Maximum likelihood estimation of totally positive Gaussian distributions.

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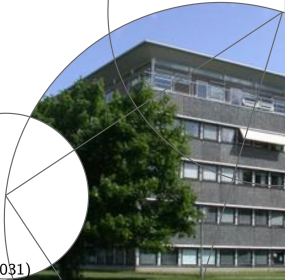
Mathematical Methods of Modern Statistics, Luminy 2017



[1] based on joint work with Caroline Uhler and Piotr Zwiernik (arXiv:1702.04031)

Positive dependence and Simpson's paradox

Two real-valued random variables X and Y are *positively associated* if if $\text{Cov}\{f(X), g(Y)\} \geq 0$ for all f, g which are non-decreasing.

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The Yule-Simpson paradox says that we may have X and Y positively associated but X and Y negatively associated conditionally on a third variable Z.

Multivariate total positivity (MTP_2) ensures this not to happen: *associations can never change sign due to changes of context.*

Multivariate total positivity for functions

Let f be a function $f : \mathcal{X} = \times_{v \in V} \mathcal{X}_v \to \mathbb{R}$ where $\mathcal{X}_v$ are either discrete or open subsets of $\mathbb{R}$.

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Definition

f is *multivariate totally positive of order two* (MTP_2) if

$$f(x)f(y) \leq f(x \wedge y)f(x \vee y) \text{ for all } x, y \in \mathcal{X}.$$

Here $\wedge$ and $\vee$ should be applied coordinatewise.

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In the bivariate case, this property is known simply as *total positivity* or TP_2 (Karlin and Rinott, 1980).

Example

For $d = 2$, $x_1 \leq x_2, y_1 \leq y_2$ the condition for MTP_2 simply becomes

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$$f(x_1, y_2)f(x_2, y_1) \leq f(x_1, y_1)f(x_2, y_2),$$

or, alternatively

$$\det \left\{ \begin{array}{cc} f(x_1, y_1) & f(x_1, y_2) \\ f(x_2, y_1) & f(x_2, y_2) \end{array} \right\} \geq 0.$$

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For $\mathcal{X} = \times_{v \in V} \mathcal{X}_v$ as before we adopt a *standard base measure* $\mu = \otimes_{v \in V} \mu_v$ where μ_v is counting measure if $\mathcal{X}_v$ is discrete and Lebesgue measure if $\mathcal{X}_v$ is an open subset of $\mathbb{R}$.

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Introduced and studied by Karlin and Rinott (1980) using results (FKG inequality) from fundamental paper by Fortuin et al. (1971).

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Mostly from Karlin and Rinott (1980):

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- Characteristic roots of a Wishart matrix W, or of $W_1 W_2^{-1}$, or $W_1(W_1 + W_2)^{-1}$, where $W_1 \perp\!\!\!\perp W_2$ (Dykstra and Hewett, 1978);

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- Many other examples...

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A wealth of probability inequalities are satisfied for MTP_2 distributions (Karlin and Rinott, 1980).

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- *If $\phi = (\phi_v)_{v \in V}$ are non-decreasing, then $Y = \phi(X)$ is MTP_2.*

Positive association and MTP_2

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Proof.

Discrete case by Fortuin et al. (1971). General case by Sarkar (1969). □

Covariance and independence

Proposition

If X is positively associated and $A, B \subseteq V$ are disjoint, then

$$X_A \perp\!\!\!\perp X_B \iff \operatorname{Cov}(X_u, X_v) = 0 \text{ for all } u \in A, v \in B.$$

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So learning MTP_2 structure may be based on correlation analysis.

Markov properties

Let P be a probability distribution on $\mathcal{X} = \times_{v \in V} \mathcal{X}_v$. The *pairwise independence graph* $\mathcal{G}(P) = (V, E)$ is defined through the relation

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We say that P is *globally Markov* w.r.t. a graph $\mathcal{G}$ if

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Further, we say that P is *faithful* to $\mathcal{G}$ if

$$A \perp_{\mathcal{G}} B \mid S \iff A \perp\!\!\!\perp_P B \mid S$$

i.e. if the independence models $\perp\!\!\!\perp_P$ and $\perp_{\mathcal{G}}$ are identical.

