## Model-Preserving Sensitivity Analysis for Families of Gaussian Distributions

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Graphical Models: Conditional Independence and Algebraic Structures

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Joint work with C. Görgen

## Plan for the Talk

Introduction

Gaussian Independence Models
Sensitivity Analysis
Model-Preserving Sensitivity Analysis

Applications
Conclusions

## Why Sensitivity Analysis?

- The accuracy of probability distributions inferred using machine-learning algorithms heavily depends on data availability and quality.
- In practical applications it is therefore fundamental to investigate the robustness of a statistical model to misspecification of some of its underlying probabilities.
- In the context of graphical models, investigations of robustness fall under the notion of sensitivity analyses.
- These analyses consist in varying some of the model's probabilities or parameters and then assessing how far apart the original and the varied distributions are.


## Gaussian Independence Models

- Let $Y$ be a $n$-dimensional Gaussian random vector with mean $\mu \in \mathbb{R}^{n}$, covariance matrix $\Sigma \in \mathbb{R}_{\text {spsd }}^{n \times n}$ and $f_{\mu, \Sigma}$ its density.
- For $A, B \subseteq[n]=\{1, \ldots, n\}$, let $\mu_{A}=\left(\mu_{i}\right)_{i \in A}$ and $\Sigma_{A, B}$ be the submatrix of $\Sigma$ with rows indexed by $A$ and columns indexed by $B$.
- For any two disjoint sets $A, B \subset[n], Y_{A}=\left(Y_{i}\right)_{i \in A}$ has density $f_{\mu_{A}, \Sigma_{A, A}}$ and $Y_{A} \mid Y_{B}=y_{B}$ has density $f_{\mu^{A \mid B}, \Sigma^{A \mid B}}$ where

$$
\begin{gathered}
\mu^{A \mid B}=\mu_{A}+\Sigma_{A, B} \Sigma_{B, B}^{-1}\left(y_{B}-\mu_{B}\right) \\
\Sigma^{A \mid B}=\Sigma_{A, A}-\Sigma_{A, B} \Sigma_{B, B}^{-1} \Sigma_{B, A} .
\end{gathered}
$$

## Gaussian Independence Models

The random vector $Y_{A}$ is said to be conditionally independent of $Y_{B}$ given $Y_{C}$ for disjoint subsets $A, B, C \subseteq[n]$ if and only if the density factorizes as

$$
f_{\mu^{A \cup B \mid C, \Sigma}, \Sigma^{A \cup B \mid C}}=f_{\mu^{A \mid C}, \Sigma^{A \mid C}} f_{\mu^{B|C, \Sigma B| C}} .
$$

and write $A \Perp B \mid C$.

## Drton et al. 2008

For a $n$-dimensional Gaussian random vector $Y$ with density $f_{\mu, \Sigma}$ and disjoint $A, B, C \subset[n]$, the conditional independence statement $A \Perp B \mid C$ is true if and only if all $(\# C+1) \times(\# C+1)$ minors of the matrix $\Sigma_{A \cup C, B \cup C}$ are equal to zero. Here, $\# C$ denotes the cardinality of the set $C$.

## Gaussian Independence Models

- Let $\mathrm{Cl}=\left\{A_{1} \Perp B_{1}\left|C_{1}, \ldots, A_{r} \Perp B_{r}\right| C_{r}\right\}$ for disjoint index sets $A_{i}, B_{i}, C_{i} \subset[n]$ and $i \in[r]$, with $r \in \mathbb{N}$.
- A Gaussian conditional independence model $\mathcal{M}_{\mathrm{CI}}$ for which all Cl statements are true is a special subset of all possible Gaussian densities $f_{\mu, \Sigma}$ :

$$
\mathcal{M}_{\mathrm{CI}} \subseteq\left\{f_{\mu, \Sigma} \mid \mu \in \mathbb{R}^{n}, \Sigma \in \mathbb{R}_{\mathrm{spsd}}^{n \times n}\right\} .
$$

- The parameter space of $\mathcal{M}_{\mathrm{CI}}$ is equal to the algebraic set

$$
\mathcal{A}_{\mathrm{Cl}}=\left\{\mu \in \mathbb{R}^{n}, \Sigma \in \mathbb{R}_{\mathrm{spsd}}^{n \times n} \mid g(\Sigma)=0 \text { for all polynomials } g\right.
$$ which are $\left(\# C_{i}+1\right) \times\left(\# C_{i}+1\right)$ minors of $\left.\Sigma_{A_{i} \cup C_{i}, B_{i} \cup C_{i}}, i \in[r]\right\}$.

