Optimizations using Deep Learning

Radu Balan, Naveed Haghani

Department of Mathematics, Applied Mathematics Applied Statistics and Scientific Computing
University of Maryland, College Park, MD

Joint work with **Maneesh Singh** (Verisk)

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Acknowledgments

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Optimization Problems

Consider a general optimization problem:

$$\begin{aligned} &\textit{minimize} && J(x;y) \\ &\textit{subject to}: && \\ &x \in D && \\ &g(x;y) \leq 0 && \\ &h(x;y) = 0 && \end{aligned}$$

where $y \in E \subset \mathbb{R}^d$ denotes a set of parameters (or input) into the optimization problem, D denotes the allowable domain for the unknown variable x, $g, h : D \times E \to \mathbb{R}$ (or $\bar{R}$) define the constraints (D can be define implicit by an indicator function constraint), and $J(x;y)$ is the objective function.

Purpose of this talk: How can deep learning solve optimization problems?

Optimization Problems
General Approaches

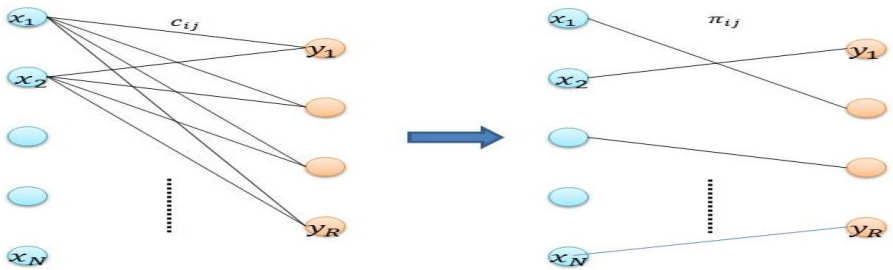
We plan to discuss three approaches to an optimization problem:

1. Deep Neural Network (DNN) as a Universal Approximator (UA)
2. Neural Network as an auxiliary function of an iterative algorithm
3. Deep Neural Network as a representation tool

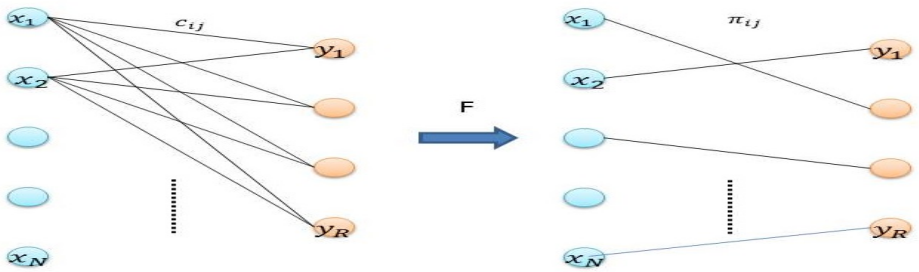
The Specific Optimization Problem

Consider a $N \times R$ cost 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 matching/assignment, namely:

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



First Approach: DNN as a Universal Approximator



The optimal solution of this (or any optimization problem) is a nonlinear map $\pi = F(C)$.

Idea: Generate optimal pairs $\{(C, \pi)\}$ and then train a Neural Network to reproduce these values.

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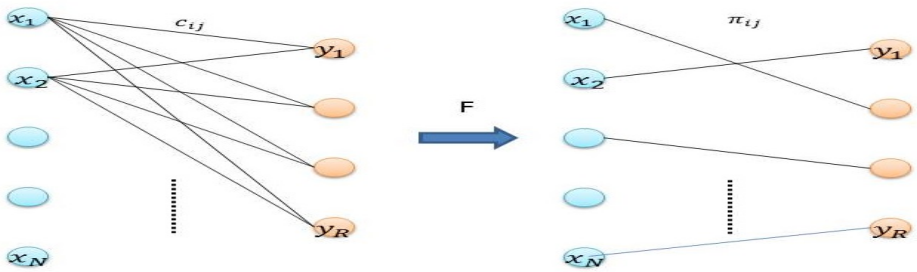

The optimal solution of this (or any optimization problem) is a nonlinear map $\pi = F(C)$.

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Issues to be discussed:

1. How to generate optimal pairs?
2. Network architecture: how many layers? how many nodes in each layer?
3. How to enforce feasibility?
4. Primal problem – what about the dual problem?

Second Approach: Emulate an Iterative Descent Algorithm

For the optimization problem $min_x\ J(x)$ use an iterative algorithm:

$$x^{(t+1)} = x^{(t)} - \alpha_t p^{(t)}$$

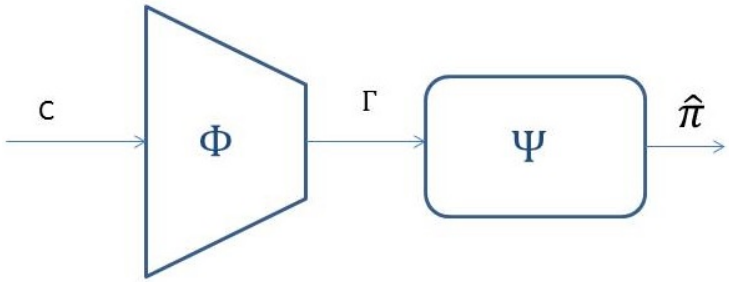
where $x^{(t)}$ is the current estimate, α_t is the step size at step t, and $p^{(t)}$ is the marching direction. Possible choices:

- Gradient Descent: $p_g^{(t)} = \nabla J(x^{(t)})$
- Newton method: $p_n^{(t)} = Hess^{(-1)} J(x^{(t)}) \nabla J(x^{(t)})$
- Mixed methods: $p^{(t)} = a_t p_g + b_t p_n + c_t p^{(t-1)}$

Idea: Implement a descent strategy, but adapt step size and learning rates using Neural Networks – Recurrent Neural Network.
See also: Google DeepMind group [Andrychowicz et.al. '16];

Third Approach: Optimization in a Representation Space

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 $\Phi : C \mapsto \Gamma$ can be learned using a Variational Auto-Encoder method.
The Optimization map $\Psi : \Gamma \mapsto \hat{\pi}$ can be implemented using a neural-network such as in the first approach.

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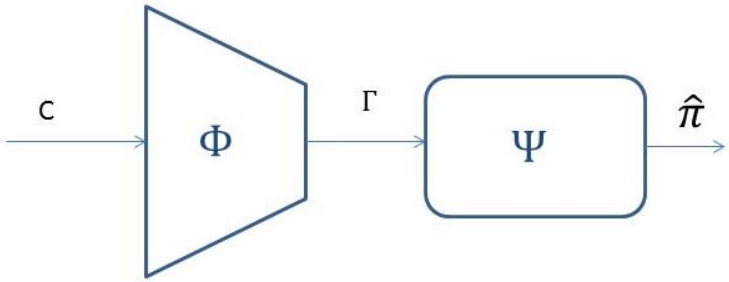


The nonlinear representation map $\Phi : C \mapsto \Gamma$ can be learned using a Variational Auto-Encoder method.
The Optimization map $\Psi : \Gamma \mapsto \hat{\pi}$ can be implemented using a neural-network such as in the first approach.
Why it makes sense? feasible solutions are graph representable – Use Graph Convolutive Networks (GCN – KipfWeiling) as a launching pad.
See also: [Nowak et.al.'18]

First Approach: DNN as a UA

Exact Solutions to Our Problem

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

Luckily, this problem admits an exact convex relaxation: the associated Linear Program produces the same optimal solution:

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

First Approach: DNN as a UA

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 $\hat{\pi}$:

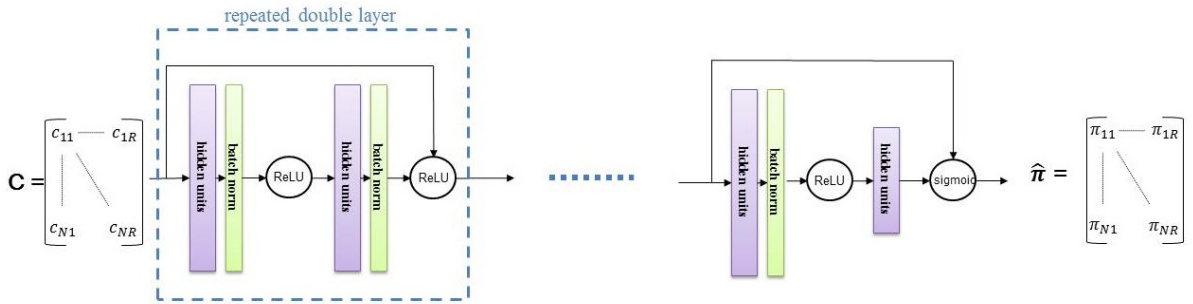
Issues to discuss:

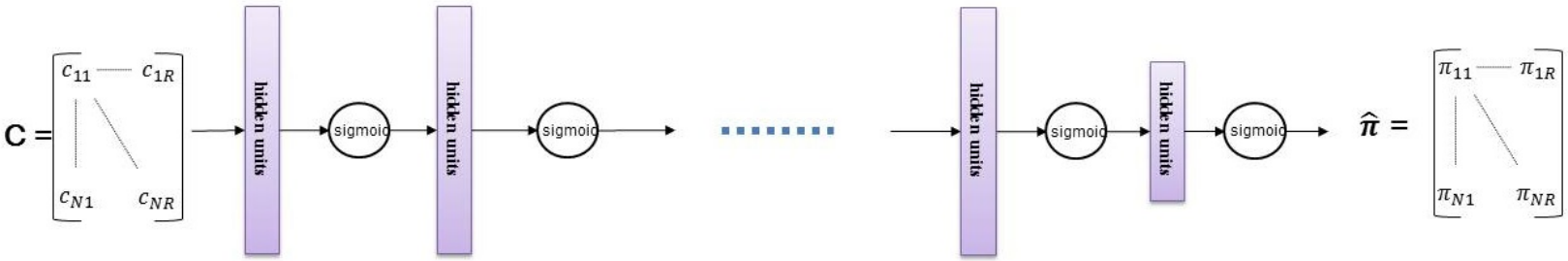
1. DNN architecture: how many layers; how many neurons per layer?
2. P, the feasibility enforcer

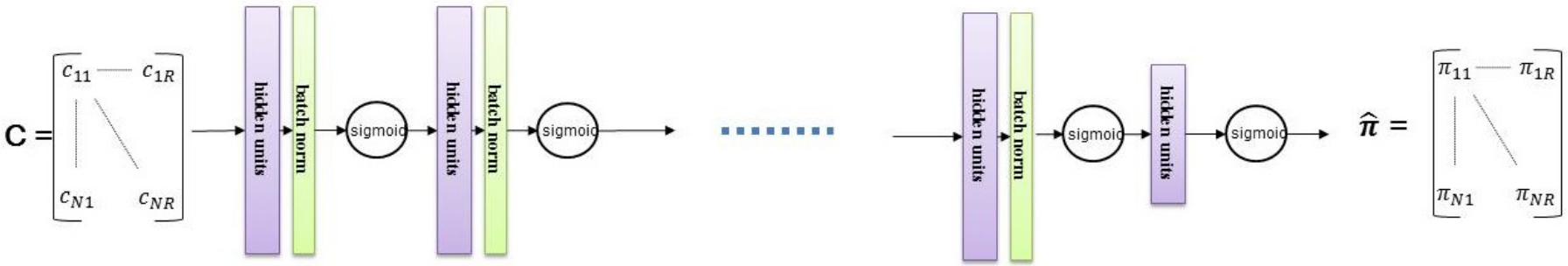
First Approach: DNN as a UA

DNNs

We study three architectures:





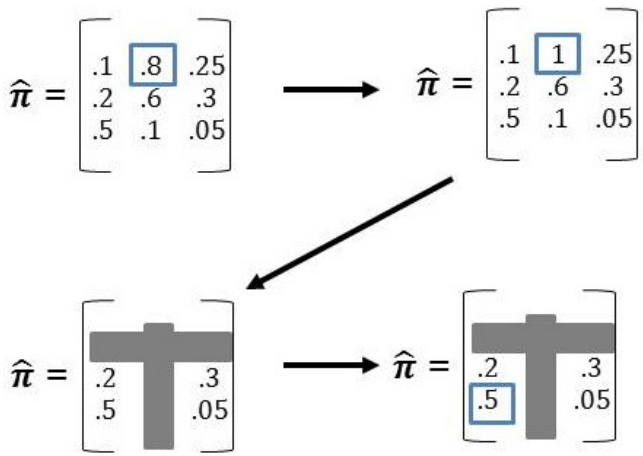


First Approach: DNN as a UA

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 $\hat{\pi}$.



