Tensor Decompositions and Their Applications

Ankur Moitra (MIT)

Simons Institute Bootcamp Tutorial, Part 1

SPEARMAN'S HYPOTHESIS

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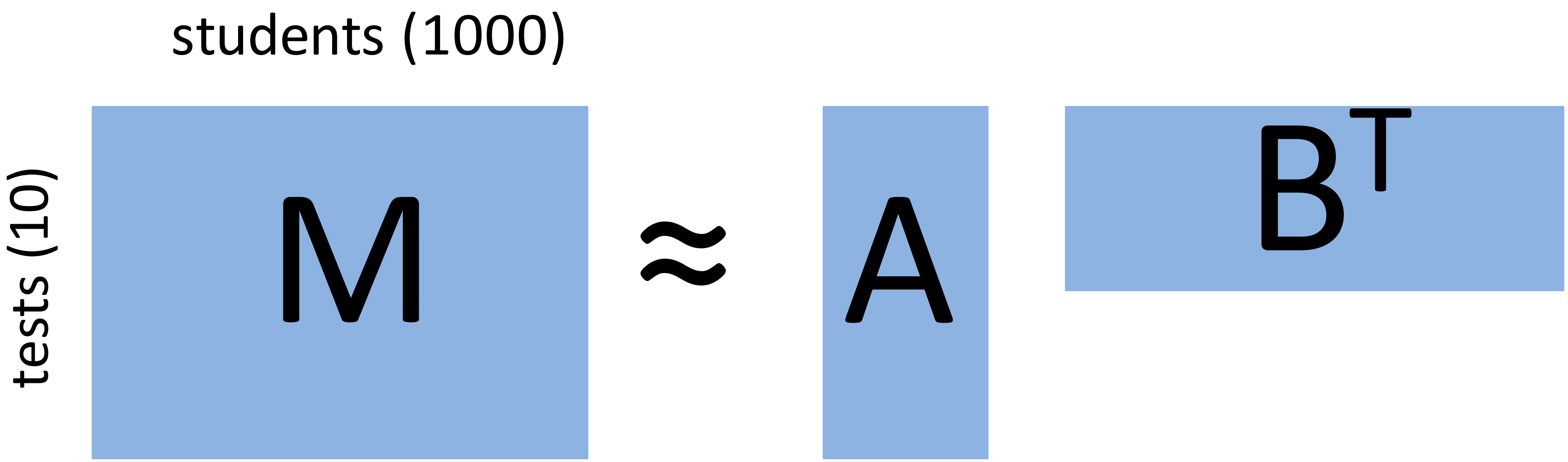

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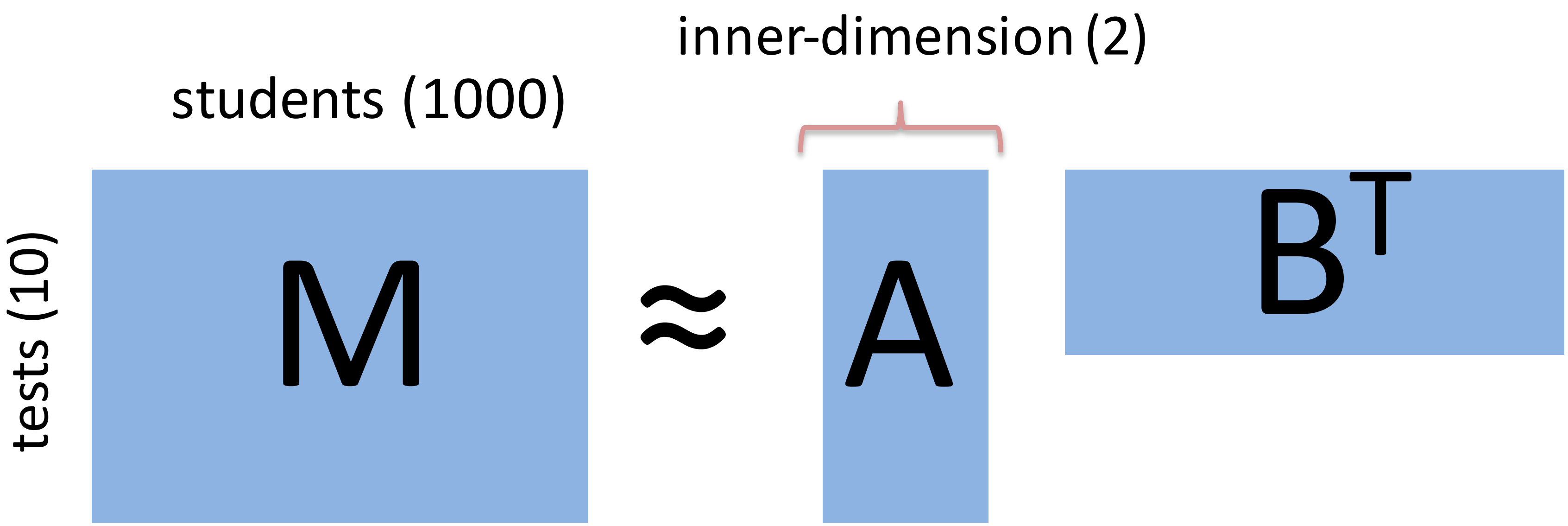

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This is called the **rotation problem**, and is a major issue in factor analysis and motivates the study of **tensor methods**…

OUTLINE

Part I: Introduction

- The Rotation Problem
- Jennrich's Algorithm

Part II: Applications

- Phylogenetic Reconstruction
- Mixtures of Gaussians
- Orbit Retrieval

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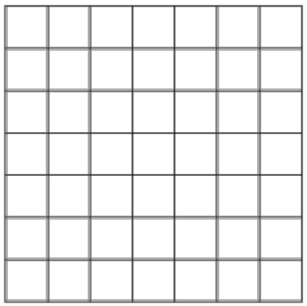
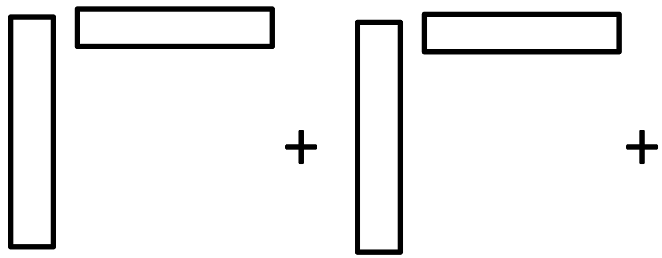
MATRIX DECOMPOSITIONS



$$M = a_1 \otimes b_1 + a_2 \otimes b_2 + \cdots + a_R \otimes b_R$$



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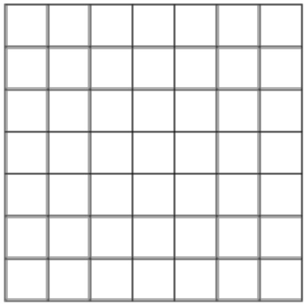

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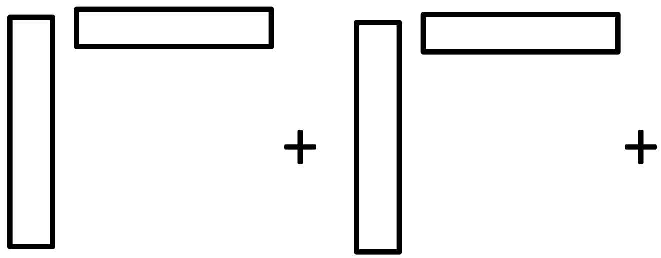
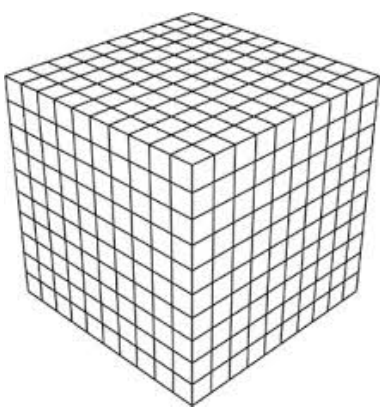


TENSOR DECOMPOSITIONS



$$T = a_1 \otimes b_1 \otimes c_1 + \cdots + a_R \otimes b_R \otimes c_R$$

(i, j, k) entry of $x \otimes y \otimes z$ is $x(i) \times y(j) \times z(k)$

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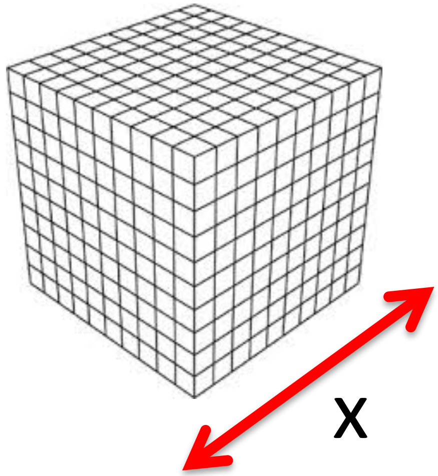
There is a simple algorithm to compute the factors too!