## Undirected Graphical Models

A Gaussian undirected graphical model for a random vector $Y=\left(Y_{i}\right)_{i \in[n]}$ is defined by an undirected graph $\mathcal{G}=(V, E)$ with vertex set $V=[n]$ and a family of densities $f_{\mu, \Sigma}$ whose covariance matrix $\Sigma$ is such that $\left(\Sigma^{-1}\right)_{i j}=0$ if and only if $(i, j) \notin E$.

The statement $Y_{2} \Perp\left\{Y_{1}, Y_{3}\right\} \mid Y_{4}$ can be represented by the undirected graph

The $2 \times 2$ minors of the submatrix


$$
\Sigma_{\{2,4\},\{1,3,4\}}=\left(\begin{array}{lll}
\sigma_{21} & \sigma_{23} & \sigma_{24} \\
\sigma_{41} & \sigma_{43} & \sigma_{44}
\end{array}\right)
$$

need to vanish. Explicitly,

$$
\sigma_{21} \sigma_{43}-\sigma_{41} \sigma_{23}=0, \sigma_{21} \sigma_{44}-\sigma_{41} \sigma_{24}=0
$$

## Gaussian Bayesian Networks

A Gaussian Bayesian network for a random vector $Y=\left(Y_{i}\right)_{i \in[n]}$ is a DAG $\mathcal{G}=(V, E)$ with $V=[n]$ and conditional Gaussian densities $f_{\mu_{i}, \sigma_{i}}$ with mean $\mu_{i}=\beta_{0 i}+\sum_{j \in \mathrm{pa}(i)} \beta_{j i} y_{j}$ and variance $\sigma_{i} \in \mathbb{R}_{+}$, with $\mathrm{pa}(i) \subseteq[i-1]$.

- Conditional independences $Y_{i} \Perp Y_{[i-1] \backslash \mathrm{pa}(i)} \mid Y_{\mathrm{pa}(i)}$
- Define
- $\beta_{0}=\left(\beta_{0 i}\right)_{i \in[n]}$ the vector of intercepts
- $B$ be the strictly upper triangular matrix with entries $B_{j i}=\beta_{j i}$ if $j \in \mathrm{pa}(i)$ and zero otherwise
- $\Phi=\operatorname{diag}\left(\sigma_{1}, \ldots, \sigma_{n}\right)$ be the diagonal matrix of the conditional variances
- Then $Y$ has Gaussian density $f_{\mu, \Sigma}$ with mean

$$
\begin{aligned}
& \mu=(I-B)^{-\top} \beta_{0} \text { and covariance matrix } \\
& \Sigma=(I-B)^{-\top} \Phi(I-B)^{-1}
\end{aligned}
$$

## Gaussian Bayesian Networks

Consider $Y_{3} \Perp Y_{1} \mid Y_{2}$

$$
1 \longrightarrow 2 \longrightarrow 3
$$

the $2 \times 2$ minors of the submatrix

$$
\Sigma_{\{2,3\},\{1,2\}}=\left(\begin{array}{ll}
\sigma_{21} & \sigma_{22} \\
\sigma_{31} & \sigma_{32}
\end{array}\right)
$$

need to vanish. Here the only vanishing minor simply corresponds to the determinant. So $g=\sigma_{21} \sigma_{32}-\sigma_{31} \sigma_{22}$ is a polynomial which must be zero.

## Sensitivity Analysis for Gaussian Models

- For a generic Gaussian random vector $Y$ with density $f_{\mu, \Sigma}$, robustness is usually studied by perturbing the mean vector $\mu$ and the covariance matrix $\Sigma$.
- Such a perturbation is carried out by defining a perturbation vector $d \in \mathbb{R}^{n}$ and a matrix $D \in \mathbb{R}^{n \times n}$ which act additively on the original mean and variance, giving rise to a vector $\tilde{Y}$ with a new distribution $f_{\mu+d, \Sigma+D}$.
- The dissimilarity between these two vectors is then usually quantified via the KL divergence.

$$
\mathrm{KL}(\tilde{Y} \| Y)=\frac{1}{2}\left(\operatorname{tr}\left(\Sigma^{-1} D\right)+d^{\top} \Sigma^{-1} d+\ln \left(\frac{\operatorname{det}(\Sigma)}{\operatorname{det}(\Sigma+D)}\right)\right) .
$$

