RCOX models: Graphical Gaussian models with edge and vertex symmetries

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Joint work with

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and

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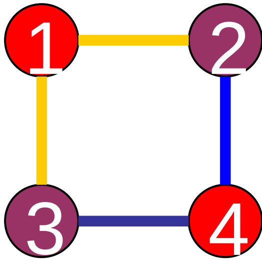
Take-home message and Outline

- **New types of graphical Gaussian models**
  - With colours; as in the logo
  - Attribute specific meanings to the colours

- **An R-package (gRc) for inference in these models**

- **Motivation**
- **RCO'X' models: RCON, RCOR, RCOP**
- **Estimation algorithms**
- **Software**

Idea…

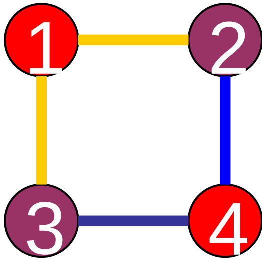


- **Apply graphical (Gaussian) models to large matrices, e.g. in gene expression**
- **Problem: d >>n, many genes few replicates**

Graphical model for $Y \sim N_d(0,\Sigma)$

- **When d >n, MLE of Σ does not exist (in saturated model)**
- **Impose restrictions on $K=\Sigma^{-1}$ to achieve more parsimonious model;**
- **In addition to conditional independence, restrict parameters to being identical**

Concentration and derived quantities



- Model for $y \sim N_d(0, \Sigma)$, $K = (k^{ij}) = \Sigma^{-1}$.
- The partial (conditional) covariance :

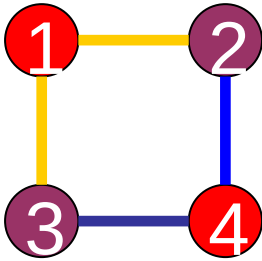
$$cov(y_i, y_j | rest) = \frac{-k^{ij}}{\det K^{ij}} \text{ where } K^{ij} = \begin{bmatrix} k^{ii} & k^{ij} \\ k^{ij} & k^{jj} \end{bmatrix}$$

- The partial (conditional) correlation:

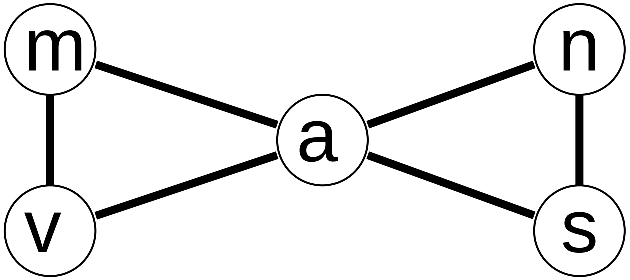
$$cor(y_i, y_j | rest) = \rho^{ij} = \frac{-k^{ij}}{\sqrt{k^{ii} k^{jj}}}$$

- Conditional independence: $y_i \perp\!\!\!\perp y_j | rest$ iff $k^{ij} = 0$

Example: Mathematics marks

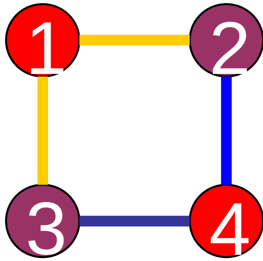


- **Mathmark data (Mardia, Kent, Bibby): 88 students marks on (a)lgebra, a(n)alysis, (m)echanics, (v)ectors and (s)tatistics**
- **Stepwise backward selection gives butterfly model**



- Convention: Black and white are neutral colours - corresponding parameters are unrestricted.

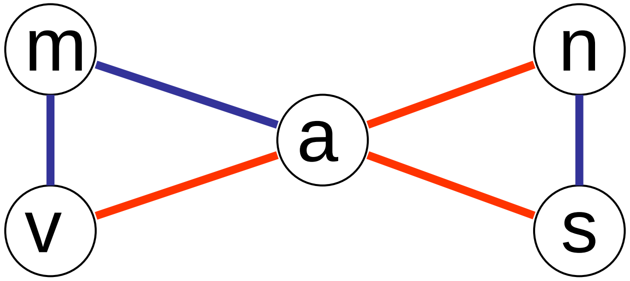
Concentrations for mathmarks



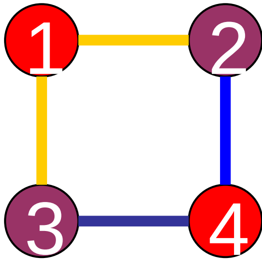
Concentrations ($\times 1000$):

	mechanics	vectors	algebra	analysis	statistics
mechanics	5.24	−2.44	−2.74	0.01	−0.14
vectors	−2.44	10.43	−4.71	−0.79	−0.17
algebra	−2.74	−4.71	26.95	−7.05	−4.70
analysis	0.01	−0.79	−7.05	9.88	−2.02
statistics	−0.14	−0.17	−4.70	−2.02	6.45

