Learning Linear Bayesian Networks with Latent Variables

Anima Anandkumar

U.C. Irvine

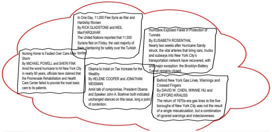
Joint work with Daniel Hsu, Adel Javanmard, and Sham Kakade.

Latent Variable Modeling

Goal: Discover hidden effects from observed measurements

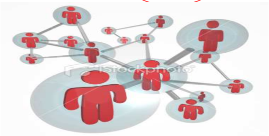
Document modeling

- Observed: words.
- Hidden: topics.



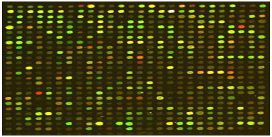
Social Network Modeling

- Observed: social interactions.
- Hidden: communities, relationships



Bio-Informatics

- Observed: gene expressions.
- Hidden: gene regulators.



Learning latent variable models: efficient methods and guarantees

Challenges and Approaches

Challenges: High-Dimensional Regime

- Identifiability: when can hidden variables be discovered?
- Design of learning algorithms with provable guarantees?
- Sample and Computational complexities?

Challenges and Approaches

Challenges: High-Dimensional Regime

- Identifiability: when can hidden variables be discovered?
- Design of learning algorithms with provable guarantees?
- Sample and Computational complexities?

Our Approach: Two Perspectives

Challenges and Approaches

Challenges: High-Dimensional Regime

- Identifiability: when can hidden variables be discovered?
- Design of learning algorithms with provable guarantees?
- Sample and Computational complexities?

Our Approach: Two Perspectives

Graphical Modeling

- Bayesian networks: Markov conditions on directed acyclic graphs.

Challenges and Approaches

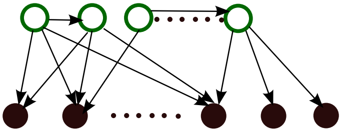
Challenges: High-Dimensional Regime

- Identifiability: when can hidden variables be discovered?
- Design of learning algorithms with provable guarantees?
- Sample and Computational complexities?

Our Approach: Two Perspectives

Graphical Modeling

- Bayesian networks: Markov conditions on directed acyclic graphs.



Method of Moments

- Linear models: linear structural equation models (SEMs)
- Tractable approaches for solving equations (convex/non-convex).

Summary of Results

Model Class

- Linear Bayesian networks with hidden variables
- Multi-Level DAGs and DAGs with effective depth one.

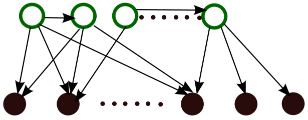
Characterize Identifiability

- Structural condition: expansion of bipartite graph from hidden to observed nodes.
- Parametric condition: satisfied for generic parameters.

Learning Method

- Learning mixing matrix: from hidden to observed nodes.

  Exploit sparsity in connections.
  ℓ_1 based method.



- Learning parameters in the hidden layer.

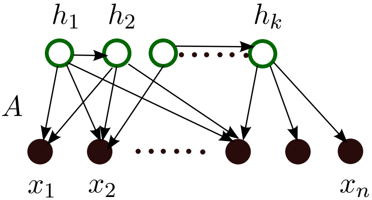
  Exploit form of moments.
  spectral method.

Outline

Linear Bayesian Networks

BN: Markov relationships on DAG

- Pa_i: parents of node i.
- $\mathbb{P}_\theta(x) = \prod_{i=1}^n \mathbb{P}_\theta(x_i | x_{\mathrm{Pa}_i})$



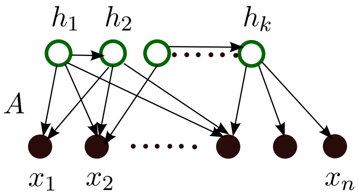
Linear Model

- n observed variables $\{x_i\}$ and k hidden variables $\{h_i\}$.
- For each observed variable: $\boxed{x_i = \sum_{j \in \mathrm{Pa}_i} a_{ij} h_j + \varepsilon_i.}$
- Condition on noise: Noise variables ε_i are uncorrelated
- Non-degeneracy: Linear indep. on hidden variables, columns of A.

