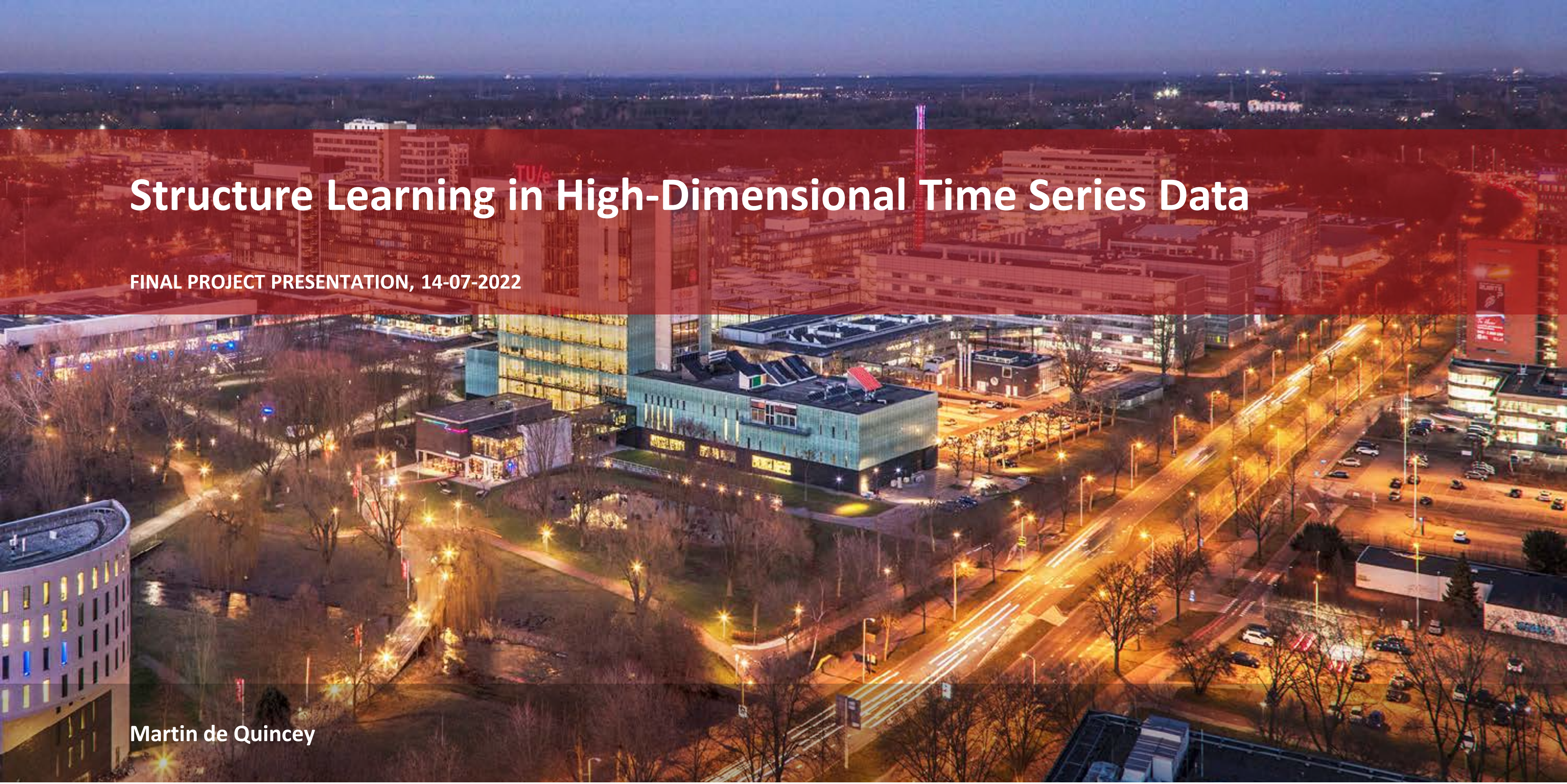

Structure Learning in High-Dimensional Time Series Data

FINAL PROJECT PRESENTATION, 14-07-2022

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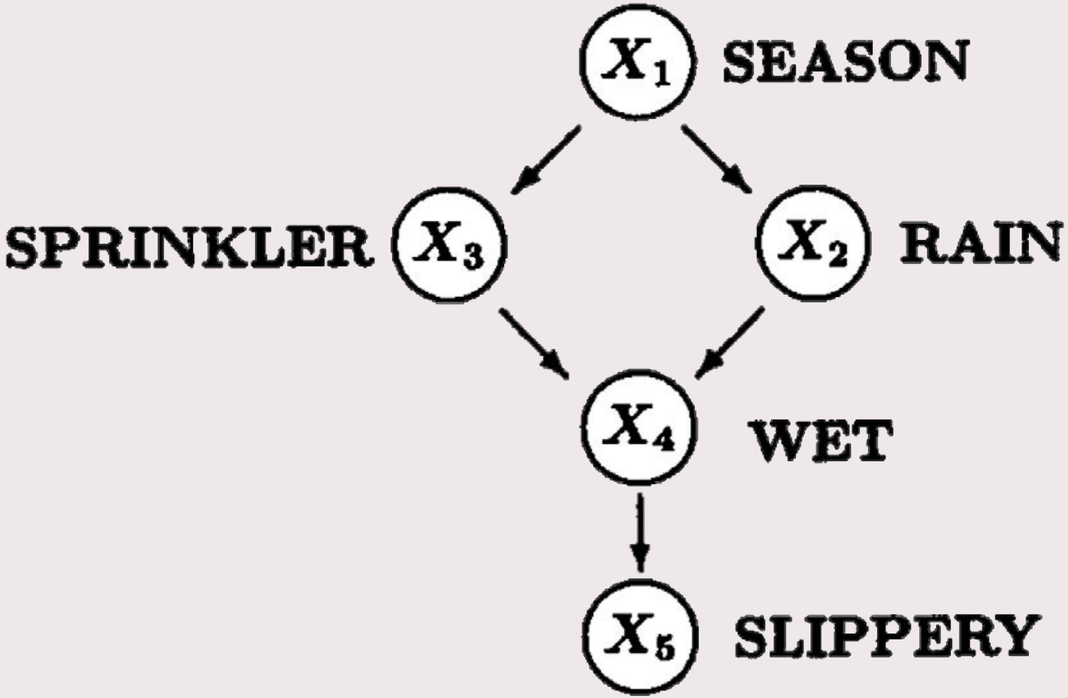
