GOLEM

- **Motivation：** NOTEARS需要$c \to \infty$时才能保证无环性，需要多次迭代，容易出现数值问题和病态问题。**可证明(a)线性高斯等方差情况下，硬约束不满足时，最小二乘最优解返回有环图；(b)GOLEM-EV最优解对应真实图结构。**

Proposition 1. *Suppose X follows a linear Gaussian model defined by Eq. (4). Then, asymptotically,*

(a) B_0 is the unique global minimizer of least squares objective under a hard DAG constraint, but without the DAG constraint, the least squares objective returns a cyclic graph.

(b) B_0 is the unique global minimizer of likelihood-EV objective (2) under soft ℓ_1 or DAG constraint.

True SEM：

- **B_0是真实图结构**
- ground truth DAG $G : X_1 \to X_2$
- $$B_0 = \begin{bmatrix} 0 & b_0 \\ 0 & 0 \end{bmatrix}, \Omega = \begin{bmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{bmatrix}, b_0 \neq 0.$$

无环性硬约束导致优化困难，硬约束不满足时，最优解返回有环图

[Ng I, Ghassami A E, Zhang K. On the role of sparsity and dag constraints for learning linear dags[J]. Advances in Neural Information Processing Systems, 2020, 33: 17943-17954.]

GOLEM

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- GOLEM证明基于**最大似然的目标函数代替最小二乘**时，只需**软稀疏性和软DAG 约束**即可在**特定假设下**渐近学习与真实DAG“等价”的 DAG。
  - GOLEM-NV：线性高斯不等方差

$$\mathcal{L}_1(B;\mathbf{x}) = \frac{1}{2}\sum_{i=1}^{d}\log\left(\sum_{k=1}^{n}\left(x_i^{(k)} - B_i^{\mathsf{T}}x^{(k)}\right)^2\right) - \log|\det(I-B)|$$

注：B为DAG $\rightarrow \boldsymbol{log|det(I-B)| = 0}$

  - GOLEM-EV：线性高斯等方差

$$\mathcal{L}_2(B;\mathbf{x}) = \frac{d}{2}\log\left(\sum_{i=1}^{d}\sum_{k=1}^{n}\left(x_i^{(k)} - B_i^{\mathsf{T}}x^{(k)}\right)^2\right) - \log|\det(I-B)|$$

软稀疏性和软DAG约束，克服ALM缺陷

- 无约束优化问题：

$$\min_{B\in\mathbb{R}^{d\times d}} \quad \mathcal{S}_i(B;\mathbf{x}) = \mathcal{L}_i(B;\mathbf{x}) + \boxed{\lambda_1\|B\|_1 + \lambda_2 h(B)}$$

$$h(B) = \operatorname{tr}\left(e^{B\circ B}\right) - d$$

GOLEM将最大似然+软DAG约束结合，取代最小二乘+硬DAG约束，优化更易求解，效果更好