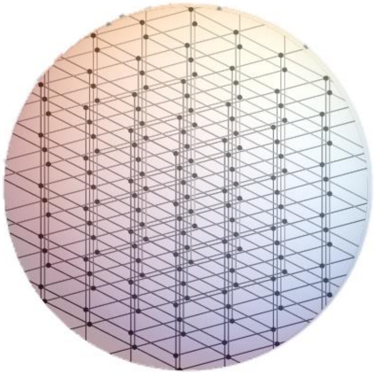

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- *Future work: other applications ?*

Outline

1. Main result
2. Choosing the forgetting factor
3. Experiments
4. Conclusion *(Bonus : GNN ?)*

Grid of forgetting factors

How to choose λ ?

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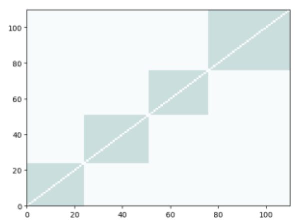

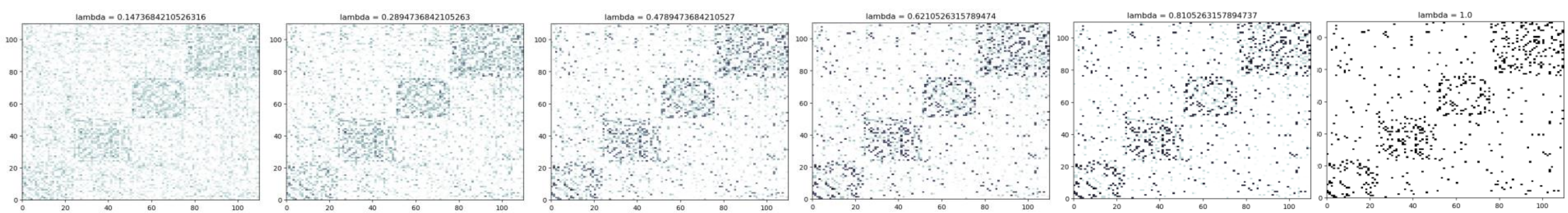

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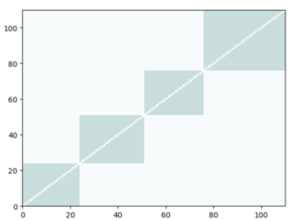
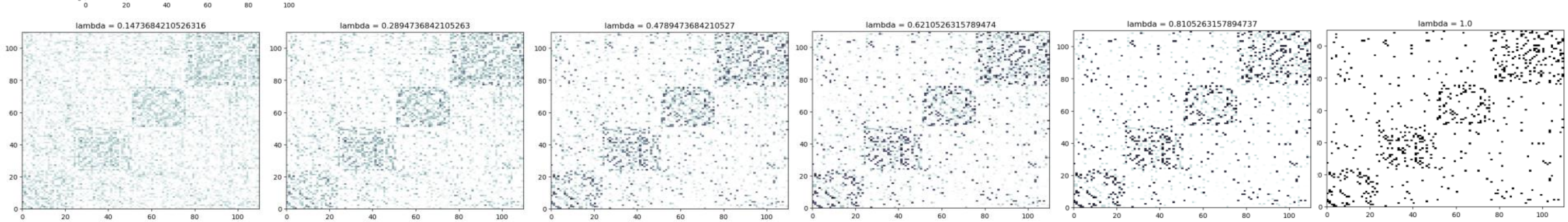


- Possible to maintain strong smoothing (small forgetting factors) without additional computational load
- Does not necessitate access to raw past data



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Lemma

Assume that $\sqrt{\lambda_i} - \sqrt{\lambda_{i-1}} \leq \gamma$ and α_n is known. Choose $\lambda_{\tilde{i}}$ such that

$$\lambda_{\tilde{i}} = \arg\min_{\lambda_i} \{\lambda_i : \forall i < j \leq N, \|\bar{A}_t(\lambda_i) - \bar{A}_t(\lambda_j)\| \leq 4\delta_1(\lambda_j)\}$$

Then with probability at least $1 - Nn^{-r}$,

$$\|\bar{A}_t(\lambda_{\tilde{i}}) - P_t\| \leq 6\delta^\star + 5\gamma\sqrt{n\alpha_n}$$

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$\mathcal{O}(\delta^\star)$ if $\gamma = \mathcal{O}((n\alpha_n\varepsilon)^{1/4})$

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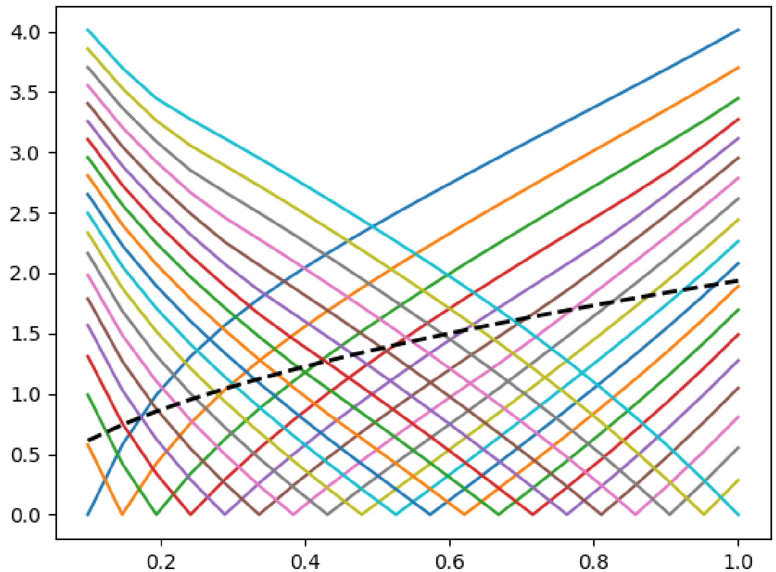