A main result

Theorem (Fallat et al. (2017))

Assume the distribution P of X is MTP_2 with strictly positive density $f > 0$. Then P is faithful to $\mathcal{G}(P)$.

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Assume the distribution P of X is MTP_2 with strictly positive density $f > 0$. Then P is faithful to $\mathcal{G}(P)$.

In other words, *for MTP_2 distributions, the pairwise independence graph yields a complete 'picture'* of the independence relations in P.

Multivariate Gaussian MTP_2 distributions

Proposition

Let $X \sim \mathcal{N}_V(0, \Sigma)$. Then X is MTP_2 if and only if $K = \Sigma^{-1}$ is a positive definite M-matrix i.e. iff

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Note also that this is a convex restriction in K.

Carcass data

Measurements of the thickness of meat and fat layers at different locations on the back of a slaughter pig on each of 344 carcasses.

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The sample correlation matrix for this data set is given by

$$S = \begin{array}{c} \\ \end{array} \begin{matrix} \text{Fat11} & \text{Meat11} & \text{Fat12} & \text{Meat12} & \text{Fat13} & \text{Meat13} \end{matrix}$$

$$S = \begin{pmatrix} 1.00 & 0.04 & 0.84 & 0.08 & 0.82 & -0.03 \\ 0.04 & 1.00 & 0.04 & 0.87 & 0.13 & 0.86 \\ 0.84 & 0.04 & 1.00 & 0.01 & 0.83 & -0.03 \\ 0.08 & 0.87 & 0.01 & 1.00 & 0.11 & 0.90 \\ 0.82 & 0.13 & 0.83 & 0.11 & 1.00 & 0.02 \\ -0.03 & 0.86 & -0.03 & 0.90 & 0.02 & 1.00 \end{pmatrix} \begin{matrix} \text{Fat11} \\ \text{Meat11} \\ \text{Fat12} \\ \text{Meat12} \\ \text{Fat13} \\ \text{Meat13} \end{matrix}$$

Empirical concentration for carcass data

and its inverse is

$$S^{-1} = \begin{pmatrix} 4.53 & 0.78 & -2.34 & -1.74 & -1.72 & 1.01 \\ 0.78 & 5.10 & -0.25 & -2.51 & -0.76 & -2.12 \\ -2.34 & -0.25 & 4.52 & 1.40 & -1.93 & -0.94 \\ -1.74 & -2.51 & 1.40 & 7.00 & -0.09 & -4.11 \\ -1.72 & -0.76 & -1.93 & -0.09 & 4.11 & 0.53 \\ 1.01 & -2.12 & -0.94 & -4.11 & 0.53 & 6.51 \end{pmatrix}$$

	Fat11	Meat11	Fat12	Meat12	Fat13	Meat13
Fat11	4.53	0.78	−2.34	−1.74	−1.72	1.01
Meat11	0.78	5.10	−0.25	−2.51	−0.76	−2.12
Fat12	−2.34	−0.25	4.52	1.40	−1.93	−0.94
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Fat13	−1.72	−0.76	−1.93	−0.09	4.11	0.53
Meat13	1.01	−2.12	−0.94	−4.11	0.53	6.51

which is clearly not quite an M-matrix.

MLestimates under MTP_2

The MLE of the correlation matrix, rounded to 2 decimals, is

$$\hat{\Sigma} = \begin{pmatrix} 1.00 & 0.10 & 0.84 & 0.09 & 0.82 & 0.09 \\ 0.10 & 1.00 & 0.11 & 0.87 & 0.13 & 0.86 \\ 0.84 & 0.11 & 1.00 & 0.09 & 0.83 & 0.09 \\ 0.09 & 0.87 & 0.09 & 1.00 & 0.11 & 0.90 \\ 0.82 & 0.13 & 0.83 & 0.11 & 1.00 & 0.11 \\ 0.09 & 0.86 & 0.09 & 0.90 & 0.11 & 1.00 \end{pmatrix}$$

