DAG LEARNING VIA SPARSE RELAXATIONS

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ABSTRACT

We propose a continuous optimization framework for discovering a latent directed acyclic graph (DAG) from observational data. Our approach optimizes over the polytope of permutation vectors, the so-called *Permutahedron*, to learn a topological ordering. Edges can be optimized jointly, or learned conditional on the ordering via a non-differentiable subroutine. Compared to existing continuous optimization approaches our formulation has a number of advantages including: 1. *validity*: optimizes over exact DAGs as opposed to other relaxations optimizing approximate DAGs; 2. *modularity*: accommodates any edge-optimization procedure, edge structural parameterization, and optimization loss; 3. *end-to-end*: either alternately iterates between node-ordering and edge-optimization, or optimizes them jointly; We demonstrate, on real-world data problems in protein-signaling and transcriptional network discovery, that our approach lies on the Pareto frontier of two key metrics, the SID and SHD.

1 INTRODUCTION

In many domains, including cell biology (Sachs et al., 2005), finance (Sanford & Moosa, 2012), and genetics (Zhang et al., 2013), the data generating process is thought to be represented by an underlying directed acylic graph (DAG). Many models rely on DAG assumptions, e.g., causal modeling uses DAGs to model distribution shifts, ensure predictor fairness among subpopulations, or learn agents more sample-efficiently (Kaddour et al., 2022). A key question, with implications ranging from better modeling to causal discovery, is how to recover this unknown DAG from observed data alone. While there are methods for identifying the underlying DAG if given additional interventional data (Eberhardt, 2007; Hauser & Bühlmann, 2014; Shanmugam et al., 2015; Kocaoglu et al., 2017; Addanki et al., 2020; Squires et al., 2020; Lippe et al., 2022), it is not always practical or ethical to obtain such data (e.g., if one aims to discover links between dietary choices and deadly diseases).

Learning DAGs from observational data alone is fundamentally difficult for two reasons. (i) *Estimation*: it is possible for different graphs to produce similar observed data, either because the graphs are Markov equivalent (they represent the same set of data distributions) or because not enough samples have been observed to distinguish possible graphs. This riddles the search space with local minima; (ii) *Computation*: DAG discovery is a costly combinatorial optimization problem over an exponentially large solution space and subject to global acyclicity constraints.

To address issue (ii), recent work has proposed continuous relaxations of the DAG learning problem. These allow one to use well-studied continuous optimization procedures to search the space of DAGs. While these methods are more efficient than combinatorial methods, the current approaches have one or more of the following downsides: 1. *Over-relaxation*: methods based on penalizing the exponential of the adjacency matrix are not guaranteed to return a valid DAG, but require post-processing to correct the graph to a DAG (Zheng et al., 2018; Yu et al., 2019; Zheng et al., 2020; Ng et al., 2020; Brouillard et al., 2020; He et al., 2021). How the learning method and the post-processing method interact with each other is not currently well-understood; 2. *Non-modularity*: continuously relaxing the DAG learning problem is often done to leverage gradient-based optimization (Zheng et al., 2018; Ng et al., 2020; Cundy et al., 2021; Charpentier et al., 2022). This requires all training operations to be differentiable, preventing the use of certain well-studied black-box estimators for learning edge functions; 3. *Error propagation*: methods that break the DAG learning problem into two stages risk propagating errors from one stage to the next (Teyssier & Koller, 2005; Bühlmann et al., 2014; Gao et al., 2020; Reisach et al., 2021; Rolland et al., 2022).

In this work, we make the following contributions to score-based methods for DAG learning:

- We note that to learn a topological ordering of a DAG (i.e., total ordering of its nodes) with d nodes, it is sufficient to optimize over the polytope of permutations of the first d natural numbers, i.e., the *Permutahedron* of order d. Whereas, prior work required expensive optimization over the polytope of bistochastic matrices: the Birkhoff polytope (or relaxations of it) (Cundy et al., 2021; Charpentier et al., 2022).
- We show how to reformulate the standard score-based optimization objective for DAG learning to leverage recent developments in sparse relaxations for discrete optimization (Niculae et al., 2018; Correia et al., 2020).
- As these sparse relaxation methods require access to MAP oracles, we derive an algorithm for constructing the top-k ranking of a score vector, a result that may be of independent interest.
- We demonstrate that working on the Permutahedron leads to improved sensitivity of the maximum a posteriori (MAP) solution to changes in optimization parameters, compared to prior approaches based on the Birkhoff polytope (i.e. the polytope of permutation matrices).

These allow us to develop a framework that addresses the issues of prior work. Specifically, our approach: 1. Optimizes over sparse distributions of DAG topological orderings (i.e., a total ordering of the nodes), ensuring all considered graphs are DAGs; 2. Separates the learning of topological orderings from the learning of edge functions, broadening the class of edge function estimators: the objective need not be differentiable (e.g. the score function proposed in Squires et al. (2020)), but even the edge optimization can be entirely black-box; 3. Alternately iterates between learning ordering and edges (if edge functions are learned via black-box regression) or optimizes them jointly. Finally, when we compare our approaches to other recent work on real-world graph discovery problems, we find that it lies on the Pareto front of two key metrics, the structural intervention distance (SID) and the structural hamming distance (SHD).

2 Related Work

The work on DAG learning can be largely categorized into four families of approaches: (a) combinatorial methods, (b) continuous relaxation, (c) order-based two-stage, (d) order-based end-to-end.

Combinatorial methods. These methods are either constraint-based, relying on conditional independence tests for selecting the sets of parents (Spirtes et al., 2000), or score-based, evaluating how well possible candidates fit the data (Geiger & Heckerman, 1994) (see Kitson et al. (2021) for a survey). Constraint-based methods, while elegant, require conditional independence testing, which is known to be a hard statistical problem Shah & Peters (2020). For this reason, we focus our attention in this paper on score-based methods. Of these, exact combinatorial algorithms exist only for small number of nodes d (Singh & Moore, 2005; Xiang & Kim, 2013; Cussens, 2011), because the space of DAGs grows superexponentially in d and finding the optimal solution is NP-hard to solve (Chickering, 1995b). Approximate methods (Scanagatta et al., 2015; Aragam & Zhou, 2015; Ramsey et al., 2017) rely on global or local search heuristics in order to scale to problems with thousands of nodes.

Continuous relaxation. To address the complexity of the combinatorial search, more recent methods have proposed relaxations that formulate DAG learning as a continuous optimization problem. To do so, the constraint on acyclicity is expressed as a smooth function and then relaxed to allow efficient optimization with gradient-based solvers (Zheng et al., 2018; Yu et al., 2019; Zheng et al., 2020; Ng et al., 2020; Brouillard et al., 2020; He et al., 2021). However, this relaxation no longer guarantees the absence of cycles at any stage of training, and solutions often require post-processing.

Order-based two-stage. The third prominent line of works learns DAGs in two-stages: (i) finding an ordering of the variables, and (ii) selecting the best scoring graph among (or marginalizing over) the structures that are consistent with the found ordering (Teyssier & Koller, 2005; Bühlmann et al., 2014; Gao et al., 2020; Reisach et al., 2021; Rolland et al., 2022). As such, these approaches work over exact DAGs, instead of relaxations. Additionally, they work on the space of orderings which is smaller and more regular than the space of DAGs (Friedman & Koller, 2003; Teyssier & Koller, 2005), while guaranteeing acyclicity. The downside of these approaches is that errors in the first stage can propagate to the second stage that is unaware of them.

Order-based end-to-end. The final line of works uses the two-stage decomposition above, but addresses the issue of error propagation by formulating an end-to-end optimization approach (Friedman & Koller, 2003; Cundy et al., 2021; Charpentier et al., 2022). In particular, Cundy et al. (2021) optimizes node ordering using the polytope of permutation matrices: the Birkhoff polytope. This method

requires $\mathcal{O}(d^3)$ time and $\mathcal{O}(d^2)$ memory complexities. To lower the time complexity, Charpentier et al. (2022) suggest to leverage another operator that drops a constraint on the permutation matrix (allowing row-stochastic matrices). Both methods introduce a mismatch between forward (based on the hard permutation) and backward (based on soft permutations) passes.

3 SETUP

3.1 THE PROBLEM

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix of n observed data inputs generated by an unknown Structural Equation Model (SEM) (Pearl, 2000). An SEM describes the functional relationships between d features as edges between nodes in a DAG $\mathcal{G} \in \mathbb{D}[d]$ (where $\mathbb{D}[d]$ is the space of all DAGs with d nodes). Each feature $\mathbf{x}_j \in \mathbb{R}^n$ is generated by some (unknown) function f_j of its (unknown) parents $\text{pa}(j)$ as: $\mathbf{x}_j = f_j(\mathbf{x}_{\text{pa}(j)})$. We keep track of whether an edge exists in the graph $\mathcal{G}$ using an adjacency matrix $\mathbf{A} \in \{0,1\}^{d \times d}$ (i.e., $\mathbf{A}_{ij} = 1$ if and only if there is a (directed) edge $i \to j$). For example, a special case is when the structural equations are linear with Gaussian noise,

$$\mathbf{y}_j = f_j\left(\mathbf{X}, \mathbf{A}_j\right) = \mathbf{X}(\mathbf{w}_j \circ \mathbf{A}_j) + \varepsilon; \quad \varepsilon \sim \mathcal{N}(0, \nu) \tag{1}$$

where $\mathbf{w}_j \in \mathbb{R}^d$, $\mathbf{A}_j$ is the jth column of $\mathbf{A}$, and ν is the noise variance. This is just to add intuition; our framework is compatible with non-linear, non-Gaussian structural equations.

3.2 OBJECTIVE

Given $\mathbf{X}$, our goal is to recover the unknown DAG that generated the observations. To do so we must learn (a) the *connectivity parameters* of the graph, represented by the adjacency matrix $\mathbf{A}$, and (b) the *functional parameters* $\mathbf{\Phi} = \{\boldsymbol{\phi}_j\}_{j=1}^d$ that define the edge functions $\{f^{\boldsymbol{\phi}_j}\}_{j=1}^d$. Score-based methods (Kitson et al., 2021) learn these parameters via a constrained optimization problem

$$\min_{\substack{\mathbf{A} \in \mathbb{D}[d] \\ \mathbf{\Phi}}} \sum_{j=1}^{d} \ell\left(\mathbf{x}_j, f^{\boldsymbol{\phi}_j}\left(\mathbf{X} \circ \mathbf{A}_j\right)\right) + \lambda \Omega(\mathbf{\Phi}), \tag{2}$$

where $\ell : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a loss that describes how well each feature $\mathbf{x}_j$ is predicted by $f^{\boldsymbol{\phi}_j}$. As in eq. (1), the adjacency matrix defines the parents of each feature $\mathbf{x}_j$ as follows $pa(j) = \{i \subseteq [d] \setminus j \mid \mathbf{A}_{ij} = 1\}$. Only these features will be used by $f^{\boldsymbol{\phi}_j}$ to predict $\mathbf{x}_j$, via $\mathbf{X} \circ \mathbf{A}_j$. The constraint $\mathbf{A} \in \mathbb{D}[d]$ enforces that the connectivity parameters $\mathbf{A}$ describes a valid DAG. Finally, $\Omega(\mathbf{\Phi})$ is a regularization term. So long as this regularizer takes the same value for all DAGs within a Markov equivalence class, the consistency results of Brouillard et al. (2020, Theorem 1) prove that the solution to Problem (2) is Markov equivalent to the true DAG, given standard assumptions.

3.3 SPARSE RELAXATION METHODS

The above objective is an NP-hard combinatorial optimization problem (Chickering, 1995a) over all possible graph structures. Our goal will be to leverage recent methods in sparse relaxation (Niculae et al., 2018; Correia et al., 2020) to replace combinatorial optimization with (more efficient) gradient-based optimization. Therefore, we rewrite the optimization problem in eq. (2) as follows.

