

On the Prior and Posterior Distributions Used in Graphical Modelling

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The Problem

A large part of the literature on the analysis of graphical models focuses on the study of the parameters of local probability distributions (such as conditional probabilities or partial correlations). However:

- Comparing models learned with different algorithms is difficult, because they maximise **different scores**, use **different estimators** for the parameters, work under **different sets of hypotheses**, etc.
- Unless the **true global probability distribution** is known it is difficult to assess the quality of the estimated models.
- The few available measures of structural difference are **completely descriptive** in nature (e.g. Hamming distance [5] or SHD [10]), and are difficult to interpret.
- When learning **causal graphical models** often the focus is not on the parameters but in the presence of particular patterns of edges in the graph (e.g. [8]).

Looking for a Solution

Focusing on graph structures \mathcal{G} sidesteps some of these problems and acknowledges causal graphical modelling literature [9].

0. We need to know more about the properties of **priors** $P(\mathcal{G})$ and **posteriors** $P(\mathcal{G} \mid \mathcal{D})$ distributions over the space of graphs, preferably as a **function of arc and edge sets**, say $P(\mathcal{G}(\mathcal{E}))$ and $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$ with $\mathcal{E} = \{(v_i, v_j), i \neq j\} \in \mathcal{O}(|\mathbf{V}|^2)$.

And then:

1. It would be good to have a measure(s) of spread for \mathcal{G} , to assess the **noisiness** of $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$ and the **informativeness** of $P(\mathcal{G}(\mathcal{E}))$.
2. Using such a measure(s), it would be interesting to study the **convergence speed** of structure learning algorithms and the influence of their tuning parameters.
3. It would also be interesting to investigate how to use higher order moments of $P(\mathcal{G}(\mathcal{E}))$ to define **new priors**.

Edge Sets as Multivariate Bernoulli

Each edge e_{ij} in an undirected graph $\mathcal{G} = (\mathbf{V}, E)$ has only two possible states and therefore can be modelled as a Bernoulli random variable:

$$e_{ij} \sim E_{ij} = \begin{cases} 1 & \text{if } e_i \in E \\ 0 & \text{otherwise} \end{cases}.$$

The natural extension of this approach is to model any set of edges as a **multivariate Bernoulli random variable** $\mathbf{B} \sim \text{Ber}_k(\mathbf{p})$. \mathbf{B} is uniquely identified by the parameter set

$$\mathbf{p} = \{p_I : I \subseteq \{1, \dots, k\}, i \neq \emptyset\}, \quad k = \frac{|\mathbf{V}|(|\mathbf{V}| - 1)}{2}$$

which represents the **dependence structure** [6] among the marginal distributions $B_i \sim \text{Ber}(p_i)$, $i = 1, \dots, k$ of the edges.

The parameter set \mathbf{p} can be estimated using a large number m of bootstrap samples as in Friedman *et al.* [2] or Imoto *et al.* [4], or MCMC samples as in Friedman & Koller [3].

Arc Sets as Multivariate Trinomial

Each arc a_{ij} in $\mathcal{G} = (\mathbf{V}, A)$ has three possible states, and therefore it can be modelled as a **Trinomial random variable** A_{ij} :

$$a_{ij} \sim A_{ij} = \begin{cases} -1 & \text{if } a_{ij} = \overleftarrow{a}_{ij} = \{v_i \leftarrow v_j\} \\ 0 & \text{if } a_{ij} \notin A, \text{ denoted with } a_{ij}^\circ . \\ 1 & \text{if } a_{ij} = \overrightarrow{a}_{ij} = \{v_i \rightarrow v_j\} \end{cases}$$

As before, the natural extension to model any set of arcs is to use a **multivariate Trinomial random variable** $\mathbf{T} \sim \text{Trin}_k(\mathbf{p})$.

However:

- the **acyclicity constraint** of Bayesian networks makes deriving exact results very difficult because it cannot be written in closed form;
- the **score equivalence** of most structure learning strategies makes inference on $\text{Trin}_k(\mathbf{p})$ tricky unless particular care is taken (i.e. both possible orientations of many arcs result in equivalent probability distributions, so the algorithms cannot choose between them).

