GraN-DAG

□ 考虑ANM数据生成机制：满足因果可识别

$$X_j := f_j(X_{\pi_j^{\mathcal{G}}}) + N_j$$

□ 考虑用NN拟合非线性函数关系：

$$X_j := f_j(X) + N_j$$

- **第j个NN参数：**

$$\phi_{(j)} \triangleq \left\{W_{(j)}^{(1)}, \ldots, W_{(j)}^{(L+1)}\right\} \text{ where } W_{(j)}^{(\ell)} \text{ is the } \ell \text{ th weight matrix of the } j \text{ th NN}$$

- **第j个NN输出（m维）：**

$$\theta_{(j)} \triangleq W_{(j)}^{(L+1)} g(\ldots g(W_{(j)}^{(2)} g(W_{(j)}^{(1)} X_{-j})) \ldots) \quad \forall j$$

□ 构造与NN深度相关的加权邻接矩阵A_ϕ：

- **第j个NN连接矩阵：** $C_{(j)} \triangleq \left|W^{(L+1)}\right| \ldots \left|W^{(2)}\right|\left|W^{(1)}\right| \in \mathbb{R}_{\geq 0}^{m \times d}$

NN输入d维
NN输出m维

- **通过$C_{(j)}$近似刻画X_i对$\theta_{(j)}$的影响：** $\sum_{k=1}^{m} (C_{(j)})_{ki} = 0$ ⟹ **$\theta_{(j)}$独立于X_i**

[Lachapelle S, Brouillard P, Deleu T, et al. Gradient-based neural dag learning[C]//In International Conference on Learning Representations (ICLR), 2020.]

GraN-DAG

□ 构造与NN深度相关的加权邻接矩阵A_ϕ：

$$(A_\phi)_{ij} \triangleq \begin{cases} \sum_{k=1}^{m} \left(C_{(j)}\right)_{ki}, & \text{if } j \neq i \\ 0, & \text{otherwise} \end{cases}$$

NN输入d维

NN输出m维

□ 优化问题：最大对数似然

A_ϕ中元素均为正

$$\max_\phi \mathbb{E}_{X\sim P_X} \sum_{j=1}^{d} \log p_j\left(X_j | X_{\pi_j^\phi}; \phi_{(j)}\right) \quad \text{s.t. } h(\phi) \triangleq \operatorname{Tr} e^{A_\phi} - d = 0$$

转为无约束优化问题，优化算法ALM

$$\max_\phi \mathcal{L}(\phi, \lambda_t, \mu_t) \triangleq \mathbb{E}_{X\sim P_X} \sum_{j=1}^{d} \log p_j\left(X_j | X_{\pi_j^\phi}; \phi_{(j)}\right) - \lambda_t h(\phi) - \frac{\mu_t}{2} h(\phi)^2$$

□ 理论保证（在样本量趋于无穷的情况下）：

当数据生成机制服从非线性高斯加性噪声模型时（噪声服从高斯分布），能证明GraN-DAG最优解对应的图结构是真实图结构。

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