General MIP Original Problem for $L \ge 2$

with artificial variable $g_{n,k',k,l}$

Parameters:

 x_{n-d} : binary vector inputs of size n × d, where n is the number of data points, d is the number of dimensions/features

 y_n : binary vector labeled outputs of size n \times 1, where n is the number of data points

Decision Variables:

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\alpha_{d,k,0}: Weight for feature d in unit k in the first hidden layer, \forall d \in D, k \in K
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 $\alpha_{k',k,l}$: Weight from the k'^{th} unit in layer l-1 to unit k in layer l, $\forall k', k \in K, l \in \{1, 2, 3, ..., L-1\}$

 $\alpha_{k',0,L}$: Weight from the k'^{th} unit in hiddenlayer L to unit output layer L+1, $\forall k' \in K$

 $\beta_{k,l}$: Bias for unit k in layer l, $\forall k \in K, l \in \{0, 1, ..., L-1\}$

 $\beta_{0,L}$: Bias in the final layer

 $h_{n,k,l}$: Binary output of unit k in layer 1, $\forall n \in \mathbb{N}, k \in \mathbb{K}, l \in \{0, 1, \dots L-1\}$

 $g_{n,k',k,l}$: Artificial Variable for decomposition, $\forall n \in \mathbb{N}, k, k' \in \mathbb{K}, l \in \{1, \dots, L-1\}$

 $g_{n,k',0,L}$: Artificial Variable for decomposition of the output layer, $\forall n \in \mathbb{N}, k' \in K$

 $z_{n,k',k,l}$: Auxilliary variable that represents $\alpha_{k',k,l}h_{n,k,(l-1)} \ \forall \ n \in \mathbb{N}, \ k', \ k \in \mathbb{K}, \ l \in \{1,2,\ldots,L-1\}$

 $z_{n,k',0,L}$: Auxilliary variable that represents $a_{k',0,L}h_{n,k,(L-1)} \ \forall \ n \in \mathbb{N}, \ k', \ k \in K$

 \hat{y}_n : Output of final layer, $\forall n \in N$

Objective:

$$\min_{\alpha,\beta,h,g,z,\hat{y},\ell} \sum_{n=1}^{N} \ell_n$$

Constraints:

$$\begin{aligned} \text{subject to} & & \sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_{0,L} \leq -\epsilon + (M+\epsilon) \hat{y}_n, \ \forall \ n \\ & & \sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_{0,L} \geq \epsilon + (m-\epsilon)(1-\hat{y}_n), \ \forall \ n \\ & & \ell_n \geq y_n - \hat{y}_n, \ \forall \ n \\ & & \ell_n \geq -y_n + \hat{y}_n, \ \forall \ n \\ & & \sum_{d=0}^{D} (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \leq -\epsilon + (M+\epsilon) h_{n,k,0}, \ \forall \ n,k \\ & & \sum_{d=0}^{D} (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \geq \epsilon + (m-\epsilon)(1-h_{n,k,0}), \ \forall \ n,k \\ & & \sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \leq -\epsilon + (M+\epsilon) h_{n,k,l}, \ \forall \ n,k,l \in \ \{1,2,\ldots,L-1\} \\ & & \sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \geq \epsilon + (m-\epsilon)(1-h_{n,k,l}), \ \forall \ n,k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \leq \alpha_{k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} - \alpha_{k',k,l} \geq m(1-g_{n,k',k,l}), \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \end{aligned}$$

$$\begin{split} &z_{n,k',k,l} \leq Mg_{n,k',k,l}, \ \forall \, n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \, n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &g_{n,k',k,l} = h_{n,k',(l-1)}, \ \forall \, n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &z_{n,k',0,L} \leq \alpha_{k',0,L}, \ \forall \, n,k' \\ &z_{n,k',0,L} \leq \alpha_{k',0,L}, \ \forall \, n,k' \\ &z_{n,k',0,L} \leq Mg_{n,k',0,L}, \ \forall \, n,k' \\ &z_{n,k',0,L} \leq Mg_{n,k',0,L}, \ \forall \, n,k' \\ &z_{n,k',0,L} \geq mg_{n,k',0,L}, \ \forall \, n,k' \\ &g_{n,k',0,L} = h_{n,k',(L-1)}, \ \forall \, n,k',k \\ &Lower \, Bound \leq \alpha_{d,k,0}, \ \alpha_{k',k,l}, \ \alpha_{k',0,L-1} \leq Upper \, Bound, \ \forall \, d,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &Lower \, Bound \leq \beta_{k,l}, \ \beta_{L-1} \leq Upper \, Bound, \ \forall \, k,l \in \ \{0,1,2,\ldots,L-1\} \\ &\int_{n,k',k,l} g_{n,k',0,L} \in \{0,1\}, \ \forall \, n,k',k,l \in \ \{0,1,\ldots,L-1\} \\ &g_{n,k',k,l}, g_{n,k',0,L} \in \{0,1\}, \ \forall \, n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &0 \leq \ell_n \leq 1, \ \forall \, n \in N \end{split}$$