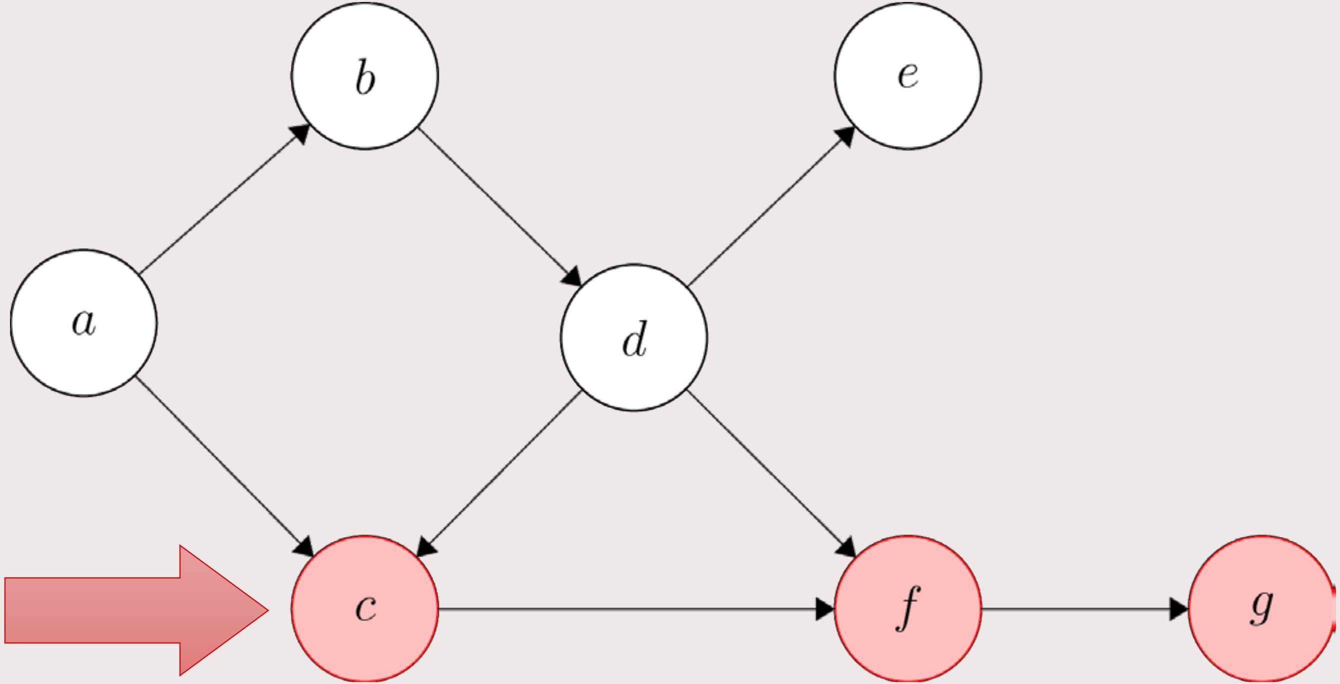
Problem Setting

- Based on time series data, learn the *structure* of a graphical model
- Arc (x, y) => x “is useful” in predicting y
- Inferred structure *must* be *acyclic*

Problem Setting – Example [1]