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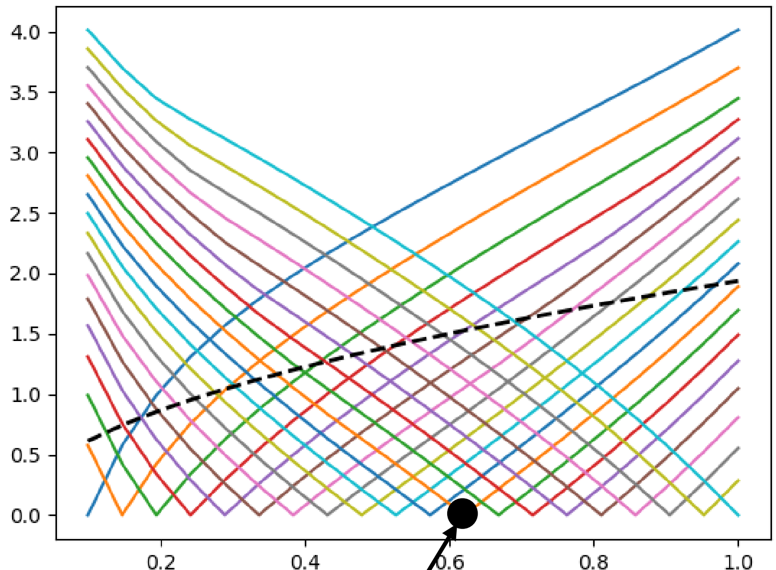

$\lambda_{\tilde{i}} \approx 0.6$

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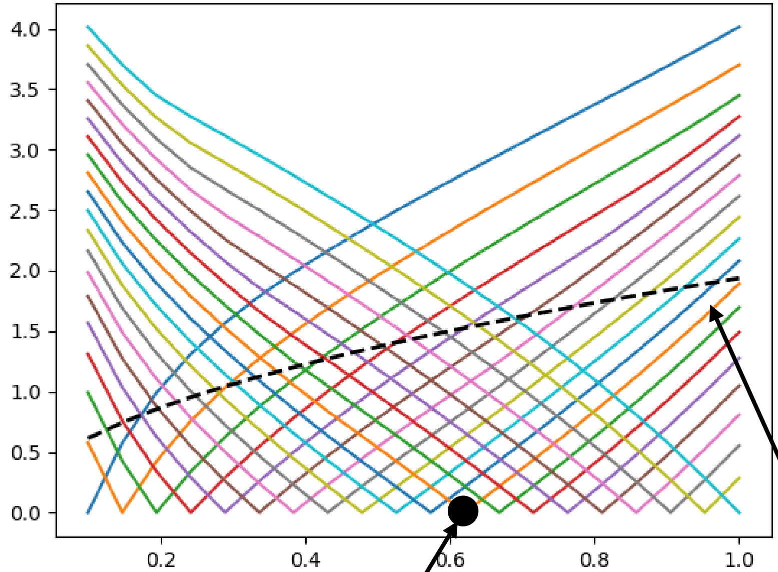

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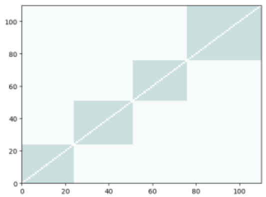
Problem :
The theoretical expression for $\delta_1(\lambda) = C_1\sqrt{n\alpha_n\lambda}$ is not tight ! Unusable in practice….

Here $C_1 = 0.5$ for illustrative purpose, in theory $C_1 \geq 289^2$! Many proof artifacts…

Method 2 : proxy for P

Method 2 : Proxy for P_t



Goal: minimize $\|\bar{A}_t(\lambda_i) - P_t\|$, but P_t unknown.

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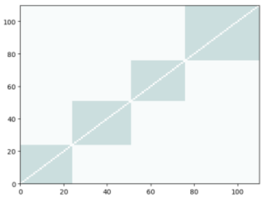

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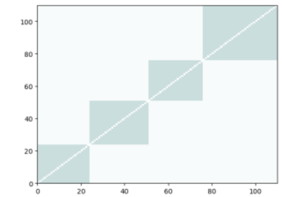

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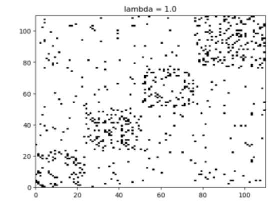

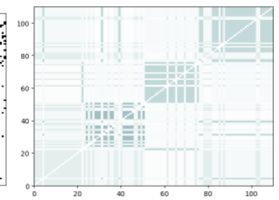

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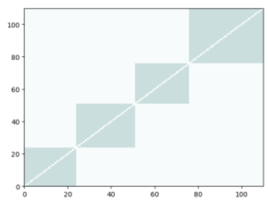

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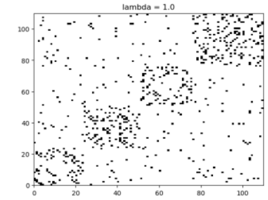

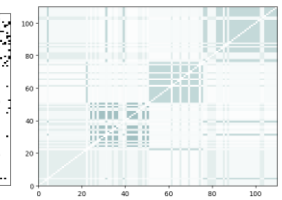

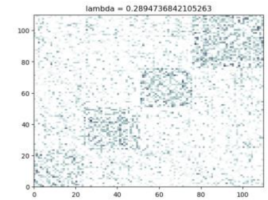

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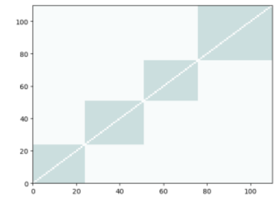

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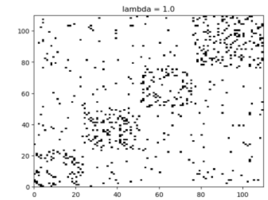

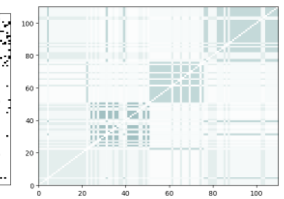

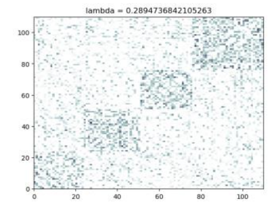

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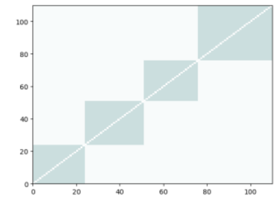

