# GLAD: Learning Sparse Graph Recovery

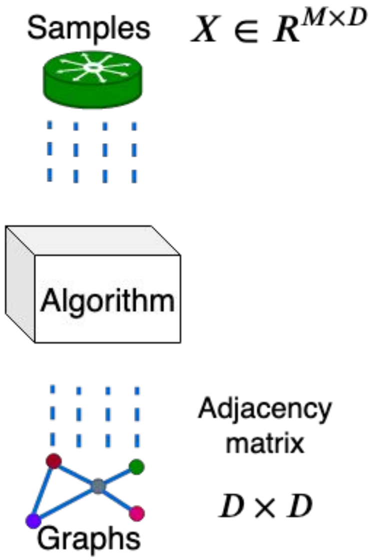
Harsh Shrivastava

*Joint work with* Xinshi Chen, Binghong Chen, Guanghui Lan, Srinvas Aluru, Han Liu, Le Song

# Objective

Recovering sparse conditional independence graph G from data

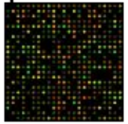
$$\Theta_{ij} = 0 \Leftrightarrow X_i \perp X_j | \, other\ variables$$



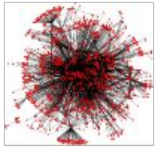
# Applications

## Biology

Gene Expression data - Microarray experiments



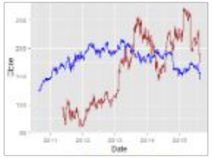
Algorithm



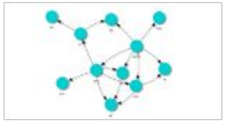
Gene regulatory network

## Finance

Time-series features



Algorithm



Relationship between assets

# Sparse Graph Recovery Problem Formulation

- Given M samples from a distribution: $X \in R^{M \times D}$
- Estimate matrix 'Θ' corresponding to the sparse graph

Objective function: L1 regularized maximum likelihood estimation

$$\widehat{\Theta} = \arg\min_{\Theta \in \mathcal{S}^d_{++}} \; -\log(\det \Theta) + \mathrm{tr}(\widehat{\Sigma}\Theta) + \rho \left\|\Theta\right\|_{1,\mathrm{off}}$$

Covariance matrix

$$\hat{\Sigma} = \frac{X^\top X}{M}$$

Regularization Parameter

# Existing Optimization Algorithms

**G-ISTA**

Proximal gradient method

**BCD**

Block coordinate descent method

**ADMM**

Alternating direction method of multipliers

$$-\log(\det \Theta) + \operatorname{tr}(\widehat{\Sigma}\Theta) + \rho \left\|Z\right\|_1 + \langle \lambda, \Theta - Z \rangle + \tfrac{1}{2}\beta \|Z - \Theta\|_F^2 .$$

Taking $U := \lambda/\beta$ as the scaled dual variable, the update rules for the ADMM algorithm are

$$\Theta_{k+1} \leftarrow \big(-Y + \sqrt{Y^\top Y + (4/\beta)I}\big)/2, \text{ where } Y = \widehat{\Sigma}/\beta - Z_k + U_k$$

$$Z_{k+1} \leftarrow \eta_{\rho/\beta}(\Theta_{k+1} + U_k), \quad U_{k+1} \leftarrow U_k + \Theta_{k+1} - Z_{k+1}$$

# Hard to Tune Hyperparameters

Tuning hyperparameters for Traditional Methods

‘Grid search’ is tedious and non-trivial

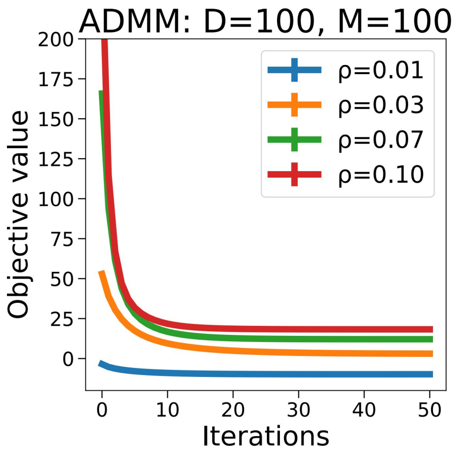
Outcomes highly sensitive to penalty parameters

