Nonparametric Density Estimation under Total Positivity

Elina Robeva
University of British Columbia

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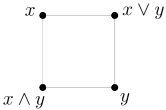
Totally Positive Distributions

- A distribution with density p on $\mathcal{X} \subseteq \mathbb{R}^d$ is *multivariate totally positive of order 2* (or MTP_2) if

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



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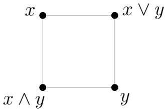


where $x \wedge y$ and $x \vee y$ are the componentwise minimum and maximum.

- MTP_2 is the same as *log-supermodular*:

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

Properties of MTP_2 distributions

Theorem (Fortuin Kasteleyn Ginibre, 1971)

MTP_2 implies positive association.

Definition

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

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

Theorem (Karlin and Rinot 1980; Lebowitz 1972)

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

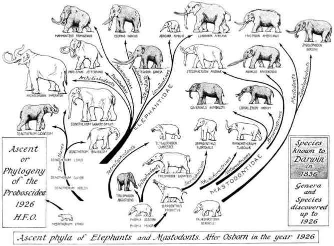
(i) *any marginal distribution is MTP_2,*

(ii) *any conditional distribution is MTP_2,*

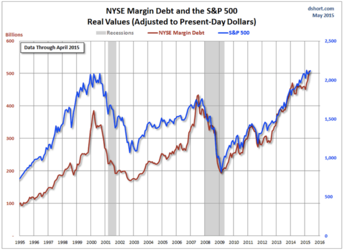
(iii) *X has the marginal independence structure*

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

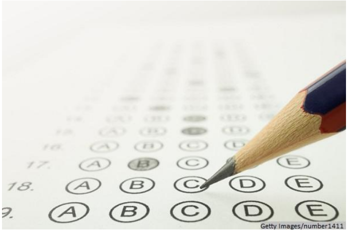
Examples of Totally Positive Distributions



[Felsenstein, 1973]



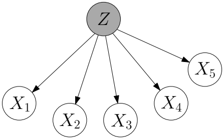
[Agrawal, Roy, and Uhler, 2019]



[Fallat, Lauritzen, Sadeghi, Uhler, Wermuth, and Zwiernik, 2016]

Examples of MTP_2 distributions

- The joint distribution of observed variables influenced by one hidden variable (in the Gaussian and binary case)



- Many models imply MTP_2:
  - Ferromagnetic Ising models
  - Order statistics of i.i.d. variables
  - Brownian motion tree models
  - Gaussian/binary (latent) tree models (e.g. single factor analysis models)

Examples of MTP_2 distributions

A Gaussian random variable $X \sim \mathcal{N}(\mu, \Sigma)$ is MTP_2 whenever Σ^{-1} is an M-matrix, i.e. its off-diagonal entries are nonpositive

$$(\Sigma^{-1})_{ij} \leq 0, \quad \forall i \neq j.$$

Very rare: out of 100,000 uniformly sampled 5×5 correlation matrices none were MTP_2. [Fallat et al., 2016].

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Data: grades of 88 students in 5 math subjects

[Mardia, Kent and Bibby, 1979, Fallat et al., 2016]

$$S = \begin{pmatrix} 305.7680 & 127.2226 & 101.5794 & 106.2727 & 117.4049 \\ 127.2226 & 172.8422 & 85.1573 & 94.6729 & 99.0120 \\ 101.5794 & 85.1573 & 112.8860 & 112.1134 & 121.8706 \\ 106.2727 & 94.6729 & 112.1134 & 220.3804 & 155.5355 \\ 117.4049 & 99.0120 & 121.8706 & 155.5355 & 297.7554 \end{pmatrix}$$

	mechanics	vectors	algebra	analysis	statistics
mechanics	305.7680	127.2226	101.5794	106.2727	117.4049
vectors	127.2226	172.8422	85.1573	94.6729	99.0120
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$$S^{-1} = 10^{-3} \cdot \begin{pmatrix} 5.2446 & -2.4351 & -2.7395 & 0.0116 & -0.1430 \\ -2.4351 & 10.4268 & -4.7078 & -0.7928 & -0.1660 \\ -2.7395 & -4.7078 & 26.9548 & -7.0486 & -4.7050 \\ 0.0116 & -0.7928 & -7.0486 & 9.8829 & -2.0184 \\ -0.1430 & -0.1660 & -4.7050 & -2.0184 & 6.4501 \end{pmatrix}$$