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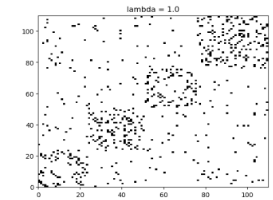

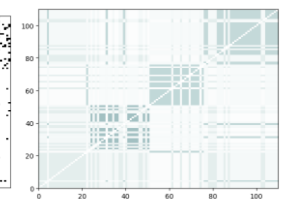

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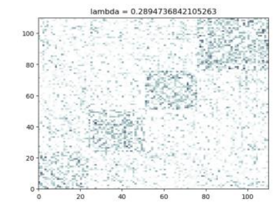
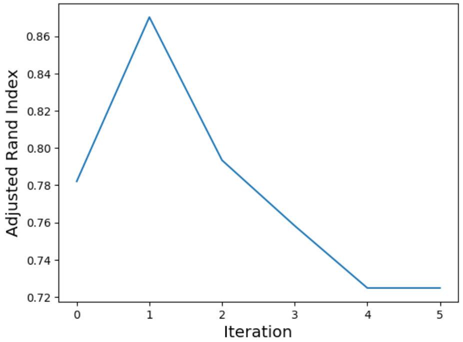


Usually diverge ! ☹



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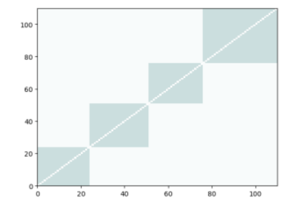
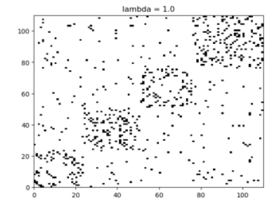
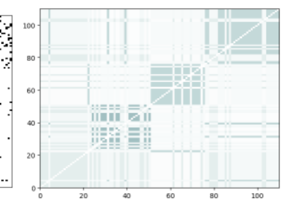
Method 2 : Proxy for P_t



Goal: minimize $\|\bar{A}_t(\lambda_i) - P_t\|$, but P_t unknown.

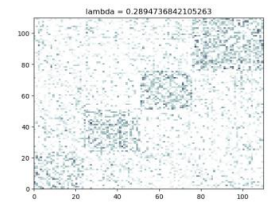
Idea: Replace it with a proxy.





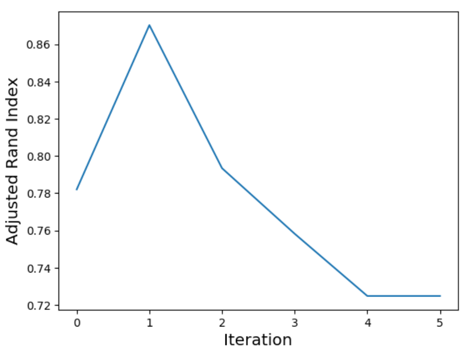
- Estimate $\hat{P}_t$ from A_t
  - ***(Spectral Clustering + maximum likelihood)***

- Minimize $\|\bar{A}_t(\lambda_i) - \hat{P}_t\|$

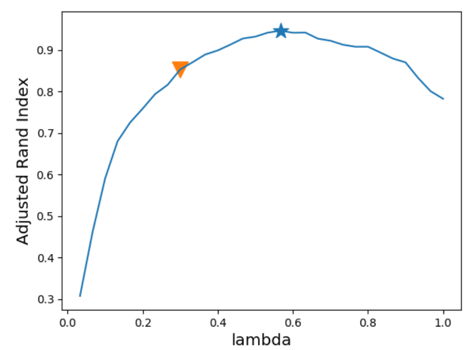


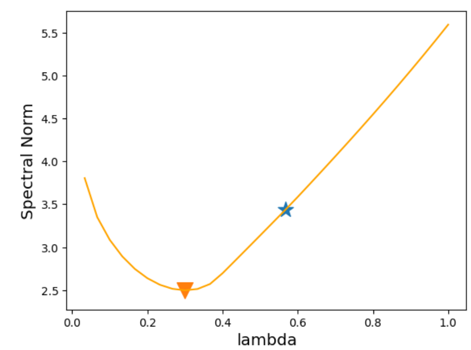
- Repeat with the new $\bar{A}_t(\lambda_i)$ and iterate ?

Usually diverge ! ☹



Explanation ? The spectral norm may not be the best criterion !





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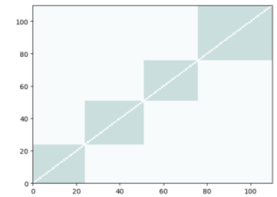

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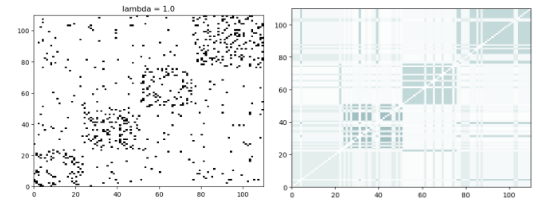

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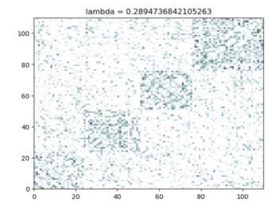

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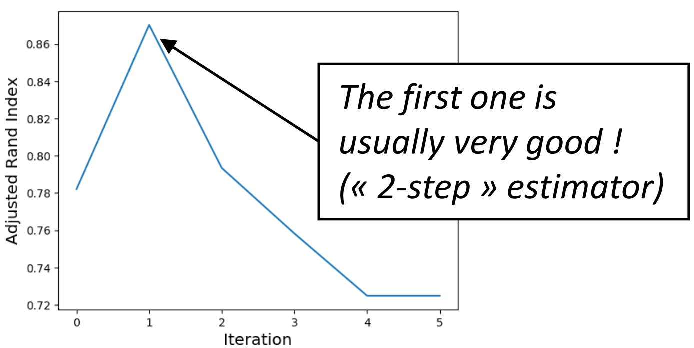

