Title

Abstract:

Keywords:

### 1 Formulation

Consider a random variable  $\mathbb{X} \in \mathbb{R}^p$  that has a sparse dependency structure among its features. This graph structure is potentially non-linear, and we want to infer the structure from a data matrix  $\mathbf{X} \in \mathbb{M}(n, p)$ .

We assume a multi-layer generative model for the structure:

$$\mathbf{X} = \varphi(\mathbf{H}_1)\mathbf{B}_1 + \mathbf{E}_x; \quad \mathbb{E} \sim \mathcal{N}_p(\mathbf{0}, \Sigma_x),$$

$$\mathbf{H}_1 = \varphi(\mathbf{H}_2)\mathbf{B}_2 + \mathbf{F}_1; \quad \mathbb{F}_1 \sim \mathcal{N}_{p_1}(\mathbf{0}, \Sigma_1),$$

$$\cdots$$

$$\mathbf{H}_{L-1} = \varphi(\mathbf{H}_L)\mathbf{B}_L + \mathbf{F}_{L-1}; \quad \mathbb{F}_{L-1} \sim \mathcal{N}_{p_{L-1}}(\mathbf{0}, \Sigma_{L-1}),$$

$$\mathbb{H}_L \sim \mathcal{N}_{p_L}(\mathbf{0}, \Sigma_L).$$

with L hidden layers, and  $\varphi(\cdot)$  being a pointwise known transformation (e.g. ReLU, sigmoid, tanh). When  $\Sigma_x$  and  $\Sigma_l$ ,  $l \in \mathcal{I}_L$  are diagonal, it is the Non-linear Gaussian Belief Network of Frey and Hinton (1999). In our case, we keep  $\Sigma_x$  non-diagonal (but sparse), while others diagonal.

The negative log-likelihood function is

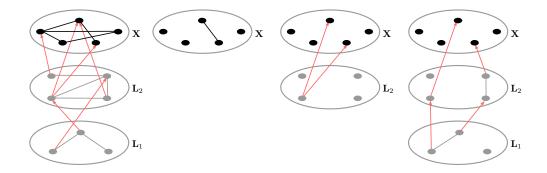
$$-\ell(\mathbf{X}|\mathcal{H}, \mathcal{B}, \Omega) = \frac{n}{2} \left[ \operatorname{Tr} \left( \mathbf{S}_x \Omega_x \right) - \log \det \Omega_x + \sum_{l=1}^{L} \left\{ \operatorname{Tr} \left( \mathbf{S}_l \Omega_l \right) - \log \det \Omega_l \right\} \right]$$

where  $\mathbf{S}_x = \mathbf{E}_x^T \mathbf{E}_x / n$ ,  $\mathbf{S}_l = \mathbf{F}_l^T \mathbf{F}_l / n$  for l = 1, ..., L-1 and  $\mathbf{S}_L = \mathbf{H}_L^T \mathbf{H}_L / n$ . Inferring the distribution of the hidden variables is difficult so we assume pointwise variational approximations:

$$h_{ij,l} \sim N(\mu_{ijl}, s_{ijl}); \quad i \in \mathcal{I}_n, j \in \mathcal{I}_{p_l}, l \in \mathcal{I}_L.$$

Collect the variational parameters in  $\mathcal{M} := \{\mathbf{M}_1, \dots, \mathbf{M}_L\}, \mathcal{S} := \{\mathbf{S}_1, \dots, \mathbf{S}_L\}$ . Now we have the variational lower-bound

$$\ell(\mathbf{X}|\mathcal{H}, \mathcal{B}, \Omega) \ge \mathbb{E}_q \ell(\mathbf{X}, \mathcal{H}|\mathcal{B}, \Omega, \mathcal{M}, \mathcal{S}) - \mathbb{E}_q \log q(\mathcal{H}|\mathbf{X}, \mathcal{B}, \Omega, \mathcal{M}, \mathcal{S})$$
(1.1)



Denote this lower bound by  $\ell_q(\mathbf{X}|\mathcal{B}, \Omega, \mathcal{M}, \mathcal{S})$ . Under the simplified model  $\Sigma_l = \sigma_l \mathbf{I}$  for  $l \in \mathcal{I}_L$ , the second term becomes (Frey and Hinton, 1999)

$$\mathbb{E}_{q} \log q(\mathcal{H}|\mathbf{X}, \mathcal{B}, \Omega, \mathcal{M}, \mathcal{S}) = \frac{1}{2} \left[ \sum_{i=1}^{n} \sum_{j=1}^{p_{l}} \sum_{l=1}^{L} \log \frac{s_{ijl}}{\sigma_{jl}} - \frac{s_{ijl}}{\sigma_{jl}} + n \log \det \Omega_{x} + \text{constant} \right].$$
(1.2)

For the first term we have

$$\mathbb{E}_{q}\ell(\mathbf{X}, \mathcal{H}|\mathcal{B}, \Omega, \mathcal{M}, \mathcal{S}) = \frac{n}{2}\mathbb{E}_{q}\left[\operatorname{Tr}(\mathbf{S}_{x}\Omega_{x}) + \sum_{l=1}^{L}\operatorname{Tr}(\mathbf{S}_{l}\Omega_{l})\right]$$
=

which simplifies to (Frey and Hinton, 1999)

$$-\left[\mathbb{E}_{q}\operatorname{Tr}(\mathbf{E}_{x}^{T}\mathbf{E}_{x}\Omega_{x})+\sum_{i=1}^{n}\sum_{j=1}^{p_{l}}\sum_{l=1}^{L-1}\frac{1}{\sigma_{jl}}\left\{(\mu_{ijl}-b_{ij,l+1}m_{ij,l+1})^{2}+b_{ij,l+1}^{2}v_{ij,l+1}\right\}+\operatorname{const}\right]$$
(1.3)

where  $m_{ijl} = \mathbb{E}_q \varphi(h_{ijl}), v_{ijl} = \mathbb{E}_q (\varphi(h_{ijl}) - m_{ijl})^2$ .