## What's the issue?

$$
1 \longrightarrow 2 \longrightarrow 3
$$

- Suppose $D$ has all zeros except for a $d \in \mathbb{R}$ in positions $(2,1)$ and $(1,2)$ such that $\Sigma+D \in \mathbb{R}_{\text {spsd }}^{3 \times 3}$.
- The graph is still valid if and only if the $2 \times 2$ minor $\left(\sigma_{21}+d\right) \sigma_{32}-\sigma_{31} \sigma_{22}$ is equal to zero.
- But this is the case if and only if $d=0$ : so if there is no perturbation.
- If alternatively the only non-zero entry of $D$ were in position $(1,1)$ then no matter what the value of $d \in \mathbb{R}$ the graph would be valid.


## Possible Solutions

- Work with the conditional Gaussian distributions.
- Perturb the matrix $\Phi$ of conditional variances which then affects $\Sigma$.
- Perturb the matrix $B$ of regression coefficients which then affects $\mu$ and $\Sigma$.
- However and critically, both these approaches lose the intuitiveness of acting directly on the unconditional mean and covariance of the Gaussian distribution.


## Our Proposal

- Consider a Gaussian model $\mathcal{M}_{\mathrm{Cl}}$ for a random vector $Y=\left(Y_{i}\right)_{i \in[n]}$ together with conditional independence assumptions $\mathrm{Cl}=\left\{A_{k} \Perp B_{k} \mid C_{k}\right.$ for $\left.k \in[r]\right\}$ as being represented by a collection of vanishing minors of its covariance matrix $\Sigma \in \mathbb{R}_{\text {spsd }}^{n \times n}$.
- Without loss suppose $\mu=0_{n}$ and write $f_{\Sigma}$.
- Let

$$
\Phi_{\Delta}: \Sigma \mapsto \Delta \circ \Sigma
$$

denote the map which sends a covariance matrix to its Schur product with a matrix $\Delta$.

- We call the map $\Phi_{\Delta}$ model-preserving if under this operation the algebraic parameter set is mapped onto itself, $\Phi_{\Delta}\left(\mathcal{A}_{\mathrm{CI}}\right) \subseteq \mathcal{A}_{\mathrm{Cl}}$.


## Variation and Covariation Matrices

We decompose the perturbation of a covariance matrix $\Sigma$ into two steps, and hence two Schur products.

1. $\Sigma$ is mapped to its Schur product with a symmetric variation matrix $\Delta \in \mathbb{R}_{\neq 0}^{n \times n}$. Some $\sigma_{i j}$ are assigned a new value $\sigma_{i j} \mapsto \delta_{i j} \sigma_{i j}$ at selected positions $(i, j)$ while all others are equal to one.

In demanding that all entries $\delta_{i j}$ are non-zero, we automatically avoid setting a non-zero covariance $\sigma_{i j} \neq 0$ to zero via multiplication by an entry of $\Delta$. This type of perturbation would force the corresponding variables to be independent, $X_{i} \Perp X_{j}$, in the perturbed model, which would clearly violate the assumptions in the original model $\mathcal{M}_{\mathrm{Cl}}$.

## Variation and Covariation Matrices

We decompose the perturbation of a covariance matrix $\Sigma$ into two steps, and hence two Schur products.
2. A Schur product between $\Delta \circ \sum_{\tilde{\sim}}$ and a symmetric covariation matrix $\tilde{\Delta} \in \mathbb{R}_{\neq 0}^{n \times n}$. This matrix $\tilde{\Delta}$ has ones in the positions $(i, j)$ whilst the others are to be set to ensure model-preservation.
$\tilde{\Delta} \circ \Delta \circ \Sigma=\left(\begin{array}{cccc}\star & \cdots & \cdots & \star \\ \vdots & \ddots & 1 & \vdots \\ \vdots & 1 & \ddots & \vdots \\ \star & \cdots & \cdots & \star\end{array}\right) \circ\left(\begin{array}{cccc}1 & \cdots & \cdots & 1 \\ \vdots & \ddots & \delta_{i j} & \vdots \\ \vdots & \delta_{j i} & \ddots & \vdots \\ 1 & \cdots & \cdots & 1\end{array}\right) \circ\left(\begin{array}{cccc}\sigma_{11} & \cdots & \cdots & \sigma_{1 n} \\ \vdots & \ddots & \sigma_{i j} & \vdots \\ \vdots & \sigma_{j i} & \ddots & \vdots \\ \sigma_{n 1} & \cdots & \cdots & \sigma_{n n}\end{array}\right)$
We need to find $\tilde{\Delta}$ such that $\tilde{\Delta} \circ \Delta \circ \Sigma \in \mathcal{A}_{\mathrm{Cl}}$. Then the map $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving.