Moment Forms and Overview of Learning

Consider (exact) second-order observed moments

$$\boxed{\mathbb{E}[xx^\top] = A\mathbb{E}[hh^\top]A^\top + \mathbb{E}[\varepsilon\varepsilon^\top].}$$



Learning

- In three stages: Denoising, unmixing and learning latent parameters
- Denoising: Separate noise ε from signal
- Unmixing : Separate mixing matrix A from hidden variables h_i. Also known as blind deconvolution/dictionary learning.
- Learning latent parameters: learn deeper layers, learn hidden structures etc.

Denoising

$$\boxed{\mathbb{E}[xx^\top] = A\mathbb{E}[hh^\top]A^\top + \mathbb{E}[\varepsilon\varepsilon^\top]}$$

- When ε_i are uncorrelated, $\mathbb{E}[\varepsilon\varepsilon^\top]$ is a diagonal matrix.
- Recall non-degeneracy conditions: Rank$(A\mathbb{E}[hh^\top]A^\top) = k$.
- Thus, denoising is Diagonal $+$ Low Rank when $n > k$, e.g. when $n > 3k$, can estimate diagonal part using off-diagonal parts.
- For details, refer to the paper.

Denoising

$$\boxed{\mathbb{E}[xx^\top] = A\mathbb{E}[hh^\top]A^\top + \mathbb{E}[\varepsilon\varepsilon^\top]}$$

- When ε_i are uncorrelated, $\mathbb{E}[\varepsilon\varepsilon^\top]$ is a diagonal matrix.
- Recall non-degeneracy conditions: $\text{Rank}(A\mathbb{E}[hh^\top]A^\top) = k$.
- Thus, denoising is Diagonal $+$ Low Rank when $n > k$, e.g. when $n > 3k$, can estimate diagonal part using off-diagonal parts.
- For details, refer to the paper.

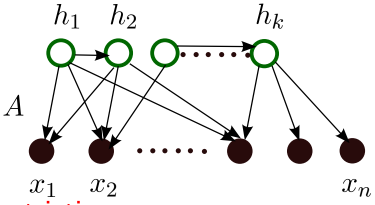
Main focus: unmixing A from $A\mathbb{E}[hh^\top]A^\top$

Some Intuitions on Blind Deconvolution

Main Task

Recover mixing matrix A from

$\boxed{A\mathbb{E}[hh^\top]A^\top}$.



Ill-posed without further restrictions

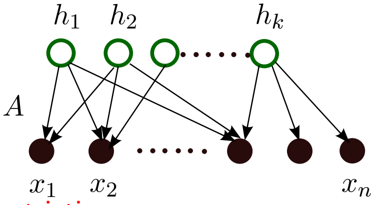
One possibility: restriction on hidden variables $\{h_i\}$

- $\mathbb{E}[hh^\top]$ is diagonal: e.g. h is the set of basis vectors in $\mathbb{R}^k$, when h is uncorrelated, can obtain diagonal covariance matrix: (ICA), or when h is drawn from Dirichlet distribution.
- No restrictions on A (other than non-degeneracy).
- Recovery through third (or higher) order moment e.g. simultaneous diagonalization, through tensor decompositions (Anandkumar et. al. 2012).

Some Intuitions on Blind Deconvolution

Main Task

Recover mixing matrix A from $\boxed{A\mathbb{E}[hh^\top]A^\top}$.



Ill-posed without further restrictions

One possibility: restriction on hidden variables $\{h_i\}$

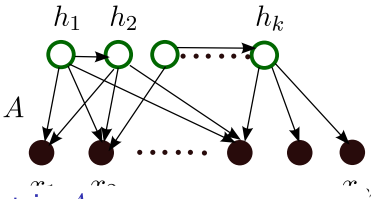
- $\mathbb{E}[hh^\top]$ is diagonal: e.g. h is the set of basis vectors in $\mathbb{R}^k$, when h is uncorrelated, can obtain diagonal covariance matrix: (ICA), or when h is drawn from Dirichlet distribution.
- No restrictions on A (other than non-degeneracy).
- Recovery through third (or higher) order moment e.g. simultaneous diagonalization, through tensor decompositions (Anandkumar et. al. 2012).

Shortcoming: cannot handle arbitrary hidden dependencies.

