Your Dreams May Come True with MTP_2...

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Hyperbolic Polynomials and Hyperbolic Programming

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Positive dependence and MTP_2 distributions

- A distribution (i.e. density function) p on $\mathcal{X} = \prod_{v \in V} \mathcal{X}_v$, with $\mathcal{X}_v \subseteq \mathbb{R}$ discrete or open subset, is **multivariate totally positive of order 2 (MTP_2)** if

$$p(x)p(y) \quad \leq \quad p(x \wedge y)p(x \vee y) \qquad \text{for all } x, y \in \mathcal{X},$$

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- 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 (FortuinKasteleynGinibre inequality, 1971, Karlin & Rinott, 1980)

MTP_2 *implies positive association.*

No Yule-Simpson Paradox under MTP_2!

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

Sentences in 4863 murder cases in Florida over the six years 1973-1978:

Murderer	Sentence: Death	Sentence: Other
Black	59	2547
White	72	2185

Victim	Murderer	Sentence: Death	Sentence: Other
Black	Black	11	2309
	White	0	111
White	Black	48	238
	White	72	2074

Overall greater proportion of white murderers receiving death sentence than black (3.2% vs. 2.3%); this trend is reversed given color of victim.

Data from: Range (1979)

Gaussian-like properties of MTP_2 distribution

Reminder: A distribution p on $\mathcal{X} \subseteq \mathbb{R}^m$ is MTP_2 if

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

Theorem (Lebowitz, 1972; Karlin and Rinott, 1980)

If X is MTP_2, then

(i) *any marginal distribution is MTP_2*

(ii) *any conditional distribution is MTP_2*

(iii) $X_A \perp\!\!\!\perp X_B \iff \mathrm{cov}(X_u, X_v) = 0$ *for all* $u \in A$, $v \in B$

Gaussian MTP_2 distributions

Theorem (Bølviken 1982, Karlin & Rinott, 1983)

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

$$K_{uv} \leq 0 \qquad \textit{for all } u \neq v.$$

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Ex: 2016 Monthly correlations of global stock markets *(InvestmentFrontier.com)*

$$S = \begin{pmatrix} 1.000 & 0.606 & 0.731 & 0.618 & 0.613 \\ 0.606 & 1.000 & 0.550 & 0.661 & 0.598 \\ 0.731 & 0.550 & 1.000 & 0.644 & 0.569 \\ 0.618 & 0.661 & 0.644 & 1.000 & 0.615 \\ 0.613 & 0.598 & 0.569 & 0.615 & 1.000 \end{pmatrix}$$

	Nasdaq	Canada	Europe	UK	Australia
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Canada	0.606	1.000	0.550	0.661	0.598
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$$S^{-1} = \begin{array}{c} \\ \end{array}$$

	Nasdaq	Canada	Europe	UK	Australia	
$S^{-1} =$	2.629	−0.480	−1.249	−0.202	−0.490	Nasdaq
	−0.480	2.109	−0.039	−0.790	−0.459	Canada
	−1.249	−0.039	2.491	−0.675	−0.213	Europe
	−0.202	−0.790	−0.675	2.378	−0.482	UK
	−0.490	−0.459	−0.213	−0.482	1.992	Australia

Sample distribution is MTP_2! If you sample a correlation matrix uniformly at random the probability of it being MTP_2 is $< 10^{-6}$!

Discrete MTP_2 distributions

Reminder: A distribution p on $\mathcal{X} \subseteq \mathbb{R}^m$ is $\mathbf{MTP_2}$ if
$$p(x)p(y) \;\le\; p(x \wedge y)p(x \vee y), \quad \text{for all } x, y \in \mathcal{X}.$$

- Distribution of 3 binary variables X, Y and Z is MTP_2 iff

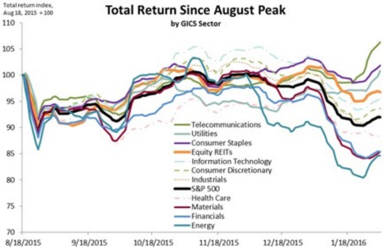
$$\begin{array}{lll} p_{001}p_{110} \le p_{000}p_{111} & p_{010}p_{101} \le p_{000}p_{111} & p_{100}p_{011} \le p_{000}p_{111} \\ p_{011}p_{101} \le p_{001}p_{111} & p_{011}p_{110} \le p_{010}p_{111} & p_{101}p_{110} \le p_{100}p_{111} \\ p_{001}p_{010} \le p_{000}p_{011} & p_{001}p_{100} \le p_{000}p_{101}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

