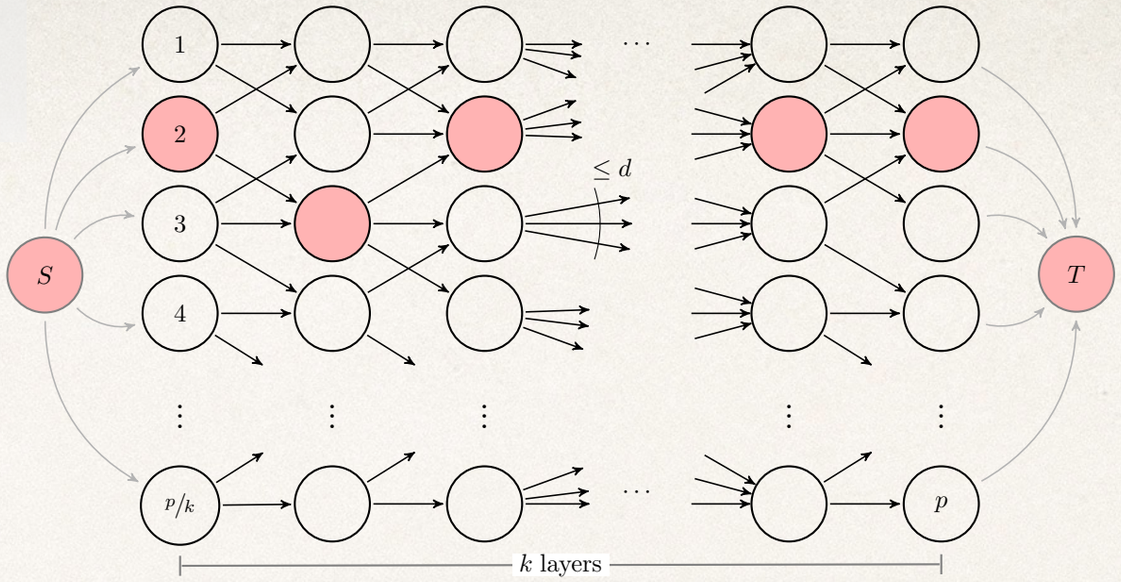
THE UNIVERSITY OF TEXAS AT AUSTIN



Stay on path: PCA along graph paths

Megasthenis Asteris
Anastasios Kyrillidis
Alexandros Dimakis

Department of Electrical and Computer Engineering

Han-Gyol Yi
Bharath Chandrasekaran

Department of Communication Sciences and Disorders

07/07/2015 - ICML

Supported by …

Setup and notation

Data:

$$\mathbf{Y} \in \mathbb{R}^{p \times n}$$

- p : number of variables.
- n : number of samples.
- In most cases, we work in the *high-dimensional regime* $n \ll p$.

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$$\hat{\mathbf{\Sigma}} = \frac{1}{n} \cdot \mathbf{Y}\mathbf{Y}^\top$$

$$\hat{\mathbf{\Sigma}} \in \mathbb{R}^{p \times p}$$

- We look for away to find: (Dis)similarities among variables, patterns of variation.

PCA and Sparse PCA (in concept)

Principal component analysis (PCA) [Jolliffe2002]

- Seeks for low-dimensional subspaces that explain well data variance.
- Classical dimensionality reduction tool.
- Numerically cheap for small- and moderate-sized problems via SVD.

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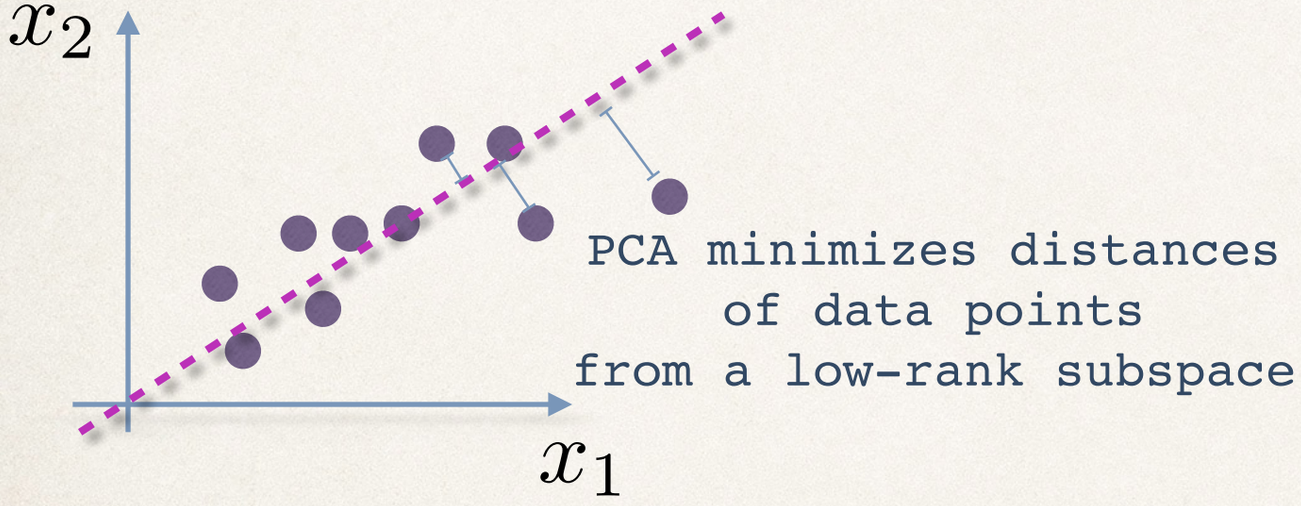

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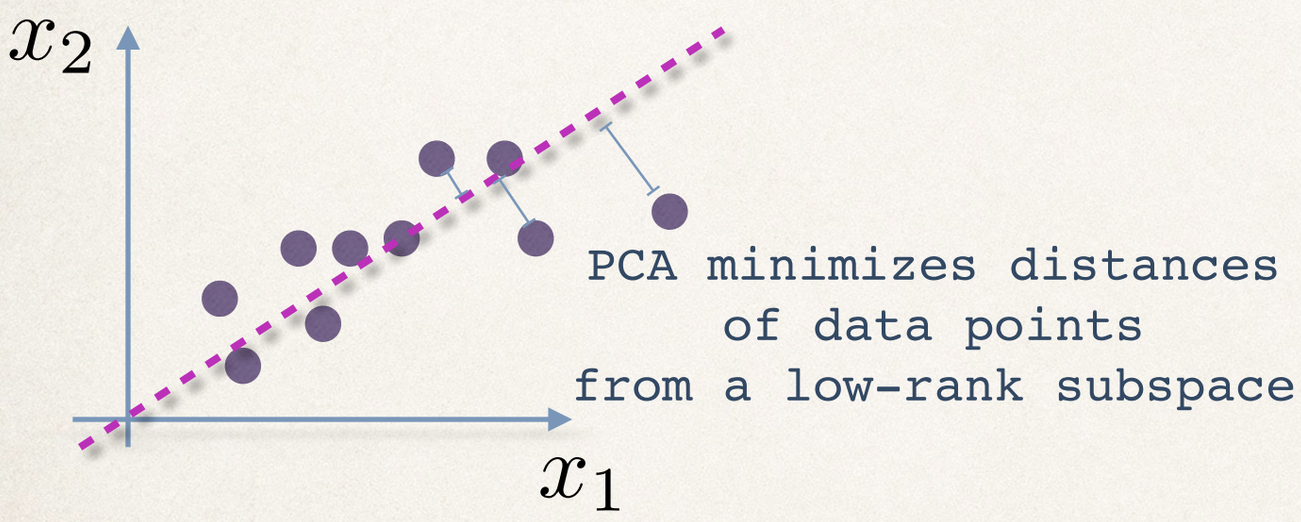