Motivation – Root Cause Analysis in Complex Systems



Formal Problem Setting

- A data-matrix $\boldsymbol{X} \in \mathbb{R}^{T \times p}$.
- Learn the structure, or joint density $\mathbb{P}(\boldsymbol{X})$
- Assumptions
  - Only depends on previous time step $t - 1$
  - Relations are *linear*
  - Random noise is *Gaussian*
  - No cyclic dependencies

Model

- Assume a Vector AutoRegressive model of order 1:

$$\boxed{\begin{gathered} X_{t,\cdot} = X_{t-1,\cdot}W + \boldsymbol{\varepsilon}, \\ X_{t,\cdot} \in \mathbb{R}^{p}, \qquad W \in \mathbb{R}^{p \times p}, \qquad \boldsymbol{\varepsilon} \sim \mathcal{N}(0, I). \end{gathered}}$$

- Objective: Given $\boldsymbol{X} \in \mathbb{R}^{T \times p}$, find most likely acyclic W

$$\widehat{W} = \arg\min_{W} \frac{1}{T-1} \sum_{t=2}^{T} \left\| X_{t,\cdot} - X_{t-1,\cdot} W \right\|_2^2 \text{ such that } W \text{ is acyclic}$$

Methodologies

- Permutation-Based
  - Greedy Random Walk
- Iterative
  - Orthogonal Matching Pursuit
- Continuous
  - NOTEARS

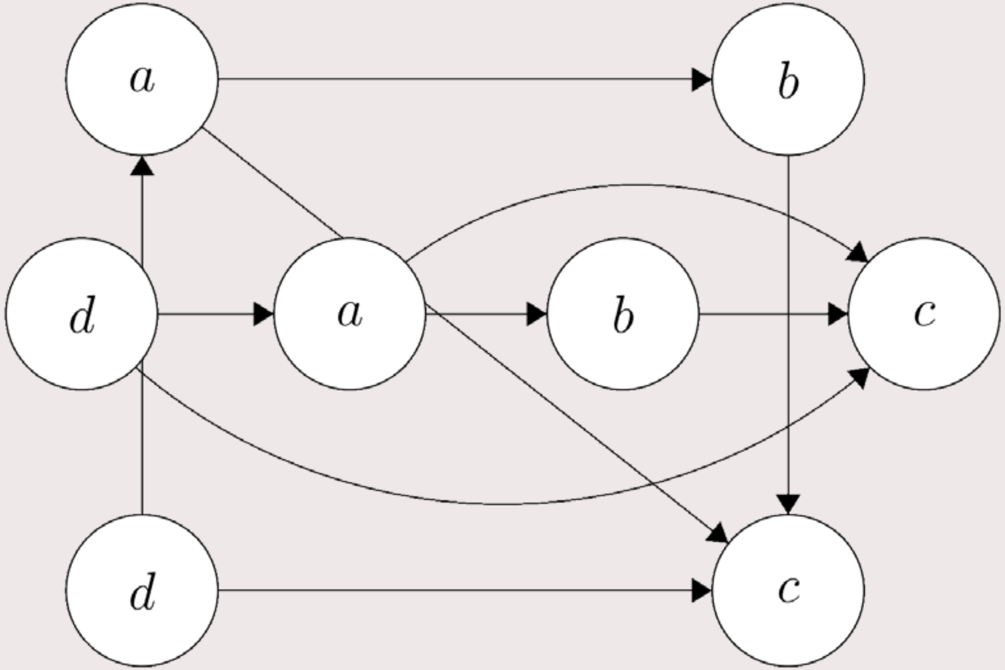
1) Orderings

- Biggest obstacle: Make sure that W is acyclic
- W is acyclic $\Leftrightarrow W = P^T U P$
- Given ordering P, we can easily find a suitable U
- New obstacle: Search the space of orderings $\mathcal{P}$ for a suitable P

1) Orderings

$$
\begin{array}{c c}
 & \begin{array}{cccc} a & b & c & d \end{array} \\
\begin{array}{c} a \\ b \\ c \\ d \end{array} & \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \end{pmatrix}
\end{array}
$$

$$
\begin{array}{c c}
 & \begin{array}{cccc} d & a & b & c \end{array} \\
\begin{array}{c} d \\ a \\ b \\ c \end{array} & \begin{pmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\end{array}
$$



1) Random Walk

- Exhaustively trying all orderings is $\mathcal{O}(p!)$
- Random walk on the set of orderings
- Possible transitions: Swapping two variables in the ordering