Let $D := |\mathbb{D}[d]|$ be the number of possible DAGs with d nodes (note that D is super-exponential in d, e.g., for $d = 10$, $D \approx 4.2 \times 10^{18}$ (Murphy et al., 2001)). Let $\boldsymbol{\psi}(\mathbf{\Phi}) \in \mathbb{R}^D$ be a vector of scores for every possible DAG (i.e., the larger the better) that depends on the functional parameters $\mathbf{\Phi}$. Our goal is to solve $\arg\max \boldsymbol{\psi}(\mathbf{\Phi})$ which is equivalent to $\arg\max_{\mathbf{z} \in \triangle^D} \boldsymbol{\psi}(\mathbf{\Phi})^\top \mathbf{z}$, where $\triangle^D := \{\mathbf{z} \in \mathbb{R}^D \mid \mathbf{z} \succeq 0, \sum_{i=1}^D z_i = 1\}$ is the D-dimensional simplex (if there are ties, then the $\arg\max$ is a set). Unfortunately, we cannot (a) enumerate $\boldsymbol{\psi}(\mathbf{\Phi}) \in \mathbb{R}^D$, and (b) learn $\mathbf{\Phi}$ via gradient-based methods, as the $\arg\max$ is not differentiable. The following sparse relaxation methods address (b).

Top-k sparsemax (Correia et al., 2020). One approach to relax $\arg\max_{\mathbf{z} \in \triangle^D} \boldsymbol{\psi}(\mathbf{\Phi})^\top \mathbf{z}$ and to allow gradient-based optimization of $\mathbf{\Phi}$ is to (i) regularize $\mathbf{z}$, and (ii) constrain the number of non-zero entries of $\mathbf{z}$,

$$\mathbf{z}^{\text{top-}k \text{ sparsemax}}(\boldsymbol{\psi}(\mathbf{\Phi})) = \underset{\mathbf{z} \in \triangle^r, \|\mathbf{z}\|_0 \leq k}{\arg\max} \; \boldsymbol{\psi}(\mathbf{\Phi})^\top \mathbf{z} - \frac{\tau}{2}\|\mathbf{z}\|_2^2, \tag{3}$$

where $\tau \in \mathbb{R}^+$ is a hyperparameter. To address (a) above, in many structure learning problems, there exists an oracle that returns the top-k scoring structures efficiently (e.g., assignment problems), with complexity t. Given such an oracle, the overall complexity of top-k sparsemax is $\mathcal{O}(t+k)$ (Correia et al., 2020). However, we are unaware of any such oracle for DAGs. We will show in Section 4 that it is possible to derive a top-k oracle for a subset of the DAG learning problem.

SparseMAP (Niculae et al., 2018). Imagine that the set of scores is low-rank: $\boldsymbol{\psi}(\boldsymbol{\Phi}) = \mathbf{B}^\top \boldsymbol{\eta}(\boldsymbol{\Phi})$ where $\mathbf{B} \in \mathbb{R}^{q \times D}$ where $q \ll D$. SparseMAP regularizes this lower-dimensional 'marginal space'

$$\mathbf{z}^{\text{sparseMAP}}(\boldsymbol{\psi}(\boldsymbol{\Phi})) \in \underset{\mathbf{z} \in \triangle^D}{\arg\max}\, \boldsymbol{\psi}(\boldsymbol{\Phi})^\top \mathbf{z} - \frac{\tau}{2}\|\mathbf{B}\mathbf{z}\|_2^2. \tag{4}$$

Given an oracle with complexity t that finds the top scoring structure, sparseMAP finds the solution in $\mathcal{O}(sd^2 + t)$ where s is the number of iterations of the active set algorithm used by sparseMAP (Nocedal & Wright, 1999). We are unaware of such an oracle for DAGs; however, by decomposing the DAG learning problem, we can find an oracle for the decomposed subproblem.

3.4 Two-Stage DAG Learning: Order, Select Edges

The key difficulty above is that the set of all valid DAGs is difficult to characterize: as soon as some edges are added, other edges are prohibited. However, note that any DAG can be generated by the following two-step procedure (Friedman & Koller, 2003): (i) Give a total ordering of the d nodes (this is called a topological ordering); (ii) Only allow an edge that is consistent with the ordering, i.e., from a node i to a node j if $\mathbf{x}_i \prec \mathbf{x}_j$. It is easy to show that any DAG can be constructed this way.

Most similar to our work, Cundy et al. (2021); Charpentier et al. (2022) use this decomposition to learn an adjacency matrix $\mathbf{A}$. Formally, any adjacency matrix $\mathbf{A}$ can be written as $\mathbf{A} = \mathbf{P}\mathbf{L}\mathbf{P}^\top$, where $\mathbf{L}$ is an upper triangular matrix and $\mathbf{P}$ is a permutation matrix. Cundy et al. (2021) learn this permutation matrix by optimizing $\arg\min_{\mathbf{P} \in \mathbb{B}[d]} \operatorname{Tr}(\boldsymbol{\Theta}^\top \mathbf{P})$, where $\mathbb{B}[d]$ is the Birkhoff polytope of $(d \times d)$- bistochastic matrices. They learn $\boldsymbol{\Theta}$ through gradient descent by relaxing the optimization problem using the Gumbel-Sinkhorn approximation (Mena et al., 2018). Charpentier et al. (2022) relax the problem even further by only requiring $\mathbf{P}$ to be row-stochastic by leveraging (SoftSort, Prillo & Eisenschlos, 2020).

4 DAG Learning via Sparse Relaxations

We now describe our framework for DAG learning, *Daguerreotype*. Figure 1 presents a schematic of the overall approach. We start showing that instead of optimizing over permutation matrices (i.e., the extreme points of the Birkhoff polytope), it is sufficient to optimize over permutation *vectors* (i.e., the extreme points of the Permutahedron). This sufficiency allows us to characterize the sensitivity of the optimal solution (i.e., the MAP) to changes in our learning parameters, in Appendix C. We then show how sparse relaxation methods can be leveraged to learn the topological ordering of a DAG. Another appealing property of this parameterization is that it allows us to always learn over valid DAGs, even when taking gradients, which is not the case for previous methods Cundy et al. (2021); Charpentier et al. (2022). It also allows us to use any arbitrary method for learning DAG edges.

4.1 Learning Orderings on the Permutahedron

Given that we can learn DAGs in two stages: (i) node ordering; (ii) edge selection; we start by defining an optimization problem for stage (i).

Given d nodes, let Σ_d be the set of all permutations of node indices $\{1, \ldots, d\}$. Given a vector $\mathbf{v} \in \mathbb{R}^d$, let $\mathbf{v}^\sigma := [\mathbf{v}^{\sigma(1)}, \ldots, \mathbf{v}^{\sigma(d)}]^\top$ be the vector of reordered $\mathbf{v}$ according to the permutation $\sigma \in \Sigma_d$. Similarly, for a matrix $\mathbf{M} \in \mathbb{R}$, let $\mathbf{M}^\sigma$ be the matrix obtained by permuting the rows and columns of $\mathbf{M}$ by σ.

Let $\mathbb{D}_{\text{C}}[d]$ be the set of *complete* DAGs (i.e., DAGs with all possible edges). Let $\mathbf{R} \in \{0,1\}^{d \times d}$ be the binary upper triangular matrix where the upper triangle is all equal to 1. Then $\mathbb{D}_{\text{C}}[d]$ can be fully enumerated given $\mathbf{R}$ and Σ_d,

$$\mathbb{D}_{\text{C}}[d] = \{\mathbf{R}^\sigma : \sigma \in \Sigma_d, \mathbf{R} \in \{0,1\}^{d \times d}, \mathbf{R}_{ij} = 0\ \forall i \geq j, \mathbf{R}_{ji} = 1\ \forall j < i\}. \tag{5}$$

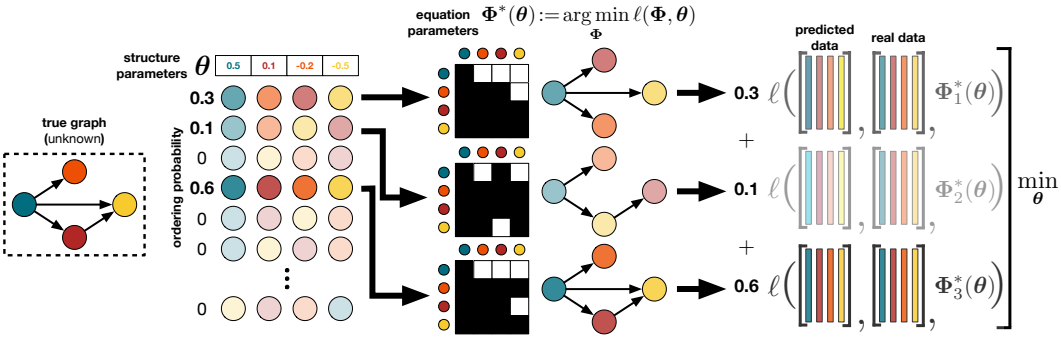

Figure 1: **Daguerreotype**: Our end-to-end approach to DAG learning works by (a) learning a sparse distribution over node orderings via structure parameters θ, and (b) learning a sparse predictor $\mathbf{w}^*$ to estimate the data. Any black-box predictor can be used to learn $\mathbf{w}^*$; differentiability is not necessary.

Note that every matrix $\mathbf{R}^\sigma = \mathbf{P}\mathbf{R}\mathbf{P}^\top$ where $\mathbf{P}$ is a permutation matrix. Therefore it is sufficient to learn σ in step (i), and then learn which edges to drop in step (ii).

Imagine now that $\boldsymbol{\theta}$ defines a score for each node, and these scores induce an ordering $\sigma(\boldsymbol{\theta})$: the larger the score, the earlier the node should be in the ordering. Formally, the following optimization problem finds such an ordering

$$\sigma(\boldsymbol{\theta}) \in \arg\max_{\sigma \in \Sigma_d} \boldsymbol{\theta}^\top \boldsymbol{\rho}^\sigma \,, \quad \text{where } \boldsymbol{\rho} = [1, 2, \ldots, d] \,. \tag{6}$$

Note that a simple oracle solves this optimization problem: sort $\boldsymbol{\theta}$ into descending order (as given by The Rearrangement Inequality (Hardy et al., 1952, Thms. 368–369)). We emphasize that we write '$\in$' in eq. (6) since the r.h.s can be a set (when components of $\boldsymbol{\theta}$ are equal).

We would like to learn the ordering $\sigma(\boldsymbol{\theta})$ by taking gradients w.r.t. $\boldsymbol{\theta}$. However, we cannot take gradients through eq. (6) because (a) $\sigma(\boldsymbol{\theta})$ is not even a function (due to it possibly being a set), and (b) even if we restrict the parameter space to not have ties, the mapping is piece-wise constant and uninformative for gradient-based learning. To fix these, Blondel et al. (2020) introduce two alterations: for (b), extend Σ_d to the convex hull of all permutations of $\boldsymbol{\rho}$, i.e., $\mathbb{P}[d] := \text{conv}\{\boldsymbol{\rho}^\sigma \mid \sigma \in \Sigma_d\}$, i.e., the order-$d$ *Permutahedron*; for (a), introduce a convex regularizer to yield

$$\boldsymbol{\mu}(\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\mu} \in \mathbb{P}[d]} \boldsymbol{\theta}^\top \boldsymbol{\mu} - \frac{\tau}{2} \|\boldsymbol{\mu}\|_2^2. \tag{7}$$

This mapping is differentiable w.r.t. $\boldsymbol{\theta}$ and, in the absence of ties, as $\tau \to 0$ we have that $\boldsymbol{\mu}(\boldsymbol{\theta}) \to \sigma(\boldsymbol{\theta})$ (Blondel et al., 2020). Unfortunately, any $\boldsymbol{\mu} \in \mathbb{P}[d]$ (except at the vertices) corresponds to an invalid 'partial' permutation, hence cannot be used directly to sort the nodes. However, we will leverage the property that any $\boldsymbol{\mu}$ can be written as a convex combination of permutations (i.e., vertices of $\mathbb{P}[d]$),

$$\boldsymbol{\mu} = \sum_{\sigma \in \Sigma_d} \alpha_\sigma \boldsymbol{\rho}^\sigma = \mathbb{E}_{\sigma \sim \boldsymbol{\alpha}}[\boldsymbol{\rho}^\sigma], \quad \text{s.t. } \alpha_\sigma \geq 0, \sum_{\sigma \in \Sigma_d} \alpha_\sigma = 1. \tag{8}$$

Note that when we use σ as a subscript, we index a vector instead of permuting it.