Second Order Properties of $Ber_k(\mathbf{p})$ and $Tri_k(\mathbf{p})$

All the elements of the **covariance matrix** Σ of an edge set \mathcal{E} are **bounded**,

$$p_i \in [0, 1] \Rightarrow \sigma_{ii} = p_i - p_i^2 \in \left[0, \frac{1}{4}\right] \Rightarrow \sigma_{ij} \in \left[0, \frac{1}{4}\right],$$

and similar bounds exist for the **eigenvalues** $\lambda_1, \dots, \lambda_k$,

$$0 \leq \lambda_i \leq \frac{k}{4} \quad \text{and} \quad 0 \leq \sum_{i=1}^k \lambda_i \leq \frac{k}{4}.$$

These bounds define a **closed convex set** in \mathbb{R}^k ,

$$\mathcal{L} = \left\{ \Delta^{k-1}(c) : c \in \left[0, \frac{k}{4}\right] \right\}$$

where $\Delta^{k-1}(c)$ is the non-standard $k - 1$ **simplex**

$$\Delta^{k-1}(c) = \left\{ (\lambda_1, \dots, \lambda_k) \in \mathbb{R}^k : \sum_{i=1}^k \lambda_i = c, \lambda_i \geq 0 \right\}.$$

Similar results hold for arc sets, with $\sigma_{ii} \in [0, 1]$ and $\lambda_i \in [0, k]$.

Minimum and Maximum Entropy

These results provide the foundation for characterising three cases corresponding to different configurations of the probability mass in $P(\mathcal{G}(\mathcal{E}))$ and $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$:

- **minimum entropy**: the probability mass is concentrated on a single graph structure. This is the best possible configuration for $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$, because only one edge set E (or one arc set A) has a non-zero posterior probability.
- **intermediate entropy**: several graph structures have non-zero probabilities. This is the case for informative priors $P(\mathcal{G}(\mathcal{E}))$ and for the posteriors $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$ resulting from real-world data sets.
- **maximum entropy**: all graph structures have the same probability. This is the worst possible configuration for $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$, because it corresponds to a non-informative prior. In other words, the data \mathcal{D} do not provide any information useful in identifying a high-posterior graph \mathcal{G} .

Properties of the Multivariate Bernoulli

In the **minimum entropy** case, only one configuration of edges E has non-zero probability, which means that

$$p_{ij} = \begin{cases} 1 & \text{if } e_{ij} \in E \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad \Sigma = \mathbf{O}$$

where \mathbf{O} is the zero matrix.

The uniform distribution over \mathbf{G} arising from the **maximum entropy** case has been studied extensively in random graph theory [1]; its two most relevant properties are that all edges e_{ij} are independent and have $p_{ij} = \frac{1}{2}$. As a result, $\Sigma = \frac{1}{4}I_k$; all edges display their maximum possible variability, which along with the fact that they are independent makes this distribution non-informative for \mathcal{E} as well as $\mathcal{G}(\mathcal{E})$.

Properties of the Multivariate Trinomial

In the **maximum entropy** case we have that [7]

$$P(\overrightarrow{a_{ij}}) = P(\overleftarrow{a_{ij}}) \simeq \frac{1}{4} + \frac{1}{4(n-1)} \rightarrow \frac{1}{4}$$

$$P(a_{ij}^{\circ}) \simeq \frac{1}{2} - \frac{1}{2(n-1)} \rightarrow \frac{1}{2}$$

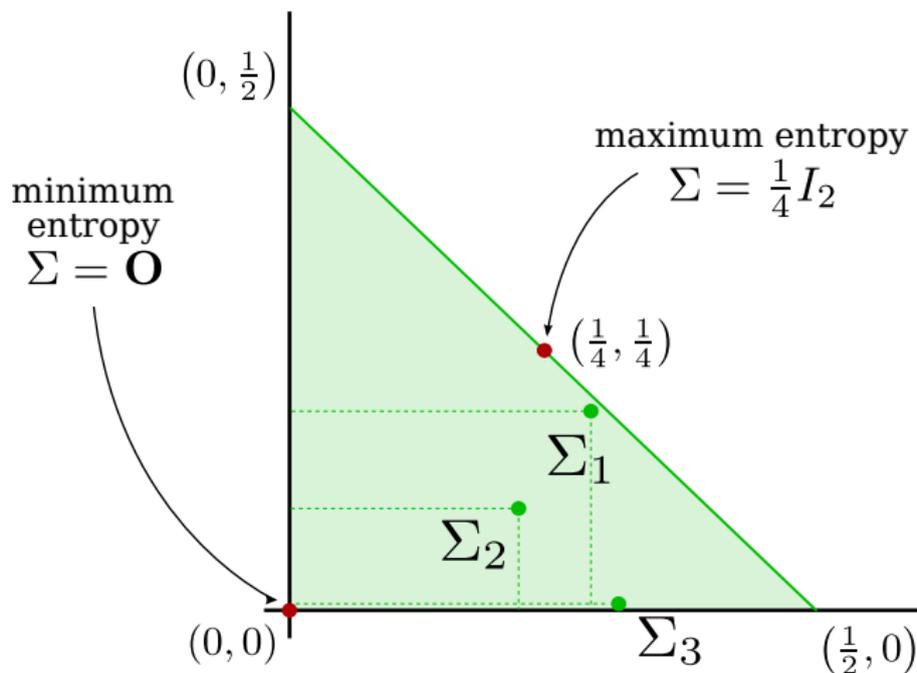
as $n \rightarrow \infty$, where n is the number of nodes of the graph. As a result, we have that