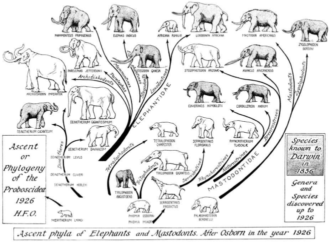
- Dataset on **EPH-gestosis** analyzed by *Wermuth & Marchetti (2014)*
  - edema (high body water retention)
  - proteinuria (high amounts of urinary proteins)
  - hypertension (elevated blood pressure)

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

- This sample distribution is MTP_2! Although when you sample 3-dim binary distributions only about 2% are MTP_2.

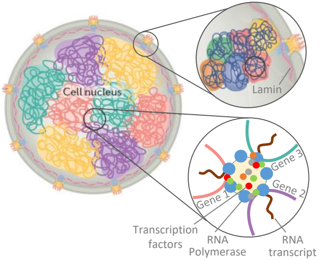
MTP_2 constraints are often implicit





$|X|$ is MTP_2 in:

- Gaussian / binary tree models
- Gaussian / binary latent tree models
    - Binary latent class models
    - Single factor analysis models



Hyperbolic MTP_2 exponential families

- An exponential family is a parametric model with density

$$p_\theta(x) \;=\; \exp\big(\langle \theta, T(x)\rangle \;-\; A(\theta)\,\big),$$

  sample space $\mathcal{X}$ with measure ν, sufficient statistics $T : \mathcal{X} \to \mathbb{R}^d$, and space of canonical parameters: $C \;=\; \big\{\theta \in \mathbb{R}^d :\; A(\theta) < +\infty\big\}$

- Gaussian distribution: $A(\theta) = -\alpha \log\det(\theta)$, $C = \mathbb{S}^p_{\succ 0}$

- Hyperbolic exponential family: $A(\theta) = -\alpha \log(f(\theta))$, f hyperbolic with hyperbolicity cone C

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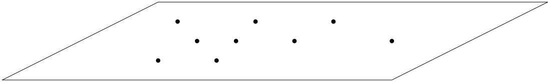
Theorem (Lauritzen, Uhler & Zwiernik, 2019)

The space of canonical parameters for any MTP_2 exponential family is given by $C \cap K$, where $K \subset \mathbb{R}$ is a closed convex cone whose dual is generated by

$$\{T(x \wedge y) + T(x \vee y) - T(x) - T(y) : \; x, y \in \mathcal{X} \textit{ differing in 2 entries}\}.$$

Density estimation

Given i.i.d. samples $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^m$ from an unknown distribution on $\mathbb{R}^m$ with density p, can we estimate p?



- parametric: assume p lies in some parametric family
  - finite-dimensional optimization problem (estimate parameters)
  - restrictive: real-world distribution might not lie in specified family
- non-parametric: assume that p lies in a non-parametric family:
  - infinite-dimensional optimization problem

ML Estimation for Gaussian MTP_2 distributions

Let $X_1, \ldots, X_n \sim \mathcal{N}(0, \Sigma)$, $S := \frac{1}{n}\sum_{i=1}^{n} X_i X_i^T$ sample covariance matrix.

Primal: Max-Likelihood:

$$\begin{array}{ll} \underset{K \succeq 0}{\text{maximize}} & \log\det(K) - \mathrm{trace}(KS) \\ \text{subject to} & K_{uv} \leq 0, \ \ \forall\, u \neq v. \end{array}$$

Dual: Min-Entropy:

$$\begin{array}{ll} \underset{\Sigma \succeq 0}{\text{minimize}} & -\log\det(\Sigma) - m \\ \text{subject to} & \Sigma_{vv} = S_{vv}, \ \Sigma_{uv} \geq S_{uv}. \end{array}$$

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- Maximum likelihood estimation under MTP_2 is a convex optimization problem with strong duality
- the global optimum is characterized by KKT conditions
- Complementary slackness implies that the MLE $\hat{K}^{-1} = \hat{\Sigma}$ satisfies $(\hat{\Sigma}_{uv} - S_{uv})\,\hat{K}_{uv} = 0 \qquad \forall u \neq v$

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- **Linear algebra:** If M is an M-matrix, then $(M^{-1})_{ij} \geq 0$ for all i, j
- Graphical model: $\hat{G}$ (support of $\hat{K}$) is in general **sparse**!!!