First Approach: DNN as a UA

Baseline solution: The Greedy Algorithm

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

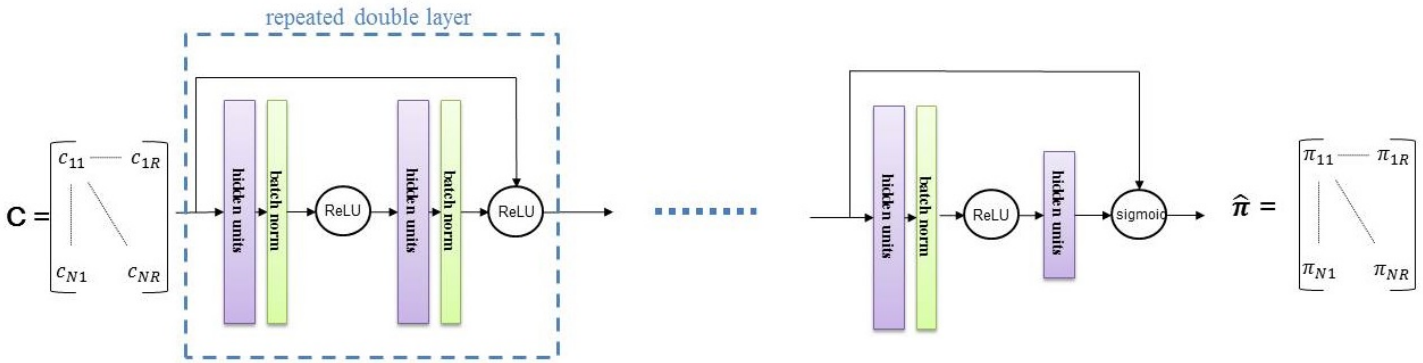
1. Initialize $E = C$ and $\hat{\pi} = 0_{N \times R}$
2. Repeat R times:
   - Find $(i, j) = argmin_{(a,b)} E_{a,b}$;
   - Set $\hat{\pi}_{i,j} = 1$, $\hat{\pi}_{i,l} = 0 \ \forall l \neq j$, $\hat{\pi}_{l,j} = 0 \ \forall l \neq i$;
   - Set $E_{i,:} = \infty$, $E_{:,j} = \infty$.

Proposition

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

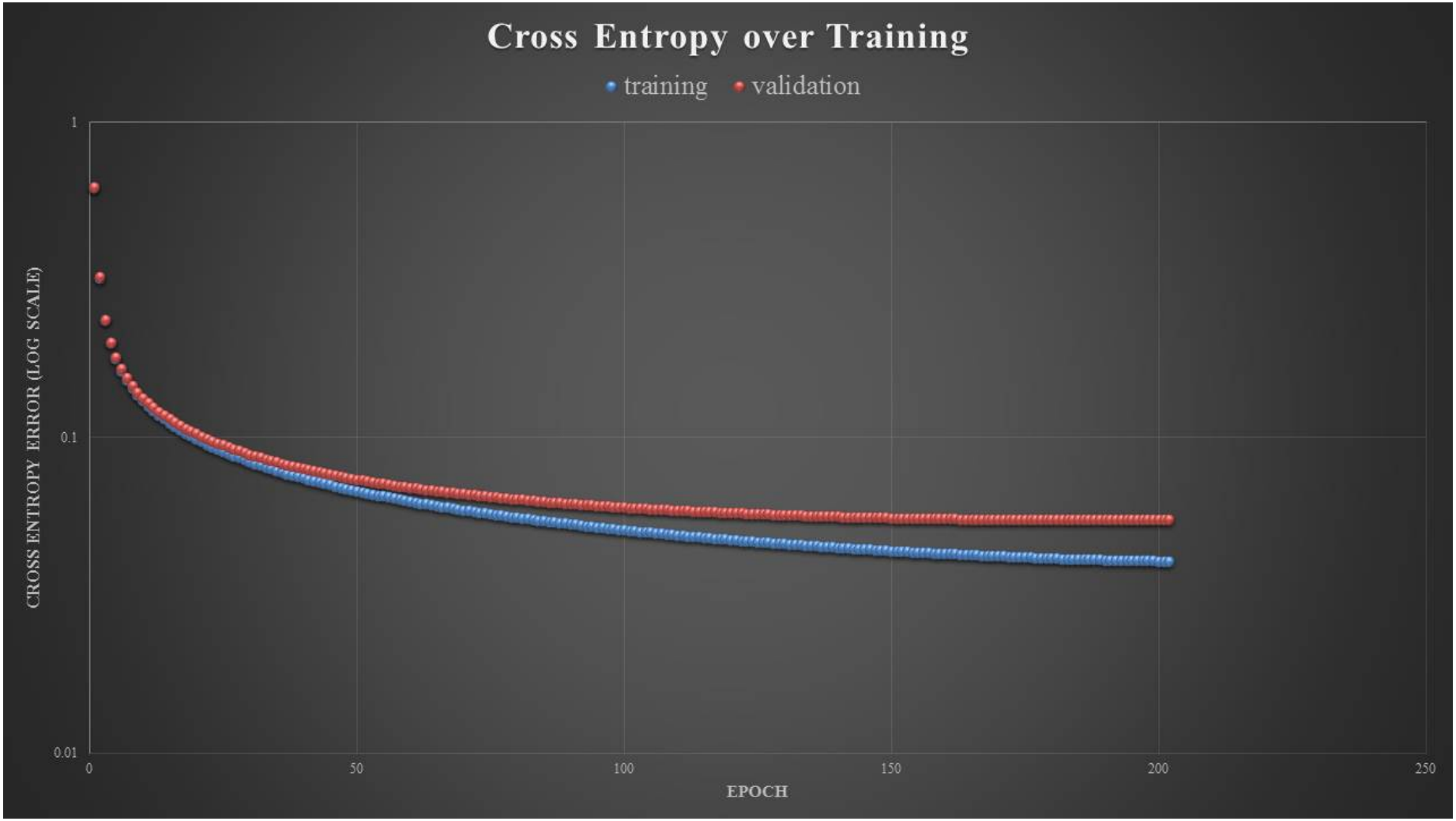
Exp.1 : $N = 5$, $R = 4$ with ReLU activation

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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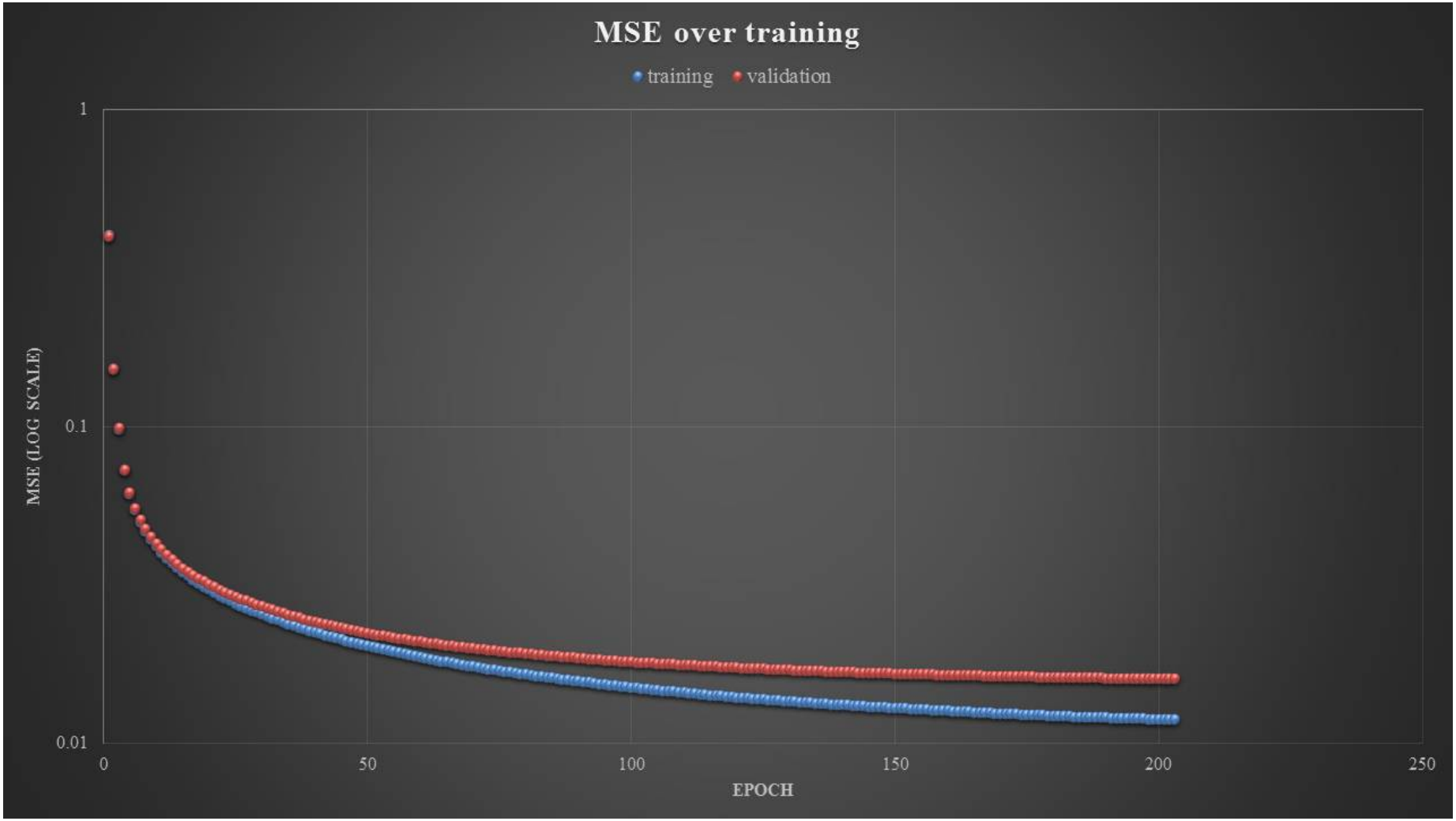