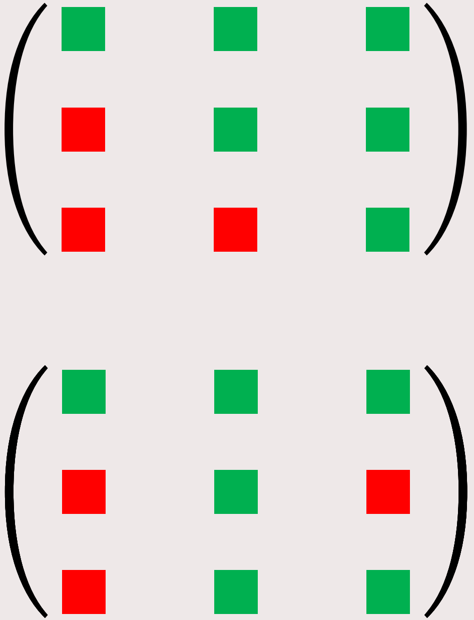
1) Greedy Random Walk

- Randomly swap the order of two variables
- Transition to this new ordering if it achieves a better score
- Iterate until time-out

1) Greedy Random Walk

: estimated ($\neq 0$) : not estimated ($= 0$)

- Ordering $(1, 2, 3)$.
- Try $(1, 3, 2)$ $\implies$ no improvement.
- Try $(2, 1, 3)$ $\implies$ improvement.
- Try $(2, 3, 1)$ $\implies$ no improvement.
- Try $(3, 2, 1)$ $\implies$ improvement.
- No improvements found.



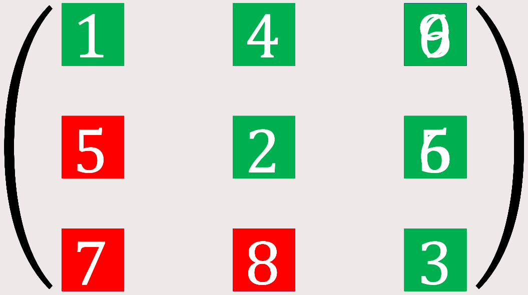
2) Orthogonal Matching Pursuit

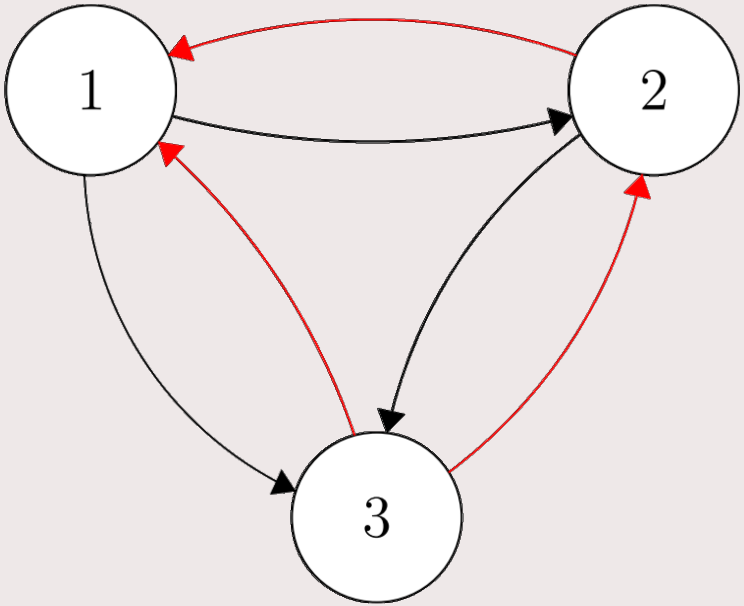
- Start with an empty matrix W
- Add the arc (i, j) yielding the largest *correlation* with the current residual:

$$(i, j) = \arg\max_{(i,j)} \frac{|\langle X_i,\ r_j \rangle|}{\|X_i\| \cdot \|r_j\|}.$$

- If this arc creates a cycle, exclude it and continue
- Continue until stopping criterion

