Algorithm 1 Minimax SGD

- 1: initialize all hyper-parameters, and initialize the primal variable θ and the dual variables \mathbf{w}_1 and
- 2: **for** t = 1 : T **do**
- sample ϵ to compute $\mathbf{v} = \mu + L\epsilon$. 3:
- sample w to compute ARD kernel matrix. 4:
- $g(\theta) = [P_{\alpha}(\mathbf{v}|\mathbf{w}), \log \frac{P(D|\mathbf{v})}{q(\mathbf{v}|\theta)}].$ $\mathbf{y} = \mathbf{e}_1 Sigmoid(\mathbf{e}_2 \epsilon + \mathbf{b}_2) + \mathbf{b}_1.$ 5:
- 6:
- update the primal variable: 7:
- $\Delta\theta = \frac{\partial g_1(\theta)}{\partial \theta} \mathbf{y} \frac{\partial g_2(\theta)}{\partial \theta}.$ $\theta = \theta \alpha \Delta \theta.$
- 9:
- update the dual variable: 10:
- $\mathbf{e}_1 = \mathbf{e}_1 + \beta \left(g_1(\theta) + 1/y \right) \frac{\partial \mathbf{y}}{\partial \mathbf{e}_1}$ 11:
- $\mathbf{e}_2 = \mathbf{e}_2 + \beta \left(g_1(\theta) + 1/y \right) \frac{\partial \mathbf{y}}{\partial \mathbf{e}_2}$
- $\mathbf{b}_1 = \mathbf{b}_1 + \beta \left(g_1(\theta) + 1/y \right) \frac{\partial \mathbf{y}}{\partial \mathbf{b}_1}$ 13:
- $\mathbf{b}_2 = \mathbf{b}_2 + \beta \left(g(\theta) + 1/y \right) \frac{\partial \mathbf{y}}{\partial \mathbf{b}_2}$ 14:

$$\begin{split} L(\theta) &= \int \log(E_{p_{\alpha}(\mathbf{w})}(p_{\alpha}(\mathbf{v}|\mathbf{w})))q(\mathbf{v}|\theta)\mathrm{d}\mathbf{v} + \int \log\frac{p_{\alpha}(\mathbf{D}|\mathbf{v})}{q(\mathbf{v}|\theta)}q(\mathbf{v}|\theta)\mathrm{d}\mathbf{v} \\ &= \int \log\left(\int p_{\alpha}(\mathbf{v}|\mathbf{w})p_{\alpha}(\mathbf{w})\mathrm{d}\mathbf{w}\right)q(\mathbf{v}|\theta)\mathrm{d}\mathbf{v} + \int \log\frac{p_{\alpha}(\mathbf{D}|\mathbf{v})}{q(\mathbf{v}|\theta)}q(\mathbf{v}|\theta)\mathrm{d}\mathbf{v} \\ &= \int \log\left(\int \frac{1}{|K_{nn}|^{1/2}}e^{-\frac{1}{2}(\mu+L\epsilon)K_{nn}^{-1}(\mu+L\epsilon)}e^{-\frac{1}{2}(\log\mathbf{w}-\mu_{0})(\mathbf{e}_{0}^{2})^{-1}(\log\mathbf{w}-\mu_{0})}\mathrm{d}\mathbf{w}\right)\frac{1}{|LL^{T}|^{1/2}}e^{-\frac{1}{2}\epsilon^{T}\epsilon}\mathrm{d}\mathbf{v} \\ &+ \int \log\frac{p_{\alpha}(\mathbf{D}|\mathbf{v})}{q(\mathbf{v}|\theta)}q(\mathbf{v}|\theta)\mathrm{d}\mathbf{v} \\ &= \int \log\left(\int \frac{1}{|K_{nn}|^{1/2}}e^{-\frac{1}{2}(\mu+L\epsilon)K_{nn}^{-1}(\mu+L\epsilon)}e^{-\frac{1}{2}(\log\mathbf{w}-\mu_{0})(\mathbf{e}_{0}^{2})^{-1}(\log\mathbf{w}-\mu_{0})}\mathrm{d}\mathbf{w}\right)\frac{1}{|LL^{T}|^{1/2}}e^{-\frac{1}{2}\epsilon^{T}\epsilon}\mathrm{d}\mathbf{v} \\ &+ \int (\log p_{\alpha}(\mathbf{D}|\mathbf{v}) - \log q(\mathbf{v}|\theta))q(\mathbf{v}|\theta)\mathrm{d}\mathbf{v} \\ &= \int \log\left(\int \frac{1}{|K_{nn}|}e^{-(\mu+L\epsilon)K_{nn}^{-1}(\mu+L\epsilon)}e^{-(\log\mathbf{w}-\mu_{0})(\mathbf{e}_{0}^{2})^{-1}(\log\mathbf{w}-\mu_{0})}\mathrm{d}\mathbf{w}\right)\frac{1}{|LL^{T}|}e^{-\epsilon^{T}\epsilon}\mathrm{d}\mathbf{v} \\ &+ \int\left(\sum_{i=1}^{n-n_{test}}\left(-\log(1+e^{-r_{i}(\mu_{i}+L_{i}\epsilon)}) + \log|LL^{T}| + \epsilon^{T}\epsilon\right)\right)\frac{1}{|LL^{T}|}e^{-\epsilon^{T}\epsilon}\mathrm{d}\mathbf{v} \\ &= \int \log\left(\int \frac{1}{|K_{nn}|}e^{-(\mu+L\epsilon)K_{nn}^{-1}(\mu+L\epsilon)}e^{-(\log\mathbf{w}-\mu_{0})(\mathbf{e}_{0}^{2})^{-1}(\log\mathbf{w}-\mu_{0})}\mathrm{d}\mathbf{w}\right)\frac{1}{|LL^{T}|}e^{-\epsilon^{T}\epsilon}\mathrm{d}(\mu+L\epsilon) \\ &+ \int\left(\sum_{i=1}^{n-n_{test}}\left(-\log(1+e^{-r_{i}(\mu_{i}+L_{i}\epsilon)}) + \log|LL^{T}| + \epsilon^{T}\epsilon\right)\right)\frac{1}{|LL^{T}|}e^{-\epsilon^{T}\epsilon}\mathrm{d}(\mu+L\epsilon) \end{split}$$