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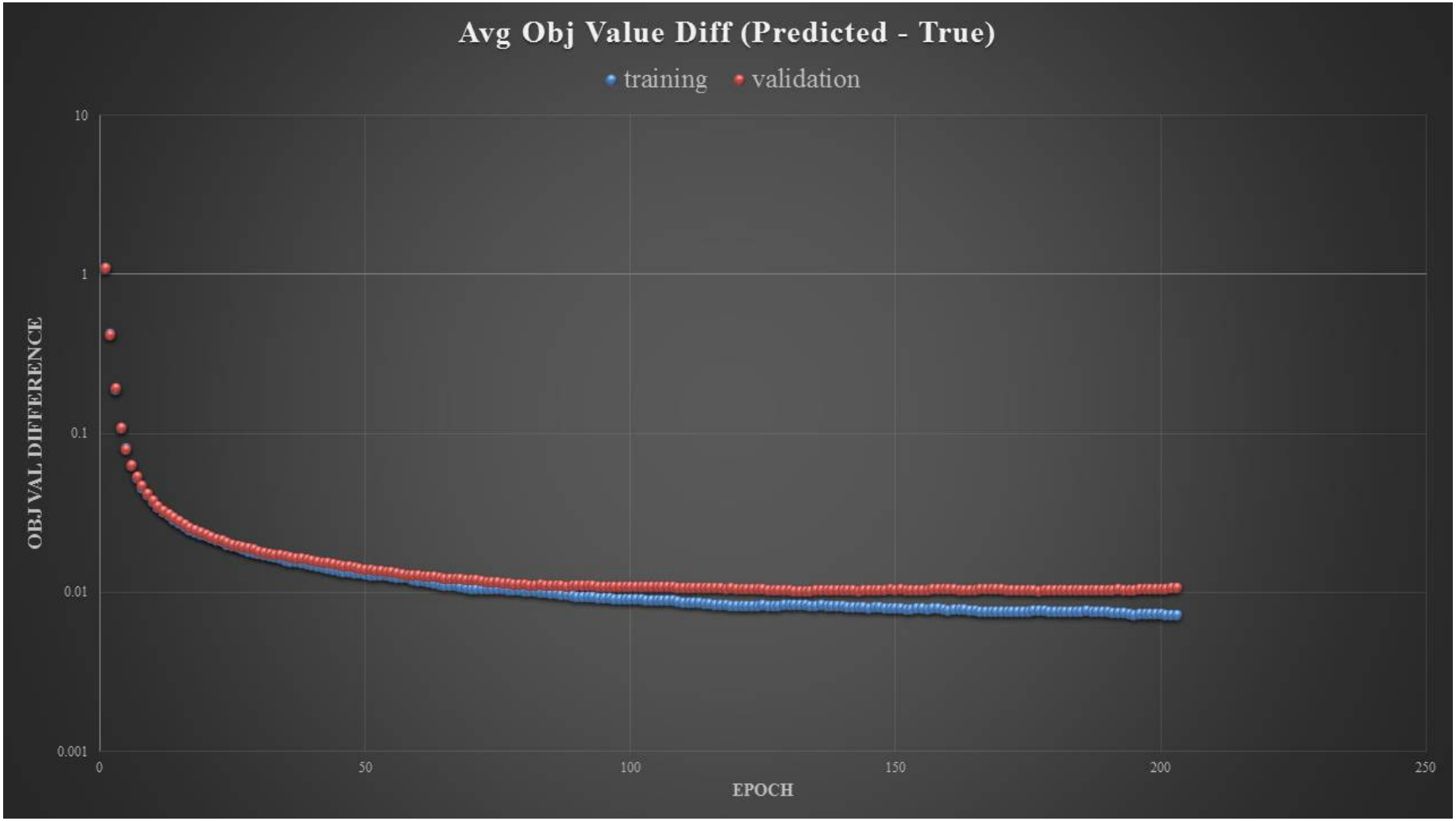

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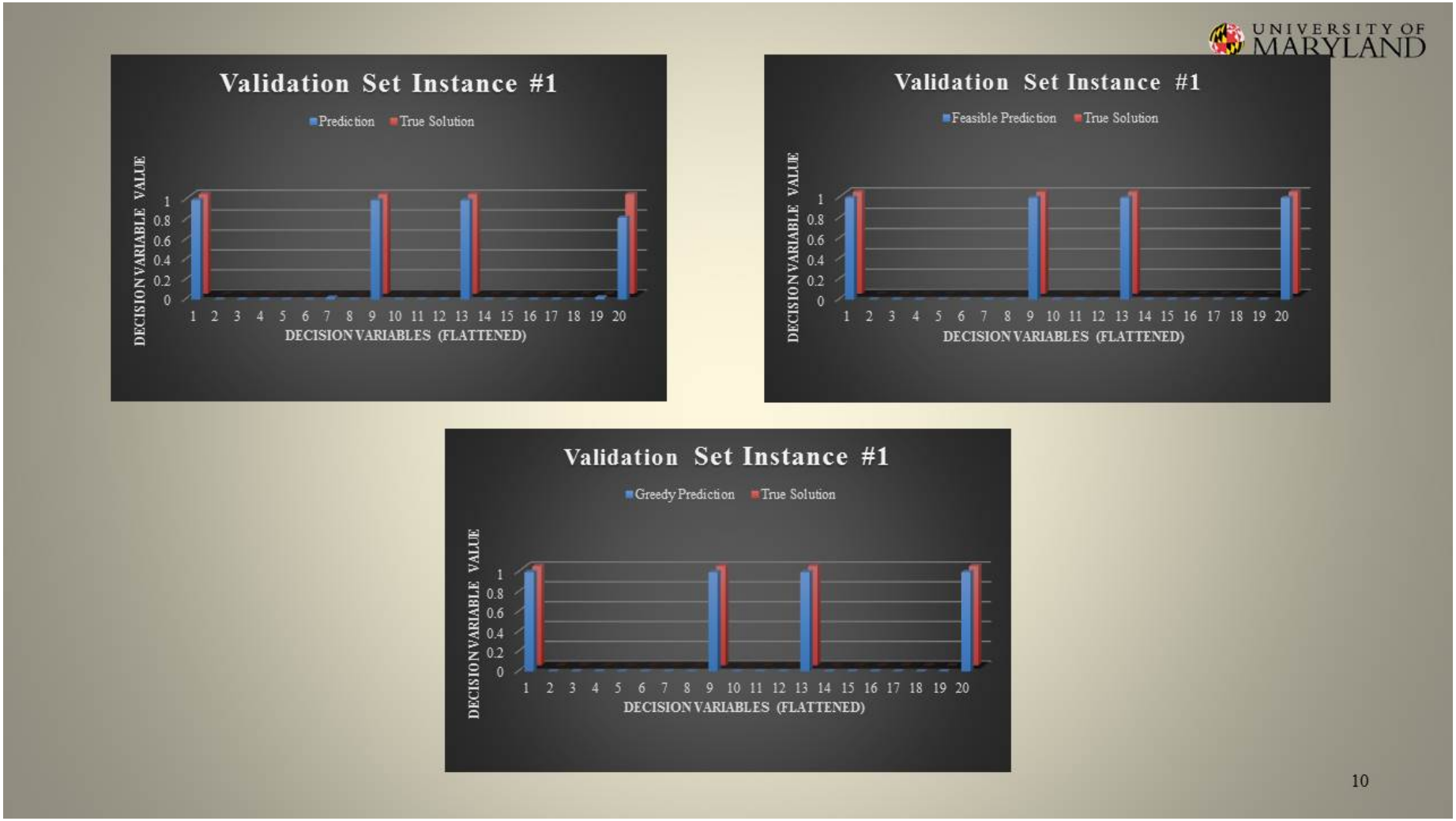

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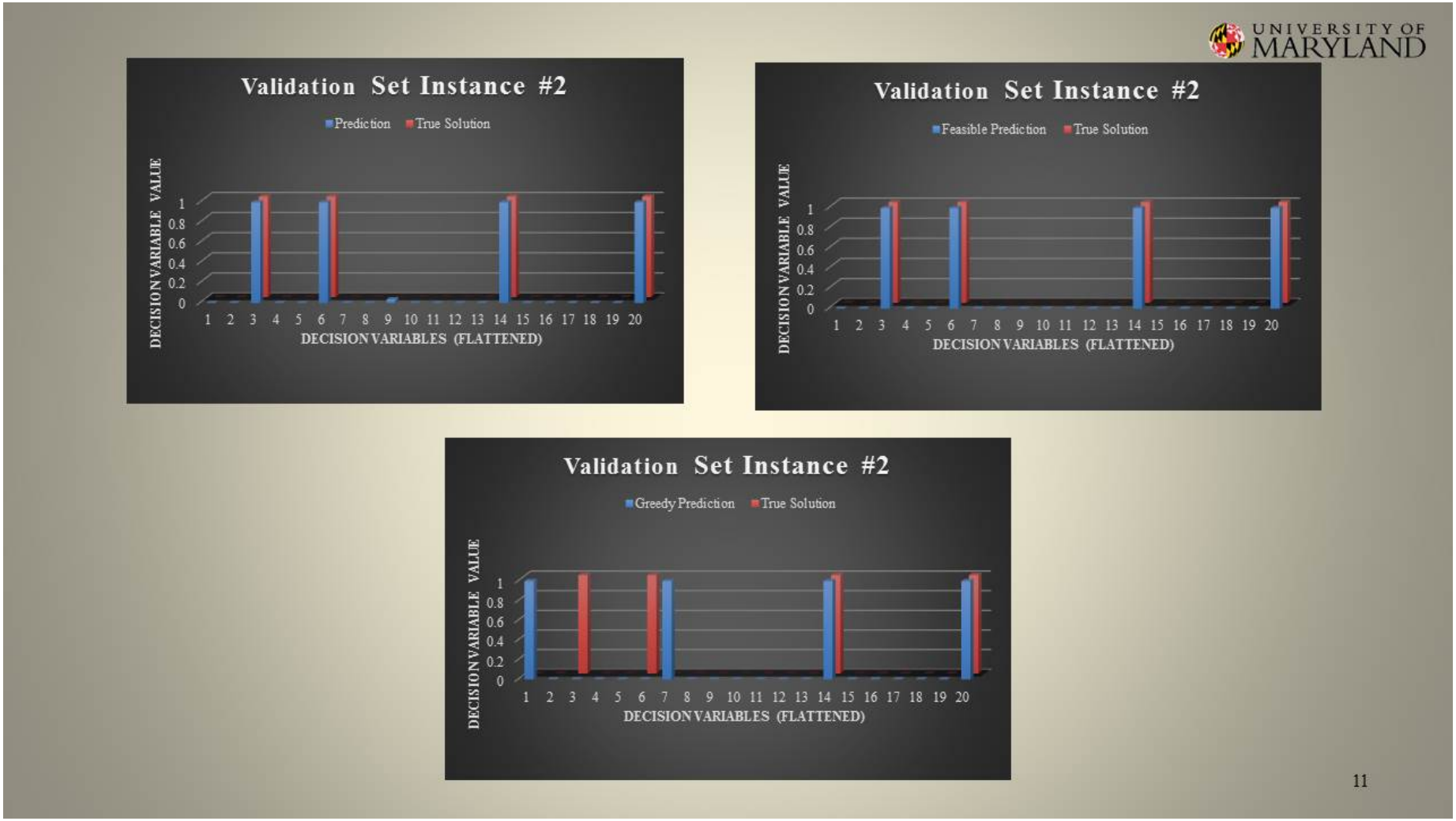
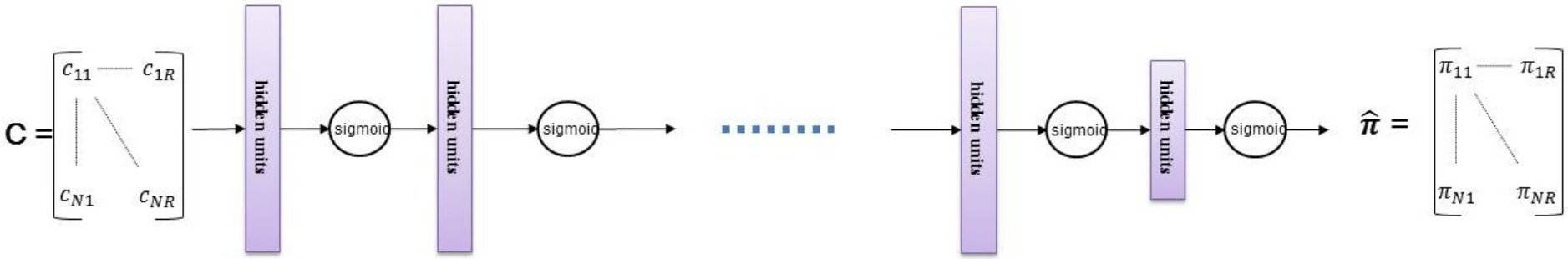