4.2 Leveraging Sparse Relaxation Methods

If we substitute $\boldsymbol{\mu}$ with its sparse decomposition $\mathbb{E}_{\sigma \sim \boldsymbol{\alpha}}[\boldsymbol{\rho}^\sigma]$, we get

$$\boldsymbol{\alpha}^{\text{sparseMAP}}(\boldsymbol{\theta}) \in \arg\max_{\boldsymbol{\alpha} \in \triangle^{|\Sigma_d|}} \boldsymbol{\theta}^\top \mathbb{E}_{\sigma \sim \boldsymbol{\alpha}}[\boldsymbol{\rho}_\sigma] - \frac{\tau}{2} \|\mathbb{E}_{\sigma \sim \boldsymbol{\alpha}}[\boldsymbol{\rho}_\sigma]\|_2^2 \,, \tag{9}$$

where $\triangle^{|\Sigma_d|}$ is the simplex over all permutations. Note that this can be solved by sparseMAP (Niculae et al., 2018)! The active set algorithm used by sparseMAP returns a sparse set of permutations and only requires access to an oracle solving eq. (6), i.e., sorting $\boldsymbol{\theta}$.[1]

[1] The sparseMAP distribution is not unique in general, it can be a polyhedral set. As described by Correia et al. (2020), the active set algorithm, when initialized with a random permutation, can be seen as a way to sample from the vertices of this solution set. Our implementation, therefore, optimizes this double loop implicitly.

Alternatively, because the only term in the regularization that matters for optimization is $\boldsymbol{\alpha}$, we can regularize it alone, and restrict the number of non-zero entries of α to k,

$$\boldsymbol{\alpha}^{\text{top-}k\text{ sparsemax}}(\boldsymbol{\theta}) \in \underset{\boldsymbol{\alpha}\in\triangle^{|\Sigma_d|}, \|\boldsymbol{\alpha}\|_0 \leq k}{\arg\max} \boldsymbol{\theta}^\top \mathbb{E}_{\sigma\sim\boldsymbol{\alpha}}[\boldsymbol{\rho}^\sigma] - \frac{\tau}{2}\|\boldsymbol{\alpha}\|_2^2 . \tag{10}$$

This is a formulation of top-k sparsemax (Correia et al., 2020). Recall that top-k sparsemax requires a top-k oracle, i.e., the set of k permutations with highest value of $\boldsymbol{\theta}^\top \boldsymbol{\rho}^\sigma$. To our knowledge, such a top-k oracle has not been presented before. We derive an efficient algorithm for this in Appendix A which may be of independent interest.

We note that top-k sparsemax optimizes over the highest-scoring permutations, while sparseMAP instead optimizes any set of permutations the marginal solution can be decomposed into. As an example, for $\boldsymbol{\theta} = \mathbf{0}$, sparseMAP returns two permutations, σ and its inverse σ^{-1}. On the other hand, because top-k sparsemax only considers k permutations, we are not guaranteed to retrieve all permutations with non-zero mass in general. In Appendix D we provide an empirical comparison of these two operators when applied to the DAG learning problem.

4.3 DAG Learning

In order to select which edges to drop from $\mathbf{R}$, we regularize the set of edge functions $\{f^{\phi_j}\}_{j=1}^d$ to be sparse via $\Omega(\boldsymbol{\Phi})$ in eq. (2), i.e., $\|\boldsymbol{\Phi}\|_0$ or $\|\boldsymbol{\Phi}\|_1$. Incorporating the sparse decompositions of eq. (9) or eq. (10) into the original problem in eq. (2) yields

$$\min_{\boldsymbol{\theta},\boldsymbol{\Phi}} \mathbb{E}_{\sigma\sim\boldsymbol{\alpha}^\star(\boldsymbol{\theta})}\left[\sum_{j=1}^d \ell\left(\mathbf{x}_j, f^{\phi_j}\left(\mathbf{X}\circ(\mathbf{R}^\sigma)_j\right)\right) + \lambda\Omega(\boldsymbol{\Phi})\right], \tag{11}$$

where $(\mathbf{R}^\sigma)_j$ is the jth column of $\mathbf{R}^\sigma$ and $\alpha^\star$ is the top-k sparsemax or the SparseMAP distribution. Notice that for both sparse operators, in the limit $\tau \to 0_+$ the distribution $\alpha^\star$ puts all probability mass on one permutation: $\sigma(\boldsymbol{\theta})$ (the sorting of $\boldsymbol{\theta}$), and thus eq. (11) is a generalization of eq. (2).

We can solve the above optimization problem for the optimal $\boldsymbol{\theta}, \boldsymbol{\Phi}$ jointly via gradient-based optimization. The downside of this, however, is that training may move towards poor permutations purely because $\boldsymbol{\Phi}$ is far from optimal. Specifically, at each iteration, the distribution over permutations $\alpha^\star(\boldsymbol{\theta})$ is updated based on functional parameters $\boldsymbol{\Phi}$ that are, on average, good for all selected permutations. In early iterations, this approach can be highly suboptimal as it cannot escape from high-error local minima. To address this, we may push the optimization over $\boldsymbol{\Phi}$ inside the objective:

$$\min_{\boldsymbol{\theta}} \mathbb{E}_{\sigma\sim\alpha^\star(\boldsymbol{\theta})}\left[\sum_{j=1}^d \ell\left(\mathbf{x}_j, f^{\boldsymbol{\Phi}^\star(\sigma)_j}\left(\mathbf{X}\circ(\mathbf{R}^\sigma)_j\right)\right)\right] \tag{12}$$

$$\text{s.t. } \boldsymbol{\Phi}^\star(\sigma) = \arg\min_{\boldsymbol{\Phi}} \sum_{j=1}^d \ell\left(\mathbf{x}_j, f^{\phi_j}\left(\mathbf{X}\circ(\mathbf{R}^\sigma)_j\right)\right) + \lambda\Omega(\boldsymbol{\Phi}).$$

This is a bi-level optimization problem (Dempe & Zemkoho; Franceschi et al., 2018) where the inner problem fits one set of structural equations $\{f^{\phi_j}\}_{j=1}^d$ per $\sigma \sim \alpha^\star(\boldsymbol{\theta})$. Note that, as opposed to many other settings (e.g. in meta-learning), the outer objective depends on $\boldsymbol{\theta}$ only through the distribution $\alpha_*(\boldsymbol{\theta})$, and not through the inner problem over $\boldsymbol{\Phi}$. In practice, this means that the outer optimization does not require gradients (or differentiability) of the inner solutions at all, saving computation and allowing for greater flexibility in picking a solver for fitting $\boldsymbol{\Phi}^\star(\sigma)$.[2] For example, for $\Omega(\boldsymbol{\Phi}) = \|\boldsymbol{\Phi}\|_1$ we may invoke any Lasso solver, and for $\Omega(\boldsymbol{\Phi}) = \|\boldsymbol{\Phi}\|_0$ we may use the algorithm of Louizos et al. (2017), detailed in Appendix B. The downside of this bi-level optimization is that it is only tractable when the support of $\alpha^\star(\boldsymbol{\theta})$ has a few permutations. Optimizing for $\boldsymbol{\theta}$ and $\boldsymbol{\Phi}$ jointly is more efficient.

[2] This computational advantage is shared with the score-function estimator (SFE, Rubinstein, 1986; Williams, 1992; Paisley et al., 2012; Mohamed et al., 2020). We are not aware of any applications of SFE to permutation learning, likely due to the #P-completeness of marginal inference over the Birkhoff polytope (Valiant, 1979; Taskar, 2004).

4.4 COMPUTATIONAL ANALYSIS

The overall complexity of our framework depends on the choice of sparse operator for learning the topological order and on the choice of the estimator for learning the edge functions. We analyze the complexity of learning topological orderings specific to our framework, and refer the reader to previous works for the analyses of particular estimators (e.g., (Efron et al., 2004)). Note that, independently from the choice of sparse operator, the space complexity of Daguerreotype is at least of the order of the edge masking matrix $\mathbf{R}$, hence $O(d^2)$. This is in line with most methods based on continuous optimization and can be improved by imposing additional constraints on the in-degree and out-degree of a node.

SparseMAP. Each sparseMAP's iteration involves a length-d argsort and a Cholesky update of a s-by-s matrix, where s is the size of the active set (number of selected permutations), bounded by the iteration number. Given a fixed number of iterations K (as in our implementation), this leads to a time complexity of $\mathcal{O}(sd \log d + s^2)$ and space complexity $\mathcal{O}(s^2 + sd)$ for sparseMAP, hence linear in d. Note that, because of Carathéodory's convex hull theorem (Reay, 1965) (which states that the solution of Problem (4) can be decomposed in at most $d+1$ permutations), the active set algorithm might converge earlier than K, leading to $s = \min(K, d+1)$ and $\mathcal{O}(d^2 \log d)$ worst-case complexity. Further, we warm-start the sorting algorithm with the last selected permutation. Both in theory and in practice, this is better than the $\mathcal{O}(d^3)$ complexity of maximization over the Birkhoff polytope.

Top-k sparsemax. Complexity for top-k sparsemax is dominated by the complexity of the top-k oracle. In our implementation, the top-k oracle has an overall time complexity $\mathcal{O}(K^2 d^2)$ and space complexity $\mathcal{O}(Kd^2)$ (as detailed in Appendix A) when searching for the best K permutations. When K is fixed, as in our implementation, this leads to an overall complexity of the top-k sparsemax operator $\mathcal{O}(d^2)$. In practice, K has to be of an order smaller than $\sqrt{d}$ for our framework to be more efficient than existing end-to-end approaches.

5 EXPERIMENTS

5.1 EXPERIMENTAL SETUP

Datasets Reisach et al. (2021) recently demonstrated that commonly studied synthetic benchmarks have a key flaw. Specifically, for linear additive synthetic DAGs, the marginal variance of each node increases the 'deeper' the node is in the DAG (i.e., all child nodes generally have marginal variance larger than their parents). They empirically show that a simple baseline that sorts nodes by increasing marginal variance and then applies sparse linear regression matches or outperforms state-of-the-art DAG learning methods. Given the triviality of simulated DAGs, here we evaluate all methods on two real-world tasks: *Sachs* (Sachs et al., 2005), a dataset of cytometric measurements of phosphorylated protein and phospholipid components in human immune system cells. The problem consists of $d = 11$ nodes, 853 observations and of the graph reconstructed by Sachs et al. (2005) as ground-truth DAG, which contains 17 edges; *SynTReN* (den Bulcke et al., 2006), a set of 10 pseudo-real transcriptional networks generated by the SynTRen simulator, each consisting of 500 simulated gene expression observations, and a DAG of $d = 20$ nodes and of e edges with $e \in \{20, \dots, 25\}$. We use the networks made publicly available by Lachapelle et al. (2020). In Appendix D we, however, compare different configurations of our method also on synthetic datasets, as they constitute an ideal test-bed for assessing the quality of the ordering learning step independently from the choice of structural equation estimator.