- **Some concentrations $\approx$ 0**
- **Some concentrations $\approx$ identical**



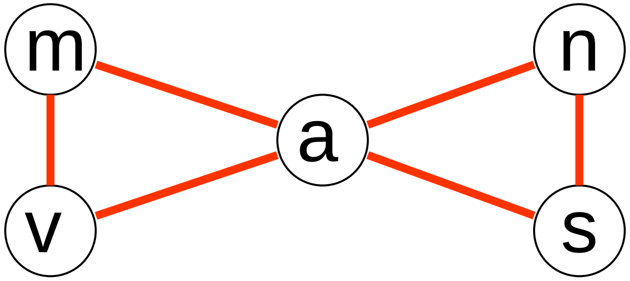
Partial correlations for mathmarks



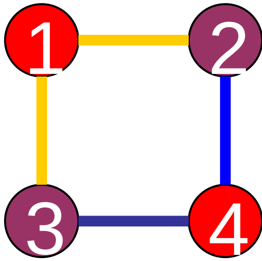
Partial correlations:

	mechanics	vectors	algebra	analysis	statistics
(m)echanics	1.00	−0.30	−0.20	0.00	0.00
(v)ectors	−0.30	1.00	−0.30	−0.10	0.00
(a)lgebra	−0.20	−0.30	1.00	−0.40	−0.40
a(n)alysis	0.00	−0.10	−0.40	1.00	−0.30
(s)tatistics	0.00	0.00	−0.40	−0.30	1.00
Partial variances	190.67	95.91	37.10	101.18	155.04

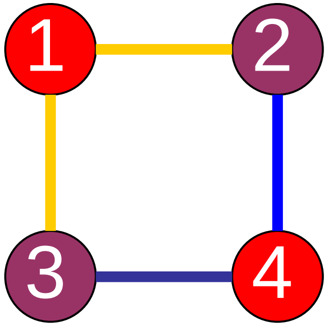
- **Some partial correlations ≈ identical**



RCON (Restricted CONcentration) models



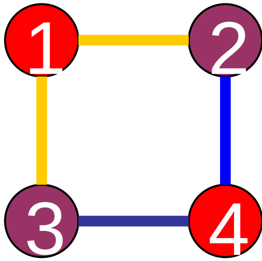
Model: $Y \sim N_d(0,\Sigma)$



$$K = \Sigma^{-1} = \begin{bmatrix} k^{11} & k^{12} & k^{13} & 0 \\ k^{12} & k^{22} & 0 & k^{24} \\ k^{13} & 0 & k^{33} & k^{34} \\ 0 & k^{24} & k^{34} & k^{44} \end{bmatrix}$$

- Markov properties as for graphical Gaussian model
- Entries of K with same colour restricted to being identical $\rightarrow$ 4 rather than 8 parameters.

# Implied restrictions (I): Equal contributions in regression



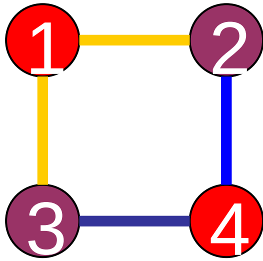
- **Regressing y_1 on y_2, y_3, y_4**

$$y_1 = a_1 - (k^{12}/k^{11})\, y_2 - (k^{13}/k^{11})\, y_3$$

- so y_2 and y_3 contribute equally because $k^{12} = k^{13}$

$$K = \Sigma^{-1} = \begin{bmatrix} k^{11} & k^{12} & k^{13} & 0 \\ k^{12} & k^{22} & 0 & k^{24} \\ k^{13} & 0 & k^{33} & k^{34} \\ 0 & k^{24} & k^{34} & k^{44} \end{bmatrix}$$