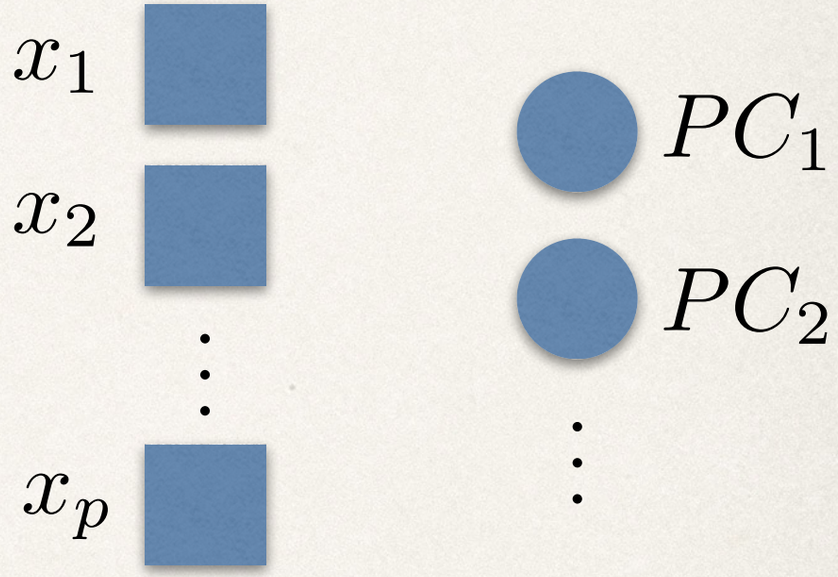

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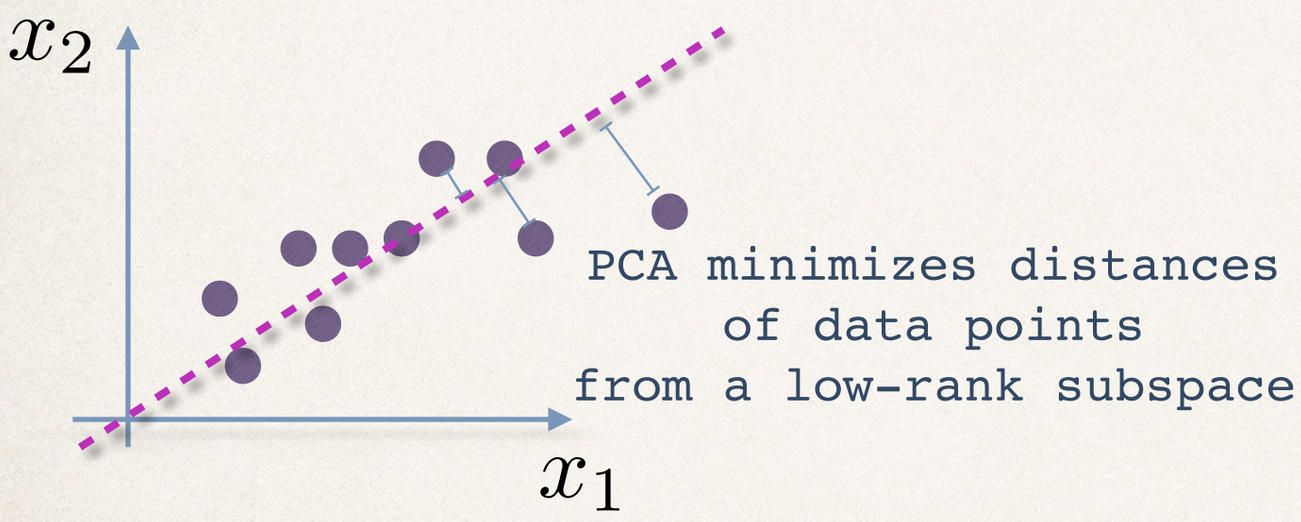

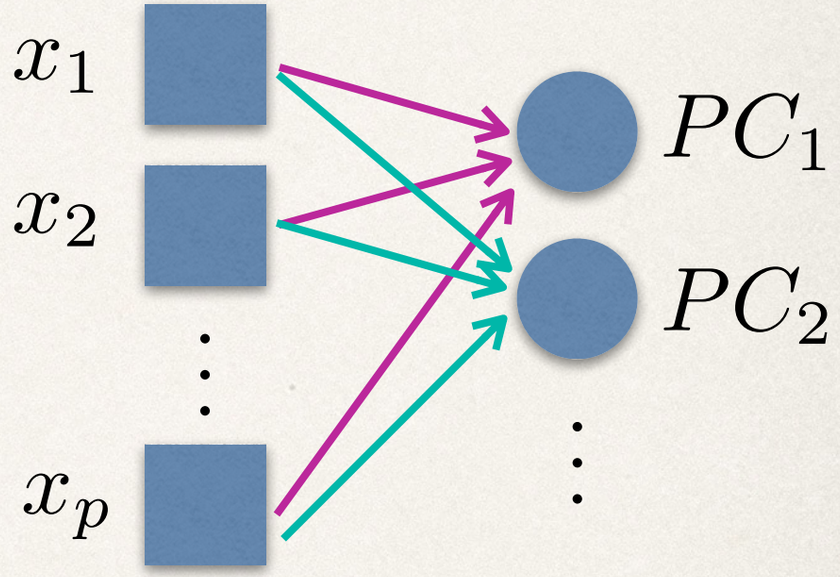

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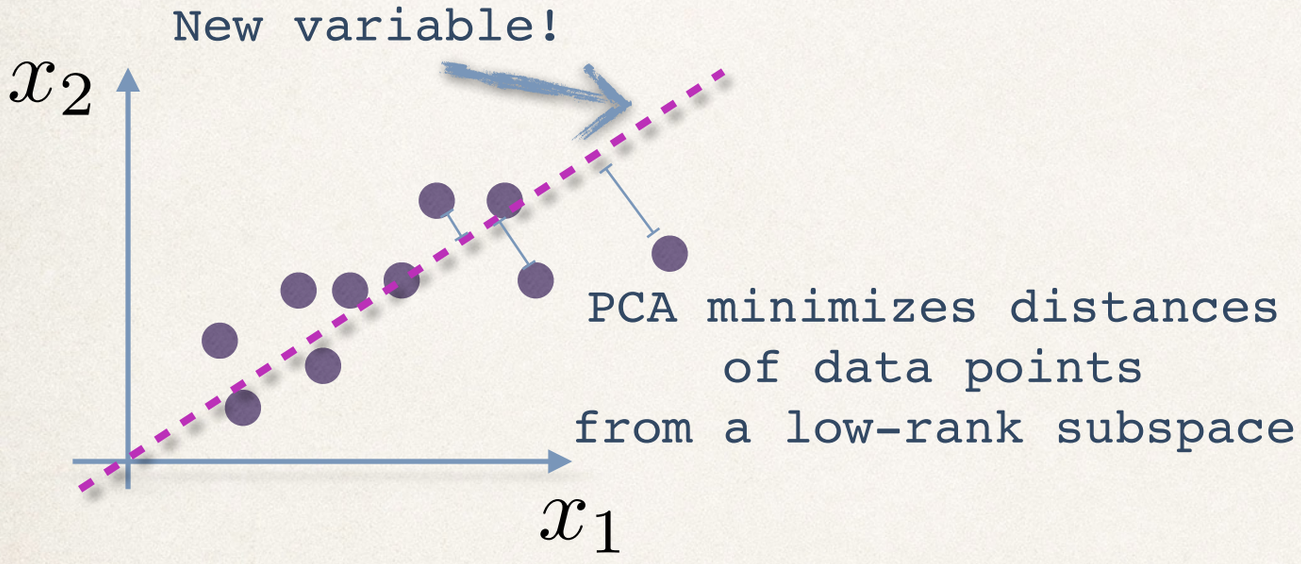

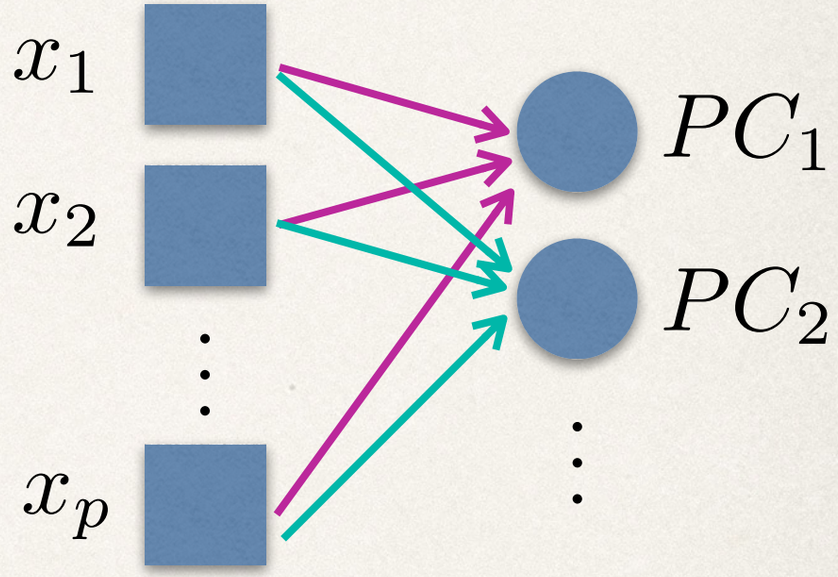

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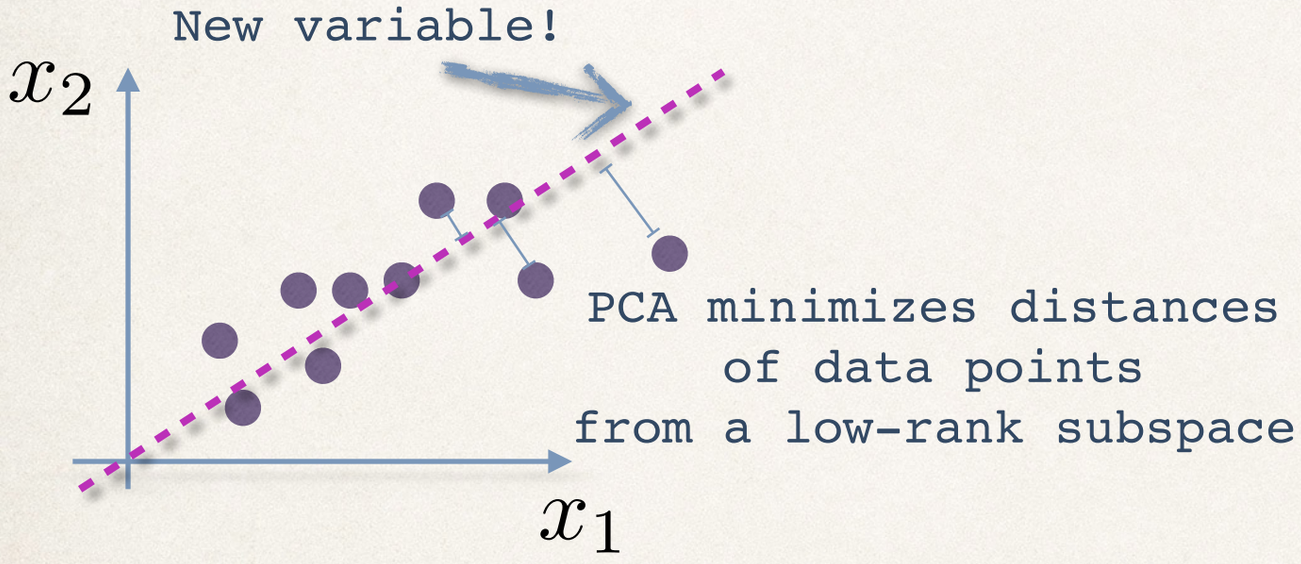

