Your Dreams May Come True with MTP_2...

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Optimization and Parsimonious Modeling
IMA

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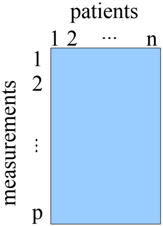
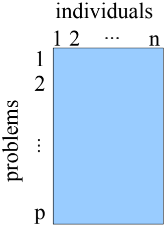
Problem

Given large data sets for example from **medical tests** or **IQ tests**, determine a sparse graph that describes the dependencies between the variables.





Two common approaches:

- **Machine Learning:** Graphical lasso
- **Applied Statistics:** Chow-Liu and subsequent stepwise selection

Overview

1. MTP_2 distributions
2. Properties of MTP_2 distributions related to sparsity
3. Models that imply MTP_2
4. Maximum likelihood estimation under MTP_2

Positive dependence and MTP_2 distributions

- A distribution (i.e. density function) p on $\mathcal{X}$ is **multivariate totally positive of order** 2 (MTP_2) if

$$p(x)p(y) \quad \leq \quad p(x \wedge y)p(x \vee y) \qquad \text{for all } x, y \in \mathcal{X} \subset \mathbb{R}^m.$$

- A random vector X is **positively associated** if for any non-decreasing functions $\phi, \psi : \mathbb{R}^m \to \mathbb{R}$

$$\mathrm{cov}\{\phi(X), \psi(X)\} \geq 0.$$

Theorem (Fortuin Kasteleyn Ginibre inequality, 1971)

MTP_2 *implies positive association.*

Discrete and Gaussian MTP_2 distribution

Example: Binary vector $X = (X_1, X_2, X_3) \in \{0,1\}^3$ is MTP_2 if and only if

$$\begin{array}{lll}
p_{001}p_{110} \le p_{000}p_{111} & p_{010}p_{101} \le p_{000}p_{111} & p_{100}p_{011} \le p_{000}p_{111} \\
p_{011}p_{101} \le p_{001}p_{111} & p_{011}p_{110} \le p_{010}p_{111} & p_{101}p_{110} \le p_{100}p_{111} \\
p_{001}p_{010} \le p_{000}p_{011} & p_{001}p_{100} \le p_{000}p_{101} & p_{010}p_{100} \le p_{000}p_{110}
\end{array}$$

Theorem (Horn and Johnson, 1991)

*A multivariate Gaussian distribution $p(x;\theta)$ is MTP_2 if and only if the inverse covariance matrix θ is an **M-matrix**, that is*

$$\theta_{ij} \le 0 \qquad \textit{for all } \; i \neq j.$$

Theorem (Karlin and Rinott, 1980)

If $p(x) > 0$ and p is MTP_2 for any pair of coordinates when the others are held constant, then p is MTP_2.

Properties of MTP_2 distribution

Theorem (FLSUWZ, 2015)

If $X = (X_1, \ldots, X_m)$ *is* MTP_2*, then*

(i) *any marginal distribution is* MTP_2

(ii) *any conditional distribution is* MTP_2

(iii) *marginal independence structure:*

$$X_i \perp\!\!\!\perp X_j \iff cov(X_i, X_j) = 0$$

(iv) *conditional independence structure:*

$$X_A \perp\!\!\!\perp X_B \mid X_C \implies X_A \perp\!\!\!\perp X_B \mid X_{C \cup \{k\}}$$

(iv) *composition property:*

$$X_A \perp\!\!\!\perp X_B \mid X_C \ and \ X_A \perp\!\!\!\perp X_D \mid X_C \implies X_A \perp\!\!\!\perp X_{B \cup D} \mid X_C$$

(iv) *singelton transitivity property:*

$$X_i \perp\!\!\!\perp X_j \mid X_C \ and \ X_i \perp\!\!\!\perp X_j \mid X_{C \cup \{k\}} \implies X_i \perp\!\!\!\perp X_k \mid X_C \ or \ X_j \perp\!\!\!\perp X_k \mid X_C$$

Occurrence of MTP_2 distributions

MTP_2 contraints appear to be extremely **restrictive**:

- 3-dim. Gaussian distributions: about 5% are MTP_2
- 4-dim. Gaussian distributions: about 0.09% are MTP_2
- 3-dim. binary distributions: about 2% are MTP_2
- 4-dim. binary distributions: about 0% are MTP_2

Constraints are less restrictive with additional Markov structure!