2) Orthogonal Matching Pursuit





: not decided yet

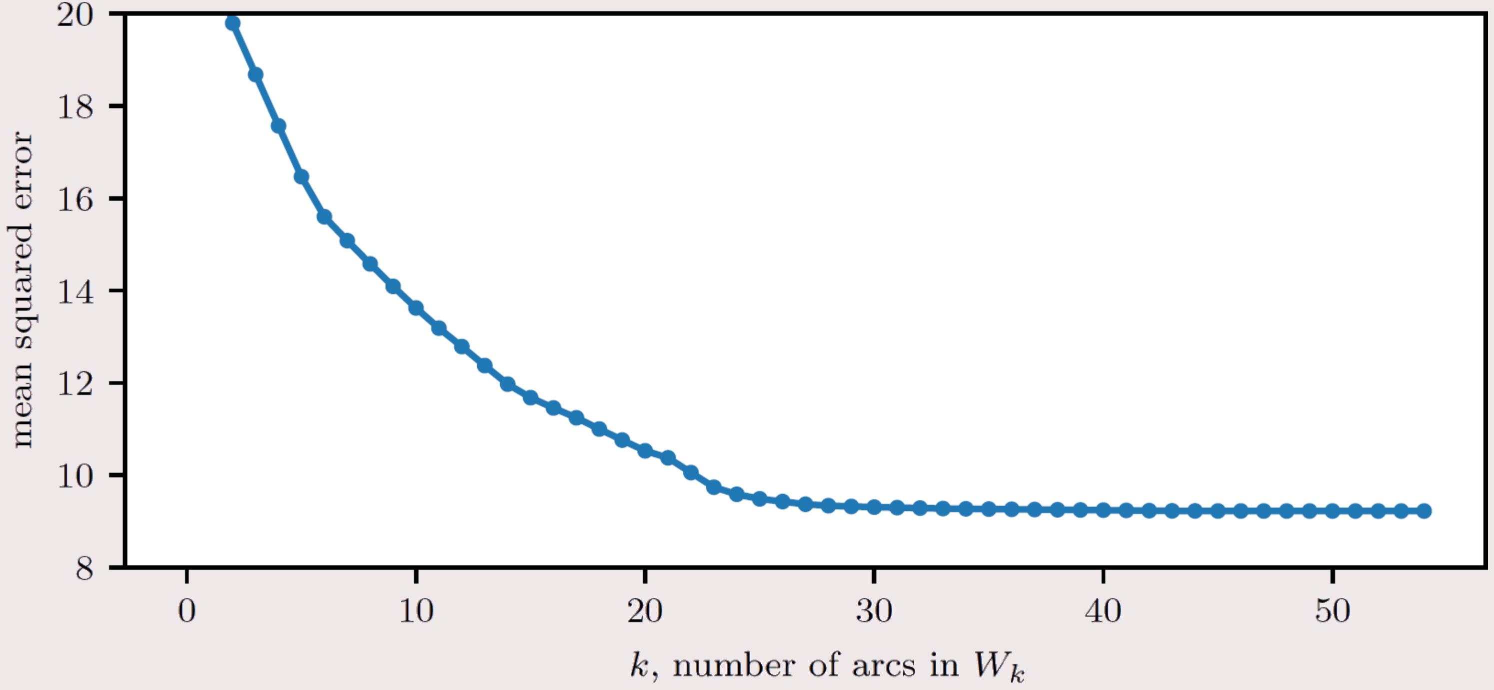
: estimated ($\neq 0$)

: not estimated ($= 0$)

2) Selecting a suitable number of arcs

- Iterative approaches constructs W one arc per iteration
- The gain in predictive performance decreases as we add more arcs
- When does adding an arc not yield sufficient gain anymore?

2) Selecting a suitable number of arcs



2) Selecting a suitable number of arcs

- Leave-one-out cross-validation

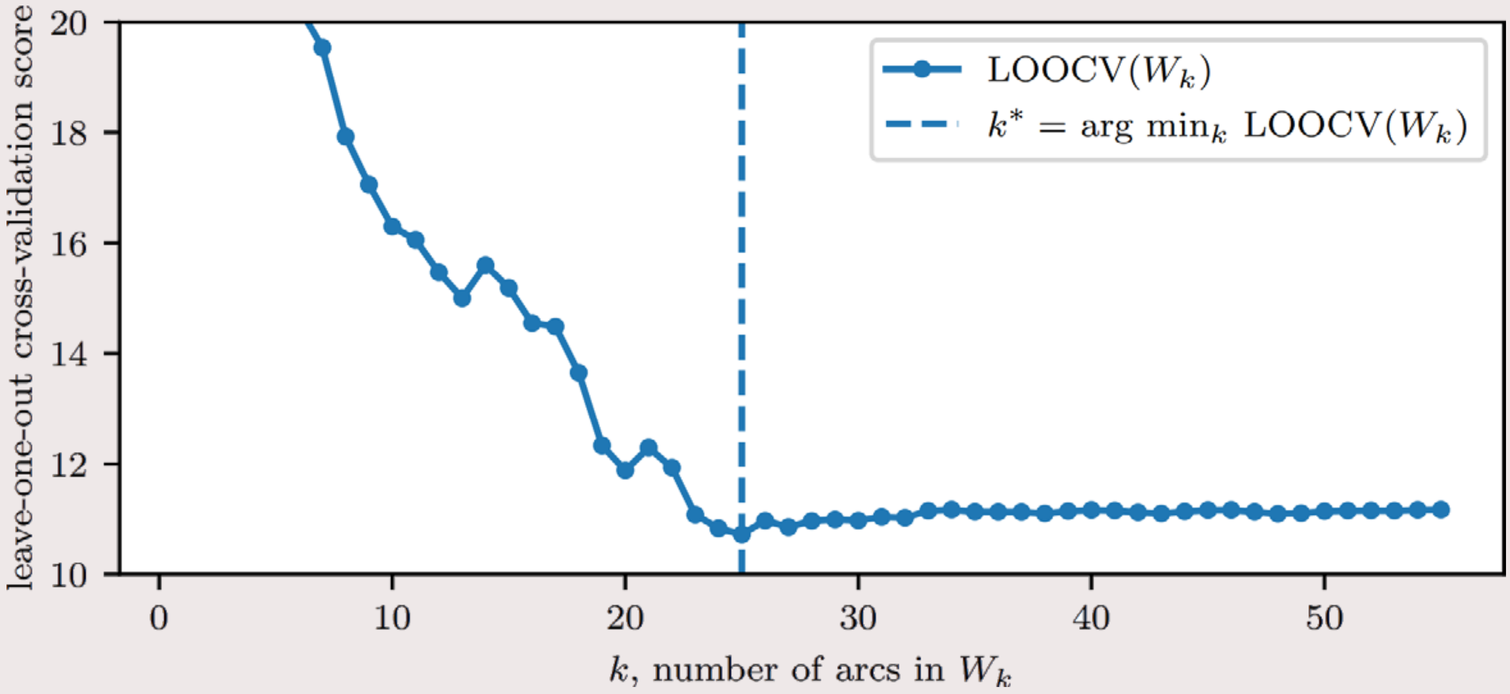
$$\mathrm{LOOCV}_t(W_k) = \left\| X_{t,\cdot} - X_{t-1,\cdot} W_k^{(-t)} \right\|_2^2$$

