
REPRESENTATION OF DISCRETE MAXIMUM ENTROPY DISTRIBUTIONS AS TENSOR NETWORKS

RESEARCH NOTES IN THE ENEXA AND QROM PROJECTS

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ABSTRACT

We here summarize results of the main report on maximum entropy distributions. The principle of maximum entropy serves as motivation for Computation Activation Networks. We then restrict to these distributions and study relative entropy minimization problems.

In the report, first discussion on the mean polytope are in Chapter 3, and the general maximum entropy problem in Chapter 4. Chapter 8 contains the discussion on maximum entropy distributions in case of boolean statistics.

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1 Introduction

1.1 Motivation

Entropy as Information Quantifier: Based on Shannons source code theorem, one can interpret entropy as an quantifier of the information content in a random variable. This has fundamental equivalences in physics and machine learning.

Maximum Entropy in Physics: E.g. Maxwell-Boltzmann distributions.

Maximum Entropy in Learning: Consider a learning problem where we want to estimate a model based on observed data. The maximum entropy problem principle approaches this problem by designing statistics of the data, which means shall be reproduced in the model, and choosing the model reproducing the means of the statistic with least structure. The entropy of a distribution quantifies the degree of structureless in a distribution and is therefore maximized to solve the learning task.

Hybrid Reasoning: Combining logical and probabilistic AI is a common aim of statistical relational AI, neuro-symbolic AI and explainable AI. Logical and probabilistic models can be treated in the tensor network formalism, which thus serves as a unifying representation language.

The maximum support problem: Factorization using the exponential represent always distributions with the maximal support (i.e. that of the base measure). Thus they do not discuss situations appearing in hybrid reasoning. We here investigate the more generic case, where distributions have different support.

1.2 Tensor Notation

Introduce here tensors, variables, contractions.

1.3 The Maximum Entropy Problem

Given a non-negative and non-vanishing base measure $\nu [X_{[d]}]$, a probability distribution is a non-negative tensor $\mathbb{P} [X_{[d]}]$ such that

$$\langle \mathbb{P} [X_{[d]}] , \nu [X_{[d]}] \rangle [\emptyset] = 1 .$$

We denote the set of such distributions by

$$\Lambda^{\delta, \text{MAX}, \nu} = \{ \mathbb{P} [X_{[d]}] : \mathbb{P} [X_{[d]}] \geq 0 [X_{[d]}] , \langle \mathbb{P} [X_{[d]}] , \nu [X_{[d]}] \rangle [\emptyset] = 1 \} .$$

The mean parameter of a distribution $\mathbb{P} [X_{[d]}]$ to a statistic $\mathcal{S} : \times_{k \in [d]} [m_k] \rightarrow \times_{s \in [n]} [p_s]$ is the vector $\mu [L] \in \mathbb{R}^p$ with the coordinates

$$\mu [L = l] = \mathbb{E} [f_l] = \langle f_l [X_{[d]}] , \mathbb{P} [X_{[d]}] , \nu [X_{[d]}] \rangle [\emptyset] .$$

The entropy of a distribution is

$$\mathbb{H}_{\nu} [\mathbb{P} [X_{[d]}]] = \langle \mathbb{P} [X_{[d]}] , \ln [\mathbb{P} [X_{[d]}]] , \nu [X_{[d]}] \rangle [\emptyset] .$$

The maximum entropy problem given a mean parameter $\mu^* [L]$ is stated by

$$\max_{\mathbb{P} [X_{[d]}] \in \Lambda^{\delta, \text{MAX}, \nu}} \mathbb{H}_{\nu} [\mathbb{P} [X_{[d]}]] \quad \text{subject to} \quad \forall_{l \in [p]} : \langle \mathbb{P} [X_{[d]}] , \mathcal{S}_l [X_{[d]}] , \nu [X_{[d]}] \rangle [L] = \mu^* [L = l] \quad (\text{P}_{\mathcal{S}, \mu, \nu})$$

1.4 Contributions

We in this paper provide tensor network representations

- Representation of distributions with maximum entropy, in case of positive realizability: Elementary activation tensors

- Representation of generic maximum entropy distributions: CP activation tensors.

Now, we want to characterize the CP rank of the activation tensors

- Depends on the face of the mean polytope, which contains the mean parameter
- We have thus a well-defined "CP rank" of faces
- Largest faces and vertices have always CP rank of 1, intermediate faces can have larger CP rank

For boolean statistics we further provide insights for boolean statistics (see Chapter 8.5):

- Example of independent statistics (see Exa. 8.28): Always elementary activation tensors (hypercubes)
- Example of partition statistics (see Exa. 8.30):
- Generic criterion for elementary activation: "Cube-like" polytopes (see Def. 8.29)

1.5 Outlook

To prepare for the presentation of our main results we introduce

- Computation-Activation Networks: A tensor network architecture, which will be used to represent maximum entropy distributions
- Mean polytopes: Polytopes, which contain all realizable mean parameter vectors.

We will then show, that dependent on the position of the mean parameter in the mean polytope, we can characterize the corresponding maximum entropy distribution by a Computation-Activation Network.