Constraints for Blind Deconvolution

Unmixing Task

Recover mixing matrix A from $\boxed{A\mathbb{E}[hh^\top]A^\top}$.



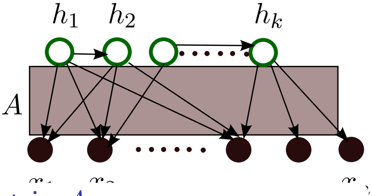
Different outlook: restriction on mixing matrix A

- No restrictions on hidden variables $\{h_i\}$ (other than non-degeneracy): can handle arbitrary hidden dependencies, e.g. correlated topic models.
- Restriction on support of A: corresponds to bipartite graph from hidden to observed layers.
- May be applicable in many settings, e.g. gene regulation, community memberships in social networks.

Constraints for Blind Deconvolution

Unmixing Task

Recover mixing matrix A from $\boxed{A\mathbb{E}[hh^\top]A^\top}$.

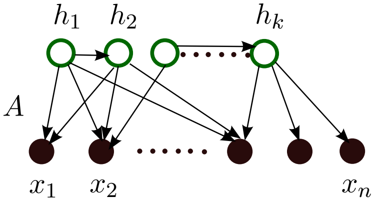


Different outlook: restriction on mixing matrix A

- No restrictions on hidden variables $\{h_i\}$ (other than non-degeneracy): can handle arbitrary hidden dependencies, e.g. correlated topic models.
- Restriction on support of A: corresponds to bipartite graph from hidden to observed layers.
- May be applicable in many settings, e.g. gene regulation, community memberships in social networks.

Sufficient Conditions for Identifiability

Unmixing Task: Recover A from $A\mathbb{E}[hh^\top]A^\top$



Structural Condition: (Additive) Graph Expansion

$$\boxed{|\mathcal{N}(S)| \geq |S| + d_{\max}, \text{ for all } S \subset [k]}$$

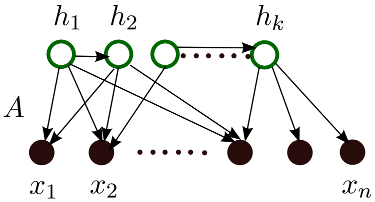
Parametric Conditions: Generic Parameters

$$\boxed{\|Av\|_0 > |\mathcal{N}_A(\mathrm{supp}(v))| - |\mathrm{supp}(v)|}$$

Identifiability Result

Under above conditions, A can be uniquely recovered from $A\mathbb{E}[hh^\top]A^\top$.

Some Intuitions Behind Identifiability Result



- Identifiability of mixing matrix under graph expansion and for generic parameters.

Intuitions

- For non-degenerate $A\mathbb{E}[hh^\top]A^\top$, we know the Col$(A)$, the column space of A.
- Under above conditions, sparsest vectors in Col(A) are columns of A, and thus identifiable.

Unmixing: search for sparse vectors in Col(A)

Outline

Tractable Algorithm for Unmixing

Unmixing Task

Recover mixing matrix A from $\boxed{A\mathbb{E}[hh^\top]A^\top}$.

Exhaustive search

$$\boxed{\min_{z\neq 0} \|Az\|_0}$$

Convex relaxation

$$\boxed{\min_z \|Az\|_1, \quad b^\top z = 1,}$$

where b is a row in A.

Change of Variables

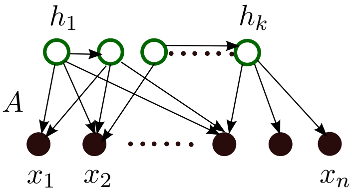
$$\boxed{\min_w \|(A\mathbb{E}[hh^\top]A^\top)^{1/2}w\|_1, \quad e_i^\top (A\mathbb{E}[hh^\top]A^\top)^{1/2}w = 1.}$$

Under "reasonable" conditions, the above program exactly recovers A

Learning Latent Space Parameters

Recall so far..

Recover mixing matrix A from $\boxed{A\mathbb{E}[hh^\top]A^\top}$.



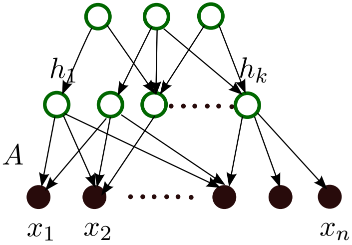
Now learning hidden structures

- In general, $\mathbb{E}[hh^\top]$ is not enough to recover joint distribution of h

Learning Multi-level DAGs

Repeat this recursively, i.e., un-mix $\mathbb{E}[hh^\top]$ to recover higher layers.