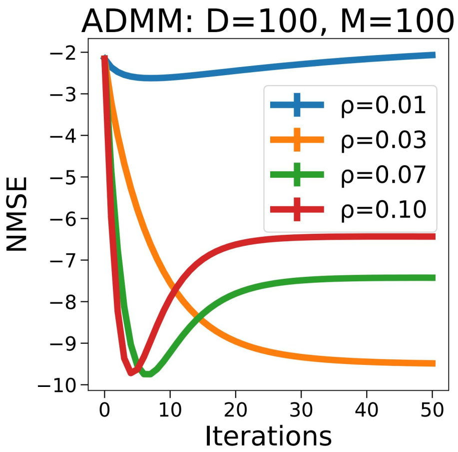
| $\rho$ \ $\beta$ | 5 | 1 | 0.5 | **0.1** | 0.01 |
|---|---|---|---|---|---|
| 0.01 | -2.51 | -2.25 | -2.06 | -2.06 | -2.69 |
| **0.03** | -5.59 | -9.05 | 9.48 | **-9.61** | -9.41 |
| 0.07 | -9.53 | -7.58 | -7.42 | -7.38 | -7.46 |
| 0.1 | -9.38 | -6.51 | -6.43 | -6.41 | -6.50 |
| 0.2 | -6.76 | -4.68 | -4.55 | -4.47 | -4.80 |

Errors of different parameter combinations

$$-\log(\det\Theta) + \mathrm{tr}(\widehat{\Sigma}\Theta) + \rho\,\|Z\|_1 + \langle\lambda, \Theta - Z\rangle + \tfrac{1}{2}\beta\|Z - \Theta\|_F^2$$

# Mismatch in Objectives




**mismatch!**

Log-determinant estimator

$\neq$

Recovery Objective (NMSE)

$$-\log(\det\Theta)+\mathrm{tr}(\widehat{\Sigma}\Theta)+\rho\,\|\Theta\|_{1,\mathrm{off}}$$

$$\|\widehat{\Theta}-\Theta^*\|_F^2\,/\|\Theta^*\|_F^2$$

# Limitations of Existing Optimization Algorithms

Limitations of the ***convex*** formulation → Consistency of estimator $\hat{\Theta}$

Based on ‘carefully chosen conditions’ like

1. Lower bound on sample size
2. Sparsity of $\Theta$
3. Degree of graph
4. Magnitude of covariance entries

Room for Improvement!

Pradeep Ravikumar, Martin J Wainwright, Garvesh Raskutti, Bin Yu, et al. High-dimensional covariance estimation by minimizing l1-penalized log-determinant divergence. Electronic Journal of Statistics, 5:935–980, 2011.

