Discrete Optimizations using Graph Deep Learning

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Combinatorial Problems
Approach

In this talk we consider the class of combinatorial problems,

$$\begin{array}{ll} \textit{maximize} & J(\Pi; \textit{Input}) \\ \text{subject to:} & \\ \Pi \in S_n & \end{array}$$

where *Input* stands for a given set input data, and S_n denotes the symmetric group of permutation matrices.

We analyze two specific objective functions:

1. Linear Assignment, $J(\Pi; C) = trace(\Pi C^T)$
2. Quadratic Assignment, $J(\Pi; A, B) = trace(A \Pi B \Pi^T)$

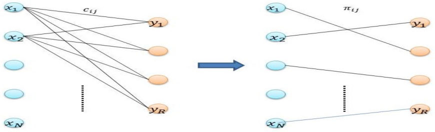
Idea: Use a two-step procedure:

1. Perform a latent representation of the Input Data using a Graph Convolutive Network;
2. Apply a direct algorithm (e.g., a greedy-type algorithm) or solve a convex optimization problem to obtain an estimate of the optimal Π.

The Linear Assignment Problem

Consider a $N \times R$ cost/reward matrix $C = (C_{i,j})_{1 \leq i \leq N, 1 \leq j \leq R}$ of non-negative entries associated to edge connections between two sets of nodes, $\{x_1, \cdots, x_N\}$ and $\{y_1, \cdots, y_R\}$ with $N \geq R$. The problem is to find the minimum cost/maximum reward matching/assignment, namely:

$$\begin{array}{cc} minimize/maximize & \sum_{i=1}^{N} \sum_{j=1}^{R} \pi_{i,j} C_{i,j} = trace(\Pi \tilde{C}^T) \\ \text{subject to:} & \\ \pi_{i,j} \in \{0,1\} \ , \ \forall i,j & \\ \sum_{i=1}^{N} \pi_{i,j} = 1 \ , \ \forall 1 \leq j \leq R & \\ \sum_{j=1}^{R} \pi_{i,j} \leq 1 \ , \ \forall 1 \leq i \leq N & \end{array}$$



Quadratic Assignment Problem

Consider two symmetric (and positive semidefinite) matrices $A, B \in \mathbb{R}^{n \times n}$. The *quadratic assignment problem* asks for the solution of

$$\begin{array}{ll} \textit{maximize} & \textit{trace}(A\Pi B\Pi^T) \\ \text{subject to:} & \\ \Pi \in S_n & \end{array}$$

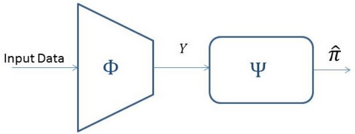
In turns this is equivalent to the minimization problem:

$$\begin{array}{ll} \textit{minimize} & \|\Pi A - B\Pi\|_F^2 \\ \text{subject to:} & \\ \Pi \in S_n & \end{array}$$

In the case A, B are graph Laplacian, an efficient solution to this optimization problem would solve the millenium problem of whether two graphs are isomorphic.

Novel Approach: Optimization in a Latent Representation Domain

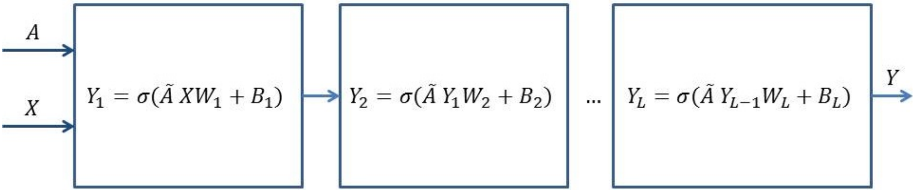
Idea: Perform a two-step procedure: (1) perform a nonlinear representation of the input data; (2) perform optimization in the representation space.



The nonlinear representation map $\Phi : \mathrm{Input\ Data} \mapsto Y$ is implemented using a GCN.
The Optimization map $\Psi : Y \mapsto \hat{\pi}$ can be implemented using a specific nonlinear map (e.g., greedy algorithm, or turning into stochastic matrix) or by solving a convex optimization problem.

Graph Convolutive Networks (GCN)

Kipf and Welling introduced a network structure that performs local processing according to a modified adjacency matrix:



Here $\tilde{A} = I + A$, where A is an input adjacency matrix, or graph weight matrix. The L-layer GCN has parameters $(W_1, B_1, W_2, B_2, \cdots, W_L, B_L)$. As activation map σ we choose the ReLU (Rectified Linear Unit).

Linear Assignment Problems using GCN

The GCN design: Consider the GCN with $N+R$ nodes, adjacency/weight matrix $\mathbf{A} = \begin{bmatrix} 0 & C \\ C^T & 0 \end{bmatrix}$ and data matrix $X = \begin{bmatrix} \nu(C(i,:)) \\ \nu(C^T(j,:)) \end{bmatrix}$.

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Key observation: When $C = uv^T$, that is, when the cost matrix is rank one then:

1. Objective Function: $J(\Pi; C) = u^T \Pi v = \langle \Pi v, u \rangle$
2. GCN output when no bias ($B_j = 0$): $\Gamma = \begin{bmatrix} \Gamma_1 \\ \Gamma_2 \end{bmatrix}$ satisfies $\Gamma_1 \Gamma_2^T = \alpha C$.