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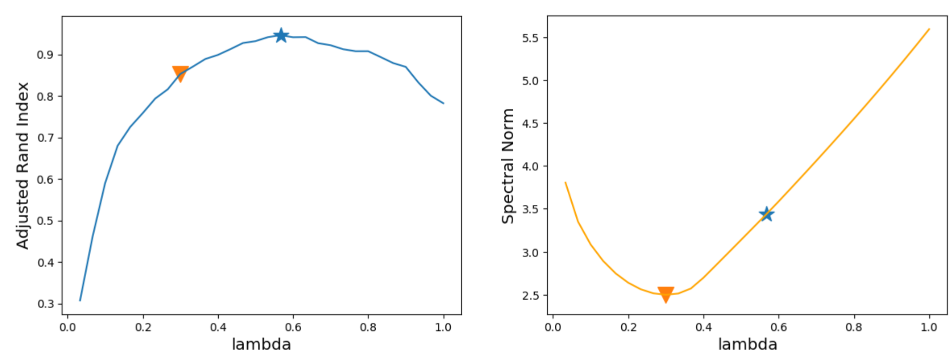
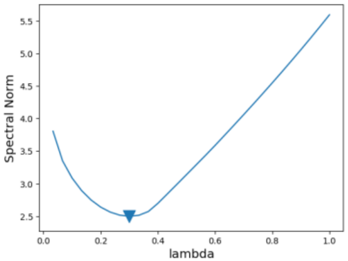


Method 3 : finite differences (in progress…)

Method 3 : Derivative and finite differences



Observation : the function $f(\lambda_i) = \|\bar{A}_t(\lambda_i) - P_t\|$ that we are trying to minimize looks convex…

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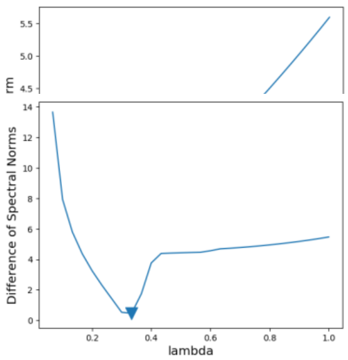

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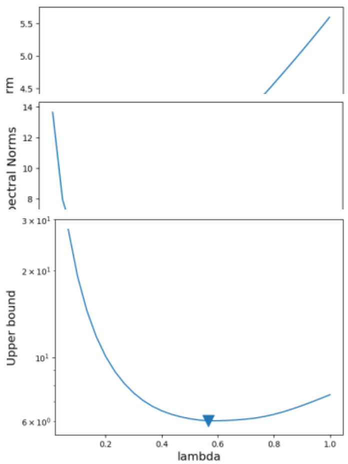

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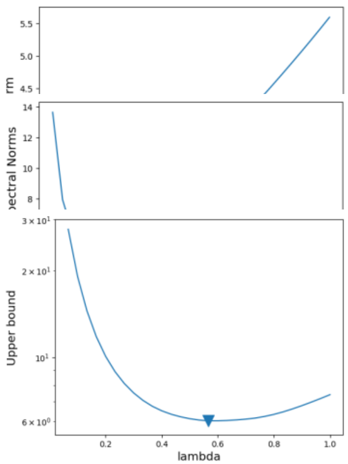

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Lemma

Assume that whp f is strongly convex and $0 < c \leq f'' \leq C$ on an interval $[\underline{\lambda}, \overline{\lambda}]$, and $\lambda^\star, \lambda_{\hat{i}} \in [\underline{\lambda}, \overline{\lambda}]$, $\lambda_i - \lambda_{i-1} = \gamma$
Then, whp, we have

$$\|\bar{A}_t(\lambda_{\hat{i}}) - P_t\| \leq 2\delta^\star + C\left(\gamma + \frac{3C\gamma + 4\delta^\star/\gamma}{c}\right)^2$$

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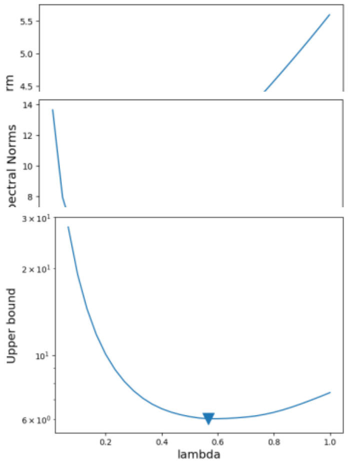

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Gives the right rate if : $\gamma = \mathcal{O}(\sqrt{\alpha_n n \varepsilon})$ $\quad c, C = \mathcal{O}((\alpha_n n)^{-1/4} \varepsilon^{-3/4})$

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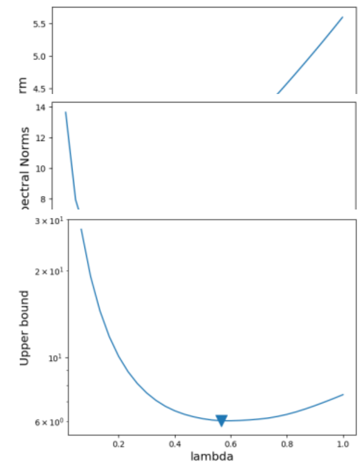

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Future work: actually proving the convexity ?