Lagrangian Relaxation and Dual

$$\zeta_{LR}(\lambda) = \min_{\alpha,\beta,h,g,z,\hat{y},\ell} \sum_{n=1}^{N} (\ell_n + \sum_{k'=0}^{K} (\sum_{k=0}^{K} (\sum_{l=1}^{L-1} (\lambda_{n,k',k,l}(g_{n,k',k,l} - h_{n,k',(l-1)}))) + \lambda_{n,k',0,L}(g_{n,k',0,L} - h_{n,k',(L-1)})))$$

$$\begin{aligned} &\text{subject to} & & \sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_{0,L} \leq -\epsilon + (M+\epsilon) \hat{y}_n, \ \forall \ n \\ & & \sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_{0,L} \geq \epsilon + (m-\epsilon)(1-\hat{y}_n), \ \forall \ n \\ & & \ell_n \geq y_n - \hat{y}_n, \ \forall \ n \\ & & \ell_n \geq -y_n + \hat{y}_n, \ \forall \ n \\ & & \sum_{d=0}^{D} (\alpha_{d,k,0} \mathbf{x}_{n,d}) + \beta_{k,0} \leq -\epsilon + (M+\epsilon)h_{n,k,0}, \ \forall \ n,k \\ & & \sum_{d=0}^{D} (\alpha_{d,k,0} \mathbf{x}_{n,d}) + \beta_{k,0} \geq \epsilon + (m-\epsilon)(1-h_{n,k,0}), \ \forall \ n,k \\ & & \sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \leq -\epsilon + (M+\epsilon)h_{n,k,l}, \ \forall \ n,k,l \in \ \{1,2,\ldots,L-1\} \\ & & \sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \geq \epsilon + (m-\epsilon)(1-h_{n,k,l}), \ \forall \ n,k,l \in \ \{1,2,\ldots,L-1\} \\ & & \sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \geq \epsilon + (m-\epsilon)(1-h_{n,k,l}), \ \forall \ n,k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \leq \alpha_{k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ & & z_{n,k',k,l} \geq mg_{n,k',k,l}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \end{aligned}$$

 $z_{n,k',0,L} \leq Mg_{n,k',0,L}, \ \forall \ n,k'$

$$\begin{split} &z_{n,k',0,L} \geq mg_{n,k',0,L}, \ \forall \ n,k' \\ &Lower \ Bound \leq \alpha_{d,k,0}, \ \alpha_{k',k,l}, \ \alpha_{k',0,L-1} \leq Upper \ Bound, \ \forall \ d,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &Lower \ Bound \leq z_{n,k',k,l}, \ z_{n,k',0,L} \leq Upper \ Bound, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &Lower \ Bound \leq \beta_{k,l}, \ \beta_{L-1} \leq Upper \ Bound, \ \forall \ k,l \in \ \{0,1,2,\ldots,L-1\} \\ &\hat{y}_n, h_{n,k,l} \in \{0,1\}, \ \forall \ n,k',k,l \in \ \{0,1,\ldots,L-1\} \\ &g_{n,k',k,l}, g_{n,k',0,L} \in \{0,1\}, \ \forall \ n,k',k,l \in \ \{1,2,\ldots,L-1\} \\ &0 \leq \ell_n \leq 1, \ \forall \ n \in N \end{split}$$

Sub-problems

$$\begin{split} \zeta_0(\lambda) &= \min_{\alpha,\beta,h} \sum_{n=0}^N (\sum_{k'=0}^K (\sum_{k=0}^K (-\lambda_{n,k',k,1} h_{n,k',0}))) \\ \text{subject to} \quad \sum_{d=0}^D (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \leq -\epsilon + (M+\epsilon) h_{n,k,0}, \ \forall \ n,k \\ \\ \sum_{d=0}^D (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \geq \epsilon + (m-\epsilon) (1-h_{n,k,0}), \ \forall \ n,k \\ \\ Lower \ Bound \leq \alpha_{d,k,0} \leq Upper \ Bound, \ \forall \ d,k \\ \\ Lower \ Bound \leq \beta_{k,0} \leq Upper \ Bound, \ \forall \ k \\ \\ h_{n,k,0} \in \{0,1\}, \ \forall \ n,k \end{split}$$

$$\zeta_{l}(\lambda) = \min_{\alpha, \beta, z, h, g} \sum_{n=0}^{N} (\sum_{k'=0}^{K} (\sum_{k=0}^{K} (\lambda_{n, k', k, l} g_{n, k', k, l} - \lambda_{n, k', k, l+1} h_{n, k', l})))$$

subject to
$$\sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \le -\epsilon + (M+\epsilon)h_{n,k,l}, \ \forall n,k$$

$$\sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \ge \epsilon + (m - \epsilon)(1 - h_{n,k,l}), \ \forall \ n, k$$

