The I-MAP Parameterization of Gaussian DAG Models

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Gaussian DAG Models and Estimation of Causal Effects

Gaussian SEMs and DAG Models

Suppose we have observations from a q-variate Gaussian random variable X, generated by a linear Gaussian Structural Equation Model (SEM) of the form

$$X = \boldsymbol{B}^T X + \epsilon, \qquad \epsilon \sim \mathcal{N}(\mathbf{0}, \boldsymbol{D}) \tag{1}$$

where $\boldsymbol{B}$ is a (q,q) matrix s.t. $\boldsymbol{B}_{ij} \neq 0$ iff $i \to j \in \mathcal{D}$, with $\mathcal{D}$ a Directed Acyclic Graph (DAG) and $\boldsymbol{D}$ a (q,q) diagonal matrix of node variances

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The linear SEM induces a Gaussian DAG model on X, i.e.

$$X \sim \mathcal{N}(\mathbf{0}, \boldsymbol{L}^{-T} \boldsymbol{D} \boldsymbol{L}^{-1})$$

where $\boldsymbol{L} = \boldsymbol{I_q} - \boldsymbol{B}$ and the joint pdf factorises according to the Markov property of $\mathcal{D}$:

$$f(x) = \prod_{j=1}^{q} d\mathcal{N}\left(x_j; -\boldsymbol{L}^T_{pa_j(\mathcal{D}),j} x_{pa_j(\mathcal{D})}, \boldsymbol{D}_{jj}\right), \quad \text{where } pa_j(\mathcal{D}) = \{i : i \to j \in \mathcal{D}\}$$

Causal effects: definition and identification

We are interested in estimating the **total causal effect** τ_{to} of a *treatment* variable X_t on an outcome variable X_o. Using the language of the *do-calculus*

$$\tau_{to} := \frac{\partial \mathbb{E}\left[X_o \mid \mathrm{do}(X_t = \tilde{x}_t)\right]}{\partial \tilde{x}_t} \tag{2}$$

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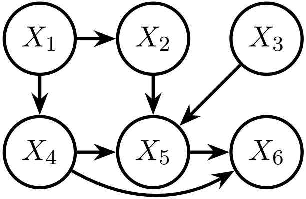
! The numerator Equation 2 requires a marginalization over a **post-intervention** distribution that we do not observe;
If $\mathcal{D}$ is known, it is possible to identify a **valid adjustment set** $z \subset [q]$ s.t. $\{t, o\} \notin z$ and

$$\mathbb{E}(X_o \mid \mathrm{do}(X_t = \tilde{x}_t) = \beta_0 + \tau_{to}\tilde{x}_t + \beta_{zo}^T \mathbb{E}(X_z) \tag{3}$$

i.e. τ_{to} corresponds to a regression coefficient in a specific regression model!

Causal effects: Example



If we are interested in τ_{46} possible valid adjustment sets are
$z_1 = \{1, 2, 3\}, z_2 = \{1, 3\}, z_3 = \{2, 3\}, z_4 = \{1\}, z_5 = \{2\}$

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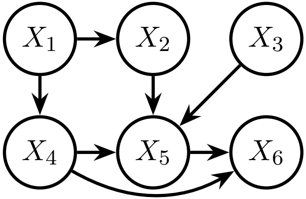

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All these valid adjustment sets would provide an unbiased estimate of the total causal effect of interest. **However**, the correspoding estimator may have different properties;

Causal effects: estimation

The regression coefficient in (3) can be very easily estimated via OLS.

Causal effects: estimation

The regression coefficient in (3) can be very easily estimated via OLS. Alternatively, in the Gaussian case, one may also

i) Obtain an estimate $(\hat{\boldsymbol{L}}, \hat{\boldsymbol{D}})$ via MLE

ii) Derive the MLE of the covariance function of the Gaussian DAG as

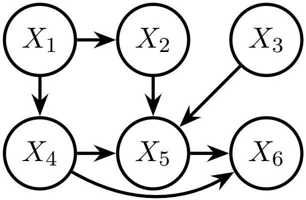
$$\hat{\boldsymbol{\Sigma}} = \hat{\boldsymbol{L}}^{-T} \hat{\boldsymbol{D}} \hat{\boldsymbol{L}}^{-1}$$