JENNRICH'S ALGORITHM

Compute $T(\cdot, \cdot, x)$



i.e. add up matrix slices

$$\sum_i x_i T_i$$

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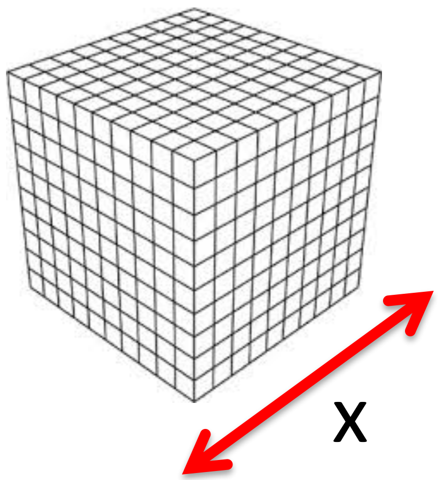

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If $T = a \otimes b \otimes c$ then $T(\cdot, \cdot, x) = \langle c, x \rangle a \otimes b$

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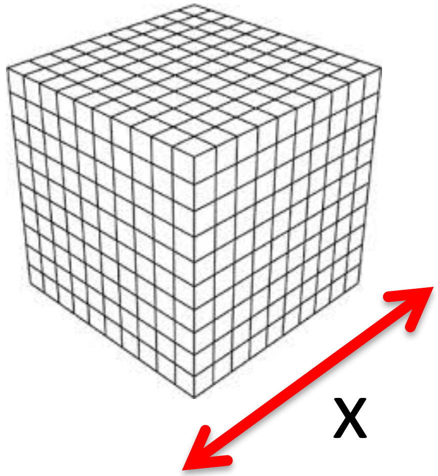

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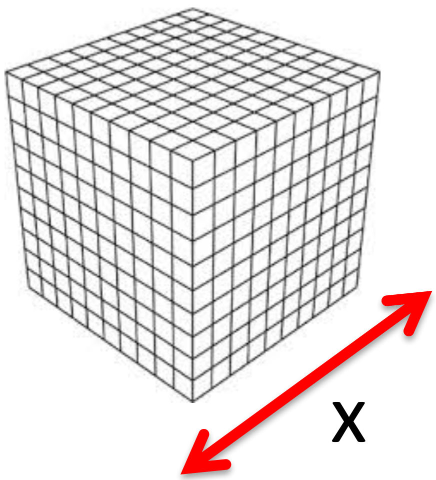

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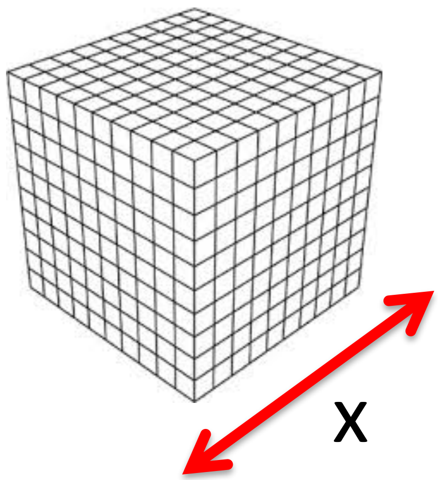
(x is chosen uniformly at random from $\mathbb{S}^{n-1}$)

JENNRICH'S ALGORITHM

$\mathrm{Diag}(\{\langle c_i, x\rangle\}_i)$

Compute $T(\cdot,\cdot,x) = A D_x B^\top$



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Claim: whp (over x,y) the eigenvalues are distinct, so the Eigendecomposition is unique and recovers a_i

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- Match up the factors (their eigenvalues are reciprocals) and find $\{c_i\}_i$ by solving a linear syst.

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Only possible if $\{a_i\}$ and $\{b_i\}$ are orthogonal, or $\mathrm{rank}(M) = 1$

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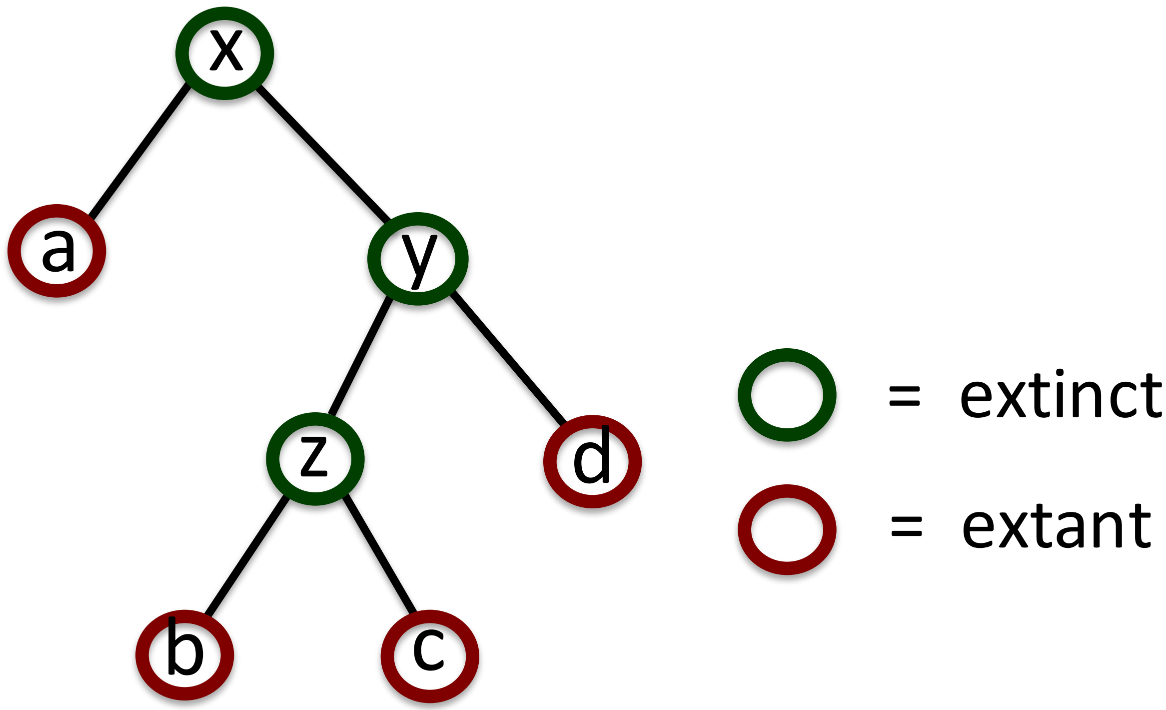
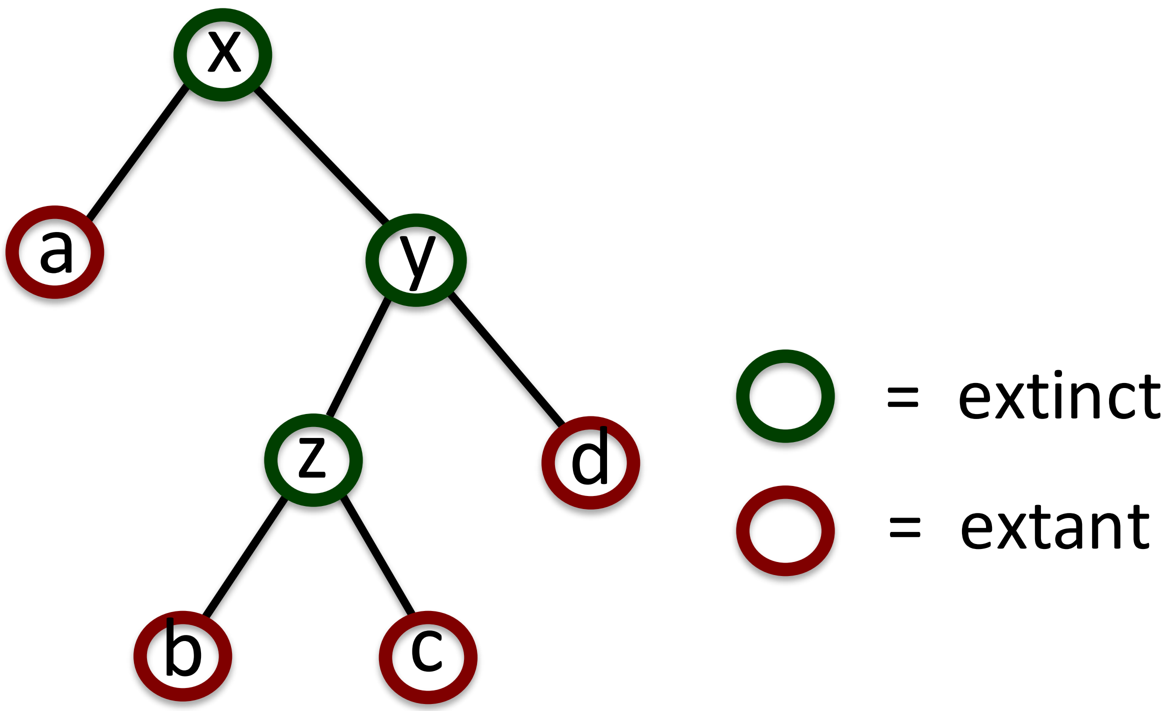