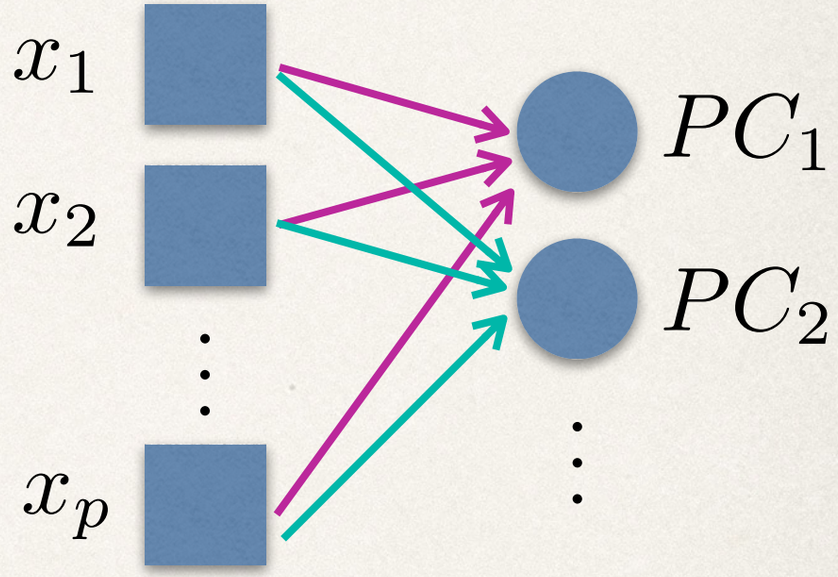

Sparse PCA [Johnstone & Lu, 2004]

- Seeks subspaces that depend only on a few variables **(sparsity)**
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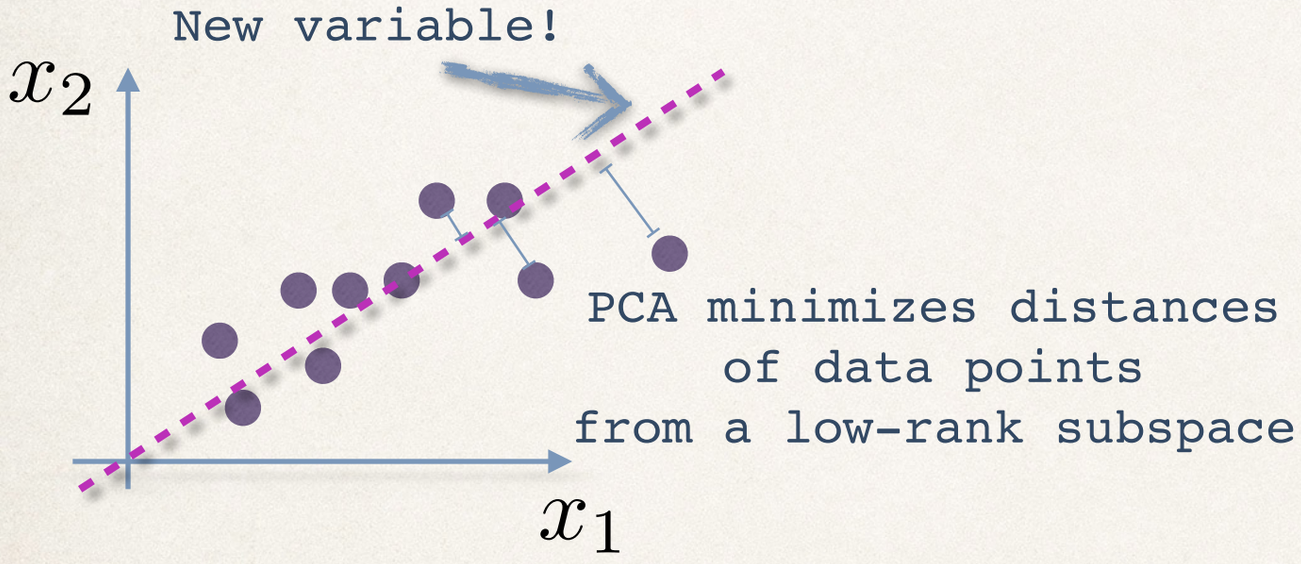

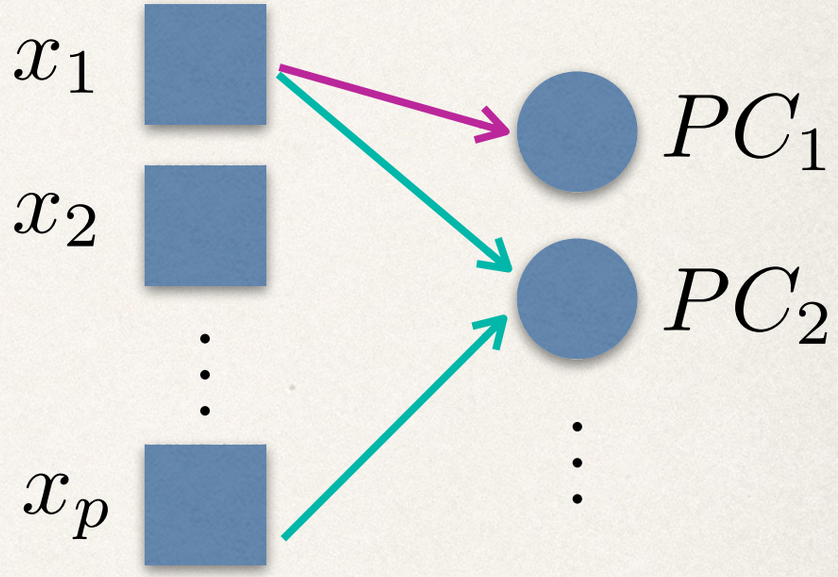

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- Given empirical covariance matrix $\hat{\mathbf{\Sigma}} = \frac{1}{n} \cdot \mathbf{Y}\mathbf{Y}^\top$, we solve:

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Maximize data variance explained by the principal factor.

to get the first principal factor.

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Sparse PCA [Johnstone & Lu, 2004; d'Aspremont et al., 2007]

- We further restrict the cardinality of principal factor as:

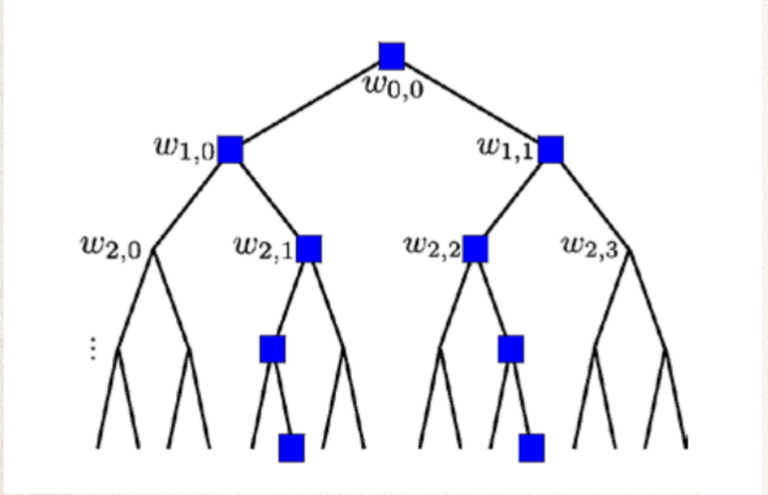
$$\begin{aligned} \underset{\mathbf{x} \in \mathbb{R}^p}{\text{maximize}} \quad & \mathbf{x}^\top \hat{\mathbf{\Sigma}} \mathbf{x} \\ \text{subject to} \quad & \|\mathbf{x}\|_2 = 1, \\ & \|\mathbf{x}\|_0 = k. \end{aligned}$$

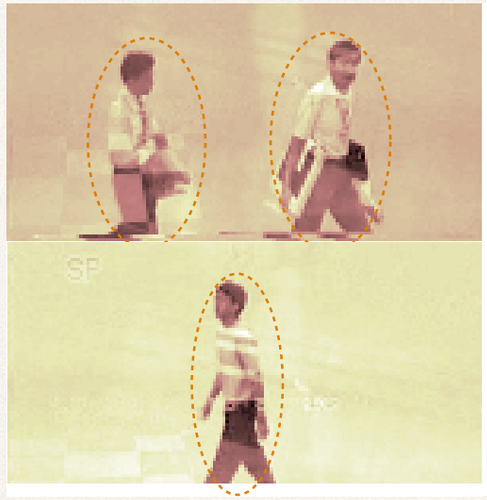
Beyond plain sparsity (to be updated)

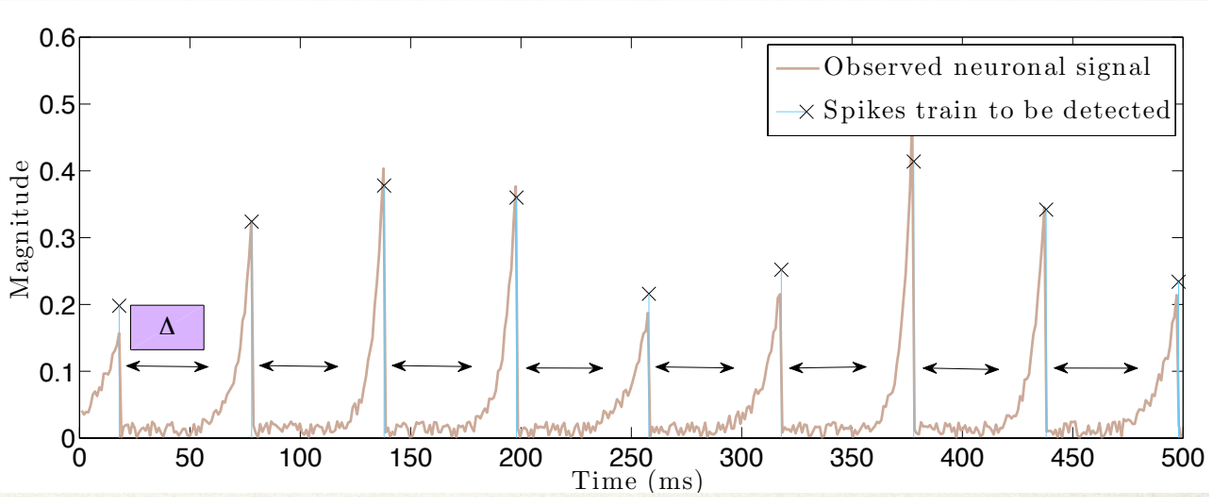
- In many cases, sparsity does not fully grasp the underlying structure

  e.g., Image processing (wavelets coeff. over trees, block sparsity),

  Neuronal signal processing, etc.
  [Baraniuk et al., 2008; Friedman et al., 2010, …]







