Permutation Invariance and Combinatorial Optimizations with Graph Deep Learning

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Permutation Invariant induced Representations

Consider the equivalence relation $\sim$ on $\mathbb{R}^{n \times d}$ indiced by the group of permutation S_n: for any $X, X' \in \mathbb{R}^{n \times d}$,

$$X \sim X' \quad \Leftrightarrow \quad X' = PX \ , \ \text{for some } P \in S_n$$

Let $\mathbb{M} = \mathbb{R}^{n \times d} / \sim$ be the quotient space endowed with the natural distance induced by Frobenius norm $\| \cdot \|_F$

$$d(\hat{X}_1, \hat{X}_2) = \min_{P \in S_n} \|X_1 - PX_2\|_F \quad , \quad \hat{X}_1, \hat{X}_2 \in \mathbb{M}.$$

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The Problem: Construct a Lipschitz embedding $\hat{\alpha} : \mathbb{M} \to \mathbb{R}^m$, i.e., an integer $m = m(n, d)$, a map $\alpha : \mathbb{R}^{n\times d} \to \mathbb{R}^m$ and a constant $L = L(\alpha) > 0$ so that for any $X, X' \in \mathbb{R}^{n\times d}$,

1. If $X \sim X'$ then $\alpha(X) = \alpha(X')$
2. If $\alpha(X) = \alpha(X')$ then $X \sim X'$
3. $\|\alpha(X) - \alpha(X')\|_2 \leq L\, d(\hat{X}, \hat{X}')$

Motivation (1)

Graph Learning Problems

Consider data graphs such as: social networks, transportation networks, citation networks, chemical networks, protein networks, biological networks, etc. Each such network is modeled as a (weighted) graph $(\mathcal{V}, \mathcal{E}, A)$ of n nodes, and a set of feature vectors $\{x_1^T, \cdots, x_n^T\} \subset \mathbb{R}^d$ that form the matrix $X = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times d}$.

Two important problems involving a map $f : (A, X) \to f(A, X)$:

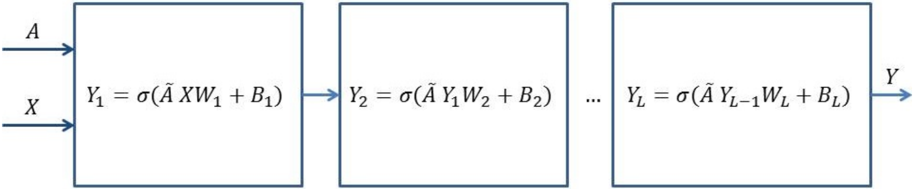
1. classification: $f(A, X) \in \{1, 2, \cdots, c\}$
2. regression/prediction: $f(A, X) \in \mathbb{R}$.

In each case we expect the task to be invariant to vertices permutation: $f(PAP^T, PX) = f(A, X)$, for every $P \in S_n$.

Motivation (2)

Graph Convolutive Networks (GCN)

Kipf and Welling ('16) introduced a network structure that performs local processing according to a modified adjacency matrix:



$\tilde{A} = I + A$, where A is the adjacency matrix, or the graph weight matrix; σ is the activation map. L-layer GCN has parameters $(W_1, B_1, \cdots, W_L, B_L)$.

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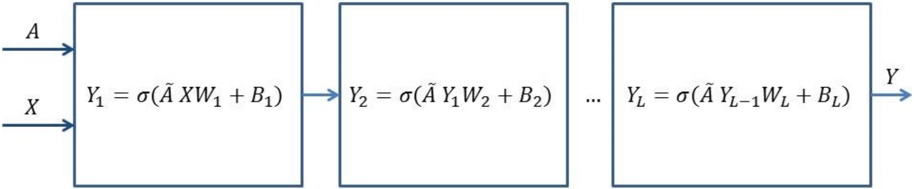


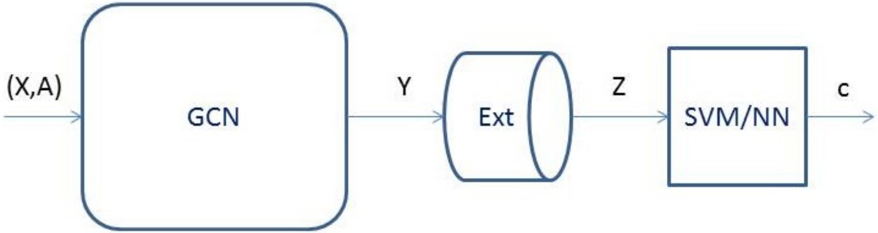
$\tilde{A} = I + A$, where A is the adjacency matrix, or the graph weight matrix; σ is the activation map. L-layer GCN has parameters $(W_1, B_1, \cdots, W_L, B_L)$.

Note the *covariance property*: for any $P \in O(n)$ (including S_n), $(A, X) \mapsto (PAP^T, PX)$ and $B_i \mapsto PB_i$ then $Y \mapsto PY$.

Motivation (3)

Deep Learning with GCN

The two learning tasks (classification or regression) can be solved by the following scheme:



where *Ext* is a permutation invariant feature extractor, and SVM/NN is a single-layer or a deep neural network (Support Vector Machine or a Fully Connected Neural Network).

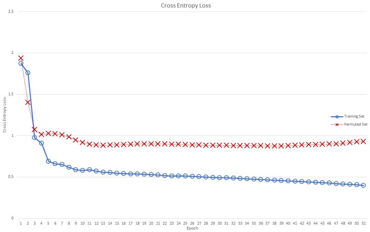
The purpose of this (part of the) talk is to analyze the *Ext* component

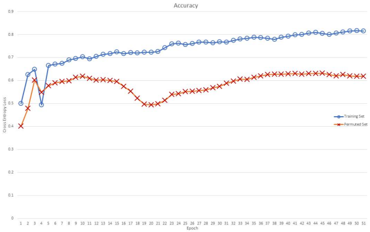
Motivation (4)

Enzyme Classification Example

Protein Dataset where task is classification into *enzyme* vs. *non-enzyme*.
Dataset: 450 enzymes and 450 non-enzymes.
Architecture (ReLU activation):

- GCN with $L = 3$ layers and $d = 25$ feature vectors in each layer;
- No Permutation Invariant Component: $Ext = Identity$
- Fully connected NN with dense 3-layers and 120 internal units.