Implied restrictions (II): Parallel regressions



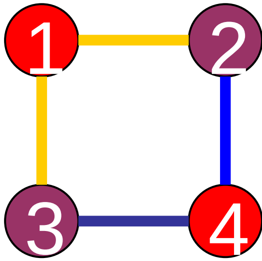
- **Regressions of y_2, y_3 on y_1, y_4 are parallel**

$$\begin{bmatrix} y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} a_2 \\ a_3 \end{bmatrix} - \begin{bmatrix} k^{22} & 0 \\ 0 & k^{33} \end{bmatrix}^{-1} \begin{bmatrix} k^{21} & k^{24} \\ k^{31} & k^{34} \end{bmatrix} \begin{bmatrix} y_1 \\ y_4 \end{bmatrix}$$

$$= \begin{bmatrix} a_2 \\ a_3 \end{bmatrix} - \begin{bmatrix} k^{21}/k^{22} & k^{24}/k^{22} \\ k^{31}/k^{33} & k^{34}/k^{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_4 \end{bmatrix}$$

- because $k^{12}=k^{13}$, $k^{24}=k^{34}$ and $k^{22}=k^{33}$

Implied restrictions (III): Partial covariances and concentrations



- This RCON model has also identical partial covariances

$$cov(y_1, y_2 | y_3, y_4) = \frac{-k^{12}}{|K^{12}|} = \frac{-k^{13}}{|K^{13}|} = cov(y_1, y_3 | y_2, y_4)$$

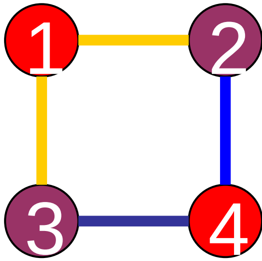
- – and identical partial correlations

$$cor(y_1, y_2 | y_3, y_4) = \frac{-k^{12}}{\sqrt{k^{11} k^{22}}} = \frac{-k^{13}}{\sqrt{k^{11} k^{33}}} = cor(y_1, y_3 | y_2, y_4)$$

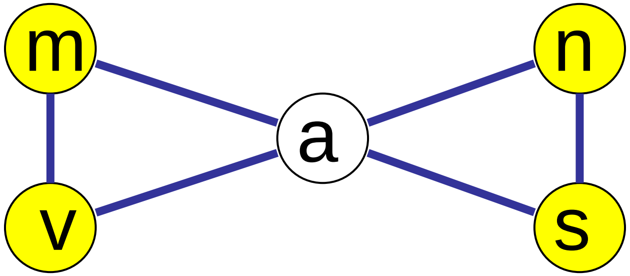
$$K = \Sigma^{-1} = \begin{bmatrix} k^{11} & k^{12} & k^{13} & 0 \\ k^{12} & k^{22} & 0 & k^{24} \\ k^{13} & 0 & k^{33} & k^{34} \\ 0 & k^{24} & k^{34} & k^{44} \end{bmatrix}$$

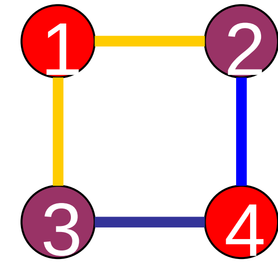
Not generally the case!!!

Example – mathematics marks



- Focus on butterfly model
  - EdgeColourClass: Edges with same colour
  - VertexColourClass: Vertices with same colour
- Note: Black and white are neutral colours; no restrictions
- Successively apply (with LR-test, 5% level)
  - JoinEdgeColourClasses()
  - JoinVertexColourClasses()





Mathematics marks...

Estimated / observed concentrations (× 1000) are

Concentrations	mechanics	vectors	algebra	analysis	statistics
mechanics	7.58	−3.49	−3.49	0.00	0.00
vectors	−3.49	7.58	−3.49	0.00	0.00
algebra	−3.49	−3.49	20.76	−3.49	−3.49
analysis	0.00	0.00	−3.49	7.58	−3.49
statistics	0.00	0.00	−3.49	−3.49	7.58
mechanics	5.24	−2.44	−2.74	0.01	−0.14
vectors	−2.44	10.43	−4.71	−0.79	−0.17
algebra	−2.74	−4.71	26.95	−7.05	−4.70
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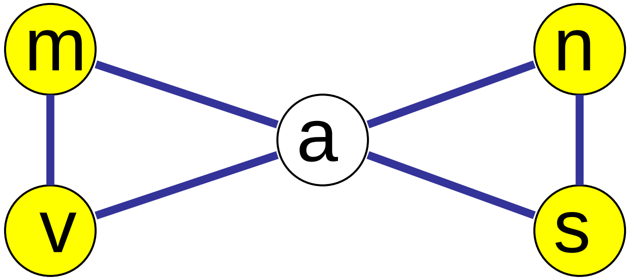
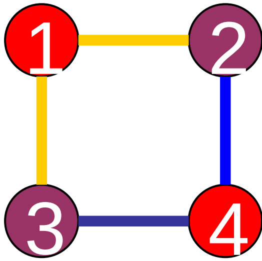