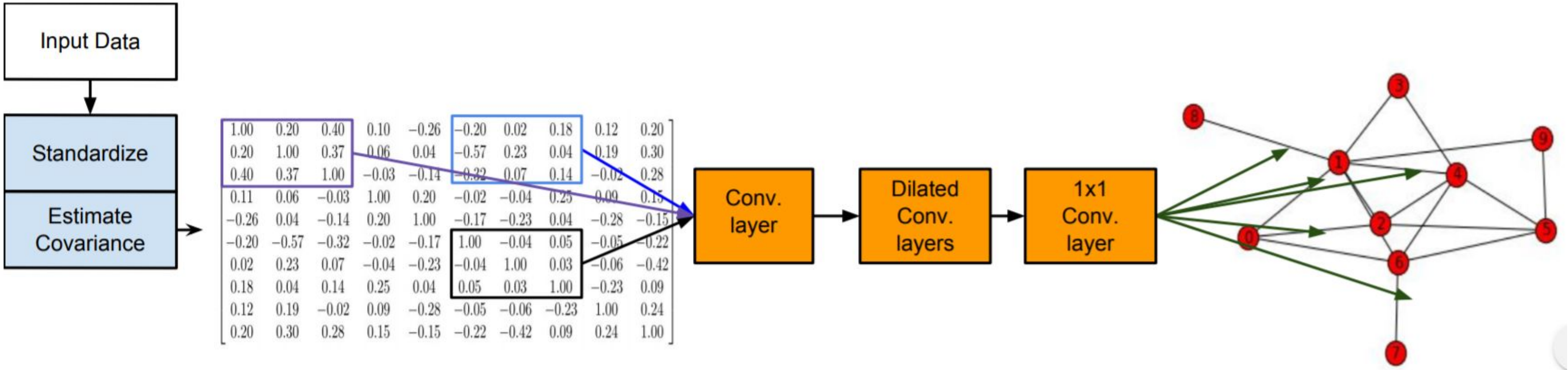
# Big Picture Question

- Given a collection of ground truth precision matrix $\Theta^*$, and the corresponding empirical covariance $\hat{\Sigma}$

- Learn an algorithm $f$ which directly produces an estimate of the precision matrix $\Theta$?

$$\min_f \frac{1}{|\mathcal{D}|} \sum_{(\hat{\Sigma}_i, \Theta_i^*) \in \mathcal{D}} \|\Theta_i - \Theta_i^*\|_F^2, \qquad s.t.\ \Theta_i = f(\hat{\Sigma}_i)$$

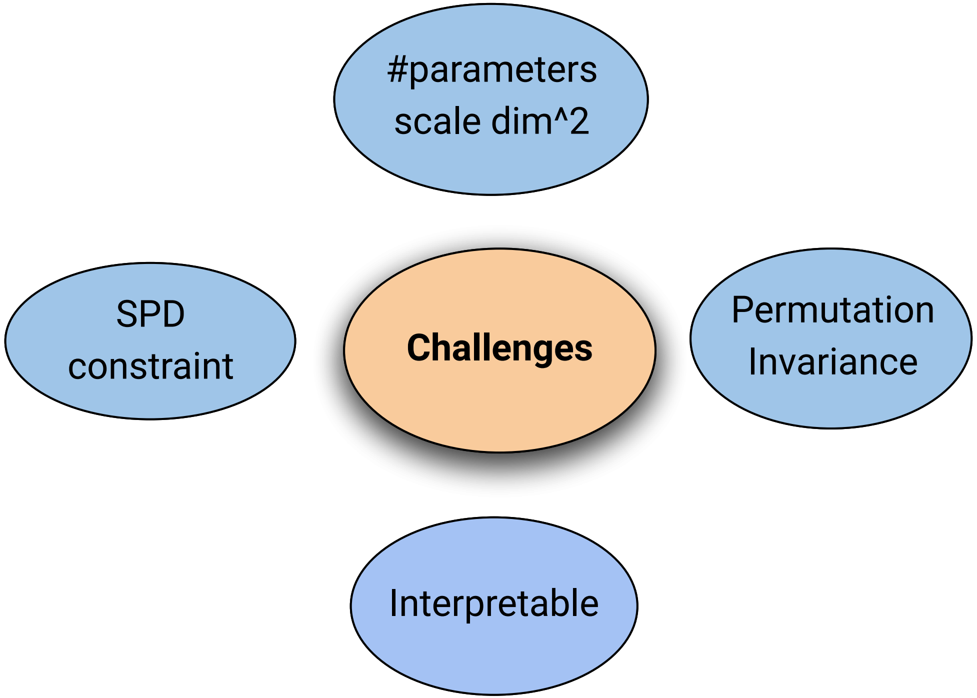
# Deep Learning Model Example



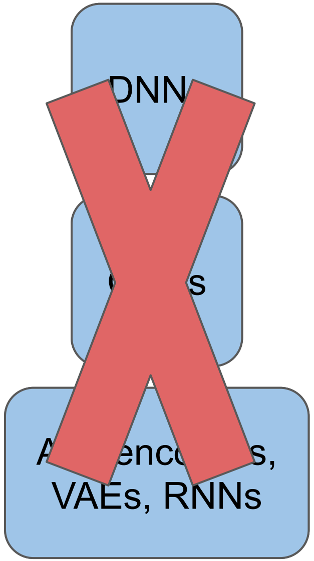

**DeepGraph (DG)**` architecture.The input is first standardized and then the sample covariance matrix is estimated. A neural network consisting of multiple dilated convolutions (Yu & Koltun, 2015) and a final 1 × 1 convolution layer is used to predict edges corresponding to non-zero entries in the precision matrix.