Baselines We benchmark our framework against state-of-the-art methods: *NoTears* (both its linear (Zheng et al., 2018) and nonlinear (Zheng et al., 2020) models), the first continuous optimization method, which optimizes the Frobenius reconstruction loss and where the DAG constraint is enforced via the Augmented Lagrangian approach; *Golem* (Ng et al., 2020), another continuous optimization method that optimizes the likelihood under Gaussian non-equal variance error assumptions regularized by *NoTears*'s DAG penalty; *CAM* (Bühlmann et al., 2014), a two-stage approach that estimates the variable order by maximum likelihood estimation based on an additive structural equation model with Gaussian noise; *NPVAR* (Gao et al., 2020), an iterative algorithm that learns topological generations and then prunes edges based on node residual variances (with the Generalized

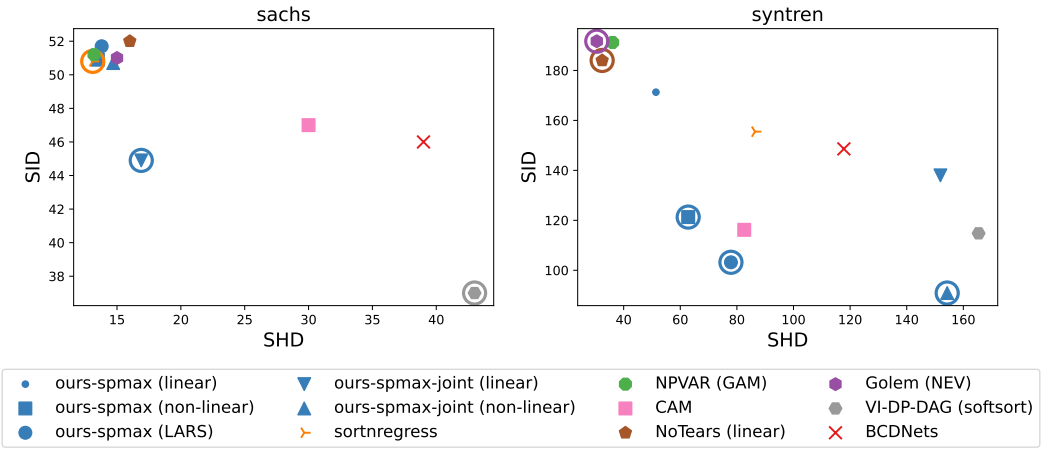

Figure 2: SHD vs SID on real datasets *Sachs* and *SynTReN*. Results are averaged over 10 seeds and the solutions lying on the Pareto front are circled.

Additive Models (Hastie & Tibshirani, 2017) regressor backend to estimate conditional variance); *sortnregress* (Reisach et al., 2021), a two-steps strategy that orders nodes by increasing variance and selects the parents of a node among all its predecessors using the Least Angle Regressor (Efron et al., 2004); *BCDNets* (Cundy et al., 2021) and *VI-DP-DAG* (Charpentier et al., 2022), the two end-to-end and probabilistic methods described in Section 3.4. Before evaluation, we post-process the graphs found by *NoTears* and *Golem* by first removing all edges with absolute weights smaller than 0.3 and then iteratively removing edges ordered by increasing weight until obtaining a DAG, as the learned graphs often contain cycles.

Metrics We compare the methods by two metrics, assessing the quality of the estimated graphs: the Structural Hamming Distance (*SHD*) between true and estimated graphs, which counts the number of edges that need to be added or removed or reversed to obtain the true DAG from the predicted one; and the Structural Intervention Distance (*SID*, Peters & Bühlmann, 2015), which counts the number of causal paths that are broken in the predicted DAG. It is standard in the literature to compute both metrics, given their complementarity: SHD evaluates the correctness of individual edges, while SID evaluates the preservation of causal orderings. We further remark here that these metrics privilege opposite trivial solutions. Because true DAGs are usually sparse (i.e., their number of edges is much smaller than the number of possible ones), SHD favors sparse solutions such as the empty graph. On the contrary, given a topological ordering, SID favors dense solutions (complete DAGs in the limit) as they are less likely to break causal paths. For this reason, we report both metrics and highlight the solutions on the Pareto front in Figure 2.

Hyper-parameters and training details We set the hyper-parameters of all methods to their default values, apart from the parameters of the Least Angle Regressor module of *sortnregress* and *Daguerreotype-LARS* that use the Bayesian Information Criterion for model selection. The default hyper-parameters of our method were tuned by Bayesian Optimization based on the performance, in terms of SHD and SID, averaged over several synthetic problems from different SEMs. More details are provided in Appendix D. For our method, we optimize the data likelihood (under Gaussian equal variance error assumptions, as derived in Ng et al. (eq. 2, 2020)) and we instantiate $f_j^{\phi_j}$ to a masked linear function (linear) or as a masked MLP with one hidden layer, 50 hidden units and sigmoid activation functions as for *NoTears-nonlinear*. Because our approach allows for modular solving of the functional parameters $\mathbf{\Phi}$, we also experiment with using Least Angle Regression (LARS) (Efron et al., 2004). We additionally apply l_2 regularizations on $\{\boldsymbol{\theta}, \mathbf{\Phi}\}$ to stabilize training, and we standardize all datasets to ensure that all variables have comparable scales.

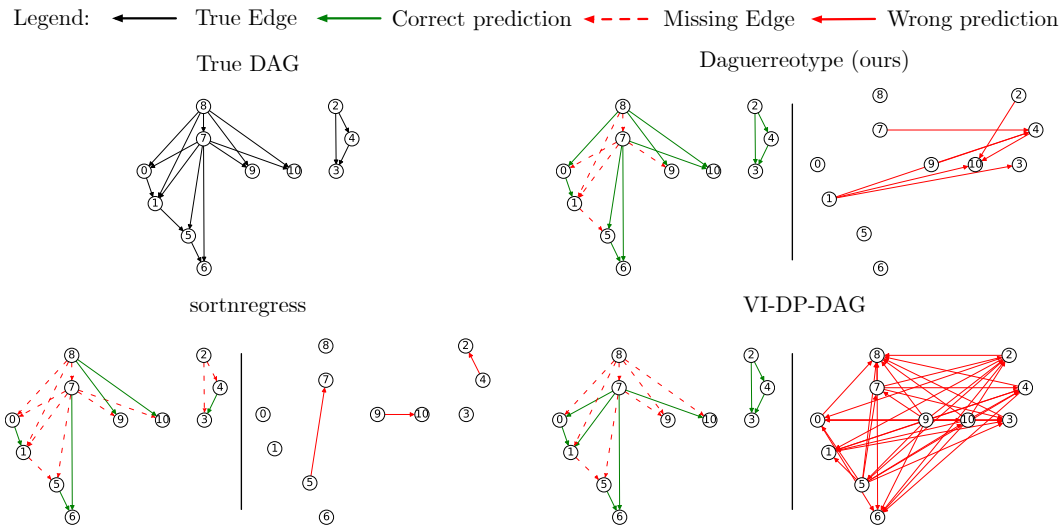

Figure 3: *Sachs*. True DAG and DAGs predicted by the best-performing methods. Daguerreotype strikes a good balance between SID and SHD; other methods focus overly on one over the other by either predicting too few (sortnregress) or too many edges (VI-DP-DAG).

5.2 Results

We report the main results in Figure 2, where we omit some baselines (e.g., Daguerreotype with sparseMAP) for sake of clarity. We present the complete comparison in Appendix D, together with additional metrics and studies on the sensitivity of Daguerreotype depending on the choice of key hyper-parameters. To provide a better idea of the learned graphs, we also plot in Figure 3 the graphs learned by the best-performing methods on *Sachs*. We observe that the solutions found by NPVAR and the matrix-exponential regularized methods (NoTears and Golem) are the best in terms of SHD, but have the worst SIDs. This can be explained by the high sparsity of their predicted graphs (see the number of edges in Tables 1 and 2). On the contrary, the high density of the solutions of VI-DP-DAG makes them among the best in terms of SID and the worst in terms of SHD. Daguerreotype provides solutions with a good trade-off between these two metrics and which lie on the Pareto front. Inevitably its performance strongly depends on the choice of edge estimator for the problem at hand. For instance, the linear estimator is better suited for *Sachs* than for *SynTReN*. In Appendix D, we assess our method's performance independently from the quality of the estimator with experiments on synthetic data where the underlying SEM is known, and the estimator can be chosen accordingly.

6 Conclusion, Limitations and Future Work

In this work, we presented *Daguerreotype* , a permutation-based method for end-to-end learning of directed acyclic graphs. While our approach shows promising results in identifying DAGs, the optimization procedure can still be improved. Alternative choices of estimators, such as Generalized Additive Models (Hastie & Tibshirani, 2017) as done in CAM and NPVAR, could be considered to improve identification. Another venue for improvement would be to include interventional datasets in training. It would be interesting to study in this context whether our framework is more sample-efficient, i.e., allows us to learn the DAG with fewer interventions or observations.

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A TOP-K ORACLE

In this section, we propose an efficient algorithm for finding the top-k scoring rankings of a vector and prove its correctness. We leverage this result in order to apply the sparsemax operator (Correia et al., 2020) to our DAG learning problem. We are not aware of existing works on this topic and believe this result is of independent interest.

A.1 NOTATION AND DEFINITIONS

Let us denote the objective function $g_{\boldsymbol{\theta}}(\sigma) = \langle \boldsymbol{\theta}, \boldsymbol{\rho}^{\sigma} \rangle$ evaluating the quality of a permutation σ, and denote one of its maximizers as $\sigma^{\star} \in \arg\max_{\sigma \in \Sigma_d} \; g_{\boldsymbol{\theta}}(\sigma)$, corresponding to the argsort of $\boldsymbol{\theta}$. Notice that we can equivalently write this objective as $g_{\boldsymbol{\theta}}(\sigma) = \langle \boldsymbol{\theta}^{\sigma}, \boldsymbol{\rho} \rangle$ by applying the permutation to $\boldsymbol{\theta}$.

Definition A.1 (Top-K permutations)**.** *We denote by $T_K(\boldsymbol{\theta}) \subset \Sigma_d$ the set of K highest-scoring permutations according to $g_{\boldsymbol{\theta}}$:*

$$T_1(\boldsymbol{\theta}) := \{\sigma^{\star}\}$$
$$T_K(\boldsymbol{\theta}) := T_{K-1}(\boldsymbol{\theta}) \cup \left\{ \sigma^K := \underset{\sigma \in \Sigma_d \setminus T_{K-1}(\boldsymbol{\theta})}{\arg\max} \; g_{\boldsymbol{\theta}}(\sigma) \right\}. \tag{13}$$

In this section, we will make use of the following definitions.

Definition A.2 (k-cycle)**.** *We note $(i_1 \; i_2 \; i_3 \; \dots \; i_k)$ a k-cycle of the components of a vector which sends in order element i_1 to element i_2, element i_2 to element i_3 and so on, and finally sends element i_k to element i_1.*

We will refer to the 2-cycle (ij) that transposes element i with element j as transposition or flip or swap, and to the 2-cycle $(ii+1)$ that transposes to consecutive elements as adjacent transposition or adjacent flip. We use $\circ$ to indicate composition of k-cycles (a.k.a. product). Propositions A.0.1 and A.0.2 give two well-known results that will be useful in what follows.

Proposition A.0.1 (k-cycles as sequences of adjacent transpositions)**.** *Applying a k-cycle is equivalent to applying a sequence of flips: $(i_1 \; i_2 \; i_3 \; \dots \; i_k)$ is equivalent to the sequence of flips of length k $(i_k \; i_{k-1}) \circ (i_k \; i_{k-2}) \circ \dots \circ (i_k \; i_1)$.*

Proposition A.0.2 (permutation transformation by adjacent transpositions)**.** *Any permutation $\sigma_1 \in \Sigma_d$ can be transformed into another permutation $\sigma_2 \in \Sigma_d$ by applying a sequence of adjacent transpositions.*

A.2 BEST-FIRST SEARCH ALGORITHM

Algorithm (1) finds the set of Kth-best scoring permutations given $\boldsymbol{\theta}$. It explores an arborescence of permutations $A = (\sigma^{\star}, \Sigma_d, E, g_{\boldsymbol{\theta}})$ (defined in Definition A.3)) and maintains a set of possible candidate permutations $P_k(\boldsymbol{\theta})$ that can be the kth-best permutation σ_k. By construction, $P_k(\boldsymbol{\theta})$ contains all (and only) the children of the top-$k-1$ permutations in the arborescence.

