Last Updated: 06/10/2021

General MIP Original Problem for $L \ge 2$

Parameters:

 $x_{n,d}$: binary vector inputs of size n \times 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:

 $\alpha_{d,k,0}$: Weight for feature d in unit k in the first hidden layer, $\forall d \in D, k \in K$

 $\alpha_{k',k,l}$: Weight from the k'^{th} unit in layer l-1 to unit k in layer l, $\forall k', k \in K, l \in \{1,2,3,\ldots,L-1\}$

 $\alpha_{k',0,1}$: 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, $\forall k \in K, l \in \{0, 1, ..., L-1\}$

 β_L : Bias in the final layer

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

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

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

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

 ℓ_n : Absolute Misclassification of data point n, $\forall n \in N$

Objective:

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

Constraints:

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

$$\begin{split} &z_{n,k',0,L} - \alpha_{k',0,L} \geq m(1 - h_{n,k',L-1}), \ \forall \ n,k' \\ &mh_{n,k',L-1} \leq z_{n,k',0,L} \leq Mh_{n,k',L-1}, \ \forall \ n,k' \\ &Lower \ Bound \leq \alpha_{d,k,0}, \ \alpha_{k',k,l}, \ \alpha_{k',0,L-1} \leq Upper \ Bound, \ \forall \ d,k,k',l \in \ \{1,2,\ldots,L-1\} \\ &Lower \ Bound \leq z_{n,k',k,l}, \ z_{n,k',0,L} \leq Upper \ Bound, \ \forall \ n,k,k',l \in \ \{1,2,\ldots,L-1\} \\ &Lower \ Bound \leq \beta_{k,l}, \ \beta_{L-1} \leq Upper \ Bound, \ \forall \ k,l \in \ \{0,1,2,\ldots,L-1\} \\ &\hat{\mathcal{Y}}_n, h_{n,k,l} \in \{0,1\}, \ \forall \ n,k,l \in \ \{0,1,\ldots,L-1\} \\ &0 \leq \ell_n \leq 1, \ \forall \ n \in N \end{split}$$

Lagrangian Relaxation and Dual

 $\sum_{l=0}^{\infty} (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \ge \epsilon + (m - \epsilon)(1 - h_{n,k,0}), \ \forall \ n, k$

$$\begin{split} \zeta_{LR}(\lambda) &= \min_{\alpha,\beta,z,h,\hat{y},\ell} \sum_{n=0}^{K} (\ell_n + (\sum_{k'=0}^{K} \sum_{k=0}^{L-1} (\lambda_{2,n,k',k,l}(-z_{n,k',k,l} + \alpha_{k',k,l} + m(1-h_{n,k',l-1})) + \lambda_{3,n,k',k,l}(mh_{n,k',l-1} - z_{n,k',k,l}) + \lambda_{4,n,k',k,l}(z_{n,k',k,l} - Mh_{n,k',l-1}) \\ & \text{subject to} \quad \sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_L \leq -\epsilon + (M+\epsilon)\hat{y}_n, \ \forall \ n \\ & \sum_{k'=0}^{K} (z_{n,k',0,L}) + \beta_L \geq \epsilon + (m-\epsilon)(1-\hat{y}_n), \ \forall \ n \\ & \ell_n \geq y_n - \hat{y}, \ \forall \ n \\ & \ell_n \geq -y_n + \hat{y}, \ \forall \ n \\ & \sum_{d=0}^{D} (\alpha_{d,k,0}x_{n,d}) + \beta_{k,0} \leq -\epsilon + (M+\epsilon)h_{n,k,0}, \ \forall \ n,k \end{split}$$

$$\sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \leq -\epsilon + (M+\epsilon)h_{n,k,l}, \ \forall n,k,l \in \{1,2,\ldots,L-1\}$$

$$\sum_{k'=0}^{K} (z_{n,k',k,l}) + \beta_{k,l} \geq \epsilon + (m-\epsilon)(1-h_{n,k,l}), \ \forall n,k,l \in \{1,2,\ldots,L-1\}$$