The Measure Theoretic Embedding

First approach: Consider the map

$$\mu : \mathbb{M} \rightarrow \mathcal{P}(\mathbb{R}^d) \quad , \quad \mu(X)(x) = \frac{1}{n}\sum_{k=1}^{n} \delta(x - x_k)$$

where $\mathcal{P}(\mathbb{R}^d)$ denotes the convex set of probability measures over $\mathbb{R}^d$, and δ denotes the Dirac measure.
Clearly $\mu(X') = \mu(X)$ iff $X' = PX$ for some $P \in S_n$.

Main drawback: $\mathcal{P}(\mathbb{R}^d)$ is infinite dimensional!

Finite Dimensional Embeddings
Architectures

Two classes of extractors:

1. Pooling Map – based on Max pooling
2. Readout Map – based on Sum pooling

Finite Dimensional Embeddings

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1. Pooling Map – based on Max pooling
2. Readout Map – based on Sum pooling

Intuition in the case $d = 1$:

Max pooling:

$$\lambda : \mathbb{R}^n \to \mathbb{R}^n \quad , \quad \lambda(x) = (x_{\pi(k)})_{k=1}^n \ , \ x_{\pi(1)} \geq x_{\pi(2)} \geq \cdots \geq x_{\pi(n)}$$

Finite Dimensional Embeddings
Architectures

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Sum pooling:

$$\sigma : \mathbb{R}^n \to \mathbb{R}^n \quad , \quad \sigma(x) = (y_k)_{k=1}^n \; , \; y_k = \sum_{j=1}^n \nu(a_k, x_j)$$

where kernel $\nu : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, e.g. $\nu(a,t) = e^{-(a-t)^2}$, or $\nu(a = k, t) = t^k$.

Pooling Mapping Approach

Fix a matrix $R \in \mathbb{R}^{d\times D}$. Consider the map:

$$\Lambda : \mathbb{R}^{n\times d} \to \mathbb{R}^{n\times D} \equiv \mathbb{R}^{nD} \quad , \quad \Lambda(X) = \lambda(XR)$$

where λ acts columnwise (reorders monotonically decreasing each column). Since $\Lambda(\Pi X) = \Lambda(X)$, then $\Lambda : \widehat{\mathbb{R}^{n\times d}} \to \mathbb{R}^{n\times D}$.

Theorem

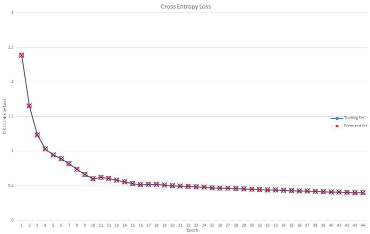
For any matrix $R \in \mathbb{R}^{n,d+1}$ so that any $n \times n$ submatrix is invertible, there is a subset $Z \subset \widehat{\mathbb{R}^{n\times d}}$ of zero measure so that $\Lambda : \widehat{\mathbb{R}^{n\times d}} \setminus Z \to \mathbb{R}^{n\times d+1}$ is faithful (i.e., injective).

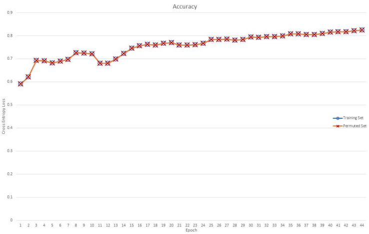
No known tight bound yet as to the minimum $D = D(n, d)$ so that there is a matrix R so that Λ is faithful (injective).
However, due to local linearity, if Λ is faithful (injective), then it is stable.

Enzyme Classification Example
Extraction with Hadamard Matrix

Protein Dataset where task is classification into *enzyme* vs. *non-enzyme*.
Dataset: 450 enzymes and 450 non-enzymes.
Architecture (ReLU activation):

- GCN with $L = 3$ layers and $d = 25$ feature vectors in each layer;
- $Ext = \Lambda$, $Z = \lambda(YR)$ with $R = [I \; Hadamard]$. $D = 50$, $m = 50$.
- Fully connected NN with dense 3-layers and 120 internal units.





Readout Mapping Approach

Kernel Sampling

Consider:

$$\Phi : \mathbb{R}^{n\times d} \to \mathbb{R}^m \quad , \quad (\Phi(X))_j = \sum_{k=1}^{n} \nu(a_j, x_k) \text{ or } (\Phi(X))_j = \prod_{k=1}^{n} \nu(a_j, x_k)$$

where $\nu : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a kernel, and $x_1, \cdots, x_n$ denote the rows of matrix X.

Known solutions: If $m = \infty$, then there exists a Φ that is globally faithful (injective) and stable on compacts.

Interesting mathematical connexion: On compacts, some kernels ν define Repreducing Kernel Hilberts Spaces (RKHSs) and yield a decomposition

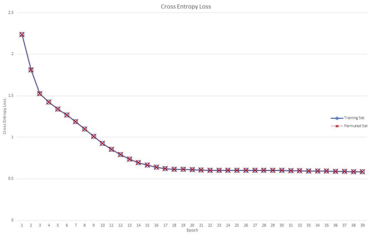
$$(\Phi(X))_j = \sum_{p\geq 1} \sigma_p f_p(a_j) g_p(X)$$

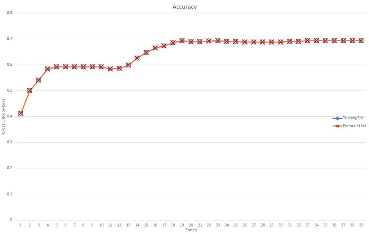
Enzyme Classification Example

Feature Extraction with Exponential Kernel Sampling

Protein Dataset where task is classification into *enzyme* vs. *non-enzyme*.
Dataset: 450 enzymes and 450 non-enzymes.
Architecture (ReLU activation):

- GCN with $L = 3$ layers and $d = 25$ feature vectors in each layer;
- $Ext : Z_j = \sum_{k=1}^{n} exp(-\pi \|y_k - z_j\|)$ with $m = 120$ and z_j random.
- Fully connected NN with dense 3-layers and 120 internal units.