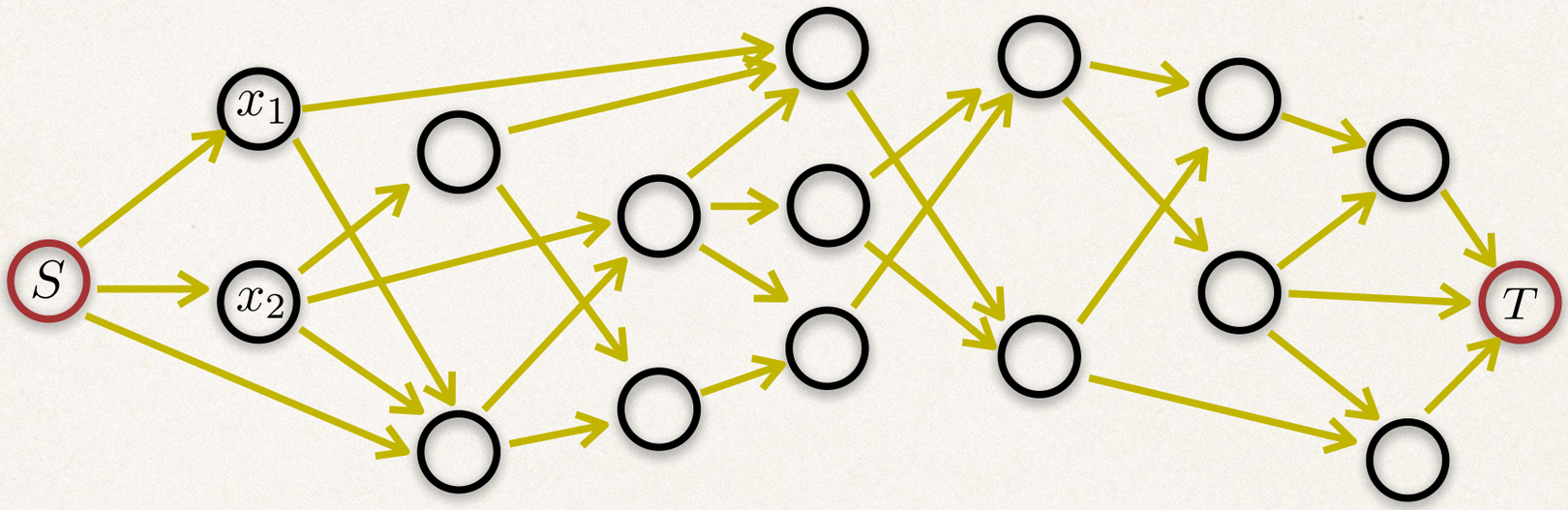
- Even within (sparse) PCA regime:

  Structured sparse PCA [Jenatton et al., 2010]

PCA on graph paths

PCA on graph paths

- Consider a *directed acyclic graph (DAG)* $G = (V, E)$ over variables.



$\mathcal{P}(G)$: collection of all $S - T$ paths.

- PCA on graph paths solves:

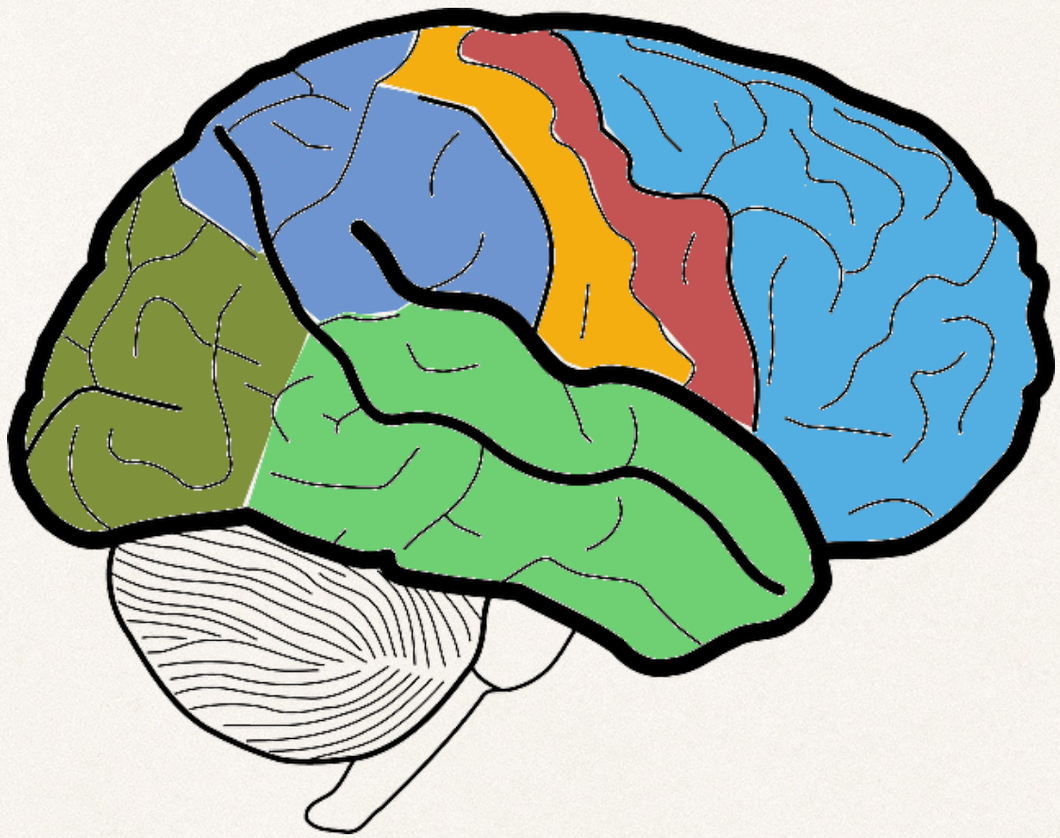
$$\begin{aligned} \underset{\mathbf{x} \in \mathbb{R}^p}{\text{maximize}} \quad & \mathbf{x}^\top \widehat{\mathbf{\Sigma}} \mathbf{x} \\ \text{subject to} \quad & \mathbf{x} \in \mathcal{X}(G). \end{aligned}$$

where:

$$\mathcal{X}(G) = \{\mathbf{x} \in \mathbb{R}^p \ : \ \|\mathbf{x}\|_2 = 1, \text{supp}(\mathbf{x}) \in \mathcal{P}(G)\}$$

Motivation (through an example)
(why?)

Find meaningful “streams” on brain



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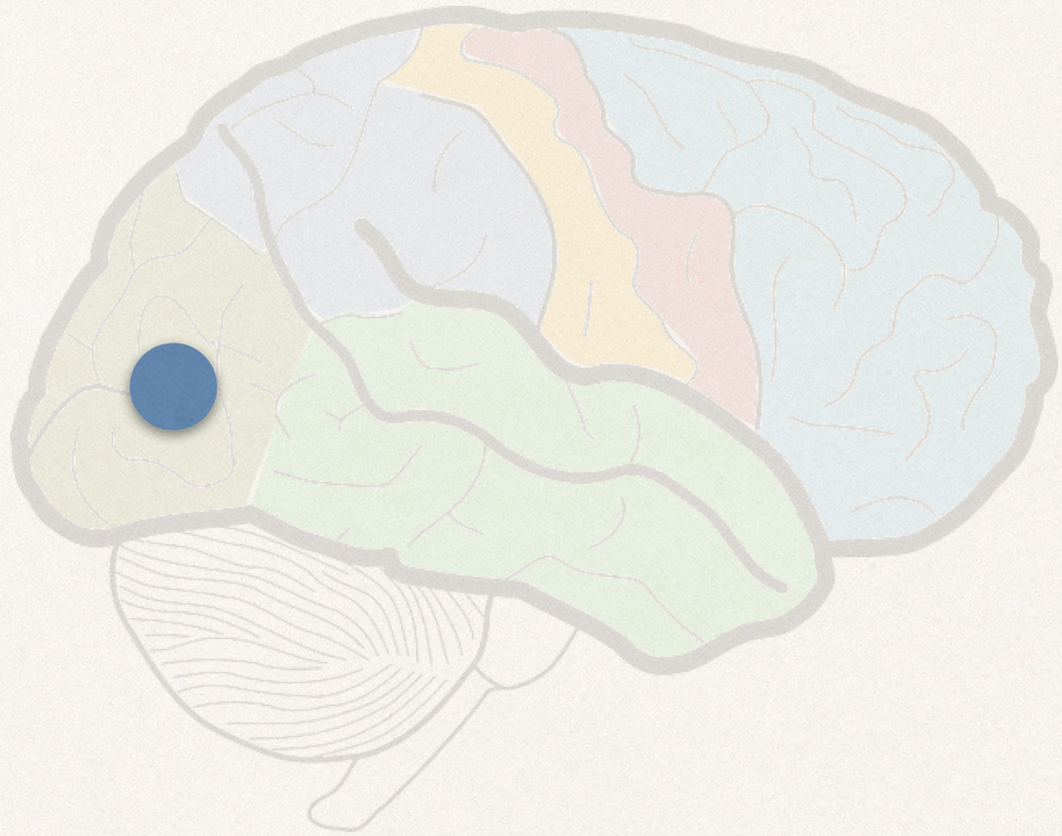