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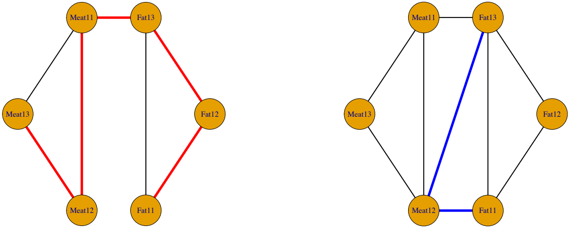
Here blue entries are those that have changed in the estimation process.

Independence graph of estimates



(a) MTP_2 constraint (b) Graphical lasso

Figure: Undirected Gaussian graphical models for `carcass` data. The thick red edges in (a) correspond to the MWSF of the correlation matrix and the blue edges in (b) to edges in the model chosen by the graphical lasso which are not in the ML graph of the MTP_2 solution. *Note that the MTP_2 constraint automatically induces sparsity.*

Basic optimization problem

Let $\mathcal{M}$ denote the convex cone of M-matrices. Then the MLE is the solution to the following optimization problem:

$$\begin{aligned} \underset{K}{\text{maximize}} \quad & \log\det(K) - \operatorname{trace}(KS) \\ \text{subject to} \quad & K \in \mathcal{M} \end{aligned} \tag{1}$$

This is a convex optimization problem, since the objective function is concave on $\mathbb{S}^p_{\succeq 0}$.

Convex duality

The dual cone to $\mathcal{M}$ is the cone $\mathcal{N}$ given as

$$\mathcal{N} = \{X \in \mathbb{S}^p \mid \exists Y \in \mathbb{S}^p_{\succ 0} \text{ with } X \leq Y \text{ and } \mathrm{diag}(X) = \mathrm{diag}(Y)\}.$$

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In other words, it holds that

$$\overline{\mathcal{N}} = \left\{ S \in \mathbb{S} \mid \langle S, K \rangle \geq 0 \text{ for all } K \in \mathcal{M} \right\} \qquad (2)$$

where $\langle A, B \rangle = \operatorname{tr}(AB)$ is the trace inner product.

Basic estimation result

Theorem (Lauritzen et al. (2017))

Consider a Gaussian MTP_2 model. Then the MLE $\hat{\Sigma}$ and $\hat{K}$ exists for a given sample covariance matrix S on V if and only if $S \in \mathcal{N}$. It is then equal to the unique element $\hat{\Sigma} \succ 0$ that satisfies the following system of equations and inequalities

$$
\begin{aligned}
\hat{k}_{uv} &\leq 0 \quad \textit{for all } u \neq v, & (3)\\
\hat{\sigma}_{vv} - s_{vv} &= 0 \quad \textit{for all } v \in V, & (4)\\
(\hat{\sigma}_{uv} - s_{uv}) &\geq 0 \quad \textit{for all } u \neq v, & (5)\\
(\hat{\sigma}_{uv} - s_{uv})\hat{k}_{uv} &= 0 \quad \textit{for all } u \neq v, & (6)
\end{aligned}
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Sparsity of the solution

The *maximum likelihood graph* (ML graph) $\hat{G}$ is the graph given by non-zero entries of $\hat{K}$.

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We then have the following

Corollary (Lauritzen et al. (2017))

Consider the Gaussian graphical model determined by $k_{uv} = 0$ for $uv \notin E(\hat{G})$, where $\hat{G}$ is the ML graph under MTP_2. Let $\bar{\Sigma}$ be the MLE of Σ under that Gaussian graphical model (without the MTP_2 constraint). Then $\hat{\Sigma} = \bar{\Sigma}$.

Proof of corollary

Proof.

