ADAPTIVE MULTIPLE OPTIMAL LEARNING FACTORS FOR NEURAL NETWORK TRAINING

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Outline

I. Multilayer perceptron review
II. Review of neural network training algorithms
III. Goals
IV. Proposed algorithm
V. Simulations
VI. Conclusions

I. MLP Review

- Widely used for function approximation and pattern recognition
  - In function approximation a function that maps between input and output is approximated
  - In pattern recognition a received signal is assigned to one of a prescribed number of classes
- Known for its special properties of approximating Bayes discriminants and universal approximation
- Function approximation is the focus of this thesis

$\mathbf{W} \rightarrow$ Input weights

$\mathbf{W_{oi}} \rightarrow$ Bypass weights

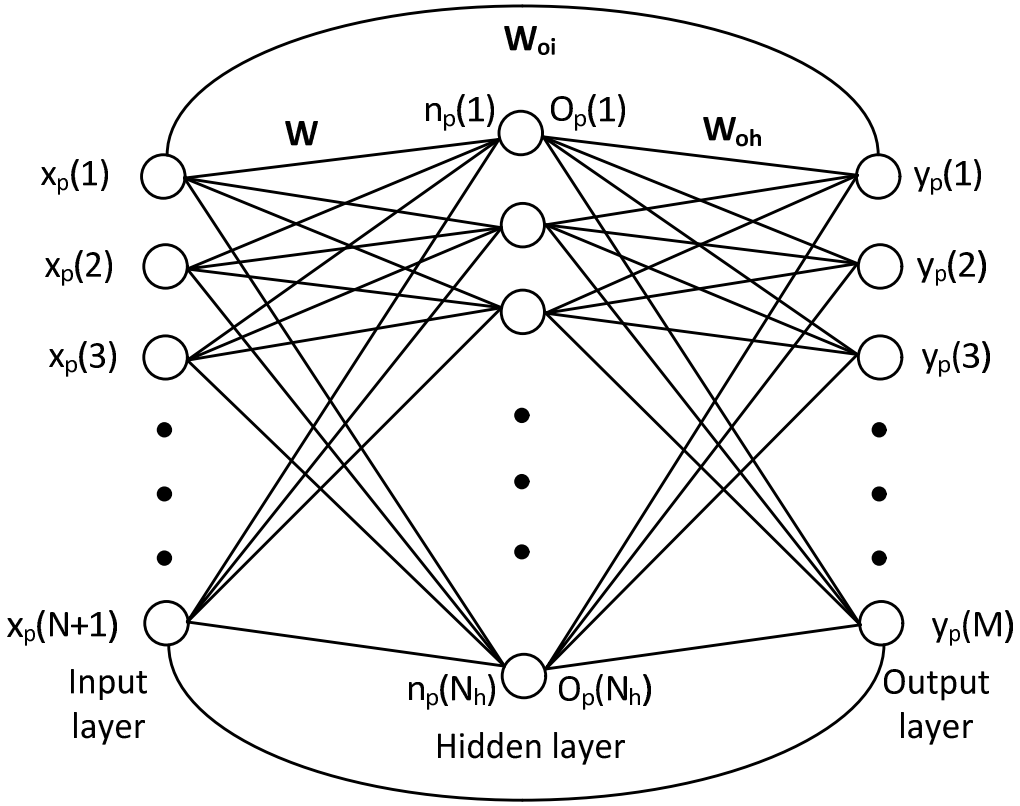
$\mathbf{W_{oh}} \rightarrow$ Output to hidden weights

$$\mathbf{n_p} = \mathbf{W} \cdot \mathbf{x_p}$$

$$O_p(k) = \frac{1}{1 + e^{-n_p(k)}}$$

$$\mathbf{y_p} = \mathbf{W_{oi}} \cdot \mathbf{x_p} + \mathbf{W_{oh}} \cdot \mathbf{O_p}$$

$$E = \frac{1}{N_v} \sum_{p=1}^{N_v} \sum_{i=1}^{M} \left[t_p(i) - y_p(i) \right]^2$$



II. Review of NN training algorithms

- Conjugate Gradient

Let, $\mathbf{w} = \mathrm{vec}\{\mathbf{W}, \mathbf{W}_{oi}, \mathbf{W}_{oh}\}$, $\mathbf{g} = \mathrm{vec}\{\mathbf{G}, \mathbf{G}_{oi}, \mathbf{G}_{oh}\}$

$$\mathbf{p} = \mathrm{vec}\{\mathbf{P}, \mathbf{P}_{oi}, \mathbf{P}_{oh}\}$$

$$\boldsymbol{p}_{k+1} = \mathbf{g}_k + \mathrm{B}_l . \boldsymbol{p}_k$$

$$\mathrm{B}_l = \frac{\mathbf{g}_{k+1}^{\mathrm{T}} \mathbf{g}_{k+1}}{\mathbf{g}_k^{\mathrm{T}} \mathbf{g}_k} \quad , \quad \mathbf{w}_{k+1} = \mathbf{w}_k + z \cdot \boldsymbol{p}_k$$

- Minimizes quadratic error functions of *n* variables in *n* steps
- No Hessian computation is required

- Levenberg Marquardt

$$\mathbf{w} \leftarrow \mathbf{w} + \mathbf{e}$$

$$\mathbf{e} = \left[\mathbf{H}' + \lambda \mathbf{I}\right]^{-1} \mathbf{g}'$$

$$h'(m,n) = \frac{\partial^2 E}{\partial w(m) \partial w(n)} \qquad g'(m) = \frac{-\partial E}{\partial w(m)}$$

- By changing λ the algorithm interpolates between steepest descent and Gauss-Newton methods
- Computationally very expensive
- Mostly used for small networks

Newton-related improved training

Newton-related algorithms usually converge faster per iteration

- Output Weight Optimization

$$\mathbf{R} = \frac{1}{N_v} \sum_{p=1}^{N_v} \mathbf{X_p} \mathbf{X_p}^T$$

$$\mathbf{C} = \frac{1}{N_v} \sum_{p=1}^{N_v} \mathbf{X_p} \mathbf{t_p}^T$$

Augmented input:

$$X_p = \begin{bmatrix} x_p \\ O_p \end{bmatrix}$$

$$\mathbf{W_o}^T = \mathbf{R}^{-1} \cdot \mathbf{C}$$

- Equivalent to Newton's method for output weights
- Computationally less expensive

- OWO-MOLF

In each iteration:

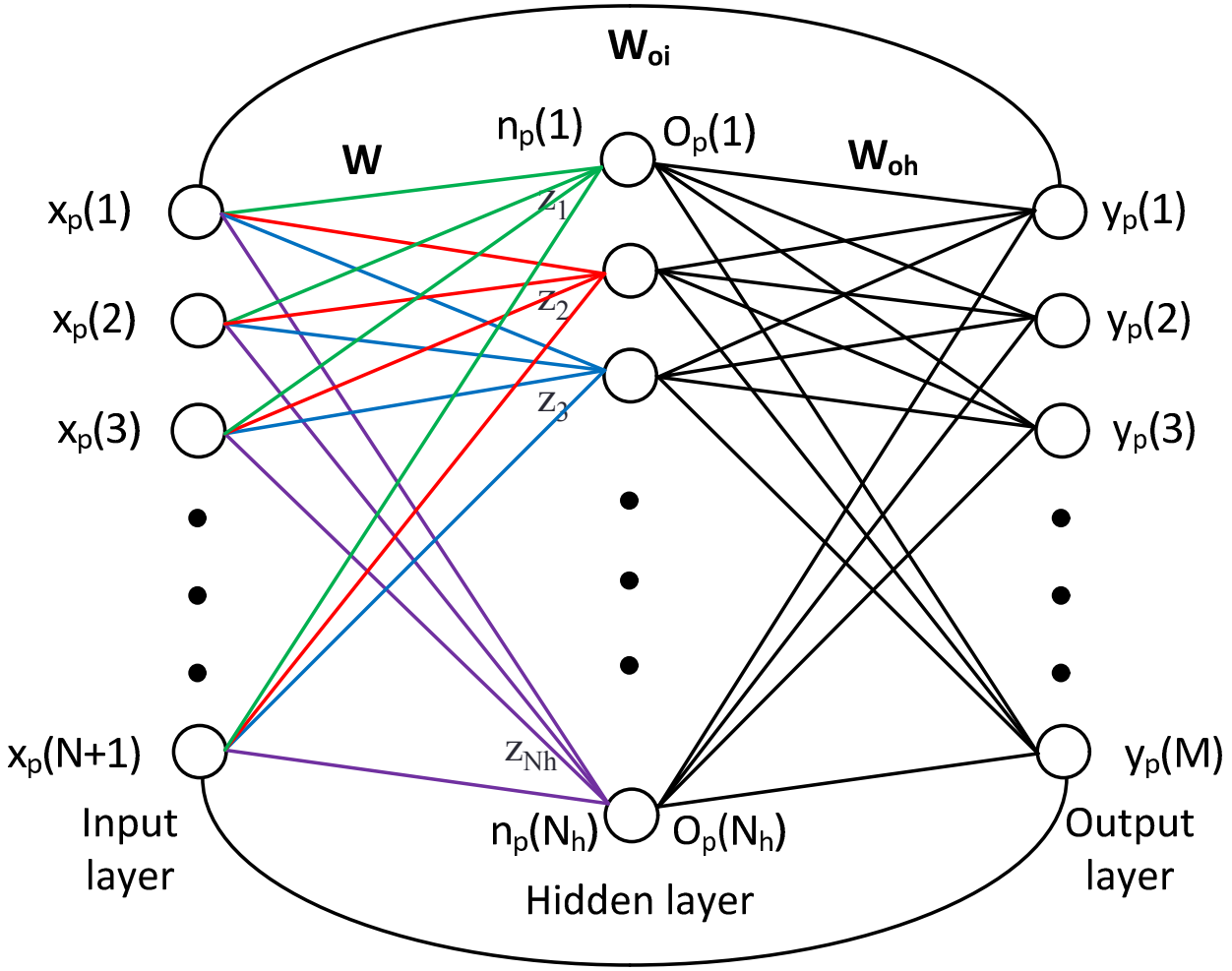
- Input weights are trained using
  - Learning factor vector **z** of size $N_h \times 1$
  - Negative gradient vector **g**

- Output weights are trained using OWO

- z_k , k^{th} element of vector **z** used to update all the weights connected to hidden unit k

$$y_p(i) = \sum_{n=1}^{N+1} w_{oi}(i,n)\, x_p(n) + \sum_{k=1}^{N_h} w_{oh}(i,k)\, f\left(\sum_{n=1}^{N+1} \left(w(k,n) + z_k\, g(k,n) \right) x_p(n) \right)$$

MOLF demonstration



- Learning factor vector **z** is computed as

$$\mathbf{z} = \mathbf{H}_{\mathbf{molf}}^{-1}\mathbf{g}_{\mathbf{molf}}$$

- Element of matrix $\mathbf{H}_{\mathbf{molf}}$,

$$h_{molf}(k, j) = \frac{\partial^2 E}{\partial z_k \partial z_j}$$

- $\mathbf{g}_{\mathbf{molf}} = \left[-\partial E/\partial z_1, -\partial E/\partial z_2 ...., -\partial E/\partial z_{N_h}\right]^T$

- OWO-MOLF trains much faster than BP

- OWO-Newton

In each iteration:

- Newton's method for input weights

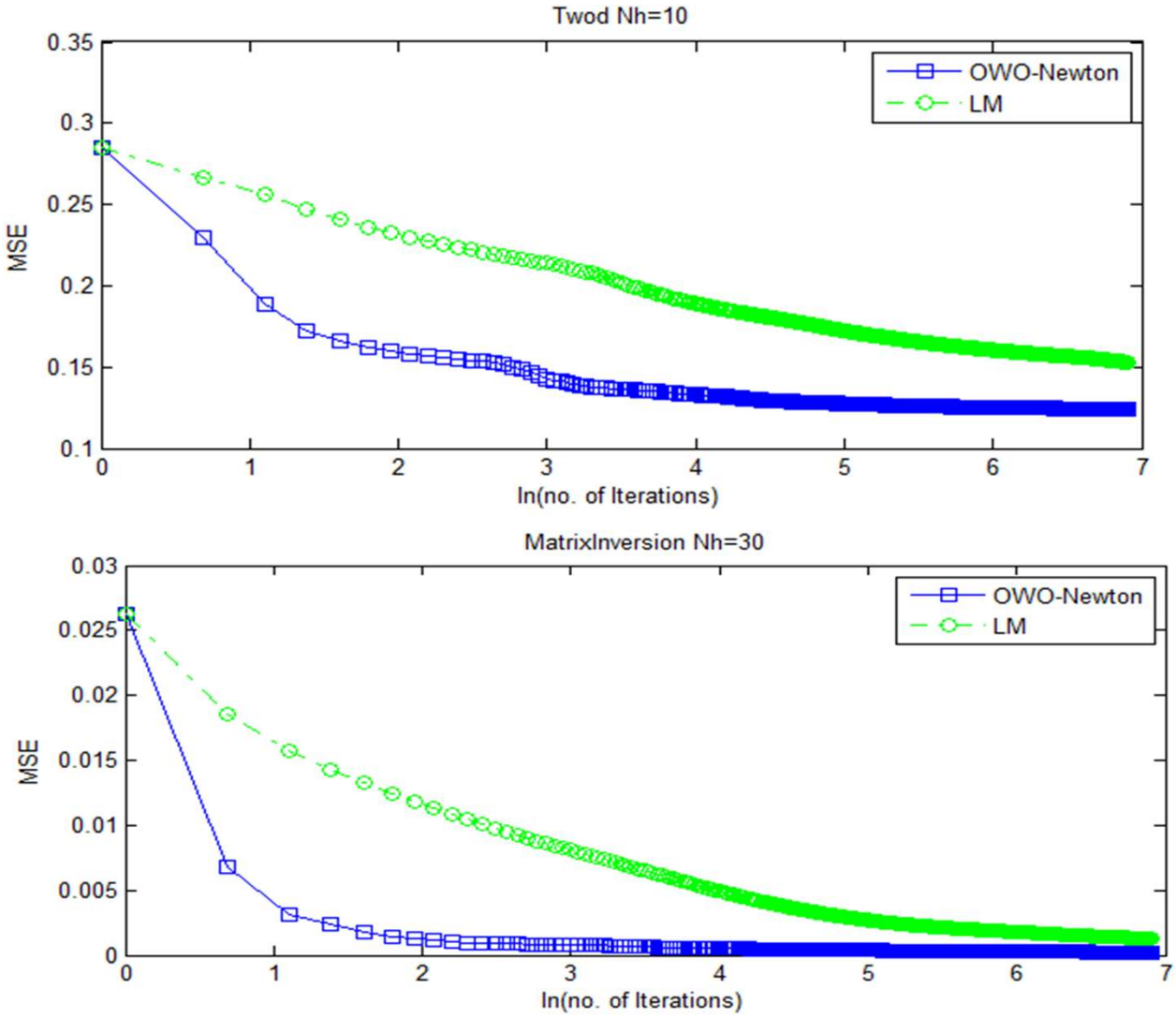
$$\mathbf{w} \leftarrow \mathbf{w} + \mathbf{e} \qquad\qquad \mathbf{w} = \text{vec}\{\mathbf{W}\}$$

$$\mathbf{e} = \mathbf{H}^{-1} \cdot \mathbf{g}$$

- $\mathbf{H}$ $\longrightarrow$ Hessian of error with respect to input weights in the network
- $\mathbf{g}$ $\longrightarrow$ negative input weight gradient vector

- Output weights are solved using OWO

- OWO-Newton has simpler and faster code than LM for similar performance



- Problems

- Little theoretical justification for using small second order modules in first order algorithms

- Second order training is computationally very expensive

- Error decrease per iteration is larger in OWO-Newton, number of multiplies per iteration is less for OWO-MOLF

- Lemmas
  - Lemma 1: Assume for quadratic E(**w**), **w** is divided into k partitions $\mathbf{w_k}$ If we minimize E with respect to **z** producing an error $E_k = E(\mathbf{w_1} + z_1\mathbf{g_1}, \mathbf{w_2} + z_2\mathbf{g_2}, ...\mathbf{w_k} + z_k\mathbf{g_k})$ and k increases by splitting an existing partition, then $E_{k+1} \leq E_k$
  - Implications
    - More learning factors means more error decrease
    - Not guaranteed since E(**w**) is not quadratic

III. Goals

- Develop a new algorithm that adapts between OWO-MOLF and OWO-Newton
- Maximize error decrease per multiply
- Simulations

IV. Adaptive Multiple Optimal Learning Factors

In each iteration:

- Input weights are trained using
  - Learning factor vector **z**
  - Negative gradient vector **g**

- Output weights are trained using OWO

- Size of **z** can vary between N_h and $N_h \times (N+1)$ in each iteration

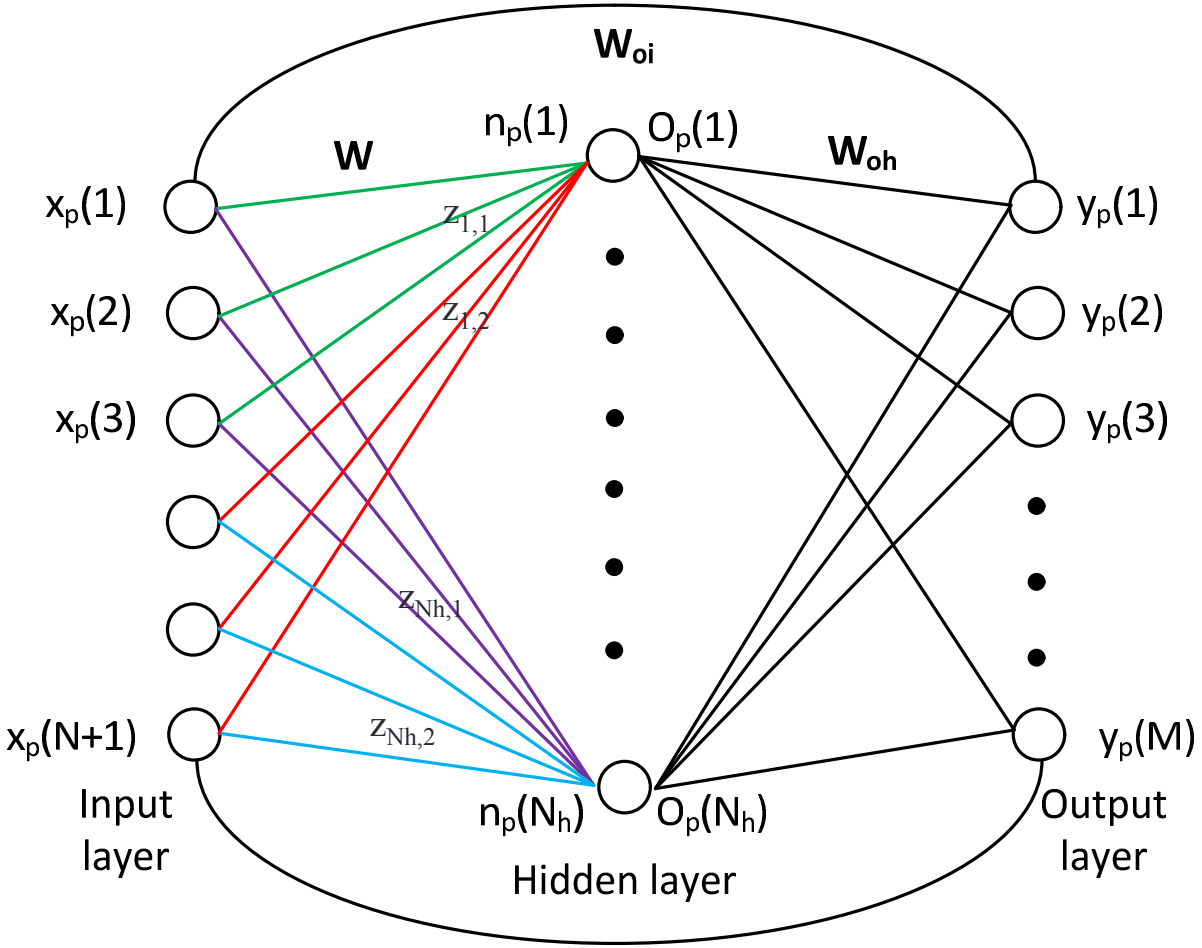
- This algorithm adapts between OWO-MOLF and OWO-Newton