Consequence: the "greedy" algorithm produces the optimal solution.

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Consequence: the "greedy" algorithm produces the optimal solution.

Network Objective: Once trained, the GCN produces a latent representation $Z = \Gamma_1 \Gamma_2^T$ close to the input cost matrix C so that the greedy algorithm applied on Z produces the optimal solution.

Quadratic Assignment Problem using GCN

Preliminary result

The GCN Design: Consider the GCN with n nodes, adjacency/weight matrix $\mathbf{A} = \begin{bmatrix} 0 & AB \\ BA & 0 \end{bmatrix}$ and data matrix $X = \begin{bmatrix} A \\ B \end{bmatrix}$.

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Key observation: When $A = uu^T$ and $B = vv^T$, that is, when the matrices are rank one then:

1. Objective function: $J(\Pi; A, B) = (u^T \Pi v)^2 = (\langle \Pi v, u \rangle)^2$
2. GCN output when no bias (($B_j = 0$): $\Gamma = \begin{bmatrix} \Gamma_1 \\ \Gamma_2 \end{bmatrix}$ satisfies $\Gamma_1 \Gamma_2^T \sim uv^T$.

Consequence: the "greedy" algorithm or the solution to the linear assignment problem associated to uv^T produces the optimal solution.

Quadratic Assignment Problem using GCN
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Consequence: the "greedy" algorithm or the solution to the linear assignment problem associated to uv^T produces the optimal solution.

Network Objective: Once trained, the GCN produces a latent representation $Z = \Gamma_1 \Gamma_2^T$ so that the linear assignment problem associated to Z produces the same optimal permutation.

Deep Neural Networks as Universal Approximators

$$
\begin{array}{cc}
\textit{minimize/maximize} & \sum_{i=1}^{N}\sum_{j=1}^{R}\pi_{i,j}C_{i,j} \\
\text{subject to:} & \\
\pi_{i,j}\in\{0,1\}\ ,\ \forall i,j & \\
\sum_{i=1}^{N}\pi_{i,j}=1\ ,\ \forall 1\leq j\leq R & \\
\sum_{j=1}^{R}\pi_{i,j}\leq 1\ ,\ \forall 1\leq i\leq N &
\end{array}
$$

Luckily, the convex relaxation (Linear Program) produces the same optimal solution:

$$
\begin{array}{cc}
\textit{minimize} & \sum_{i=1}^{N}\sum_{j=1}^{R}\pi_{i,j}C_{i,j} \\
\text{subject to:} & \\
0\leq\pi_{i,j}\leq 1\ ,\ \forall i,j & \\
\sum_{i=1}^{N}\pi_{i,j}=1\ ,\ \forall 1\leq j\leq R & \\
\sum_{j=1}^{R}\pi_{i,j}\leq 1\ ,\ \forall 1\leq i\leq N &
\end{array}
$$

Deep Neural Networks as Universal Approximators

Architectures

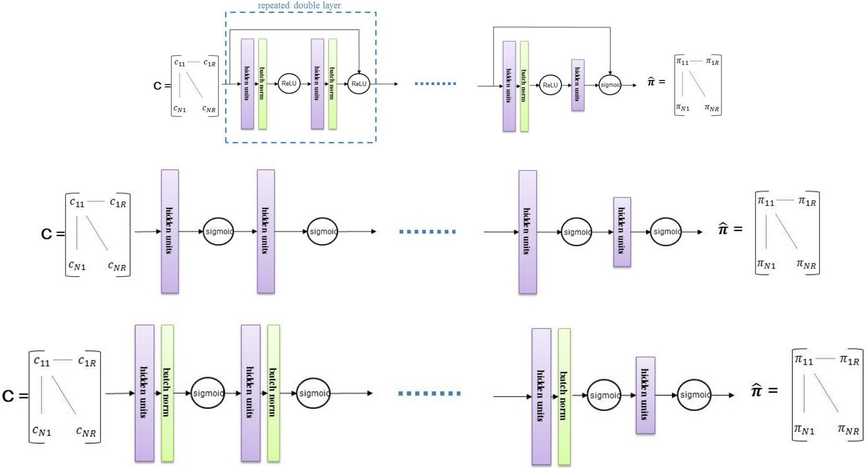
The overall system must output feasible solutions $\hat{\pi}$. Our architecture compose two components: (1) a deep neural network (DNN) that outputs a (generally) unfeasible estimate $\bar{\pi}$; (2) an enforcer (P) of the feasibility conditions that outputs the estimate $\hat{\pi}$:

Issues:

1. DNN architecture: how many layers; how many neurons per layer?
2. P, the feasibility enforcer

Deep Neural Networks as Universal Approximators
DNNs

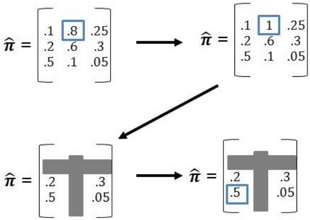
We studied three architectures:



Deep Neural Networks as Universal Approximators
Feasibility Enforcer P

An "optimal" feasibility condition enforcer would minimize some "distance" to the feasibility set. However this may be a very computationally expensive component. An intermediate solution is to alternate between different feasibility conditions (equalities and inequalities) until convergence.
Instead we opt for a simpler and "greedier" approach:

Repeat R times:
1. Find (i,j) the largest entry in $\bar{\pi}$
2. Set $\hat{\pi}_{i,j} = 1$; set to 0 other entries in row i and column j;
3. Remove row i and column j from both $\bar{\pi}$ and $\hat{\pi}$.