For now: the upper bound $\delta_1(\lambda) + \delta_2(\lambda)$ has **the right strong convexity** on $[a\lambda^\star, b\lambda^\star]$ …

Outline

1. Main result
2. Choosing the forgetting factor
3. Experiments
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Illustration on synthetic data

Quality of clustering $\longleftrightarrow$ $\|\bar{A}_t - P_t\| \leq \|\bar{A}_t - \bar{P}_t\| + \|\bar{P}_t - P_t\| \leq \delta_1(\lambda) + \delta_2(\lambda)$

$\lambda^\star = \mathcal{O}(\sqrt{n\alpha_n\varepsilon})$

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$\boxed{\lambda^\star = \mathcal{O}(\sqrt{n\alpha_n\varepsilon})}$

$n = 500,$

$k = 5,$

$\alpha = \mathcal{O}(\frac{\log(n)}{n}),$

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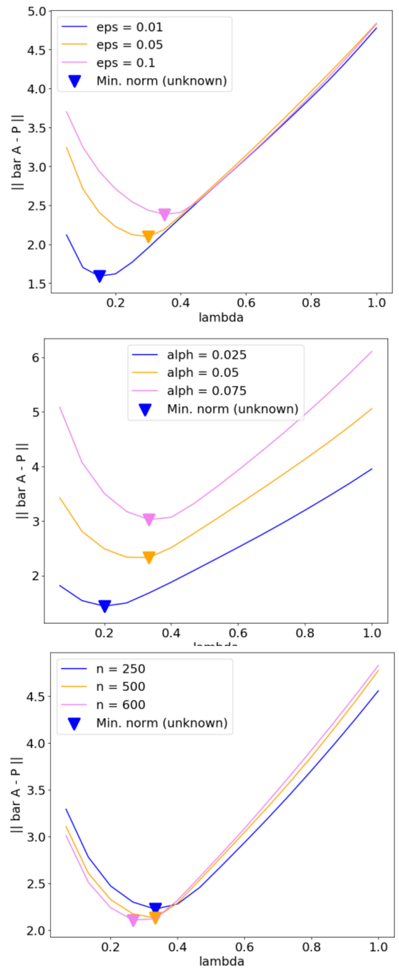

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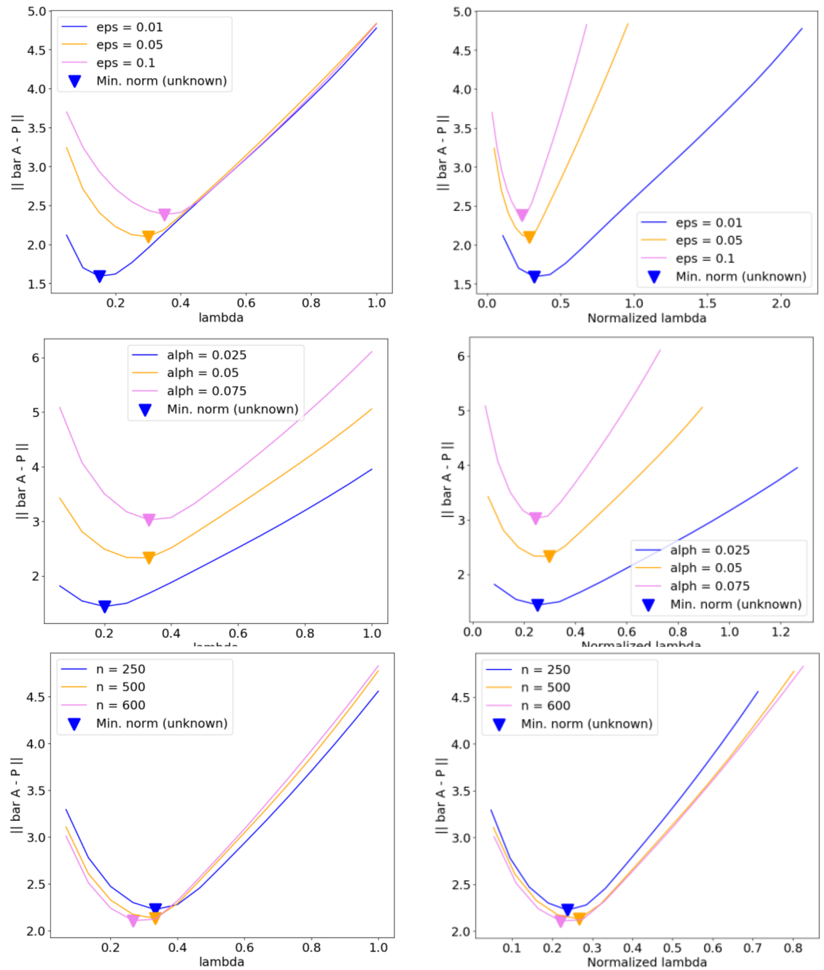