#### 1.1 Objective function

Our goal is to solve a penalized version of the variational lower bound in (1.1):

$$-\frac{2}{n}\ell_q(\mathbf{X}|\mathcal{B}, \Omega, \mathcal{M}, \mathcal{S}) + \sum_{l=1}^{L} \lambda_{nl} \|\mathbf{B}_l\|_1 + \gamma_n \|\Omega_x\|_{1,\text{off}}$$

We take the greedy strategy of solving two-layer problems successively. This means molte-carlo sequential EM: first solve for the variational parameters  $(\mathbf{M}_1, \mathbf{S}_1) = ((\mu_{ij,1}, s_{ij,1}))$ , in the E step, then solve for  $(\mathbf{B}_1, \Omega_x)$  in the M step, and continue until convergence. After convergence is reached, go to the next layer. Similar to Bengio et al. (2007); Hinton and Salakhutdinov (2006).

The objective function for a two-layer model, with the top layer being the observed data  $\mathcal{X}$ , is:

$$\operatorname{Tr}\left[\frac{1}{n}(\mathbf{X} - \varphi(\mathbf{H})\mathbf{B})^{T}(\mathbf{X} - \varphi(\mathbf{H})\mathbf{B})\Omega_{x}\right] + \log \det \Omega_{x} + \lambda_{n} \|\mathbf{B}\|_{1} + \gamma_{n} \|\Omega_{x}\|_{1,\text{off}}.$$

When  $\varphi$  is identity, this becomes a sparse factor model (refs). However for non-linear  $\varphi$  optimizing this becomes difficult. To tackle this, we use a variational approximation of the objective function. We assume the following hierarchical generative model for the hidden variables and associated variational parameters:

$$h_{ij} \sim N(\mu_{ij}, \sigma_{ij}^2),$$

$$\mu_{ij} \sim \sum_{k=1}^{K} I_{mk} N(\mu_{mk}, \sigma_{mk}^2); \quad I_{mk} = \text{Ber}(\pi_{mk})$$

$$\log \sigma_{ij} \sim \sum_{k=1}^{K} I_{sk} N(\mu_{sk}, \sigma_{sk}^2); \quad I_{sk} = \text{Ber}(\pi_{sk}).$$
(1.4)

Thus in total there are 6K generative parameters. Following the framework of hierarchical variational models (refs), we replace the negative loglikelihood  $-l(\mathbf{x};\theta)$  by a hierarchical evidence lower bound (HELBO)  $-\bar{l}(\mathbf{x};\theta)$ , defined as:

$$\bar{l}(\mathbf{x}; \boldsymbol{\eta}) = \mathbb{E}_2 l(\mathbf{x}, \mathbf{h}_{\varphi}; \boldsymbol{\eta}) + \mathbb{E}_1 KL(q(\mathbf{m}, \mathbf{s}|\mathbf{x}) || p(\mathbf{m}, \mathbf{s})) + KL(q(\boldsymbol{\vartheta}|\mathbf{z}) || p(\boldsymbol{\vartheta})),$$

with  $\mathbb{E}_1$  and  $\mathbb{E}_2$  denoting expectations over the distributions of  $(\mathbf{m}, \mathbf{s})$  only and both the latent data and variational parameter distributions, respectively. Our desired set of parameter estimates (variational as well as generative) are defined as the minimizer of a penalized version of this HELBO:

$$\hat{\boldsymbol{\eta}} = \underset{\boldsymbol{\eta}}{\operatorname{arg\,min}} \left[ \frac{1}{n} \sum_{i=1}^{n} \bar{l}(\mathbf{x}_{i}; \boldsymbol{\eta}) + \lambda_{n} \|\mathbf{B}\|_{1} + \gamma_{n} \|\Omega_{x}\|_{1, \text{off}} \right]. \tag{1.5}$$

#### 1.2 Computational algorithm

Our objective function in (1.5) is not convex in general. However, with the variational specifications in (1.4) it is bi-convex with respect to the variational and generative components of our parameter vector.

**Proposition 1.1.** The objective function in (1.5) is bi-convex with respect to the variational parameters  $\vartheta$  and generative parameters  $\theta$ .

**E-step:** we solve for the variational parameters by minimizing the following (take  $\mathbf{H}_{\varphi} \equiv \varphi(\mathbf{H})$ )

$$\mathcal{F}(\mathbf{M}, \mathbf{S}) = \mathbb{E}_{q} \operatorname{Tr} \left[ \frac{1}{n} (\mathbf{X} - \mathbf{H}_{\varphi} \mathbf{B})^{T} (\mathbf{X} - \mathbf{H}_{\varphi} \mathbf{B}) \Omega_{x} \right]$$

$$= \operatorname{Tr} \left[ \left\{ \frac{1}{n} (\mathbf{X} - \mathbf{M}_{\varphi} \mathbf{B})^{T} (\mathbf{X} - \mathbf{M}_{\varphi} \mathbf{B}) + \mathbf{B}^{T} \mathbf{V}_{\varphi} \mathbf{B} \right\} \Omega_{x} \right]$$

$$= \left[ \sum_{j=1}^{p} \sum_{j'=1}^{p} \omega_{jj'} \left\{ \frac{1}{n} (\mathbf{X}_{j} - \mathbf{M}_{\varphi} \mathbf{B}_{j})^{T} (\mathbf{X}_{j'} - \mathbf{M}_{\varphi} \mathbf{B}_{j'}) + \mathbf{B}_{j}^{T} \mathbf{V}_{\varphi} \mathbf{B}_{j'} \right\} \right]$$

$$= \sum_{j,j'=1}^{p} \omega_{jj'} \left\{ -\frac{2}{n} \mathbf{X}_{j}^{T} \mathbf{M}_{\varphi} \mathbf{B}_{j'} + \mathbf{B}_{j}^{T} \left( \frac{1}{n} \mathbf{M}_{\varphi}^{T} \mathbf{M}_{\varphi} + \mathbf{V}_{\varphi} \right) \mathbf{B}_{j'} \right\} + c$$