“Tree of Life”

PHYLOGENETIC RECONSTRUCTION



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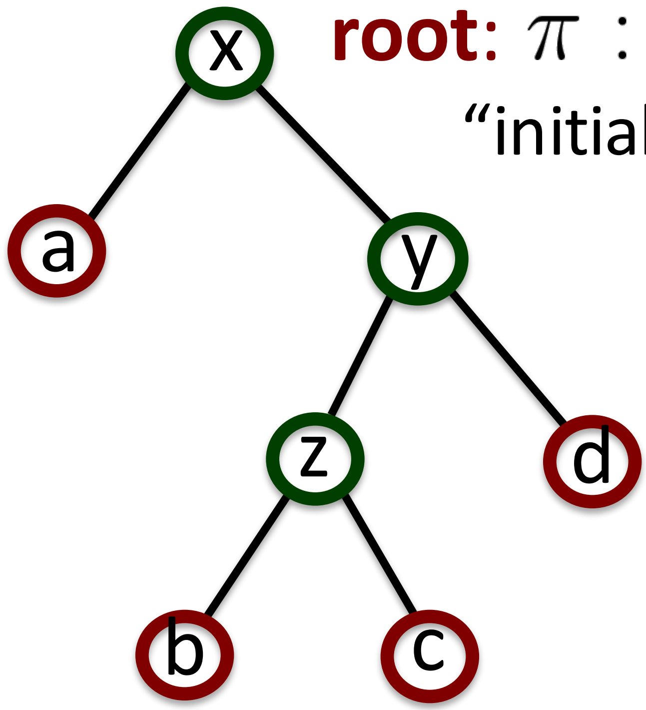
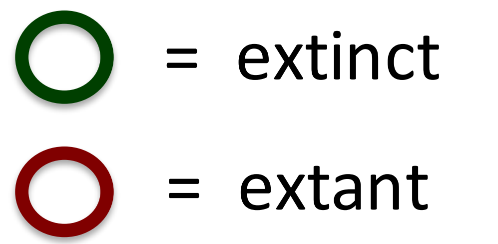


root: $\pi : \Sigma \to \mathbb{R}^+$

"initial distribution"



Σ = alphabet

PHYLOGENETIC RECONSTRUCTION

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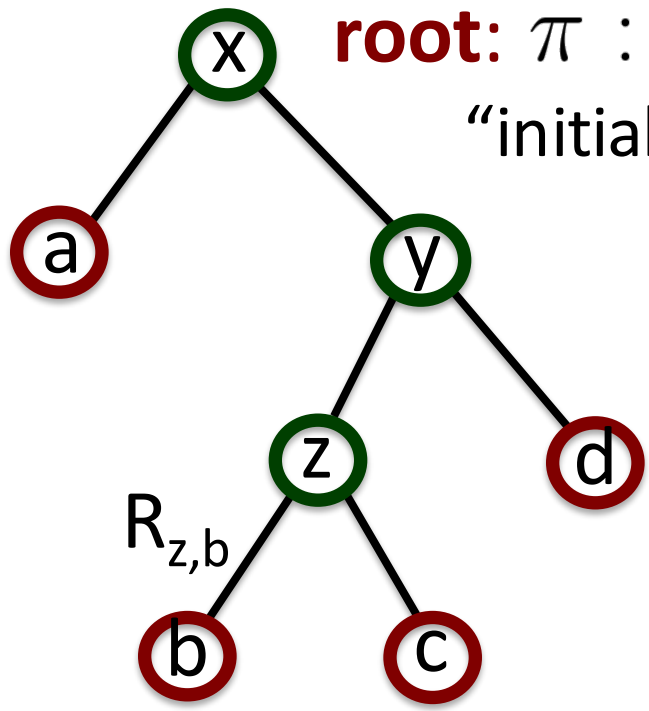

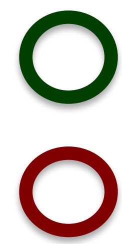

= extinct

= extant

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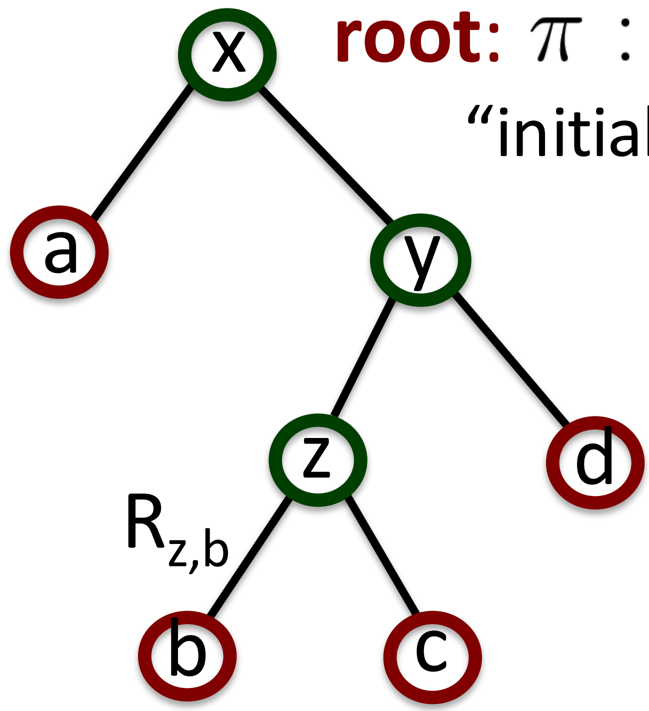
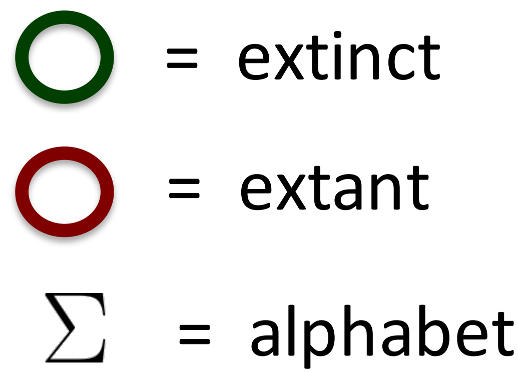
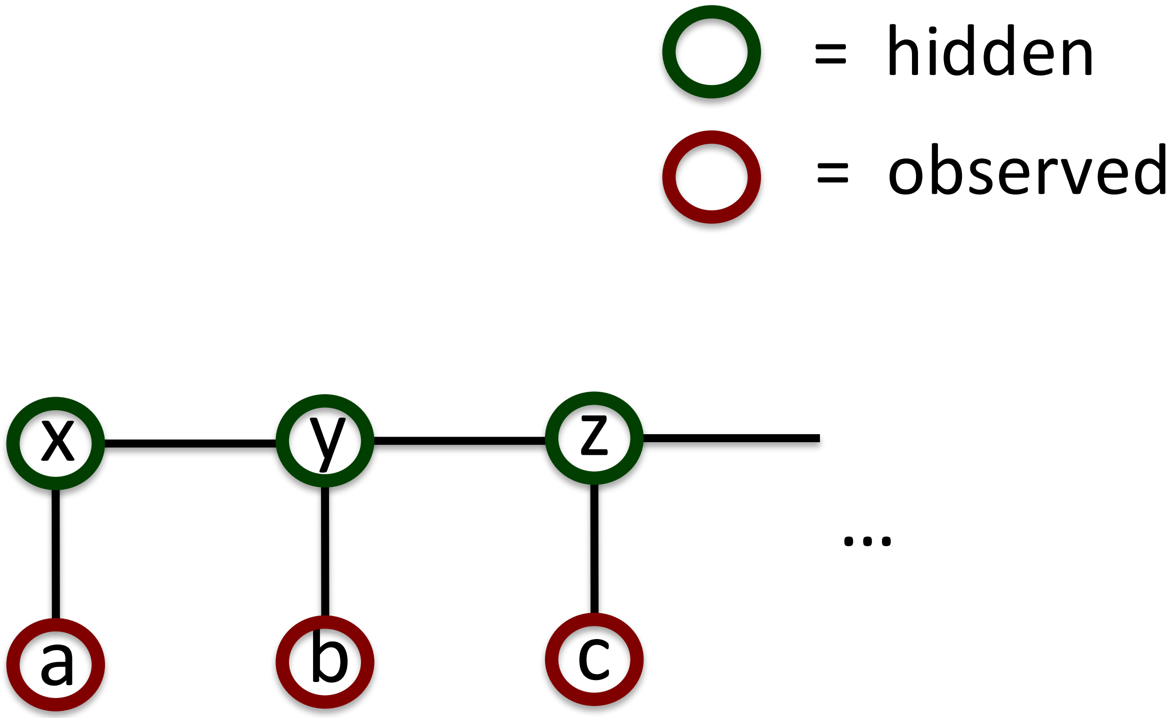