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Examples of MTP_2 distributions

Data: 2016 monthly correlations of global stock markets

[*InvestmentFrontier.com*; Agrawal, Roy, and Uhler, 2019]

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

	Nasdaq	Canada	Europe	UK	Australia
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Europe	0.731	0.550	1.000	0.644	0.569
UK	0.618	0.661	0.644	1.000	0.615
Australia	0.613	0.598	0.569	0.615	1.000

$$S^{-1} = \begin{pmatrix} 2.629 & -0.480 & -1.249 & -0.202 & -0.490 \\ -0.480 & 2.109 & -0.039 & -0.790 & -0.459 \\ -1.249 & -0.039 & 2.491 & -0.675 & -0.213 \\ -0.202 & -0.790 & -0.675 & 2.378 & -0.482 \\ -0.490 & -0.459 & -0.213 & -0.482 & 1.992 \end{pmatrix}$$

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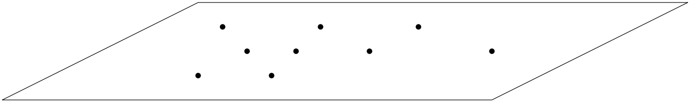
Density estimation

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



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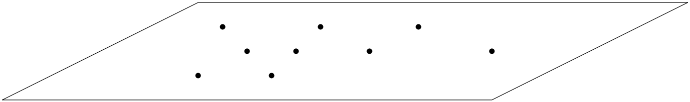
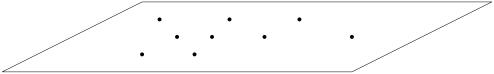


- non-parametric: assume that p lies in a non-parametric family, e.g. impose shape-constraints on p (convex, log-concave, monotone, etc.)
  - infinite-dimensional problem
  - need constraints that are:
    - strong enough so that there is no spiky behavior
    - weak enough so that function class is large

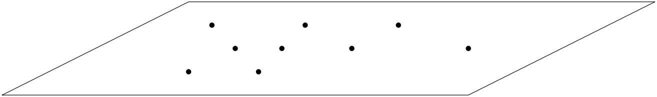
Shape-constrained density estimation



- monotonically decreasing densities: [Grenander 1956, Rao 1969]
- convex densities: [Anevski 1994, Groeneboom, Jongbloed, and Wellner 2001]
- **log-concave** densities: [Cule, Samworth, and Stewart 2008, Dümbgen et al. 2009, ...]
- generalized additive models with shape constraints: [Chen and Samworth 2016]

- **totally positive (and log-concave) densities**

Maximum Likelihood Estimation under MTP_2



Given i.i.d. samples $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ with weights $w = (w_1, \ldots, w_n)$ (where $w_1, \ldots, w_n \geq 0$, $\sum w_i = 1$) from a distribution p on $\mathbb{R}^d$, can we estimate p?

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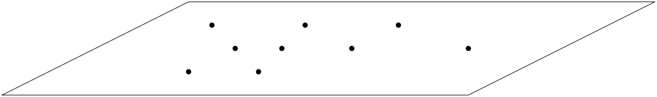

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$$\begin{aligned} \text{maximize}_p \quad & \sum_{i=1}^{n} w_i \log(p(x_i)) \\ \text{s.t.} \quad & p \text{ is an } \text{MTP}_2 \text{ density.} \end{aligned}$$

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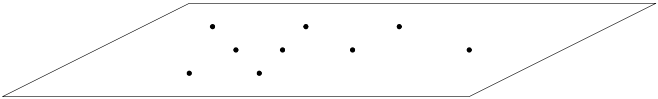

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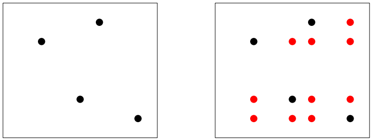
Problem: likelihood is unbounded, MTP_2 constraint is too weak for MLE to exist.



Maximum Likelihood Estimation under MTP_2

To ensure that the likelihood function is bounded, we impose the condition that p is log-concave.

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A function $f : \mathbb{R}^d \to \mathbb{R}$ is *log-concave* if its logarithm is concave.