where  $(\mathbf{M}_{\varphi})_{ik} = \mathbb{E}_q \varphi(h_{ik})$  for  $i \in \mathcal{I}_n, k \in \mathcal{I}_q$ , and  $\mathbf{V}_{\varphi} = \mathbb{E}_q[(\mathbf{H}_{\varphi} - \mathbf{M}_{\varphi})^T (\mathbf{H}_{\varphi} - \mathbf{M}_{\varphi})/n]$ . Differentiating with respect to entries of  $\mathbf{M}$  we now have

$$\frac{\partial \mathcal{F}}{\partial \mu_{ik}} = \sum_{j,j'=1}^{p} \omega_{jj'} \left[ -\frac{2}{n} x_{ij} \frac{dm_{ik}}{d\mu_{ik}} b_{j'k} + \frac{1}{n} \left\{ 2b_{jk} \left( 2m_{ik} + \sum_{i' \neq i} m_{i'k} \right) \frac{dm_{ik}}{d\mu_{ik}} b_{j'k} \right\} + \mathbf{tbd} \right]$$

Using chain rule, we get the derivatives with respect to the component vectors:

$$\frac{\partial \mathcal{F}}{\partial \mu} = \mathbf{b}^T \frac{\partial \mathcal{F}}{\partial (\mu \mathbf{b})}; \quad \frac{\partial \mathcal{F}}{\partial \sigma} = \mathbf{t} \mathbf{b} \mathbf{d}; \quad \frac{\partial \mathcal{F}}{\partial b_k} = \mathbf{a}^T \frac{\partial \mathcal{F}}{\partial (b_k \mathbf{a})}.$$

**M-step:** First generate data  $\mathbf{H}_{\varphi}$  using the variational parameters  $(\mathbf{M}, \mathbf{S})$ . Then obtain  $\mathbf{B}, \Omega_x$  by solving a penalized LS problem:

$$\{\hat{\mathbf{B}}, \hat{\Omega}_x\} = \underset{\mathbf{B}, \Omega_x}{\operatorname{arg \, min}} \operatorname{Tr}(\mathbf{S}_x^{\varphi} \Omega_x) + \log \det \Omega_x + \|\mathbf{B}\|_1 + \|\Omega_x\|_{\operatorname{off}, 1}.$$

# 2 Theoretical properties

#### 2.1 Concentration bounds for a two-layer model

Define equivalence classes,  $\boldsymbol{\theta} = \text{vec}(\mathbf{B}, \Omega_{x,\text{off}})$ ,  $\boldsymbol{\vartheta}$  denoting the variational parameters,  $\boldsymbol{\eta} = (\boldsymbol{\theta}, \boldsymbol{\vartheta})$ . Then we are minimizing

$$\mathbb{E}_{q}\left[l(\mathbf{x};\mathbf{z},\boldsymbol{\eta}) + \mathrm{KL}(q(\mathbf{z}|\boldsymbol{\vartheta}_{1})||p(\mathbf{z})) + \mathrm{KL}(r(\boldsymbol{\vartheta}_{1}|\mathbf{z};\boldsymbol{\vartheta})||q(\boldsymbol{\vartheta}_{1};\boldsymbol{\vartheta}))\right] + P(\boldsymbol{\theta}).$$

define the negative hierarchical ELBO by  $\bar{l}(\cdot)$ . We consider a  $\ell_1$ -penalty

$$P(\boldsymbol{\theta}) = \rho_1 \|\boldsymbol{\beta}\|_1 + \rho_2 \|\boldsymbol{\omega}\|_1 = \lambda P_{\alpha}(\boldsymbol{\theta})$$

by reparameterizing the penalties:  $\lambda = \rho_1 + \rho_2, \alpha = \rho_1/\lambda$ .

Conditions 1, 2, 3 same as those in SPINN paper.

Define 
$$V_n(\eta) = \mathbb{E}\bar{l}(\mathbf{x}; \eta) - \bar{l}(\mathbf{X}; \eta)$$
,  $\mathcal{E}(\eta|\eta_0)$ ,  $\bar{\mathcal{E}}(\eta|\eta_0)$  as in Städler et al. (2010).

**Theorem 2.1.** Define the event

$$\mathcal{T} = \left\{ \mathcal{X} : \sup_{\boldsymbol{\eta}} \frac{|V_n(\boldsymbol{\eta}_0^{\boldsymbol{\eta}}) - V_n(\boldsymbol{\eta})|}{\lambda_0 \vee (P_\alpha(\boldsymbol{\theta} - \boldsymbol{\theta}_0^{\boldsymbol{\eta}}) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0^{\boldsymbol{\eta}}\|_2)} \leq T\lambda_0 \right\}$$

for  $T \ge 1, \lambda_0 > 0$ . Then for the solution  $\hat{\eta}$  defined in **tbd** that is calculated using a fixed sample  $\mathcal{X} \in \mathcal{T}$ , we have

$$\mathcal{E}(\hat{\boldsymbol{\eta}}) + \frac{\lambda - 2T\lambda_0}{2} \|\hat{\boldsymbol{\theta}}_{S^c}\|_1 \le \left[ (\lambda + 2T\lambda_0)(\alpha\sqrt{s_\beta} + (1 - \alpha)\sqrt{s_\omega})c_0 \right]^2$$

for some constant  $c_0 > 0$ .

**Condition 4.** The gradient of  $\bar{l}(\cdot)$  with respect to the model parameters is bounded above:

$$\|\nabla_{\boldsymbol{\eta}}\bar{l}(\mathbf{x};\boldsymbol{\eta})\|_{\infty} \leq G(\mathbf{x})$$

for some function  $G: \mathbb{R}^p \to \mathbb{R}^+$ . Further, there exists c' > 0 such that

$$|\bar{l}(\mathbf{x}; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}, \boldsymbol{\eta}')| \mathbb{I}(G(\mathbf{x}) \leq M)) \leq c'$$

for any  $M \geq 0$  and  $\eta, \eta'$ .