iii) Compute the MLE of τ_{to} as

$$\hat{\tau}_{to} = (\hat{\boldsymbol{\Sigma}}_{z^*,z^*})^{-1} \hat{\boldsymbol{\Sigma}}_{z^*,o}$$

where $z^* = t \cup z$ and z

Causal effects: Best Valid Adjustment set



Henckel et al. (2022): graphical characterization of **best valid adjustment set** $\mathcal{O}_{to}(\mathcal{D})$ as the one minimising asymptotic variance of the corresponding OLS estimator:

$$\mathcal{O}_{to}(\mathcal{D}) = \mathsf{pa}_{\mathcal{D}}\left(\mathsf{med}_{\mathcal{D}}(X_t, X_o) \cup X_o\right) \setminus \{X_t \cup \mathsf{med}_{\mathcal{D}}(X_t, X_o)\}$$

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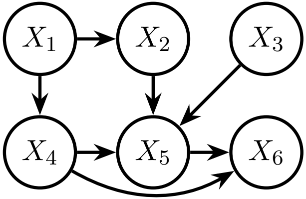

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In our example, $\mathcal{O}_{46}(\mathcal{D}) = \{2, 3\}$

Causal effects: unknown causal structure

If $\mathcal{D}$ is **not** known, one may:

i) Learn $\mathcal{D}$ from data using a **causal discovery** algorithm such as the PC-algorithm;

ii) Identify a valid adjustment set from the learnt DAG, and use it to estimate τ_{to};

Problem: Causal discovery algorithm return Markov equivalence classes of DAGs
Solution: Enumerate all the possible causal effects compatible with the Markov equivalence class (IDA, Maathuis et al. 2009)

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! This approach would still not account for the uncertainty in the estimation of the Markov equivalence class $\implies$ **Bayesian approaches**

Bayesian Causal Discovery and Causal Effect Estimation

In the Bayesian setting, causal discovery can be tackled as a Bayesian Model Selection task, and causal effect estimation under DAG uncertainty as a Bayesian Model Averaging (BMA) estimation problem;

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Let $\boldsymbol{X}$ be a (n, q) matrix of observations from a causal Gaussian DAG Model. We are interested in the posterior distribution

$$p((\boldsymbol{L}, \boldsymbol{D}), \mathcal{D}|\boldsymbol{X}) = p(\boldsymbol{L}, \boldsymbol{D}|\mathcal{D}, \boldsymbol{X})p(\mathcal{D}|\boldsymbol{X}) \tag{4}$$

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As the causal effect is a function of the parameters, by sampling from the posterior distribution (4), we can also approximate the posterior distribution over τ_{to} and hence obtain a BMA estimate of τ.

Bayesian Causal Discovery: A simple model

A typical model for Bayesian causal effect estimation under DAG uncertainty in the Gaussian setting is the following:

$$\boldsymbol{X}_{i\cdot}|(\boldsymbol{L}, \boldsymbol{D}), \mathcal{D} \sim \mathcal{N}_q\left(\boldsymbol{0}, \boldsymbol{L}^{-T}\boldsymbol{D}\boldsymbol{L}^{-1}\right) \qquad i \in [n]$$
$$(\boldsymbol{L}, \boldsymbol{D})|\mathcal{D} \sim \text{DAG-Wishart}(\boldsymbol{a}(\mathcal{D}), \boldsymbol{U})$$
$$p(\mathcal{D}) \propto \omega^{|\mathcal{S}_\mathcal{D}|}(1-\omega)^{\frac{q(q-1)}{2}-|\mathcal{S}_\mathcal{D}|}$$

where the DAG-Wishart prior (Ben-David, 2015) is a prior on the Cholesky space of a DAG $\mathcal{D}$, with hyperparameters $\boldsymbol{a}(\mathcal{D}) = (\boldsymbol{a}_1(\mathcal{D}), \dots, \boldsymbol{a}_q(\mathcal{D}))$ and a (q, q) s.p.d. matrix $\boldsymbol{U}$, while $\omega \in (0, 1)$ is a prior probability of edge inclusion.