2 The mean polytope

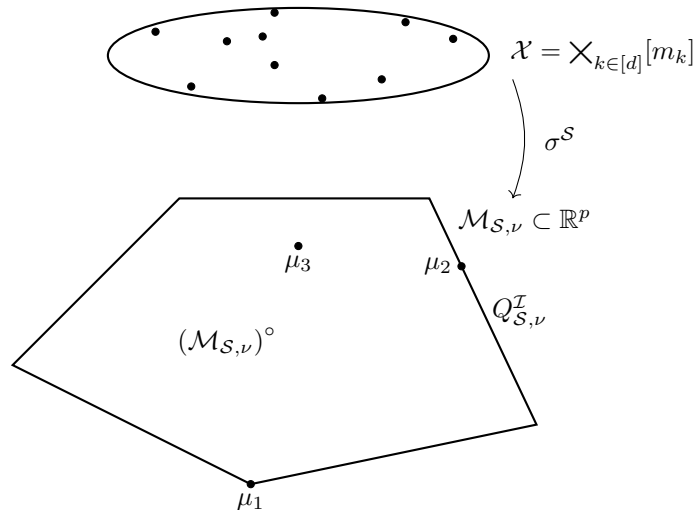
The mean polytope is the set of mean parameters to any distribution. To ease the notation, we use the selection encoding $\sigma^S [X_{[d]}, L]$ of a statistic

$$\sigma^S [X_{[d]}, L = l] = \mathcal{S}_l [X_{[d]}] .$$

We define it as

$$\mathcal{M}_{\mathcal{S}, \nu} = \{ \langle \mathbb{P}, \sigma^S, \nu \rangle [L] : \mathbb{P} [X_{[d]}] \in \Lambda^{\delta, \text{MAX}, \nu} \} ,$$

where we denote by $\Lambda^{\delta, \text{MAX}, \nu}$ the set of all probability distributions representable with respect to ν .



2.1 Convex hull

Lemma 1. *For any statistic \mathcal{S} and base measure ν , the set of mean parameters is the convex hull of the set*

$$\mathcal{N}_{\mathcal{S},\nu} = \{\sigma^{\mathcal{S}}[X_{[d]} = x_{[d]}, L] : x_{[d]} \in \bigtimes_{k \in [d]} [m_k], \nu[X_{[d]} = x_{[d]}] \neq 0\}$$

that is $\mathcal{M}_{\mathcal{S},\nu} = \text{conv}(\mathcal{N}_{\mathcal{S},\nu})$.

Proof. This follows from

$$\Lambda^{\delta, \text{MAX}, \nu} = \text{conv} \left(\frac{1}{\nu[X_{[d]} = x_{[d]}]} \cdot \epsilon_{x_{[d]}}[X_{[d]}] : x_{[d]} \in \bigtimes_{k \in [d]} [m_k], \nu[X_{[d]} = x_{[d]}] \neq 0 \right).$$

and for any vertex of this simplex we have

$$\left\langle \frac{1}{\nu[X_{[d]} = x_{[d]}]} \cdot \epsilon_{x_{[d]}}[X_{[d]}], \sigma^{\mathcal{S}}[X_{[d]}, L], \nu[X_{[d]}] \right\rangle [L] = \sigma^{\mathcal{S}}[X_{[d]} = x_{[d]}, L].$$

□

Thus the polytope of mean parameters depends on the base measure only through its support.

2.2 Faces

Let us now continue with the investigation of the faces of the mean parameter polytope.

Definition 1. *We say that the convex hull of a subset $\mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}} \subset \mathcal{N}_{\mathcal{S},\nu}$ is a face, if and only if there is a face normal vector $\theta_{\mathcal{I}}[L] \in \mathbb{R}^p$ such that*

$$\mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}} = \text{argmax}_{\mu[L] \in \mathcal{N}_{\mathcal{S},\nu}} \langle \mu[L], \theta_{\mathcal{I}}[L] \rangle [\emptyset].$$

we denote $Q_{\mathcal{S},\nu}^{\mathcal{I}} = \text{conv}(\mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}})$.

We notice, that each face itself is a convex polytope. What is more, we can characterize these as mean parameter polytopes with respect to refined base measures to be defined next.

Definition 2. *The face measure to the face $Q_{\mathcal{S},\nu}^{\mathcal{I}}$ of $\mathcal{M}_{\mathcal{S},\nu}$ is the boolean tensor $\nu^{\mathcal{S},\mathcal{I}}[X_{[d]}]$ with coordinates to $x_{[d]} \in \bigtimes_{k \in [d]} [m_k]$ by*

$$\nu^{\mathcal{S},\mathcal{I}}[X_{[d]} = x_{[d]}] = \begin{cases} \nu[X_{[d]} = x_{[d]}] & \text{if } \mathcal{S}(x_{[d]}) \in \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}} \\ 0 & \text{else} \end{cases}.$$

We now specify the mean parameter polytope to any face using the face measure as a refinement of the base measure.

Lemma 2. *For any face $Q_{\mathcal{S},\nu}^{\mathcal{I}}$ of $\mathcal{M}_{\mathcal{S},\nu}$ we have*

$$Q_{\mathcal{S},\nu}^{\mathcal{I}} = \mathcal{M}_{\mathcal{S},\nu^{\mathcal{S},\mathcal{I}}}.$$

Proof. For any $x_{[d]} \in \bigtimes_{k \in [d]} [m_k]$ we have $\nu^{\mathcal{S},\mathcal{I}}[X_{[d]} = x_{[d]}] \neq 0$ if and only if $\mathcal{S}(x_{[d]}) \in \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}$ and $\nu[X_{[d]} = x_{[d]}] \neq 0$. Thus we have

$$\begin{aligned} Q_{\mathcal{S},\nu}^{\mathcal{I}} &= \text{conv}(\mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}) \\ &= \text{conv}(\sigma^{\mathcal{S}}[X_{[d]} = x_{[d]}, L] : \mathcal{S}(x_{[d]}) \in \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}, \nu[X_{[d]} = x_{[d]}] \neq 0) \\ &= \text{conv}(\sigma^{\mathcal{S}}[X_{[d]} = x_{[d]}, L] : \nu^{\mathcal{S},\mathcal{I}}[X_{[d]} = x_{[d]}] \neq 0) \\ &= \mathcal{M}_{\mathcal{S},\nu^{\mathcal{S},\mathcal{I}}}. \end{aligned}$$

□

Representability of a distribution with respect to face measures is an equivalent condition for the mean parameter of a distribution to be on a face, as we show next.