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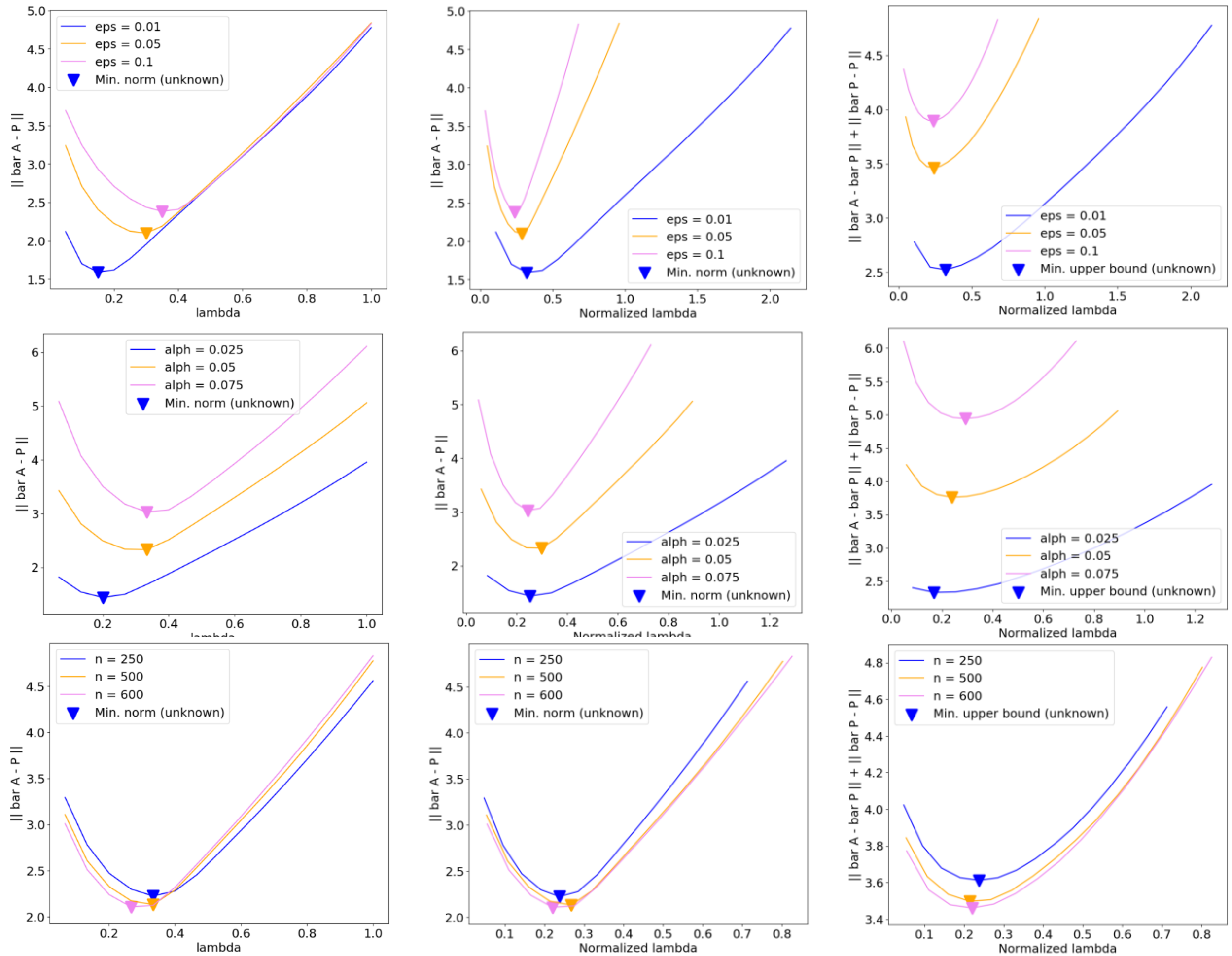

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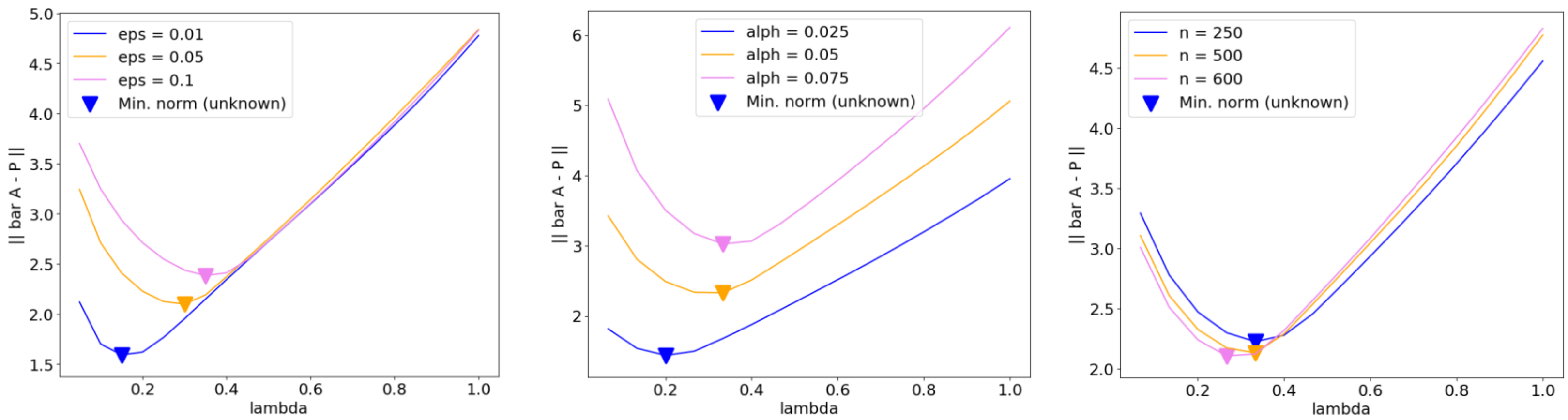