RCOR (Restricted CORrelation) models

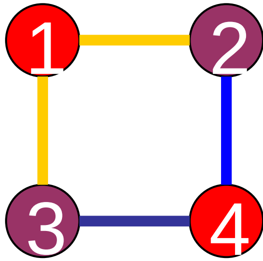


- Restricting concentrations not scale-invariant: Identical concentrations of $y \sim N(0,\Sigma)$ not generally preserved for $Ay \sim N(0,A\Sigma A)$, where A is diagonal

- Hence RCON models are only of interest in cases where the scale of measurement for different variables are comparable

- Alternatively: Focus on restricted partial correlations

RCOR (restricted correlation) models



Write –K as

$$\begin{bmatrix} \eta^{11} & 0 & 0 & 0 \\ 0 & \eta^{22} & 0 & 0 \\ 0 & 0 & \eta^{33} & 0 \\ 0 & 0 & 0 & \eta^{44} \end{bmatrix} \begin{bmatrix} 1 & \rho^{12} & \rho^{13} & 0 \\ \rho^{12} & 1 & 0 & \rho^{24} \\ \rho^{13} & 0 & 1 & \rho^{34} \\ 0 & \rho^{24} & \rho^{34} & 1 \end{bmatrix} \begin{bmatrix} \eta^{11} & 0 & 0 & 0 \\ 0 & \eta^{22} & 0 & 0 \\ 0 & 0 & \eta^{33} & 0 \\ 0 & 0 & 0 & \eta^{44} \end{bmatrix}$$

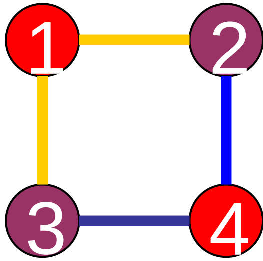
= A_η C_ρ A_η where

A_η : diagonal with positive entries (inverse partial standard deviations)

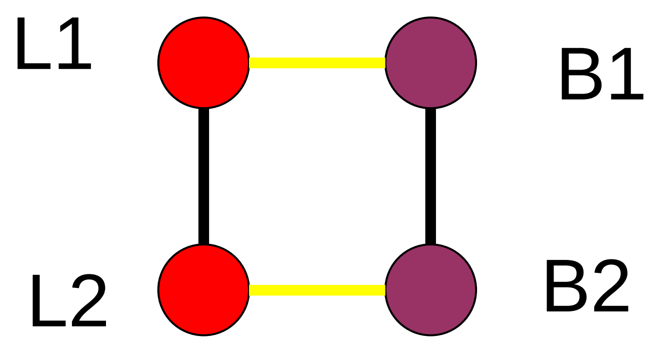
C_ρ : has 1s on diagonal (partial correlations)

- Entries of (A_η, C_ρ) restricted according to colouring
- Scale invariant - if vertices with same colour are rescaled identically

RCOP models ('P' for permution symmetry)



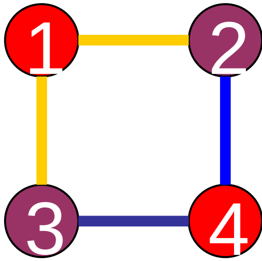
Fret's head: Length and breadth of head of first and second son:

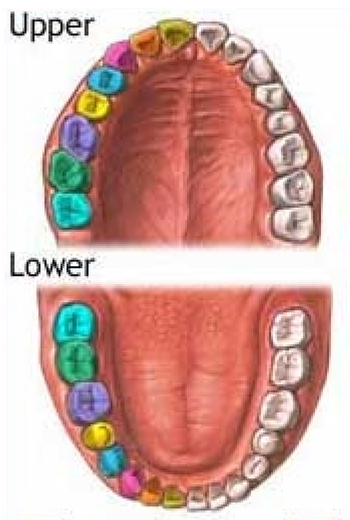


Complete symmetry between first and second son

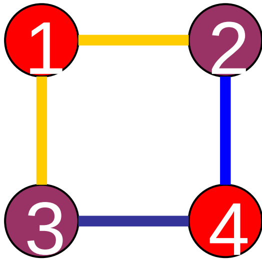
- Both RCON and RCOR
- RCOP-model (defined by permutations)
- Studied by Helene Neufeld (poster session)