Ultrametric matrices and inverse M-matrices

- U is **ultrametric**: $U_{ii} \geq U_{ij} = U_{ji} \geq \min(U_{ik}, U_{jk}) \geq 0$ for all i, j, k.

Theorem (Dellacherie, Martinez and San Martin, 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.

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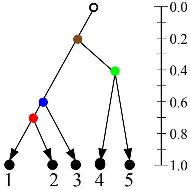
New proof: Construct primal & dual feasible point by single-linkage clustering

$$S = \left(\begin{array}{ccc|cc} 1 & 0.7 & 0.6 & 0.2 & 0.1 \\ 0.7 & 1 & 0.5 & 0.1 & -0.5 \\ 0.6 & 0.5 & 1 & -0.3 & 0.1 \\ \hline 0.2 & 0.1 & -0.3 & 1 & 0.4 \\ 0.1 & -0.5 & 0.1 & 0.4 & 1 \end{array}\right) \rightarrow \left(\begin{array}{ccc|cc} 1 & 0.7 & 0.6 & 0.2 & 0.2 \\ 0.7 & 1 & 0.6 & 0.2 & 0.2 \\ 0.6 & 0.6 & 1 & 0.2 & 0.2 \\ \hline 0.2 & 0.2 & 0.2 & 1 & 0.4 \\ 0.2 & 0.2 & 0.2 & 0.4 & 1 \end{array}\right)$$



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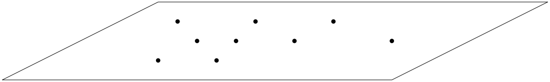

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- non-parametric: assume that p lies in a non-parametric family:
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  - need constraints that are:
    - strong enough so that there is no spiky behavior
    - weak enough so that function class is large

Shape-constrained density estimation

- monotonically decreasing densities: [Grenander 1956, Rao 1969]
- convex densities: [Anevski 1994, Groeneboom, Jongbloed, and Wellner 2001]
- **log-concave** densities: [Cule, Samworth, and Stewart 2010]
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- Maximum liklihood estimation under MTP_2: Given i.i.d. samples $X = \{x_1, ..., x_n\} \subset \mathbb{R}^m$,

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$$p \text{ log-concave.}$$

Log-concave density estimation

- Log-concavity is natural assumption: ensures density is continuous and includes many distributions: Gaussian, Uniform(a, b), Gamma(k, θ) for $k \geq 1$, Beta(a, b) for $a, b \geq 1$, etc.

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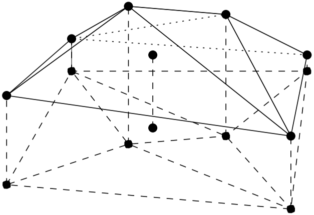
Theorem (Cule, Samworth and Stewart, 2008)

When $n \geq m + 1$, a log-concave MLE $\hat{p}$ exists and is unique with probability 1. Moreover, $\log(\hat{p})$ is a tent-function supported on the convex hull of the data. **Finite-dimensional optimization problem!**



ML estimation under log-concavity and MTP_2 / LLC

Questions:

- When does the MLE under log-concavity and MTP_2 / LLC exist? Is it unique?
- What is the shape of the MLE under log-concavity and MTP_2 / LLC?
  - Is the MLE always exp(tent function)?
- Can we compute the MLE?