## Example

Consider $Y_{3} \Perp Y_{2} \mid Y_{1}$ and perturb $\sigma_{21}$. Then

$$
\Delta=\left(\begin{array}{lll}
1 & \delta & 1 \\
\delta & 1 & 1 \\
1 & 1 & 1
\end{array}\right)
$$

and the only vanishing minor of $\Delta \circ \Sigma$ takes the form $\delta \sigma_{12} \sigma_{32}-\sigma_{31} \sigma_{22}$. This polynomial is equal to zero in either of three cases

- $\sigma_{22}$ is covaried by $\delta$;
- $\sigma_{31}$ and $\sigma_{13}$ are covaried by $\delta$
- $\sigma_{22}, \sigma_{31}, \sigma_{13}, \sigma_{32}$ and $\sigma_{23}$ are covaried by $\delta$.

The associated covariation matrices $\tilde{\Delta}$ are,

$$
\left(\begin{array}{lll}
1 & 1 & 1 \\
1 & \delta & 1 \\
1 & 1 & 1
\end{array}\right), \quad\left(\begin{array}{lll}
1 & 1 & \delta \\
1 & 1 & 1 \\
\delta & 1 & 1
\end{array}\right), \quad\left(\begin{array}{lll}
1 & 1 & \delta \\
1 & \delta & \delta \\
\delta & \delta & 1
\end{array}\right) .
$$

For these $\tilde{\Delta}$, we have that $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving.
Consider $\tilde{\Delta}_{\{2,3\},\{1,2\}} \circ \Delta_{\{2,3\},\{1,2\}}$. Then the matrices are equal to

$$
\left(\begin{array}{ll}
\delta & \delta \\
1 & 1
\end{array}\right), \quad\left(\begin{array}{ll}
\delta & 1 \\
\delta & 1
\end{array}\right), \quad\left(\begin{array}{ll}
\delta & \delta \\
\delta & \delta
\end{array}\right) .
$$

## Some Notation

For any symmetric matrix $D \in \mathbb{R}^{n \times n}$ and two index sets
$A, B \subseteq[n]$, we henceforth denote with $\left\lfloor D_{A, B}\right\rfloor^{1}$ the symmetric, full dimension $n \times n$ matrix where:

- all positions indexed by $A$ and $B$ are equal to the corresponding entries in $D$;
- entries not indexed by $A$ and $B$ are set to ensure symmetry;
- all other entries are equal to one.

Let $D \in \mathbb{R}^{3 \times 3}$ and suppose

$$
D_{\{1,2\},\{2,3\}}=\left(\begin{array}{ll}
1 & \delta \\
1 & \delta
\end{array}\right)
$$

Then

$$
\left\lfloor D_{\{1,2\},\{2,3\}}\right\rfloor^{1}=\left(\begin{array}{lll}
1 & 1 & \delta \\
1 & 1 & \delta \\
\delta & \delta & 1
\end{array}\right)
$$

## Covariation Matrices

For a single-parameter variation matrix $\Delta$ with $\delta_{i j}=\delta_{j i}=\delta$, we say that the covariation matrix $\tilde{\Delta}$ is

- total if $\tilde{\Delta} \circ \Delta=\delta \mathbb{1}_{[n],[n]}$;
- partial if $\tilde{\Delta} \circ \Delta=\left\lfloor\delta \mathbb{1}_{A \cup C, B \cup C}\right\rfloor^{1}$.
- row-based if $\tilde{\Delta} \circ \Delta=\left\lfloor\delta \mathbb{1}_{E, B \cup C}\right\rfloor^{1}$ for a subset $E \subseteq A \cup C$;
- column-based if $\tilde{\Delta} \circ \Delta=\left\lfloor\delta \mathbb{1}_{A \cup C, F}\right\rfloor^{1}$ for a subset $F \subseteq B \cup C$.

