# Estimating high-dimensional directed acyclic graphs with the PC-algorithm

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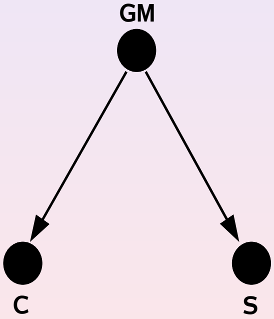
# Overview

1. DAG and its skeleton
2. PC-algorithm
3. Consistency
4. Simulation
5. Application

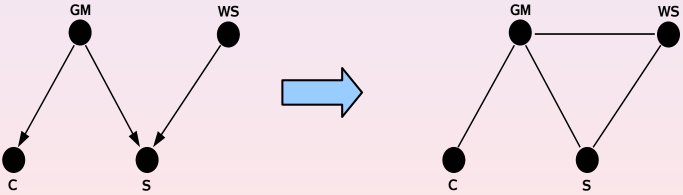
# Directed Acyclic Graphs (DAGs)



- Nodes: Random Variables
- Edges: Some Dependence
- Recursive factorization: $f(GM, C, S) = f(GM)f(C|GM)f(S|GM)$
- We assume Multivariate Normal Distribution

# Directed Global Markov Property

- DAG implies conditional independence relations
- $C \perp S | GM \iff C, S$ are separated by $GM$ in $(G_{An(C \cup S \cup GM)})^m$



- Ancestral set
- Moralize
- Drop directions

# Faithfulness

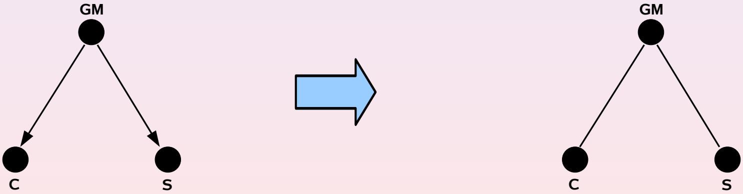
Conditional independence relations implied by DAG

=

Conditional independence relations of distribution

# Skeleton of a DAG

- Ignore directions of arrows
- Edge between two nodes $A$ and $B$ $\iff$ $A, B$ are dependent given every subset of remaining nodes



# The PC-algorithm for finding a DAG

- **Finding the skeleton:**

```
Form complete graph $G$
$l = -1$
repeat
    $l = l + 1$
    repeat
        select (new) ordered pair of adjacent nodes $A, B$ in $G$
        select (new) neighborhood $N$ of $A$ with size $l$ (if possible)
        if $A, B$ are cond. indep. given $N$
            save $N$ in $\mathbf{N}$
            delete edge $A, B$ in $G$
    until all ordered pairs have been tested
until all neighborhoods are of size smaller than $l$
```

- **Finding the DAG:** The skeleton can be directed using **N** and four simple rules.

# Sample Version of the PC-algorithm

- Real World: Cond. Indep. Relations $A \perp B|S$ are not known
- Instead: Test for partial correlation $\rho_{AB|S} = 0$ (due to Gaussian assumption)

**Therefore:**
Remove edge if test for $\rho_{AB|S} = 0$ cannot be rejected for some $S$ on level $\alpha$.

# Consistency: Assumptions

$n$: Number of samples, $p$: Number of nodes

- Multivariate Normality, Faithfulness
- Nodes: $p_n = O(n^a)\ 0 \leq a < \infty$ (**high-dimensional**)
- Max number of neighbors is $O(n^{1-b})\ 0 < b \leq 1$ (**sparse**)
- Bounded partial correlations ($0 < d < \frac{b}{2}$):
  $\inf\{|\rho_{ij|\mathbf{k}}|; \rho_{ij|\mathbf{k}} \neq 0\} \geq c_n,\ c_n^{-1} = O(n^d)$ (**larger than** $\frac{1}{\sqrt{n}}$)
  $\sup\{|\rho_{ij|\mathbf{k}}|\} \leq M < 1$

# Consistency: Main Result

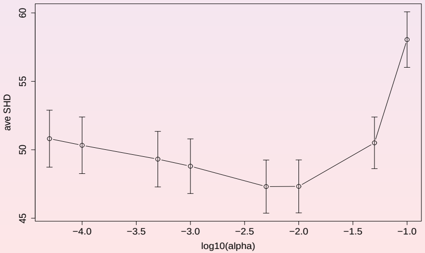
**Under these assumptions:**

There exists some $\alpha_n \rightarrow 0$ $(n \rightarrow \infty)$ so that

$P$(estimated DAG = true DAG) $= 1 - O(\exp(-Cn^{1-2d})) \rightarrow 1$
$(n \rightarrow \infty) \quad \text{for} \quad 0 < C < \infty$

# Choice of $\alpha$

- Structural Hamming Distance (SHD) measures distance between estimated and true graph.
- Over a wide range of parameters the average SHD is minimized for significance levels between $\alpha = 0.005$ and $\alpha = 0.001$.
- In practice: Either choose default values for $\alpha$ or generate priority list of edges

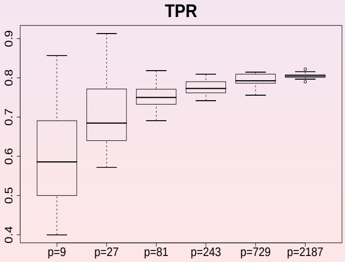


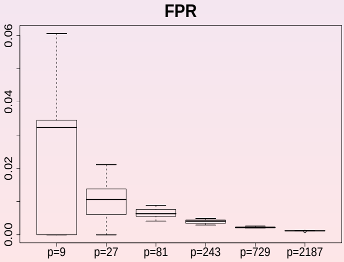
# Performance

**Computing Time:** $p = 1000, n = 1000, E[N] = 8 \rightarrow t \sim 1h$
**Estimation:**

- Number of variables $p$ increases exponentially
- Number of samples $n$ increases linearly
- Expected size of neighborhood $E[N] = \sqrt{n}$ increases sublinearly

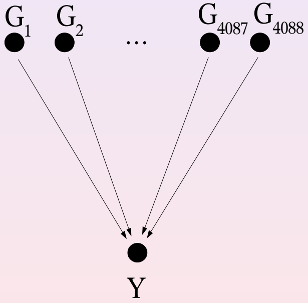
Then: TPR increases, FPR decreases





# Application

Production of Riboflavin (Vitamin $B_2$) in Bacillus Subtilis

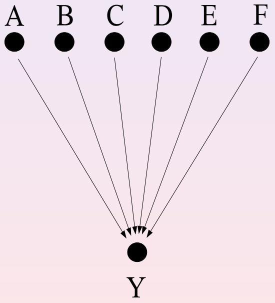


- **Goal:** Maximize output of Riboflavin $Y$ by manipulating genes
- Data obtained by Affymetrix B. subtilis GeneChips from DSM Nutritional Products
- Number of Variables $p = 4088$, number of samples $n = 50$

Which genes have an influence on $Y$?

# Application 2

## Result



- Small number of stable candidates extracted
- They are a subset of genes found with other techniques (Lasso, Elastic Net,. . . )
- Findings promising from a biological point of view
- Experimental testing in progress

# Conclusion

- DAG, Skeleton, Dependence
- PC-algorithm finds true DAG/skeleton consistently (under some assumptions)
- PC-algorithm is fast for sparse graphs
- More information:  
  M. Kalisch and P. Bühlmann  
  Estimating High-Dimensional Directed Acyclic Graphs with the PC-algorithm  
  JMLR 8 (2007)
- R-package `pcalg` for the PC-algorithm (including robust version)