$$z_{n,k',k,l} \leq \alpha_{k',k,l}, \ \forall n,k',k,l \in \{1,2,\ldots,L-1\}$$

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

$$Lower Bound \leq \alpha_{d,k,0}, \ \alpha_{k',k,l}, \ \alpha_{k',0,L} \leq Upper Bound, \ \forall d,k,k',l \in \{0,1,\ldots,L-1\}$$

$$Lower Bound \leq z_{n,k',k,l}, \ z_{n,k',0,L} \leq Upper Bound, \ \forall n,k,k',l \in \{1,2,\ldots,L-1\}$$

$$Lower Bound \leq \beta_{k,l}, \ \beta_{L} \leq Upper Bound, \ \forall k,l \in \{0,1,2,\ldots,L-1\}$$

$$\hat{y}_{n}, \ h_{n,k,l} \in \{0,1\}, \ \forall n,k,l \in \{0,1,\ldots,L-1\}$$

$$0 \leq \ell_{n} \leq 1, \ \forall n \in N$$

Sub-problems

$$\begin{split} \zeta_0(\lambda) &= \min_{\alpha,\beta,h} \sum_{n=0}^N (\sum_{k'=0}^K (\sum_{k=0}^K h_{n,k',0} (-m\lambda_{2,n,k',k,1} + m\lambda_{3,n,k',k,1} - M\lambda_{4,n,k',k,1}))) + \mu_1 \sum_{d=0}^D (\sum_{k=0}^K (|\alpha_{d,k,0}|)) \\ &\text{subject to} \quad \sum_{d=0}^D (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \leq -\epsilon + (M+\epsilon) h_{n,k,0}, \ \forall \ n,k \\ &\qquad \qquad \sum_{d=0}^D (\alpha_{d,k,0} x_{n,d}) + \beta_{k,0} \geq \epsilon + (m-\epsilon) (1-h_{n,k,0}), \ \forall \ n,k \\ &\qquad \qquad Lower \ Bound \leq \alpha_{d,k,0} \leq Upper \ Bound, \ \forall \ d,k \\ &\qquad \qquad Lower \ Bound \leq \beta_{k,0} \leq Upper \ Bound, \ \forall \ k \end{split}$$

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

$$\zeta_{l}(\lambda) = \min_{z,\beta,h,\alpha} \sum_{n=0}^{N} (\sum_{k'=0}^{K} (\sum_{k=0}^{K} (z_{n,k',k,l}(-\lambda_{2,n,k',k,l} + \lambda_{4,n,k',k,l}) + h_{n,k',l}(-m\lambda_{2,n,k',k,l+1} + m\lambda_{3,n,k',k,l+1} - M\lambda_{4,n,k',k,l+1}) + \alpha_{k',k,l}(\lambda_{2,n,k',k,l}))))$$

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

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

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

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

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

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

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

$$\zeta_{L-1}(\lambda) = \min_{z,\beta,h,\alpha} \sum_{n=0}^{N} (\sum_{k'=0}^{K} (\sum_{k=0}^{K} (z_{n,k',k,L-1}(-\lambda_{2,n,k',k,L-1} + \lambda_{4,n,k',k,L-1}) + \alpha_{k',k,L-1}(\lambda_{2,n,k',k,L-1})) + h_{n,k',L-1}(-m\lambda_{2,n,k',0,L} + m\lambda_{3,n,k',0,L}) + m\lambda_{3,n,k',0,L}(-m\lambda_{2,n,k',k,L-1}) + \alpha_{k',k,L-1}(\lambda_{2,n,k',k,L-1}) + \alpha_{k',k,L-1}(\lambda_{2,n$$