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- Log-concavity is a natural assumption because it ensures the density is continuous and includes many known families of parametric distributions.
- Log-concave families:
  - Gaussian;
  - Uniform(a, b);
  - Gamma(k, θ) for $k \geq 1$;
  - Beta(a, b) for $a, b \geq 1$.
- Maximum likelihood estimation under log-concavity is a well-studied problem (Cule et al. 2008, Dümbgen et al. 2009, Schuhmacher et al. 2010, ...).

Maximum Likelihood Estimation under Log-Concavity

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Theorem (Cule, Samworth and Stewart 2008)

- *With probability 1, a log-concave maximum likelihood estimator $\hat{p}$ exists and is unique as long as there are at least $d+1$ samples.*

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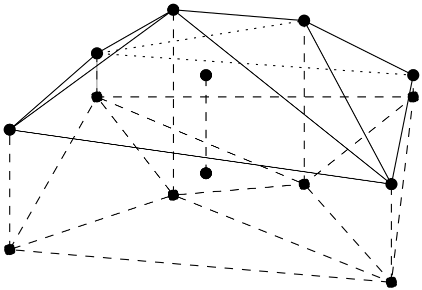
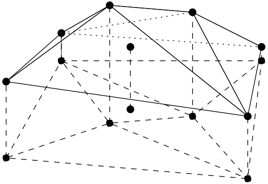
Theorem (Cule, Samworth and Stewart 2008)

- *With probability 1, a log-concave maximum likelihood estimator $\hat{p}$ exists and is unique as long as there are at least $d+1$ samples.*
- *Moreover, $\log(\hat{p})$ is a 'tent-function' supported on the convex hull of the data $P(X) = conv(x_1, \ldots, x_n)$.*



Optimizing over Tent Functions



Given points $X = \{x_1, \dots, x_n\}$ and heights $y = (y_1, \dots, y_n) \in \mathbb{R}^n$, the *tent function*

$$h_{X,y} : \mathbb{R}^d \to \mathbb{R}$$

is the smallest concave function such that $h_{X,y}(x_i) \geq y_i$ for all i. Thus, $\hat{p} = \exp(h_{X,y})$ for some y.

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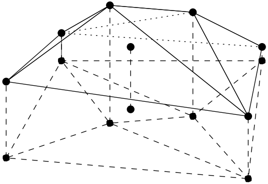

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INFINITE DIMENSIONAL

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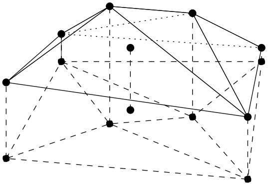

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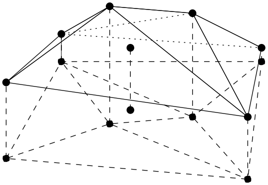

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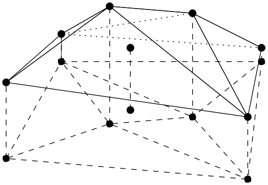

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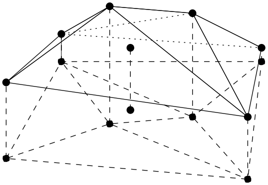

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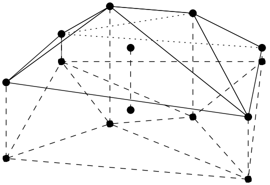

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$$\max_{y \in \mathbb{R}^n} \quad \sum_{i=1}^{n} w_i y_i - \int \exp(h_{X,y}(t))dt$$

INFINITE DIMENSIONAL

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Maximum Likelihood Estimation under Log-concavity and MTP_2

Questions:

1. Does the MLE under log-concavity and MTP_2 exist with probability 1 and, if so, is it unique?
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   2.1 What is the support of the MLE?
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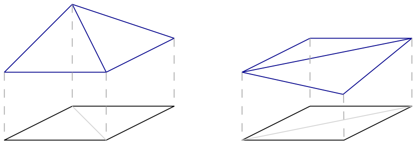


Existence and Uniqueness of the MLE

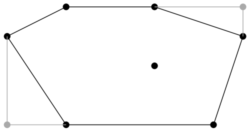
Theorem (R., Sturmfels, Tran, Uhler, 2018)

- *The maximum likelihood estimator under log-concavity and MTP_2 exists and is unique with probability 1 as long as there are at least 3 samples.*
- *Furthermore, the MLE is a consistent estimator.*

Proof uses convergence properties for log-concave distributions, and does not shed light on the shape of the MLE.

The Support of the MLE

Support of MLE = "Min-max convex hull" of X.