$$\mathrm{LOOCV}(W_k) = \frac{1}{T-1} \sum_{t=2}^{T} \mathrm{LOOCV}_t(W_k)$$

- How to choose a suitable number of arcs?

$$k^* = \arg\min_k \mathrm{LOOCV}(W_k)$$

2) Selecting a suitable number of arcs



3) NOTEARS

- Paper from 2015 by Xun Zheng et al. [2]

- Translated the problem from

$$\min_W \frac{1}{T-1}\sum_{t=2}^{T}\left\|X_{t,\cdot} - X_{t-1,\cdot}W\right\|_2^2$$
$$\text{such that } W \text{ is acyclic,}$$

to

$$\min_W \frac{1}{T-1}\sum_{t=2}^{T}\left\|X_{t,\cdot} - X_{t-1,\cdot}W\right\|_2^2$$
$$\text{such that } h(W) = 0.$$

- $h(W) = 0 \Leftrightarrow W$ is acyclic.

Experimental Results

1. Vary number of variables $p \in \{5, 10, 15, 25, 50\}$.

2. Generate ten acyclic W with a total of $s = 3p$ arcs per value of p

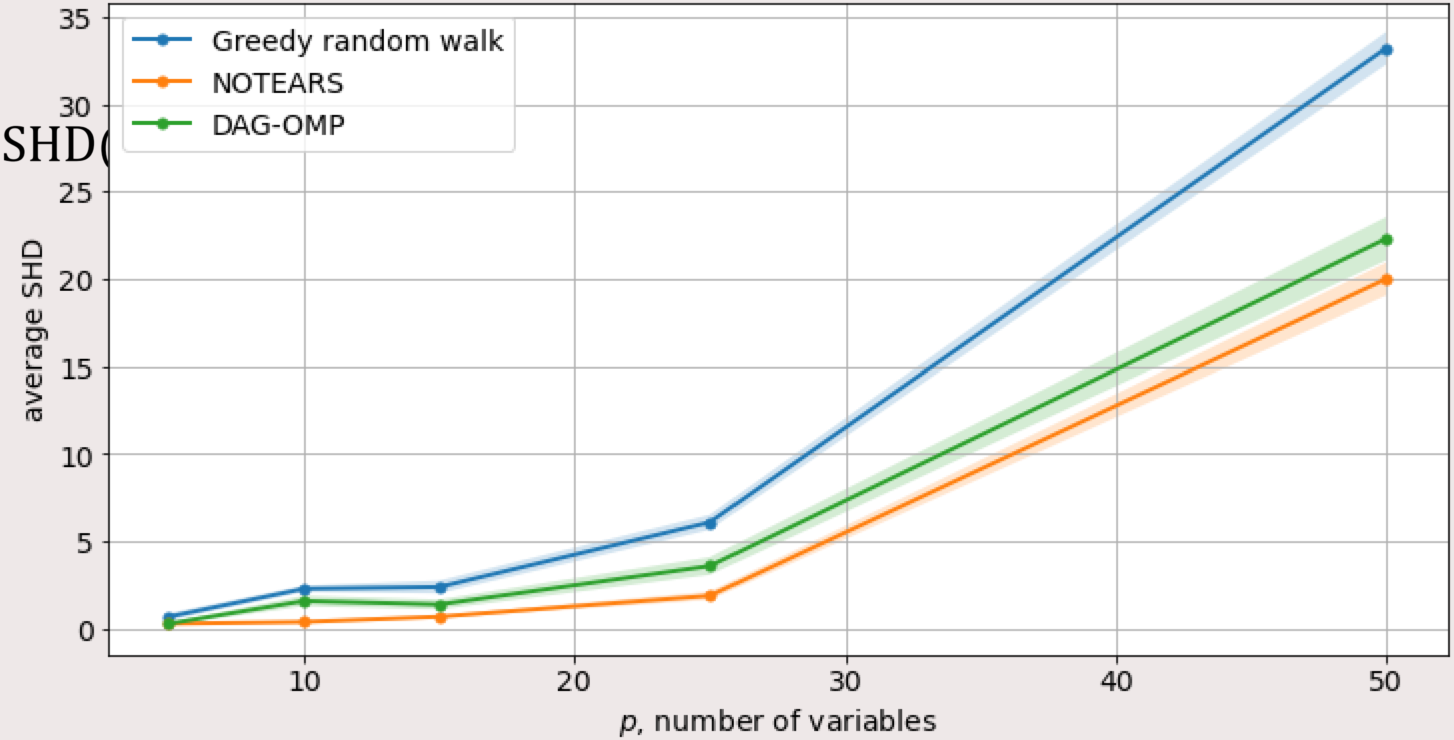
3. Generate ten data matrices $\boldsymbol{X}$ of 1000 time steps