Readout Mapping Approach

Polynomial Expansion - Quadratics

Another interpretation of the moments for $d = 1$: coefficients of linear expansion

$$P(X) = \frac{1}{n}\sum_{k=1}^{n}(X - x_k)^n = X^n + \sum_{k=1}^{n} a_k X^{n-k}$$

Readout Mapping Approach

Polynomial Expansion - Quadratics

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$$P(X)=\frac{1}{n}\sum_{k=1}^{n}(X-x_k)^n = X^n+\sum_{k=1}^{n} a_k X^{n-k}$$

For $d>1$, consider the quadratic d-variate polynomial:

$$\begin{aligned} P(Z_1,\cdots,Z_d) &= \prod_{k=1}^{n}\left((Z_1-x_k(1))^2+\cdots+(Z_d-x_k(d))^2\right) \\ &= \sum_{p_1,\ldots,p_d=0}^{2n} a_{p_1,\ldots,p_d} Z_1^{p_1}\cdots Z_d^{p_d} \end{aligned}$$

Encoding complexity:

$$m = O\left(\begin{array}{c} 2n+d \\ d \end{array}\right) \sim (2n)^d.$$

Algebraic Embedding

Encoding using Complex Roots

Idea: Consider the case $d = 2$. Then each $x_1, \cdots, x_n \in \mathbb{R}^2$ can be replaced by n complex numbers $z_1, \cdots, z_n \in \mathbb{C}$, $z_k = x_k(1) + ix_k(2)$. Then consider the complex polynomial:

$$Q(z) = \prod_{k=1}^{n}(z - z_k) = z^n + \sum_{k=1}^{n} \sigma_k z^{n-k}$$

which requires n complex numbers, or $2n$ real numbers.

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which requires n complex numbers, or $2n$ real numbers.
For $d > 3$ encode each combination of two columns of $X \in \mathbb{R}^{n \times d}$: Total of $d(d-1)/2$ combinations, each using $2n$ real numbers.

Encoding complexity: $m = nd(d-1)$

Combinatorial Optimization Problems
Approach

Consider the class of combinatorial problems,

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

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, $J(\Pi; A, B) = trace(A \Pi B \Pi^T)$

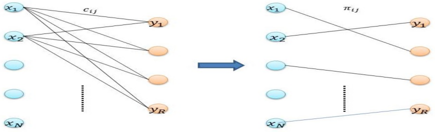
Idea: Use a two-step procedure:

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:

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



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

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

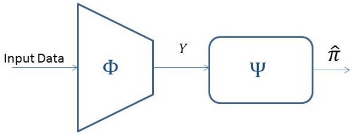
In turns this is equivalent to the minimization problem:

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

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

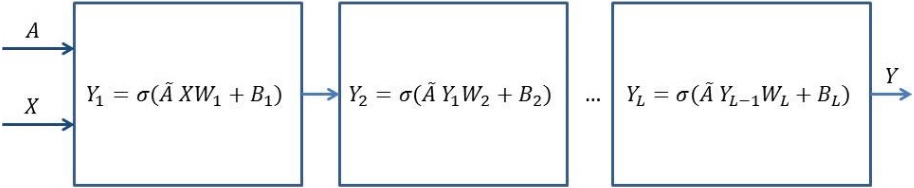
Idea: Perform a two-step procedure: (1) perform a nonlinear representation of the input data; (2) perform optimization in the representation space.



The nonlinear representation map $\Phi : \text{Input Data} \mapsto Y$ 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 $X = \begin{bmatrix} A \\ B \end{bmatrix}$.

Quadratic Assignment Problem using GCN

Preliminary result

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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 $\hat{\pi}$:

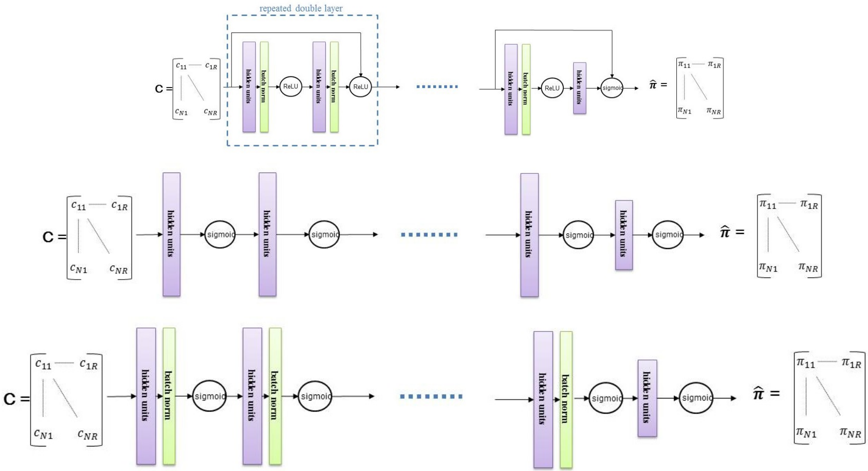
Issues:

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

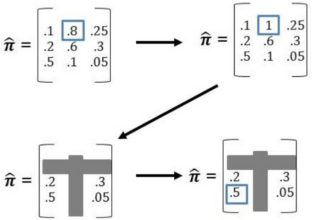
Feasibility Enforcer P

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:

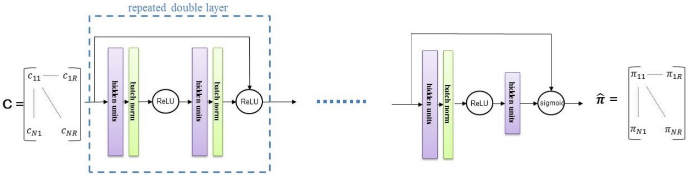
1. Initialize $E = C$ and $\hat{\pi} = 0_{N \times R}$
2. Repeat R times:
   - Find $(i, j) = argmin_{(a,b)} E_{a,b}$;
   - Set $\hat{\pi}_{i,j} = 1$, $\hat{\pi}_{i,l} = 0 \ \forall l \neq j$, $\hat{\pi}_{l,j} = 0 \ \forall l \neq i$;
   - Set $E_{i,:} = \infty$, $E_{:,j} = \infty$.