$$z_{n,k',k,l} \leq \alpha_{k',k,l}, \ \forall \ n,k',k$$

$$z_{n,k',k,l} - \alpha_{k',k,l} \ge m(1 - g_{n,k',k,l}), \ \forall \ n,k',k$$

$$z_{n,k',k,l} \leq Mg_{n,k',k,l}, \ \forall \ n,k',k$$

$$z_{n,k',k,l} \ge mg_{n,k',k,l}, \ \forall \ n,k',k$$

Lower Bound $\leq a_{k',k,l} \leq Upper$ Bound, $\forall k', k$

Lower Bound $\leq z_{n,k',k,l} \leq Upper Bound, \ \forall \ n,k,k'$

Lower Bound $\leq \beta_{k,l} \leq Upper Bound, \ \forall \ k$

$$h_{n,k,l}, g_{n,k',k,l} \in \{0,1\}, \ \forall \ n,k,k'$$

$$\zeta_{L-1}(\lambda) = \min_{\alpha,\beta,z,h,g} \sum_{n=0}^{N} (\sum_{k'=0}^{K} (\sum_{k=0}^{K} (\lambda_{n,k',k,L-1}g_{n,k',k,L-1}) - \lambda_{n,k',0,L}h_{n,k',L-1}))$$

subject to
$$\sum_{k'=0}^{K} (z_{n,k',k,L-1}) + \beta_{k,L-1} \le -\epsilon + (M+\epsilon)h_{n,k,L-1}, \ \forall \ n,k$$

$$\sum_{k'=0}^{K} (z_{n,k',k,L-1}) + \beta_{k,L-1} \ge \epsilon + (m-\epsilon)(1 - h_{n,k,L-1}), \ \forall \ n, k$$

$$z_{n,k',k,L-1} \le \alpha_{k',k,L-1}, \ \forall \ n,k',k$$

 $z_{n,k',k,L-1} - \alpha_{k',k,L-1} \ge m(1 - g_{n,k',k,L-1}), \ \forall \ n,k',k$

 $z_{n,k',k,L-1} \leq Mg_{n,k',k,L-1}, \ \forall \ n,k',k$

 $z_{n,k',k,L-1} \ge mg_{n,k',k,L-1}, \ \forall \ n,k',k$

Lower Bound $\leq a_{k',k,L-1} \leq Upper$ Bound, $\forall k', k$

Lower Bound $\leq z_{n,k',k,L-1} \leq Upper$ Bound, $\forall n,k,k'$

Lower Bound $\leq \beta_{k,L-1} \leq Upper Bound, \ \forall \ k$

 $h_{n,k,L-1}, g_{n,k',k,L-1} \in \{0,1\}, \ \forall \ n,k,k'$

$$\zeta_{L}(\lambda) = \min_{\alpha, \beta, z, g, \hat{y}, \ell} \sum_{n=0}^{N} (\ell_{n} + \sum_{k'=0}^{K} (\lambda_{n, k', 0, L} g_{n, k', 0, L}))$$

subject to
$$\sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_{0,L} \le -\epsilon + (M+\epsilon)\hat{y}_n, \ \forall \ n$$

$$\sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_{0,L} \ge \epsilon + (m - \epsilon)(1 - \hat{y}_n), \ \forall \ n$$

$$\ell_n \ge y_n - \hat{y}_n, \ \forall \ n$$

$$\ell_n \geq -y_n + \hat{y}_n, \ \forall \ n$$

$$z_{n,k',0,L} \le \alpha_{k',0,L}, \ \forall \ n,k'$$

$$z_{n,k',0,L} - \alpha_{k',0,L} \ge m(1 - g_{n,k',0,L}), \ \forall \ n,k'$$

$$z_{n,k',0,L} \leq Mg_{n,k',0,L}, \ \forall \ n,k'$$

$$z_{n,k',0,L} \ge mg_{n,k',0,L}, \forall n,k'$$

 $Lower \ Bound \leq \alpha_{k',\,0\,,\,L} \leq Upper \ Bound, \ \forall \ k'$

Lower Bound
$$\leq z_{n,k',0,L} \leq Upper$$
 Bound, $\forall n, k'$

Lower Bound
$$\leq \beta_{0,L} \leq Upper Bound$$

$$\hat{y}_n, g_{n,k',0,L} \in \{0,1\}, \ \forall \ n, k'$$

$$0 \le \ell_n \le 1, \ \forall \ n$$

$$z_{L} = \max_{\lambda \in \mathbb{R}^{m_{1}}} \zeta_{0}(\lambda) + \sum_{l=1}^{L-2} (\zeta_{l}(\lambda)) + \zeta_{L-1}(\lambda) + \zeta_{L}(\lambda)$$

Vrishabh's Notes

- Not sure if the $z \le \alpha$ constraints are in the right subproblems. They're in their respective layers, but since neither z nor α are in the dualized constraints, should they be in the final "master" dual problem?
- Not sure if it's okay to have $h_{n,k',l}$ in the objective, but $h_{n,k,l}$ in the constraints for $\zeta_0(\lambda), \zeta_l(\lambda)$, and $\zeta_{L-1}(\lambda)$. The variables don't necessarily align