**Theorem 2.2.** For the choice of  $\lambda_0$ :

$$\lambda_0 = (20 + c_1)^{1/2} \frac{\log n}{\sqrt{n}} \left[ \frac{\sqrt{2c_2K}}{m_\alpha} + \log\left(\frac{n\sqrt{c_2K}\log n}{m_\alpha}\right) \sqrt{\log(2d)} \right],\tag{2.1}$$

and any  $T \geq 1$ , the event  $\mathcal{T}$  happens with probability  $\geq$ 

$$1 - c_3 \log n \exp \left[ -\frac{nT^2 \lambda_0^2}{c_4^2 K \log n} \right] - \frac{c_5 \sqrt{K}}{n^{3/2} \log n}, \tag{2.2}$$

for some constants  $c_1, c_2, c_3, c_4, c_5 > 0$ , and sample size condition  $n \log n \ge m_{\alpha}(c_2 K)^{-1/2}$ .

Using theorems 2.1 and 2.2 a concentration bound on both the excess risk and weights of irrelevant nodes is now immediate.

Corollary 2.3. Suppose conditions 1-4 are satisfied, and we have sample size n so that  $n \log n \ge m_{\alpha}(c_2K)^{-1/2}$ . Then for random  $\mathcal{X}$  and  $\lambda_n \ge 2\lambda_0$ , with  $\lambda_0$  defined as (2.1), we have

$$\mathcal{E}(\hat{\boldsymbol{\eta}}) + \frac{\lambda_n - 2\lambda_0}{2} \|\hat{\boldsymbol{\theta}}_{S^c}\|_1 \le c_0^2 m_\alpha^2 (\lambda_n + 2\lambda_0)^2 s$$

with probability larger than or equal to

$$1 - c_3 \log n \exp \left[ -\frac{n\lambda_0^2}{c_4^2 K \log n} \right] - \frac{c_5 \sqrt{K}}{n^{3/2} \log n}.$$

#### 2.2 Multi-layer sparse latent model

## 3 Proofs of main results

Proof of Proposition 1.1. Since our penalties are convex, we only need to prove the biconvexity of the HELBO. For this we first simplify its squared error part. For  $j, j' \in \mathcal{I}_p$ , consider  $\mathbf{X}_j$  to be the  $j^{\text{th}}$  column of  $\mathbf{X}$ ,  $\mathbf{b}_j$  to be the  $j^{\text{th}}$  row of  $\mathbf{B}$ , and  $\omega_{jj'}$  to be the  $(j,j')^{\text{th}}$  element of  $\Omega_x$ .

$$\frac{1}{n}\operatorname{Tr}[(\mathbf{X} - \mathbf{H}_{\varphi}\mathbf{B})(\mathbf{X} - \mathbf{H}_{\varphi}\mathbf{B})^{T}\Omega_{x}] = \frac{1}{n}\sum_{j,j'=1}^{p}\omega_{jj'}(\mathbf{X}_{j} - \mathbf{H}_{\varphi}\mathbf{b}_{j})^{T}(\mathbf{X}_{j'} - \mathbf{H}_{\varphi}\mathbf{b}_{j'})$$
(3.1)

Now substitute  $\mathbf{H}_{\varphi} = \mathbf{M} + \mathbf{S} \odot \mathbf{E}_h$ , where the elements of  $\mathbf{E}_h$  are independently drawn from N(0,1), and  $\odot$  denotes element-wise multiplication. Simplifying, we have

$$(\mathbf{X}_{j} - \mathbf{H}_{\varphi}\mathbf{b}_{j})^{T}(\mathbf{X}_{j'} - \mathbf{H}_{\varphi}\mathbf{b}_{j'}) = \mathbf{X}_{j}^{T}\mathbf{X}_{j'} - 2\mathbf{X}_{j}^{T}(\mathbf{M} + \mathbf{S} \odot \mathbf{E}_{h})\mathbf{b}_{j'} + \mathbf{b}_{j}^{T}(\mathbf{S} \odot \mathbf{E}_{h})\mathbf{b}_{j'} + 2\mathbf{b}_{j}^{T}\mathbf{M}^{T}(\mathbf{S} \odot \mathbf{E}_{h})\mathbf{b}_{j'} + \mathbf{b}_{j}^{T}(\mathbf{S} \odot \mathbf{E}_{h})^{T}(\mathbf{S} \odot \mathbf{E}_{h})\mathbf{b}_{j'}$$

Taking expectation over the first-level variational distribution,

$$\mathbb{E}_{1}[(\mathbf{X}_{j} - \mathbf{H}_{\varphi}\mathbf{b}_{j})^{T}(\mathbf{X}_{j'} - \mathbf{H}_{\varphi}\mathbf{b}_{j'})] = \mathbf{X}_{j}^{T}\mathbf{X}_{j'} - 2\mathbf{X}_{j}^{T}\mathbf{M}\mathbf{b}_{j'} + \mathbf{b}_{j}^{T}\mathbf{M}^{T}\mathbf{M}\mathbf{b}_{j'} + \sum_{i=1}^{n} \mathbf{b}_{j}^{T}\mathbf{S}_{i}^{T}\mathbf{S}_{i}\mathbf{b}_{j'}$$

Now substitute

$$\mathbf{M} = \sum_{k=1}^{K} I_{mk} (\mu_{mk} \mathbf{J}_{n \times q} + \sigma_{mk} \mathbf{J}_{n \times q} \odot \mathbf{E}_{mk}),$$

$$\mathbf{S} = \exp \left[ \sum_{k=1}^{K} I_{sk} (\mu_{sk} \mathbf{J}_{n \times q} + \sigma_{sk} \mathbf{J}_{n \times q} \odot \mathbf{E}_{sk}) \right],$$

and take expectation over the second-level variational distributions.

$$\mathbb{E}_{2}[(\mathbf{X}_{j} - \mathbf{H}_{\varphi}\mathbf{b}_{j})^{T}(\mathbf{X}_{j'} - \mathbf{H}_{\varphi}\mathbf{b}_{j'})] = \mathbf{X}_{j}^{T}\mathbf{X}_{j'} - 2\sum_{k} \pi_{mk}\mu_{mk}\mathbf{X}_{j}^{T}\mathbf{J}_{n\times q}\mathbf{b}_{j'}$$

$$+ n\mathbf{b}_{j}^{T}\mathbf{b}_{j'}\sum_{k} \pi_{mk}(\mu_{mk}^{2} + \sigma_{mk}^{2})$$

$$+ n\mathbf{b}_{j}^{T}\mathbf{b}_{j'}\sum_{k} \pi_{sk} \exp[2(\mu_{sk} + \sigma_{sk}^{2})]. \tag{3.2}$$

For the last term we use the fact that if  $x \sim N(\mu, \sigma^2)$  then  $\mathbb{E}e^{tx} = e^{t\mu + t^2\sigma^2/2}$ .