The MLE of Σ under the Gaussian graphical model with graph $\hat{G}$ is the unique element $\bar{\Sigma} \succ 0$ that satisfies the following system of equations:

$$\begin{aligned} \bar{\sigma}_{vv} - s_{vv} &= 0 \text{ for all } v \in V, \\ \bar{\sigma}_{uv} - s_{uv} &= 0 \text{ for all } uv \in E(\hat{G}), \\ k_{uv} &= 0 \text{ for all } uv \notin E(\hat{G}). \end{aligned}$$

The estimation theorem says that also $\hat{\Sigma}$ satisfies these equations and hence we must have $\bar{\Sigma} = \hat{\Sigma}$. □

Ultrametric matrices and inverse M-matrices

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$$u_{ij} \geq \min(u_{ik}, u_{jk}) \text{ for all } i, j, k.$$

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We then have the following known result.

Theorem (Dellacherie et al. (2014))

Let U be an ultrametric matrix with strictly positive entries on the diagonal. Then U is non-singular if and only if no two rows are equal. Moreover, if U is non-singular, then U^{-1} is an M-matrix.

Single linkage matrix

By invariance, we may without loss of generality assume that instead of S we consider R given as $r_{uv} = s_{uv}/\sqrt{s_{uu}s_{vv}}$ so in particular $r_{uu} = 1$ for all u.

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If R is positive semidefinite with $r_{ii} = 1$, we define G^+ as the graph determined by positive entries of R. Define further a matrix Z by

$$z_{ij} \quad := \quad \max_P \min_{uv \in P} r_{uv}, \tag{7}$$

where maximum is taken over paths in G^+ between i and j.

Single linkage matrix

By invariance, we may without loss of generality assume that instead of S we consider R given as $r_{uv} = s_{uv}/\sqrt{s_{uu}s_{vv}}$ so in particular $r_{uu} = 1$ for all u.

If R is positive semidefinite with $r_{ii} = 1$, we define G^+ as the graph determined by positive entries of R. Define further a matrix Z by

$$z_{ij} := \max_{P} \min_{uv \in P} r_{uv}, \tag{7}$$

where maximum is taken over paths in G^+ between i and j.

Z is the *single-linkage* matrix based on R and is known from cluster analysis.

Example

Suppose that

$$R = \begin{bmatrix} 1 & -0.5 & 0.5 & 0.6 \\ -0.5 & 1 & 0.4 & -0.1 \\ 0.5 & 0.4 & 1 & 0.2 \\ 0.6 & -0.1 & 0.2 & 1 \end{bmatrix}$$

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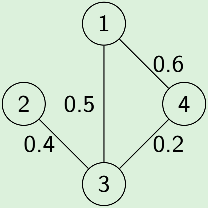
Then G^+ and Z are given by



$$Z = \begin{bmatrix} 1 & 0.4 & 0.5 & 0.6 \\ 0.4 & 1 & 0.4 & 0.4 \\ 0.5 & 0.4 & 1 & 0.5 \\ 0.6 & 0.4 & 0.5 & 1 \end{bmatrix}.$$

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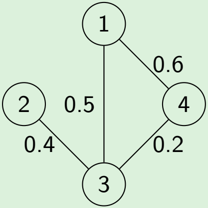

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Note that $Z \geq R$, Z is invertible, and Z^{-1} is an M-matrix.

Single linkage and ultrametric

Proposition (Lauritzen et al. (2017))

Let R be a symmetric $p \times p$ positive semidefinite matrix satisfying $r_{ii} = 1$ for all $i = 1, \ldots, p$. Then the single-linkage matrix Z based on R is an ultrametric matrix with $z_{ij} \geq r_{ij}$ for all $i \neq j$. If, in addition, $r_{ij} < 1$ for all $i \neq j$, then Z is nonsingular and therefore an inverse M-matrix.

Existence of the MLE

Theorem (Slawski and Hein (2015))

Consider a Gaussian MTP_2 model and let R be the sample correlation matrix. If $r_{ij} < 1$ for all $i \neq j$ then the MLE $\hat{\Sigma}$ (and $\hat{K}$) exists and it is unique. In particular, if the number n of observations satisfies $n \geq 2$, then the MLE exists with probability 1.

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Proof.