By construction total, partial, row- and column-based covariations ensure symmetry. Henceforth, we assume that the perturbed matrix $\tilde{\Delta} \circ \Delta \circ \Sigma$ is also positive semidefinite, so that
$\tilde{\Delta} \circ \Delta \circ \Sigma \in \mathbb{R}_{\text {spsd }}^{n \times n}$.

## One Independence Statement $\mathrm{CI}=\{A \Perp B \mid C\}$

- If $(i, j),(j, i) \notin(A \cup C, B \cup C)$ then the map $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving for a covariation $\tilde{\Delta}=\mathbb{1}_{[n],[n]}$.
- If $C=\emptyset$ then the map $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving for $\tilde{\Delta}=\mathbb{1}_{[n],[n]}$.
- The map $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving for total and partial covariation matrices $\tilde{\Delta}$.

For total covariation matrices, $\delta>0$. For partial covariations this may not have to be enforced, but it is rare to investigate the effect of changing the sign. Furthermore, increasing interest on covariance matrices whose entries are positive.

## One Independence Statement $\mathrm{CI}=\{A \Perp B \mid C\}$

The map $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving in the following cases:

- if $(i, j)$ or $(j, i) \in(A, B)$ for a row-based covariation $\tilde{\Delta}$ whenever $i \in E \subseteq A$, and for a column-based covariation $\tilde{\Delta}$ whenever $j \in F \subseteq B$;
- if $(i, j)$ or $(j, i) \in(A, C)$ for a row-based covariation $\tilde{\Delta}$ whenever $i \in E \subseteq A$, and for a column-based covariation $\tilde{\Delta}$ whenever $F=C$;
- if $(i, j)$ or $(j, i) \in(C, B)$ for a row-based covariation $\tilde{\Delta}$ whenever $E=C$, and for a column-based covariation $\tilde{\Delta}$ whenever $i \in F \subseteq B$;
- if $(i, j)$ and $(j, i) \in(C, C)$ for a row-based covariation $\tilde{\Delta}$ whenever $E=C$, and for a column-based covariation $\tilde{\Delta}$ whenever $F=C$.


## Multiple CI Statements

Consider $Y_{4} \Perp Y_{\{1,2\}} \mid Y_{3}$ and $Y_{\{2,4\}} \Perp Y_{5} \mid Y_{3}$. The associated submatrices are

$$
\left(\begin{array}{lll}
\sigma_{31} & \sigma_{32} & \sigma_{33} \\
\sigma_{41} & \sigma_{42} & \sigma_{43}
\end{array}\right) \text { and } \quad\left(\begin{array}{ll}
\sigma_{23} & \sigma_{25} \\
\sigma_{33} & \sigma_{35} \\
\sigma_{43} & \sigma_{45}
\end{array}\right) .
$$

Suppose the entry $\sigma_{43}$ is perturbed by $\delta$ and pick two $\tilde{\Delta}$. Then

$$
\left(\begin{array}{lllll}
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & \delta & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1
\end{array}\right) \circ\left(\begin{array}{lllll}
1 & 1 & 1 & 1 & 1 \\
1 & 1 & \delta & 1 & 1 \\
1 & \delta & \delta & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1
\end{array}\right) \circ\left(\begin{array}{lllll}
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & \delta & 1 \\
1 & 1 & \delta & 1 & 1 \\
1 & 1 & 1 & 1 & 1
\end{array}\right)=\left(\begin{array}{lllll}
1 & 1 & 1 & 1 & 1 \\
1 & 1 & \delta & 1 & 1 \\
1 & \delta & \delta^{2} & \delta & 1 \\
1 & 1 & \delta & 1 & 1 \\
1 & 1 & 1 & 1 & 1
\end{array}\right)
$$

## Multiple CI Statements

$$
\begin{aligned}
& \text { Let } \mathrm{CI}=\left\{A_{1} \Perp B_{1}\left|C_{1}, \ldots, A_{r} \Perp B_{r}\right| C_{r}\right\}, A=\cup_{k \in[r]} A_{k}, \\
& B=\cup_{k \in[r]} B_{k} \text { and } C=\cup_{k \in[r]} C_{k} .
\end{aligned}
$$

- Standard conditional independences can be eliminated from Cl ;
- We introduced a notion of separable Cls for which we can define covariations independently
- total and partial covariations are model-preserving.