For 3-dim. Gaussian distributions:

- if $1 \perp\!\!\!\perp 2 \mid 3$: 25% are MTP_2,
- if in addition $1 \perp\!\!\!\perp 3 \mid 2$: 50% are MTP_2,
- if $1 \perp\!\!\!\perp 2 \perp\!\!\!\perp 3$: 100% are MTP_2.

Example: EPH-gestosis

Dataset collected 40 years ago in a study on "Pregnancy and Child Development" by the German Research Foundation and recently analyzed by *Wermuth and Marchetti (2014)*.

EPH-gestosis: disease syndrome for pregnant women; three symptoms

- edema (high body water retention)
- proteinuria (high amounts of urinary proteins)
- hypertension (elevated blood pressure)

Observed counts:

$$\begin{bmatrix} n_{000} & n_{010} & n_{001} & n_{011} \\ n_{100} & n_{110} & n_{101} & n_{111} \end{bmatrix} = \begin{bmatrix} 3299 & 107 & 1012 & 58 \\ 78 & 11 & 65 & 19 \end{bmatrix}.$$

This sample distribution is MTP_2!

Example: Math grades

Data: grades of 88 students in

`Mechanics`, `Vectors`, `Algebra`, `Analysis`, `Statistics`

$$S = \begin{array}{cc} & \begin{array}{ccccc} \text{mechanics} & \text{vectors} & \text{algebra} & \text{analysis} & \text{statistics} \end{array} \\ & \left(\begin{array}{rrrrr} 305.7680 & 127.2226 & 101.5794 & 106.2727 & 117.4049 \\ 127.2226 & 172.8422 & 85.1573 & 94.6729 & 99.0120 \\ 101.5794 & 85.1573 & 112.8860 & 112.1134 & 121.8706 \\ 106.2727 & 94.6729 & 112.1134 & 220.3804 & 155.5355 \\ 117.4049 & 99.0120 & 121.8706 & 155.5355 & 297.7554 \end{array}\right) \begin{array}{l} \text{mechanics} \\ \text{vectors} \\ \text{algebra} \\ \text{analysis} \\ \text{statistics} \end{array} \end{array}$$

$$S^{-1} = 10^{-3} \cdot \begin{array}{cc} & \begin{array}{ccccc} \text{mechanics} & \text{vectors} & \text{algebra} & \text{analysis} & \text{statistics} \end{array} \\ & \left(\begin{array}{rrrrr} 5.2446 & -2.4351 & -2.7395 & 0.0116 & -0.1430 \\ -2.4351 & 10.4268 & -4.7078 & -0.7928 & -0.1660 \\ -2.7395 & -4.7078 & 26.9548 & -7.0486 & -4.7050 \\ 0.0116 & -0.7928 & -7.0486 & 9.8829 & -2.0184 \\ -0.1430 & -0.1660 & -4.7050 & -2.0184 & 6.4501 \end{array}\right) \begin{array}{l} \text{mechanics} \\ \text{vectors} \\ \text{algebra} \\ \text{analysis} \\ \text{statistics} \end{array} \end{array}$$

Although sample distribution is not quite MTP_2, any fitted reasonable Gaussian graphical model is MTP_2

MTP_2 constraints are often implicit

Pairwise interaction model for a graph $G = (V, E)$:

$$p(x) = \frac{1}{Z} \prod_{i \in V} \psi_i(x_i) \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j),$$

where ψ_{ij} positive functions, Z the normalizing constant.

Theorem (FLSUWZ, 2015)

p is MTP_2 if and only if ψ_{ij} are MTP_2 functions.

- **Example:** Ferromagnetism in Ising models

$$\psi_{ij}(x_i, x_j) = \exp(-\theta_{ij} x_i x_j), \quad \theta_{ij} \leq 0$$

Signed MTP_2 distributions

A Gaussian / discrete random vector $X = (X_1, \dots, X_m)$ has a **signed MTP_2 distribution** if and only if:

- **Discrete:** The distribution of X is MTP_2 up to a permutation of the values in each $\mathcal{X}_i$
- **Gaussian:** There exists a diagonal matrix $D \in \{-1, +1\}^m$ such that DX is MTP_2.