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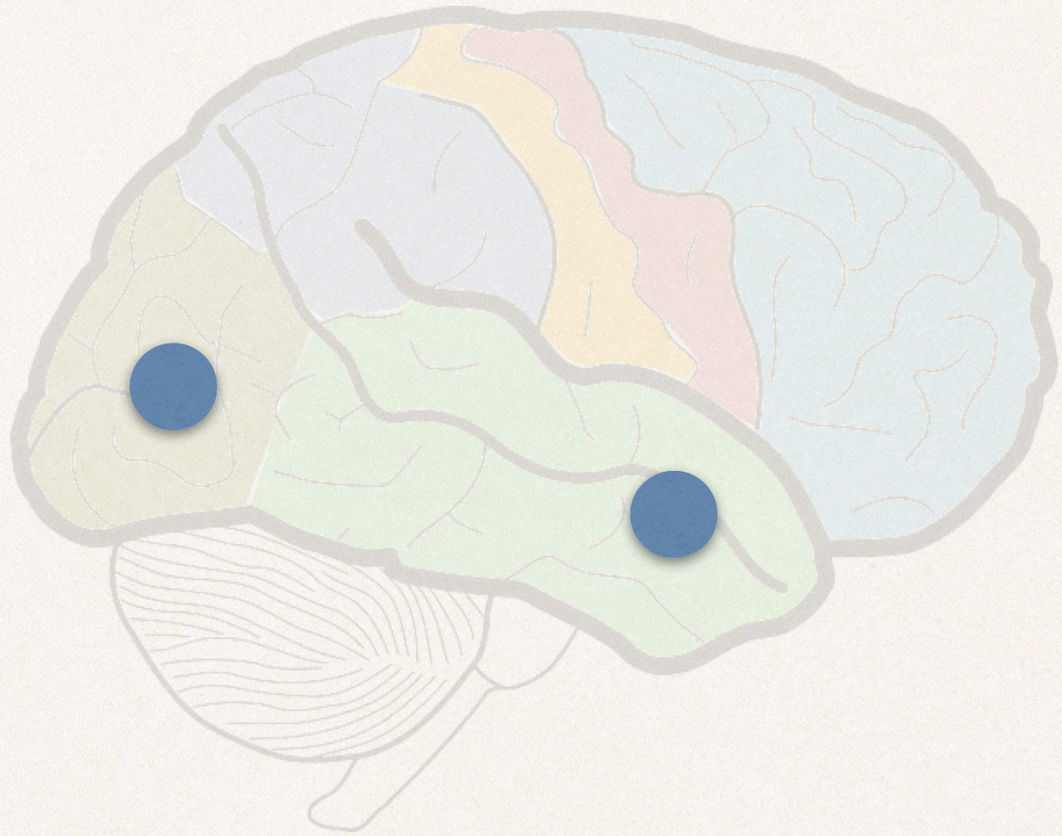

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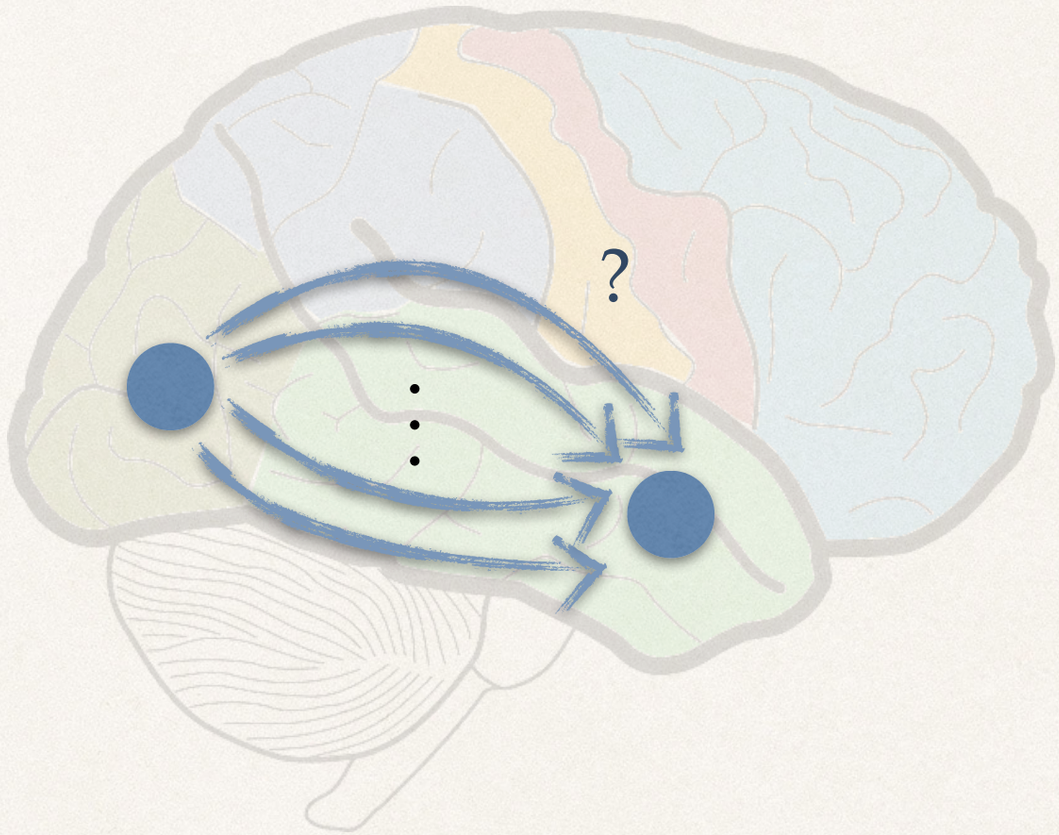