In each sample, we observe a symbol (Σ) at each extant (◯) node where we sample from π for the root, and propagate it using $R_{x,y}$, etc

HIDDEN MARKOV MODELS



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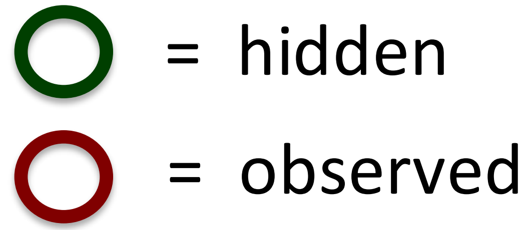

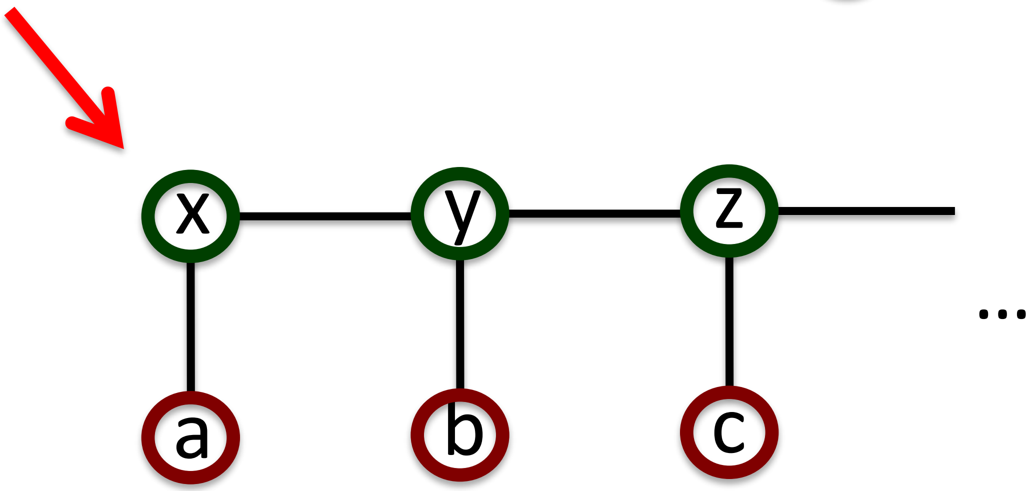

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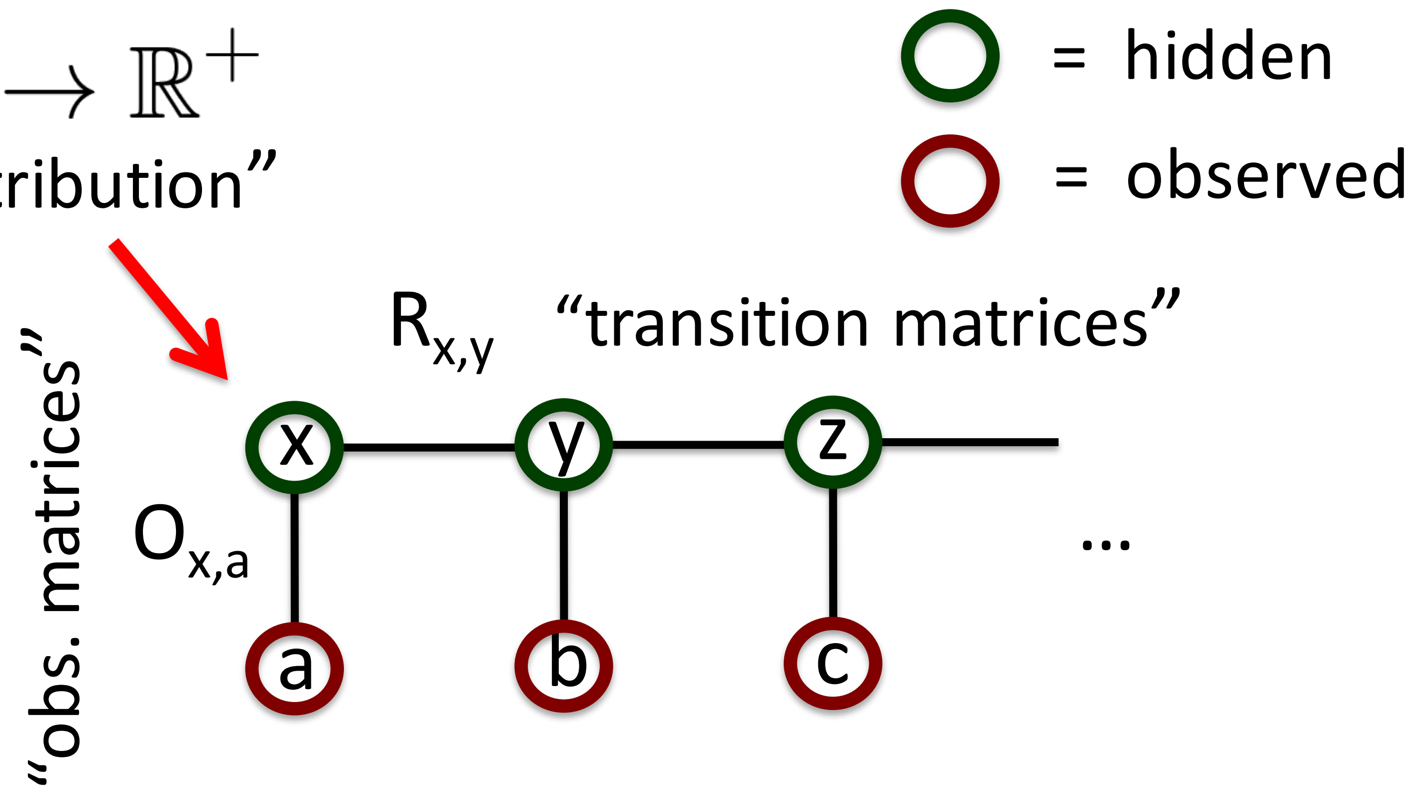

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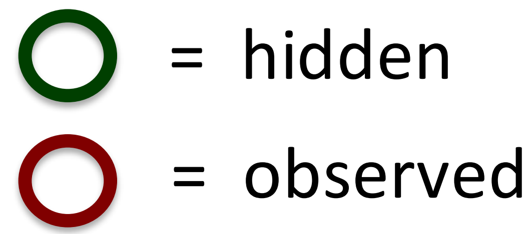

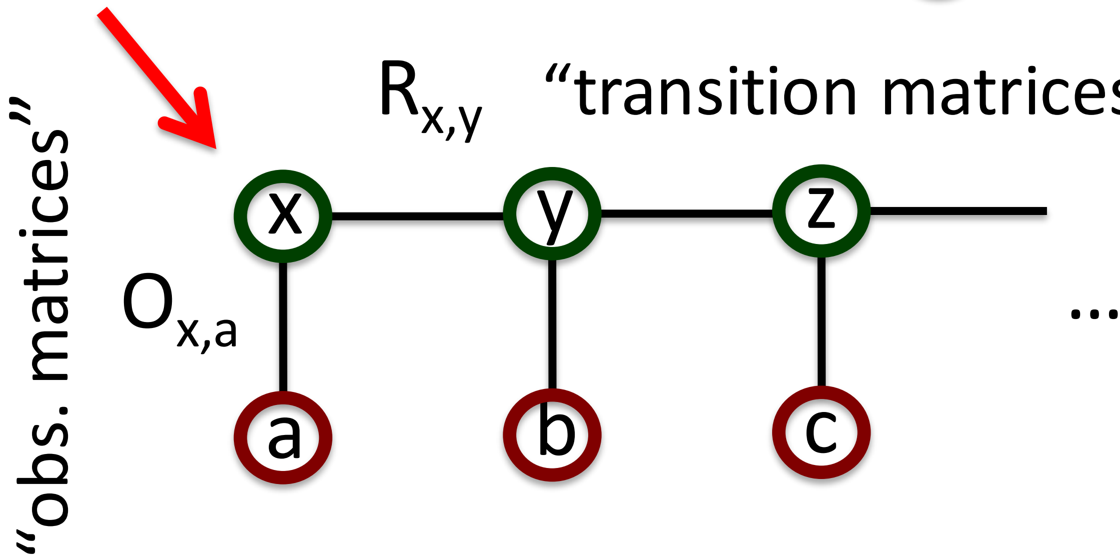

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[Steel, 1994]: The following is a distance function on the edges

$$d_{x,y} = -\ln|\det(P_{x,y})| + \frac{1}{2}\prod_{\sigma \text{ in } \Sigma} \pi_{x,\sigma} - \frac{1}{2}\prod_{\sigma \text{ in } \Sigma} \pi_{y,\sigma}$$

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(It's not even obvious it's nonnegative!)