Proposition

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

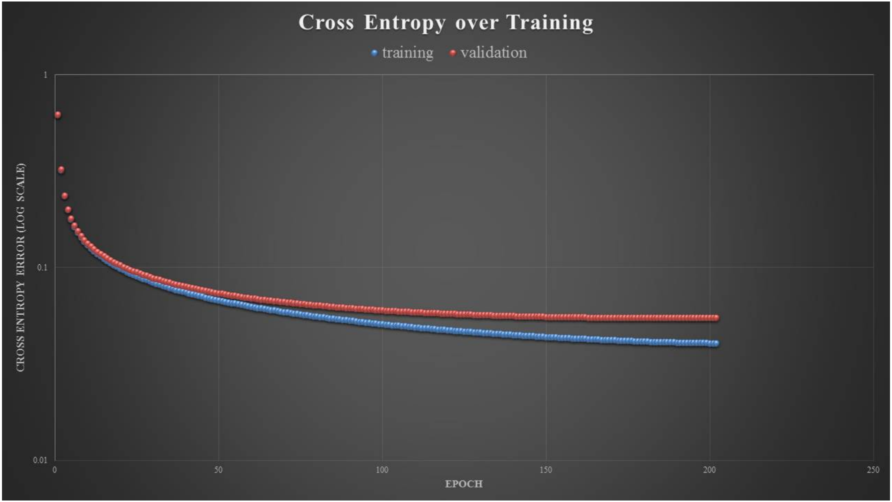
Exp.1 : $N = 5$, $R = 4$ with ReLU activation

First architecture:

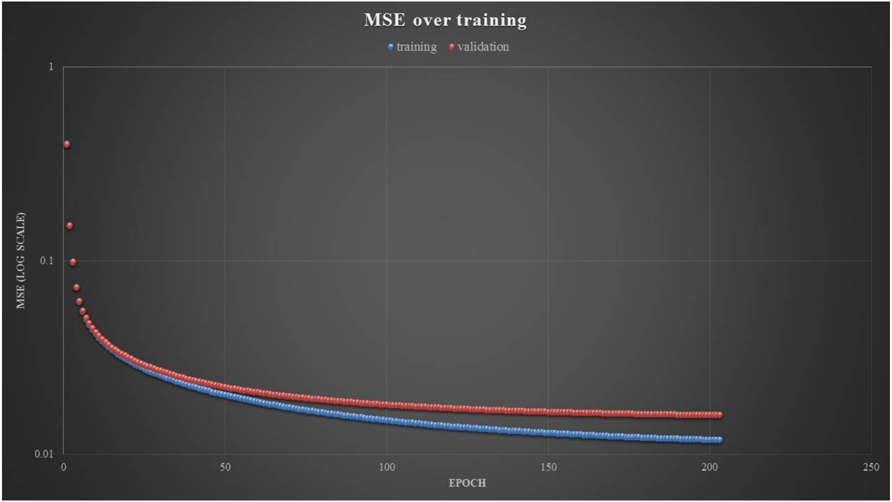


- Number of internal layers: 9
- Number of hidden units per layer: 250
- Batch size: 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 1 million random instances $U(0,1)$ i.i.d.
- Validation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

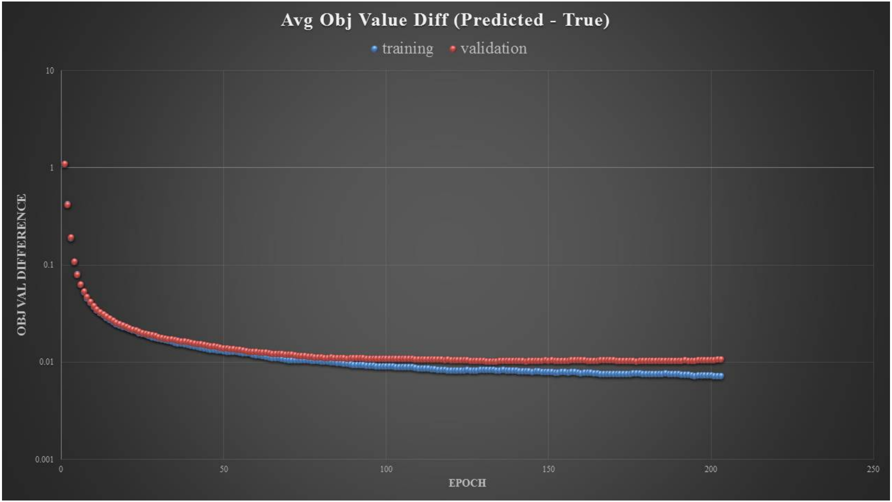
Exp.1 : $N = 5$, $R = 4$ with ReLU activation



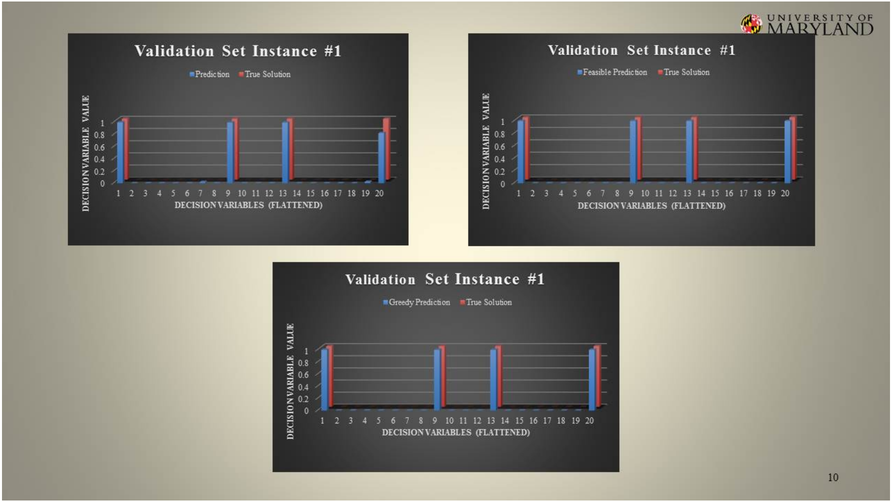
Exp.1 : $N = 5$, $R = 4$ with ReLU activation