Lemma 3. *If and only if for a distribution $\mathbb{P}[X_{[d]}] \in \Lambda^{\delta, \text{MAX}, \nu}$ and a face \mathcal{I} we have*

$$\langle \sigma^{\mathcal{S}}[X_{[d]}, L], \mathbb{P}[X_{[d]}], \nu[X_{[d]}] \rangle [L] \in Q_{\mathcal{S}, \nu}^{\mathcal{I}},$$

then $\mathbb{P}[X_{[d]}]$ is representable with respect to the base measure

$$\nu^{\mathcal{S}, \mathcal{I}}[X_{[d]}].$$

Proof. We have

$$\mu[L] = \sum_{x_{[d]}} \mathbb{P}[X_{[d]} = x_{[d]}] \cdot \nu[X_{[d]} = x_{[d]}] \cdot \gamma^{\mathcal{S}}[X_{[d]} = x_{[d]}, L].$$

Let now $\theta_{\mathcal{I}}[L]$ be a face normal to the face $Q_{\mathcal{S}, \nu}^{\mathcal{I}}$. We then have

$$\langle \mu[L], \theta_{\mathcal{I}}[L] \rangle [\emptyset] = \sum_{x_{[d]} \in \times_{k \in [d]} [m_k]} \mathbb{P}[X_{[d]} = x_{[d]}] \cdot \nu[X_{[d]} = x_{[d]}] \cdot \langle \gamma^{\mathcal{S}}[X_{[d]} = x_{[d]}, L], \theta_{\mathcal{I}}[L] \rangle [\emptyset].$$

Now if and only if $\mathbb{P}[X_{[d]} = x_{[d]}] \cdot \nu[X_{[d]} = x_{[d]}]$ is supported only for $x_{[d]}$ with $\mathcal{S}(x_{[d]}) \in \mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}$ we have that

$$\langle \mu[L], \theta_{\mathcal{I}}[L] \rangle [\emptyset] = \max_{\mu[L] \in \mathcal{M}_{\mathcal{S}, \nu}} \langle \mu[L], \theta_{\mathcal{I}}[L] \rangle [\emptyset]$$

which is equal to $\mu[L] \in Q_{\mathcal{S}, \nu}^{\mathcal{I}}$. Thus, if and only if $\mu[L] \in Q_{\mathcal{S}, \nu}^{\mathcal{I}}$ then $\mathbb{P}[X_{[d]}]$ is only supported at $x_{[d]}$ in the support of $\nu^{\mathcal{S}, \mathcal{I}}[X_{[d]}]$. □

Let us now investigate tensor network representations of face measures, based on the basis encoding $\beta^{\mathcal{S}}$ of a statistic.

Theorem 1 (Face measure representation). *For any face $Q_{\mathcal{S}, \nu}^{\mathcal{I}}$ of \mathcal{M} we have*

$$\nu^{\mathcal{S}, \mathcal{I}}[X_{[d]}] = \langle \beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}], \kappa^{\mathcal{I}}[Y_{[p]}], \nu[X_{[d]}] \rangle [X_{[d]}]$$

where

$$\kappa^{\mathcal{I}}[Y_{[p]}] = \sum_{\mu \in \mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}} \epsilon_{\mu}[Y_{[p]}].$$

Proof. For any $\mu \in \mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}$ the tensor

$$\tau^{\mu}[X_{[d]}] = \langle \beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}], \epsilon_{\mu}[Y_{[p]}] \rangle [X_{[d]}]$$

is the indicator of the preimage of μ under $\sigma^{\mathcal{S}}$. Since preimages the elements in $\mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}$ are disjoint, the support of $\tau^{\mu}[X_{[d]}]$ is disjoint and their sum

$$\sum_{\mu \in \mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}} \tau^{\mu}[X_{[d]}]$$

is the indicator of the preimage of $Q_{\mathcal{S}, \nu}^{\mathcal{I}}$ under $\sigma^{\mathcal{S}}$. The face measure obeys thus

$$\begin{aligned} \nu^{\mathcal{S}, \mathcal{I}}[X_{[d]}] &= \left\langle \left(\sum_{\mu \in \mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}} \tau^{\mu}[X_{[d]}] \right), \nu[X_{[d]}] \right\rangle [X_{[d]}] \\ &= \sum_{\mu \in \mathcal{N}_{\mathcal{S}, \nu}^{\mathcal{I}}} \langle \beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}], \epsilon_{\mu}[Y_{[p]}], \nu[X_{[d]}] \rangle [X_{[d]}] \\ &= \langle \beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}], \kappa^{\mathcal{I}}[Y_{[p]}], \nu[X_{[d]}] \rangle [X_{[d]}] \end{aligned}$$

□

More general, we define face representability with respect to any hypergraph.