Symmetry models in nature



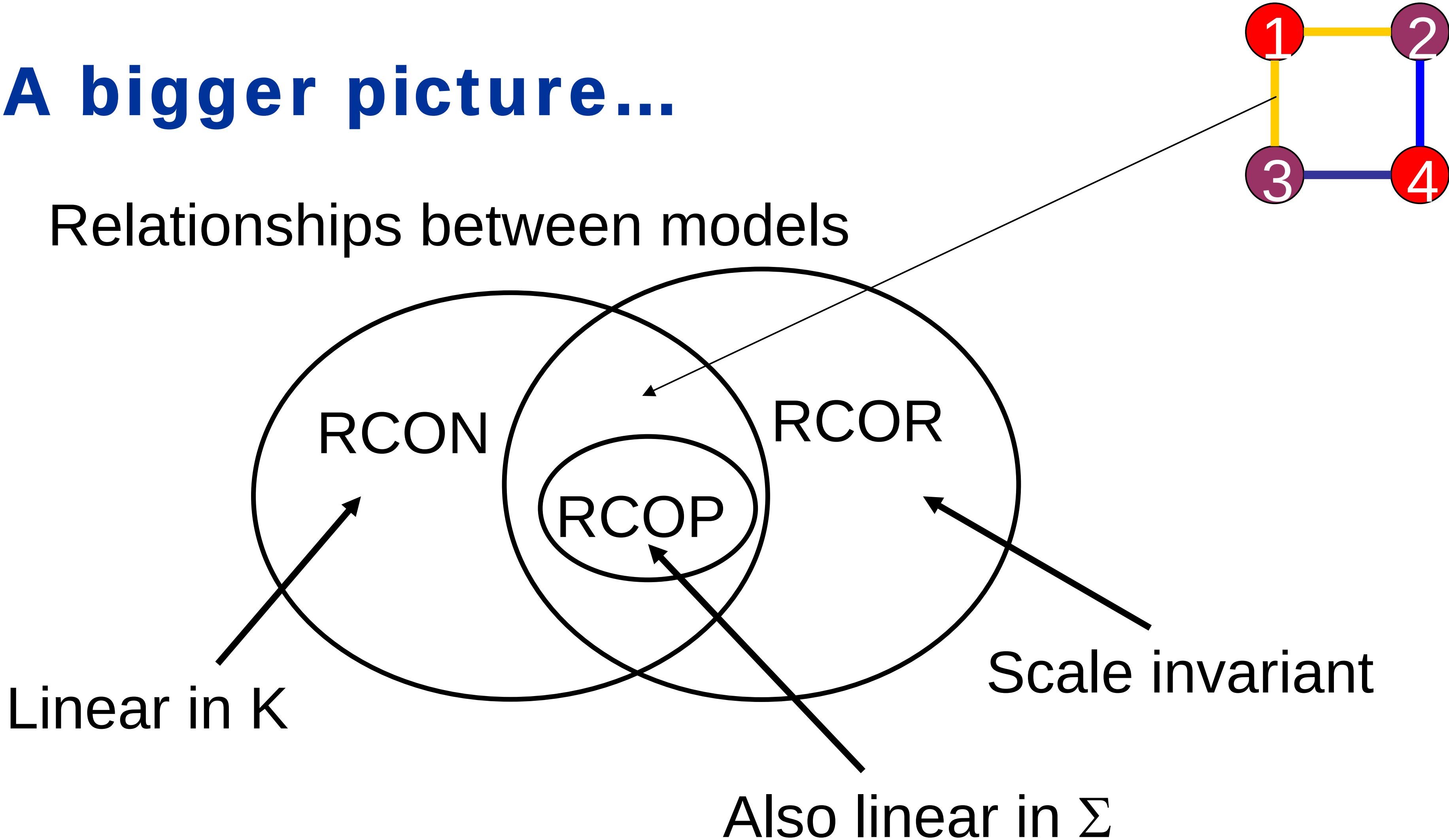


Further…

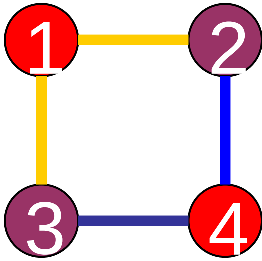


A bigger picture…

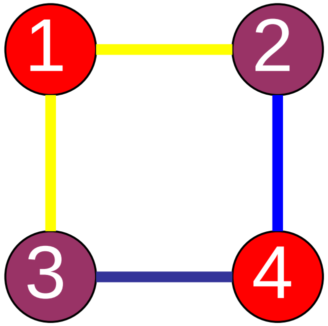
Relationships between models



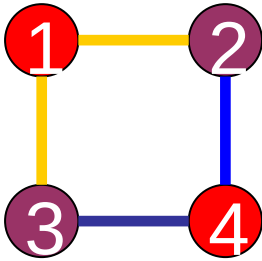
Specification of RCON / RCOR models



- **Generators of model**
  - Edge colour classes:
    EC **=** ***{{1,2}{1,3}} {{2,4}{3,4}}***
  - Vertex colour classes:
    VC **=** ***{1,4}{2,3}***
- **(EC,VC) specifies RCON / RCOR model**



RCON Estimation - Sufficient statistics



For EdgeCC s={{1,2}{1,3}}

$$T^s = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

For vertexCC s={1,4}

$$T^s = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Let W ~ Wishart(f,Σ)

RCON regular exponential family; linear in K:

Then

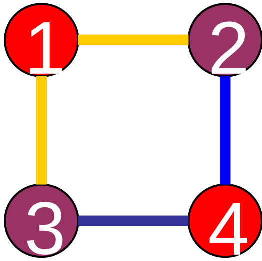
$$2 \log L = f \log |K| - tr(KW)$$
$$= f \log |K| - \Sigma_s \theta_s tr(T^s W)$$

So $\{t^s = tr(T^s W)\}$ is a set of sufficient statistics

Equated with expectations

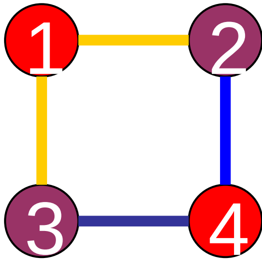
$$\{t^s\} = \{f\ tr(T^s \Sigma)\}$$

Estimation in RCON models - Modified Newton