The right hand side of (3.2) is quadratic in **B**, and the quadratic terms all have positive coefficients. Thus, in conjunction with (3.1) we can easily conclude that the negative log-likelihood is convex in (**B**,  $\Omega_x$ ) for fixed  $\vartheta$ . Other terms in the HELBO do not depend either **B** or  $\Omega_x$ , the same holds for it as well.

Proof of Theorem 2.1. Just prove an equivalent lemma of Städler et al. (2010). Details **tbd**.

Other details similar to Thm 1 of Städler et al. (2010).

By definition we now have that

$$\bar{l}(\mathbf{X}; \hat{\boldsymbol{\eta}}) + \lambda P_{\alpha}(\hat{\boldsymbol{\theta}}) \leq \bar{l}(\mathbf{X}; \boldsymbol{\eta}_0) + \lambda P_{\alpha}(\boldsymbol{\theta}_0)$$

for any  $\eta_0 \in \mathcal{Q}_0$ . Adding  $\mathcal{E}(\hat{\boldsymbol{\eta}}) = \mathbb{E}\bar{l}(\mathbf{x}; \hat{\boldsymbol{\eta}}) - \mathbb{E}\bar{l}(\mathbf{x}; \boldsymbol{\eta}_0)$  on both sides, we get

$$\mathcal{E}(\hat{\boldsymbol{\eta}}) + \lambda P_{\alpha}(\hat{\boldsymbol{\theta}}) \leq |V_{n}(\boldsymbol{\eta}_{0}) - V_{n}(\hat{\boldsymbol{\eta}})| + \lambda P_{\alpha}(\boldsymbol{\theta}_{0})$$

$$\leq T\lambda_{0} \left( \lambda_{0} \vee (P_{\alpha}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}_{0}) + ||\hat{\boldsymbol{\vartheta}} - \boldsymbol{\vartheta}_{0}||_{2}) \right) + \lambda P_{\alpha}(\boldsymbol{\theta}_{0})$$
(3.3)

on the set  $\mathcal{T}$ . There are three cases now.

Case I. Suppose  $\lambda_0 \geq P_{\alpha}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}_0) + \|\hat{\boldsymbol{\vartheta}} - \boldsymbol{\vartheta}_0\|_2$ . Then rearranging the terms in (3.3) we have

$$\mathcal{E}(\hat{\boldsymbol{\eta}}) + \lambda P_{\alpha}(\hat{\boldsymbol{\theta}}_{S^c}) \leq T\lambda_0^2 + \lambda P_{\alpha}(\hat{\boldsymbol{\theta}}_S - \boldsymbol{\theta}_{0,S}) \leq T\lambda_0^2 + \lambda\lambda_0$$

since  $\lambda_0 \geq P_{\alpha}(\hat{\boldsymbol{\theta}}_S - \boldsymbol{\theta}_{0,S})$ .

Case II. Suppose  $\lambda_0 < P_{\alpha}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}_0) + \|\hat{\boldsymbol{\vartheta}} - \boldsymbol{\vartheta}_0\|_2$ . Then after some rearrangement we get

$$\begin{split} \mathcal{E}(\hat{\boldsymbol{\eta}}) + (\lambda - T\lambda_0) P_{\alpha}(\hat{\boldsymbol{\theta}}_{S^c}) &\leq T\lambda_0 \|\hat{\boldsymbol{\vartheta}} - \boldsymbol{\vartheta}_0\|_2 + T\lambda_0 P_{\alpha}(\hat{\boldsymbol{\theta}}_S - \boldsymbol{\theta}_{0,S}) + \lambda (P_{\alpha}(\boldsymbol{\theta}_{0,S}) - P_{\alpha}(\hat{\boldsymbol{\theta}}_S)) \\ &\leq T\lambda_0 \|\hat{\boldsymbol{\vartheta}} - \boldsymbol{\vartheta}_0\|_2 + (\lambda + T\lambda_0) P_{\alpha}(\hat{\boldsymbol{\theta}}_S - \boldsymbol{\theta}_{0,S}) \end{split}$$

Proof of Theorem 2.2. We follow an approach similar to Städler et al. (2010) and Feng and Simon (2017) to obtain probability bounds for truncated versions and tails of the quantity  $|V_n(\boldsymbol{\eta}_0^{\boldsymbol{\eta}}) - V_n(\boldsymbol{\eta})|$  after proper scaling.

Part I: Bounding truncated parts. Define the following:

$$\bar{V}_n(\boldsymbol{\eta}) := \mathbb{E}[\bar{l}(\mathbf{x}; \boldsymbol{\eta})\mathbb{I}(G(\mathbf{x}) \leq M_n)] - \frac{1}{n} \sum_{i=1}^n \bar{l}(\mathbf{x}_i; \boldsymbol{\eta})\mathbb{I}(G(\mathbf{x}_i) \leq M_n)$$

so that

$$|\bar{V}_n(\boldsymbol{\eta}) - \bar{V}_n(\boldsymbol{\eta}_0)| \leq \mathbb{E}[|\bar{l}(\mathbf{x};\boldsymbol{\eta}) - \bar{l}(\mathbf{x};\boldsymbol{\eta}_0)|\mathbb{I}(G(\mathbf{x}) \leq M_n)] + \frac{1}{n} \sum_{i=1}^n |\bar{l}(\mathbf{x}_i;\boldsymbol{\eta}) - \bar{l}(\mathbf{x}_i;\boldsymbol{\eta}_0)|\mathbb{I}(G(\mathbf{x}_i) \leq M_n)$$
(3.4)