Definition A.3 (Arborescence)**.** *Given the vector $\boldsymbol{\theta} \in \mathbb{R}^d$, we define the arborescence $A = (\sigma^{\star}, \Sigma_d, E, g_{\boldsymbol{\theta}})$ with $\sigma^{\star}$ the root vertex, Σ_d the set of vertices, E the set of arcs and $g_{\boldsymbol{\theta}} : \Sigma_d \to \mathbb{R}$ scoring a vertex, constructed such that:*

Level 1 *the root is one (arbitrary) optimal permutation $\sigma^{\star} \in \arg\max_{\sigma \in \Sigma_d} \; g_{\boldsymbol{\theta}}(\sigma)$;*

Level H the children of a vertex σ are all the permutations that are obtained by applying a score-non-increasing adjacent transposition to σ.

We denote by child(σ) the children of a vertex (which are $d-1$ for the root, and at most $d-2$ for the others), and by parent(σ) the (unique) parent of a vertex.

Figure A.2 shows an example of this structure for the permutations of 4 nodes. Remark that, as defined, the arborescence covers all possible permutations $\sigma \in \Sigma_d$ because of Proposition A.0.2.

Theorem A.1 (Correctness of Algorithm (1))**.** *Given $\boldsymbol{\theta} \in \mathbb{R}^d$ and $K \in \mathbb{N}$, Algorithm (1) returns $T_K(\boldsymbol{\theta})$.*

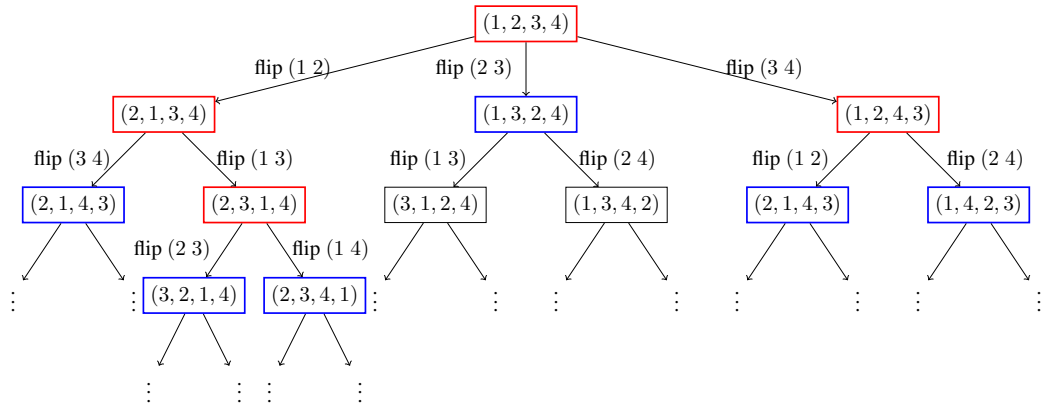

Figure 4: Example of permutation arborescence $A = ((1, 2, 3, 4), \Sigma_4, E, g_\theta)$ for a possible $\boldsymbol{\theta} \in \mathbb{R}^4$. We mark on an arc the flip that is applied to the parent to get to the child. Supposing that we are at iteration $k = 5$ of Algorithm 1, we plot the best permutations found so far ($T_4(\boldsymbol{\theta})$) within a red box, the candidate permutations ($P_5(\boldsymbol{\theta})$) to be the 5th-best one within a blue box, and the ones that are not considered yet within a black box. Remark that (i) permutations can appear multiple times in the structure (e.g., $(2, 1, 4, 3)$) but not on a single directed path and always at the same level in the structure.

Algorithm 1: Top-K permutations.

Data: $K \in \mathbb{N}^+$, $\boldsymbol{\theta} \in \mathbb{R}^d$, arborescence $A = (\sigma^\star, \Sigma_d, E, g_{\boldsymbol{\theta}})$
Result: top K permutations $T_K(\boldsymbol{\theta})$
$T_K(\boldsymbol{\theta}) \leftarrow \emptyset$;
$P_1(\boldsymbol{\theta}) \leftarrow \emptyset$; `/* initialize set of best candidates`
$k \leftarrow 1$;
while $k \leq K$ **do**
  if $k = 1$ **then**
    $\sigma_k \leftarrow \sigma^\star$;
  end
  else
    $\sigma_k \leftarrow \arg\max_{\sigma \in P_k(\boldsymbol{\theta})} g_{\boldsymbol{\theta}}(\sigma)$; `/* k-best permutation`
    $P_{k+1}(\boldsymbol{\theta}) \leftarrow P_k(\boldsymbol{\theta}) \setminus \{\sigma_k\}$; `/* remove k-best from candidates`
  end
  $P_{k+1}(\boldsymbol{\theta}) \leftarrow P_k(\boldsymbol{\theta}) \cup \text{child}(\sigma_k)$; `/* add children of k-best as possible candidates`
  $T_K(\boldsymbol{\theta}) \leftarrow T_K(\boldsymbol{\theta}) \cup \{\sigma_k\}$;
  $k \leftarrow k + 1$;
end

We prove this result by induction in the following sections. Firstly, we prove that the 2nd-best permutation is indeed obtained by applying an adjacent transposition to $\sigma^\star$ (base case). Secondly, we show that if $P_k(\boldsymbol{\theta})$ contains the kth-best solution, then $P_{k+1}(\boldsymbol{\theta})$ contains the $k+1$th-best one.

A.3 Minimal flip

In this section, we want to show that the flips that give the minimal objective reduction are the ones swapping consecutive elements (i.e., an adjacent transposition).

Let $S_2(\sigma)$ the set of permutations that differ from a permutation σ in exactly two elements. In other words, $S_2(\sigma)$ is the set of permutations obtained by swapping any two-elements of σ. Let us write the objective gap from the optimal solution $\forall \sigma^{(i\ j)} \in S_2(\sigma^\star)$, noting $(i\ j)$ the indices of the elements

that have been swapped in $\sigma^\star$:

$$g_{\boldsymbol{\theta}}(\sigma^\star) - g_{\boldsymbol{\theta}}(\sigma^{(i\ j)}) = \left\langle \boldsymbol{\theta}^{\sigma^\star} - \boldsymbol{\theta}^{\sigma^{(i\ j)}}, \boldsymbol{\rho} \right\rangle \tag{14}$$

$$= (\boldsymbol{\theta}_i^{\sigma^\star} - \boldsymbol{\theta}_i^{\sigma^{(i\ j)}})\boldsymbol{\rho}_i + (\boldsymbol{\theta}_j^{\sigma^\star} - \boldsymbol{\theta}_j^{\sigma^{(i\ j)}})\boldsymbol{\rho}_j \tag{15}$$

$$= (\boldsymbol{\theta}_i^{\sigma^\star} - \boldsymbol{\theta}_j^{\sigma^\star})\boldsymbol{\rho}_i + (\boldsymbol{\theta}_j^{\sigma^\star} - \boldsymbol{\theta}_i^{\sigma^\star})\boldsymbol{\rho}_j \tag{16}$$

$$= (\boldsymbol{\theta}_i^{\sigma^\star} - \boldsymbol{\theta}_j^{\sigma^\star})(\boldsymbol{\rho}_i - \boldsymbol{\rho}_j) \tag{17}$$

Notice that this gap is always non-negative, whether $i < j$ or $i > j$. Without loss of generality, in the following we consider that $i < j$, hence $\boldsymbol{\theta}_i^{\sigma^\star} \leq \boldsymbol{\theta}_j^{\sigma^\star}$ and $\boldsymbol{\rho}_i < \boldsymbol{\rho}_j$ by construction. The minimum of the gap is given by the permutation that minimizes both terms of the RHS of Eq. (17):

$$\min_{\sigma^{(i\ j)} \in S_2(\sigma^\star)} g_{\boldsymbol{\theta}}(\sigma^\star) - g_{\boldsymbol{\theta}}(\sigma^{(i\ j)}) = \min_{i<j} (\boldsymbol{\theta}_i^{\sigma^\star} - \boldsymbol{\theta}_j^{\sigma^\star})(\boldsymbol{\rho}_i - \boldsymbol{\rho}_j) \tag{18}$$

$$= \min_i \boldsymbol{\theta}_i^{\sigma^\star} - \boldsymbol{\theta}_{i+1}^{\sigma^\star}. \tag{19}$$

We will refer to $(i\ i{+}1)$ such that $i = \arg\min_i \boldsymbol{\theta}_i^{\sigma^\star} - \boldsymbol{\theta}_{i+1}^{\sigma^\star}$ as the minimal flip.

A.4 Non-increasing trajectory

We now want to prove that no other change to $\sigma^\star$ will result in a smaller reduction in the objective, i.e. in a permutation with a higher score than the one obtained by applying the minimal flip. For that, we can show that $\forall \sigma \in \Sigma_d$, there exists a sequence of flips from $\sigma^\star$ to σ such that each flip reduces (or does not change) the objective function. Algorithm (2) describes a method for finding one such non-increasing sequence from the source $\sigma^\star$ to a target σ' permutation. It consists in iteratively modifying the source as follows:

1. finding the ordered set D of components that differ in the two permutations;
2. naming the index of the first different element i (i.e. $\sigma_i^\star \neq \sigma_i'$);
3. in source, pulling up the element σ_i', by applying to D the cycle that starts with $\sigma_i^\star$ and ends with σ_i'.

We can then leverage Proposition (A.0.1) to convert the sequence of cycles into a sequence of element flips. The constructed trajectory is then non-decreasing as it never places an element at a lower index than its final, which would require applying a score-increasing operation to push it back to its final position.

Algorithm 2: Non-increasing sequence of k-cycles.

Data: target $\sigma' \in \Sigma_d$
Result: sequence of cycles C (non-increasing) trajectory
$\sigma \leftarrow \sigma^\star$; /* start from source
$C \leftarrow ()$; /* sequence of cycles
$D \leftarrow [i \in [1, \dots, d] \mid \sigma_i \neq \sigma_i']$; /* ordered set of different components
while $D \neq \emptyset$ **do**
  $i \leftarrow D[1]$;
  $e \leftarrow \sigma_i'$; /* first different element of target
  $j \leftarrow \sigma_e$; /* corresponding index in source
  $\sigma \leftarrow \sigma^{(D[1]\ D[2]\ \dots\ D[j])}$; /* apply j-cycle to first different elements
  $C \leftarrow C \circ (D[1]\ D[2]\ \dots\ D[j])$; /* add new cycle to trajectory
  $D \leftarrow [i \in [1, \dots, d] \mid \sigma_i \neq \sigma_i']$
end

As the objective reduction of each swap is greater or equal to the reduction given by the minimal flip, it follows that $\sigma^{(i\ i+1)} \in S_2(\sigma^\star)$ such that $i = \arg\min_{i'} \boldsymbol{\theta}_{i'}^{\sigma^\star} - \boldsymbol{\theta}_{i'+1}^{\sigma^\star}$ is the second highest scoring permutation. This indeed proves that $\sigma_2 \in P_1(\boldsymbol{\theta})$, as $P_1(\boldsymbol{\theta})$ is the set of permutations one adjacent transposition away from $\sigma^\star$, to which $\sigma^{(i\ i+1)}$ belongs.

A.5 Induction from $K-1$ to K

Now that we have shown the base case for the 2nd-best permutation, we can prove Theorem (A.1) by induction.