* DeepGraph-39 model from Fig.2 of “Learning to Discover Sparse Graphical Models” by Belilovsky et. al.

# Challenges in Designing Learning Models




Traditional Approaches



# GLAD: DL model based on Unrolled Algorithm

## Alternating Minimization (AM) algorithm: Objective function

$$\widehat{\Theta}_\lambda, \widehat{Z}_\lambda := \arg\min_{\Theta, Z \in \mathcal{S}^d_{++}} -\log(\det \Theta) + \mathrm{tr}(\widehat{\Sigma}\Theta) + \rho \|Z\|_1 + \frac{1}{2}\lambda \|Z - \Theta\|_F^2$$

## AM: Update Equations (Nice closed form updates!)

$$\Theta^{\mathrm{AM}}_{k+1} \leftarrow \frac{1}{2}\Big(-Y + \sqrt{Y^\top Y + \frac{4}{\lambda} I}\Big), \text{ where } Y = \frac{1}{\lambda}\widehat{\Sigma} - Z^{\mathrm{AM}}_k$$

$$Z^{\mathrm{AM}}_{k+1} \leftarrow \eta_{\rho/\lambda}(\Theta^{\mathrm{AM}}_{k+1}), \quad \text{where } \eta_{\rho/\lambda}(\theta) := \mathrm{sign}(\theta)\max(|\theta| - \rho/\lambda, 0)$$

**Modifications**

Unroll to fixed #iterations 'K'

Treat it as a deep model

# GLAD: Training

*Loss function:* Frobenius norm with discounted cumulative reward

$$\min_f \quad \text{loss}_f := \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K}\gamma^{K-k}\left\|\Theta_k^{(i)} - \Theta^{*(i)}\right\|_F^2$$

*Optimizer for training:* 'Adam'. Learning rate chosen between [0.01, 0.1] in conjunction with Multi-step LR scheduler.

*Gradient Computation through matrix square root in the GLADcell:*

For any SPD matrix *X*: $X = X^{1/2}X^{1/2}$

Solve Sylvester's equation for $d(X^{1/2})$:

$$dX = d(X^{1/2})X^{1/2} + X^{1/2}d(X^{1/2})$$

# Use Neural Networks for (ρ, λ)

$$\lambda \leftarrow \Lambda_{nn}(\|Z - \Theta\|_F^2, \lambda)$$

$$\rho_{ij} = \rho_{nn}(\Theta_{ij}, \widehat{\Sigma}_{ij}, Z_{ij})$$

# of layers = **2**
Hidden unit size = **3**

**Minimalist designing of Neural Networks**

# of layers = **4**
Hidden unit size = **3**

Non-Linearity:
Hidden layers = ‘*tanh*’
Final layer = ‘*sigmoid*’

# GLAD

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**Algorithm 1:** GLAD

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**Function** `GLADcell` $(\widehat{\Sigma}, \Theta, Z, \lambda)$**:**

$\quad \lambda \leftarrow \Lambda_{nn}(\|Z - \Theta\|_F^2, \lambda)$

$\quad Y \leftarrow \lambda^{-1}\widehat{\Sigma} - Z$

$\quad \Theta \leftarrow \frac{1}{2}\left(-Y + \sqrt{Y^\top Y + \frac{4}{\lambda}I}\right)$