- The input weights connected to each hidden unit are grouped into N_g groups

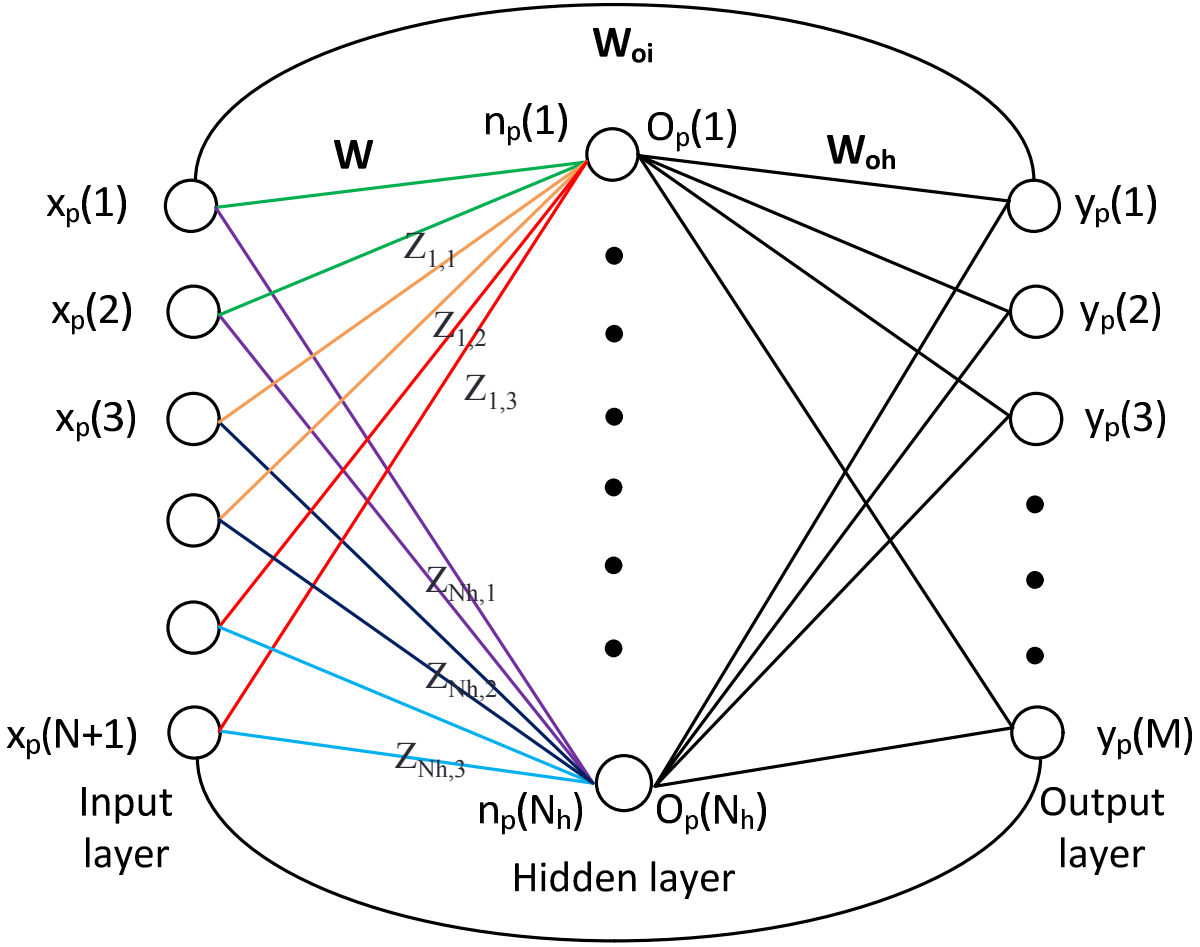
- An unique learning factor is computed for each of this groups

- $z_{k,C}$ is an element of **z** used to update all the input weights that belong to the group C of hidden unit k.

Adaptive MOLF with N_g=2



Adaptive MOLF with N_g=3



- Grouping of input weights

- Grouping is done based on the curvature $\mathbf{H_w}$ of the error function calculated with respect to input weights

- The elements of $\mathbf{H_w}$ can be calculated as,

$$h_w(k,n) = \frac{\partial^2 E}{\partial w(k,n)^2} = \frac{2}{N_v} \sum_{i=1}^{M} w_{oh}(i,k)^2 \sum_{p=1}^{N_v} f'(n_p(k))^2 x_p(n)^2$$

- How is the number of groups changed

- Goal is to vary number of groups so that the error change per multiply is maximized
- Number of groups per hidden unit increases as the error change per multiply (EPM) increases and vice versa.

$$EPM(i_t) = \frac{E(i_t - 1) - E(i_t)}{M(i_t)}$$

- $M(i_t)$ stands for number of multiplies in iteration i_t
- $EPM(i_t)$ is the error per multiply in iteration i_t
- $E(i_t)$ it the error computer in iteration i_t
- i_t is the current iteration number.