Exp.2 : $N = 10$, $R = 8$ with sigmoid activation

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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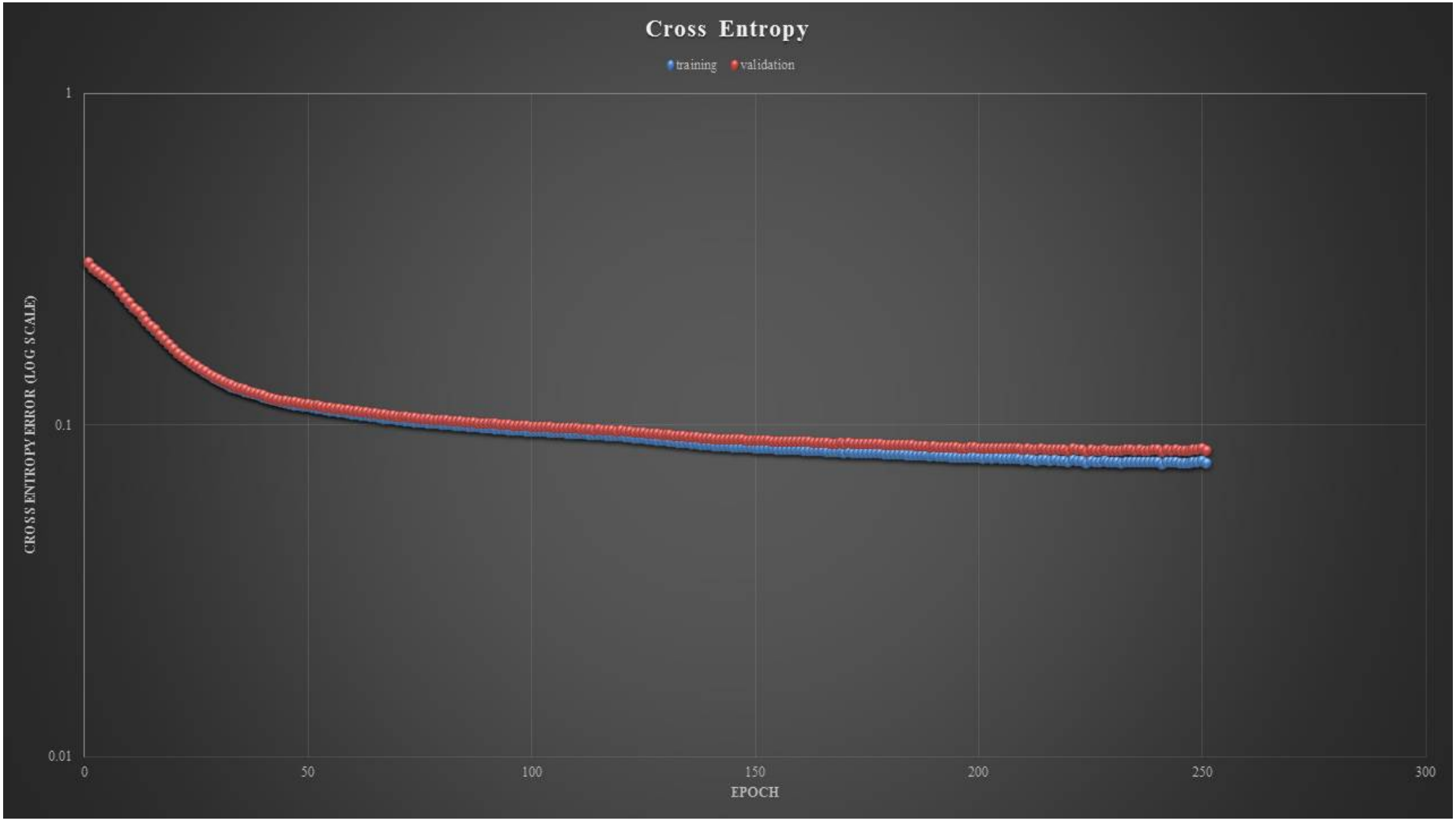

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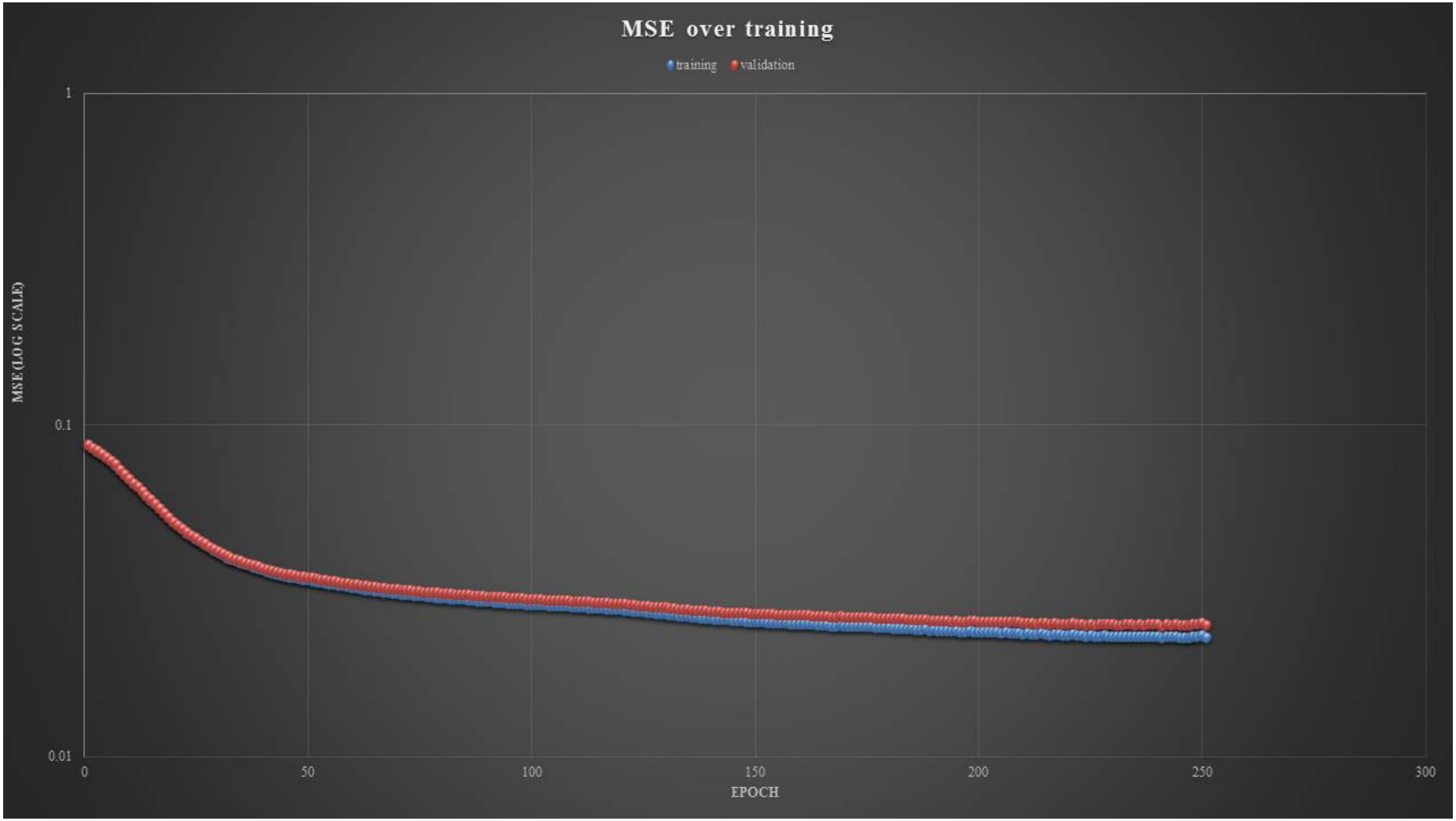

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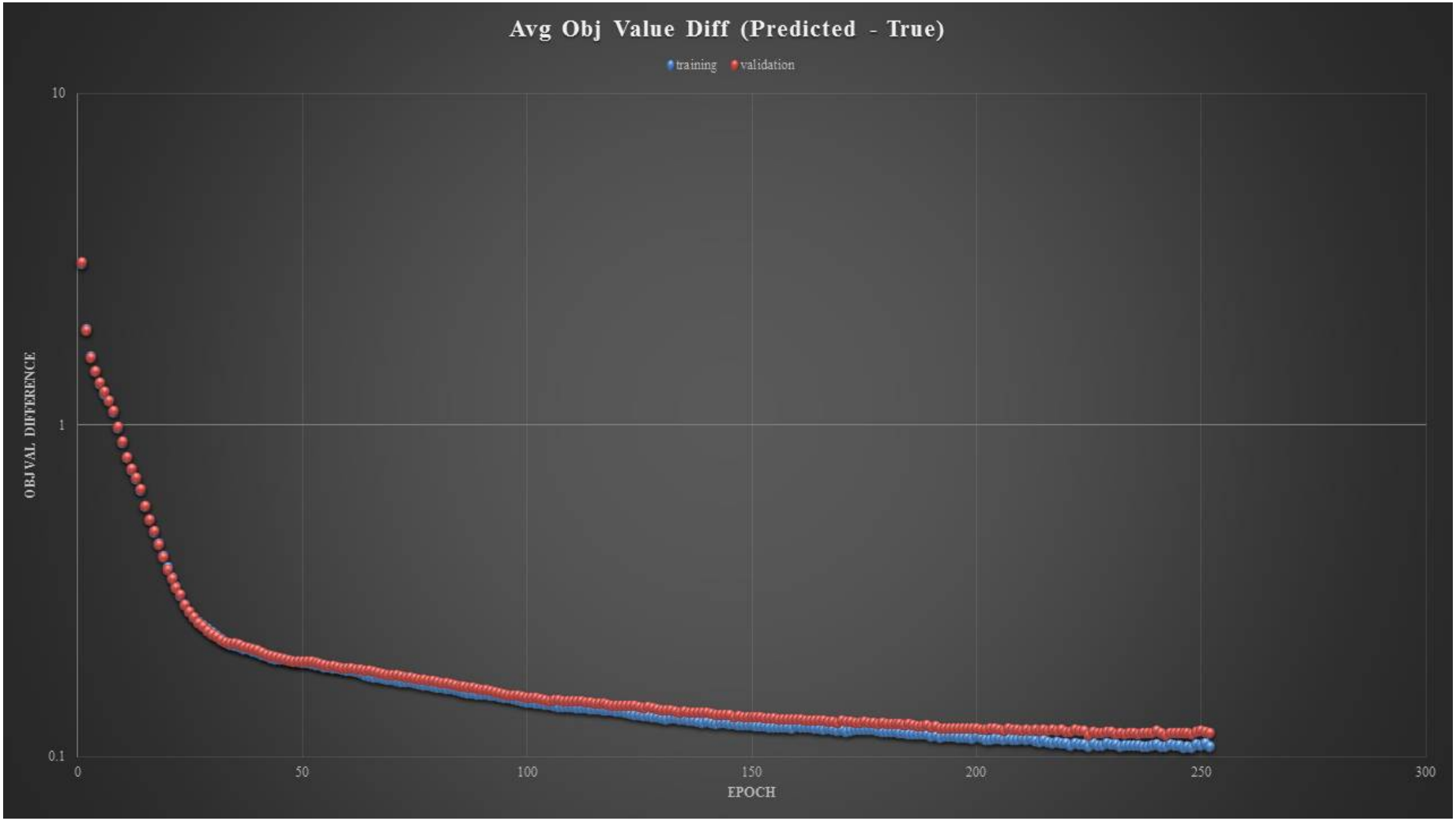