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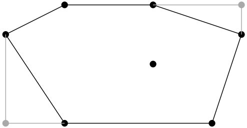

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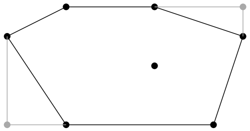

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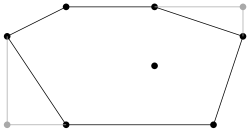

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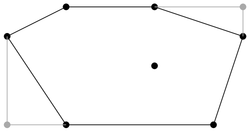

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Lemma

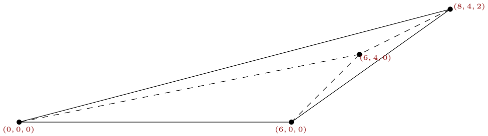
Let $X = \{x_1, \ldots, x_n\}$. If $X \subseteq \mathbb{R}^2$ or $X \subseteq \prod_{i=1}^{d} \{a_i, b_i\}$, then,

$$MMconv(X) = conv(MM(X)).$$

$\Longrightarrow$ we can compute $\text{MMconv}(X)$ for $X \subseteq \mathbb{R}^2$ and $X \subseteq \prod_{i=1}^{d} \{a_i, b_i\}$.

The Min-Max Convex Hull

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



It turns out that

$$\mathrm{MM}(X) = X.$$

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conv(MM(X)) is **not min-max closed**!

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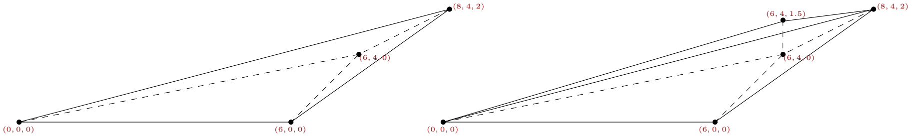

It turns out that

$$\mathrm{MM}(X) = X.$$

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

This is because:

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

Therefore,

$$\mathrm{conv}(\mathrm{MM}(X)) \subsetneq \mathrm{MMconv}(X).$$

Computing $MMconv(X)$

Theorem (The 2-D Projections Theorem)

For any finite subset $X \subseteq \mathbb{R}^d$,

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

$$\pi_{ij} : \mathbb{R}^d \to \mathbb{R}^2, \quad x \mapsto (x_i, x_j).$$

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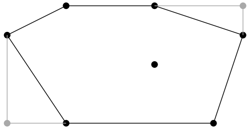
Corollary (Queyranne and Tardella, 2006)

A convex polytope C in $\mathbb{R}^d$ is min-max closed if and only if it is defined by a finite collection of bimonotone linear inequalities.

A linear inequality is *bimonotone* if it has the form

$$a_i x_i + a_j x_j + b \le 0, \quad \text{where} \quad a_i a_j \le 0.$$



Back to Log-concave and MTP_2 Maximum Likelihood Estimation

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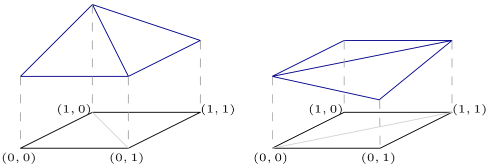
Supermodular Tent Functions

Recall that $p = \exp(h)$ is $\mathbf{MTP}_2$ if and only if h is **supermodular**, i.e.

$$h(x) + h(y) \leq h(x \wedge y) + h(x \vee y), \qquad \text{for all } x, y \in \mathbb{R}^d.$$

Theorem (R., Sturmfels, Tran, Uhler, 2018)

Let $X \subset \mathbb{R}^d$ be a finite set of points. A tent function h is supermodular if and only if all of the walls of the subdivision h induces are **bimonotone***.*



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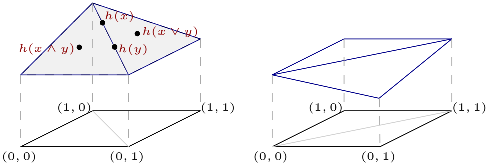

Remark

To find the best $h_{X,y}$, need to optimize over heights y that induce bimonotone subdivisions.

- *In general not convex.*
- *Example:* $X = \{0,1\} \times \{0,1\} \times \{0,1,2\}$.

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When is the MLE the exponential of a tent function?