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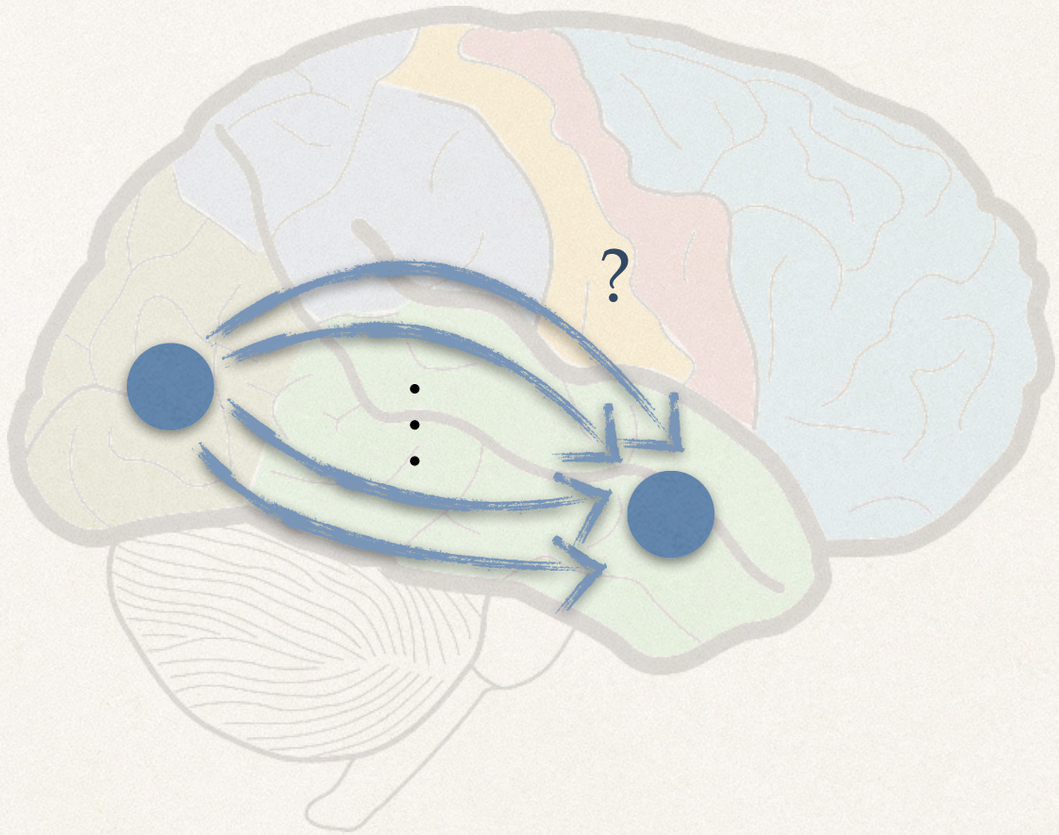
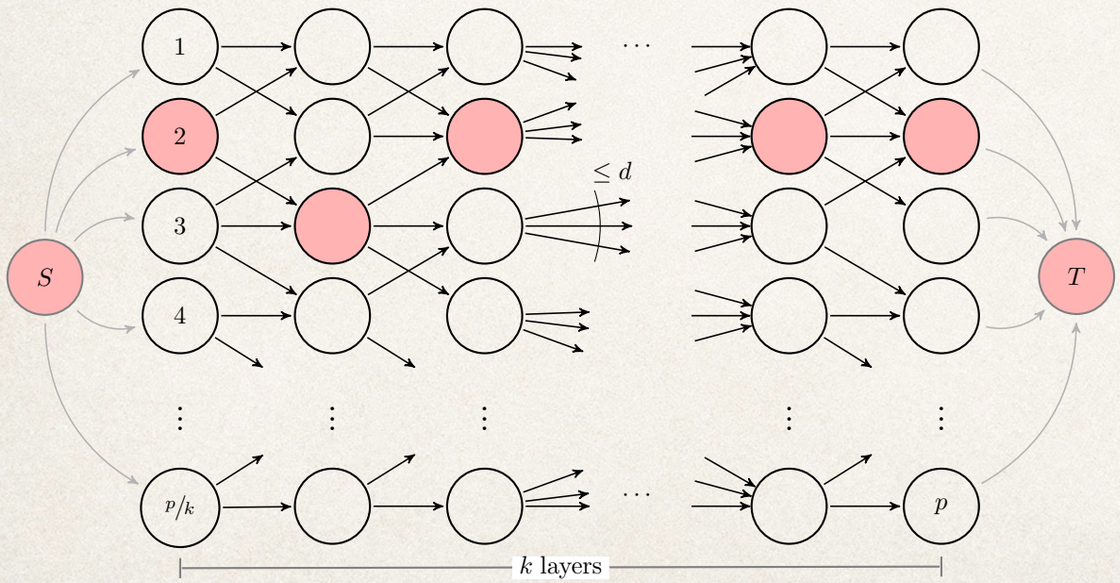
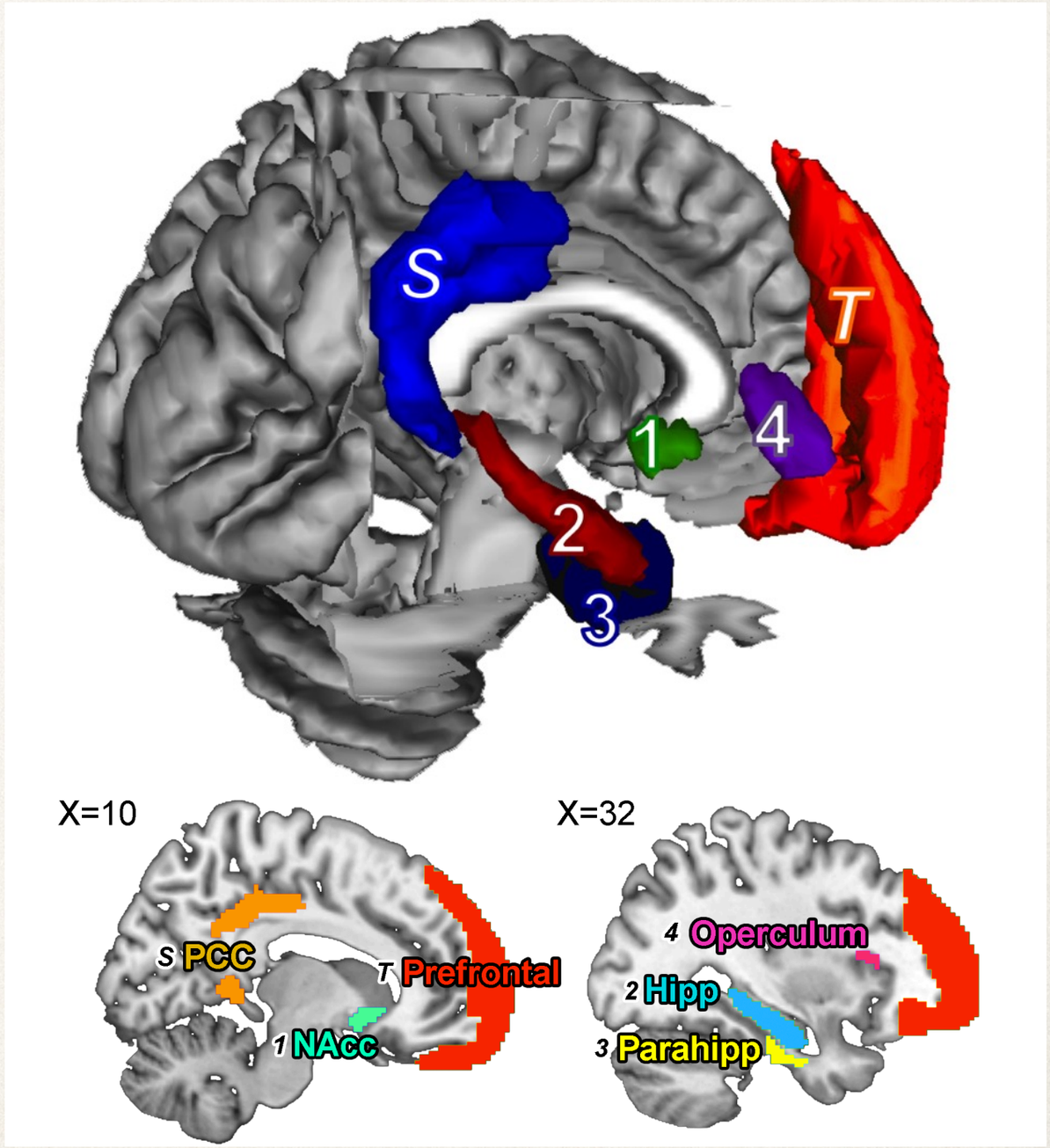


e.g., two stream hypothesis

Brain fMRI networks (preliminary results)

- Resting state fMRI dataset.*
- 111 regions of interest (ROIs) (variables), extracted based on Harvard-Oxford Atlas [Desikan et al., 2006].
- Graph extracted based on Euclidean distances between center of mass of ROIs.

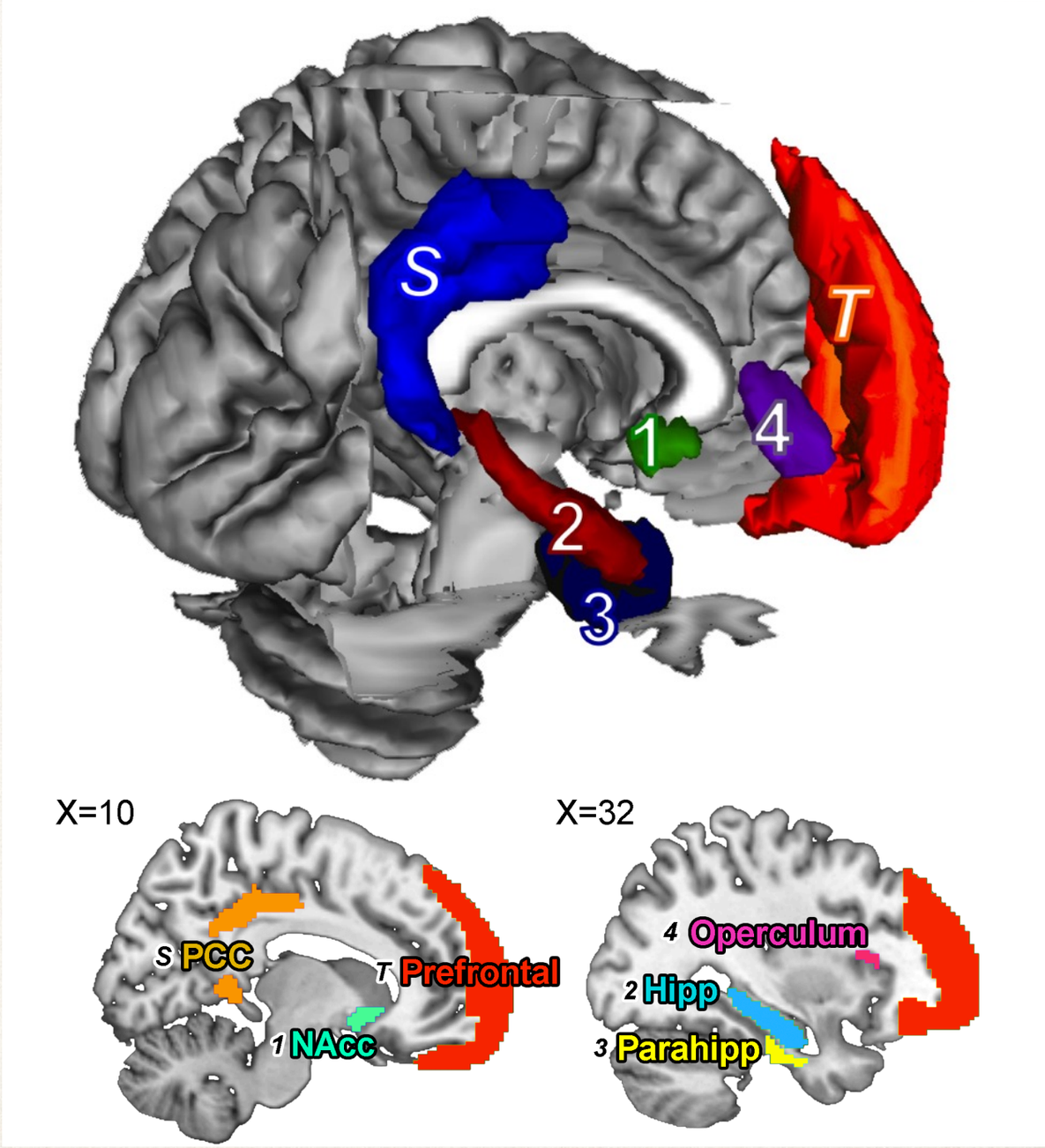




**Human Connectome Project, WU-Minn Consortium.*

Brain fMRI networks (preliminary results)

- Setup: 6 layers (sparsity)
- Starting node S:
  Posterior cingulate cortex
- Ending node T:
  Prefrontal cortex
- Path:
  1. Nucleus accumbens
  2. Hippocampus
  3. Parahippocampal gyrus
  4. Frontal operculum
- **All of them core neural components of the memory network.**



Αλγόριθμοι - Algorithms

(how?)

Graph-truncated power method

Algorithm 1 Graph-Truncated Power Method

input $\widehat{\mathbf{\Sigma}} \in \mathbb{R}^{p \times p},\ G = (V, E),\ \mathbf{x}_0 \in \mathbb{R}^p$

1: $i \leftarrow 0$
2: **repeat**
3: $\quad \mathbf{w}_i \leftarrow \widehat{\mathbf{\Sigma}} \mathbf{x}_i$
4: $\quad \mathbf{x}_{i+1} \leftarrow \mathrm{Proj}_{\mathcal{X}(G)}(\mathbf{w}_i)$
5: $\quad i \leftarrow i + 1$
6: **until** Convergence/Stop Criterion

output $\mathbf{x}_i$

- Similar to truncated power method of [Yuan & Zhang, 2013].