Suppose that Algorithm (1) correctly finds $T_{K-1}(\boldsymbol{\theta})$. We can show that the Kth-best permutation σ_K is then in the set of candidates $P_K(\boldsymbol{\theta})$. By contradiction, if $\sigma_K \notin P_K(\boldsymbol{\theta})$, it must be one of these two cases:

- $\sigma_K \in T_{K-1}(\boldsymbol{\theta})$, then σ_K cannot also be the Kth-best permutation;
- $\sigma_K \notin T_{K-1}(\boldsymbol{\theta})$, and as $g_{\boldsymbol{\theta}}(\text{parent}(\sigma_K)) \geq g_{\boldsymbol{\theta}}(\sigma_K)$ (by construction) and $\text{parent}(\sigma_K) \notin T_{K-1}(\boldsymbol{\theta})$ (otherwise σ_K would be in $P_K(\boldsymbol{\theta})$), then there exists at least one solution that is better than σ_K and that is not in $T_{K-1}(\boldsymbol{\theta})$, so σ_K cannot be the Kth-best permutation.

This concludes our proof.

A.6 Computational analysis

Finding $\sigma^\star$ requires sorting a vector of size d (hence $O(d \log d)$ complexity). Then, at each iteration k of Algorithm (1), the maximum of $P_k(\boldsymbol{\theta})$ needs to be found, which requires $O(dk)$ complexity as $|P_k(\boldsymbol{\theta})| \leq (d-2)k$, and $O(d)$ adjacent flip operations are applied to it.

The most expensive operation is checking that the selected best candidate is not already in $T_{k-1}(\boldsymbol{\theta})$. At worst, this requires going through the whole $P_k(\boldsymbol{\theta})$ and comparing them in order to all top-k solutions, so no more than $K \times |P_K(\boldsymbol{\theta})|$ comparisons of cost $O(d)$ each.

This leads to an overall time complexity of $O(K^2 d^2)$. The space complexity is dominated by the size of $P_k(\boldsymbol{\theta})$, which contains at most Kd vectors of size d, leading to $O(Kd^2)$.

B L0 Regularization

In the linear and non-linear variants of Daguerreotype , we implement the regularization term Ω_ξ of the inner problem of Eq. (12) with an approximate L0 regularizer. The exact L0 norm

$$||\mathbf{w}||_0 = \sum_{i=1}^{n} \mathbf{1}_{w_j \neq 0} \tag{20}$$

counts the number of non-zero entries of $\mathbf{w} \in \mathbb{R}^n$ and, when used as regularizer, it favors sparse solutions without injecting other priors. However, its combinatorial nature and its non-differentiability make its optimization intractable. Following Louizos et al. (2017), we reparameterize (20) by introducing a set of binary variables $\mathbf{z} \in \{0,1\}^n$ and letting $\mathbf{w} = \hat{\mathbf{w}} \circ \mathbf{z}$, sothat $||\mathbf{w}||_0 = \sum z_i$. Next, we let $\mathbf{z} \sim p(\mathbf{z}; \boldsymbol{\pi}) = \text{Bernoulli}(\boldsymbol{\pi})$ where $\boldsymbol{\pi} \in [0,1]^d$. For linear SEMs, we can now reformulate the Inner Problem (12) as follows:

$$\min_{\hat{\mathbf{w}}, \boldsymbol{\pi}} \sum_{j=1}^{d} \left(\mathbb{E}_{z_j \sim p(z_j|\pi_j)} \left[\ell \left(\mathbf{x}_j, f_j^{\hat{w}_j \circ z_j} \left(\mathbf{X}, (\mathbf{M}^\sigma)_j \right) \right) \right] + \xi \sum_{i=1}^{d} \pi_{ji} \right); \tag{21}$$

where now the decision (inner) variables are intended to be matrices and $\xi \geq 0$ is a hyperparameter. In the non-linear (MLP) case, we achieve sparsity at the graph level by group-regularizing the parameters corresponding to each input variable. In the experiments, we optimize (21) using the one-sample Monte Carlo straight-through estimator and set the final functional parameters as

$$\mathbf{w}_* = \hat{\mathbf{w}}_* \circ \text{MAP}\left[p(\,\cdot\,; \boldsymbol{\pi})\right] = \hat{\mathbf{w}}_* \circ H\left(\boldsymbol{\pi} - \frac{1}{2}\mathbf{1}\right); \tag{22}$$

where H is the Heaviside function. We leave the implementation of more sophisticated strategies, such as the relaxation with the hard-concrete distribution presented in (Louizos et al., 2017) or other estimators (e.g. Paulus et al., 2020; Niepert et al., 2021), to future work.

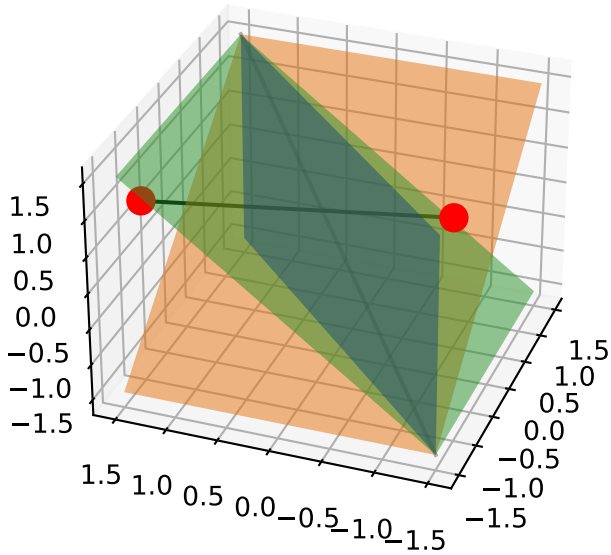

Figure 5: Representation of the degeneracy hyper-planes in $\mathbb{R}^3$ and of two-parameter points (in red) whose connecting segment intersects two hyper-planes.

C Characterization and sensitivity of the vector parametrization

In this section, we provide some intuition into the behavior of our score vector parameterization in the space of complete DAGs. More precisely, we look at the Maximum A Posteriori (MAP) complete DAG

$$M^{\sigma^*} \in \mathbb{D}_{\mathrm{C}}[d] \quad \text{where} \quad \sigma^* \in \arg\max \langle \boldsymbol{\theta}, \boldsymbol{\rho}_\sigma \rangle \tag{23}$$

and how it varies as a function of the score vector $\boldsymbol{\theta} \in \mathbb{R}^d$. The permutation σ^* is a MAP state (or mode) of both the sparseMAP and the sparsemax distributions (as well as the standard categorical/softmax distribution). For brevity, we shall rename $M^{\sigma^*} := M(\boldsymbol{\theta})$ in the following.

We choose to work on the space of complete DAGs because there is a one-to-one correspondence between topological orderings and complete DAGs. This is not generally true when analyzing the space of DAGs, as a permutation does not uniquely identify a DAG and vice versa.

C.1 Preliminary

For the results of this section, we will use the following relationship between transpositions (adjacent or not) and SHD.

Proposition C.0.1 (SHD difference after a flip)**.** *Consider $\boldsymbol{\theta} \in \mathbb{R}^d$ and $\boldsymbol{\theta}'$ which is obtained by applying a flip $(i\ j)$ with the convention that $i < j$. All the edges from nodes between i and j directed towards i or j need to be reversed. Thus, the SHD between complete DAGs $\mathrm{SHD}(M(\boldsymbol{\theta}), M(\boldsymbol{\theta}')) = 2(j-i)-1$. (because no new undirected edges are added, no undirected edges are removed, and $2(j-i)-1$ edges are reversed).*

From Proposition (C.0.1) we deduce that the SHD difference after applying an adjacent flip is $\mathrm{SHD}(M(\boldsymbol{\theta}), M(\boldsymbol{\theta}')) = 1$.

C.2 Analysis

Recall that σ^* sorts the elements of $\boldsymbol{\theta}$ in increasing order. Then, the points $\boldsymbol{\theta} \in \mathbb{R}^d$ where $\arg\max \langle \boldsymbol{\theta}, \boldsymbol{\rho}_\sigma \rangle$ is non-singleton (degeneracy) are exactly those that have at least one tie among their

entries (i.e., $\exists\, i, j$ such that $\boldsymbol{\theta}_i = \boldsymbol{\theta}_j$). Following this simple observation, we can populate $\mathbb{R}^d$ with $\binom{d}{2}$ hyper-planes (of dimensionality $d-1$), and call them $H_{i,j}$ with $i < j$, such that $\forall \boldsymbol{\theta} \in H_{i,j}, \boldsymbol{\theta}_i = \boldsymbol{\theta}_j$. Intersections of such hyper-planes are lower dimensional subspaces where more than 2 entries of $\boldsymbol{\theta}$ are equal. For $d = 3$, Figure 5 depicts the $\binom{3}{2} = 3$ hyper-planes in orange, green and blue, and their intersection (a line) in gray.

The hyper-planes $\{H_{i,j}\}_{i<j}$'s delimit exactly $d!$ open cones of the form $C = \{\boldsymbol{\theta} \in \mathbb{R}^d | \boldsymbol{\theta}_1^\sigma < \boldsymbol{\theta}_2^\sigma < \cdots < \boldsymbol{\theta}_d^\sigma, \sigma \in \Sigma_d\}$, i.e., each cone is the space of all points that give the same MAP permutation and do not contain any ties.

This partition of the space allows us to reason about the sensitivity of our MAP estimates to changes to the parameters. For instance, as the points of a cone do not have any ties, changes to the score vector do not affect SHD: $\forall \boldsymbol{\theta} \in C, \boldsymbol{\theta}' \in C\ \mathrm{SHD}(M(\boldsymbol{\theta}), M(\boldsymbol{\theta}')) = 0$.

We first analyze the sensitivity to single-entry changes, hence assessing how much an entry of $\boldsymbol{\theta}$ can be individually perturbed without changing its MAP. Proposition C.0.2 provides the entry-wise ranges in which the optimal solution set does not change.

Proposition C.0.2 (Entry-wise intervals)**.** *For any $\boldsymbol{\theta} \in \mathbb{R}^d$ and $\varepsilon_i \in \mathbb{R}$, $\arg\max \langle \boldsymbol{\theta}^\sigma, \boldsymbol{\rho} \rangle = \arg\max \langle \boldsymbol{\theta}^\sigma + \varepsilon_i \mathbf{e}_i, \boldsymbol{\rho} \rangle$ if and only if:*

- $\forall i \in [2, \ldots, d-1]$, $\varepsilon_i \in (\boldsymbol{\theta}_{i-1}^{\sigma^\star} - \boldsymbol{\theta}_i^{\sigma^\star}, \boldsymbol{\theta}_{i+1}^{\sigma^\star} - \boldsymbol{\theta}_i^{\sigma^\star})$;
- $i = 1$, $\varepsilon_i \in (-\infty, \boldsymbol{\theta}_{i+1}^{\sigma^\star} - \boldsymbol{\theta}_i^{\sigma^\star})$;
- $i = d$, $\varepsilon_i \in (\boldsymbol{\theta}_{i-1}^{\sigma^\star} - \boldsymbol{\theta}_i^{\sigma^\star}, \infty)$

where $\mathbf{e}_i$ denotes the i-th standard unit vector and $\sigma^\star \in \arg\max \langle \boldsymbol{\theta}, \boldsymbol{\rho}^\sigma \rangle$.

We can relate this result to changes in terms of SHD, by making the following observation: if we gradually increase one coordinate $\boldsymbol{\theta}_i$ initially ranked $\sigma_i^\star$, its rank changes in the optimal ordering as soon as it becomes greater than the coordinate right after it in the ordering, entailing an adjacent transposition between the two coordinates[3]. Greater perturbations entail a longer sequence of adjacent transpositions. By Proposition C.0.1, this implies an increase in SHD of 1 for each transposition. Visually, the SHD increases by 1 every time the perturbed vector crosses a hyper-plane along its perturbation direction, as this corresponds to swapping two components that are adjacent when optimally sorted.