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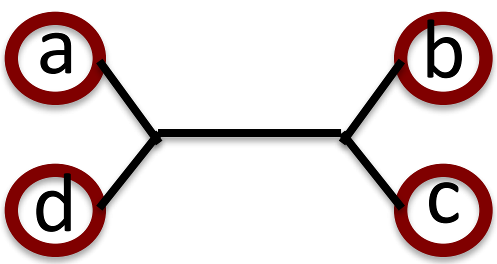

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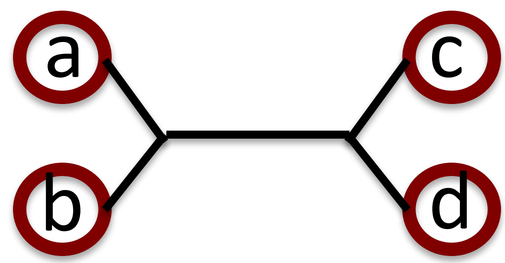

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to reconstruction the topology

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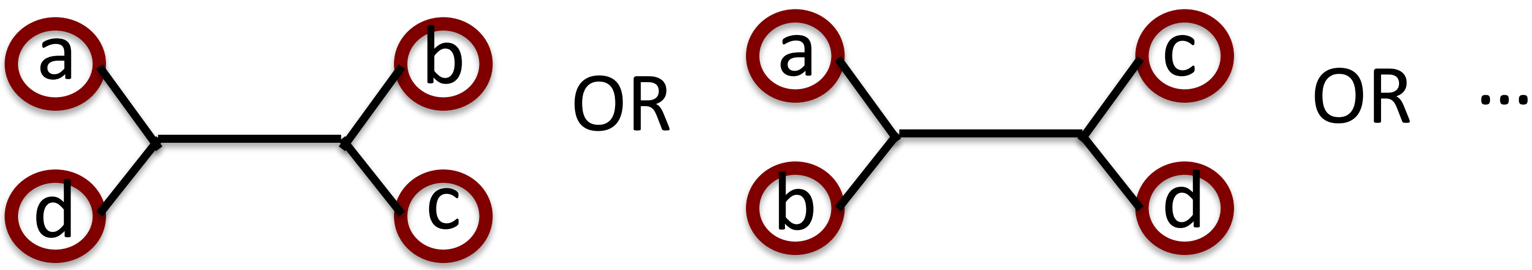

to reconstruction the topology, from polynomially many samples

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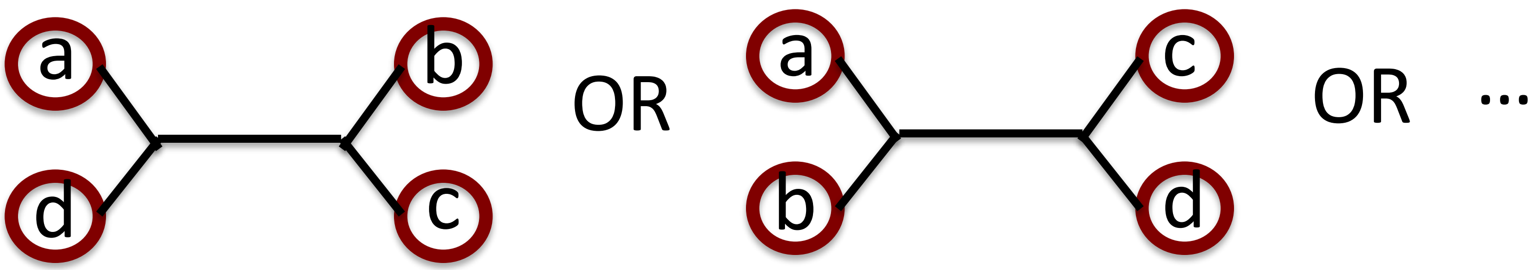

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For many problems (e.g. HMMs) finding the transition matrices is the main issue…

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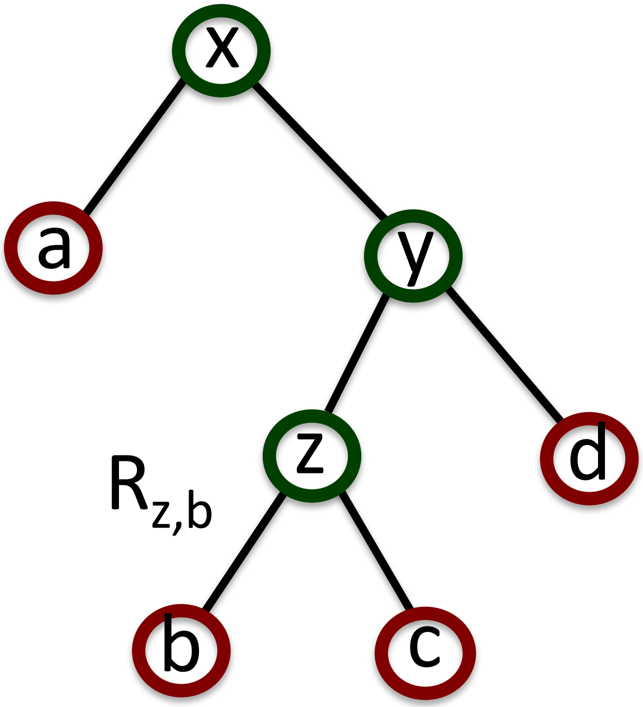

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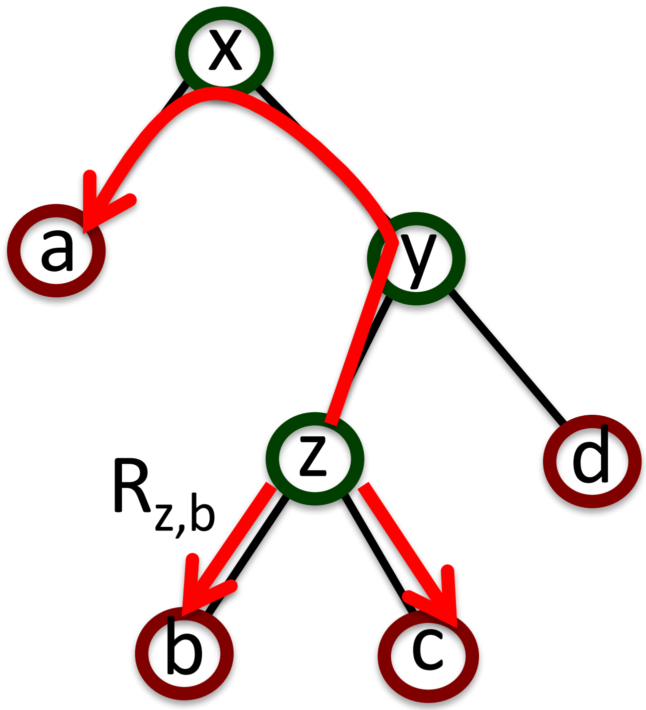