The following models are signed MTP_2:

- Gaussian / binary pairwise interaction models on trees
- Binary latent class models (*Allman, Rhodes, Sturmfels & Zwiernik, 2013*)
- Gaussian / binary latent tree models
    - Single factor analysis models

ML Estimation for Gaussian graphical models

Primal: Max-Likelihood:

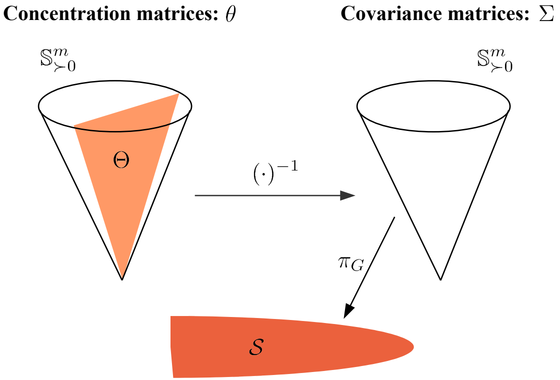
$$\underset{\theta \succeq 0}{\text{maximize}} \quad \log\det(\theta) - \mathrm{trace}(\theta S)$$

$$\text{subject to} \quad \theta_{uv} = 0, \ \ \forall\, uv \notin E, u \neq v.$$

Dual: Min-Entropy: $G = (V, E)$

$$\underset{\Sigma \succeq 0}{\text{minimize}} \quad -\log\det(\Sigma) - m$$

$$\text{subject to} \quad \Sigma_{uv} = S_{uv}, \ \ \forall\, uv \in E, \text{ and } u = v.$$



ML Estimation for Gaussian MTP_2 distributions

Primal: Max-Likelihood:

$$\underset{\theta \succeq 0}{\text{maximize}} \quad \log\det(\theta) - \mathrm{trace}(\theta S)$$
$$\text{subject to} \quad \theta_{uv} \leq 0, \;\; \forall\, u \neq v.$$

Dual: Min-Entropy:

$$\underset{\Sigma \succeq 0}{\text{minimize}} \quad -\log\det(\Sigma) - m$$
$$\text{subject to} \quad \Sigma_{vv} = S_{vv}, \; \Sigma_{uv} \geq S_{uv}.$$

Theorem

The MLE based on S exists if and only if there exists $\Sigma \succ 0$ with $\Sigma \geq S$. It is then equal to the unique element $\hat{\theta} = \hat{\Sigma}^{-1} \succ 0$ that satisfies the following system of equations and inequalities

(a) *Primal feasibility:* $\hat{\theta}_{uv} \leq 0 \;\; \forall u \neq v,$

(b) *Dual feasibility:* $\hat{\Sigma}_{vv} - S_{vv} = 0 \;\; \forall v, \quad \hat{\Sigma}_{uv} - S_{uv} \geq 0 \;\; \forall u \neq v$

(c) *Complimentary slackness:* $(\hat{\Sigma}_{uv} - S_{uv})\,\hat{\theta}_{uv} = 0 \;\; \forall u \neq v.$

Note: We get sparsity for free!!

ML Estimation for Gaussian MTP_2 distributions

Theorem (Slawski and Hein, 2015)

The MLE in a Gaussian MTP_2 model exists with probability 1 when $n \geq 2$.