$\quad$ **For** *all* $i, j$ **do**

$\qquad \rho_{ij} = \rho_{nn}(\Theta_{ij}, \widehat{\Sigma}_{ij}, Z_{ij})$

$\qquad Z_{ij} \leftarrow \eta_{\rho_{ij}}(\Theta_{ij})$

$\quad$ **return** $\Theta, Z, \lambda$

**Function** `GLAD` $(\widehat{\Sigma})$**:**

$\quad \Theta_0 \leftarrow (\widehat{\Sigma} + tI)^{-1}, \lambda_0 \leftarrow 1$

$\quad$ **For** $k = 0$ *to* $K - 1$ **do**

$\qquad \Theta_{k+1}, Z_{k+1}, \lambda_{k+1}$

$\qquad \leftarrow$ `GLADcell` $(\widehat{\Sigma}, \Theta_k, Z_k, \lambda_k)$

$\quad$ **return** $\Theta_K, Z_K$

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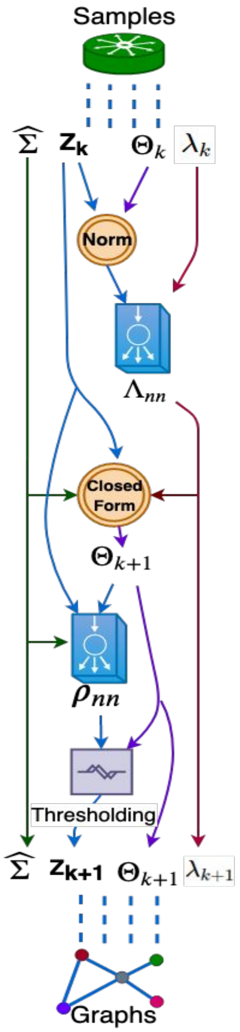
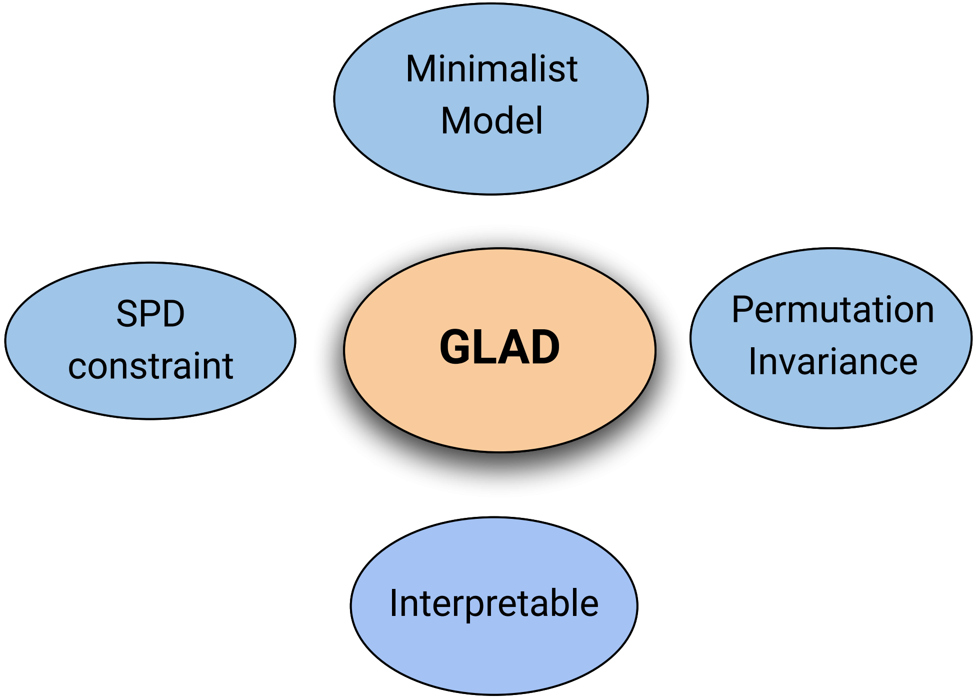
GLADcell




GLAD

Using algorithm structure as inductive bias for designing unrolled DL architectures

# Desiderata for GLAD




**Algorithm 1:** GLAD

**Function** GLADcell$(\widehat{\Sigma}, \Theta, Z, \lambda)$**:**

- $\lambda \leftarrow \Lambda_{nn}(\|Z - \Theta\|_F^2, \lambda)$
- $Y \leftarrow \lambda^{-1}\widehat{\Sigma} - Z$
- $\Theta \leftarrow \frac{1}{2}\big(-Y + \sqrt{Y^\top Y + \frac{4}{\lambda} I}\big)$
- **For** *all* $i, j$ **do**
  - $\rho_{ij} = \rho_{nn}(\Theta_{ij}, \widehat{\Sigma}_{ij}, Z_{ij})$
  - $Z_{ij} \leftarrow \eta_{\rho_{ij}}(\Theta_{ij})$
- **return** $\Theta, Z, \lambda$