DAG-Wishart prior: properties

The DAG-Wishart prior has many useful properties:

- It's conjugate, so that

$$p(\boldsymbol{L}, \boldsymbol{D} | \boldsymbol{X}, \boldsymbol{\mathcal{D}}) \sim \text{DAG-Wishart}\left(\boldsymbol{a}(\mathcal{D}) + n, \boldsymbol{U} + \boldsymbol{X}^T \boldsymbol{X}\right)$$

- Its **marginal likelihood** $p(\boldsymbol{X}|\mathcal{D})$ is **available in closed form** and **decomposable**
- Sampling from $p(\boldsymbol{L}, \boldsymbol{D}|\boldsymbol{X}, \boldsymbol{\mathcal{D}}$ occurs by direct sampling.
- Nice selection consistency properties in high-dimensions (Cao et al. 2019);
- The hyperparameters can be chosen in a way that guarantees **score equivalence**, i.e. that Markov equivalent DAGs are assigned the same marginal likelihood (Peluso & Consonni, 2020);

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When doing causal inference, our ultimate goal is testing or estimating causal effects
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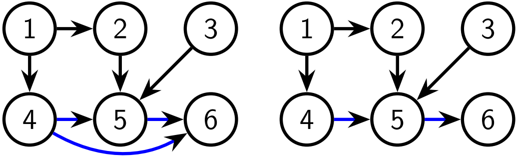

Figure: In the first DAG, $\tau_{46} = \boldsymbol{L}_{45}\boldsymbol{L}_{56} - \boldsymbol{L}_{46}$, in the second $\tau_{46} = \boldsymbol{L}_{45}\boldsymbol{L}_{56}$

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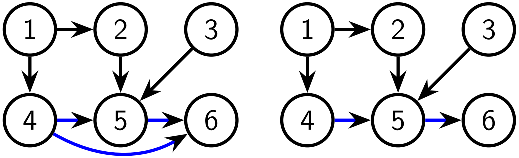


Figure: In the first DAG, $\tau_{46} = \boldsymbol{L}_{45}\boldsymbol{L}_{56} - \boldsymbol{L}_{46}$, in the second $\tau_{46} = \boldsymbol{L}_{45}\boldsymbol{L}_{56}$

Solution: Novel parameterization, the **I-MAP parameterization**, which always contains a **single parameter** corresponding to the total causal effect of interest;

The I-MAP parameterization

Minimal Independence MAPs: Constructive procedure

Suppose X is a Gaussian q-variate random vector and let π be an ordering of the variables. For any π, the joint pdf can be written as

$$f(x) = \prod_{j=1}^{q} f(x_j | x_{a_j(\pi)})$$

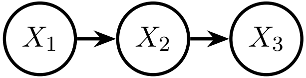
where $a_j(\pi)$ denotes all the variables that precede j in π;
If X is Markov w.r.t. to a DAG $\mathcal{D}$, then a set of conditional independencies $\mathcal{I}(\mathcal{D})$ holds, and for each j we can cancel out conditionally indep. variables from $a_j(\pi)$, so that

$$f(x) = \prod_{j=1}^{q} f(x_j | x_{\mathsf{S}_j(\mathcal{D},\pi)}) \qquad S_j(\mathcal{D},\pi) \subseteq a_j(\pi)$$

Def: A **Minimal Independence Map** (I-MAP) is the DAG $\mathcal{D}^*_\pi$ obtained by drawing, for each $j \in [p]$ an edge $k \to j$ if $k \in S_j(\mathcal{D},\pi)$

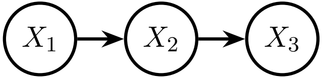
Minimal Independence MAPs: Example

Suppose that our random vector X is Markov w.r.t to the following DAG, implying only that $X_1 \perp X_3 \mid X_2$:

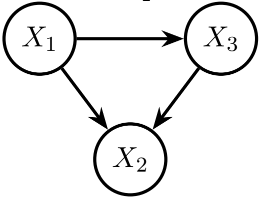


If we consider the two orderings $\pi_1 = X_1 \prec X_2 \prec X_3$ and $\pi_2 = X_1 \prec X_3 \prec X_2$, we obtain the following minimal I-MAPs:

$\mathcal{D}^*_{\pi_1}$



$\mathcal{D}^*_{\pi_2}$



Minimal I-MAPs: Comments

Different orderings imply different Minimal I-MAPs;