To get an upper bound on the right hand side of (3.4), we start by bounding the entropy of the functional class  $\mathcal{E}_r$ , r > 0:

$$\Theta_r := \{ \boldsymbol{\eta} = (\boldsymbol{\theta}, \boldsymbol{\vartheta}) : P_{\alpha}(\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_2 \le r \}$$
$$\mathcal{E}_r := \{ \bar{l}(\mathbf{x}; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}; \boldsymbol{\eta}_0) \mathbb{I}(G(\mathbf{x}) \le M_n) : \boldsymbol{\eta} \in \Theta_r \}$$

with respect to the empirical norm  $||h||_{P_n} = \sqrt{\sum_{i=1}^n h^2(\mathbf{x}_i)/n}$ .

**Lemma 3.1.** For a collection of functions  $\mathcal{H}$  taking values in  $\mathcal{X}$ , denote its metric entropy by  $H(\cdot, \mathcal{H}, \|.\|_{P_n})$ . Then for any  $u, r, M_n > 0$  and some  $c_0 > 0$  the following holds:

$$H(u, \mathcal{E}_r, ||.||_{P_n}) \le \frac{(5+c_0)r^2M_n^2}{u^2}\log\left(1+\frac{du^2}{r^2M_n^2}\right)$$

Leveraging the bound in Lemma 3.1, we now prove that a symmetrized version of the truncated empirical process is small with high probability.

**Lemma 3.2.** Assume fixed **X**, and Rademacher random variables  $W_i$ ,  $i \in \mathcal{I}_n$  (defined as  $P(W_i = 1) = P(W_i = -1) = 1/2$ ). Also define

$$\delta = (5 + c_0)^{1/2} \frac{M_n}{\sqrt{n}} \left[ \frac{\sqrt{2c_1 K}}{m_\alpha} + \log\left(\frac{n\sqrt{c_1 K} M_n}{m_\alpha}\right) \sqrt{\log(2d)} \right]$$
(3.5)

for constants  $c_0, c_1 > 0$ , and  $m_{\alpha} := \alpha \vee (1 - \alpha)$ . Then for any  $r > 0, T \geq 1$  we have

$$P\left(\sup_{\boldsymbol{\eta}\in\Theta_r}\left|\frac{1}{n}\sum_{i=1}^n W_i(\bar{l}(\mathbf{x}_i;\boldsymbol{\eta}) - \bar{l}(\mathbf{x}_i;\boldsymbol{\eta}_0))\mathbb{I}(G(\mathbf{x}) \leq M_n)\right| \geq Tr\delta\right)$$

$$\leq C\exp\left[-\frac{nT^2\delta^2 m_{\alpha}^2(r^2 \vee 1)}{C_1^2KM_n^2}\right]$$

for constants  $C, C_1 > 0$  and sample size  $n > m_{\alpha} (M_n \sqrt{c_1 K})^{-1}$ .

Using (3.4) and Corollary 3.4 in van de Geer (2000), we now obtain the bound:

$$P\left(\sup_{\boldsymbol{\eta}\in\Theta_r}|\bar{V}_n(\boldsymbol{\eta})-\bar{V}_n(\boldsymbol{\eta}_0)|\geq Tr\delta\right)\leq 5C\exp\left[-\frac{nT^2\delta^2m_\alpha^2(r^2\vee 1)}{16C_1^2KM_n^2}\right].$$
 (3.6)

Finally, the following lemma bounds a scaled version of  $|\bar{V}_n(\eta) - \bar{V}_n(\eta_0)|$  over the full parameter space  $\Theta$ .

**Lemma 3.3.** Let  $\lambda_0 = 2\delta$ . Then for any  $T \ge 1$  we have

$$P\left(\sup_{\boldsymbol{\eta}} \frac{|\bar{V}_n(\boldsymbol{\eta}_0) - \bar{V}_n(\boldsymbol{\eta})|}{\lambda_0 \vee (P_\alpha(\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_2)} \ge T\lambda_0\right) \le C_2 \log n \exp\left[-\frac{nT^2\delta^2}{C_3^2KM_n^2}\right].$$

Pat II: Bounding the tails. Using taylor expansion, we have

$$\begin{split} |\bar{l}(\mathbf{x}; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}; \boldsymbol{\eta}_0)| \mathbb{I}(G(\mathbf{x}) > M_n) &\leq G(\mathbf{x}) \mathbb{I}(G(\mathbf{x}) > M_n) (\|\boldsymbol{\theta} - \boldsymbol{\theta}_0)\|_1 + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_1) \\ &\leq \frac{\sqrt{6K}}{m_{\alpha}} G(\mathbf{x}) \mathbb{I}(G(\mathbf{x}) > M_n) (P_{\alpha}(\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_2) \\ \Rightarrow \frac{|\bar{l}(\mathbf{x}; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}; \boldsymbol{\eta}_0)| \mathbb{I}(G(\mathbf{x}) > M_n)}{P_{\alpha}(\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_2} &\leq \frac{\sqrt{6K}}{m_{\alpha}} G(\mathbf{x}) \mathbb{I}(G(\mathbf{x}) > M_n) \end{split}$$