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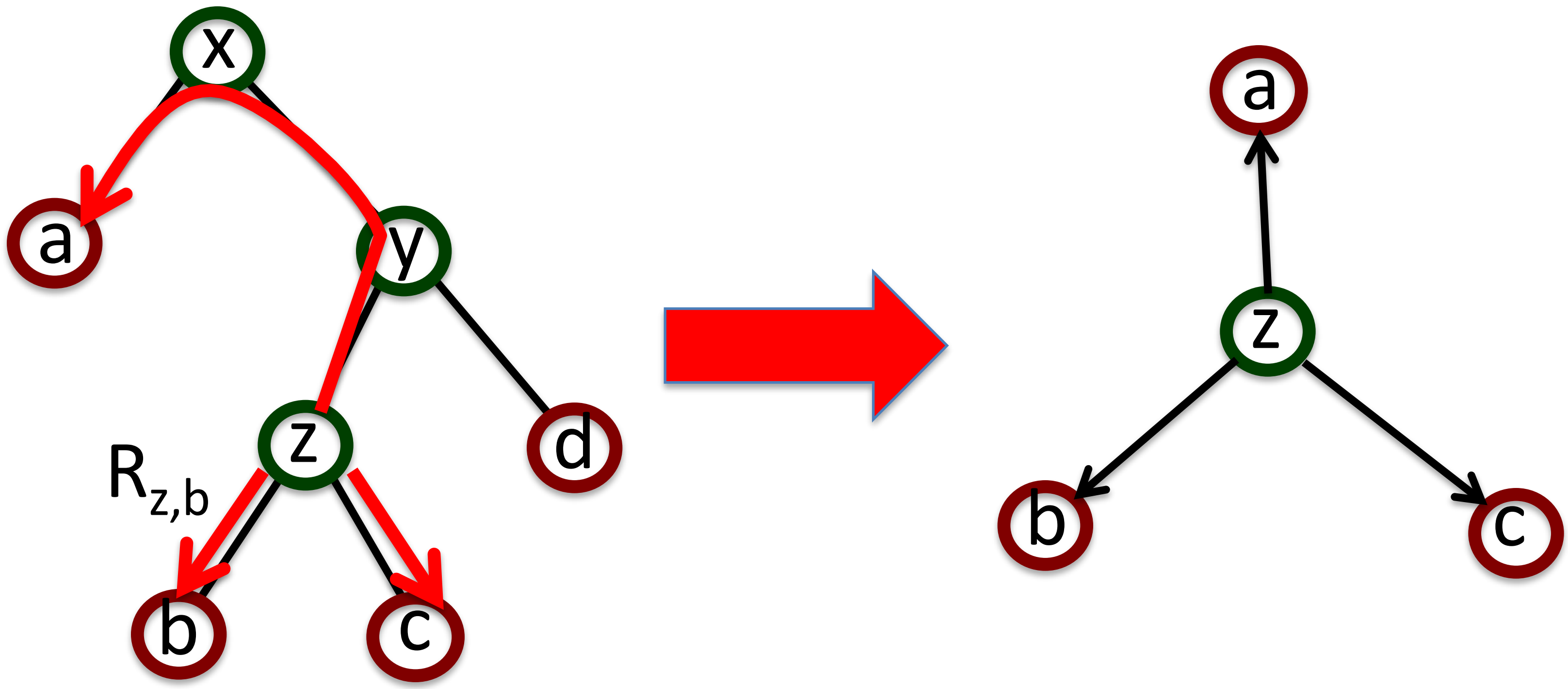

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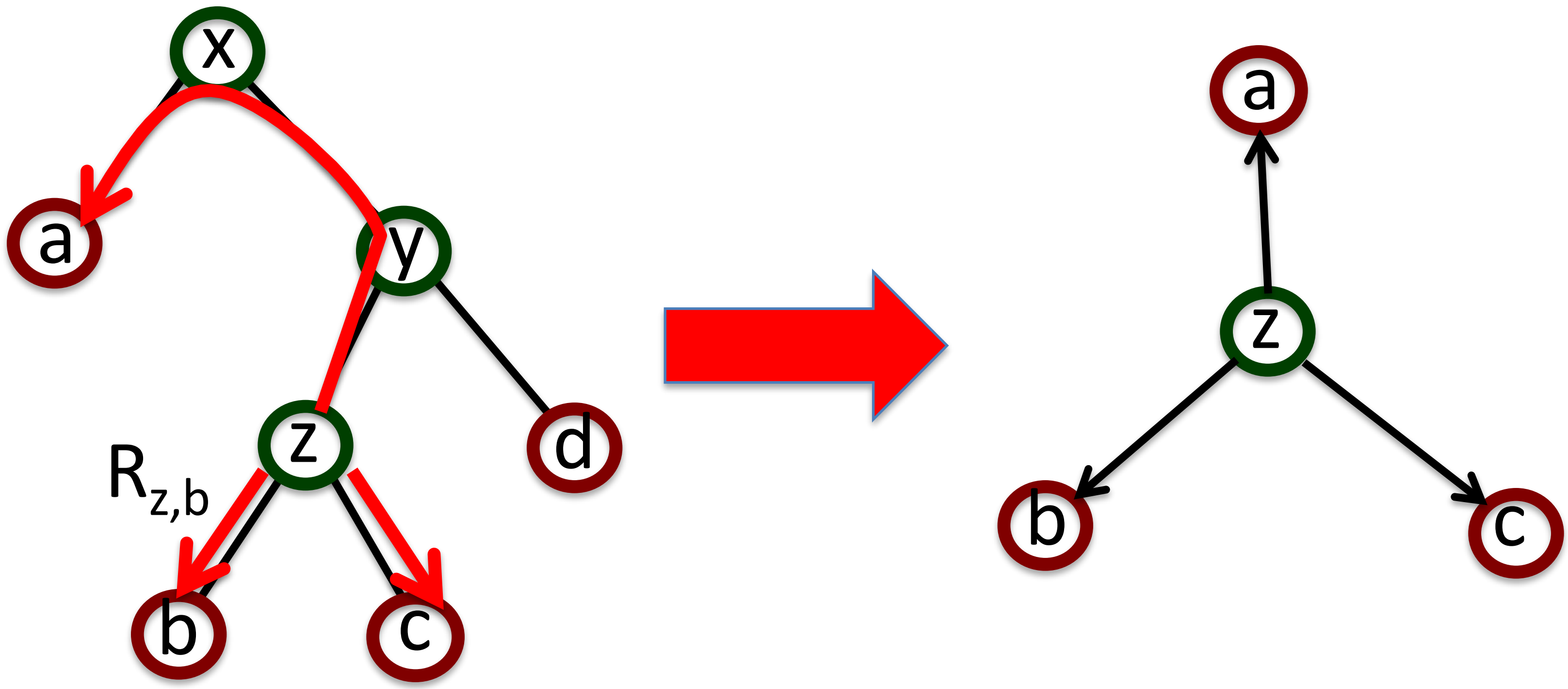
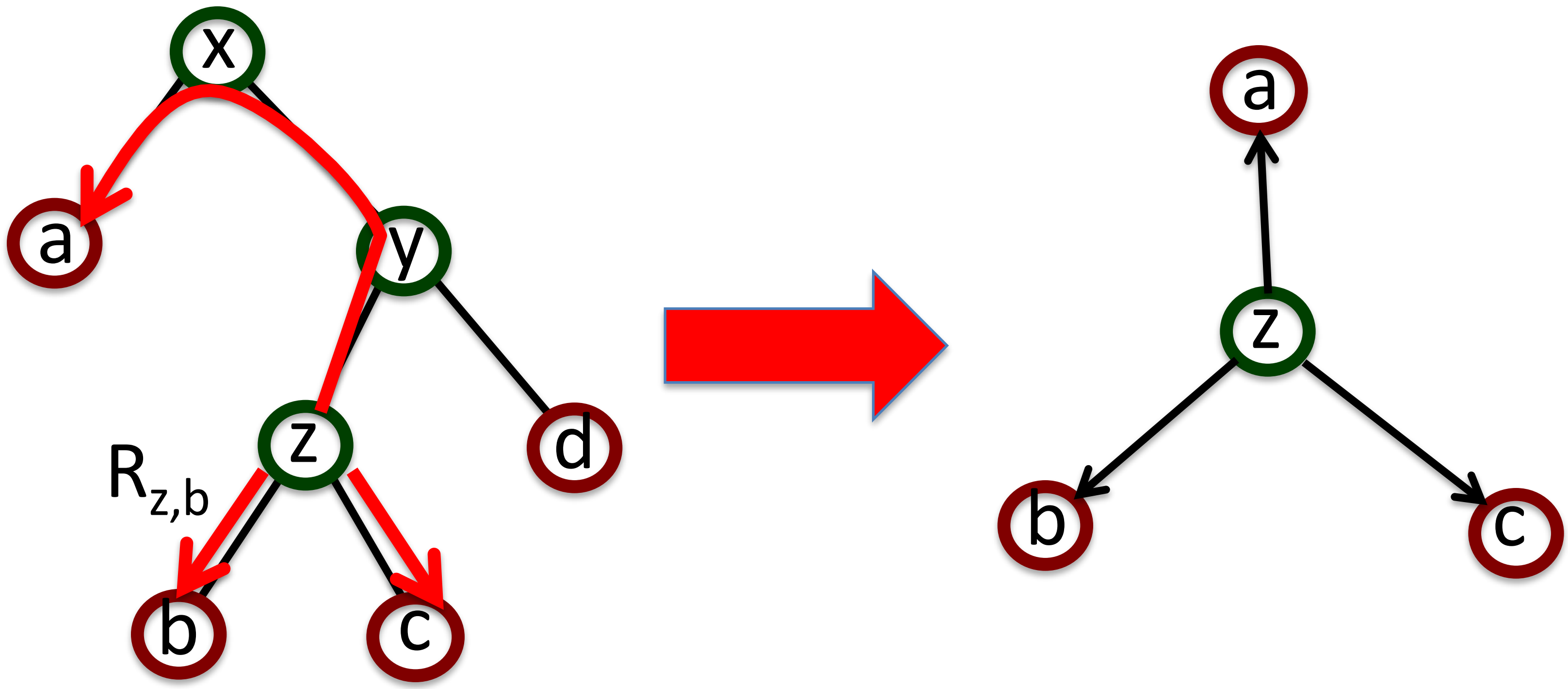