Definition 3. Let \mathcal{G} be a hypergraph which nodes include $[p]$. We say that a face $Q_{\mathcal{S},\nu}^{\mathcal{I}}$ is representable by \mathcal{G} if and only if there is a set \mathcal{U} of basis vectors with

$$\mathcal{U} : \mathcal{U} \cap \mathcal{N}_{\mathcal{S},\nu} = \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}$$

and there is a tensor network $\tau^{\mathcal{G}}$ with respect to the hypergraph \mathcal{G} such that

$$\langle \tau^{\mathcal{G}} \rangle [Y_{[p]}] = \sum_{v \in \mathcal{U}} \epsilon_v [Y_{[p]}] .$$

Lemma 4. If any only if a face is representable by a hypergraph \mathcal{G} we have

$$\nu^{\mathcal{S},\mathcal{I}} [X_{[d]}|\emptyset] \in \Lambda^{\mathcal{S},\mathcal{G},\nu} .$$

Proof. For any \mathcal{U} with $\mathcal{U} : \mathcal{U} \cap \mathcal{N}_{\mathcal{S},\nu} = \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}$ and tensor network $\tau^{\mathcal{G}}$ respecting the assumptions of Def. 3 we have

$$\begin{aligned} \langle \langle \tau^{\mathcal{G}} \rangle [Y_{[p]}] , \beta^{\mathcal{S}} [Y_{[p]}, X_{[d]}] \rangle [X_{[d]}] &= \left\langle \sum_{v \in \mathcal{U}} \epsilon_v [Y_{[p]}] , \beta^{\mathcal{S}} [Y_{[p]}, X_{[d]}] \right\rangle [X_{[d]}] \\ &= \left\langle \sum_{v \in \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}} \epsilon_v [Y_{[p]}] , \beta^{\mathcal{S}} [Y_{[p]}, X_{[d]}] \right\rangle [X_{[d]}] . \end{aligned}$$

Here we used in the second equation that only the vertices in $\mathcal{N}_{\mathcal{S},\nu}$ are in the image of \mathcal{S} . It follows, that

$$\nu^{\mathcal{S},\mathcal{I}} [X_{[d]}|\emptyset] = \langle \langle \tau^{\mathcal{G}} \rangle [Y_{[p]}] , \beta^{\mathcal{S}} [Y_{[p]}, X_{[d]}] , \nu [X_{[d]}] \rangle [X_{[d]}|\emptyset]$$

and thus $\nu^{\mathcal{S},\mathcal{I}} [X_{[d]}|\emptyset] \in \Lambda^{\mathcal{S},\mathcal{G},\nu}$. \square

Let us now investigate, which normalized face measures can be computed using \mathcal{S} and a hypergraph \mathcal{G} .

Example 1 (Vertices). Vertices $Q_{\mathcal{S},\nu}^{\mathcal{I}}$ are proper faces of affine dimension 0, that is they consist in single vectors. Since all vertices are in the image $\sigma^{\mathcal{S}}(\mathcal{X})$, there exists an index tuple $x_{[d]} \in \mathcal{X}$ such that $\nu [X_{[d]} = x_{[d]}] = 1$ and

$$Q_{\mathcal{S},\nu}^{\mathcal{I}} = \{\sigma^{\mathcal{S}} [X_{[d]} = x_{[d]}, L]\} .$$

Then $\kappa^{\mathcal{I}} [Y_{[p]}]$ is the one-hot encoding of the by an interpretation map I assigned index to $\sigma^{\mathcal{S}} [X_{[d]} = x_{[d]}, L]$, that is

$$\kappa^{\mathcal{I}} [Y_{[p]}] = \epsilon_{I^{-1}(\sigma^{\mathcal{S}} [X_{[d]} = x_{[d]}, L])} [Y_{[p]}] .$$

In particular, the activation core is elementary and the face measure to any vertex is in $\Lambda^{\mathcal{S},\text{EL},\nu}$.

Extending Example 1, we can provide a coarse estimation of the hypergraph \mathcal{G} required to decompose $\kappa^{\mathcal{I}}$ for generic faces $Q_{\mathcal{S},\nu}^{\mathcal{I}}$.

Lemma 5. Any face $Q_{\mathcal{S},\nu}^{\mathcal{I}}$ is representable by a CP graph with hidden rank $r = |\mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}|$.

Proof. We enumerate the vertices by a variable I with dimension r , i.e. $\mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}} = \{v^i[L] : i \in [r]\}$. Then we define core tensors $\tau^l [Y_l, I]$

$$\tau^l [Y_l, I = i] = \epsilon_{v^i[L=l]} [Y_l] .$$

Then we have

$$\sum_{v \in \mathcal{N}_{\mathcal{S},\nu}^{\mathcal{I}}} \epsilon_v [Y_{[p]}] = \langle \{\tau^l [Y_l, I] : l \in [p]\} \rangle [Y_{[p]}]$$

and thus have found a tensor network representing the face $Q_{\mathcal{S},\nu}^{\mathcal{I}}$. \square

Let us notice that in many cases the bound provided by Lem. 5 is loose. By Example 2 we provide with the maximal face an example, where the CP rank is given by the tensor space dimension, whereas the generic CP rank is one and the normalized face measure is thus still in $\Lambda^{\mathcal{S},\text{EL}}$.

Example 2 (Maximal face). *The maximal face $Q_{\mathcal{S},\nu}^{\emptyset} = \mathcal{M}_{\mathcal{S},\nu}$ coincides with the mean polytope itself and is given by the choice $\theta_{\emptyset}[L] = 0[L]$. In this case the corresponding activation tensor to the face measure is trivial, that is*

$$\kappa^{\emptyset}[Y_{[p]}] = \mathbb{I}[Y_{[p]}] .$$

κ^{\emptyset} is elementary and the normalized face measure $\nu^{\mathcal{S},\emptyset}$ to the maximal face is in $\Lambda^{\mathcal{S},\text{EL}}$.