Deep Neural Networks as Universal Approximators

Baseline solution: The Greedy Algorithm

The "greedy" enforcer can be modified into a "greedy" optimization algorithm:

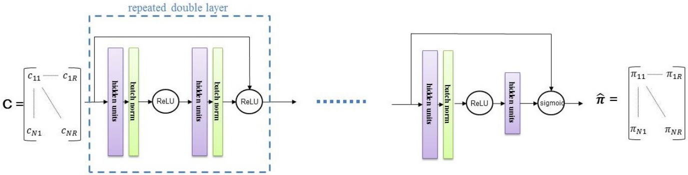
1. Initialize $E = C$ and $\hat{\pi} = 0_{N \times R}$
2. Repeat R times:
   - Find $(i, j) = argmin_{(a,b)} E_{a,b}$;
   - Set $\hat{\pi}_{i,j} = 1$, $\hat{\pi}_{i,l} = 0 \ \forall l \neq j$, $\hat{\pi}_{l,j} = 0 \ \forall l \neq i$;
   - Set $E_{i,:} = \infty$, $E_{:,j} = \infty$.

Proposition

The greedy algorithm produces the optimal solution if there is a positive number $\lambda > 0$ and two nonnegative vectors u, v such that $C = \lambda 1 \cdot 1^T - u \cdot v^T$.

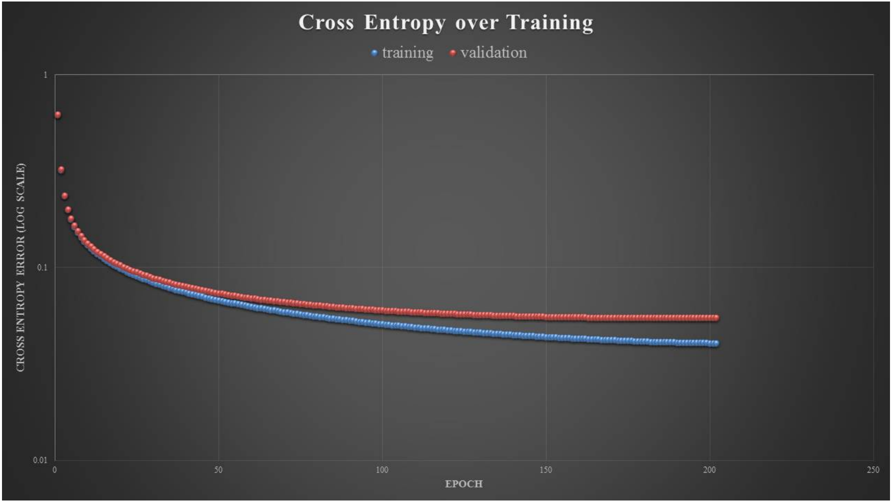
Exp.1 : $N = 5$, $R = 4$ with ReLU activation

First architecture:



- Number of internal layers: 9
- Number of hidden units per layer: 250
- Batch size: 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 1 million random instances $U(0,1)$ i.i.d.
- Validation set: 20,000 random instances.

Exp.1 : $N = 5$, $R = 4$ with ReLU activation



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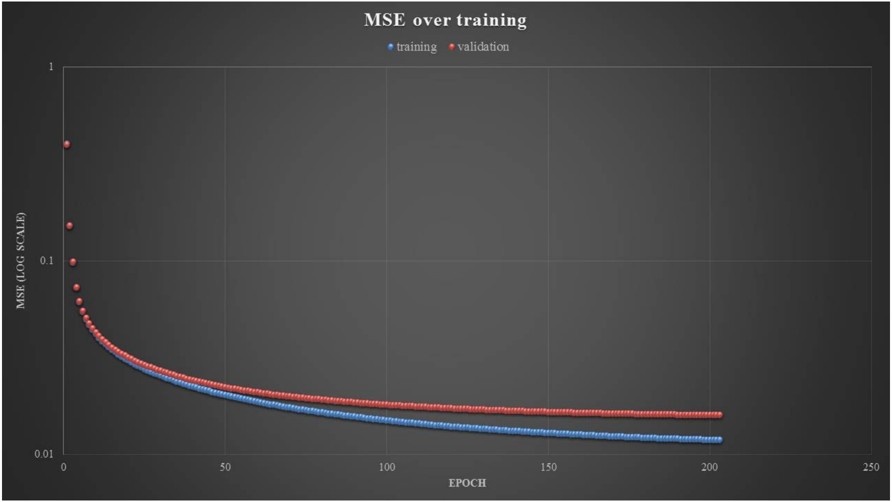