- Derivation of adaptive MOLF algorithm

$$y_p(i) = \sum_{n=1}^{N+1} x_p(n) w_{oi}(k,n) + \sum_{k=1}^{N_h} w_{oh}(i,k) f\left(\sum_{C=1}^{N_g} \sum_{a=R(C-1)+1}^{R(C)} x_p(i_k(a)) \left[w(k,i_k(a)) + z_{k,C} g(k,i_k(a)) \right] \right)$$

$$R(C) = C \times Gs(C)$$

$$Gs(0) = 0$$

- C is the group index
- **Gs** is an array of $N_g \times 1$ elements, these elements contains the sizes of all group the belong to a hidden unit
- $\mathbf{I_k}$ contains input indices ordered in such a way that the index n of input to which weight w(k,n) with higher curvatures are connected will come first.

- $\mathbf{I_k} = [n_1, n_2, n_3 \ldots\ldots, n_{N+1}]$ where $n_1, n_2, n_3 \ldots\ldots, n_{N+1}$ are input indices such that $h_w(k,n_1) \geq h_w(k,n_2) \geq h_w(k,n_3) \ldots\ldots\ldots\ldots \geq h_w(k,n_{N+1})$

- Hessian and negative gradient elements

$$g_{Amolf}(k,C) = \frac{-\partial E}{\partial z_{k,C}} = \frac{2}{N_v} \sum_{p=1}^{N_v} \sum_{i=1}^{M} \left(t_p(i) - y_p(i)\right) \frac{\partial y_p(i)}{\partial z_{k,C}}$$

$$\frac{\partial y_p(i)}{\partial z_{k,C}} = w_{oh}(i,k) f'\left(n_p(k)\right) \Delta n_p(k,C)$$

$$\Delta n_p(k,C) = \sum_{a=R(C-1)+1}^{R(C)} x_p\left(i_k(a)\right) g\left(k, i_k(a)\right)$$

$$h_{Amolf}(k,C_1,j,C_2) = \frac{2}{N_v} \sum_{i=1}^{M} w_{oh}(i,k) w_{oh}(i,j) \sum_{p=1}^{N_v} f'\left(n_p(k)\right) f'\left(n_p(j)\right) \Delta n_p(k,C_1) \Delta n_p(j,C_2)$$

- The elements of the 2 dimensional Hessian $\mathbf{H_{Amolf}}$ are found from $h_{Amolf}(k,C_1,j,C_2)$ as

$$h_{Amolf}\left((k-1)N_g + C_1, (j-1)N_g + C_2\right) = h_{Amolf}\left(k, C_1, j, C_2\right)$$

- Elements of negative gradient column vector $\mathbf{g_{Amolf}}$ are calculated from $g_{Amolf}(k,C)$ as,

$$g_{Amolf}\left((k-1)N_g + C\right) = g_{Amolf}\left(k, C\right)$$

$$\mathbf{z} = \mathbf{H}_{\mathbf{Amolf}}^{-1} \cdot \mathbf{g}_{\mathbf{Amolf}}$$

- The input weights **W** are updated as follows,

$$w\left(k, i_k\left(a\right)\right) = w\left(k, i_k\left(a\right)\right) + z_{k,C}\, g\left(k, i_k\left(a\right)\right)$$

where,

$$[(C\text{-}1) \times Gs(C\text{-}1)] + 1 \leq a \leq [C \times Gs(C)]$$

- Lemma 2: $E\text{-}E_{MOLF}$ and $E\text{-}E_{aMOLF}$ denote the error decrease due to the Newton steps of OWO-MOLF and adaptive MOLF respectively, then $E\text{-}E_{MOLF} \leq E\text{-}E_{aMOLF}$

- Lemma 3: OWO-Newton is a limiting case of the adaptive MOLF algorithm as the k groups of adaptive MOLF are split until $k=N_h \cdot (N+1)$

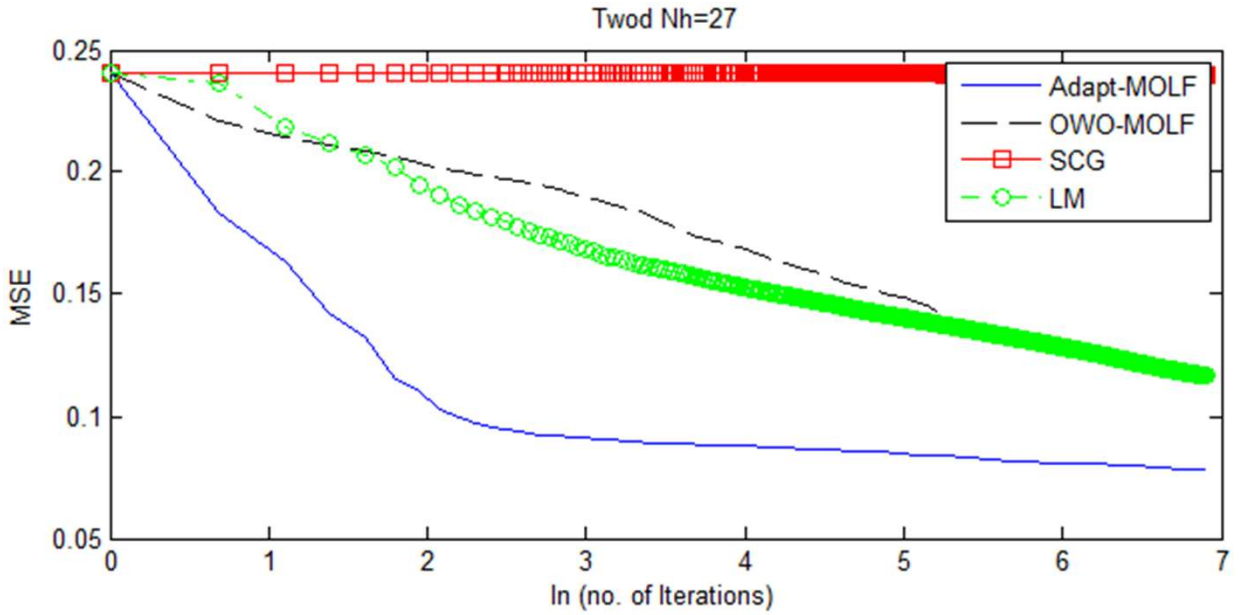
- Adaptive MOLF Hessian and gradients can be generated from Gauss-Newton Hessian and gradients as follows