For comparison, we can apply the same reasoning to the matrix parametrization of the linear assignment problem, deployed by Cundy et al. (2021) for learning permutation matrices. In this context, we can leverage the edge sensitivity analysis reviewed in Michael et al. (2020, Equations 6-7). As a general remark, it is not as intuitive to determine the entry-wise intervals for this problem, not only because we have d^2 variables instead of d but especially because it requires solving a different assignment problem per entry. Furthermore, the minimal perturbation that changes the MAP does not necessarily result in flipping two adjacent nodes, entailing an SHD relative to the optimal permutation of at least 1. Consider, for example, the following 3×3 matrix parameter:

$$\boldsymbol{\Theta} = \begin{pmatrix} 16 & 16 & 15 \\ 5 & 16 & 10 \\ 16 & 9 & 10 \end{pmatrix}$$

Its optimal permutation matrix corresponds to the rank $(3, 1, 2)$ with a score of 29. The minimal perturbations on $\boldsymbol{\Theta}_{1,3}$ or $\boldsymbol{\Theta}_{3,2}$ that change the MAP result in the solution $(2, 1, 3)$ which has an SHD of 3 w.r.t. the optimal (and the second best score of 31). For problems of scale larger than this example, the resulting SHD can take values up to $2d - 3$ for non-adjacent transpositions.

We now generalize and formalize this relationship between perturbations and SHD changes for general vector perturbations (global sensitivity). Theorem (C.1) upper bounds the SHD between complete DAGs of any pair of score vectors by the number of hyper-planes crossed by the segment connecting them.

[3] A similar reasoning also applies when decreasing the value of one coordinate instead.

Theorem C.1 (Global sensitivity)**.** *For any $\boldsymbol{\theta} \in \mathbb{R}^d$ and $\boldsymbol{\theta}' \in \mathbb{R}^d$*

$$\mathrm{SHD}(M(\boldsymbol{\theta}), M(\boldsymbol{\theta}')) \leq \int_{t\in[0,1]} \sum_i \sum_{j>i} \delta_{H_{i,j}}(\boldsymbol{\theta} + t(\boldsymbol{\theta}' - \boldsymbol{\theta}))\, \mathrm{d}t \tag{24}$$

where $\delta_A(x)$ is the (generalized) Dirac delta that evaluates to infinity if $x \in A$ and 0 otherwise.

Proof. Let us first consider the case where $\boldsymbol{\theta} \in C$ and $\boldsymbol{\theta}' \in C'$, i.e., the two vectors do not contain ties. Let us denote σ (respectively σ') the permutation that sorts the components of a point of C (C') by increasing order. The minimal-length sequence of adjacent flips that need to be applied to σ to obtain σ' has a length equal to the number of times the segment connecting their parameters crosses a hyper-plane. Then the SHD between their complete DAGs equals the minimal number of adjacent flips, which proves the result. When either $\boldsymbol{\theta}$ or $\boldsymbol{\theta}'$ lies on a hyper-plane, the minimal required number of adjacent flips might be smaller, hence the upper bound in Theorem C.1. □

In Figure 5, the segment connecting the two red dots intersects the green and blue hyperplanes and hence the resulting complete DAGs will have an SHD of at most 2 (in fact, exactly 2 in this case).

This intuitive characterization links the SHD distance in the complete DAG space to a partition of $\mathbb{R}^d$ resulting from the "sorting" operator (i.e. the MAP, or maximizer of the linear program) of the score vector $\boldsymbol{\theta}$. This implies that, during optimization, if $\boldsymbol{\theta}_k$ are in the interior of any cone (which happens almost surely) then it is very likely that updating the parameters results in small changes to the SHD unless the parameters have all similar values. In contrast, updates to the matrix parameter of the linear assignment problem are more likely to return

A deeper analysis of the vector parameterization is the object of future work, as we hope it can fuel further improvements in the optimization algorithm, such as better initialization strategies or reparameterization. For instance, optimizing in $\mathbb{S}_r^{d-1}$ (over polar coordinates) would expose the role of the radius r as similar to the temperature parameter for the distributions we consider (the smaller the radius, the higher the "temperature"). Typically, the temperature is left constant during training or annealed, suggesting this might be advantageous also in our scenario. We leave the exploration of this strategy to future work.

D Additional experiments

We provide a detailed description of the experimental setup and report additional results. The method is implemented in (PyTorch, Paszke et al., 2019), and the code used for carrying out the experiments is included in the supplementary material. All experiments were run on a machine with 16 cores and $32Gb$ of RAM.

Daguerreotype 's optimization and evaluation For our method, we optimize the data likelihood (under Gaussian equal variance error assumptions, as derived in Ng et al. (Equation 2, 2020)) We optimize the bilevel Problem (12) when not specified otherwise. We report results for the following three variants of Daguerreotype , where the black-box estimator of the graph is instantiated

(linear) with L0 regularization, $f_j^{\boldsymbol{\phi}_j}(\mathbf{X}, \mathbf{A}_j) = \mathbf{X}\,(\boldsymbol{\phi}_j \circ \mathbf{A}_j)$ and $w_j \in \mathbb{R}^d$;

(non-linear) with L0 regularization, $f_j^{\boldsymbol{\phi}_j}(\mathbf{X}, \mathbf{A}_j) = h_j\left(g_j^{\boldsymbol{\phi}_j}(\mathbf{X}, \mathbf{A}_j)\right)$, with h_j a locally connected MLP with one hidden layer, 50 hidden units and sigmoid activation function, $g_j^{\boldsymbol{\phi}_j}$ a linear layer with $d \times 50$ hidden units (50 per parent i) and masking out all non-parents of j (according to $\mathbf{A}_j$), and $\boldsymbol{\phi}_{ji} = \|g_{ji}^{\boldsymbol{\phi}_j}\|_2$ as for *NoTears* (non-linear);

(LARS) with Least Angle Regression (LARS) (Efron et al., 2004), $f_j^{\boldsymbol{\phi}_j}(\mathbf{X}, \mathbf{A}_j) = \mathbf{X}\,(\boldsymbol{\phi}_j \circ \mathbf{A}_j)$ and $\boldsymbol{\phi}_j \in \mathbb{R}^d$.

We additionally apply a l_2 regularization on $\{\boldsymbol{\theta}, \boldsymbol{\phi}\}$ to stabilize training, and we standardize all datasets to ensure that all variables have comparable scales.

With any variant, the outer problem is optimized for $5,000$ maximum iterations by gradient descent and early-stopped when approximate convergence is reached. When using the (linear) and (non-linear) back-ends, the graph of each permutation is optimized also by gradient descent, for $1,000$ epochs and also with an early-stopping mechanism based on approximate convergence. After training, the graph for the mode permutation is further fine-tuned, and the final evaluation is carried out with this model.

We also experiment with the approximated, but faster, joint optimization of $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ in Problem (2) instead of the bilevel formulation, when we add the suffix *joint* to the method name. In this case, as we need a differentiable graph estimator for jointly updating the ordering and the graph, we instantiate the method only with the (linear) and (non-linear) back-ends. These models are optimized by gradient descent for $5,000$ epochs and with an early-stopping mechanism based on approximate convergence.

The default hyper-parameters of our methods were chosen as follows. We set the sparse operators' temperature $\tau = 1$ and $K = 100$, the strength of the l_2 regularizations to 0.0005, and tuned the learning rates for the outer and inner optimization $\in [10^{-4}, 10^{-1}]$ and pruning strength $\lambda \in [10^{-6}, 10^{-1}]$. The tuning was carried out by Bayesian Optimization using (Optuna, Akiba et al., 2019) for 50 trials on synthetic problems, consisting of data generated from different types of random graphs (Scale-Free, Erdős–Rényi, BiPartite) and of noise models (e.g., Gaussian, Gumbel, Uniform) with 20 nodes and 20 or 40 expected edges. For each setting, three datasets are generated by drawing a DAG, its edge weights uniformly in $[-2, -0.5] \cup [0.5, 2]$, and $1,000$ data points. A set of hyper-parameters is then evaluated by averaging its performance on all the generated datasets, and the tuning is carried out to minimize SHD and SID jointly. The default value of a hyper-parameter was then set to be the average value among those lying on the Pareto front and rounded up to have a single significant digit.

Baseline optimization and evaluation All baseline methods are optimized using the codes released by their authors, apart from *CAM* that is included in the Kalainathan & Goudet (Causal Discovery Toolbox, 2019). Before evaluation, we post-process the graphs found by *NoTears* and *Golem* by first removing all edges with absolute weights smaller than 0.3 and then iteratively removing edges ordered by increasing weight until obtaining a DAG, as the learned graphs often contain cycles. For the probabilistic baselines (*VI-DP-DAG* and *BCDNets*), we make use of the mode model (in particular, the mode permutation matrix) for evaluation.

We set the hyper-parameters of all methods to their default values, released together with the source code, apart from the parameters of the Least Angle Regressor module of *sortnregress* that uses the Bayesian Information Criterion for model selection.

Additional results on real-world tasks In Figures 6, 7, and Tables 1 and 2 we extend the evaluation on real-world tasks provided in the main text. More precisely, we report the results also for Daguerreotype with sparseMAP, and provide additional metrics for comparison: the *F1* score using the existence of an edge as the positive class and the number of predicted edges to assess the density of the solutions.

Sparsemax vs sparseMAP comparison In Figure 8, we report an analysis of the effect of Daguerreotype 's hyper-parameter K on the quality of the learned DAG. Recall that this parameter corresponds to the maximal number of selected permutations for **sparsemax** and to the maximal number of iterations of the active set algorithm for **sparseMAP**, and that is the principal parameter that controls the computational cost of the ordering learning step in our framework. This analysis is carried out on data generated by a linear SEM from a scale-free graph with equal variance Gaussian noise. We choose this simple setting for two reasons: the true DAG can be identified from (enough) observational data only (Proposition 7.5, Peters et al., 2017); provided with the true topological ordering, the LARS estimator can identify the true edges. In this setting, we can then assess the quality of sparsemax and sparseMAP independently from the quality of the estimator. For reference, in Figure 8 we also report the performance of optimizing LARS with a random ordering or with a true one.

We observe that sparsemax and sparseMAP provide MAP orderings that are significantly better than random ones for $K > 2$. For K big enough, these orderings give DAGs that are almost as good as when knowing the variable ordering. The gap from DAG-true's performance can be explained by the non-convexity of the search space and Daguerreotype getting stuck in local minima. We further observe that sparsemax generally provides better solutions than sparseMAP's at a comparable

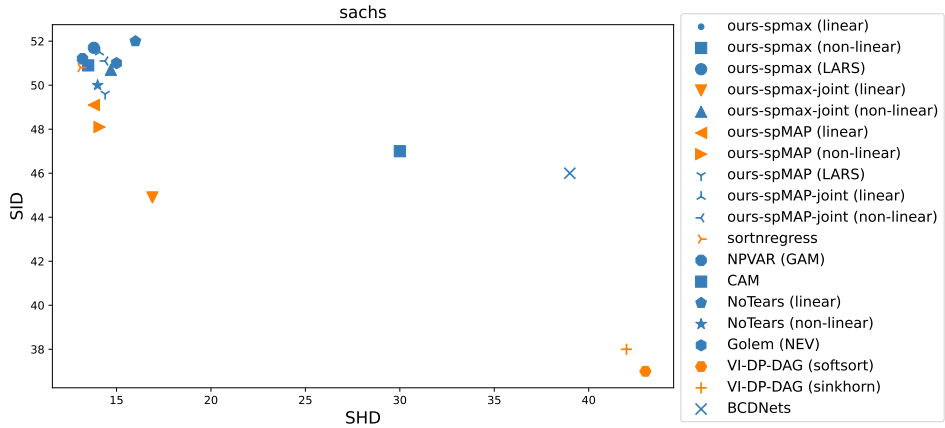

Figure 6: SHD vs SID on *Sachs*. The solutions lying on the Pareto front are colored in orange and the others in blue.