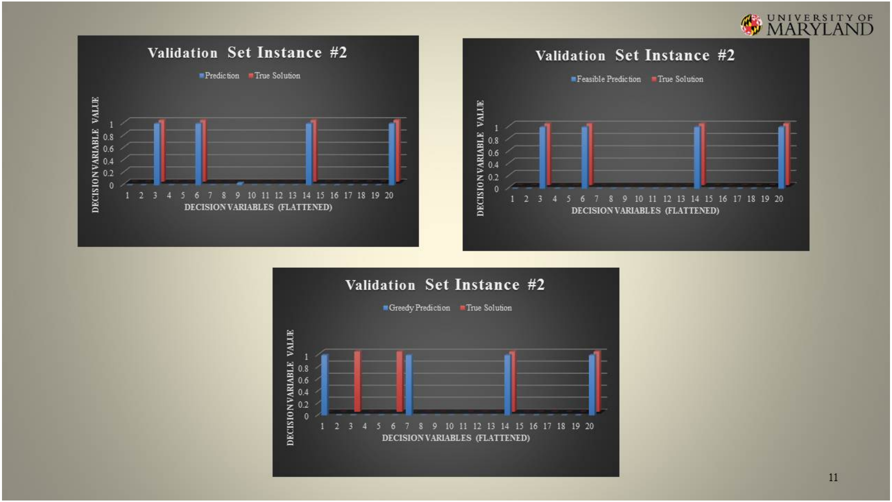
Exp.1 : $N = 5$, $R = 4$ with ReLU activation



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

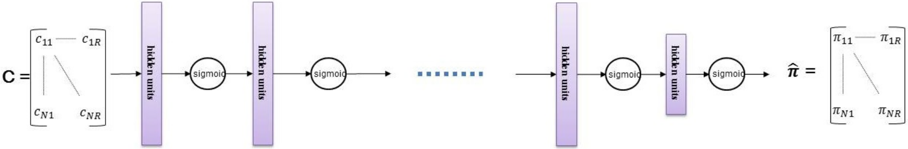


Exp.1 : $N = 5$, $R = 4$ with ReLU activation



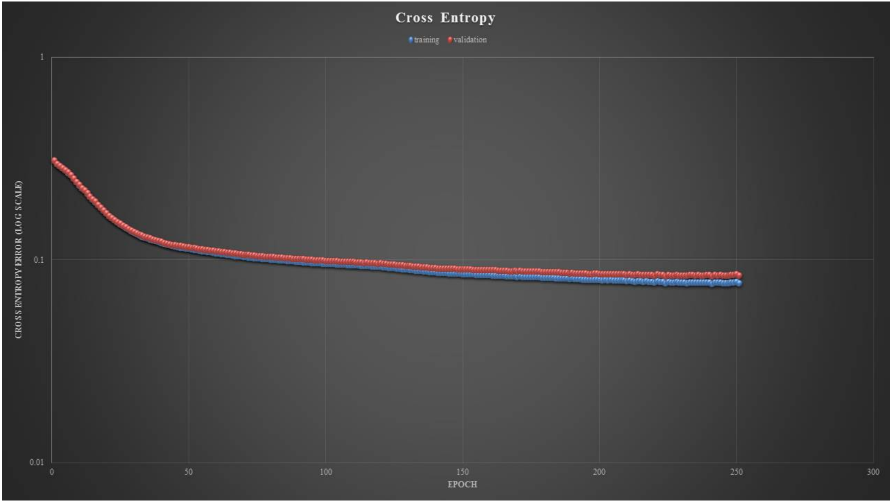
Exp.2 : $N = 10$, $R = 8$ with sigmoid activation

Second architecture:

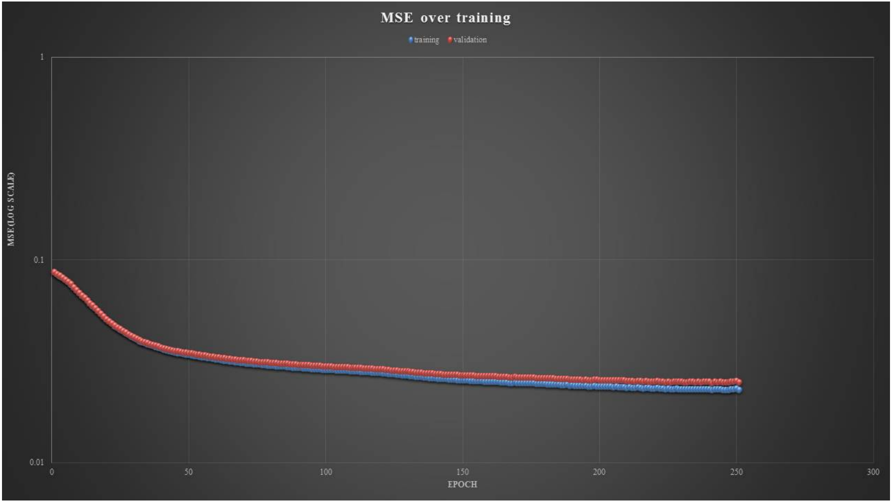


- Number of internal layers: 10
- Number of hidden units per layer: 250
- No Batch; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 1 million random instances $U(0, 1)$ i.i.d.
- Validation set: 20,000 random instances.