**Function** GLAD$(\widehat{\Sigma})$**:**

- $\Theta_0 \leftarrow (\widehat{\Sigma} + tI)^{-1}, \lambda_0 \leftarrow 1$
- **For** $k = 0$ *to* $K - 1$ **do**
  - $\Theta_{k+1}, Z_{k+1}, \lambda_{k+1}$
  - $\leftarrow$GLADcell$(\widehat{\Sigma}, \Theta_k, Z_k, \lambda_k)$
- **return** $\Theta_K, Z_K$

**GLAD: G**raph recovery **L**earning **A**lgorithm using **D**ata-driven training

# Experiments: Convergence

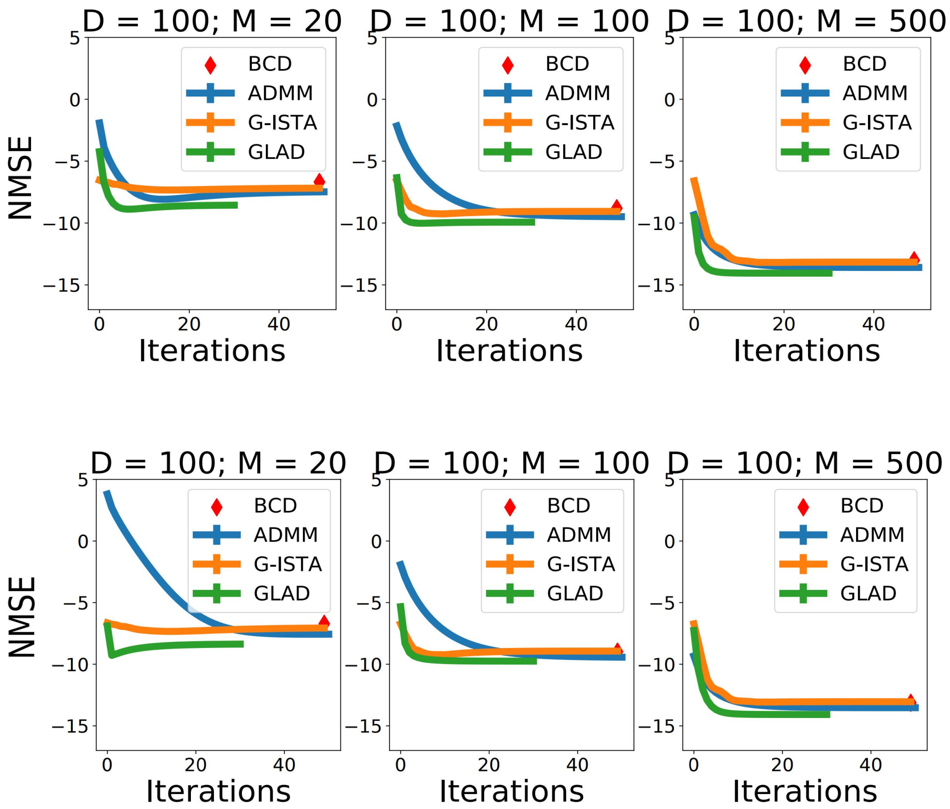
Train/finetuning using 10 random graphs

Test on 100 random graphs

GLAD vs traditional methods

Fixed Sparsity level s=0.1

Mixed Sparsity level s ~U(0.05, 0.15)