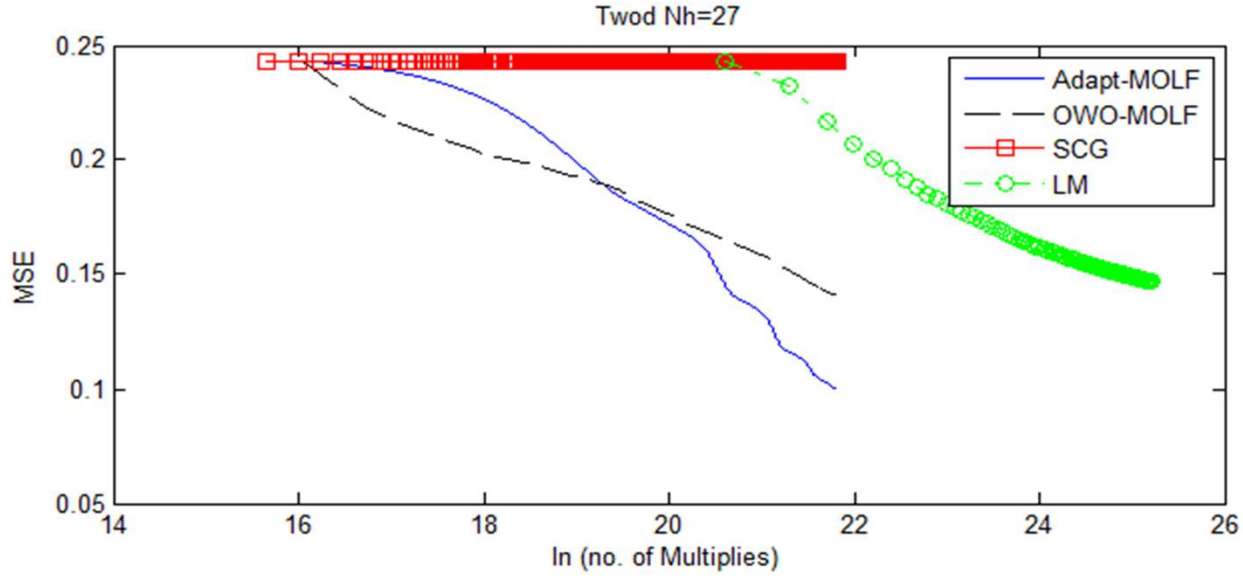
$$g_{\text{Amolf}}(k,C) = \sum_{a=R(C-1)+1}^{R(C)} g(k,i_k(a))^2$$

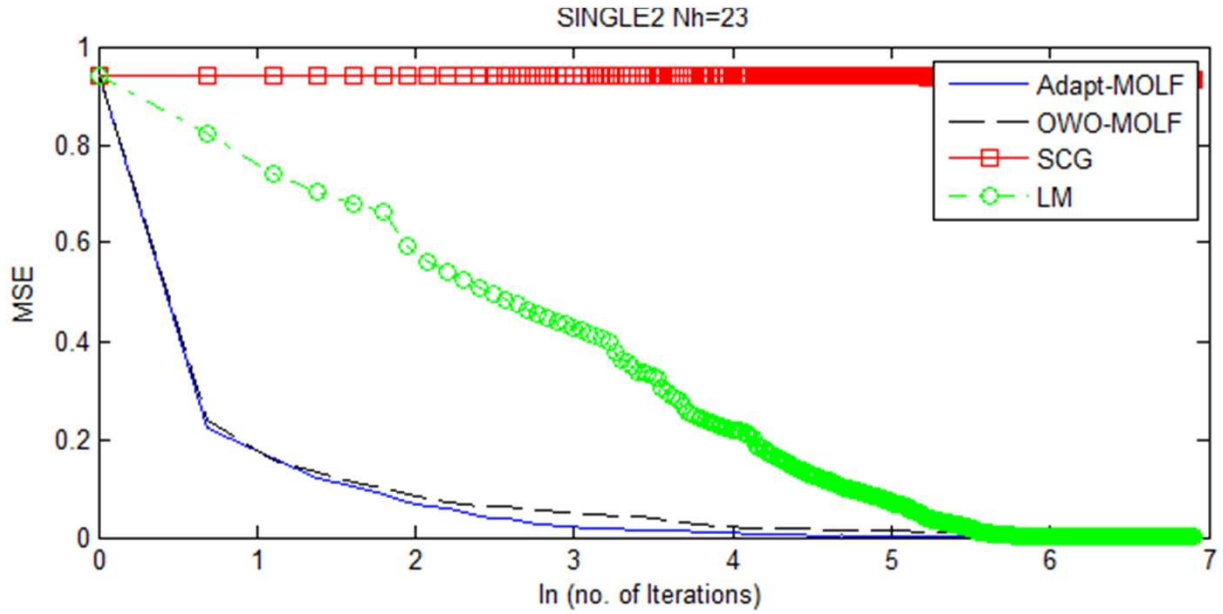
$$h_{\text{Amolf}}(k,C_1,j,C_2) = \sum_{a=R(C_1-1)+1}^{R(C_1)} \sum_{b=R(C_2-1)+1}^{R(C_2)} h(k,i_k(a),j,i_j(b)) g(k,i_k(a)) g(j,i_j(b))$$