- **Use convergent (!) algorithm of Jensen, Johansen and Lauritzen (1991):**
- **Maximize 1/L (instead of logL) cyclically over one parameter at the time by Newton iteration.**
- **In exponential families we have**
  - $\exp(t(y)\theta-\psi(\theta))$
  - $l^* = 1/L = \exp(-t(y)\theta+\psi(\theta))$

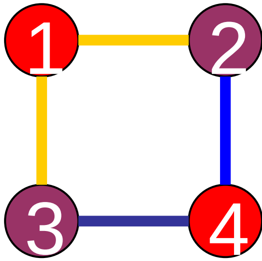
Modified Newton



- **Let $\Delta=E(t(y))-t(y)$.**
- **Then**
  - $(l^*)' = \exp(-t(y)\theta+\psi(\theta))\Delta$
  - $(l^*)'' = \exp(-t(y)\theta+\psi(\theta))[Var(t(y)) + \Delta^2]$
- **Newton step becomes:**
- $\theta \leftarrow \theta - (l^*)'/ (l^*)'' = \theta - \Delta / (Var(t(y)) + \Delta^2)$

- **For RCON models**
  - $E(T^s W)=f\ tr(T^s \Sigma)$
  - $Var(T^s W) = f\ tr(T^s \Sigma T^s \Sigma)$

Estimation – RCOR - short version



RCOR model is generally not a linear exponential family

$\log L = f/2 \log |C_\rho| + f \log |A_\eta| - \mathrm{tr}(A_\eta C_\rho A_\eta W)/2$

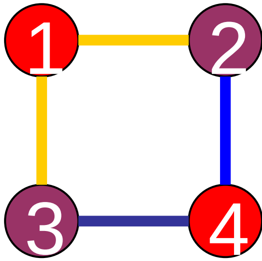
Linear exponential family for fixed η; likelihood equations quadratic for fixed ρ.

Existence/uniqueness of MLE not clear. But unique maximum in ρ for fixed η and unique maximum in η for fixed ρ.