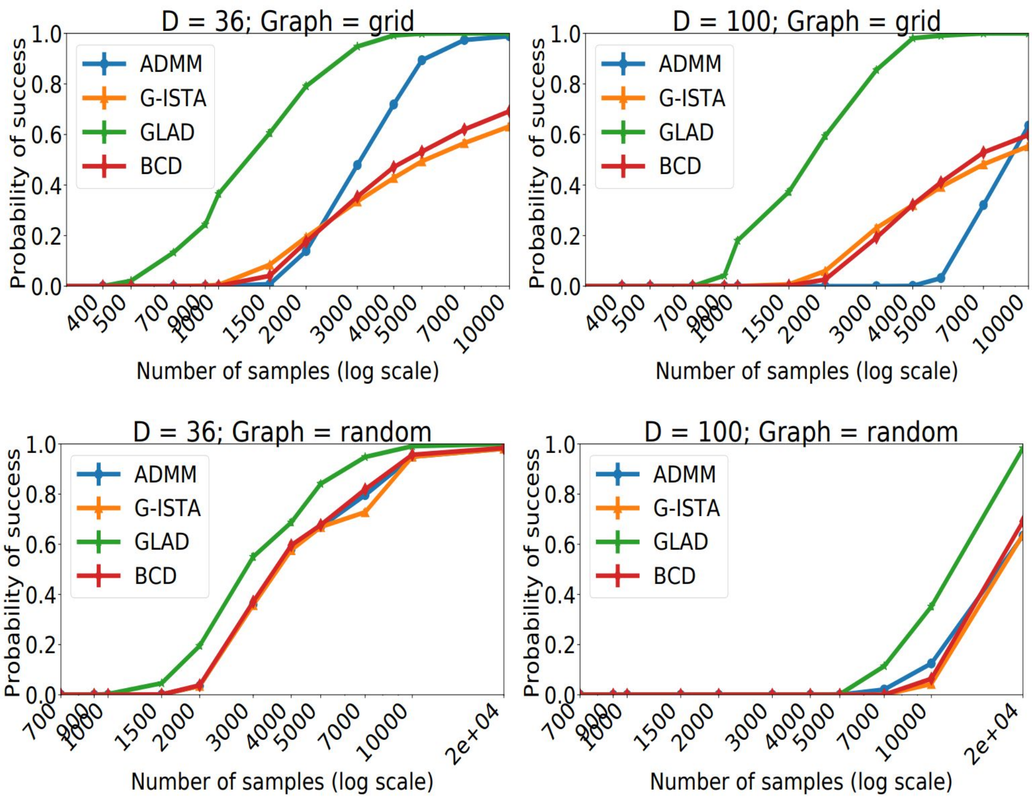


# Experiments: Recovery probability

Sample complexity for model selection consistency

PS is non-zero if all graph edges are recovered with correct signs

GLAD able to recover true edges with considerably fewer samples



# Experiments: Data Efficiency

GLAD vs DG-39*

Training graphs
100 vs 100,000

# of parameters
<25 vs >>>25

Runtime
< 30 mins vs
several hours

| Methods | M=15 | M=35 | M=100 |
|---|---|---|---|
| BCD | 0.578±0.006 | 0.639±0.007 | 0.704±0.006 |
| DeepGraph-39 | 0.664±0.008 | 0.738±0.006 | 0.759±0.006 |
| DG-39+P | 0.672±0.008 | 0.740±0.007 | 0.771±0.006 |
| **GLAD** | 0.788±0.003 | 0.811±0.003 | 0.878±0.003 |

**AUC**` on 100 test graphs with dimension=39, Gaussian random graph sparsity=0.05 and edge values sampled from ~U(-1, 1).

* DeepGraph-39 model from “Learning to Discover Sparse Graphical Models” by Belilovsky et. al.

` Table 1. of Belilovsky et. al.

# Gene Regulation Data: SynTReN details

Synthetic gene expression data generator creating biologically plausible networks

Models biological & correlation noises

SynTReN

The topological characteristics of generated networks closely resemble transcriptional networks