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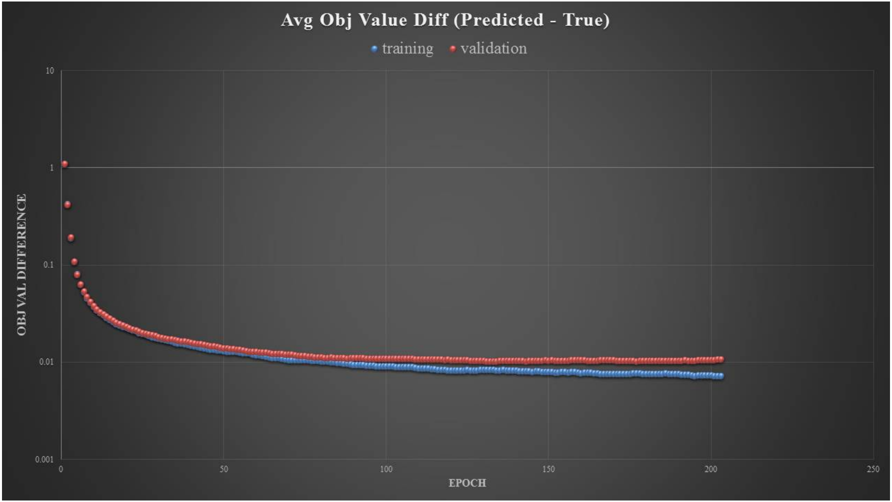

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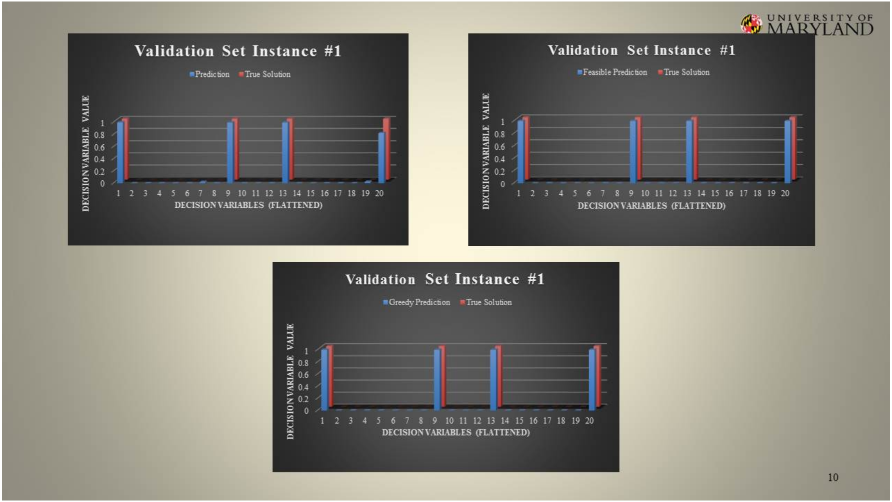

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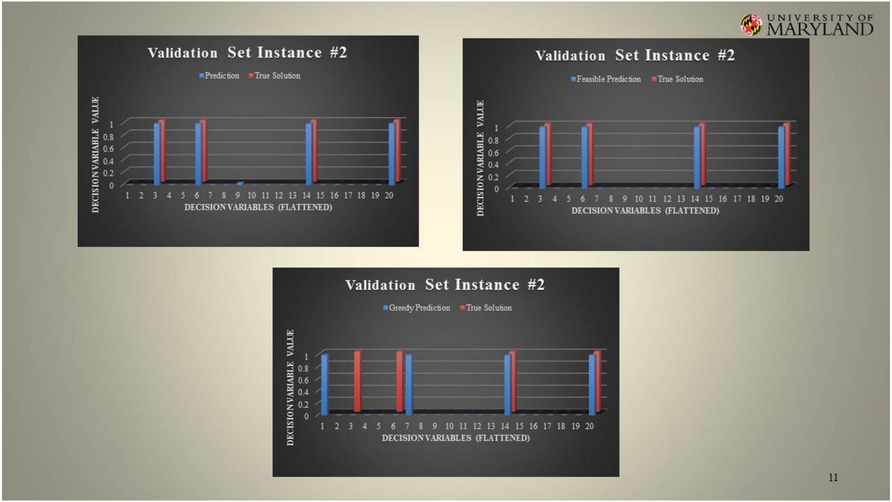
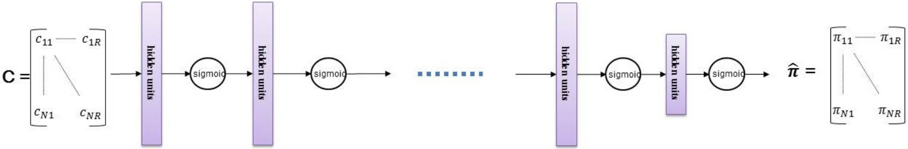


Exp.2 : $N = 10$, $R = 8$ with sigmoid activation

Second architecture:



- Number of internal layers: 10
- Number of hidden units per layer: 250
- No Batch; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1-\pi_{i,j})(-log(1-\hat{\pi}_{i,j}))$
- Training data set: 1 million random instances $U(0,1)$ i.i.d.
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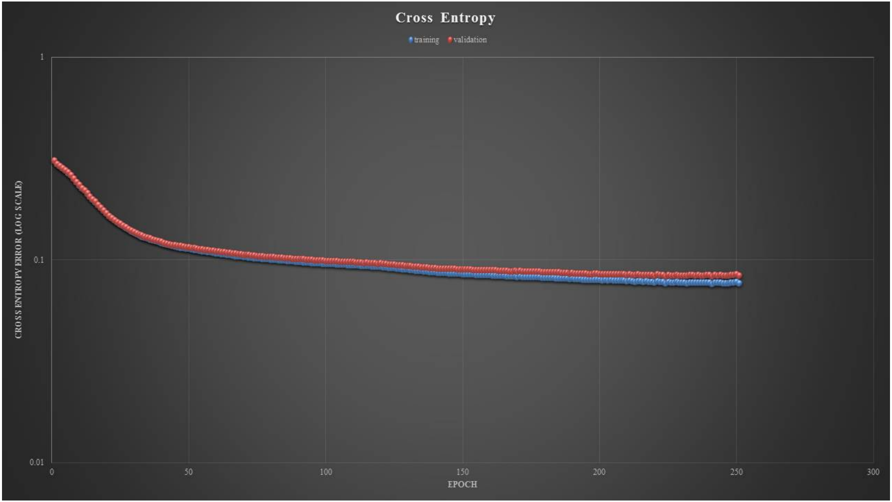
Exp.2 : $N = 10$, $R = 8$ with sigmoid activation



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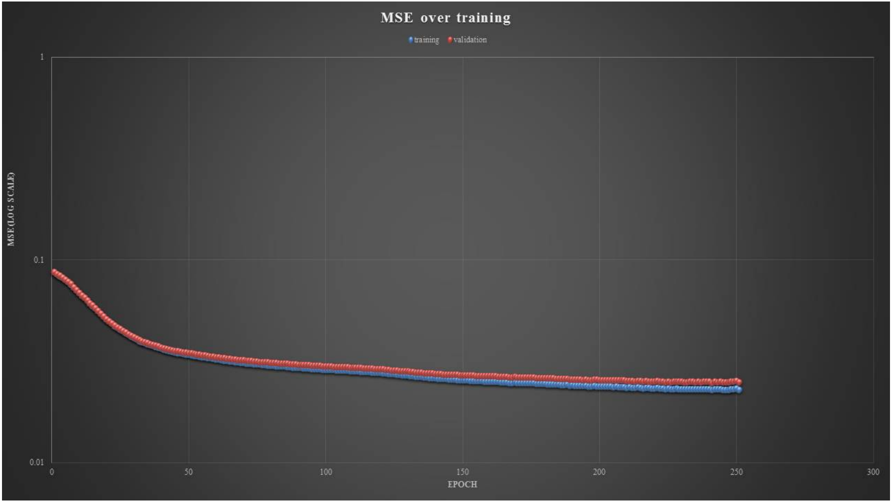

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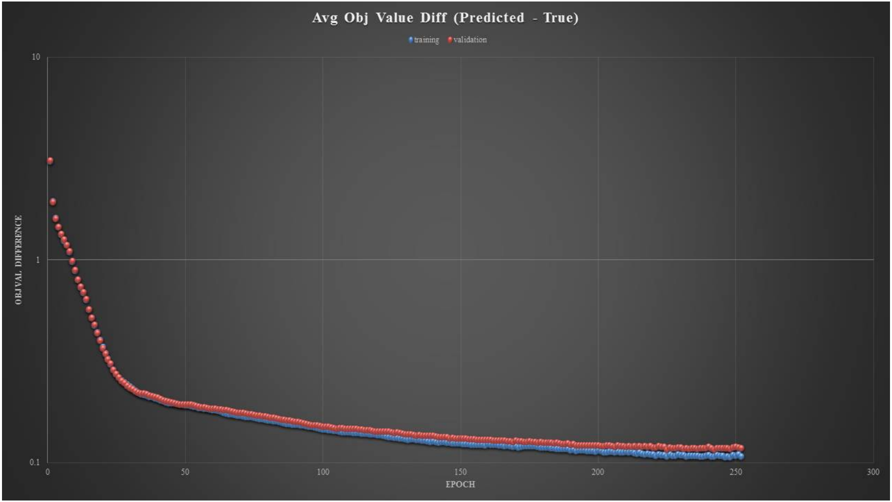