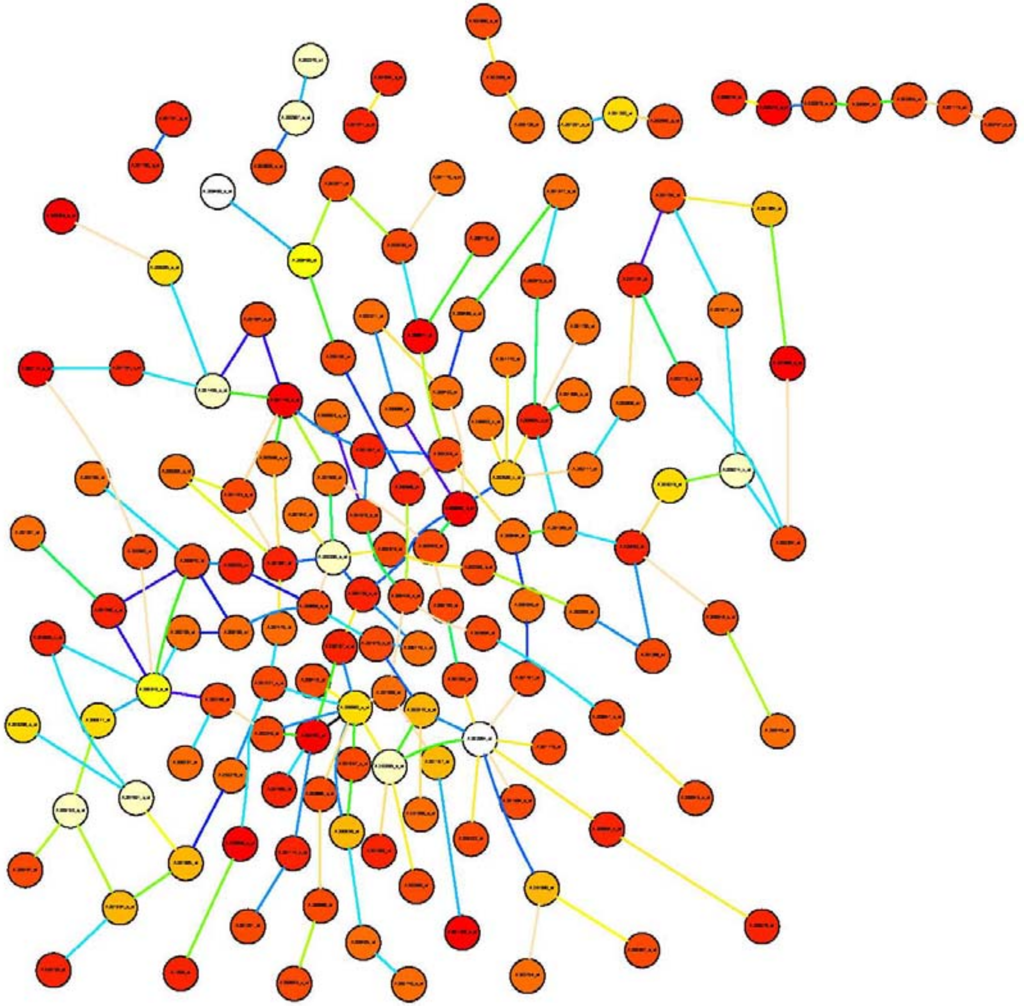
Suggests alternating algorithm

1. For given η, estimate ρ using modified Newton as for RCON
2. For given ρ, estimate η by solving system of 2nd degree equations (cyclically)

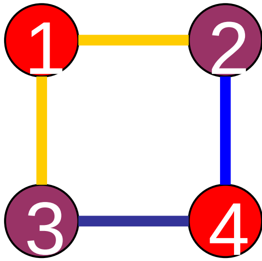
Larger model: Breast cancer genes



- **58 cases, 150 genes**
- **7 VCC, 10 ECC: 17 parameters**
- **Fitting with gRc: 0.3 sec**
- **380 parms**
- **Fitting with gRc: 1.1 sec**
- **Model selection is a big issue…**



Summing up



- SH +Lauritzen: Graphical Gaussian models with edge and vertex symmetries. *(RSSB, To appear)*
- SH + Lauritzen (2007). Inference in graphical Gaussian models with edge and vertex symmetries with the gRc package for R *(J. Stat. Soft)*
- gRc package in R (‘c’ for colour) on CRAN