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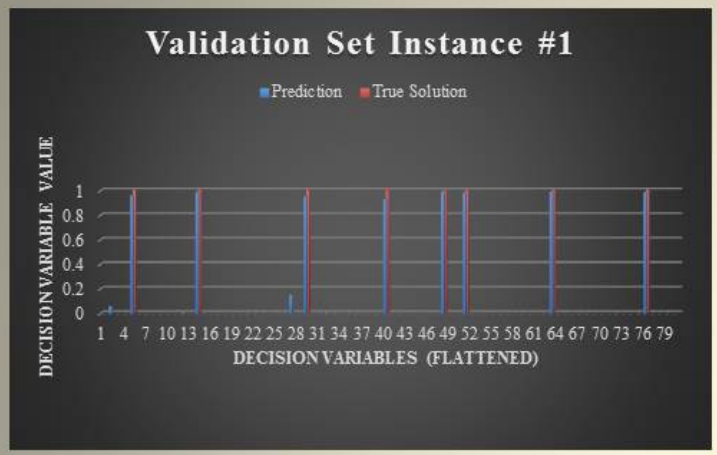

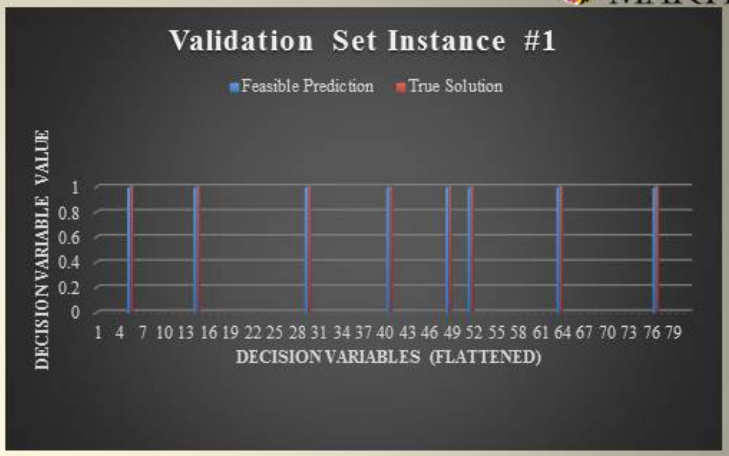

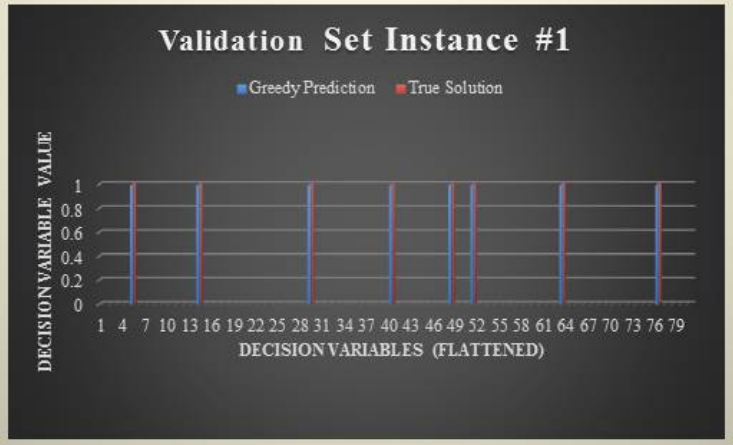

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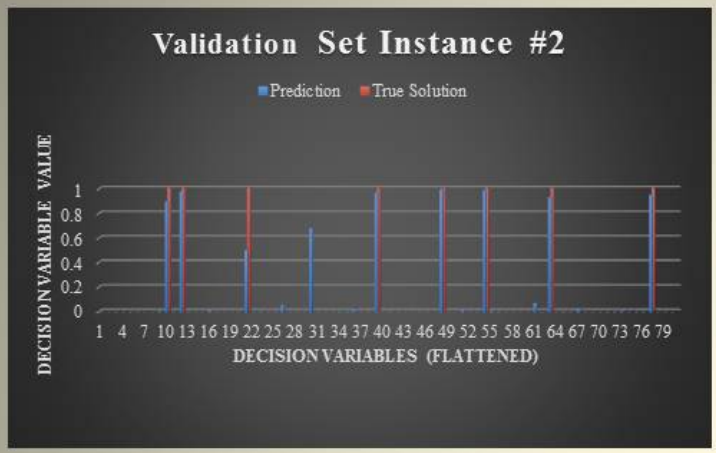

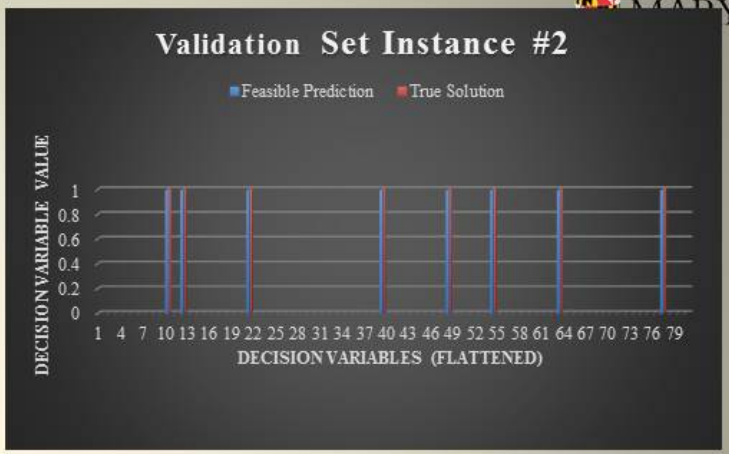

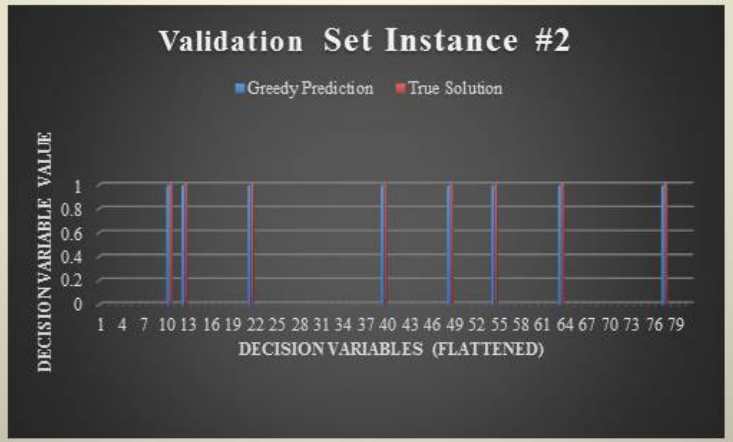

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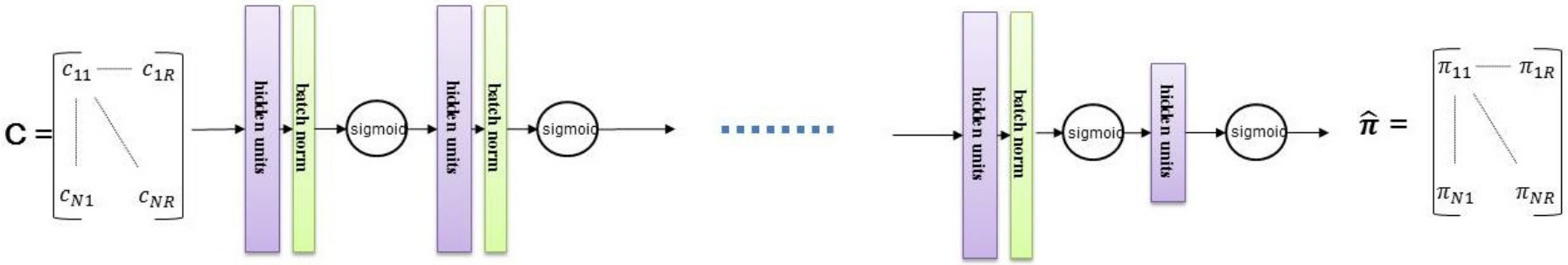
Exp.3 : $N = 5,\ R = 4$ with sigmoid activation

Second architecture:



- Number of internal layers: 10
- Number of hidden units per layer: 250
- Batch size 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
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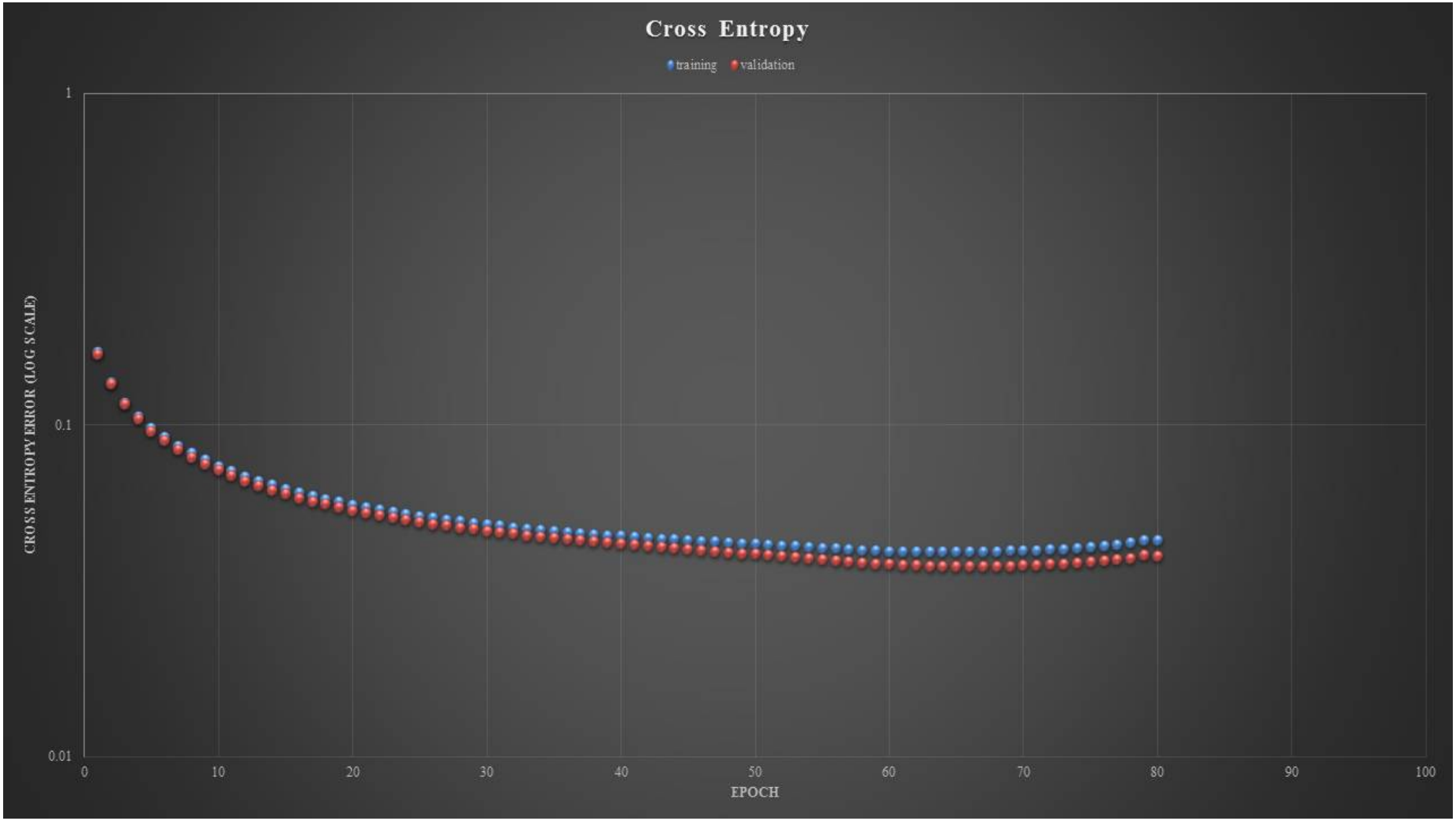