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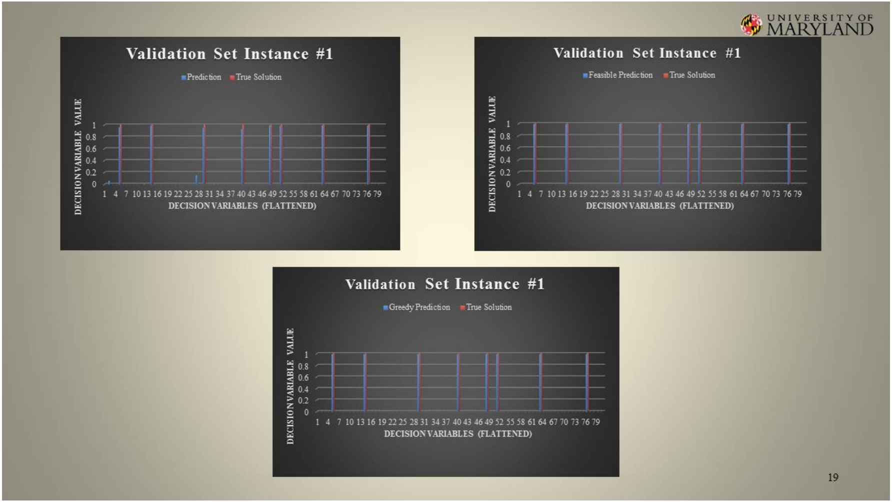
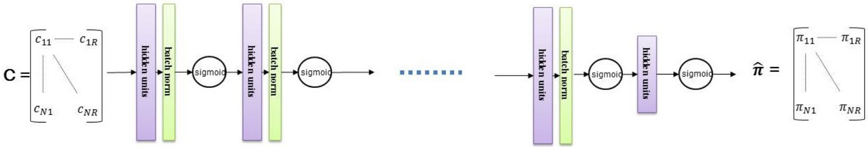


Exp.2 : $N = 10$, $R = 8$ with sigmoid activation

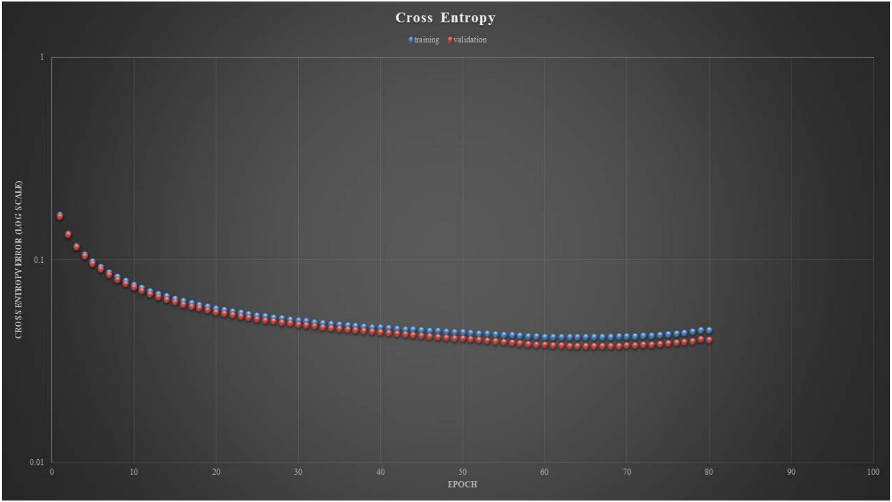
Exp.3 : $N = 5$, $R = 4$ with sigmoid activation

Second architecture:

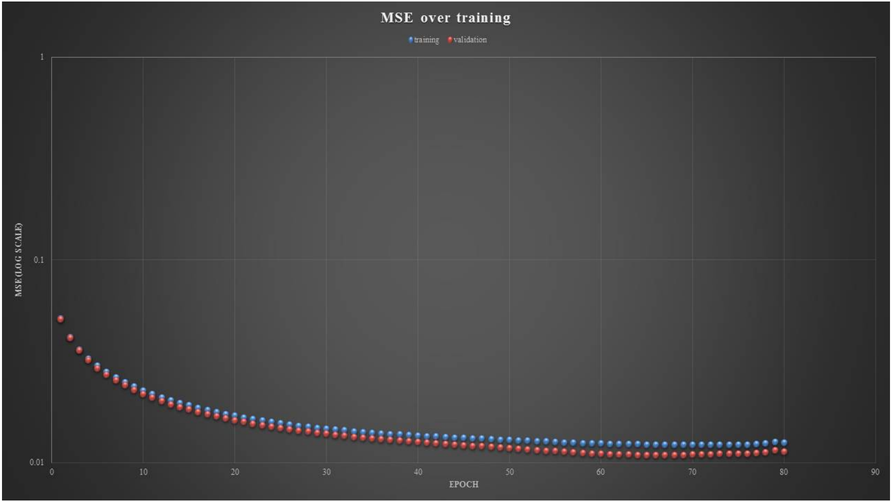


- Number of internal layers: 10
- Number of hidden units per layer: 250
- Batch size 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 500,000 random instances $U(0, 1)$ i.i.d.
- Validation set: 20,000 random instances.

Exp.3 : $N = 5$, $R = 4$ with sigmoid activation



Exp.3 : $N = 5$, $R = 4$ with sigmoid activation



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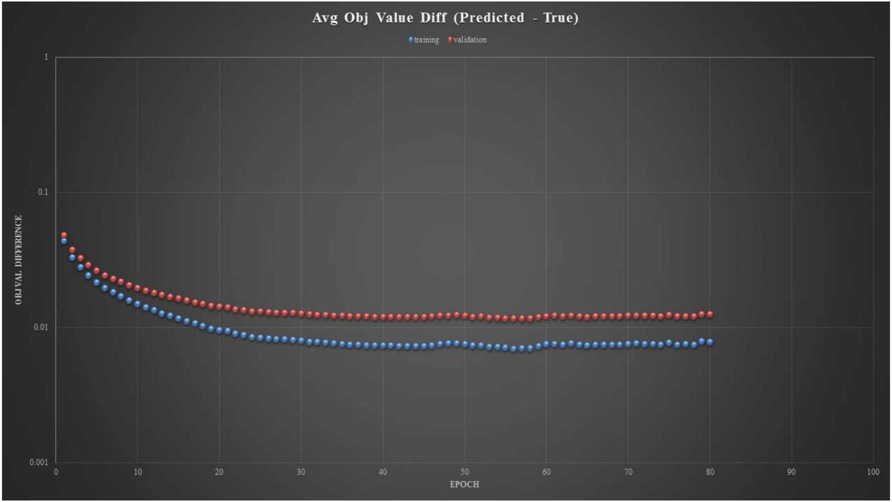