Now since  $\mathbf{x} = \varphi(\mathbf{z})^T \mathbf{B} + \boldsymbol{\epsilon}$  and  $\varphi(\cdot)$  is bounded, we have the bound

$$G(\mathbf{x}) \le k_1(\|\epsilon\| + k_2); \quad k_1, k_2 > 0,$$

so that

$$P\left(\sup_{\eta} \frac{|V_{n}(\eta_{0}) - V_{n}(\eta)|\mathbb{I}(G(\mathbf{x}) > M_{n})}{\lambda_{0} \vee (P_{\alpha}(\boldsymbol{\theta} - \boldsymbol{\theta}_{0}) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_{0}\|_{2})} \geq T\lambda_{0}\right)$$

$$\leq P\left(\frac{\sqrt{K}}{n} \sum_{i=1}^{n} k_{3}(\|\boldsymbol{\epsilon}_{i}\| + k_{4})\mathbb{I}(\|\boldsymbol{\epsilon}_{i}\| > M_{n} - k_{5}) + \mathbb{E}[k_{3}(\|\boldsymbol{\epsilon}\| + k_{4})\mathbb{I}(\|\boldsymbol{\epsilon}\| > M_{n} - k_{5})] \geq T\lambda_{0}\right)$$

$$\leq \frac{(\sqrt{K} + 1)\mathbb{E}[k_{3}(\|\boldsymbol{\epsilon}\| + k_{4})\mathbb{I}(\|\boldsymbol{\epsilon}\| > M_{n} - k_{5})]}{T\lambda_{0}}$$

$$(3.7)$$

using Markov inequality.

Since  $\epsilon \sim \mathcal{N}(\mathbf{0}, \Omega_x^{-1})$ , i.e. sub-gaussian, we have the following tail bound:

$$\mathbb{E}[k_3(\|\epsilon\| + k_4)\mathbb{I}(\|\epsilon\| > M_n - k_5)] \le k_6 \exp(-k_7 M_n^2),$$

using constants  $k_6, k_7 > 0$  depending on  $\Omega_x$  only. Now take  $M_n = \log n$ . Using (3.5) and  $\lambda_0 = 2\delta$  it is easy to see that  $\lambda_0 \succeq \log n/\sqrt{n}$ . Putting everything back in (3.7) we thus have a probability bound on the tail of the empirical process:

$$P\left(\sup_{\boldsymbol{\eta}} \frac{|V_n(\boldsymbol{\eta}_0) - V_n(\boldsymbol{\eta})|\mathbb{I}(G(\mathbf{x}) > M_n)}{\lambda_0 \vee (P_\alpha(\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_2)} \ge T\lambda_0\right) \le \frac{k_8(\sqrt{K} + 1)\sqrt{n}}{n^2 \log n} \le \frac{k_9\sqrt{K}}{n^{3/2} \log n}. \quad (3.8)$$

Now, we combine the conclusions of parts I and II, taking  $M_n = \log n$  to conclude the proof.

# 4 Proofs of auxiliary lemmas

*Proof of Lemma 3.1.* For any  $\eta, \eta' \in \Theta$ , due to the mean value theorem there exists  $\eta''$  so that

$$\left\| \nabla_{\boldsymbol{\eta}} \bar{l}(\mathbf{x}; \boldsymbol{\eta}) \right\|_{\boldsymbol{\eta} = \boldsymbol{\eta}''} \right\|_{\infty} = \frac{|\bar{l}(\mathbf{x}; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}; \boldsymbol{\eta}')|}{\|\boldsymbol{\eta} - \boldsymbol{\eta}'\|_{1}}.$$
(4.1)

Define  $e_{\eta}(\mathbf{x}) = |\bar{l}(\mathbf{x}; \eta) - \bar{l}(\mathbf{x}; \eta_0)|\mathbb{I}(G(\mathbf{x}) \leq M_n)$ . Then, combining (4.1) with Condition (4) we get

$$|e_{\eta}(\mathbf{x}) - e_{\eta'}(\mathbf{x})| \leq |\bar{l}(\mathbf{x}; \eta) - \bar{l}(\mathbf{x}; \eta')| \mathbb{I}(G(\mathbf{x}) \leq M_n)$$

$$\leq M_n(\|\boldsymbol{\theta} - \boldsymbol{\theta}'\|_1 + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}'\|_1)$$

$$\leq M_n(\|\boldsymbol{\theta} - \boldsymbol{\theta}'\|_1 + \sqrt{6K}\|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}'\|_2)$$
(4.2)

so that for u > 0,

$$H(u, \mathcal{E}_r, \|.\|_{P_n}) \le H\left(\frac{u}{M_n}, \left\{\boldsymbol{\vartheta} : \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}_0\|_2 \le \frac{r}{\sqrt{6K}}\right\}, \|.\|_2\right) + H\left(\frac{u}{M_n}, \left\{\boldsymbol{\theta} : \|\boldsymbol{\theta} - \boldsymbol{\theta}_0\|_1 \le r\right\}, \|.\|_2\right)$$

$$(4.3)$$

The first term is bounded above by  $6K \log(5rM_n/(\sqrt{6K}u))$  (Städler et al., 2010). Also  $\log x/x \le 1/e$  for any x > 0 implies that

$$6K \log \left(\frac{5rM_n}{\sqrt{6K}u}\right) = 3K \log \left(\frac{25r^2M_n^2}{6Ku^2}\right) \le \frac{25r^2M_n^2}{2eu^2} \le \frac{5r^2M_n^2}{u^2}$$

For the second term, we use Lemma 2.6.11 in van der Vaart and Wellner (1996) to obtain

$$H\left(\frac{u}{M_n}, \{\boldsymbol{\theta} : \|\boldsymbol{\theta} - \boldsymbol{\theta}_0\|_1 \le r\}, \|.\|_2\right) \le \frac{c_0 r^2 M_n^2}{u^2} \log\left(1 + \frac{du^2}{r^2 M_n^2}\right)$$

for some  $c_0 > 0$ . Now putting everything back in (4.3) we have the needed.