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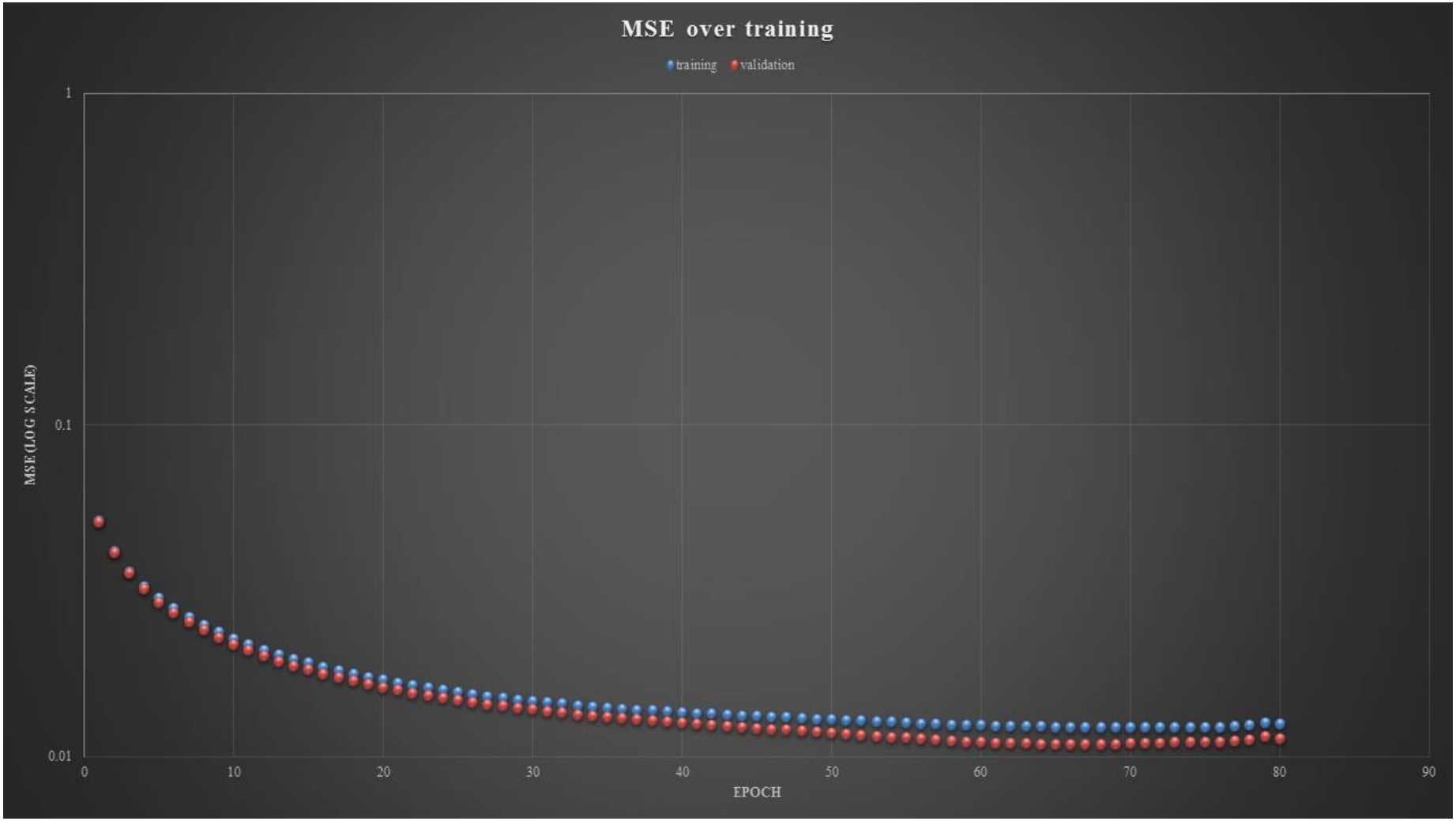

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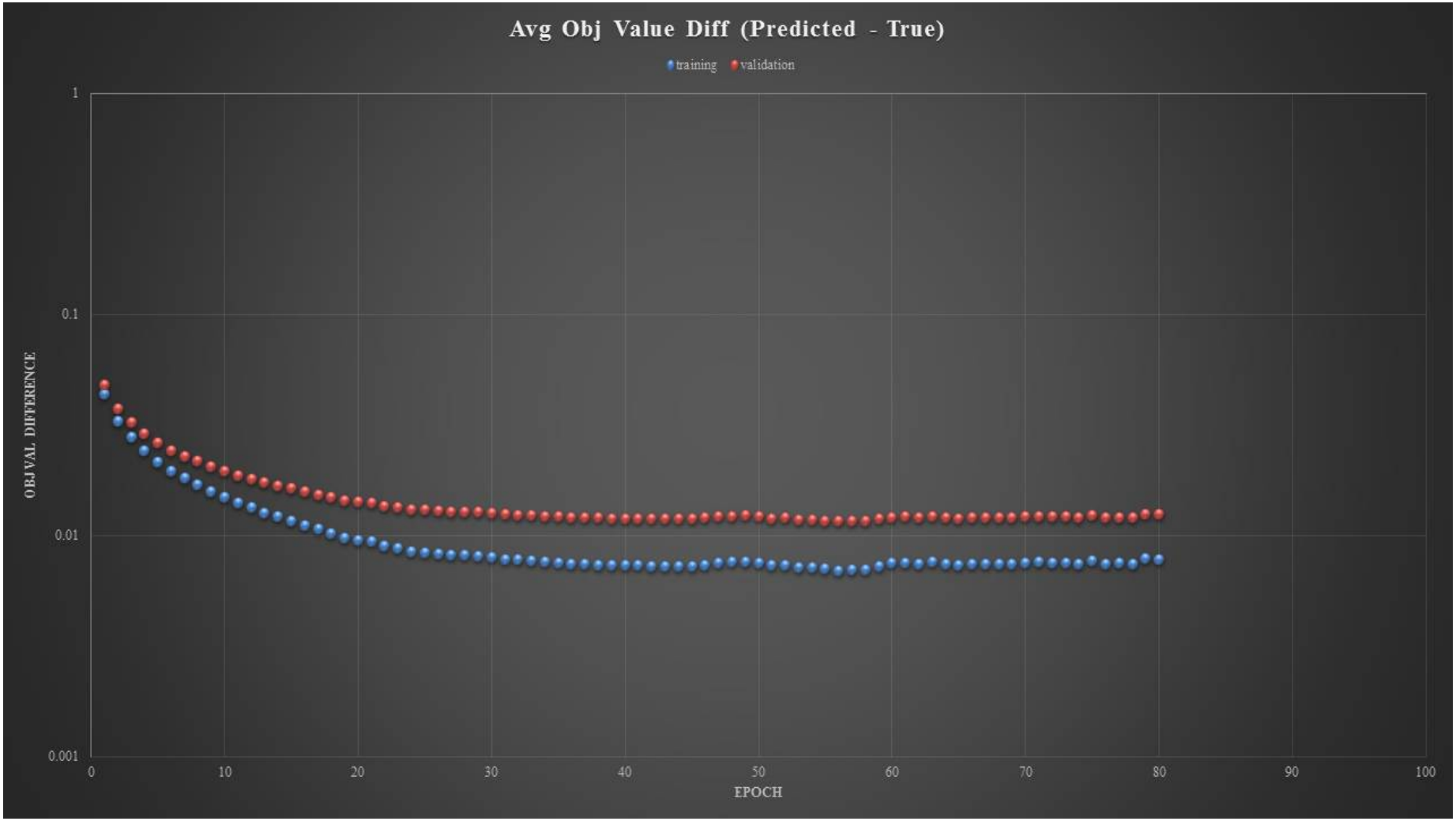
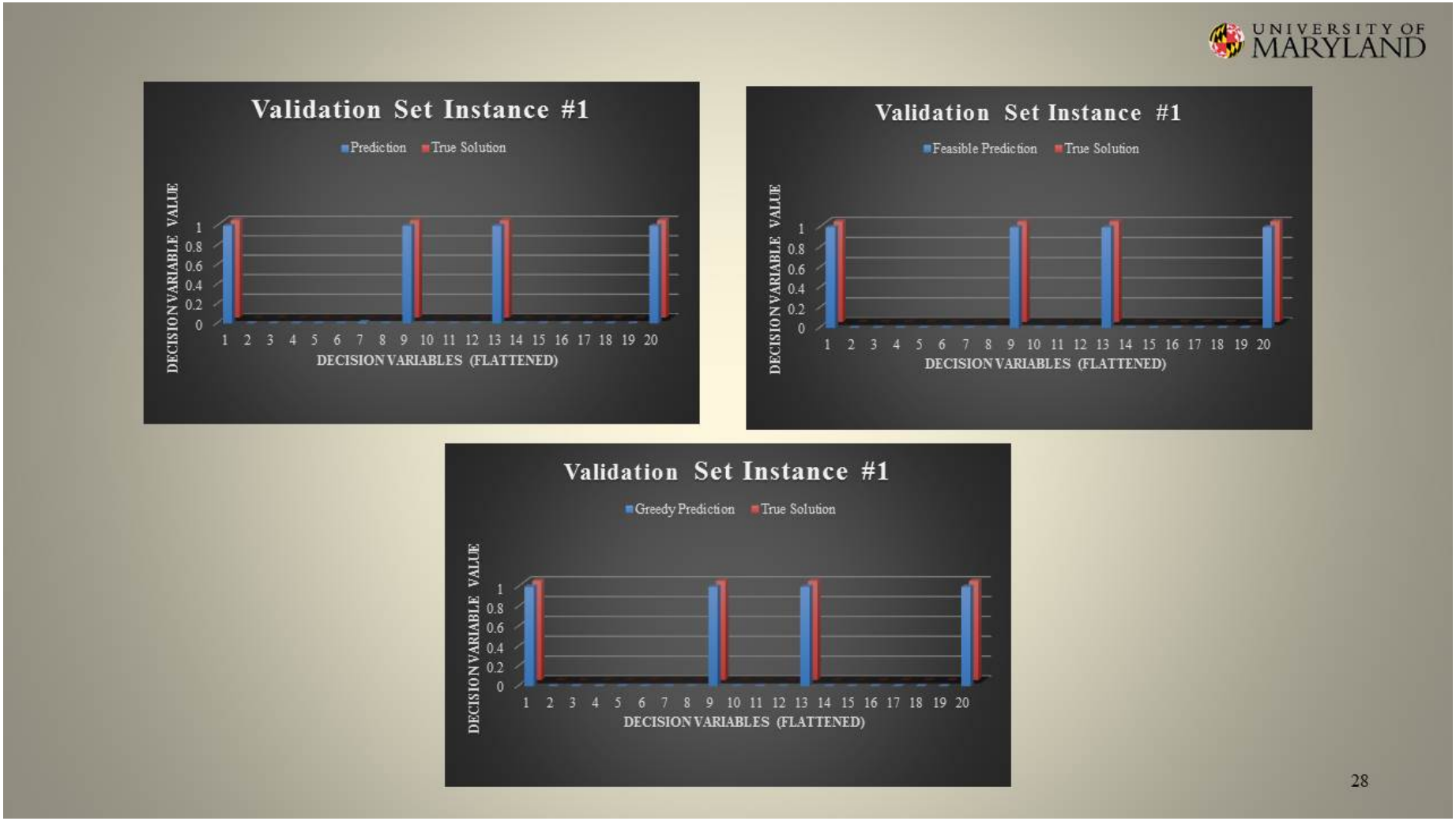