Let us now introduce relative interiors, which enables us to find disjoint partitions of the mean polytope.

Definition 4 (Relative Interior). *Let $\mathcal{U} \subset \mathbb{R}^p$ be an arbitrary set and \mathcal{L} be the affine hull of \mathcal{U} . Then the relative interior, denoted $(\mathcal{U})^{\circ}$ is the interior of \mathcal{U} in the subspace \mathcal{L} .*

Lemma 6. *Any polytope is a disjoint union of the relative interiors of its faces, that is*

$$\mathcal{M}_{\mathcal{S},\nu} = \bigcup_{\mathcal{I} \subset [n]} (Q_{\mathcal{S},\nu}^{\mathcal{I}})^{\circ} .$$

Proof. For any $\mu \in \mathcal{M}_{\mathcal{S},\nu}$ we find a face such that $\mu \in Q_{\mathcal{S},\nu}^{\mathcal{I}}$. If $\mu \notin (Q_{\mathcal{S},\nu}^{\mathcal{I}})^{\circ}$, then there is a face $Q_{\mathcal{S},\nu}^{\tilde{\mathcal{I}}} \subset Q_{\mathcal{S},\nu}^{\mathcal{I}}$ of smaller affine dimension such that $\mu \in Q_{\mathcal{S},\nu}^{\tilde{\mathcal{I}}}$. When continuing this process we reach a face such that $\mu \in (Q_{\mathcal{S},\nu}^{\mathcal{I}})^{\circ}$, since the faces with affine dimension 0 are vertices and they coincide with their relative interior because they contain a single vector. \square

Definition 5. *To each $\mu \in \mathcal{M}_{\mathcal{S},\nu}$ we denote the unique face $Q_{\mathcal{S},\nu}^{\mathcal{I}}$ with $\mu \in (Q_{\mathcal{S},\nu}^{\mathcal{I}})^{\circ}$ by $Q_{\mathcal{S},\nu}^{\mathcal{I}(\mu)}$.*

3 Main results: Tensor network representation of maximum entropy distributions

Given the mean polytope discussion we now characterize the tensor network representation of maximum entropy distributions.

3.1 Computation-Activation Networks

Given a statistic $\mathcal{S} : \times_{k \in [d]} [m_k] \rightarrow \times_{s \in [n]} [p_s]$ we build its basis encoding tensor

$$\beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}] = \sum_{x_{[d]} \in \times_{k \in [d]} [m_k]} \epsilon_{\mathcal{S}(x_{[d]})}[Y_{[p]}] \otimes \epsilon_{x_{[d]}}[X_{[d]}] .$$

A computation network is any representation of $\beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}]$ as a tensor network. These can be constructed in the case statistics being a composition of connective functions.

An activation tensor is $\tau[Y_{[p]}]$ and the Computation Activation Network of \mathcal{S} and τ the tensor

$$\mathbb{P}[X_{[d]}] = \langle \beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}], \tau[Y_{[p]}] \rangle [X_{[d]}|\emptyset] .$$

We are interested in decomposition formats of $\tau[Y_{[p]}]$, where we use sets of tensor networks $\mathcal{T}^{\mathcal{G}}$ on a hypergraph \mathcal{G} . The family of by \mathcal{S} and a \mathcal{G} computable distributions are

$$\Lambda^{\mathcal{S},\mathcal{G}} = \{ \langle \beta^{\mathcal{S}}[Y_{[p]}, X_{[d]}], \tau[Y_{\mathcal{V}}] \rangle [X_{[d]}|\emptyset] : \tau[Y_{\mathcal{V}}] \in \mathcal{T}^{\mathcal{G}} \} .$$

3.2 Maximum entropy on the interior

A classical result states, that the maximum entropy distribution is in the exponential family $\Gamma^{\mathcal{S},\nu}$ (see e.g. Koller and Friedman).

Theorem 2. *If and only if μ^* is in the relative interior of $\mathcal{M}_{\mathcal{S},\nu}$, then the unique solution of the maximum entropy problem is the distribution*

$$\mathbb{P}^{\mathcal{S},\mu^*,\nu}[X_{[d]}] \in \Gamma^{\mathcal{S},\nu}$$

with $\langle \mathbb{P}^{\mathcal{S},\mu^*,\nu}[X_{[d]}], \sigma^{\mathcal{S}}[X_{[d]}, L] \rangle [L] = \mu^*[L]$.

Proof. By The 3.3 in Wainwright and Jordan, since by assumption

$$\mu[L] \in (\mathcal{M}_{S,\nu})^\circ,$$

there is a canonical parameter θ with

$$\langle \mathbb{P}^{S,\theta,\nu}[X_{[d]}], \sigma^S[X_{[d]}, L], \nu[X_{[d]}] \rangle [L] = \mu[L].$$

For any other feasible distribution $\tilde{\mathbb{P}}[X_{[d]}]$ we also have $\langle \tilde{\mathbb{P}}[X_{[d]}], \sigma^S[X_{[d]}, L], \nu[X_{[d]}] \rangle [L] = \mu[L]$ and thus

$$\begin{aligned} \mathbb{H}_\nu[\tilde{\mathbb{P}}, \mathbb{P}^{(S,\theta,\nu)}] &= -\langle \tilde{\mathbb{P}}, \ln[\mathbb{P}^{(S,\theta,\nu)}[X_{[d]}]], \nu[X_{[d]}] \rangle [\emptyset] \\ &= -\langle \tilde{\mathbb{P}}, \sigma^S[X_{[d]}, L], \theta[L], \nu[X_{[d]}] \rangle [\emptyset] + A^{(S,\nu)}(\theta) \\ &= -\langle \theta[L], \mu[L] \rangle [\emptyset] + A^{(S,\nu)}(\theta) \\ &= \mathbb{H}_\nu[\mathbb{P}^{(S,\theta,\nu)}]. \end{aligned}$$