Log-$L^\natural$-concave (LLC) functions

- A function $f : \mathbb{R}^m \to \mathbb{R}$ is MTP_2 if

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- A function $f : \mathbb{R}^m \to \mathbb{R}$ is log-$L^\natural$-concave (LLC) if

$$f(x)f(y) \leq f((x + \alpha \mathbf{1}) \wedge y)\, f(x \vee (y - \alpha \mathbf{1})) \quad \forall \alpha \geq 0 \text{ and } x, y \in \mathbb{R}^m.$$

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Theorem (Murota, 2008)

A function $f : \mathbb{Z}^m \to \mathbb{R}$ is LLC if and only if it is log-concave, i.e.,

$$f(x)f(y) \leq f\left(\left\lfloor \frac{x+y}{2} \right\rfloor\right) f\left(\left\lceil \frac{x+y}{2} \right\rceil\right) \quad \textit{for all } x, y \in \mathbb{Z}^m.$$

Ex.: A Gaussian distribution with covariance matrix Σ is LLC if and only if $K = \Sigma^{-1}$ is a diagonally dominant M-matrix, i.e.,

$$K_{ij} \leq 0 \text{ for all } i \neq j \quad \text{and} \quad \sum_{j=1}^{m} K_{ij} \geq 0 \text{ for all } i = 1, \ldots m.$$

Existence and uniqueness of the MLE

Theorem (Robeva, Sturmfels, Tran and Uhler, 2018)

Let $X_1, \ldots, X_n$ be i.i.d samples from a distribution with density f_0 supported on a full-dimensional subset of $\mathbb{R}^m$. The following hold with probability one:

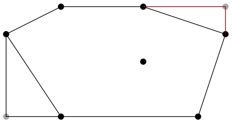
- *If $n \geq 3$, the MTP_2 log-concave MLE exists and is unique.*
- *If $n \geq 2$, the LLC log-concave MLE exists and is unique.*

- This result is in contrast with existence of the MLE under log-concavity, where $n \geq m + 1$ samples are needed for existence
- Proof uses convergence properties for log-concave distributions, and does not shed light on the shape of the MLE.

Support of the MLE

Under MTP_2 we need the density to be nonzero at additional points:

$\implies$ "Min-max convex hull" of X



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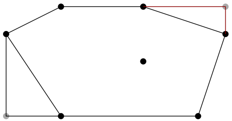

- $\mathbf{MM}(X) :=$ smallest min-max closed set S containing X, i.e. $x, y \in S \Rightarrow x \wedge y, x \vee y \in S$
- $\mathbf{MMconv}(X) :=$ smallest min-max closed & convex set containing X

Is it always true that $\mathbf{MMconv}(X) = \mathbf{conv}(\mathbf{MM}(X))$?

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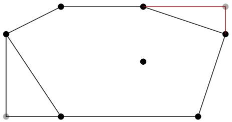

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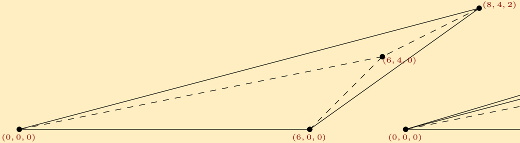
Is it always true that MMconv$(X) = \mathbf{conv}(\mathbf{MM}(X))$?

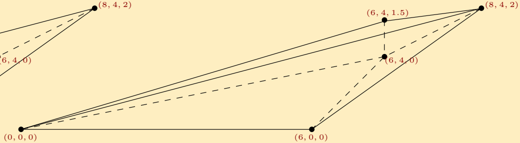
Lemma

If $X \subseteq \mathbb{R}^2$ or $X \subseteq \{0,1\}^m$, then $MMconv(X) = conv(MM(X))$.

Support of the MLE in higher dimensions

Ex: Consider $X = \{(0,0,0),(6,0,0),(6,4,0),(8,4,2)\} \subseteq \mathbb{R}^3$.



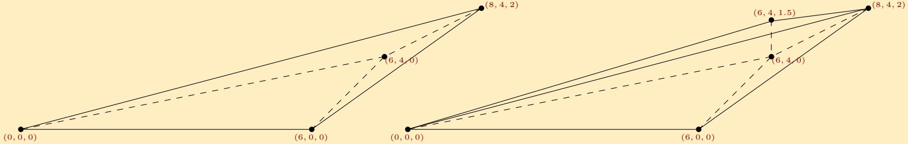


- $\mathrm{MM}(X) = X$
- But $\mathrm{conv}(\mathrm{MM}(X))$ is not min-max closed!

$$(6,4,3/2) = \max\{(6,4,0),(6,3,3/2)\} \notin \mathrm{conv}(\mathrm{MM}(X)).$$

Support of the MLE in higher dimensions

Ex: Consider $X = \{(0,0,0),(6,0,0),(6,4,0),(8,4,2)\} \subseteq \mathbb{R}^3$.