Objective:

$$\min \mathcal{L}(\theta) = \min_{g_{\theta}} \max_{\mathbf{y}_{v}} g_{1}(\theta)\mathbf{y}_{v} + 1 + \log(-\mathbf{y}_{v}) - g_{2}(\theta)$$

Gradients w.r.t the primal variables:

$$\frac{\partial \mathcal{L}(\theta)}{\partial \theta} \ = \ \left(\frac{\partial \mathcal{L}(\theta)}{\partial \mu}, \frac{\partial \mathcal{L}(\theta)}{\partial L}\right)^T.$$

з Here,

$$\begin{array}{lcl} \frac{\partial \mathcal{L}(\theta)}{\partial \mu} & = & \mathbf{y}_v \frac{\partial g_1(\theta)}{\partial \mu} - \frac{\partial g_2(\theta)}{\partial \mu} \\ & = & \mathbf{y}_v \frac{\partial g_1(\theta)}{\partial \mu} - \left(\frac{\partial \log P(\mathbf{D}|\mathbf{v})}{\partial \mu} - \frac{\partial \log q(\mathbf{v}|\theta)}{\partial \mu} \right) \end{array}$$

4 where

$$\frac{\partial g_1(\theta)}{\partial \mu} = \frac{\partial P_{\alpha}(\mathbf{v}|\mathbf{w})}{\partial \mu} = \exp\left(-\frac{1}{2}(\mu + L\epsilon)^T K^{-1}(\mu + L\epsilon)\right) K^{-1}(\mu + L\epsilon),$$

$$\frac{\partial \log P(\mathbf{D}|\mathbf{v})}{\partial \mu} = \left(\mathbf{0}_{1 \times n_{test}}, \left[\frac{y_i}{1 + \exp(y_i(\mu_i + L_i \epsilon))}\right]_{i:n_{test} + 1 - > n}\right)^T$$

$$\frac{\partial \log q(\mathbf{v}|\boldsymbol{\theta})}{\partial \boldsymbol{\mu}} = \mathbf{0}$$

5 Besides,

$$\begin{array}{lcl} \frac{\partial \mathcal{L}(\theta)}{\partial L} & = & \mathbf{y}_v \frac{\partial g_1(\theta)}{\partial L} - \frac{\partial g_2(\theta)}{\partial L} \\ & = & \mathbf{y}_v \frac{\partial g_1(\theta)}{\partial L} - \left(\frac{\partial \log P(\mathbf{D}|\mathbf{v})}{\partial L} - \frac{\partial \log q(\mathbf{v}|\theta)}{\partial L}\right) \end{array}$$

6 where

$$\frac{\partial g_1(\theta)}{\partial L} = \frac{P_{\alpha}(\mathbf{v}|\mathbf{w})}{\partial L} = \exp\left(-\frac{1}{2}(\mu + L\epsilon)^T K^{-1}(\mu + L\epsilon)\right) \frac{\partial (\mu + L\epsilon)^T K^{-1}(\mu + L\epsilon)}{\partial L},$$

$$\frac{\partial \log P(\mathbf{D}|\mathbf{v})}{\partial L} = \left(\mathbf{0}_{n_{test} \times n}, \left[\frac{y_i}{1 + \exp(y_i(\mu_i + L_i \epsilon))} \epsilon^T\right]_{i:n_{test} + 1 - > n}\right)^T$$

$$\frac{\partial \log q(\mathbf{v}|\theta)}{\partial L} = (L^T)^{-1}$$

7 References