*Proof of Lemma 3.2.* Continuing from the right hand side of (4.2), we have for any  $\eta, \eta' \in \Theta_r$ ,

$$|\bar{l}(\mathbf{x}; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}; \boldsymbol{\eta}')|^{2} \mathbb{I}(G(\mathbf{x}) \leq M_{n}) \leq 6KM_{n}^{2} \left( \|\boldsymbol{\theta} - \boldsymbol{\theta}'\|_{1} + \|\boldsymbol{\vartheta} - \boldsymbol{\vartheta}'\|_{2} \right)^{2}$$

$$\leq \frac{6KM_{n}^{2}}{m_{\alpha}^{2}} \left( P_{\alpha}(\boldsymbol{\theta} - \boldsymbol{\theta}_{0}) + \|\boldsymbol{\eta} - \boldsymbol{\eta}_{0}\|_{2} + P_{\alpha}(\boldsymbol{\theta}' - \boldsymbol{\theta}_{0}) + \|\boldsymbol{\eta}' - \boldsymbol{\eta}_{0}\|_{2} \right)^{2}$$

$$\leq \frac{24KM_{n}^{2}r^{2}}{m_{\alpha}^{2}}$$

Now applying second part of Condition 4 we get

$$\frac{1}{n} \sum_{i=1}^{n} |\bar{l}(\mathbf{x}_i; \boldsymbol{\eta}) - \bar{l}(\mathbf{x}_i; \boldsymbol{\eta}')|^2 \mathbb{I}(G(\mathbf{x}) \le M_n) \le \frac{c_1 K M_n^2(r^2 \wedge 1)}{m_\alpha^2} := R_n^2.$$
 (4.4)

Also, say  $\tilde{R}_n^2 = c_1 K M_n^2 r^2 / m_\alpha^2$ . Now using Lemma 3.1 we have

$$\int_{r/n}^{R_n} H^{1/2}(u, \mathcal{E}_r, ||.||_{P_n}) du \leq \int_{r/n}^{\tilde{R}_n} H^{1/2}(u, \mathcal{E}_r, ||.||_{P_n}) du 
\leq (5 + c_0)^{1/2} \int_{r/n}^{\tilde{R}_n} \frac{r M_n}{u} \log^{1/2} \left( 1 + \frac{du^2}{r^2 M_n^2} \right) du$$
(4.5)

There are three cases now.

Case I: If  $\tilde{R}_n/rM_n < 1$ , we have

$$\int_{r/n}^{\tilde{R}_n} \frac{1}{u} \log^{1/2} \left( 1 + \frac{du^2}{r^2 M_n^2} \right) du \le \sqrt{\log(2d)} \log \left( \frac{n\tilde{R}_n}{r} \right)$$

Case II: If  $1 < (nM_n)^{-1}$ , we have

$$\begin{split} \int_{r/n}^{\tilde{R}_n} \frac{1}{u} \log^{1/2} \left( 1 + \frac{du^2}{r^2 M_n^2} \right) du &\leq \sqrt{\log d} \int_{r/n}^{\tilde{R}_n} \frac{du}{u} + \int_{r/n}^{\tilde{R}_n} \frac{1}{u} \log^{1/2} \left( \frac{2u^2}{r^2 M_n^2} \right) du \\ &\leq \sqrt{\log(d)} \log \left( \frac{n\tilde{R}_n}{r} \right) + \int_{r/n}^{\tilde{R}_n} \frac{1}{u} \frac{\sqrt{2}u}{r M_n} du \\ &\leq \sqrt{\log(d)} \log \left( \frac{n\tilde{R}_n}{r} \right) + \frac{\sqrt{2}\tilde{R}_n}{r M_n} \end{split}$$

using the fact that  $\log x/x < 1/e < 1$  for any x > 0.

Case II: If  $(nM_n)^{-1} < 1 < \tilde{R}_n/rM_n$ , we have

$$\begin{split} \int_{r/n}^{\tilde{R}_n} \frac{1}{u} \log^{1/2} \left( 1 + \frac{du^2}{r^2 M_n^2} \right) du &= \sqrt{\log d} \int_{r/n}^{\tilde{R}_n} \frac{du}{u} + \int_{r/n}^1 \frac{1}{u} \log^{1/2} \left( 1 + \frac{u^2}{r^2 M_n^2} \right) du + \\ \int_1^{\tilde{R}_n} \frac{1}{u} \log^{1/2} \left( 1 + \frac{u^2}{r^2 M_n^2} \right) du \\ &\leq \sqrt{\log(2d)} \log \left( \frac{n\tilde{R}_n}{r} \right) + \frac{\sqrt{2}\tilde{R}_n}{r M_n} \end{split}$$

Now  $n > m_{\alpha}(M_n \sqrt{c_1 K})^{-1}$  implies  $n\tilde{R}_n/r > 1$  so  $\log(n\tilde{R}_n/r) > 0$ . Thus we can combine all three cases to get the common upper bound:

$$\int_{r/n}^{R_n} H^{1/2}(u, \mathcal{E}_r, ||.||_{P_n}) du \leq (5 + c_0)^{1/2} \left[ \sqrt{2} \tilde{R}_n + r M_n \log \left( \frac{n \sqrt{c_1 K} M_n}{m_\alpha} \right) \sqrt{\log(2d)} \right] \\
= (5 + c_0)^{1/2} r M_n \left[ \frac{\sqrt{2c_1 K}}{m_\alpha} + \log \left( \frac{n \sqrt{c_1 K} M_n}{m_\alpha} \right) \sqrt{\log(2d)} \right] \tag{4.6}$$

Take  $\delta$  as in (3.5). We now apply Lemma 3.2 in van de Geer (2000) on the functional class  $\mathcal{E}_r$ . Combining (4.4) and (4.6), all conditions of the lemma are satisfied. Thus we obtain

$$P\left(\sup_{\boldsymbol{\eta}\in\Theta_r}\left|\frac{1}{n}\sum_{i=1}^nW_i(\bar{l}(\mathbf{x}_i;\boldsymbol{\eta})-\bar{l}(\mathbf{x}_i;\boldsymbol{\eta}_0))\mathbb{I}(G(\mathbf{x})\leq M_n)\right|\geq\delta\right)\leq C\exp\left[-\frac{n\delta^2}{C^2R_n^2}\right]$$

by applying the lemma. Now replace  $\delta$  by  $Tr\delta$  and substitute for  $R_n^2$  from right hand side of (4.4) to get the needed.

*Proof of Lemma 3.3.* The proof follows using a peeling argument similar to the proof of Lemma 4 in Feng and Simon (2017) and Lemma 2 in Städler et al. (2010). We leave the details to the reader.  $\Box$ 

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