The single linkage matrix Z based on R is feasible both for the primal and dual problem. Hence the optimization problem has a (unique) solution. □

Properties of the maximum likelihood graph

Theorem (Lauritzen et al. (2017))

Let $MWSF(R)$ be the maximum weight spanning forest of R. Then with probability one, it holds that $MWSF(R) \subseteq \hat{G}$, where $\hat{G} = G(\hat{K})$ is the ML graph.

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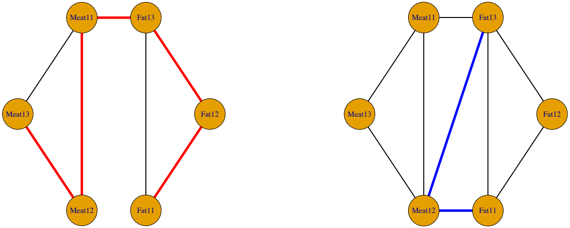
Proof.

(sketch): Add MWSF(R) to $\hat{G}$ and show that $\hat{\Sigma}$ is also the MLE for the graphical model with graph MWSF(R) $\cup\, \hat{G}$. Now this happens with probability zero unless MWSF(R) $\subseteq \hat{G}$. □

Carcass data revisited



(a) MTP_2 constraint (b) Graphical lasso

Figure: Undirected Gaussian graphical models for `carcass` data. The thick red edges in (a) correspond to the MWSF of the correlation matrix and the blue edges in (b) to edges in the model chosen by the graphical lasso which are not in the ML graph of the MTP_2 solution.

Signed MTP_2 distributions

Definition

A distribution of X is *signed MTP_2* if there is a diagonal matrix D with $d_{ii} \in \{-1, 1\}$ so that $Y = DX$ is MTP_2.

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Then change signs along the tree to obtain $\tilde{X}$ with all pairwise correlations along edges positive.

Finally estimate under MTP_2 based on $\tilde{X}$.

Personality traits

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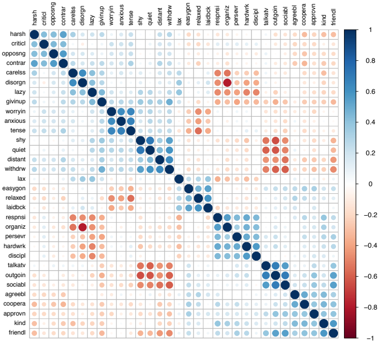

Figure: Correlation matrix of personality traits from the data set described in Malle and Horowitz (1995).

Personality traits

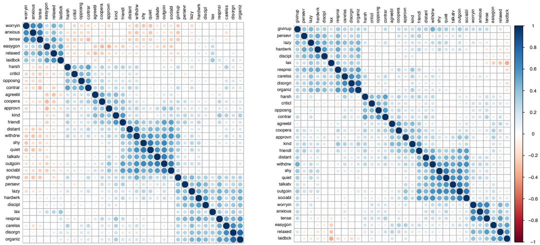

Figure: The correlation matrix of the data set on personality traits after performing the sign switches using the Chow-Liu tree is shown on the left. The correlation matrix resulting from switching the signs of the 16 (negative) traits that constitute the first block of variables in the previous figure is shown on the right.

Personality traits

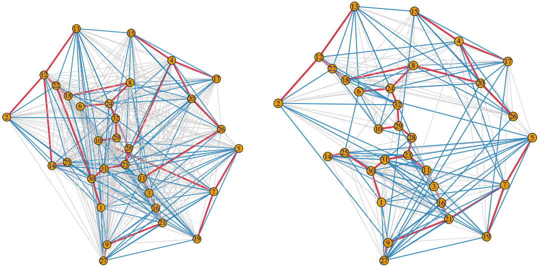

Figure: The graphical models resulting from estimation under MTP_2 under the two correlation matrices. The thin gray edges correspond to the edges of the EC graph that are not part of the ML graph. The blue edges represent edges of the ML graph that are not part of the minimum weight spanning tree. The latter is represented by thick red edges.

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