Exp.3 : $N = 5,\ R = 4$ with sigmoid activation



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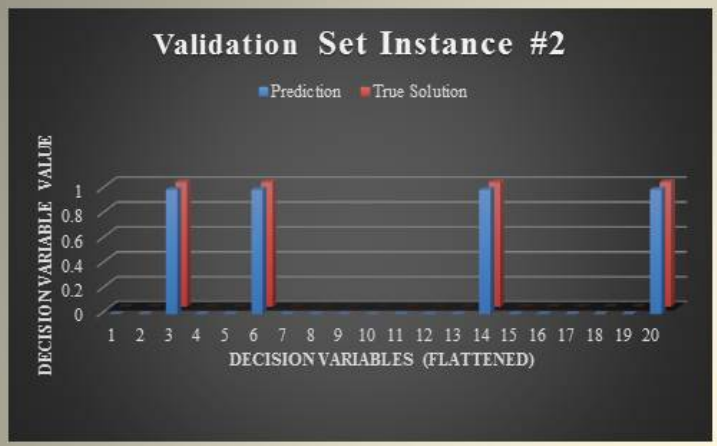
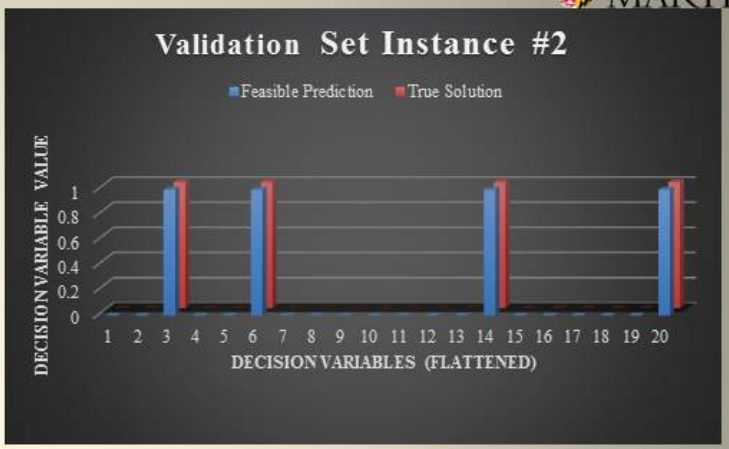
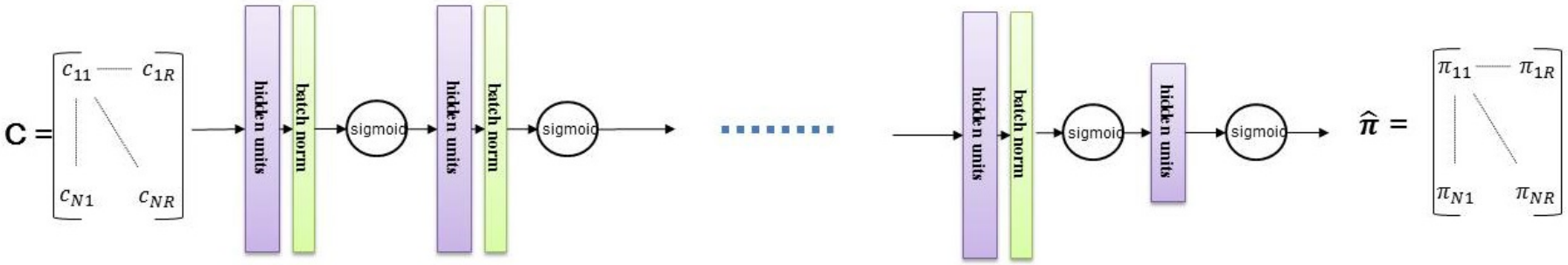




Exp.4 : $N = 10$, $R = 8$ with sigmoid activation

Second architecture:



- Number of internal layers: 10
- Number of hidden units per layer: 300
- Batch size 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
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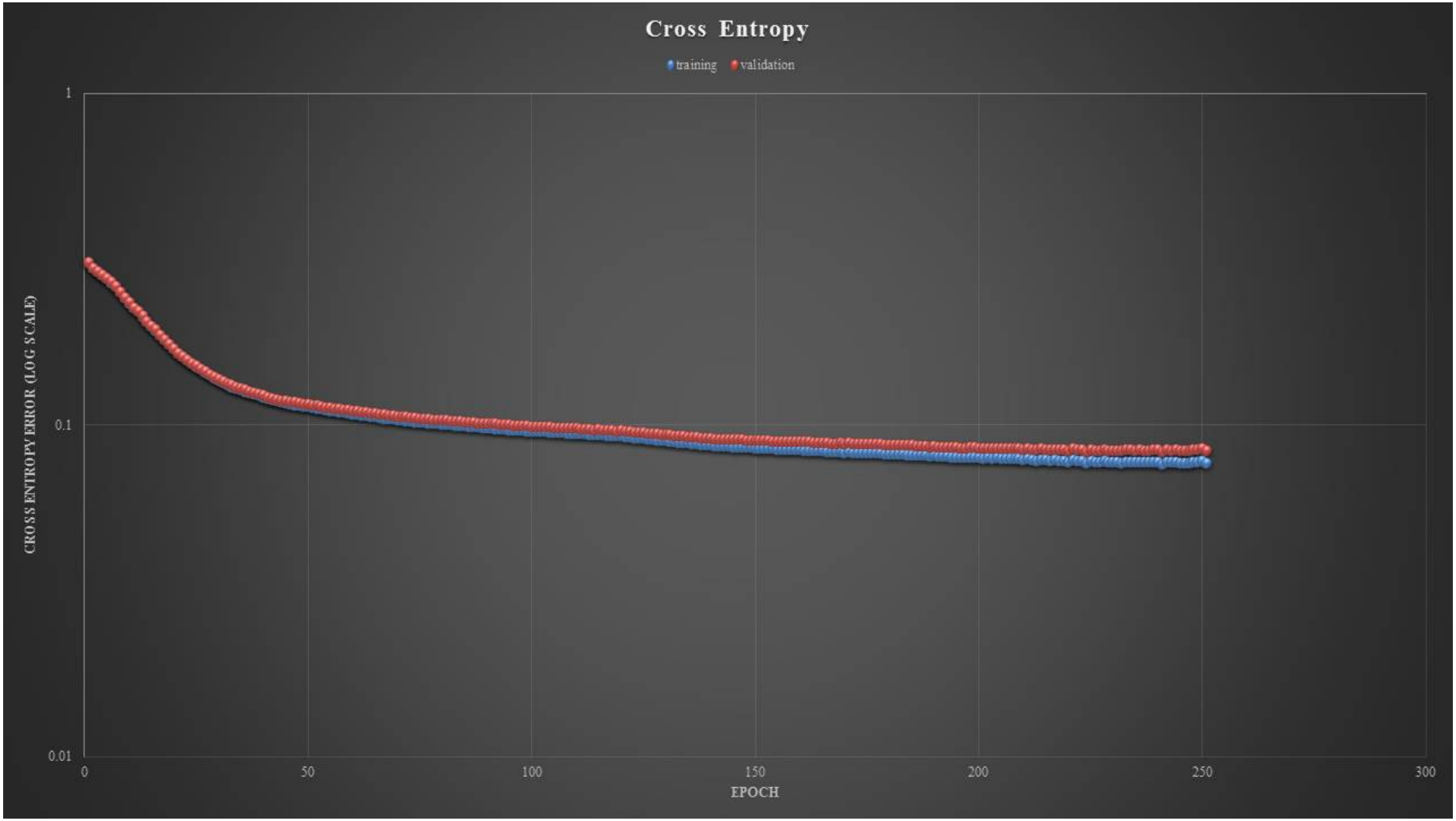

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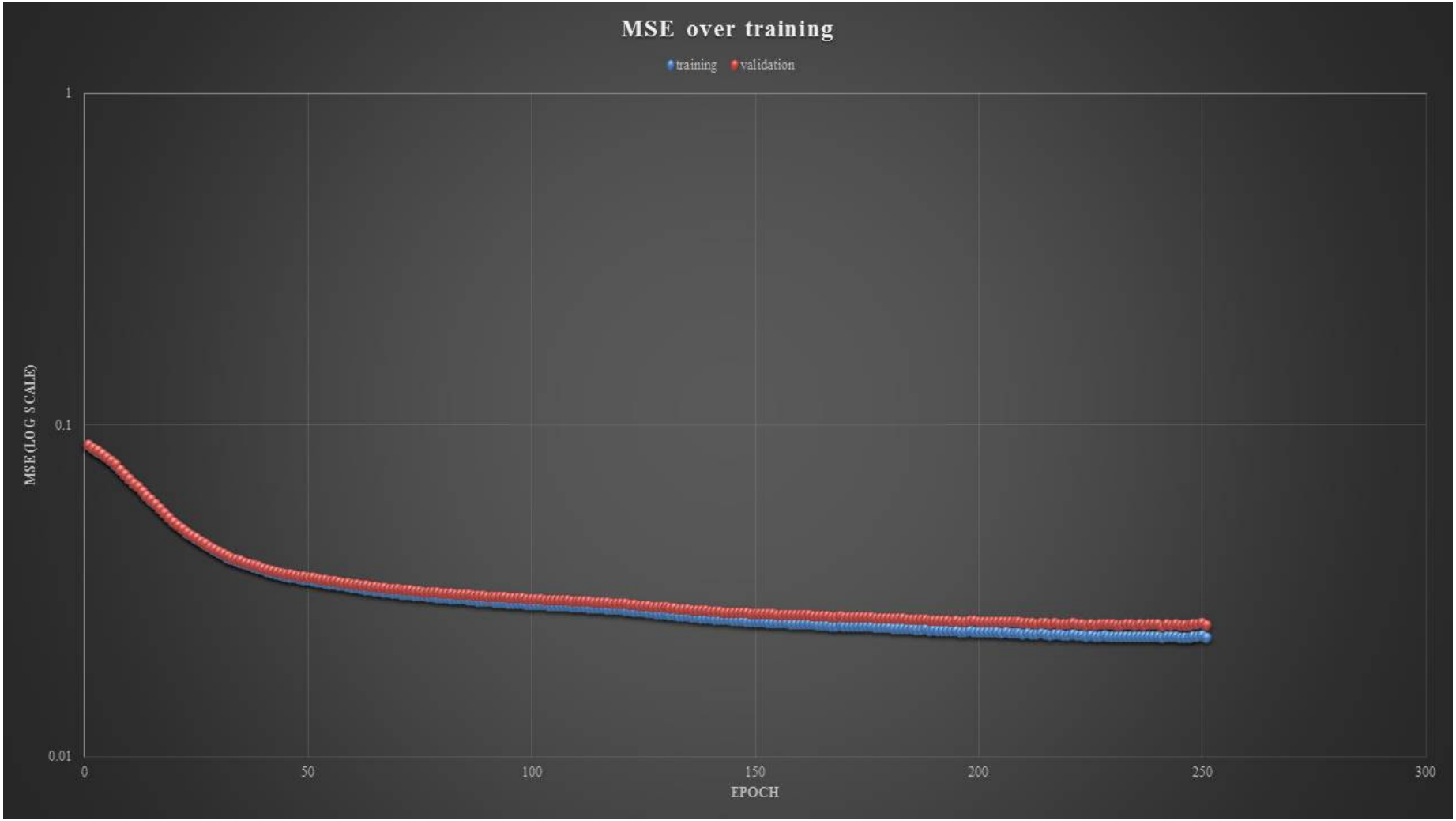