## Multiple CI Statements

$$
\begin{aligned}
& \text { Let } \mathrm{CI}=\left\{A_{1} \Perp B_{1}\left|C_{1}, \ldots, A_{r} \Perp B_{r}\right| C_{r}\right\}, A=\cup_{k \in[r]} A_{k}, \\
& B=\cup_{k \in[r]} B_{k} \text { and } C=\cup_{k \in[r]} C_{k} .
\end{aligned}
$$

- Standard conditional independences can be eliminated from Cl ;
- We introduced a notion of separable Cls for which we can define covariations independently
- total and partial covariations are model-preserving.

The map $\Phi_{\tilde{\Delta} \circ \Delta}$ is model-preserving for a row-based or a column-based covariation matrix $\tilde{\Delta}$ if

$$
\tilde{\Delta}_{A \cup C, B \cup C} \circ \Delta_{A \cup C, B \cup C}=\left(\left\lfloor\tilde{\Delta}_{A \cup C, B \cup C} \circ \Delta_{A \cup C, B \cup C}\right\rfloor^{1}\right)_{A \cup C, B \cup C} .
$$

## Multi-way Sensitivity Analysis

Compositions of model-preserving maps are model-preserving. In particular, for any two matrices $\Delta$ and $\Delta^{\prime}$ we have $\Phi_{\Delta}\left(\Phi_{\Delta^{\prime}}\right)=\Phi_{\Delta \circ \Delta^{\prime}}$.

- We can write $\Delta=\Delta^{1} \circ \Delta^{2} \circ \cdots \circ \Delta^{n}$ where every $\Delta^{k}$ enforces a single-parameter variation.
- We can covary every single-parameter variation $\Delta^{k}$ by a matrix $\tilde{\Delta}^{k}$ using any covariation.
- Because the Schur product is commutative, this induces a map

$$
\Phi_{\tilde{\Delta}^{1} \circ \Delta^{1} \circ \tilde{\Delta}^{2} \circ \Delta^{2} \circ \ldots \circ \tilde{\Delta}^{n} \circ \Delta^{n}}=\Phi_{\tilde{\Delta}^{1} \circ \tilde{\Delta}^{2} \circ \ldots \circ \tilde{\Delta}^{n} \circ \Delta^{1} \circ \Delta^{2} \circ \ldots \circ \Delta^{n}}=\Phi_{\tilde{\Delta} \circ \Delta}
$$

where $\tilde{\Delta}=\tilde{\Delta}^{1} \circ \tilde{\Delta}^{2} \circ \cdots \circ \tilde{\Delta}^{n}$ is the covariation matrix for $\Delta$.

## Divergence Quantification - KL Divergence

The KL divergence between $Y$ and $\tilde{Y}$ in model-preserving sensitivity analyses can be written as

$$
\mathrm{KL}(\tilde{Y} \| Y)=\frac{1}{2}\left[\operatorname{tr}\left(\Sigma^{-1}(\tilde{\Delta} \circ \Delta \circ \Sigma)\right)-n+\log \frac{\operatorname{det}(\Sigma)}{\operatorname{det}(\tilde{\Delta} \circ \Delta \circ \Sigma)}\right]
$$

For total covariation matrices KL divergence has the following simple closed-form formula.

$$
\mathrm{KL}(\tilde{Y} \| Y)=\frac{1}{2}(n(\delta-\log (\delta)-1))
$$

where $\delta=\prod_{i \in[n]} \delta_{i}$ for a multi-way variation.

## Divergence Quantification - Frobenius Norm

- The Frobenius norm between zero-mean Gaussians $Y$ and $Y^{\prime}$ is

$$
F\left(Y, Y^{\prime}\right)=\operatorname{tr}\left(\left(\Sigma-\Sigma^{\prime}\right)^{\top}\left(\Sigma-\Sigma^{\prime}\right)\right) .
$$

- Let $\tilde{\Delta} \circ \Delta=\left(\delta_{i j}\right)_{i j}$ be model-preserving. Then

$$
\begin{equation*}
F(Y, \tilde{Y})=\sum_{i, j \in[n]}\left(1-\delta_{i j}\right)^{2} \sigma_{i j}^{2} \tag{1}
\end{equation*}
$$