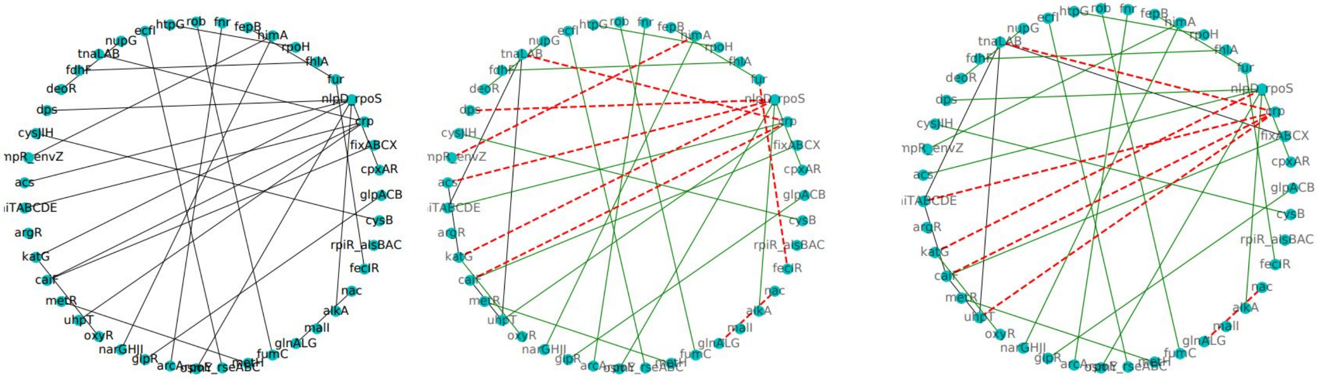
Contains instances of Ecoli bacteria and other true interaction networks

# Gene Regulation Data: Ecoli network predictions

GLAD trained on Erdos-Renyi graphs of dimension=25.

# of train/valid graphs were 20/20.

1 batch of M samples were taken per graph




(a) True graph

(b) **M=10**, fdr=0.613, tpr=0.913, fpr=0.114

(c) **M=100**, fdr=0.236, tpr=0.986, fpr=0.024

Recovered graph structures for a sub-network of the E. coli consisting of 43 genes and 30 interactions with increasing samples. All noises sampled ~U(0.01, 0.1) Increasing the samples reduces the fdr by discovering more true edges.

# Theoretical Analysis: Assumptions

**Assumption 1.** *Let the set* $S = \{(i,j) : \Theta^*_{ij} \neq 0, i \neq j\}$. *Then* $card(S) \leq s$.

**Assumption 2.** $\Lambda_{\min}(\Sigma^*) \geq \epsilon_1 > 0$ *(or equivalently* $\Lambda_{\max}(\Theta^*) \leq 1/\epsilon_1$*),* $\Lambda_{\max}(\Sigma^*) \leq \epsilon_2$ *and an upper bound on* $\|\widehat{\Sigma}\|_2 \leq c_{\widehat{\Sigma}}$.

Assumption 1 just upper bounds sparsity.

Assumption 2 guarantees that ϴ* exists.

# Theoretical Analysis: Linear Convergence of AM

## Recalling AM

An adaptive sequence of penalty parameters should achieve a better error bound

$\Theta_{k+1}^{\text{AM}} \leftarrow \frac{1}{2}\Big($ … $\frac{1}{\lambda}\widehat{\Sigma} - Z_k^{\text{AM}}$

$Z_{k+1}^{\text{AM}} \leftarrow \eta_{\rho/\lambda}(\Theta_{k+1}^{\text{AM}})$, where $\eta_{\rho/\lambda}(\theta) := \text{sign}(\theta)\max(|\theta| - \rho/\lambda, 0)$

**Theorem 1.** *Under the assumptions 1 & 2,* …

**Summary**

Optimal parameter values depends on the prediction error. Hard to choose manually

*… n and m is the number of … linear convergence rate for optimization objective defined in … algorithm satisfies,*

AM has linear convergence rate. Can run for fixed iterations with reasonable error margins

$$\|\Theta_k^{\text{AM}} \ldots \sqrt{\frac{(\log d)/m}{\min(\frac{1}{(d+s)}, \frac{\lambda}{d^2})}}\Bigg),$$

*where* $0 < C_\lambda < 1$ *is* …

# Conclusion

Unrolled DL architecture, GLAD, for sparse graph recovery

Empirically, GLAD is able to reduce sample complexity

Empirical evidence that learning can improve graph recovery

Highlighting the potential of using algorithms as inductive bias for DL architectures

Thank you!