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Theorem (The 2-D Projections Theorem)

Let $\pi_{ij} : \mathbb{R}^m \to \mathbb{R}$, $x \mapsto (x_i, x_j)$. Then for any finite subset $X \subseteq \mathbb{R}^m$,

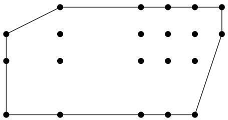
$$MMconv(X) = \bigcap_{1 \le i < j \le m} \pi_{ij}^{-1}\left(conv(\pi_{ij}(MM(X))\right).$$

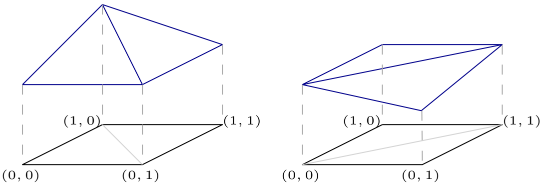
Exponentials of tent functions $h_{X,y}$

Theorem (Robeva, Sturmfels, Tran and Uhler, 2018)

Let $X \subset \mathbb{R}^m$ be a finite set of points. The exponential of a tent function $h_{X,y}$ is MTP_2 if and only if all of the walls of the subdivision h induces are **bimonotone**.

A linear inequality $a \cdot x + b \leq 0$ is bimonotone if it has the form $a_i x_i + a_j x_j + b \leq 0$, where $a_i a_j \leq 0$.



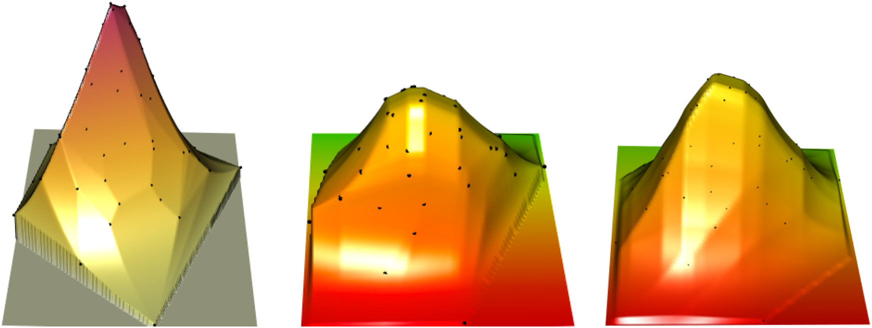


Shape of the MLE

Theorem (Robeva, Sturmfels, Tran and Uhler, 2018)

If $X \subseteq \mathbb{R}^2$ or $X \subseteq \{0,1\}^m$ ($X \subseteq \mathbb{Q}^m$), then the MTP_2 (LLC) MLE is of the form exp(tent function) and the set of MTP_2 (LLC) tent pole heights define a convex polytope.

$\Longrightarrow$ We can use the conditional gradient method to compute the MLE



Conclusions

- We conjecture that the MTP_2-MLE is always the exponential of a tent function (we provide conjectured tent pole locations)
- LLC estimate provides an MTP_2 estimate (might not be the MLE)
- Total positivity constraints are often implicit and reflect real processes
  - ferromagnetism
  - latent tree models
- Total positivity represents interesting shape constraint for non-parametric density estimation: broad enough class to be of interest in applications, constrained enough to obtain good density estimates with few samples
- MTP_2 / LLC is well-suited for high-dimensional applications

References

MTP2 distributions not only have broad applications for data analysis, but also lead to interesting new problems in combinatorics, geometry & algebra.

- Fallat, Lauritzen, Sadeghi, Uhler, Wermuth, & Zwiernik: Total positivity in Markov structures, *Annals of Statistics* 45 (2017)
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- Robeva, Sturmfels, Tran & Uhler: Maximum likelihood estimation for totally positive log-concave densities (arXiv:1806.10120)
- Lauritzen, Uhler, & Zwiernik: Total positivity in structured binary distributions (to appear on the arXiv today!)

Thank you!