NOTEARS-MLP+SOB

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□ 通过MLP或正交级数拟合非线性关系：

$$W(f) = W(f_1, \ldots, f_d) \in \mathbb{R}^{d\times d} \qquad f_j : \mathbb{R}^d \to \mathbb{R} \qquad f_j \in H^1(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$$

$H^1(\mathbb{R}^d)$定义：f_j和其偏导数均为平方可积函数

- **通过偏导数定义非线性因果效应：** $[W(f)]_{kj} := \|\partial_k f_j\|_{L^2}.$

$$f_j \text{ is independent of } X_k \text{ if and only if } \|\partial_k f_j\|_{L^2} = 0.$$

- **考虑MLP对f进行拟合：**

$$\text{MLP}(u; A^{(1)}, \ldots, A^{(h)}) = \sigma(A^{(h)}\sigma(\cdots A^{(2)}\sigma(A^{(1)}u))),$$

$$A^{(\ell)} \in \mathbb{R}^{m_\ell \times m_{\ell-1}}, \quad m_0 = d.$$ **输入u为d维**

Proposition 1. *Consider the function class $\mathcal{F}$ of all MLPs that are independent of u_k and the function class $\mathcal{F}_0$ of all MLPs such that the kth column of $A^{(1)}$ consists of all zeros. Then $\mathcal{F} = \mathcal{F}_0$.*

$$A^{(1)}_{bk} = 0 \text{ for each } b.$$

命题表明：MLP输出独立于输入的第k维u_k的充要条件为MLP的第1层权重矩阵$A^{(1)}$的第k列均为0。

[Zheng X, Dan C, Aragam B, et al. Learning sparse nonparametric dags[C]//International Conference on Artificial Intelligence and Statistics. PMLR, 2020: 3414-3425.]

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- **每个变量用1个MLP拟合，共拟合d个MLP：**

Let $\theta_j = (A_j^{(1)}, \ldots, A_j^{(h)})$ denote the parameters for the jth MLP and $\theta = (\theta_1, \ldots, \theta_d)$.

- **提出独立于MLP深度的加权邻接矩阵表示：**

$$[W(\theta)]_{kj} = \| kth - column(A_j^{(1)}) \|_2$$

- **NOTEARS-MLP目标函数：**

$$\min_{\theta} \quad \frac{1}{n} \sum_{j=1}^{d} \ell(\mathbf{x}_j, \mathrm{MLP}(\mathbf{X}; \theta_j)) + \lambda \|A_j^{(1)}\|_{1,1}$$

$$\text{subject to} \quad h(W(\theta)) = 0. \qquad \mathbf{X} = [\mathbf{x}_1 | \cdots | \mathbf{x}_d] \in \mathbb{R}^{n \times d}$$

求加权邻接矩阵W方式：在MLP训练完后，取出每个MLP第1层参数矩阵，计算得W，然后取阈值0.3得到邻接矩阵

训练d个MLP，只通过MLP的第1层参数表征无环性约束

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