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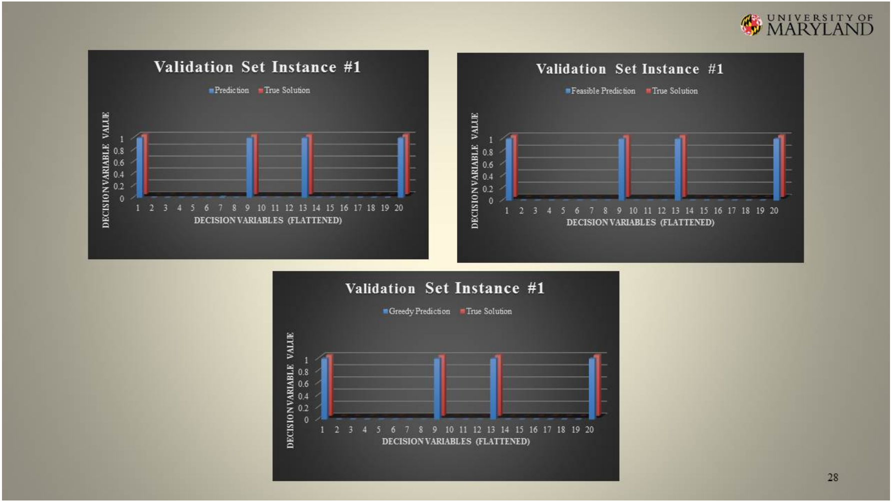

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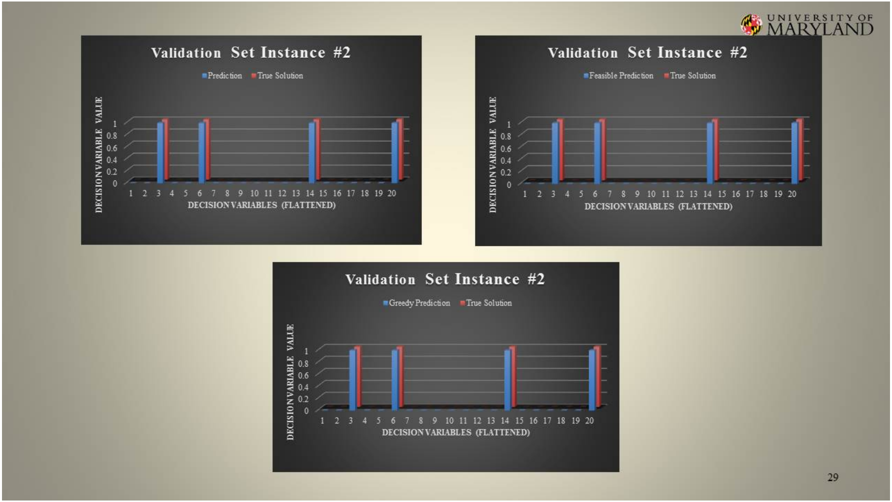
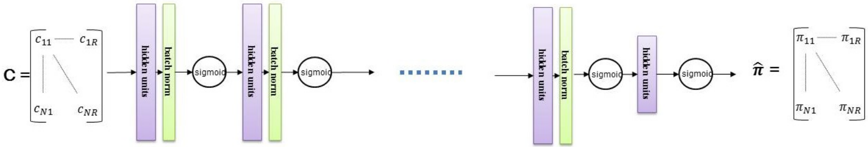


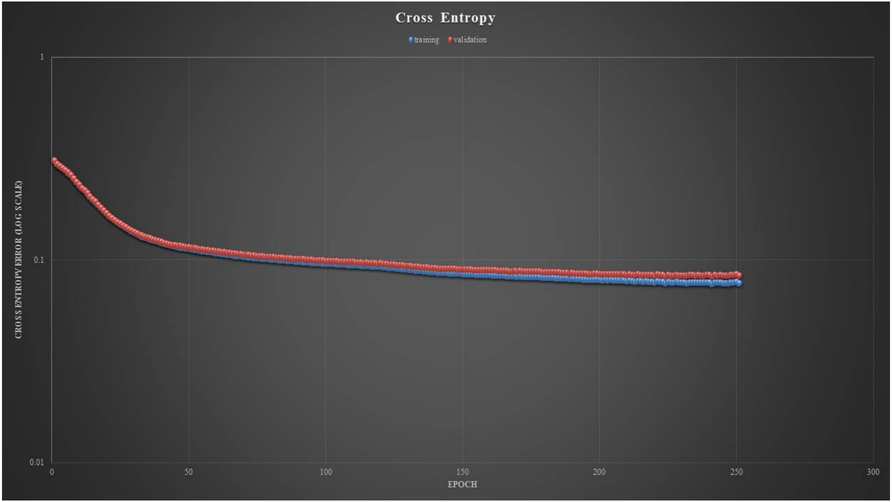
Exp.4 : $N = 10$, $R = 8$ with sigmoid activation

Second architecture:



- Number of internal layers: 10
- Number of hidden units per layer: 300
- Batch size 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 500,000 random instances $U(0,1)$ i.i.d.
- Validation set: 20,000 random instances.