With the Gibbs inequality we have if $\tilde{\mathbb{P}} \neq \mathbb{P}^{(S,\theta,\nu)}$

$$\mathbb{H}_\nu[\mathbb{P}^{(S,\hat{\theta},\nu)}] - \mathbb{H}_\nu[\tilde{\mathbb{P}}] = \mathbb{H}_\nu[\tilde{\mathbb{P}}, \mathbb{P}^{(S,\hat{\theta},\nu)}] - \mathbb{H}_\nu[\tilde{\mathbb{P}}] > 0$$

and thus $\mathbb{H}_\nu[\tilde{\mathbb{P}}] < \mathbb{H}_\nu[\mathbb{P}^{(S,\hat{\theta},\nu)}]$. Therefore, if $\tilde{\mathbb{P}}$ does not coincide with $\mathbb{P}^{(S,\hat{\theta},\nu)}$, it is not a maximum entropy distribution. \square

3.3 Main result

Our main result generalizes the maximum entropy characterization of Thm. 2 to arbitrary mean parameters.

Theorem 3 (Generic characterization of Maximum Entropy Solutions). *Let S be a statistic and ν a base measure. For any $\mu[L]$ the maximum entropy problem has a feasible distribution, if and only if $\mu[L] \in \mathcal{M}_{S,\nu}$. In case $\mu[L] \in \mathcal{M}_{S,\nu}$ denote the unique face of $\mathcal{M}_{S,\nu}$ with μ in its relative interior by $Q_{S,\nu}^{\mathcal{I}}$ (see Def. 4). Then the solution of the maximum entropy problem is the member*

$$\mathbb{P}^{(S, B^{S,\nu^{\mathcal{I}},\mathcal{I}}(\mu), \nu^{S,\mathcal{I}})}$$

of the exponential family $\Gamma^{S,\nu^{\mathcal{I},\mathcal{I}}}$, where $\nu^{S,\mathcal{I}}$ is the face measure (see Def. 2). If for a hypergraph \mathcal{G} the face is representable with respect to \mathcal{G} (see Def. 3), then the maximum entropy distribution is in $\Lambda^{S,\hat{\mathcal{G}},\nu}$.

To prepare for the proof of this theorem we first show in an auxiliary lemma that we can reduce the set of feasible distributions in Problem $(P_{S,\mu,\nu})$.

Lemma 7. *For any $\mu[L] \in \mathcal{M}_{S,\nu}$ and a face $Q_{S,\nu}^{\mathcal{I}}$ with $\mu[L] \in (Q_{S,\nu}^{\mathcal{I}})^\circ$ we have that the solutions of $P_{S,\mu,\nu}$ and $P_{S,\mu,\nu^{S,\mathcal{I}}}$ coincide.*

Proof. By Lem. 3 all feasible distributions are representable by the with the face measure refined base measure. We have that any for $P_{S,\mu,\nu}$ feasible distribution $\mathbb{P}[X_{[d]}]$ satisfies

$$\langle \mathbb{P}[X_{[d]}], \nu^{S,\mathcal{I}} \rangle [\emptyset] = 1$$

and thus $\mathbb{P}[X_{[d]}] \in \Lambda^{S,\nu^{S,\mathcal{I}}}$. Conversely, any $\mathbb{P}[X_{[d]}] \in \Lambda^{S,\nu^{S,\mathcal{I}}}$ satisfies

$$\langle \mathbb{P}[X_{[d]}], \nu^{S,\mathcal{I}} \rangle [\emptyset] = \langle \mathbb{P}[X_{[d]}], \nu \rangle [\emptyset] = 1$$

and thus $\mathbb{P}[X_{[d]}] \in \Lambda^{S,\nu}$. Problem $P_{S,\mu,\nu}$ is thus equal to

$$\operatorname{argmax}_{\mathbb{P}[X_{[d]}] \in \Lambda^{S,\nu^{S,\mathcal{I}}}} \mathbb{H}_\nu[\mathbb{P}[X_{[d]}]] \quad \text{subject to} \quad \forall l \in [p] : \langle \mathbb{P}[X_{[d]}], \mathcal{S}_l[X_{[d]}], \nu[X_{[d]}] \rangle [L] = \mu^*[L = l]$$

We further have that any $\mathbb{P}[X_{[d]}] \in \Lambda^{S,\nu^{S,\mathcal{I}}}$

$$\mathbb{H}_\nu[\mathbb{P}[X_{[d]}]] = \mathbb{H}_{\nu^{S,\mathcal{I}}}[\mathbb{P}[X_{[d]}]]$$

and arrive together with the above equivalence at the claim. \square

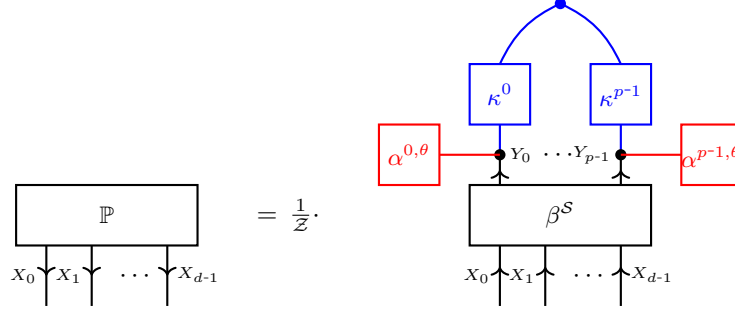


Figure 1: Tensor network decomposition of maximum entropy distributions to the constraint $\mu[L] = \langle \mathbb{P}, \sigma^S \rangle [L]$. Blue: Constraint activation cores κ^l in a CP decomposition, representing the face measure to the minimal face, such that $\mu \in Q_{S, \nu}^{\mathcal{I}}$. Red: Probabilistic activation cores $\alpha^{l, \theta} [Y_l]$ in an elementary decomposition, where each leg core is a scaled exponentials evaluated on the enumerated image $\text{im}(s_l)$.