- For standard sensitivity analyses $\mathrm{F}\left(Y, Y^{\prime}\right)=\operatorname{tr}\left(D^{\top} D\right)$.
- We can rank methods:
- $\mathrm{F}\left(Y, \tilde{Y}_{\text {total }}\right) \geq \mathrm{F}\left(Y, \tilde{Y}_{\text {partial }}\right)$
- $\mathrm{F}\left(Y, \tilde{Y}_{\text {partial }}\right) \geq \mathrm{F}\left(Y, \tilde{Y}_{\text {row }}\right)$
- $\mathrm{F}\left(Y, \tilde{Y}_{\text {partial }}\right) \geq \mathrm{F}\left(Y, \tilde{Y}_{\text {column }}\right)$
- $\mathrm{F}\left(Y, \tilde{Y}_{\text {column }}\right) \geq \mathrm{F}\left(Y, \tilde{\gamma}_{\text {standard }}\right)$
- $\mathrm{F}\left(Y, \tilde{Y}_{\text {row }}\right) \geq \mathrm{F}\left(Y, \tilde{\gamma}_{\text {standard }}\right)$


## A First Example

$$
\Sigma=\left(\begin{array}{cccc}
1 & 2 & 2 & 7 \\
2 & 5 & 5 & 17 \\
2 & 5 & 6 & 19 \\
7 & 17 & 19 & 63
\end{array}\right)
$$

One conditional independence statement, $Y_{3} \Perp Y_{1} \mid Y_{2}$, vanishing minor $\sigma_{12} \sigma_{23}-\sigma_{22} \sigma_{13}=0$. Thus only variations of the parameters $\sigma_{21}, \sigma_{22}, \sigma_{31}$ and $\sigma_{32}$ may break the conditional independence structure of this model.

## KL Divergence



Figure: black $=$ standard variation; blue $=$ full; red $=$ partial; green $=$ row-based; pink $=$ column-based.

## Frobenius Norm



Figure: black $=$ standard; blue $=$ full; red $=$ partial; green $=$ row-based; pink $=$ column-based.

## Two-way Sensitivity



Figure: KL divergence (top) and Frobenius norm (bottom) for multi-way variation of the parametes $\sigma_{22}$ and $\sigma_{32}$

## Real-World Application

Metabolomic information of 77 individuals: 47 of them suffering of cachexia, whilst the remaining do not. Cachexia is a metabolic syndrome characterized by loss of muscle with or without loss of fat mass.
We focus on only six metabolics: Adipate (A), Betaine (B), Fumarate (F), Glucose (GC), Glutamine (GM) and Valine (V).


## Real-World Application

$\left.\begin{array}{ccccccc} & \text { B } & \text { V } & \text { GC } & \text { GM } & \text { A } & \text { F } \\ \text { B } & 304 & 3262 & 220 & 2963 & 414 & 208 \\ \text { V } & \begin{array}{cccccc} \\ \text { GC }\end{array} & 98456 & 6637 & 89431 & 12489 & 6279 \\ \text { GM } & 220 & 6637 & 3950 & 53223 & 1693 & 839 \\ \text { A } & 2963 & 89431 & 53223 & 3050126 & 65012 & 31858 \\ \text { F } & 12489 & 1695 & 65012 & 7279 & 1791 \\ 208 & 6279 & 839 & 31858 & 1791 & 1124\end{array}\right)$
$\left.\begin{array}{cccccc} & \\ \text { B } & \text { V } & \text { GC } & \text { GM } & \text { A } & \text { F } \\ \text { V } \\ \text { GC } \\ \text { GC } \\ \text { GM } \\ \text { A } & (1004 & 0 & 310 & 168 & 51 \\ 1004 & 38647 & 0 & 11923 & 10192 & 1974 \\ 0 & 0 & 109 & 376 & 0 & 77 \\ 310 & 11923 & 376 & 8952 & 3144 & 1092 \\ 168 & 10192 & 0 & 3144 & 5171 & 520 \\ 51 & 1974 & 77 & 1092 & 520 & 192\end{array}\right)$

## KL Divergence



Figure: We use the color code black = standard variation; blue = full; red = partial; green = row-based; pink = column-based.

## Frobenius Norm



Figure: black $=$ standard variation; blue $=$ full; red $=$ partial; green $=$ row-based; pink = column-based.

## Conclusions

- A new approach to sensitivity analysis which does not break the conditional independence structure of the model;
- The effect of changing additional entries may (or may not) increase the divergence between the original and the varied distributions, depending on the form of the matrix
- For standard analyses, the theory of interval matrices can tell us for which variations the matrix is still positive-semidefinite
- An R package implementing these methods (as well as standard ones) is currently being developed.