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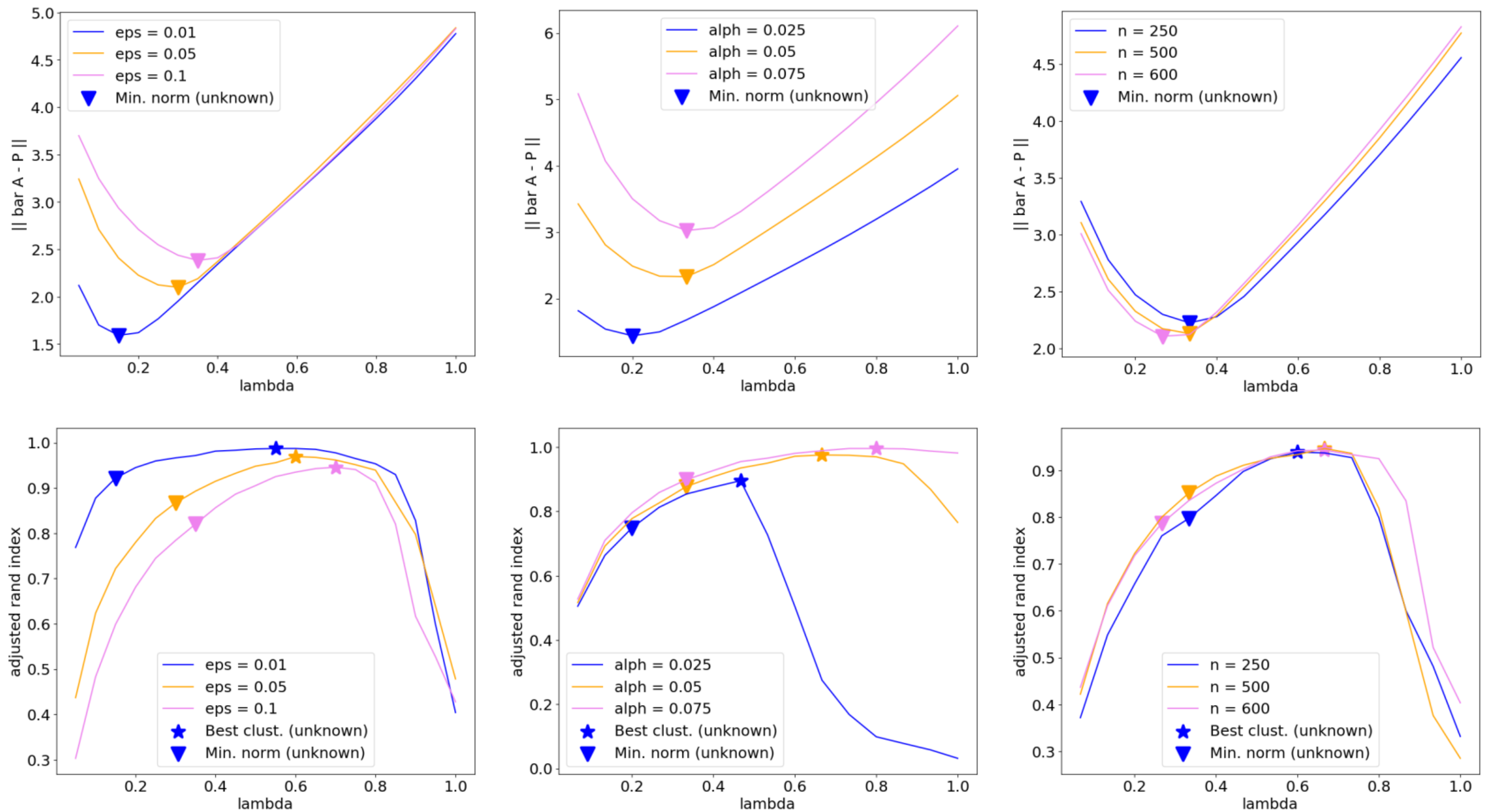
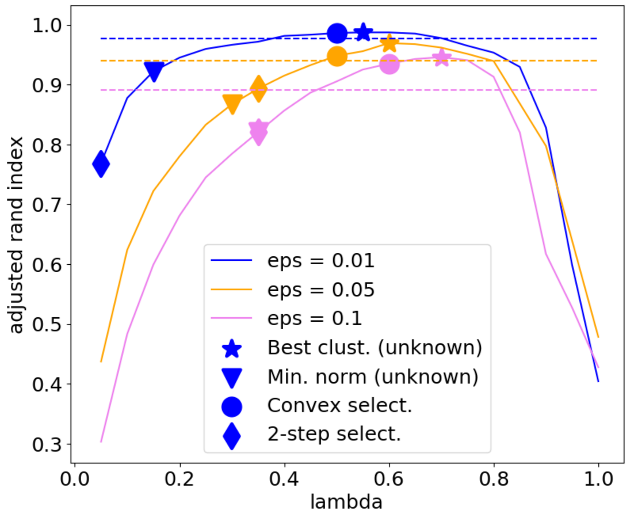
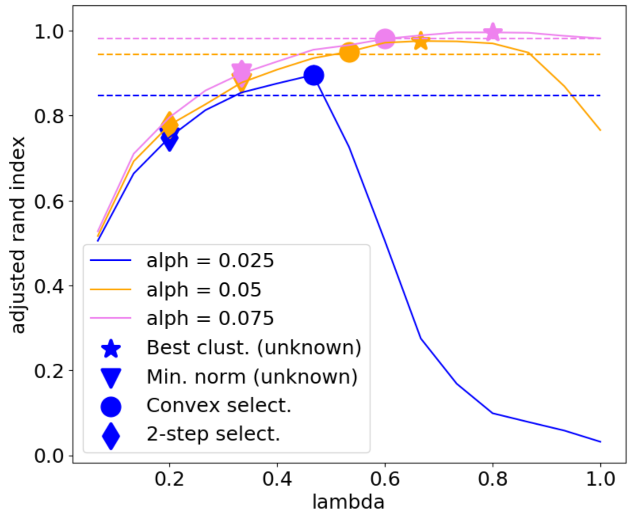
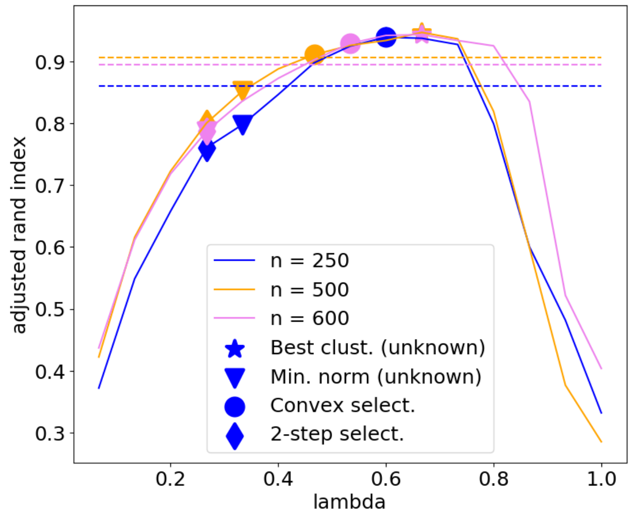


Illustration on synthetic data

Choice of forgetting factor, comparison with uniform average:







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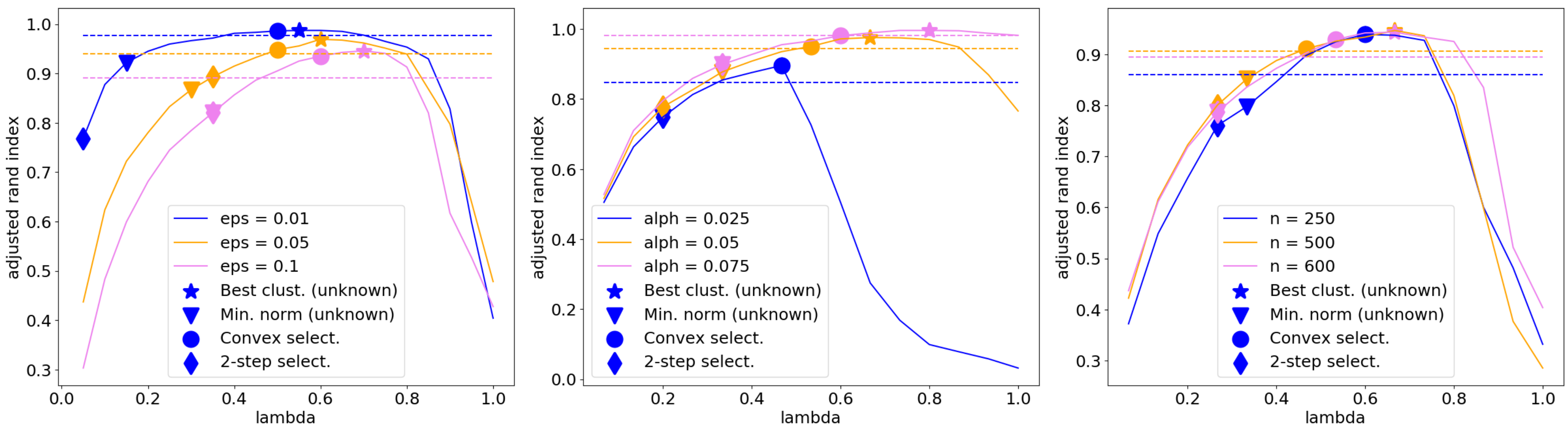

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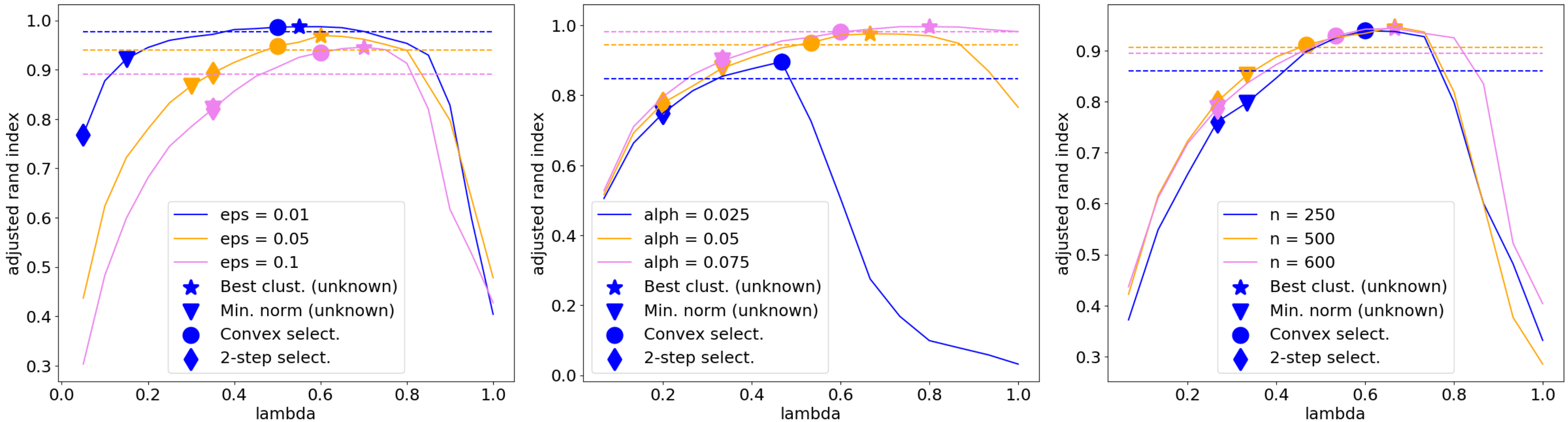

- Choice by « proxy » of P_t often does not work… (tends to privilege low λ)
- Choice by « finite differences » is even better than the (unknown) best uniform average

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Conclusion, outlooks

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- **Improved Non-asymptotic guarantees** for smoothed Spectral Clustering for Dynamic Stochastic Block Model
  - ***Non-asymptotic guarantees for the sparse case !!***

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- **Detectability threshold** *à la* statistical physic of the difficult model !!

Done $\begin{cases} \alpha = \mathcal{O}(1/n) \\ \varepsilon = \mathcal{O}(1/\log(n)^2) \end{cases}$

Todo: $\begin{cases} \alpha = \mathcal{O}(1/n) \\ \varepsilon = cte \end{cases}$

Bonus : Universal invariant and equivariant Graph Neural Networks

N. Keriven[1], Gabriel Peyré[1]

[1]Ecole Normale Supérieure, Paris

Universal Invariant and Equivariant GNN

Graph

$$W \in \mathbb{R}^{n \times n}, P \star W := P^\top W P$$

Universal Invariant and Equivariant GNN

Graph	**Higher-order** tensor
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Characterized by [Maron et al 2018]: basis does not depend on n !!

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$\mathbb{R}^{n^k} \to \mathbb{R}$ $\quad$ $\mathbb{R}^{n^k} \to \mathbb{R}^n$

Linear equivariant
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Equivariant bias
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Characterized by [Maron et al 2018]: basis does not depend on n !!

Thm: GNNs are **universal approximators** of invariant (resp. equivariant) continuous functions.

Universal Invariant and Equivariant GNN

Graph

$W \in \mathbb{R}^{n \times n}, P \star W := P^\top W P$

Higher-order tensor

$W \in \mathbb{R}^{n^k}, P \star W := \dots$

Invariant functions (graph -> scalar)

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- Case **invariant** already known *[Maron 2019]*, high k is necessary !

Thank you !

Preprints are coming soon !

data-ens.github.io

Enter the data challenges!
Come to the colloquium!
Come to the Laplace seminars!