Joint distribution over (a, b, c):

$$\sum_{\sigma} \mathbb{P}[z=\sigma]\mathbb{P}[a|z=\sigma] \otimes \mathbb{P}[b|z=\sigma] \otimes \mathbb{P}[c|z=\sigma]$$

[Chang, 1996]: The model is identifiable (if R's are full rank)



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(It's now used as a hard problem to build cryptosystems!)

THE POWER OF CONDITIONAL INDEPENDENCE

[Phylogenetic Trees/HMMS]: (joint distribution on leaves a, b, c)

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MIXTURES OF SPHERICAL GAUSSIANS

Let's see another powerful application of tensor methods to learning mixtures of spherical Gaussians

$$\sum_{i=1}^{k} w_i \mathcal{N}(\mu_i, \sigma^2 I, x)$$

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Can we reconstruct the parameters in polynomial time?

Theorem [Hsu, Kakade, 2013]: There is an algorithm that has polynomial run time/sample complexity that works when the μ_i's have full rank

smallest singular value

Running time and sample complexity depend on $1/\sigma_{min}$

Main Lemma: If σ^2 is known then the tensor

$$T = \sum_{i=1}^{k} w_i \mu_i \otimes \mu_i \otimes \mu_i$$

can be expressed through the empirical moments of the mixture

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Again, there is a low rank tensor that can be computed from samples whose tensor decomposition reveals the parameters we want to learn

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Case #1: If a, b, c are distinct then we have

$$\mathbb{E}[x_a x_b x_c] = \Big(\sum_{i=1}^{k} w_i \mu_i \otimes \mu_i \otimes \mu_i \Big)_{a,b,c}$$

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Case #2: If a = b ≠ c then we have

$$\mathbb{E}[x_a x_b x_c] = \left(\sum_{i=1}^{k} w_i \mu_i \otimes \mu_i \otimes \mu_i \right)_{a,b,c} + \sigma^2 \left(\sum_{i=1}^{k} w_i \mu_i \right)_c$$

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$$T = \mathbb{E}[x \otimes x \otimes x] - \sigma^2 \sum_{j=1}^{d} M_j \quad \text{with}$$

$$M_j = \left(\mathbb{E}[x] \otimes e_j \otimes e_j + e_j \otimes \mathbb{E}[x] \otimes e_j + e_j \otimes e_j \otimes \mathbb{E}[x]\right)$$

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Now use Jennrich's Algorithm

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[Mixtures of Spherical Gaussians]: (corrections of third moment)

$$\mathbb{E}[x \otimes x \otimes x] - \sigma^2 \sum_{j=1}^{d} M_j$$

following **[Hsu, Kakade, 2013]**

THE POWER OF CONDITIONAL INDEPENDENCE

[Pure Topic Models/LDA]: (joint distribution on first three words)

$$\sum_j \mathbb{P}[\text{topic} = j] A_j \otimes A_j \otimes A_j$$

following **[Anandkumar, Hsu, Kakade, 2012]**

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[Pure Topic Models/LDA]: (joint distribution on first three words)

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[Community Detection]: (counting stars)

$$\sum_j \mathbb{P}[C_x = j] \Big(C_A \Pi\Big)_j \otimes \Big(C_B \Pi\Big)_j \otimes \Big(C_C \Pi\Big)_j$$

following **[Anandkumar, Ge, Hsu, Kakade, 2014]**

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ORBIT RETRIEVAL

What if we want to learn the parameters of generative model with a continuous latent variable?

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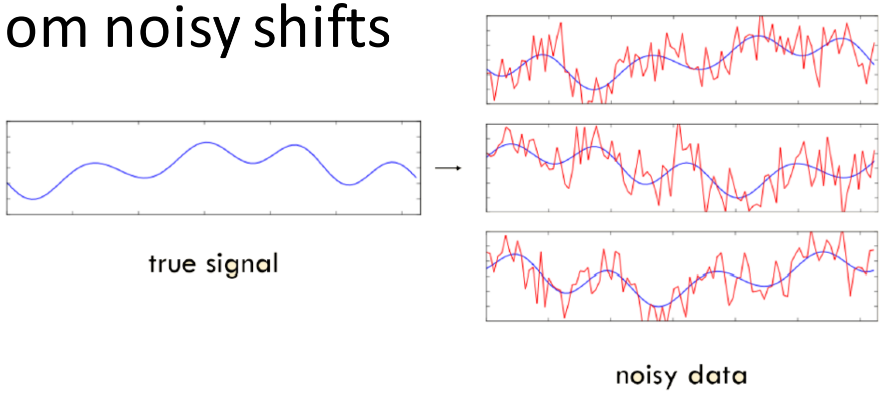
What if we want to learn the parameters of generative model with a continuous latent variable?

Multireference Alignment

Recover a signal from random noisy shifts



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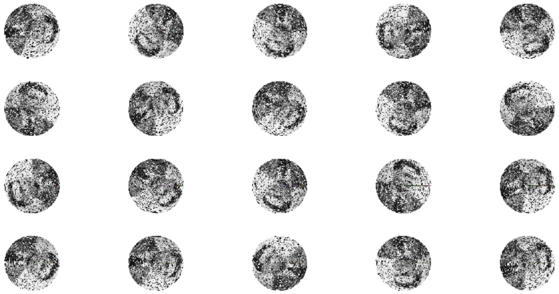
Global Registration

Estimate positions from rigid motions



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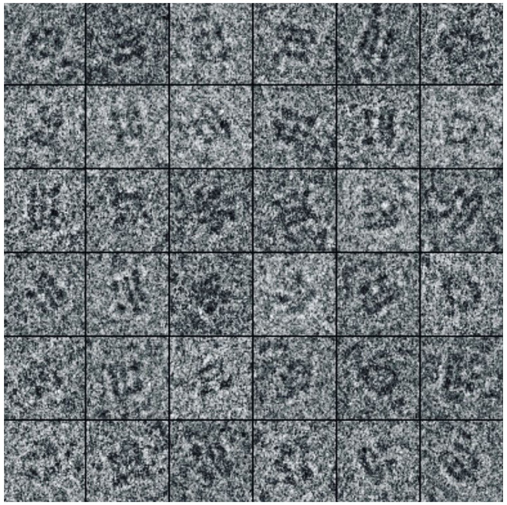
Cryo-electron microscopy

Determine 3D structure from random noisy 2D projections



ORBIT RETRIEVAL

Definition: An **orbit retrieval** problem is specified by a group G and a linear homomorphism

$$\rho : G \to GL(\mathbb{R}^d)$$

We get noisy observations under the group action

$$\rho(g) \cdot x + \eta$$

where g is chosen from the Haar measure on G and η is Gaussian noise

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Goal: Recover some $\widehat{x}$ that is close to the orbit

$$\{\rho(g) \cdot x | g \in G\}$$

ORBIT TENSOR DECOMPOSITION

In many settings we can estimate

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What about for non-abelian groups?