If π is topological of $\mathcal{D}$ (i.e., if $i \to j \in \mathcal{D}$ implies that $i \prec j$ (i precedes j) in π), then the Minimal I-MAP corresponds to the data-generating DAG;

Otherwise it is a strictly denser DAG whose Markov property implies a subset of the conditional independencies originally implied by the DAG;

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In the **Gaussian case**, one can obtain the parameters of the minimal I-MAP $(\boldsymbol{L}_\pi, \boldsymbol{D}_\pi)$ by permuting the rows and column of $\boldsymbol{\Sigma}_\mathcal{D}$ according to the ordering π, and then computing the LDL decomposition of the permuted covariance matrix
If π is not topological of $\mathcal{D}$, the I-MAP parameters $(\boldsymbol{L}_\pi, \boldsymbol{D}_\pi)$ will have a strictly larger number of non-null elements, **but** the **free parameters** will be the same;

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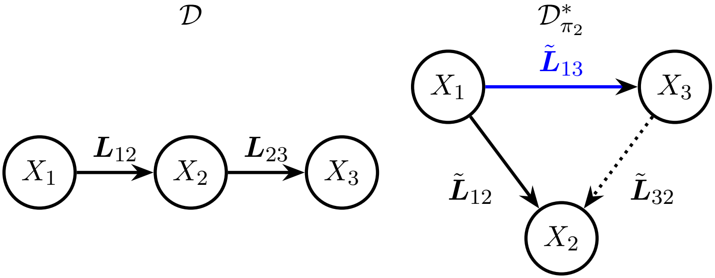
Our **I-MAP Parameterization** involves the free parameters of a **specific** minimal I-MAP

I-MAP constraints: Example

Let's consider again the 3-nodes DAG and its minimal I-MAP for π_2:



For the minimal I-MAP to represent the same model as the $\mathcal{D}$, it must hold that

$$\tilde{\boldsymbol{L}}_{32} = -\frac{\tilde{\boldsymbol{L}}_{13}\tilde{\boldsymbol{D}}_{22}}{\tilde{\boldsymbol{L}}_{12}\tilde{\boldsymbol{D}}_{33}}$$

The Optimal I-MAP: Definition

Let

- $\mathcal{D}$ be such that the treatment node X_t is an ancestor of the outcome node X_o;
- π^* be an ordering of the variables such that (i) π^* is topological of $\mathcal{D}$ and (ii) X_t and X_o are separated only by their mediators;
- $\tilde{\pi}$ be the ordering obtained from a topological ordering π and moving all the mediators of X_t and X_o after X_o, preserving their relative ordering relation

We call $\tilde{\mathcal{D}} := \mathcal{D}^*_{\tilde{\pi}}$ the **optimal I-MAP** of $\mathcal{D}$. It holds that

$$\mathsf{pa}_{\tilde{\mathcal{D}}}(X_o) = \tilde{z} = \mathcal{O}(X_t, X_o, \mathcal{D}) \quad \text{and} \quad \tilde{\boldsymbol{L}}_{\mathsf{pa}_o(\tilde{\mathcal{D}}),o} = -(\hat{\boldsymbol{\Sigma}}_{\tilde{z},\tilde{z}})^{-1}\hat{\boldsymbol{\Sigma}}_{\tilde{z},o}$$

The parameter of the edge $t \to o \in \tilde{\mathcal{D}}$ corresponds to the **total causal effect** of interest;

The Optimal I-MAP: Example

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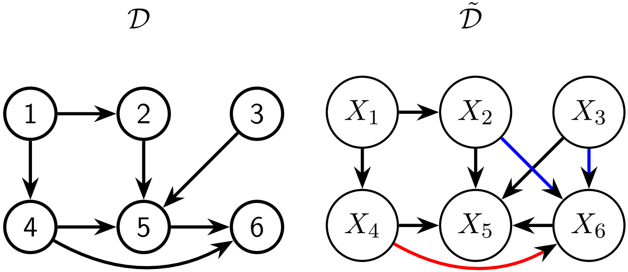