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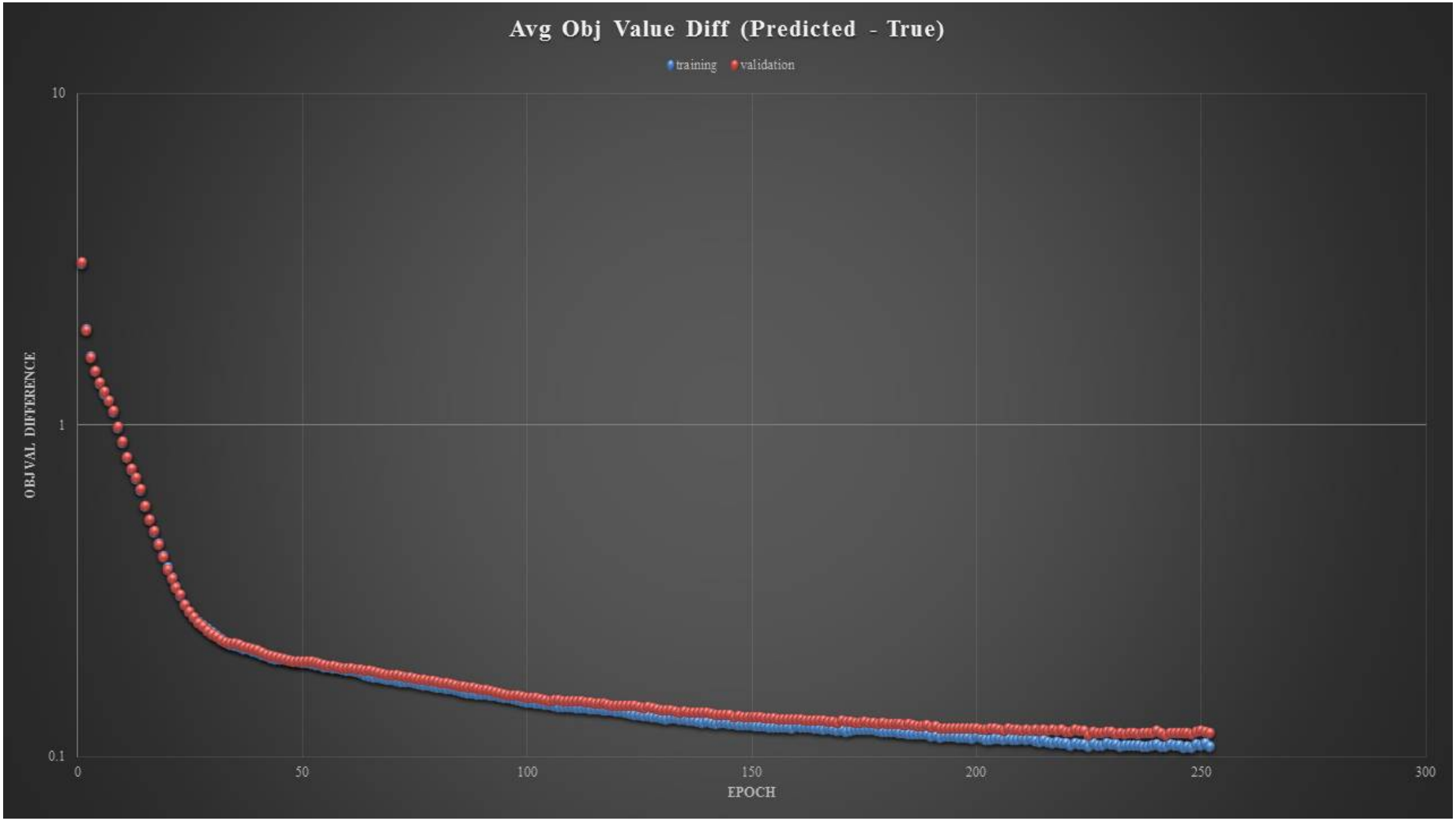

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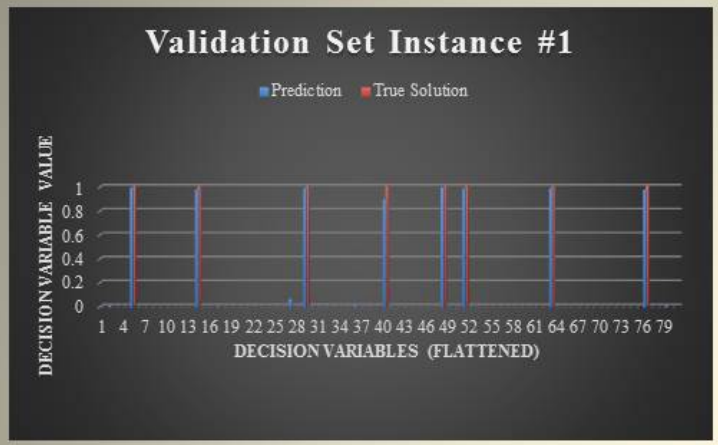

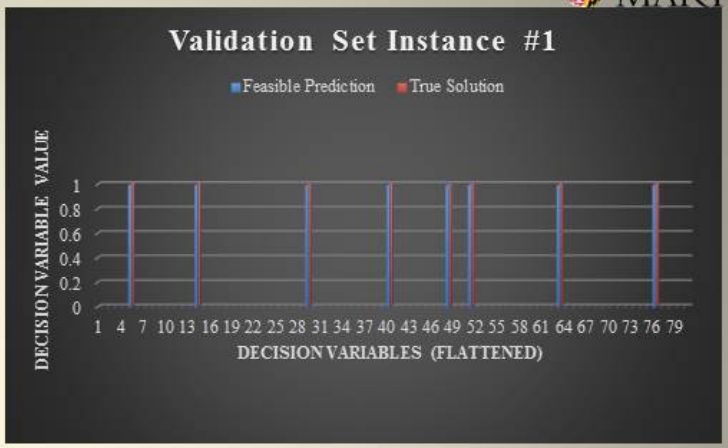

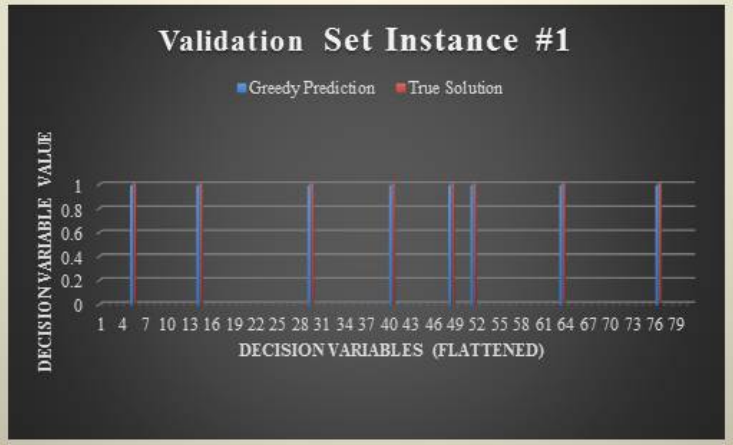

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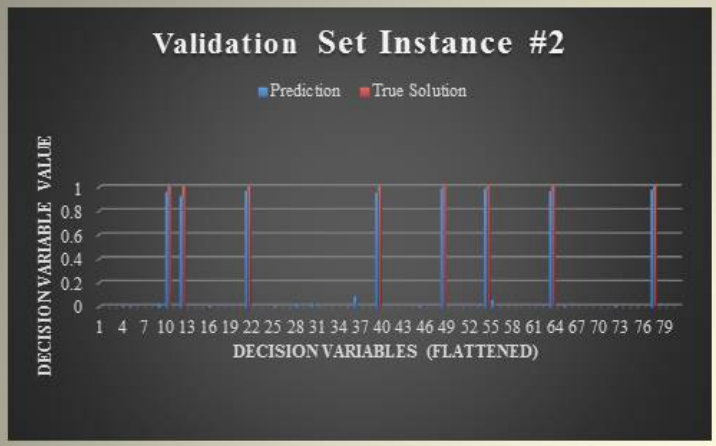
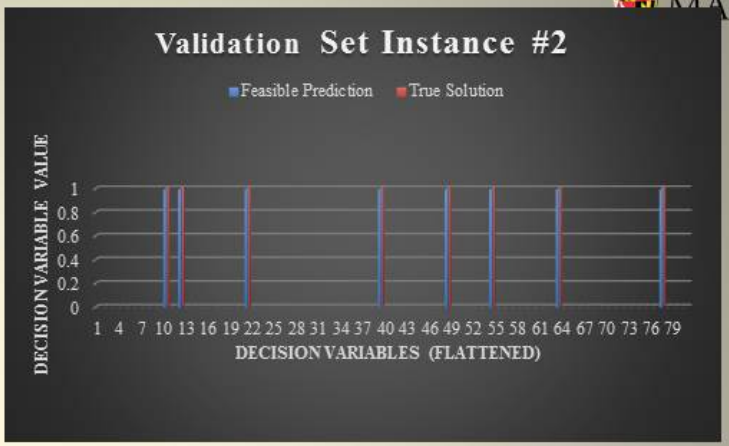
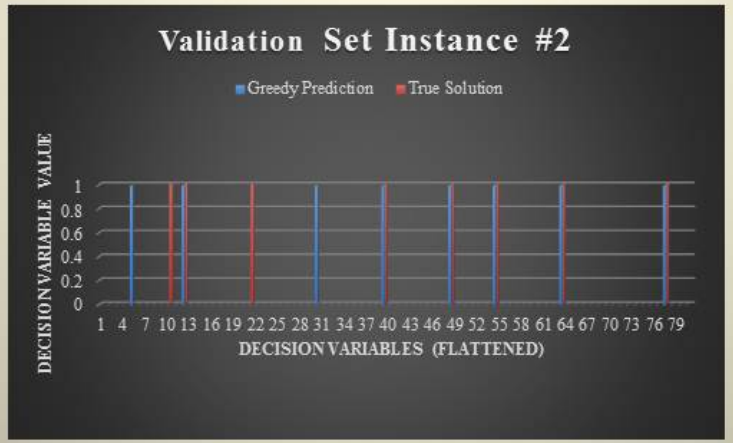
Exp.4 : $N = 10$, $R = 8$ with sigmoid activation







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