Theorem (LUZ, 2016)

Let S be a sample correlation matrix and $\hat{\theta}$ the MLE of the concentration matrix in the Gaussian MTP_2 model. Let $G_{MST}(S)$ be the maximal spanning tree of S and $G(\hat{\theta})$ the concentration graph. Then

$$G_{MST}(S) \subset G(\hat{\theta}).$$

Algorithm: *Input:* Sample correlation matrix S
Output: Graph under Gaussian signed MTP_2 model

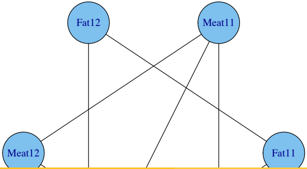
- Let $D \in \{-1, 1\}^p$ diagonal s.t. Chow-Liu tree of DSD is positive
- Compute MLE $\hat{\Sigma}$ based on DSD under Gaussian MTP_2 model
- Output $G(\hat{\Sigma}^{-1})$

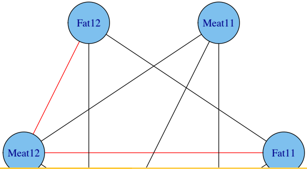
Example: Carcass

344 measurements of the thickness of meat and fat layers at different locations of a slaughter pig

$$
S^{-1} = \begin{array}{c} \\ \end{array}
\begin{array}{cccccc|c}
\text{Fat11} & \text{Meat11} & \text{Fat12} & \text{Meat12} & \text{Fat13} & \text{Meat13} & \\
0.40 & \color{red}{0.04} & -0.23 & -0.07 & -0.19 & \color{red}{0.05} & \text{Fat11} \\
\color{red}{0.04} & 0.15 & -0.01 & -0.06 & -0.05 & -0.06 & \text{Meat11} \\
-0.23 & -0.01 & 0.51 & \color{red}{0.07} & -0.23 & -0.05 & \text{Fat12} \\
-0.07 & -0.06 & \color{red}{0.07} & 0.14 & -0.00 & -0.09 & \text{Meat12} \\
-0.19 & -0.05 & -0.23 & -0.00 & 0.54 & \color{red}{0.03} & \text{Fat13} \\
\color{red}{0.05} & -0.06 & -0.05 & -0.09 & \color{red}{0.03} & 0.16 & \text{Meat13}
\end{array}
$$

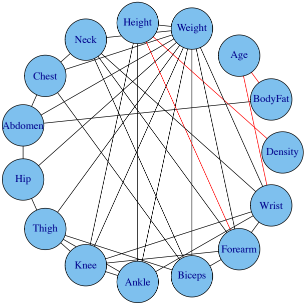
$$
S = \begin{array}{cccccc|c}
\text{Fat11} & \text{Meat11} & \text{Fat12} & \text{Meat12} & \text{Fat13} & \text{Meat13} & \\
11.34 & 0.74 & 8.42 & 2.06 & 7.66 & \color{red}{-0.76} & \text{Fat11} \\
0.74 & 32.97 & 0.67 & 35.94 & 2.01 & 31.97 & \text{Meat11} \\
8.42 & 0.67 & 8.91 & 0.31 & 6.84 & \color{red}{-0.60} & \text{Fat12} \\
2.06 & 35.94 & 0.31 & 51.79 & 2.18 & 41.47 & \text{Meat12} \\
7.66 & 2.01 & 6.84 & 2.18 & 7.62 & 0.38 & \text{Fat13} \\
\color{red}{-0.76} & 31.97 & \color{red}{-0.60} & 41.47 & 0.38 & 41.44 & \text{Meat13}
\end{array}
$$



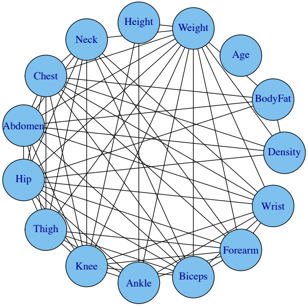


Example: BodyFat

241 observations on 15 variables: age, weight, height, percentage of body fat, body density, and the circumferences of various body parts.



Under MTP_2 constraint



Using glasso

Conclusions and future work

- MTP_2 constraints reflect real processes and models
  - ferromagnetism
  - latent class models with positive associations
  - latent Gaussian/binary tree models
- they lead to some beautiful theory (exponential families, convexity, combinatorics, semialgebraic geometry)
- they are useful in high-dimensional settings

References

- Fallat, Lauritzen, Sadeghi, Uhler, Wermuth, and Zwiernik: Total positivity in Markov structures (arXiv:1510.01290)
- Lauritzen, Uhler, and Zwiernik: Totally positive exponential families and graphical models (on the arXiv shortly)

Thank you!