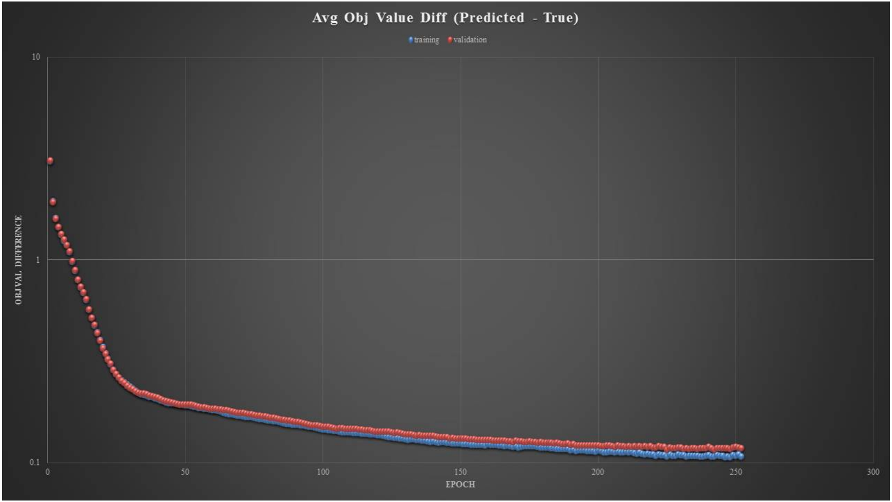
Exp.2 : $N = 10$, $R = 8$ with sigmoid activation



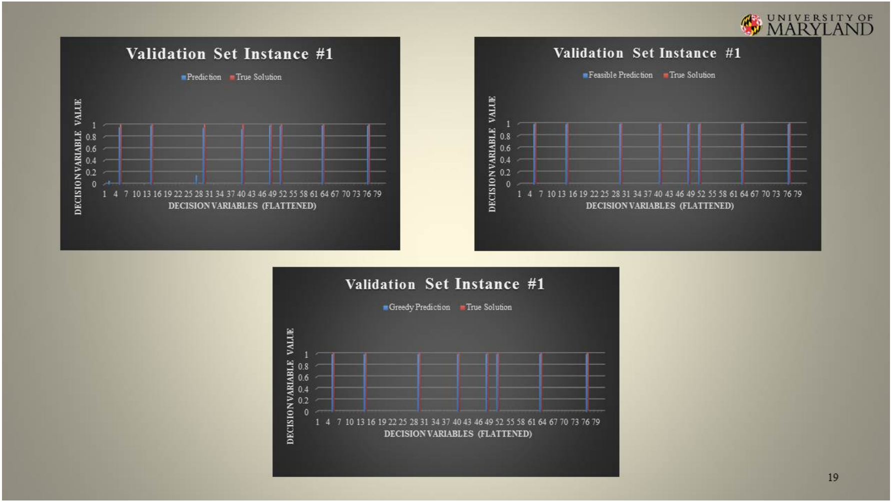
Exp.2 : $N = 10$, $R = 8$ with sigmoid activation



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



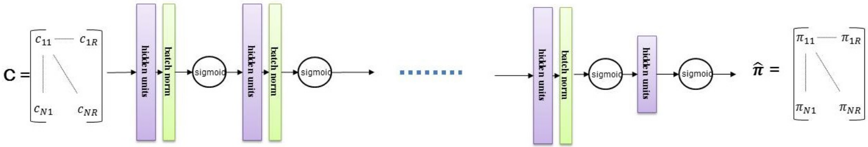
Exp.2 : $N = 10$, $R = 8$ with sigmoid activation



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

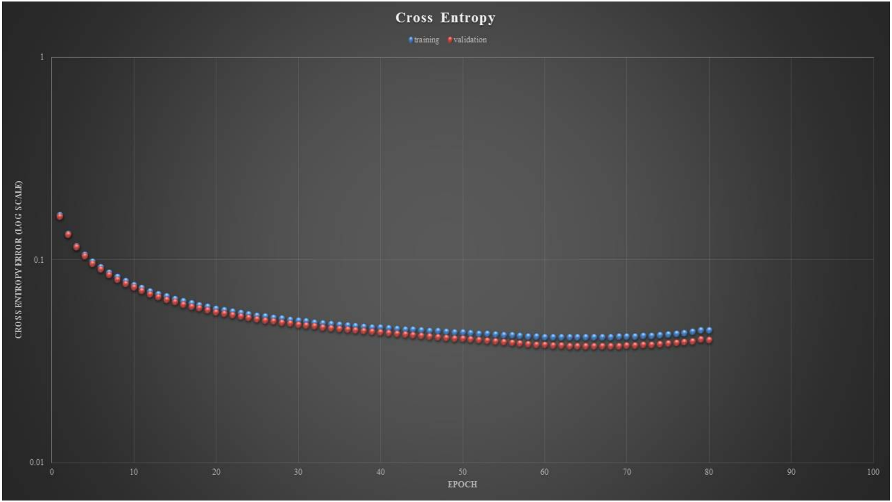
Exp.3 : $N = 5$, $R = 4$ with sigmoid activation

Second architecture:

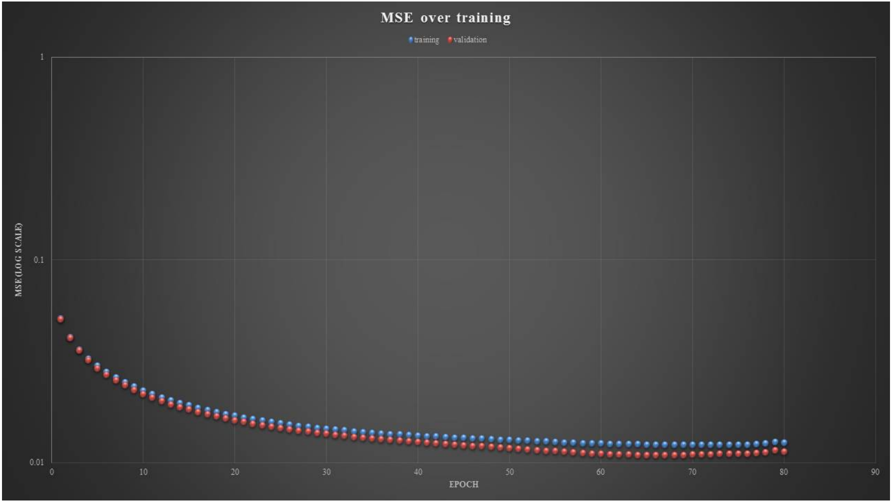


- Number of internal layers: 10
- Number of hidden units per layer: 250
- Batch size 200; ADAM optimizer
- Loss function: cross-entropy:
  $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 500,000 random instances $U(0,1)$ i.i.d.
- Validation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