Proof of Thm. 3. Feasibility Claim: If and only if $\mu[L] \in \mathcal{M}_{S, \nu}$ then there is by definition a by ν representable $\mathbb{P}[X_{[d]}]$ reproducing $\mu[L]$. Thus if and only if $\mu[L] \in \mathcal{M}_{S, \nu}$ there is a feasible distribution for the maximum entropy problem.

Characterization Claim: We use the following argumentation to show the second claim:

- By Lem. 6 for any μ we find a unique face $Q_{S, \nu}^{\mathcal{I}}$.
- By Lem. 7 we can reduce the maximum entropy problem $P_{S, \mu, \nu^S, \mathcal{I}}$ to the base measure $\nu^{S, \mathcal{I}}$.
- By Lem. 2 the face $Q_{S, \nu}^{\mathcal{I}}$ coincides with the polytope $\mathcal{M}_{S, \langle \nu, \nu^S, \mathcal{I} \rangle} [X_{[d]}]$ and in particular μ is in the relative interior of that polytope.
- We can now apply Thm. 2 and get a characterization of the maximum entropy solution as a member of the exponential family.

Representation Claim: By Def. 3 we find a tensor network on \mathcal{G} representing the face measure. We contract the activation vectors of the exponential family on this tensor network (see Figure 1) and get an activation tensor network on \mathcal{G} representing the maximum entropy distribution. \square

4 Characterization for boolean statistics

We here study the face CP ranks in case of boolean statistics. We further show that any elementary Computation-Activation Network to boolean statistics is a maximum entropy distribution.

For boolean statistics $\mathcal{F} : \times_{k \in [d]} [m_k] \rightarrow \times_{l \in [p]} [2]$ the mean polytope is a subset of the cube $[0, 1]^p$. In this case, any boolean vector in $\mathcal{M}_{\mathcal{F}, \nu}$ is a vertex. It follows, that any distribution reproducing a mean parameter $\mu[L]$ on the relative interior of $\mathcal{M}_{\mathcal{F}, \nu}$ is positive with respect to ν .

We apply the exponential distribution characterization of the maximum entropy distribution and get that the maximum entropy distribution is in $\Lambda^{S, \text{EL}}$, if and only if the face measure is in $\Lambda^{S, \text{EL}}$. This is exactly the case, when the face is an intersection of the mean polytope with a face of the cupe $[0, 1]^p$.

4.1 Set of maximum entropy distributions

Theorem 4. Any distribution in $\Lambda^{\mathcal{F}, \text{EL}}$ is a maximum entropy distribution. Any maximum entropy distribution is realized by $\Lambda^{\mathcal{F}, \text{EL}}$ if and only if the mean parameter is on an relative interior of a cube-like face.

Proof. First claim by decomposing any elementary tensor into exponential and hard activation core. Second claim by characterization of elementary faces by cube-likeness. \square

The mean parameters, which can be realized by a distribution in $\Lambda^{\mathcal{F}, \text{EL}}$ are those, which are on the relative interior of the intersection of the mean polytope with a face of the cube.

4.2 Example

Add examples: Partition Statistics - Simplices, (Logically) Independent formulas - Hypercubes

Example 3 (Maximum entropy distribution with non-elementary activation cores). *Consider two atomic variables X_0 and X_1 and a statistic \mathcal{F} consisting in the formulas*

$$f_0 = (X_0 \wedge X_1) \quad , \quad f_1 = (X_0 \Rightarrow X_1)$$

with the coordinatewise expressions

$$f_0 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad , \quad f_1 = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} .$$

We can think of X_0 as a feature on an invoice, and X_1 as a feature on the accounting proposal.

From this we have

$$\begin{aligned} \beta^{(f_0, f_1)} [Y_0 = 0, Y_1 = 0, X_0, X_1] &= \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \quad , \quad \beta^{(f_0, f_1)} [Y_0 = 0, Y_1 = 1, X_0, X_1] = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \quad , \\ \beta^{(f_0, f_1)} [Y_0 = 1, Y_1 = 0, X_0, X_1] &= \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \beta^{(f_0, f_1)} [Y_0 = 1, Y_1 = 1, X_0, X_1] = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} . \end{aligned}$$

Since the only vanishing slice of $\beta^{\mathcal{F}}$ with respect to the head variables is that to $y_{0,1} = (1, 0)$, the vertices of the mean polytope are the vectors to the other head indices. The mean polytope is the convex hull of these vertices

$$\mathcal{M}_{(f_0, f_1)} = \text{conv} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right) .$$

This polytope has a non cube-like face (sketched blue in Figure 2), which is the convex hull of the vertices $[0 \ 0]^T$, $[1 \ 1]^T$. This face is parametrized by the (CP-rank 2) hard activation core

$$\kappa^{(0,0),(1,1)} [Y_0, Y_1] = \epsilon_{(0,0)} [Y_0, Y_1] + \epsilon_{(1,1)} [Y_0, Y_1] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and has the face measure

$$\left\langle \kappa^{(0,0),(1,1)} [Y_0, Y_1], \beta^{\mathcal{F}} [Y_0, Y_1, X_0, X_1] \right\rangle [X_0, X_1] = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} .$$