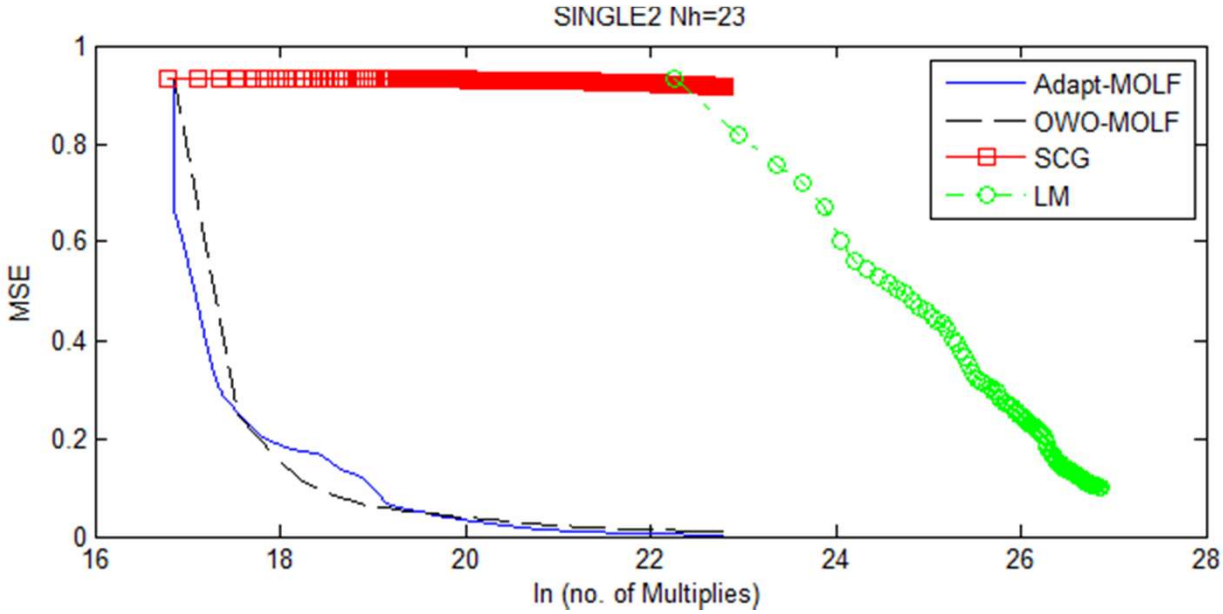
V. Simulations

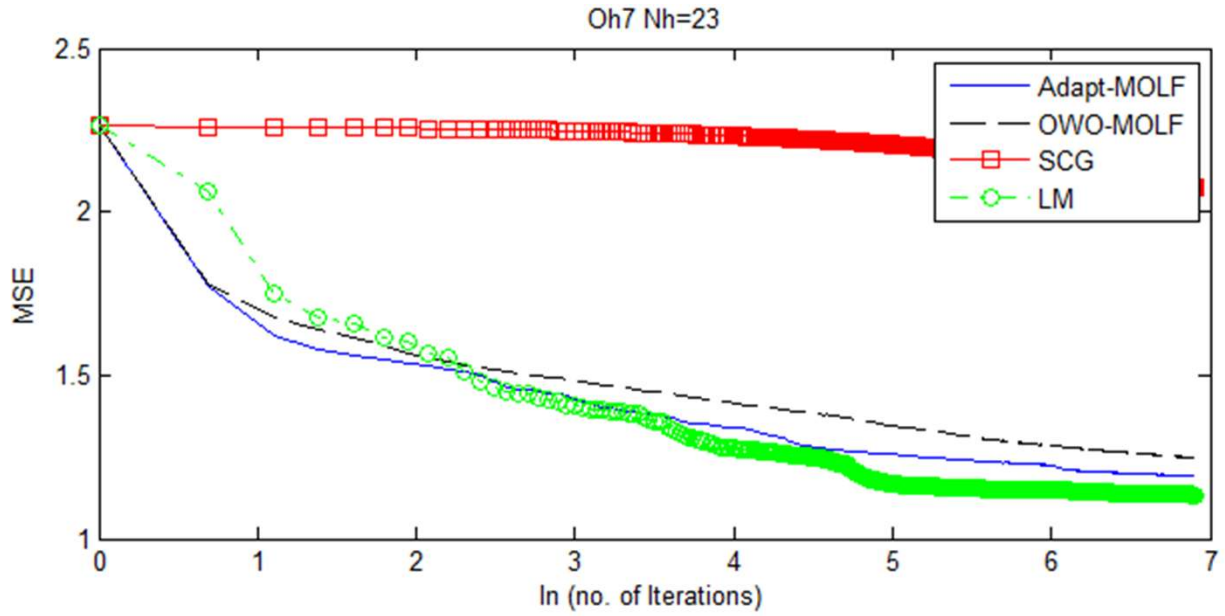
- Training is done on the entire data set 10 times with 10 different initial networks. The average MSE from this 10-fold training is shown in the plots below.

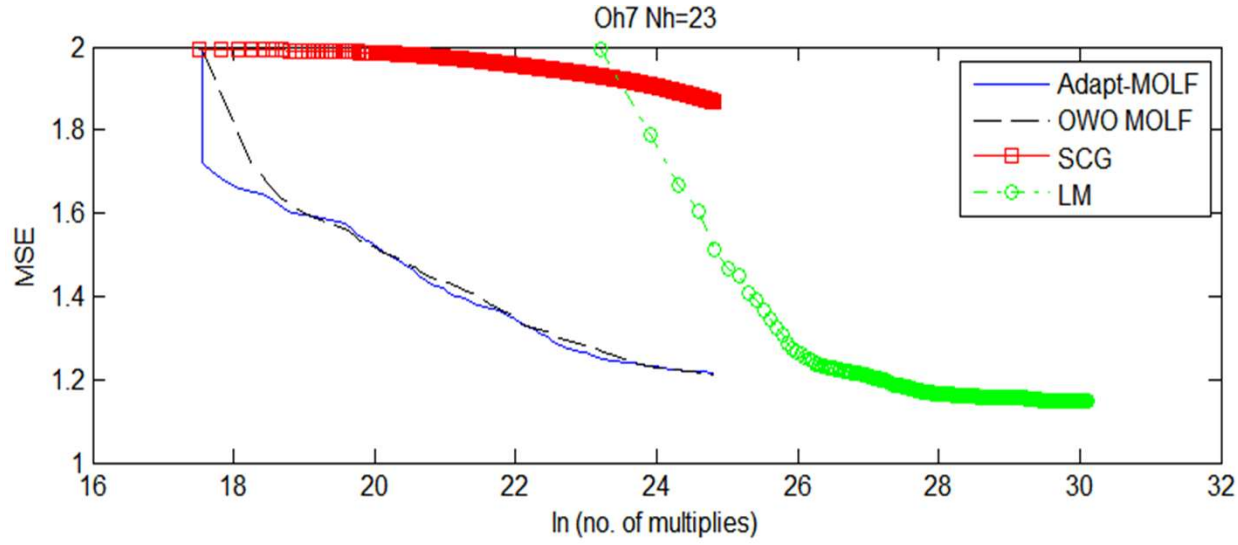

Twod Nh=27
MSE
ln (no. of Iterations)
Adapt-MOLF
OWO-MOLF
SCG
LM
0.25
0.2
0.15
0.1
0.05
0
1
2
3
4
5
6
7