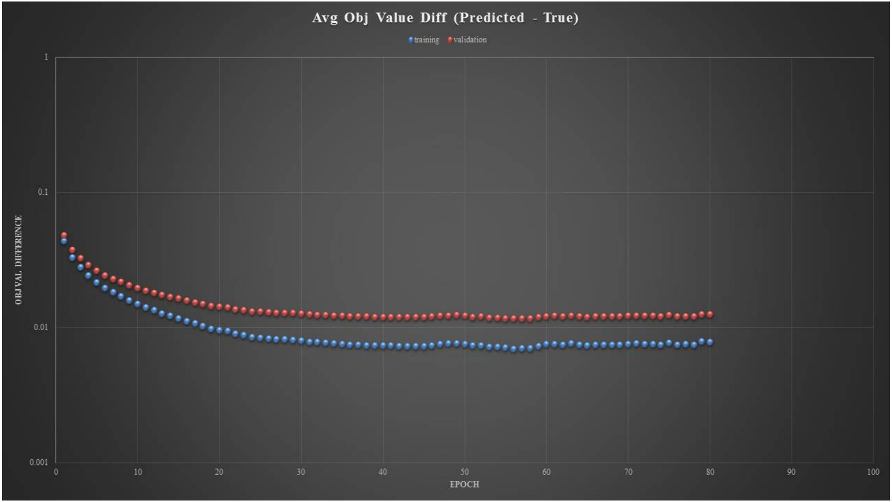
Exp.3 : $N = 5$, $R = 4$ with sigmoid activation



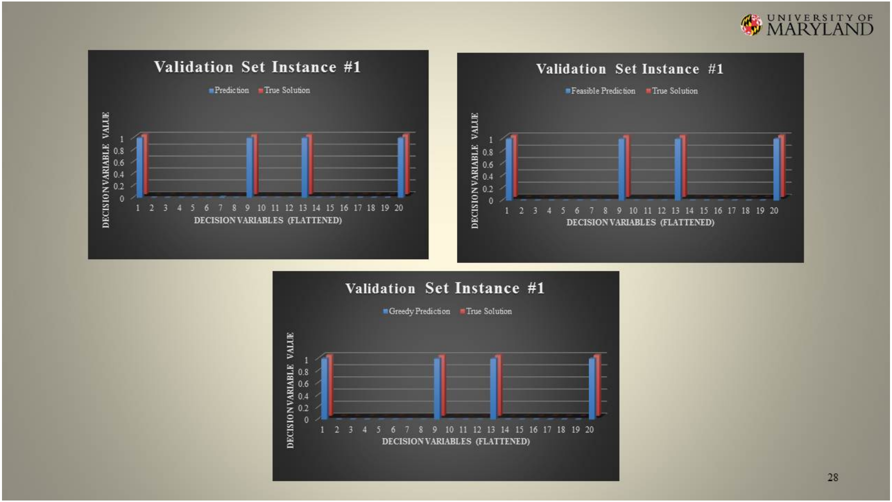
Exp.3 : $N = 5$, $R = 4$ with sigmoid activation



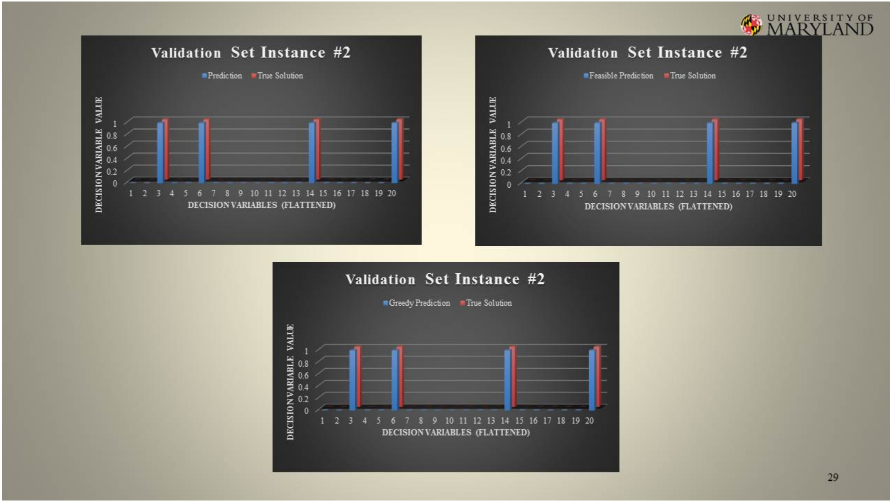
Exp.3 : $N = 5$, $R = 4$ with sigmoid activation



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

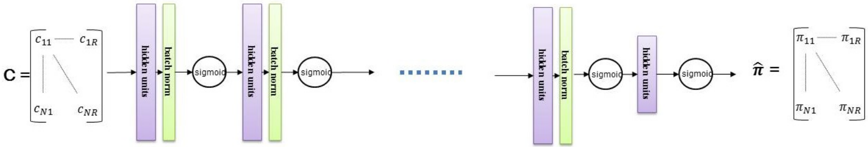


Exp.3 : $N = 5$, $R = 4$ with sigmoid activation



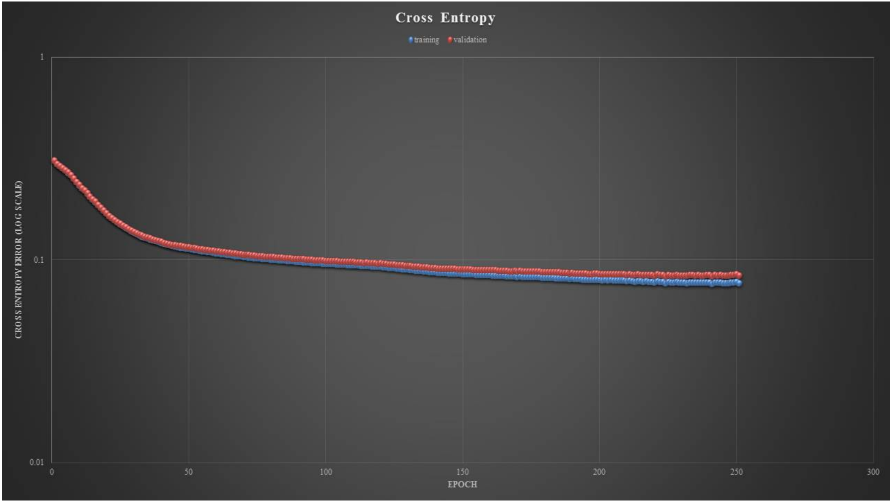
Exp.4 : $N = 10$, $R = 8$ with sigmoid activation