Theorem (R., Sturmfels, Tran, Uhler 2018)

If $X \subseteq \mathbb{R}^2$ or $X \subseteq \prod_{i=1}^{d} \{a_i, b_i\}$, then the MLE is the exponential of a tent function

$$p^* = \exp(h_{\tilde{X},y}),$$

where $\tilde{X} = MM(X)$.

Finding the MLE

Theorem (R., Sturmfels, Tran, Uhler 2018)

If $X \subseteq \mathbb{R}^2$ or $X \subseteq \prod_i \{a_i, b_i\}$, then the set of heights for which $\exp(h_{\tilde{X},y})$ is MTP_2 is a convex polytope $\mathcal{S}$.
Therefore, we can use, e.g. the conditional gradient method, to find y^*.

$$\begin{array}{ll} \text{maximize}_y & \displaystyle\sum_{i=1}^{n} w_i y_i - \int \exp(h_{\tilde{X},y}) \\ \text{s.t.} & y \in \mathcal{S}. \end{array}$$

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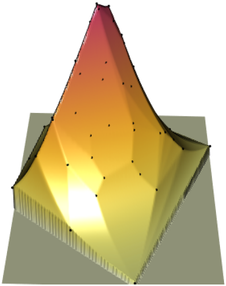
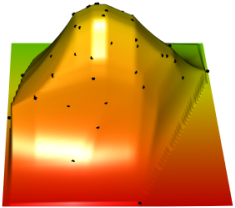
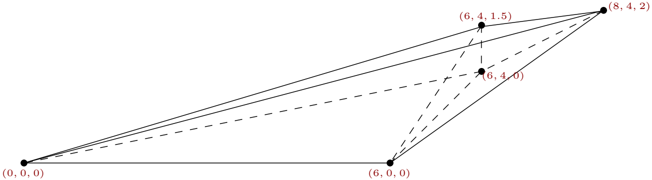




What is the shape of the MLE in the general case?

Let $X = \{(0,0,0), (6,0,0), (6,4,0), (8,4,2), (6,4,\frac{3}{2})\}$, $w = \frac{1}{28}(15,1,1,1,10)$. The log-concave MLE is not MTP_2.



The MTP_2 and log-concave MLE is exp(tent function) on $X \cup \{(6,3,\frac{3}{2}), (7.5,4,\frac{3}{2})\}$ with subdivision as above.

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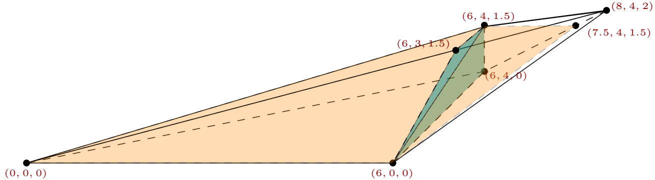

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Sample complexity for log-concave density estimation

- $\mathcal{F}_d$ = set of log-concave and MTP_2 densities in $\mathbb{R}^d$
- $h^2(f,g) = \int(\sqrt{f} - \sqrt{g})^2$ Hellinger distance
- $\hat{p}_n$ = log-concave MLE from n samples

Theorem (Kim and Samworth, 2014)

(a). *Upper bound for $d = 2, 3$:*

$$\sup_{p_0 \in \mathcal{F}_2} \mathbb{E}_{p_0}[h^2(p_0, \hat{p}_n)] = \mathcal{O}(n^{-\frac{2}{d+1}} \log n).$$

(b). *Lower bound for $d \geq 2$:*

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Theorem (Carpenter et al., 2018)

When $d \geq 4$:

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Problem

When $d \geq 3$:

(a). *Upper bound?*

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(b). *Lower bound:*

$$\inf_{\tilde{p}_n} \sup_{p_0 \in \mathcal{F}_d} \mathbb{E}_{p_0}[h^2(p_0, \tilde{p}_n)] \geq c_2 poly(d) n^{-\frac{2}{3}}$$

No curse of dimensionality?

Conclusion

MLE

- Is the MLE always exp(tent function)?
- Rates for $d \geq 3$?
- Faster algorithms for finding the MLE?

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- Min-max closure of sample, $\mathrm{MM}(X)$, convolved with standard Gaussian is MTP_2.
  [with Ali Zartash, 2019]
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  [with Ali Zartash, 2019]
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- Test statistics for MTP_2 distributions?
- Multivariate total positivity of higher orders (i.e. MTP_k)?

Thank you!

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