4. Estimate $\widehat{W}$ using all three methods

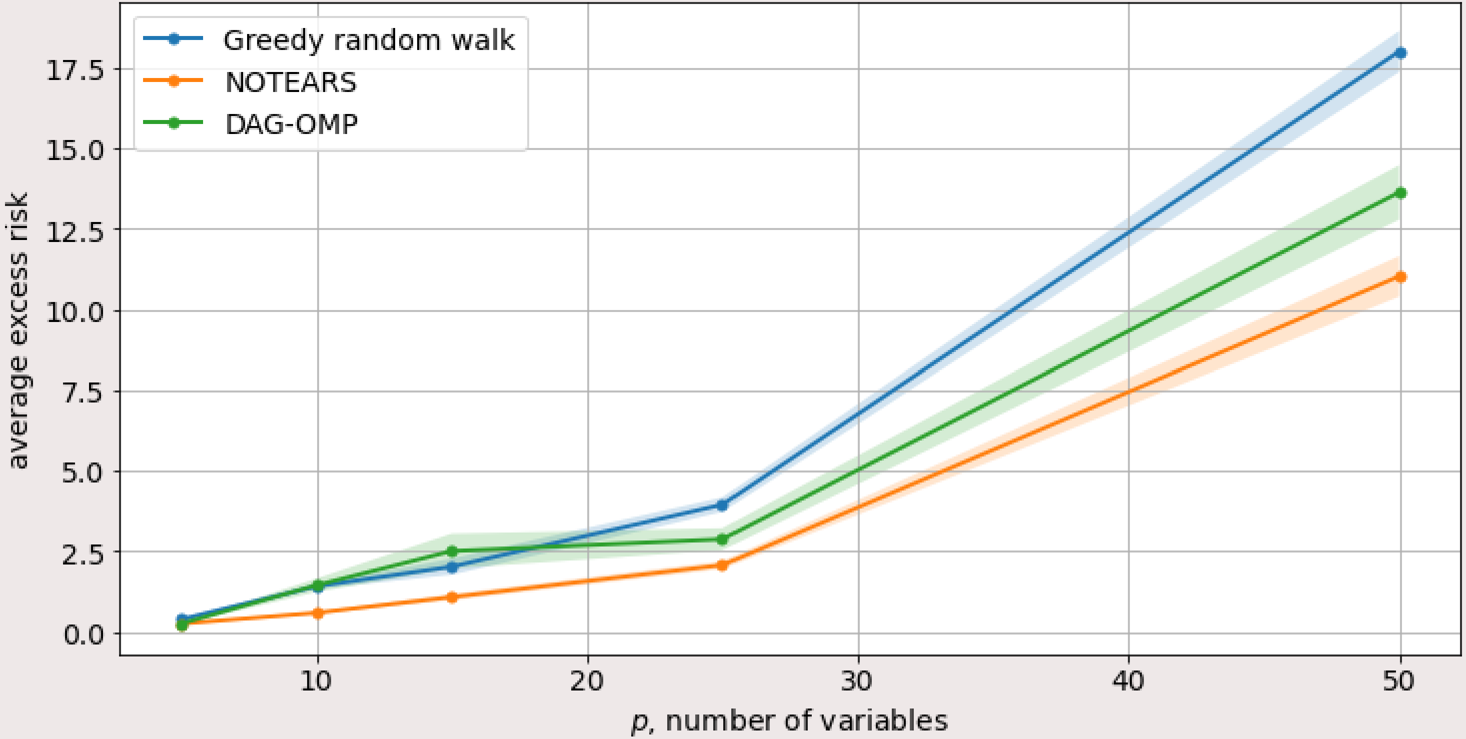
5. Compare Structural Hamming Distance and Excess Expected Loss