Learning Latent Space Parameters



Recall so far..

Recover mixing matrix A from

$\boxed{A\mathbb{E}[hh^\top]A^\top}$.

Now learning hidden structures

- In general, $\mathbb{E}[hh^\top]$ is not enough to recover joint distribution of h

Learning Multi-level DAGs

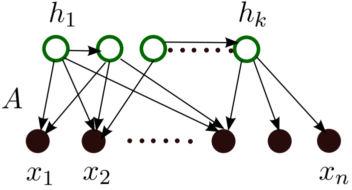
Repeat this recursively, i.e., un-mix $\mathbb{E}[hh^\top]$ to recover higher layers.

Learning DAGs with Effective Depth 1

Effective Depth 1

Each hidden variable is connected to at least one observed variable.

Linear Structural Equations



- Recall, $\boxed{x = Ah + \varepsilon}$
- Now additionally, $h_j = \sum_{i \in \mathrm{Pa}_j} \lambda_{ji} h_i + \eta_j$, or

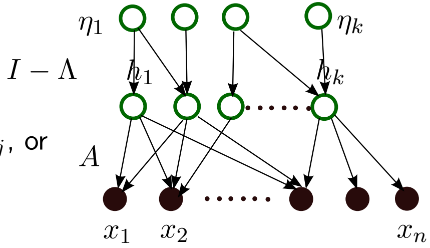
  $\boxed{h = \Lambda h + \eta}$
- This implies that $\boxed{x = A(I - \Lambda)^{-1}\eta + \varepsilon}$
- η_i are uncorrelated: $\mathbb{E}[\eta\eta^\top]$ is diagonal.

Spectral approach for learning

Learning DAGs with Effective Depth 1

Effective Depth 1

Each hidden variable is connected to at least one observed variable.



Linear Structural Equations

- Recall, $\boxed{x = Ah + \varepsilon}$
- Now additionally, $h_j = \sum_{i \in \mathrm{Pa}_j} \lambda_{ji} h_i + \eta_j$, or

  $\boxed{h = \Lambda h + \eta}$
- This implies that $\boxed{x = A(I-\Lambda)^{-1}\eta + \varepsilon}$
- η_i are uncorrelated: $\mathbb{E}[\eta\eta^\top]$ is diagonal.

Spectral approach for learning

Learning DAGs with Effective Depth 1

$$\boxed{x = A(I-\Lambda)^{-1}\eta + \varepsilon}$$

- Employ spectral approach to learn $A(I-\Lambda)^{-1}$.
- Therefore, $\boxed{\mathbb{E}[xx^\top] = A(I-\Lambda)^{-1}\mathbb{E}[\eta\eta^\top](A(I-\Lambda)^{-1})^\top + \mathbb{E}[\varepsilon\varepsilon^\top]}$
- Similarly for third order moment, $\mathbb{E}[xx^\top\langle\lambda, x\rangle] =$ $\boxed{A(I-\Lambda)^{-1}\mathbb{E}[\eta\eta^\top\langle\eta, A^\top\lambda\rangle](A(I-\Lambda)^{-1})^\top + \mathbb{E}[\varepsilon\varepsilon^\top\langle\lambda, \varepsilon\rangle]}$
- Simultaneous diagonalization of second and third order moments: through SVD or tensor decompositions.
- Un-mix A from $A(I-\Lambda)^{-1}$ through ℓ_1 optimization.

Learning both structure and parameters of depth-1 DAGs

Outline

Conclusion

Learning Linear Latent Bayesian Networks

- Considered learning with arbitrary hidden variable dependencies
- Constraints on the mixing matrix: expansion of bipartite graph from hidden to observed layer, generic parameters and non-degeneracy.
- Established identifiability of mixing matrix.
- Recovering mixing matrix through ℓ_1 optimization.
- Able to learn multi-level DAGs and DAGs with effective depth 1

Outlook: Learning over-complete basis

- When more hidden variables than observed variables
- Require higher order moments
- Interesting questions on identifiability and efficient algorithms.