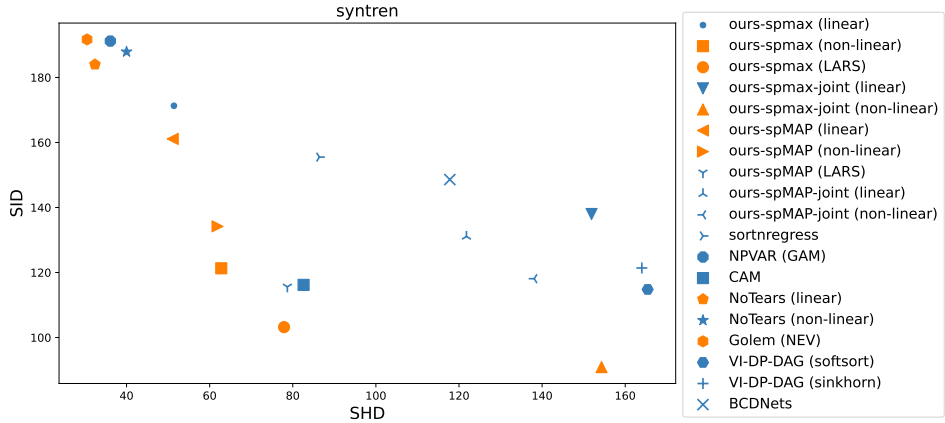

Figure 7: SHD vs SID on *SynTReN*. The solutions lying on the Pareto front are colored in orange and the others in blue.

training time. The only settings where this is not the case are for $d = 30$ and $K > 35$. Notice that sparseMAP's performance peaks at $K = 35$ and degrades for higher K in this setting. This phenomenon can be due to the inclusion of unnecessary orderings to sparseMAP's set, which ends up hurting training.

We further study in Figures 9 and 10 the effect of the pruning strength, (controlled by λ) on the performance of both operators on the real datasets. For this experiment, we instantiate Daguerreotype with the linear estimator and train it by joint optimization. As a general remark, when strongly penalizing dense graphs (higher λ) SHD generally improves and SID degrades. On Sachs, the two operators do not provide significantly different results, while on SynTReN we find that sparsemax provides better SHD for comparable SID.

Table 1: *Sachs*. We report Structural Hamming Distance (SHD, the lower the better), Structural Interventional Distance (SID, the lower the better), (F1, the higher the better), and the number of predicted edges for all methods.

Method	SHD ↓	SID ↓	F1 ↑	# edges
NoTears (linear)	16.0	52.0	0.095	4
NoTears (non-linear)	14.0	50.0	0.320	8
Golem (NEV)	15.0	51.0	0.190	4
VI-DP-DAG (softsort)	43.0	37.0	0.265	51
VI-DP-DAG (sinkhorn)	42.0	38.0	0.269	50
BCDNets	39.0	46.0	0.196	34
sortnregress	13.1	50.8	0.377	9.0
CAM	30.0	47.0	0.28	33.0
NPVAR (GAM)	13.2	51.2	0.344	9.6
Daguerreotype -spmax (linear)	13.8	51.6	0.323	7.7
Daguerreotype -spMAP (linear)	13.8	49.1	0.309	7.6
Daguerreotype -spmax (LARS)	13.8	51.7	0.316	9.5
Daguerreotype -spMAP (LARS)	14.4	49.6	0.275	9.2
Daguerreotype -spmax (non-linear)	13.5	50.9	0.348	7.1
Daguerreotype -spMAP (non-linear)	14.1	48.1	0.32	7.4
Daguerreotype -spmax-joint (linear)	16.9	44.9	0.36	16.1
Daguerreotype -spMAP-joint (linear)	14.1	51.5	0.244	6.8
Daguerreotype -spmax-joint (non-linear)	14.7	50.7	0.265	8.6
Daguerreotype -spMAP-joint (non-linear)	14.4	51.1	0.236	5.0

Table 2: *SynTReN*. We report Structural Hamming Distance (SHD, the lower the better), Structural Interventional Distance (SID, the lower the better), Topological Ordering Pearson Correlation (TOPC, the higher the better), (F1, the higher the better) number of predicted edges all averaged over the 10 networks.

Method	SHD ↓	SID ↓	F1 ↑	# edges
NoTears (linear)	32.4	184.0	0.157	17.7
NoTears (non-linear)	40.0	187.9	0.165	28.1
Golem (NEV)	30.5	191.7	0.152	15.4
VI-DP-DAG (softsort)	165.4	114.8	0.109	175.7
VI-DP-DAG (sinkhorn)	164.0	121.4	0.104	173.6
BCDNets	117.8	148.6	0.113	119.0
sortnregress	86.4	156.0	0.151	89.8
CAM	82.6	116.0	0.192	86.6
NPVAR (GAM)	36.1	191.0	0.184	26.0
Daguerreotype -spmax (linear)	51.4	171.0	0.182	44.5
Daguerreotype -spMAP (linear)	51.1	161.0	0.211	47.2
Daguerreotype -spmax (LARS)	77.9	103.0	0.238	86.0
Daguerreotype -spMAP (LARS)	78.7	116.0	0.212	83.8
Daguerreotype -spmax (non-linear)	62.8	121.0	0.245	65.1
Daguerreotype -spMAP (non-linear)	61.9	134.0	0.255	65.5
Daguerreotype -spmax-joint (linear)	152.0	138.0	0.104	161.0
Daguerreotype -spMAP-joint (linear)	122.0	131.0	0.139	131.0
Daguerreotype -spmax-joint (non-linear)	154.0	90.9	0.149	169.0
Daguerreotype -spMAP-joint (non-linear)	138.0	118.0	0.143	150.0

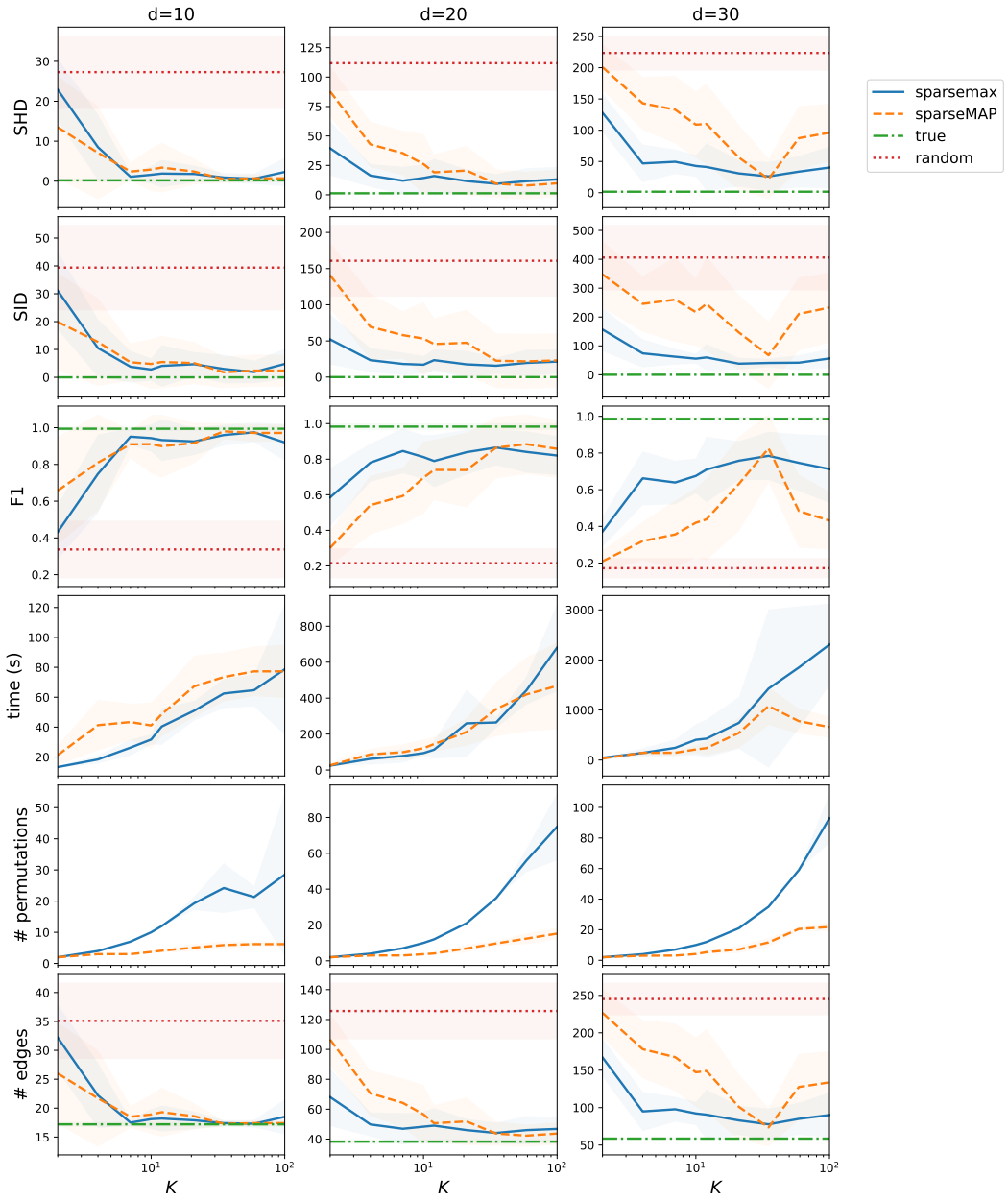

Figure 8: Comparison of different strategies for learning topological orderings, on data ($1,000$ samples) generated from a linear SEM with Scale-Free graph and Gaussian noise, and a varying number of nodes d. In order from top to bottom, we plot SHD, SID, F1, training time in seconds, number of permutations, and number of predicted edges (all at the end of training) as a function of the sparse operators' parameter K, which corresponds to the maximal number of sampled permutations for **sparsemax** and to the maximal number of iterations of the active set algorithm for **sparseMAP**. We also include two simple variants of Daguerreotype , where the ordering is fixed to one true ordering (**true**) or to a random one (**random**). Results are averaged over 10 seeds.

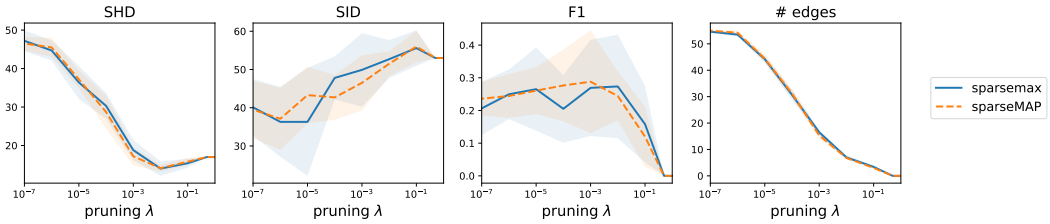

Figure 9: *Sachs*. Effect of L0 pruning intensity (controlled by λ) on SHD, SID, F1 and number of learned edges for Daguerreotype jointly optimizing a linear estimator and the topological ordering distribution either with sparsemax (**sparsemax**) or sparseMAP (**sparseMAP**).

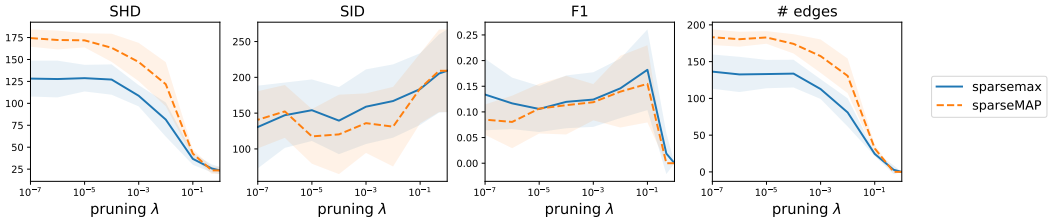

Figure 10: *SynTReN*. Effect of L0 pruning intensity (controlled by λ) on SHD, SID, F1 and number of learned edges for Daguerreotype jointly optimizing a linear estimator and the topological ordering distribution either with sparsemax (**sparsemax**) or sparseMAP (**sparseMAP**).