Exp.4 : $N = 10$, $R = 8$ with sigmoid activation



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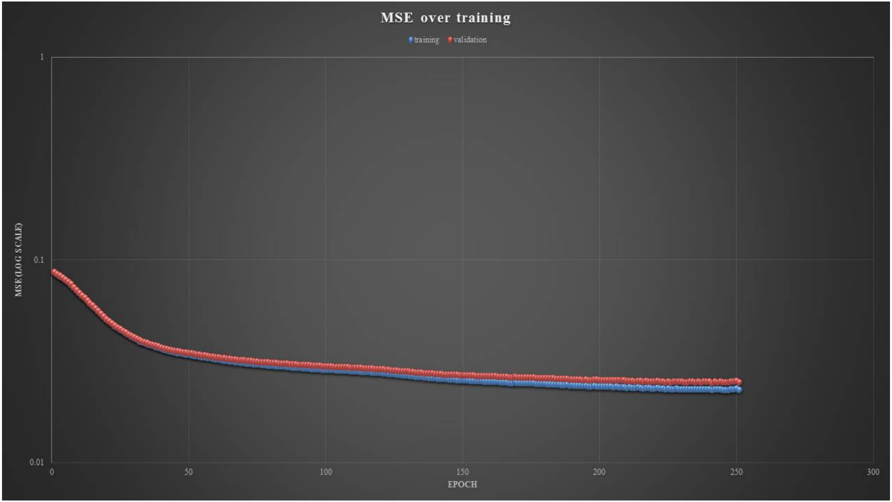

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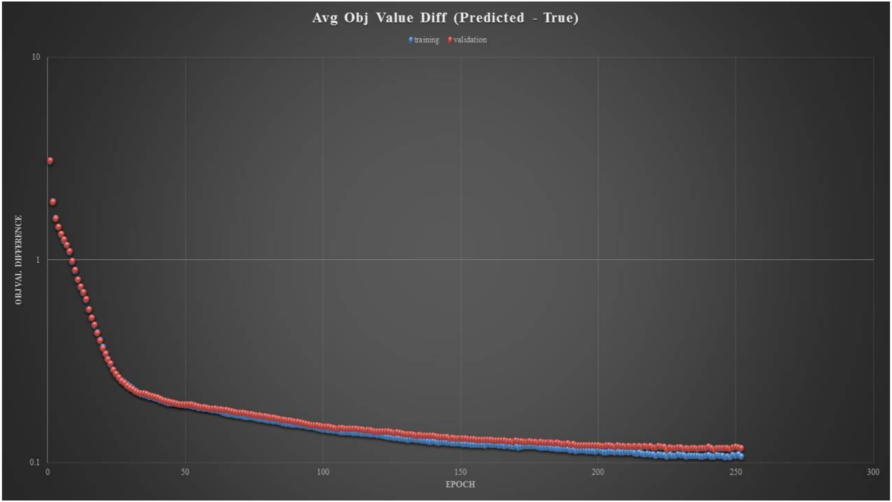

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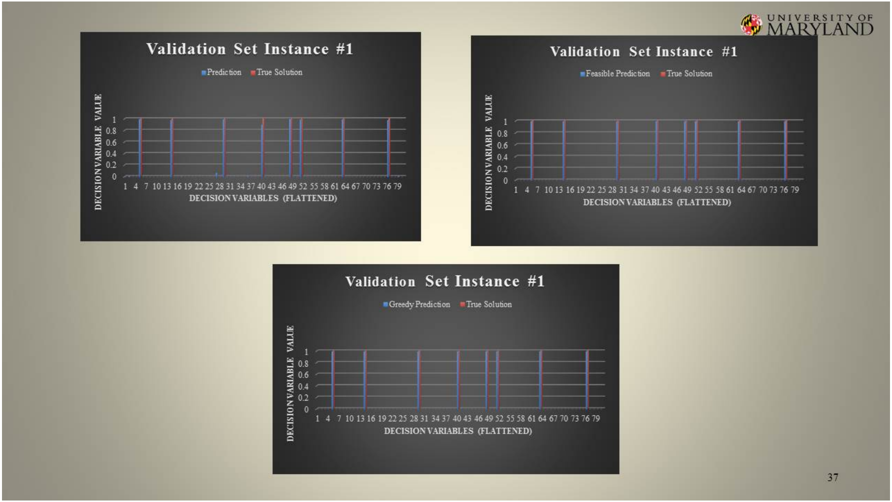

Exp.4 : $N = 10$, $R = 8$ with sigmoid activation

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