Second architecture:

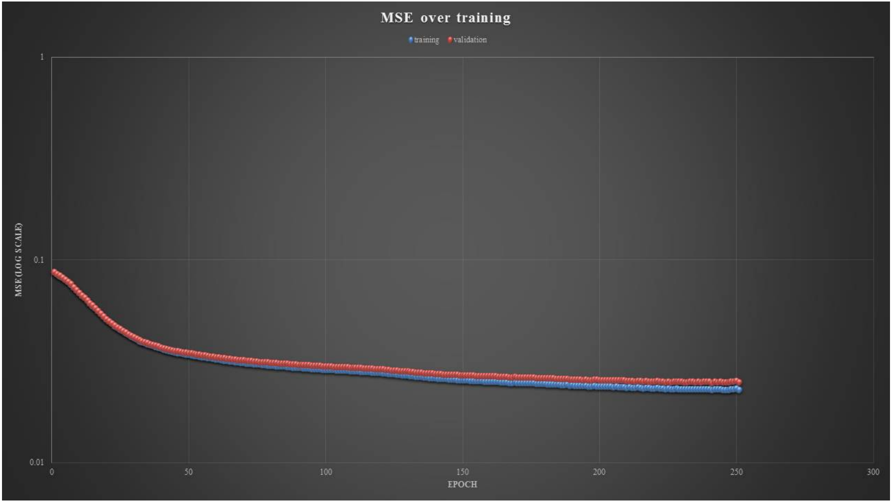


- Number of internal layers: 10
- Number of hidden units per layer: 300
- Batch size 200; ADAM optimizer
- Loss function: cross-entropy: $\sum_{i,j} \pi_{i,j}(-log(\hat{\pi}_{i,j})) + (1 - \pi_{i,j})(-log(1 - \hat{\pi}_{i,j}))$
- Training data set: 500,000 random instances $U(0,1)$ i.i.d.
- Validation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

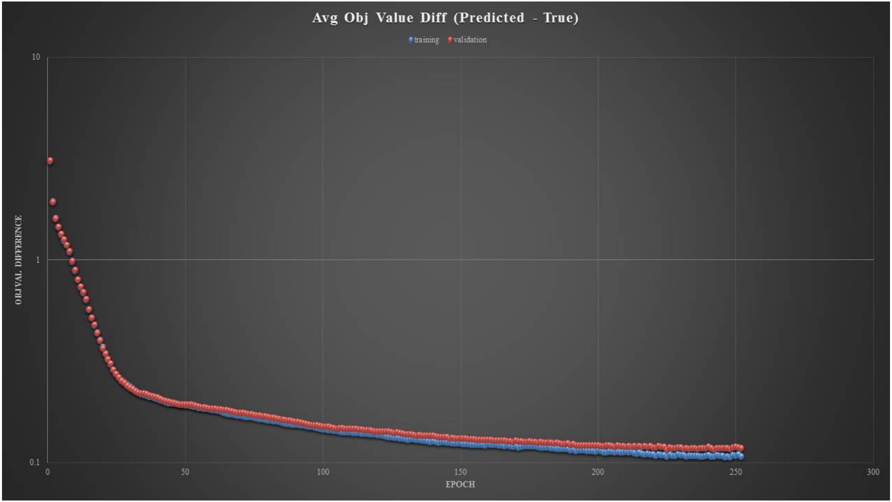
Exp.4 : $N = 10$, $R = 8$ with sigmoid activation



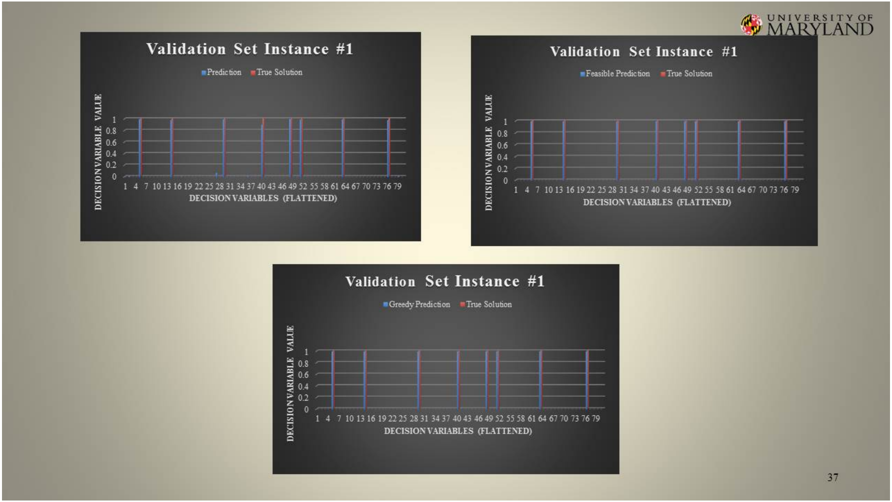
Exp.4 : $N = 10$, $R = 8$ with sigmoid activation



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



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



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

Bibliography

1. M. Andrychowicz, M. Denil, S.G. Colmenarejo, M.W. Hoffman, D. Pfau, T. Schaul, B. Shillingford, N.de Freitas, *Learning to learn by gradient descent by gradient descent*, arXiv:1606.04474v2 [cs.NE]
2. T.N. Kipf, M. Welling, *Variational Graph Auto-Encoder*, arXiv:1611.07308 [stat.ML]
3. A. Nowak, S. Villar, A. Bandeira, J. Bruna, *Revised Note on Learning Quadratic Assignment with Graph Neural Network*, arXiv: 1706.07450 [stat.ML]