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- Main difference with previous work: projection operation

$$\mathrm{Proj}_{\mathcal{X}(G)}(\mathbf{w}) \in \arg \min_{\mathbf{x} \in \mathcal{X}(G)} \frac{1}{2} \|\mathbf{x} - \mathbf{w}\|_2^2$$

(defined later)

Low dim. sample and project

Algorithm 2 Low-Dimensional Sample and Project

input $\widehat{\mathbf{\Sigma}} \in \mathbb{R}^{p \times p}$, $G = (V, E)$, $r \in [p]$, $\epsilon > 0$

$[\mathbf{Q}, \mathbf{\Lambda}] \leftarrow \texttt{svd}(\widehat{\mathbf{\Sigma}}, r)$

$\mathbf{V} \leftarrow \mathbf{Q}\mathbf{\Lambda}^{1/2}$ $\quad \{\widehat{\mathbf{\Sigma}}_r \triangleq \mathbf{V}\mathbf{V}^\top\}$

$\mathcal{C} \leftarrow \emptyset$ $\quad \{\text{Candidate solutions}\}$

for $i = 1 : O(\epsilon^{-r} \cdot \log p)$ **do**

  $\mathbf{c}_i \leftarrow$ uniformly sampled from $\mathbb{S}^{r-1}$

  $\mathbf{w}_i \leftarrow \mathbf{V}\mathbf{c}_i$

  $\mathbf{x}_i \leftarrow \text{Proj}_{\mathcal{X}(G)}(\mathbf{w}_i)$

  $\mathcal{C} = \mathcal{C} \cup \{\mathbf{x}_i\}$

end for

output $\widehat{\mathbf{x}}_r \leftarrow \arg\max_{\mathbf{x} \in \mathcal{C}} \|\mathbf{V}^\top \mathbf{x}\|_2^2$

- Based on Spannogram algorithm by [Asteris et al, 2014].

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Projection operator

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$$\mathbf{w}^\top \mathbf{x} = \sum_{i\in\pi} w_i x_i \leq \sum_{i\in\pi} w_i^2 = \widehat{\mathbf{w}}^\top \mathbf{1}_\pi$$

where: $\pi \in \mathcal{P}(G)$, $\widehat{w}_i = w_i^2, \forall i \in [p]$ and, $\mathbf{1}_\pi \in \{0,1\}^p$ denotes the characteristic of π. For fixed π, equality is achieved for:

$$\mathbf{x}_\pi = \mathbf{w}_\pi / \|\mathbf{w}_\pi\|_2 \qquad \text{and} \qquad \mathbf{x}_{\pi^c} = 0$$

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- "Equivalent" problem: $\pi(\mathbf{w}) \in \arg\max_{\pi\in\mathcal{P}(G)} \widehat{\mathbf{w}}^\top \mathbf{1}_\pi$

i.e., **solving the longest (weighted) path problem.**

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- By Cauchy-Schwarz:

$$\mathbf{w}^\top \mathbf{x} = \sum_{i\in\pi} w_i x_i \leq \sum_{i\in\pi} w_i^2 = \widehat{\mathbf{w}}^\top \mathbf{1}_\pi$$

where: $\pi \in \mathcal{P}(G)$, $\widehat{w}_i = w_i^2, \forall i \in [p]$ and, $\mathbf{1}_\pi \in \{0,1\}^p$ denotes the characteristic of π. For fixed π, equality is achieved for:

$$\mathbf{x}_\pi = \mathbf{w}_\pi / \|\mathbf{w}_\pi\|_2 \qquad \text{and} \qquad \mathbf{x}_{\pi^c} = 0$$

- "Equivalent" problem: $\pi(\mathbf{w}) \in \arg\max_{\pi\in\mathcal{P}(G)} \widehat{\mathbf{w}}^\top \mathbf{1}_\pi$

i.e., **solving the longest (weighted) path problem.**

- For DAGs, this problem can be solved in $O(p+|E|)$ time, *i.e.*, linear in the size of the graph.

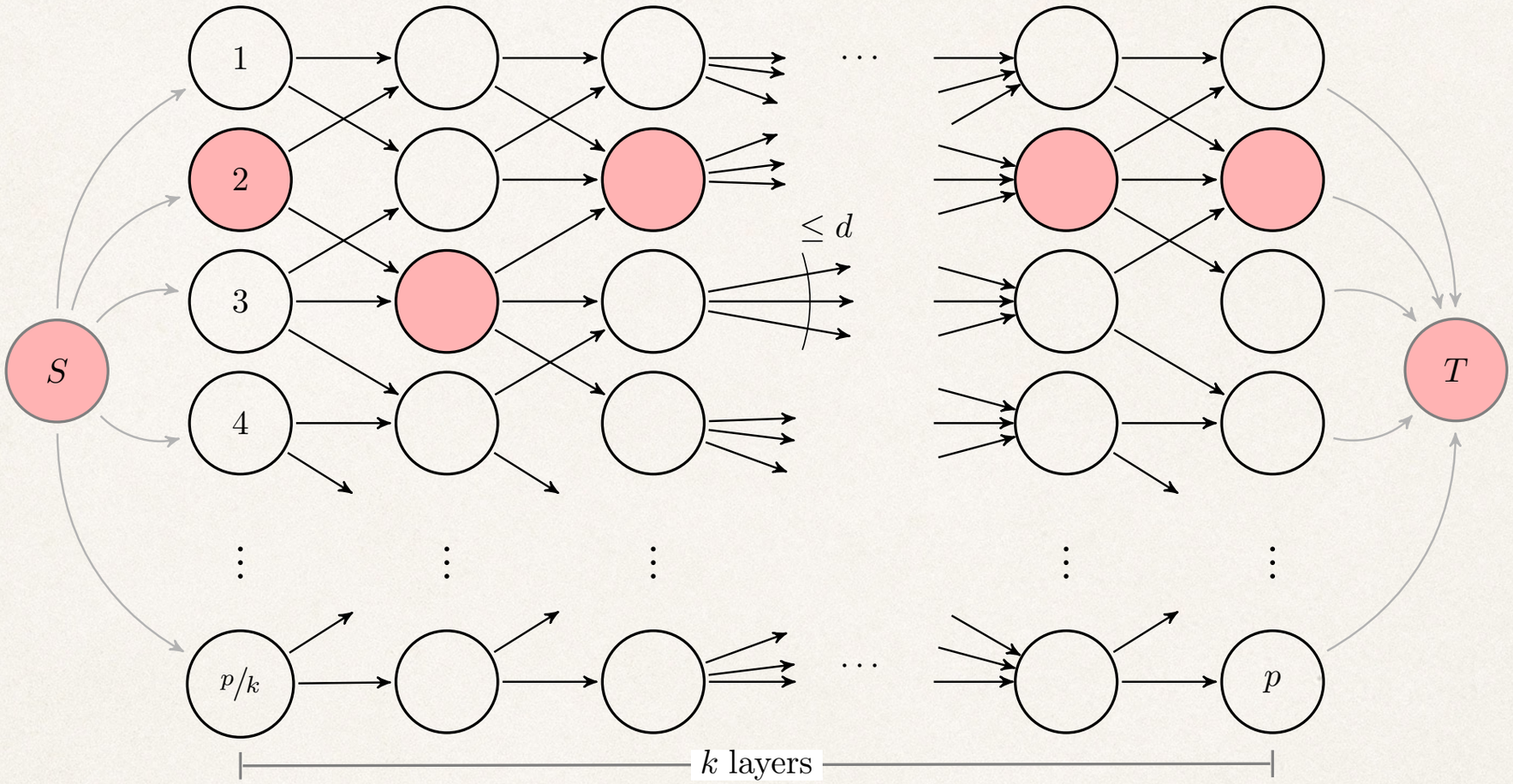
Θεωρία - Theory

(why it works?)

Data model and assumptions

- The layer graph:

$\mathcal{X}(G)$



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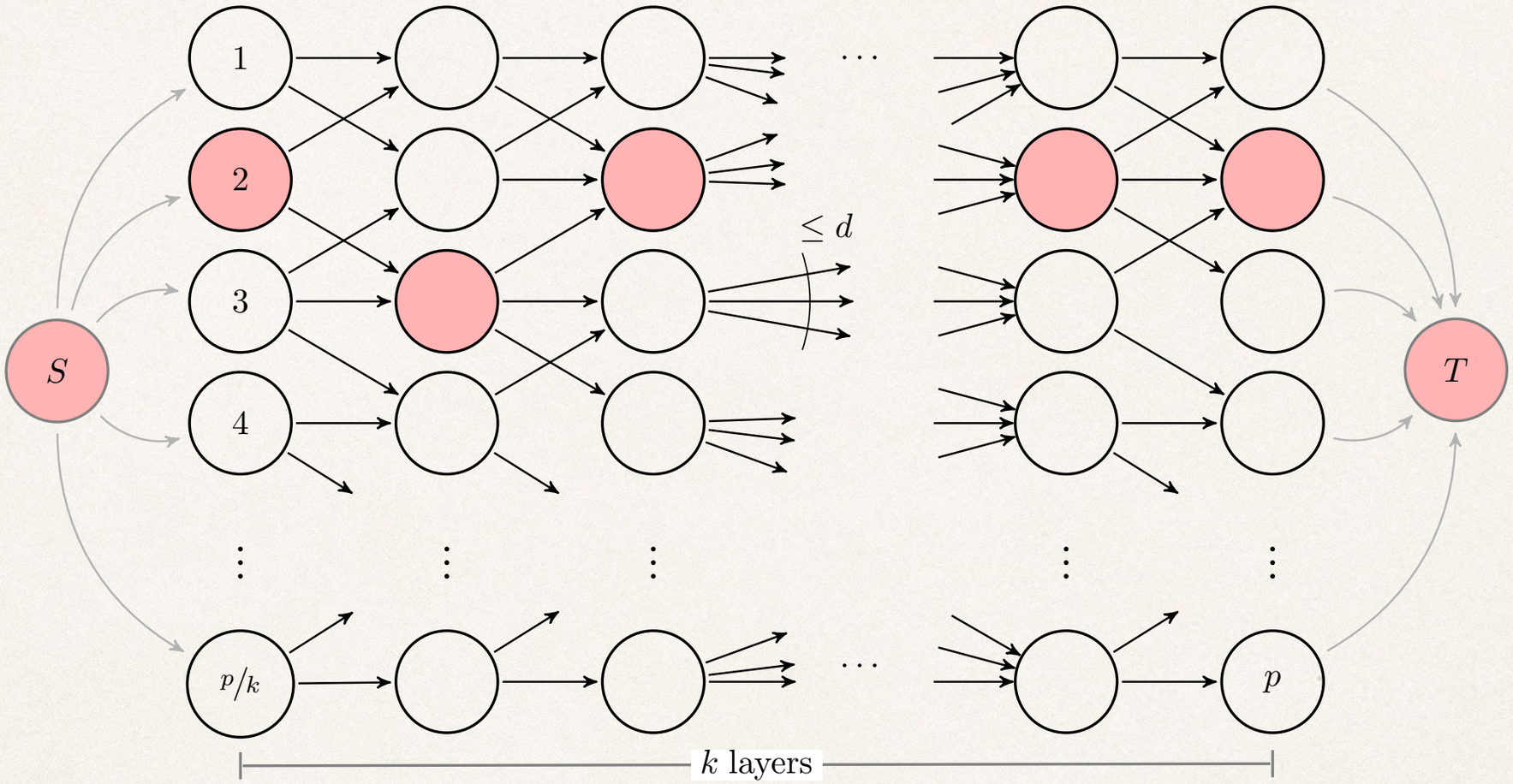