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

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

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

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

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

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

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

$$\zeta_L(\lambda) = \min_{z,\alpha,\beta,\hat{y},\ell} \sum_{n=0}^{N} (\ell_n + (\sum_{k'=0}^{K} z_{n,k',0,L}(-\lambda_{2,n,k',0,L} - \lambda_{3,n,k',0,L} + \lambda_{4,n,k',0,L}) + \alpha_{k',0,L}(\lambda_{2,n,k',0,L}))) + \mu_3 \sum_{k=0}^{K} (|\alpha_{k',0,L}|))$$

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

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

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

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

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

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 $\leq \beta_L \leq Upper Bound$

$$\hat{y}_n \in \{0, 1\}, \ \forall \ n$$

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

$$z_{\rm L} = \max_{\lambda \in \mathbb{R}^m_+ l = 1}^{L-2} (\zeta_l(\lambda)) + \zeta_{L-1}(\lambda) + \zeta_0(\lambda) + \zeta_L(\lambda) + \sum_{n=0}^{N} (\sum_{k'=0}^{K} (\sum_{k=0}^{K} (\sum_{l=1}^{K} m \lambda_{2,n,k',k,l})) + m \lambda_{2,n,k',0,L})$$

Notes and Questions for 05/03/2021

- Lagrange Dual
 - Clean up the formulation to merge the $z_{n,k',k,l}$ and respective $h_{n,k',l}$
 - Specifically general to have a sub problem for the first layer, middle layers and output layer separately.
- · Read up on MIP and NN papers
 - Laurent El-Ghaoui (UC Berkeley)

Notes and Questions for 05/11/2021

- Lagrange Dual
 - Min in the sub problems over the decision variables
 - Decompose the first subproblem
- Read up on MIP and NN papers/textbooks
 - Specifically, subgradient descent in lagrange decomposition problems.

Notes:

- Subgradient vector of $\zeta_{LR}(\lambda)$, s^t , consists of the dualized constraints at λ^t
- 1. Choose a starting point for all λ
 - 2. Let $s^t = b Ax^t$ of the $\zeta(\lambda^t)$. If $s^t = 0$, stop
 - 3. $\lambda^{t+1} = \max(0, \lambda^t + \gamma^t s^t)$ where γ is the step size
 - 4. Increment t and go to 2.

Referenced from: Lagrangian Relaxation: An overview; Discrete Mathematics for Bioinformatics WS 07/08, G. W. Klau, 18. Dezember 2007, 14:21

Solving the Lagrangian Dual (5)

Held and Karp proposed the following formula for adapting the stepsize:

$$\gamma^{t} = \mu^{t} \frac{Z^{*} - Z(\lambda^{t})}{\sum_{i=1}^{m} (b_{i} - \sum_{j=1}^{n} a_{ij} x^{t})^{2}} ,$$

where

- Z* is the value of the best solution for the original problem found so far
- μ^t is a decreasing adaption parameter with $0 < \mu^0 \le 2$ and

$$\mu^{t+1} = \begin{cases} \alpha \mu^t & Z_D \text{ did not increase in the last } T \text{ iterations} \\ \mu^t & \text{otherwise} \end{cases}$$

with parameters $0 < \alpha < 1$ and T > 1.

- the denominator is the square of the length of the subgradient vector $b Ax^t$.
- General Notes:
 - Subgradient vs Cutting Plane? (Prof. Luedtke's Slides)
 - Bundle Method? (Prof. Luedtke's Slides)
 - Verify if our problem is convex (Since the relaxation is till a MIP, I'm guessing it's nonconvex)
 - <u>Ballstep Subgradient Method</u> (https://www.researchgate.net/publication/220442497 Lagrangian Relaxation via Ballstep Subgradient Methods) "can provide a solution to the problem at no extra cost". Scope for not just giving us the bounds? Example was for "Lagrangian relaxation of convex programs"

Notes and Questions for 06/01/2021

- Global Dependence (Introduction to Linear Optimization Bertsimas, Tsitsikilis)
- Code up the problems (Langrangian Dual Method-Implementation)