Any mean parameter μ on the interior of that face can be parametrized by a scalar $\lambda \in (0, 1)$

$$\mu_\lambda [L] = [\lambda \quad \lambda]^T .$$

With the canonical parameters $\theta [L] \in \mathbb{R}^2$ of the maximum entropy distributions on this face by

$$\mathbb{P} [X_0, X_1] = \frac{1}{1 + \exp [\theta [L = 0] + \theta [L = 1]]} \begin{bmatrix} 0 & 0 \\ 1 & \exp [\theta [L = 0] + \theta [L = 1]] \end{bmatrix}$$

we get the correspondence by the sigmoid

$$\lambda = \frac{1}{1 + \exp [-(\theta [L = 0] + \theta [L = 1])] .$$

Note, that the hard activation core $\kappa^{(0,0),(1,1)} [Y_0, Y_1]$ to the blue face is the only non-elementary activation core. While the vertices have always elementary cores, the further non-vertex faces have elementary activation cores

$$\kappa^{(0,0),(1,0),(1,1)} [Y_0, Y_1] = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \mathbb{I} [Y_0] \otimes \mathbb{I} [Y_1] \quad , \quad \kappa^{(0,0),(1,0)} [Y_0, Y_1] = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} = \mathbb{I} [Y_0] \otimes \epsilon_0 [Y_1] \quad ,$$

$$\kappa^{(1,0),(1,1)} [Y_0, Y_1] = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} = \epsilon_0 [Y_0] \otimes \mathbb{I} [Y_1] .$$

The maximum entropy distributions to mean parameters on the interior of all other faces than the blue face are represented by Computation-Activation Networks with only elementary activation cores.

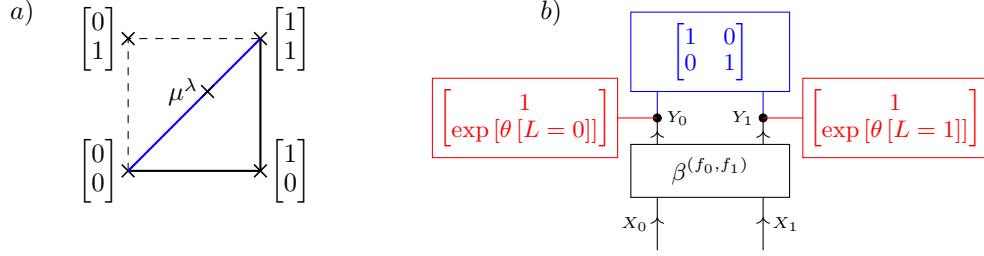


Figure 2: a) Mean polytope of the statistic $\mathcal{F} = (X_0 \wedge X_1, X_0 \Rightarrow X_1)$ (thick), as a subset of the cube $[0, 1]^2$ (dashed). The blue line is the face of the polytope, which is not cube like, that is not an intersection of the polytope with the faces of the polytope. We further define for $\lambda \in (0, 1)$ a mean parameter $\mu_\lambda[L] = [\lambda \lambda]^T$ which is on the interior of the blue face. b) Corresponding Computation-Activation Network being the maximum entropy distribution reproducing $\mu_\lambda[L]$, when λ is the sigmoid of $\theta[L = 0] + \theta[L = 1]$.

5 Mean as a Statistic

We in this section take the perspective of estimating a maximum entropy distribution given observed data.

The mean parameter μ_D given a dataset can be understood as a statistic of the dataset. We here show that for the family of maximum entropy distributions this statistic is a minimal sufficient statistic.

The family of maximum entropy distributions is the set

$$\{\mathbb{P}^\mu[X_{[d]}] : \mu \in \mathcal{M}_{\mathcal{S}, \nu}\}$$

which has been characterized above by a union of exponential families with respect to face measures.

Taking a frequentist perspective we now understand datasets by random variables $X_{[d] \times [m]}$, where for $j \in [m]$ the variables $X_{[d], j}$ are drawn i.i.d. from a maximum entropy distribution. The mean statistic is then a tensor

$$\mu_D[X_{[d] \times [m]}, L]$$

with coordinates

$$\mu_D[X_{[d] \times [m]} = x_{[d] \times [m]}, L] = \frac{1}{m} \sum_{j \in [m]} \sigma^S[X_{[d], j} = x_{[d], j}, L].$$

Theorem 5. *The mean statistic is sufficient for the family of maximum entropy distributions (\mathcal{S}, ν) .*

Proof. It suffices to show that the likelihood is a function of μ_D . Let us choose a face \mathcal{I} of $\mathcal{M}_{\mathcal{S}, \nu}$, then the likelihood is different from 0 if and only if the empirical distribution is representable with respect to the face measure. This is the case if and only if μ_D is on the face. In case that μ_D is on the face, then the likelihood of any distribution on that face exponential family is

$$\exp \left[m \cdot \left(\langle \mu_D[X_{[d] \times [m]}, L], \theta[L] \rangle [\emptyset] - A^{(\mathcal{S}, \nu)}(\theta) \right) \right]$$

We have thus shown that the likelihood is always a function of μ_D . □

6 Outlook

This is relevant for Parameter Estimation: Instabilities when fitting a mean parameter on a non cube-like face.

Border-rank development to resolve the issue. CITE

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