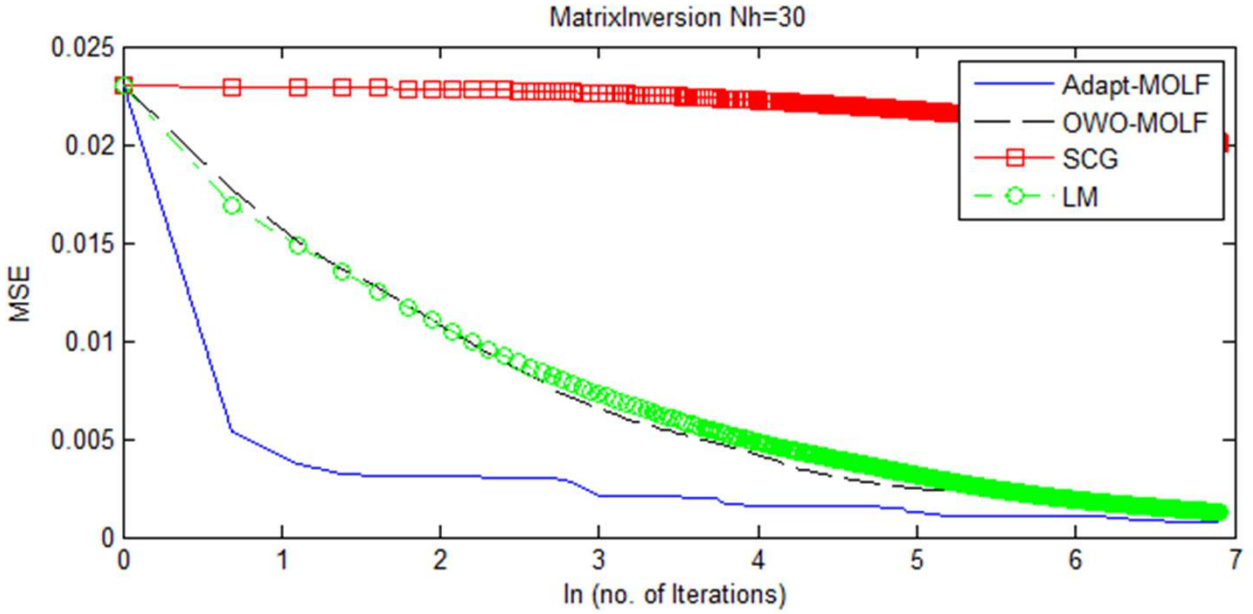

Twod Nh=27
MSE
ln (no. of Multiplies)
Adapt-MOLF
OWO-MOLF
SCG
LM
0.25
0.2
0.15
0.1
0.05
14
16
18
20
22
24
26

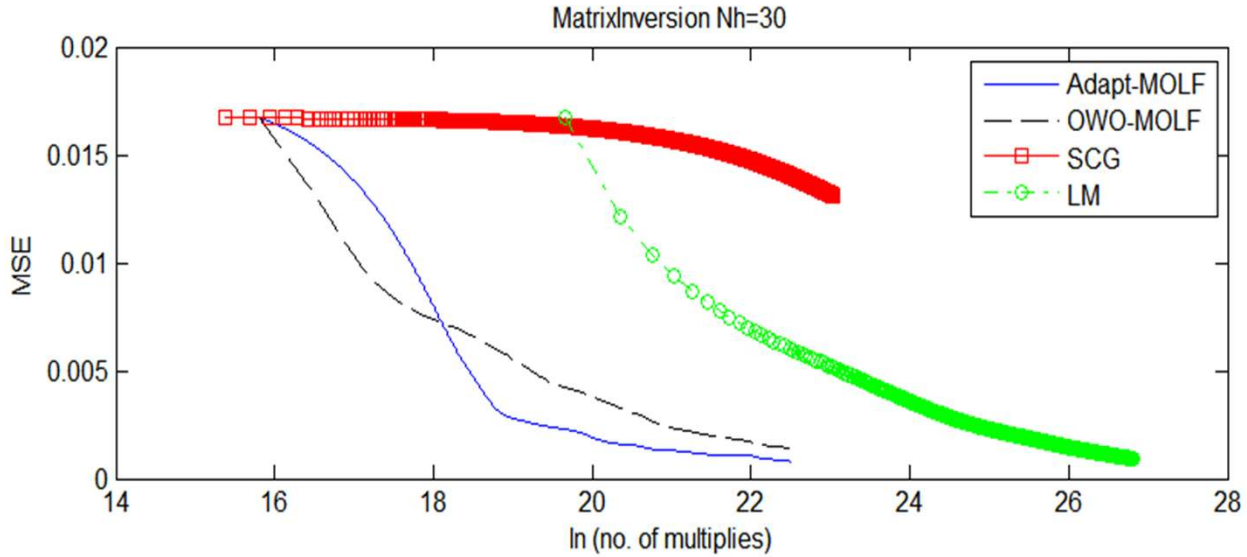

SINGLE2 Nh=23
Adapt-MOLF
OWO-MOLF
SCG
LM
MSE
ln (no. of Iterations)


SINGLE2 Nh=23
Adapt-MOLF
OWO-MOLF
SCG
LM
MSE
ln (no. of Multiplies)


Oh7 Nh=23
MSE
ln (no. of Iterations)
Adapt-MOLF
OWO-MOLF
SCG
LM
2.5
2
1.5
1
0
1
2
3
4
5
6
7


Oh7 Nh=23
MSE
ln (no. of multiplies)
Adapt-MOLF
OWO MOLF
SCG
LM
2
1.8
1.6
1.4
1.2
1
16
18
20
22
24
26
28
30
32


MatrixInversion Nh=30
MSE
ln (no. of Iterations)
Adapt-MOLF
OWO-MOLF
SCG
LM
0.025
0.02
0.015
0.01
0.005
0
0
1
2
3
4
5
6
7


MatrixInversion Nh=30
MSE
ln (no. of multiplies)
Adapt-MOLF
OWO-MOLF
SCG
LM
0.02
0.015
0.01
0.005
0
14
16
18
20
22
24
26
28

K-fold validation and testing

Data Set		Adaptive MOLF	OWO-MOLF	SCG	LM
Twod.tra	E_{trn}	0.0888	0.1554	1.0985	0.2038
	E_{tst}	0.1172	0.1731	1.0945	0.2205
Single2.tra	E_{trn}	0.0042	0.0151	3.5719	0.0083
	E_{tst}	0.2319	0.1689	3.6418	0.0178
Mattrn.tra	E_{trn}	0.0011	0.0027	4.2400	0.0022
	E_{tst}	0.0013	0.0032	4.3359	0.0027
Oh7.tra	E_{trn}	1.2507	1.3205	4.1500	1.1602
	E_{tst}	1.4738	1.4875	4.1991	1.4373

VI. Conclusions

- The number of learning factors needed by a training algorithm is addressed and adaptively optimized
- The adaptive MOLF algorithm is superior to the OWO-MOLF algorithm in terms of error decrease per iteration and often in terms of error decrease per multiply
- The proposed algorithm interpolates between OWO-MOLF and OWO-Newton

Thank you

Questions