When interested in τ_{46} the Optimal I-MAP includes the **best valid adjustment set** $z^* = \{4, 2, 3\}$ as the parent set of the outcome node, and $\tilde{\boldsymbol{L}}_{46}$ is the corresponding parameter in the I-MAP parameterization;

I-MAP Parameterization: Further technical results

We fully characterise the connection between the canonical Gaussian DAG Model parameterization and our I-MAP parameterization.
We developed a **fast** procedure that transform the parameters $(\boldsymbol{L}, \boldsymbol{D})$ of a Gaussian DAG Model into the corresponding parameters of the I-MAP parameterization, using only $m := |\text{med}_{\mathcal{D}}(t, o)|$ steps of **Gaussian elimination**.
The same procedure can be also used in computer algebra systems to derive the **constraints** that hold among the parameters of the I-MAP parameterization.

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The same procedure can be also used in computer algebra systems to derive the **constraints** that hold among the parameters of the I-MAP parameterization.

In practice, identifying the constraints of the I-MAP parameterization remains quite inconvenient;

Bayesian Model Specification on the I-MAP

The statistical model can be written as

$$\boldsymbol{X} \mid \boldsymbol{\Sigma}_{\mathcal{D}}, \mathcal{D} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\mathcal{D}})$$
$$\boldsymbol{\Sigma}_{\mathcal{D}} = \tilde{\boldsymbol{L}}^{-T} \tilde{\boldsymbol{D}} \tilde{\boldsymbol{L}}^{-1}$$

The parameter prior must then be defined only on the free-parameters of the I-MAP parameterization. For instance, in the simplest case, we may specify for any $j \in [q]$ and any pair i, j such that $\boldsymbol{L}_{ij}$ is a free parameter:

$$\tilde{\boldsymbol{L}}_{ij} \mid \mathcal{D} \sim \mathcal{N}(0, \sigma_0^2)$$
$$\tilde{\boldsymbol{D}}_{jj} \mid \mathcal{D} \sim \text{Inv-Gamma}(\nu_0/2, \nu_0\sigma_0/2)$$

The DAG prior can be specified as before

$$p(\mathcal{D}) =\propto \omega^{|\mathcal{S}_{\mathcal{D}}|}(1-\omega)^{\frac{q(q-1)}{2} - |\mathcal{S}_{\mathcal{D}}|}$$

Bayesian Model Specification: Comments

Because of the constraints holding among the parameters of the I-MAP parameterization, computing the marginal likelihood becomes a difficult task;

Solution: We propose to use a Laplace approximation centered on the MLE of the I-MAP $(\tilde{\boldsymbol{L}}^{\mathsf{MLE}}, \tilde{\boldsymbol{D}}^{\mathsf{MLE}})$, leading to a **BIC**-style approximation of the marginal likelihood;

As deriving the said constraints is computationally costly, even evaluating the likelihood and deriving the MLE can be difficult

We thus first estimate the MLE of the DAG parameters $(\boldsymbol{L}, \boldsymbol{D})$ and then use our Gaussian elimination procedure to derive $(\tilde{\boldsymbol{L}}^{\mathsf{MLE}}, \tilde{\boldsymbol{D}}^{\mathsf{MLE}})$ by the **invariance property** of MLE;

Similarly, sampling from the posterior $p(\tilde{\boldsymbol{L}}, \tilde{\boldsymbol{D}} | \boldsymbol{X}, \mathcal{D})$ occurs via Importance Sampling, by first sampling from a DAG-Wishart distribution and then resampling the transformed samples with weights given by the two priors ratio;

Conclusions

- We propose an alternative parameterization of Gaussian DAG Models, the I-MAP parameterization, that always contains a causal effect of interest as a single parameter;
- Our parameterization allows for full control over the specification over the prior distribution on the causal effect of interest in a Bayesian setting;
- As the I-MAP parameterization involves constraints among the parameters, we developed both a procedure to (more easily) derive those constraints, and a procedure to quickly transform the parameters of a Gaussian DAG model in the typical parameterization to the ones of the I-MAP parameterization;
- The second procedure can be used to both derive an approximation to the marginal likelihood and to sample from the posterior distribution over the parameters.
- As numerical experiments are still unsatisfactory, we are currently exploring new possibilities for the approximation of the marginal likelihood

Thank you!

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https://alesmascaro.github.io

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