- Number of paths:

$$|\mathcal{P}(G)| = \frac{p-2}{k} \cdot d^{k-1} \leq \binom{p-2}{k}$$

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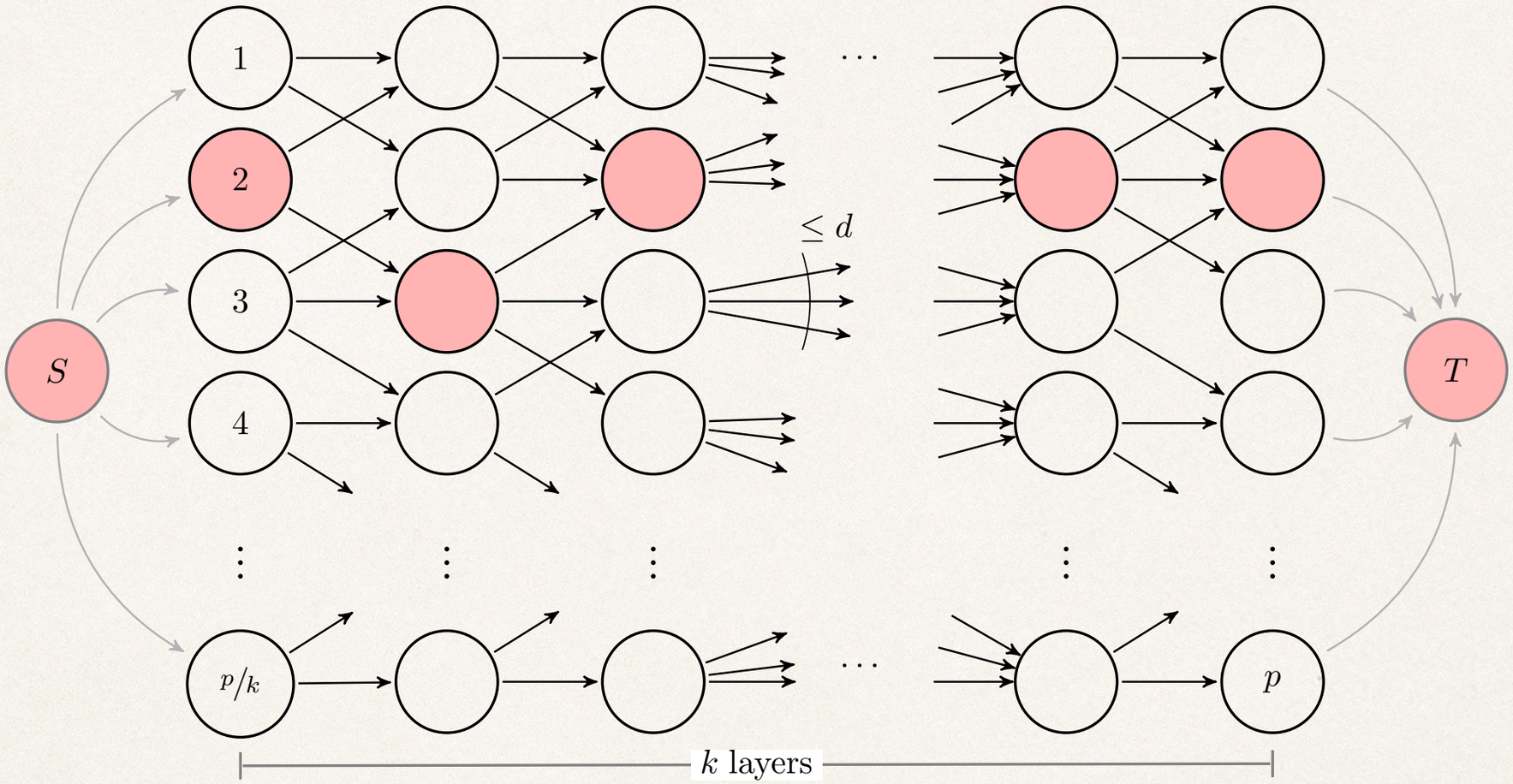

- Number of paths:

$$|\mathcal{P}(G)| = \frac{p-2}{k} \cdot d^{k-1} \leq \binom{p-2}{k} \qquad \beta > 0$$

- Spike along a path: $\boldsymbol{\Sigma} = \mathbf{I}_p + \beta \cdot \mathbf{x}_\star \mathbf{x}_\star^\top$ and draw samples $\sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$.

Lower bound

Theorem 1 (Lower Bound). *Consider a (p, k, d)-layer graph G on p vertices, with $k \geq 4$, and $\log d \geq 4H(3/4)$. Let $\{\mathbf{y}_i\}_{i=1}^n$ be a sequence of n random observations, independently drawn according to probability density function*

$$\mathcal{D}_p(\mathbf{x}_\star) = \mathcal{N}\big(\mathbf{0}, \mathbf{I}_p + \beta \cdot \mathbf{x}_\star \mathbf{x}_\star^\top\big),$$

for some $\beta > 0$. There exists $\mathbf{x}_\star \in \mathcal{X}(G)$ such that for every estimator $\widehat{\mathbf{x}}$,

$$\mathbb{E}_{\mathcal{D}_p^{(n)}(\mathbf{x}_\star)}\left[\|\widehat{\mathbf{x}}\widehat{\mathbf{x}}^\top - \mathbf{x}_\star \mathbf{x}_\star^\top\|_{\mathrm{F}}\right] \geq \frac{1}{2\sqrt{2}} \cdot \sqrt{\min\left\{1,\ \frac{C' \cdot (1+\beta)}{\beta^2} \cdot \frac{1}{n}\left(\log \frac{p-2}{k} + \frac{k}{4}\log d\right)\right\}}.$$

- *I.e.,* the minimax error is bounded away from zero, unless:

$$n = \Omega\left(\log \frac{p}{k} + k \log d\right) \qquad \left(\text{vs. } \Omega\left(k \log \frac{p}{k}\right)\right)$$

- Proof based on a **non-trivial local packing set construction** in Fano inequality.

Upper bound

- Upper bound is based on the estimator:

$$\begin{aligned} \underset{\mathbf{x}\in\mathbb{R}^p}{\text{maximize}} \quad & \mathbf{x}^\top \widehat{\mathbf{\Sigma}} \mathbf{x} \\ \text{subject to} \quad & \mathbf{x} \in \mathcal{X}(G). \end{aligned}$$

Theorem 2 (Upper bound). *Consider a (p,k,d)-layer graph G and $\mathbf{x}_\star \in \mathcal{X}(G)$. Let $\{\mathbf{y}_i\}_{i=1}^n$ be a sequence of n i.i.d. $\mathcal{N}(\mathbf{0},\mathbf{\Sigma})$ samples, where $\mathbf{\Sigma} \succeq \mathbf{0}$ with eigenvalues $\lambda_1 > \lambda_2 \geq \ldots$, and principal eigenvector $\mathbf{x}_\star$. Let $\widehat{\mathbf{\Sigma}}$ be the empirical covariance of the n samples, $\widehat{\mathbf{x}}$ the estimate of $\mathbf{x}_\star$ obtained via* (3)*, and $\epsilon \triangleq \|\widehat{\mathbf{x}}\widehat{\mathbf{x}}^\top - \mathbf{x}_\star\mathbf{x}_\star^\top\|_{\mathrm{F}}$. Then,*

$$\mathbb{E}[\epsilon] \leq C \cdot \frac{\lambda_1}{\lambda_1 - \lambda_2} \cdot \frac{1}{n} \cdot \max\left\{\sqrt{nA},\, A\right\},$$

where $A = O\big(\log \frac{p-2}{k} + k \log d\big)$.

- Analysis not restricted to the spiked covariance model.
- Thus:

$$n = \Theta\left(\log \frac{p}{k} + k \log d\right)$$

Conclusions (to be updated)

This paper:

- Introduces new Sparse PCA formulation: set of feasible supports determined by paths on DAGs.
- Proposes two efficient algorithmic solutions for the case of longest weighted paths.
- Provides lower and upper bounds for the case of layer graph model.

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- Introduces new Sparse PCA formulation: set of feasible supports determined by paths on DAGs.
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Future work:

- Other graph models, beyond longest paths?
- Practical upper bounds, “connected” with algorithms proposed.
- Further investigation for more applications.