$$E(A_{ij}) = P(\overrightarrow{a_{ij}}) - P(\overleftarrow{a_{ij}}) = 0,$$

$$\text{VAR}(A_{ij}) = 2P(\overrightarrow{a_{ij}}) \simeq \frac{1}{2} + \frac{1}{2(n-1)} \rightarrow \frac{1}{2},$$

$$\begin{aligned} |\text{COV}(A_{ij}, A_{kl})| &= 2 [P(\overrightarrow{a_{ij}}, \overrightarrow{a_{kl}}) - P(\overrightarrow{a_{ij}}, \overleftarrow{a_{kl}})] \\ &\simeq 4 \left[\frac{3}{4} - \frac{1}{4(n-1)} \right]^2 \left[\frac{1}{4} + \frac{1}{4(n-1)} \right]^2 \rightarrow \frac{9}{64}. \end{aligned}$$

A Geometric Representation of Entropy in \mathcal{L}



The space of the eigenvalues \mathcal{L} for two edges in an undirected graph.

Univariate Measures of Variability

- The **generalised variance**, $\text{VAR}_G(\Sigma) = \det(\Sigma) = \prod_{i=1}^k \lambda_i \in [0, \frac{1}{4^k}]$.
- The **total variance** (or **total variability**)

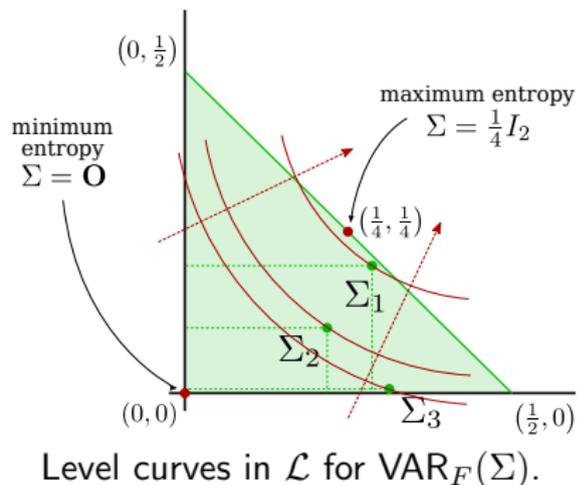
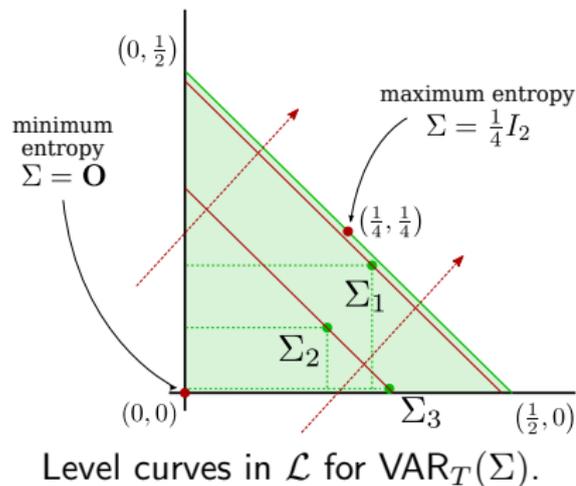
$$\text{VAR}_T(\Sigma) = \text{tr}(\Sigma) = \sum_{i=1}^k \lambda_i \in \left[0, \frac{k}{4}\right].$$

- The squared **Frobenius matrix norm**

$$\text{VAR}_F(\Sigma) = \left\| \Sigma - \frac{k}{4} I_k \right\|_F^2 = \sum_{i=1}^k \left(\lambda_i - \frac{k}{4} \right)^2 \in \left[\frac{k(k-1)^2}{16}, \frac{k^3}{16} \right].$$

All of these measures **can be rescaled to vary in the $[0, 1]$ interval** and to associate high values to networks whose structure displays a high entropy. The equivalent measures of variability for **directed acyclic graphs** can be derived in the same way, and they can be similarly normalised.

Structure Variability: Level Curves



Conclusions and Open Problems

- First and second order properties of $P(\mathcal{G}(\mathcal{E}))$ and $P(\mathcal{G}(\mathcal{E}) \mid \mathcal{D})$ can be often derived in **closed form**, and have a **geometric interpretation**.
- First and second order properties of the uniform $P(\mathcal{G}(\mathcal{E}))$ on directed acyclic graphs can be a basis for **simulations** and the definition of new priors; could they translate to the uniform prior over **decomposable undirected graphs**?
- Is there a way of identifying **paths** using covariance matrix decompositions?
- **Shrinking** the covariance matrix affects $P(e_{ij})$ and $P(a_{ij})$ as well, and it is possible to use it for regularisation purposes. Applications to Bayesian model averaging and significant edges/arcs identification?

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