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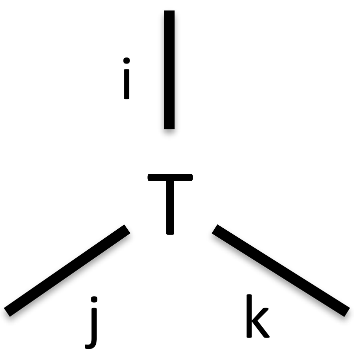
third order tensors have three legs



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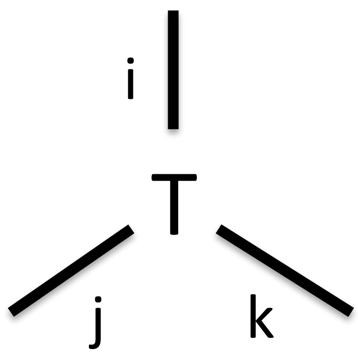

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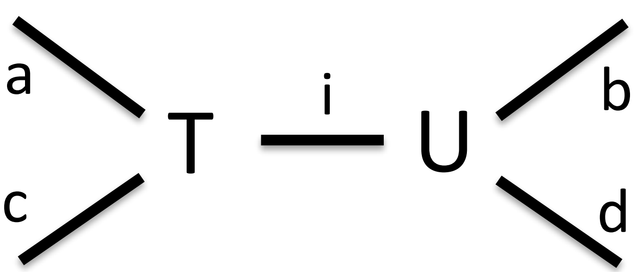
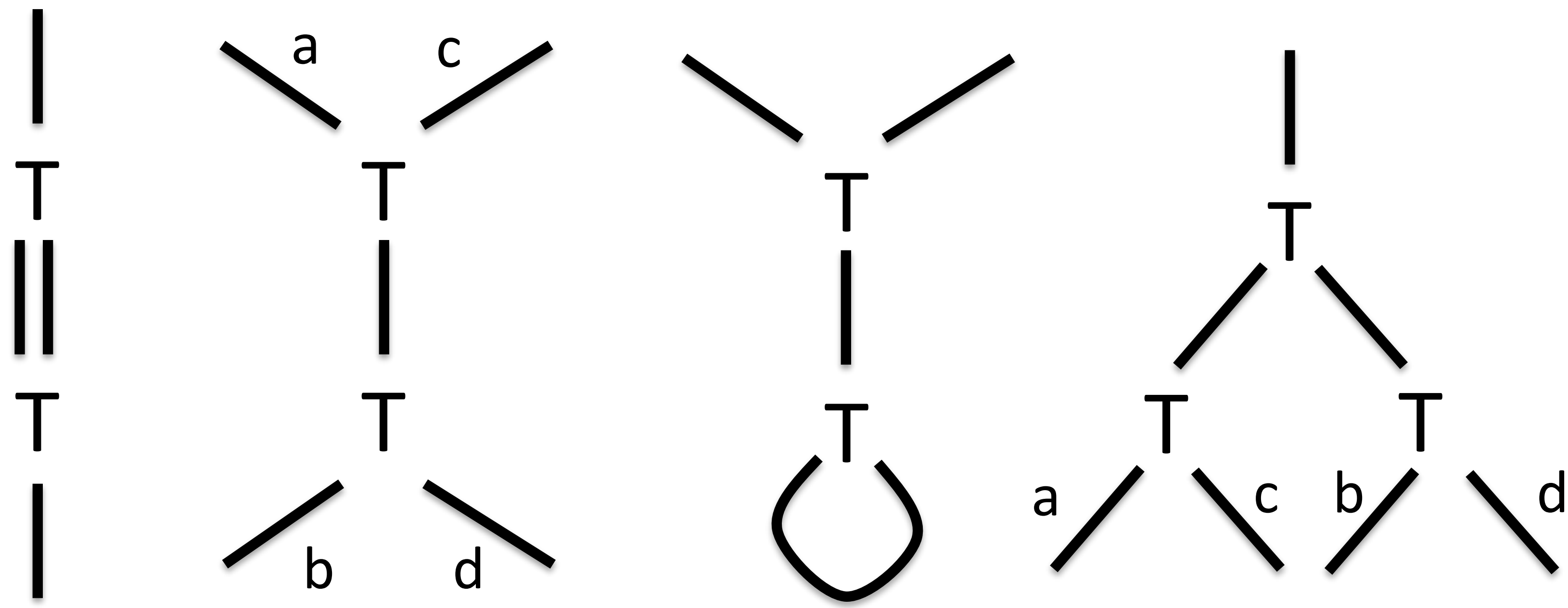
tensors can be attached by summing over connected indices



$$B_{a,b,c,d} = \sum_i T_{a,c,i} U_{b,d,i}$$

REVISITING PRIOR WORK

Prior work implicitly uses this framework



See **[Richard, Montanari]**, **[Barak, Moitra]**, **[Hopkins, Shi, Steurer]**, **[Hopkins et al.]**, **[Hopkins, Shi, Steurer]** for applications to tensor principal component analysis, tensor completion, decomposing random overcomplete third order tensors, etc

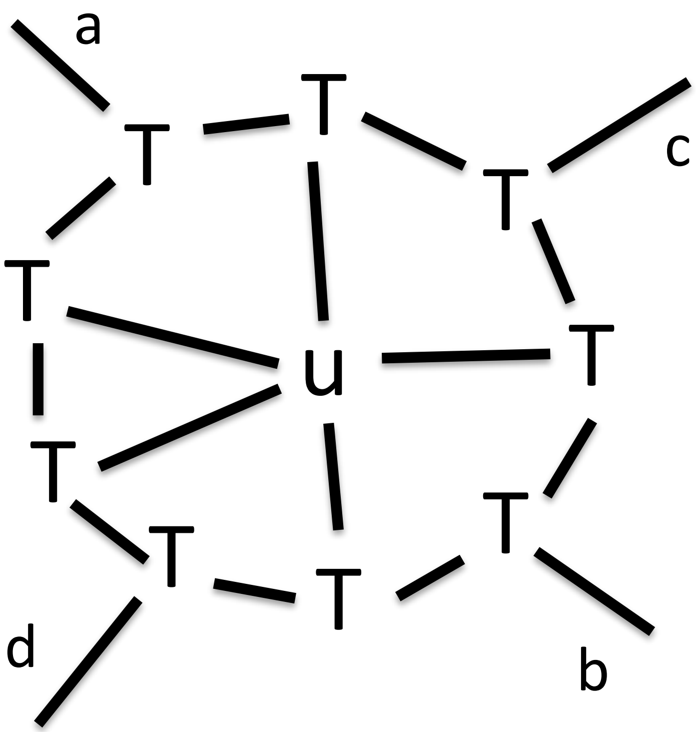
SPECTRAL METHODS FROM TENSOR NETS

Given input tensor T

- **Step #1:** Build a new tensor B by connecting copies of T according to the tensor network
- **Step #2:** Flatten B to form a symmetric matrix M
- **Step #3:** Compute the leading eigenvector of M

THE BLUEPRINT

We give a spectral method based on the following tensor network



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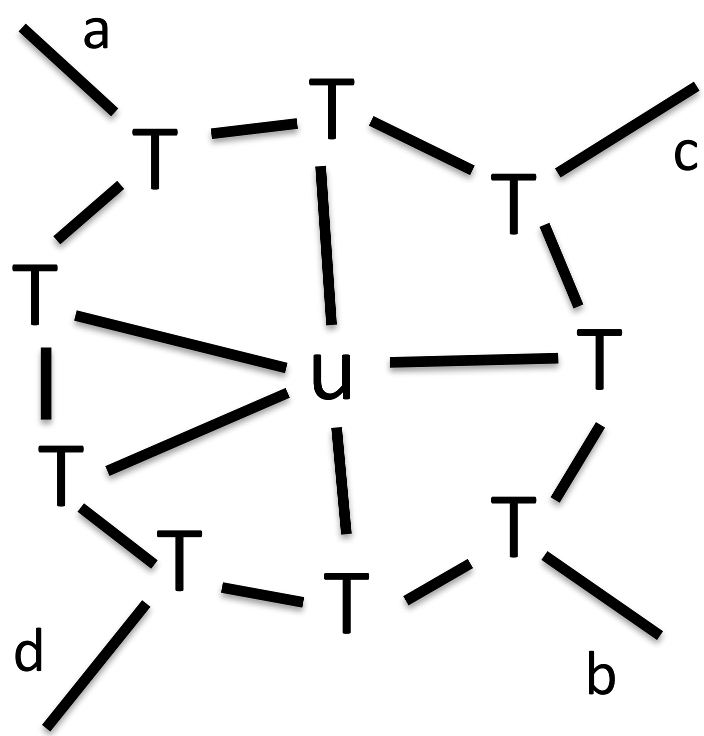

Smaller tensor networks fail for this problem

TUTORIAL OUTLINE

Part I: Tensor Decompositions and Their Applications

Part II: Robust and Computationally Efficient Parameter Estimation

Part III: Noise Models in Supervised Learning and Connections to Fairness

Part IV: Provable Algorithms for Inverse Problems in the Sciences?

Summary:

- Tensor decompositions are unique under more general conditions than matrix decompositions
- Jennrich's Algorithm
- Applications to Phylogenetic Reconstruction, HMMs, Mixtures of Gaussians, Topic Models, …
- **Are there tensor methods that work with group structure?**

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Thanks! Any Questions?