Structural Hamming Distance

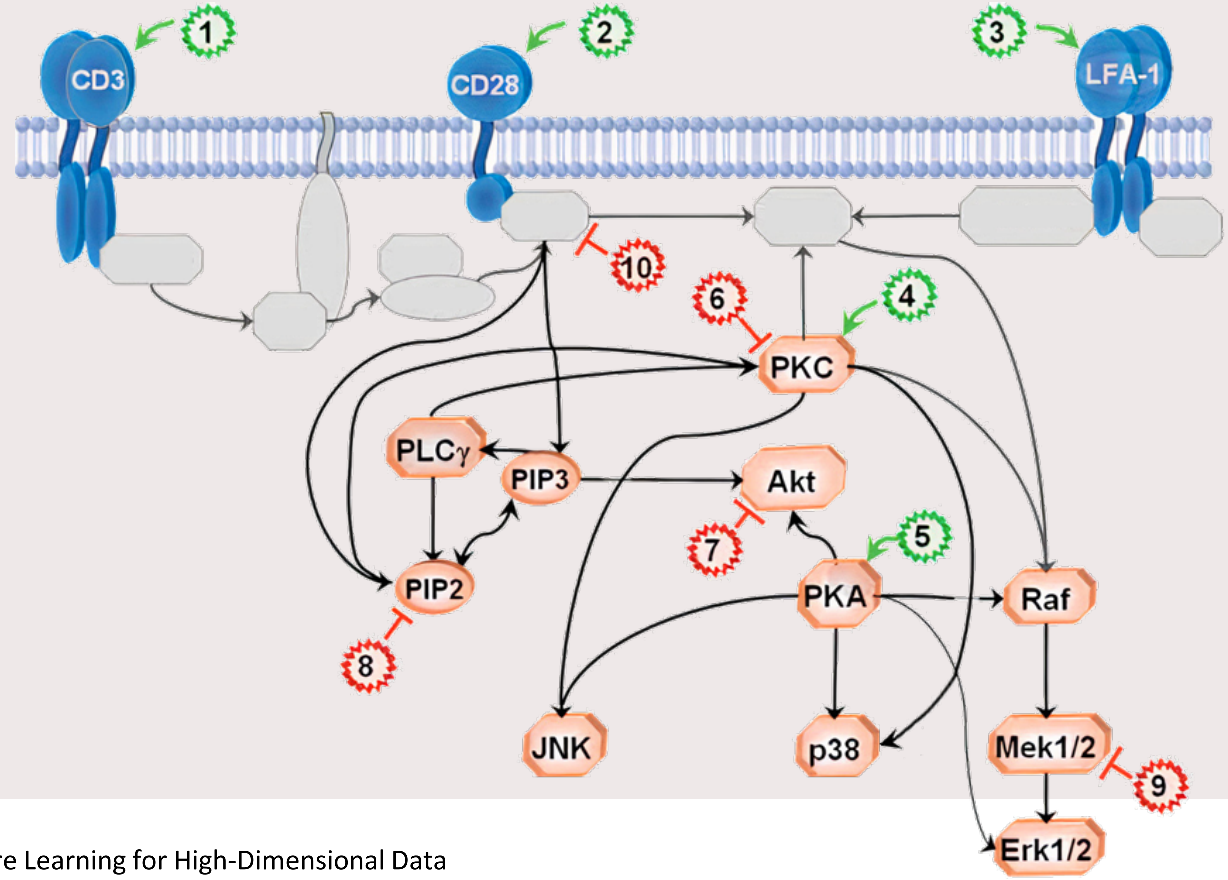
- SHD(



Expected Excess Risk



Recovering causal pathways using structure learning



Recovering causal pathways using structure learning

Method	Predicted arcs	TP (out of 20)	SHD	Empirical Risk
Random Walk	*13*	*6*	*21*	*5.037*
Regular MH	*15*	*7*	*21*	*5.051*
Greedy MH	17	**8**	21	**4.998**
NOTEARS	16	**8**	22	5.032
DAG-OMP	17	**8**	21	5.000
DAG-OLS-V	*14*	*7*	***20***	*5.156*

TU/e

Conclusions

- Structure learning for high-dimensional data
- Two methods competitive with state of the art
- Greedy Random Walk
  - Performs well on sparse graphs
  - Competitive in low-dimensional settings
- Orthogonal Matching Pursuit
  - Method is very fast ($\approx 1{,}000$ times faster than NOTEARS)
  - Competitive in high-dimensional settings

Future Directions

- Extending the model
- Investigate regularization
- Statistical guarantees

References

[1] Pearl, J. (1997). Causality: Models, Reasoning, and Inference, Second Edition, p.15.

[2] Zheng, X., Aragam, B., Ravikumar, P., Xing, E. (2018) DAGs with NO TEARS: Continuous Optimization for Structure Learning. *Proceedings of the 32nd International Conference on Neural Information Processing Systems.* p.9492-9503.