

Learning and generalization characteristics of the random vector Functional-link net

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Abstract

In this paper we explore and discuss the learning and generalization characteristics of the random vector version of the Functional-link net and compare these with those attainable with the GDR algorithm. This is done for a well-behaved deterministic function and for real-world data. It seems that 'overtraining' occurs for stochastic mappings. Otherwise there is saturation of training.

Keywords. Neural net; Functional-link net; functional mapping; generalized delta rule; auto-enhancement; overtraining and generalization.

1. Introduction

Of all the capabilities ascribable to neural-net computing, there is none more noteworthy than that of *supervised learning*. The work of Hornik, Stinchcombe and White [1], Funahashi [2] and Cardaliaguet and Euvrard [3] indicate that the multi-layer generalized *PERCEPTRON* feedforward net with linear links and appropriate nonlinear activation at nodes can serve as a computational model of functional mappings $f(x)$ from R^N to R . Such existence theorems do not address issues such as learning and generalization, and different approaches to those matters can be adopted with correspondingly different results in practice.

In the past, we have explored variations [4, 5] on the feedforward net architecture, inspired primarily by the work of Giles and Maxwell [13] on high-order neural networks. Our idea is that often it might be helpful to abstract and replace substantial parts of an otherwise massive net with use of Functional-links. Functional-link (FL) nets can be implemented in various ways, one of which is the random vector (RV) approach [7, 8]. This paper is concerned with the learning and generalization characteristics of the random-vector implementation of the FL net. These are described and discussed comparatively with corresponding characteristics of the backpropagation-of-error (BP) [9] net for two types of situations; one for which a

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deterministic causal mapping does exist and another involving *real world* noisy data. In this work the BP net is also referred to interchangeably as the generalized delta rule (GDR) net.

In the neural-network supervised learning task, the generic idea is that such a net can synthesize a network computational model of a known function *if that function does indeed exist*. The learning procedure is based on a finite number of known instances of the *presumed functional mapping*, and it is assumed and hoped that the computational network model so learned is not only capable of replicating the known instances of the mapping but is also valid for the infinitude of all the other points in the neighborhoods of the exemplars.

In practice many things can go awry. For example, there may be, in fact, no deterministic function and the exemplars might be merely a set of random pairings of points. In such a case the training set of mappings can still be learned very well, but any test set will exhibit the random scatter inherent to the stochastic process used to generate the data. If a net does not have enough available adjustable parameters or if the learning process is terminated prematurely, then both the training set and test set errors may be large. On the other hand if the net has too many adjustable parameters or if the net is *over-trained*, then the training set error may be deceptively low without comparable performance attainable for the test set points.

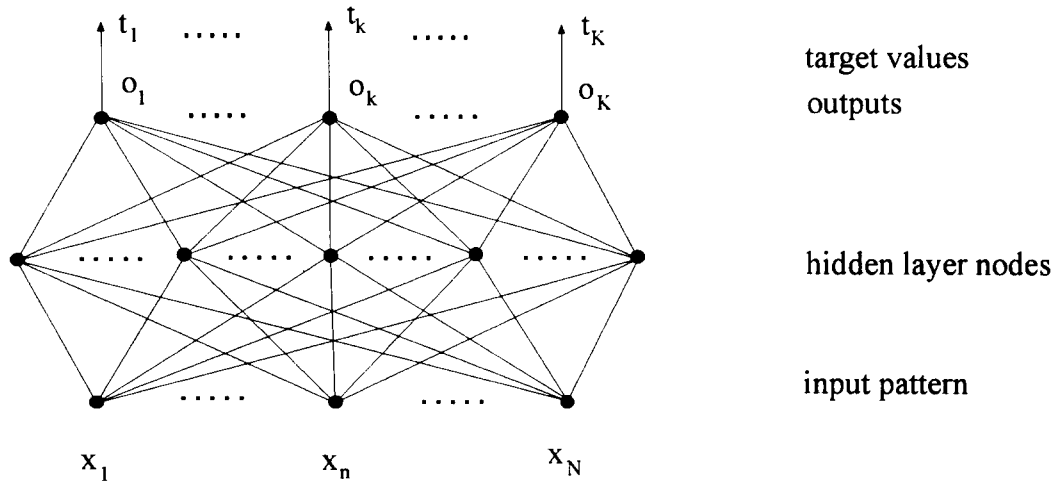
2. Brief review of the random vector Functional-link approach

The basic GDR concept is illustrated in *Fig. 1(a)* for a mapping from an N -dimensional space to K -dimensional space. There are J nodes in the hidden layer and the action of the net may be understood in terms of two successive mappings or transformations. The action of the initial mapping, from the input to the hidden layer, is to transform the description of the input pattern vectors from the original one in input space into another description in *internal representation* space. In that new representation, the next mapping is a linear one. In the GDR or BP approach, all the network parameters are successively adjusted until the known mappings are replicated to the desired accuracy for all the vector parts provided as the *training set*.

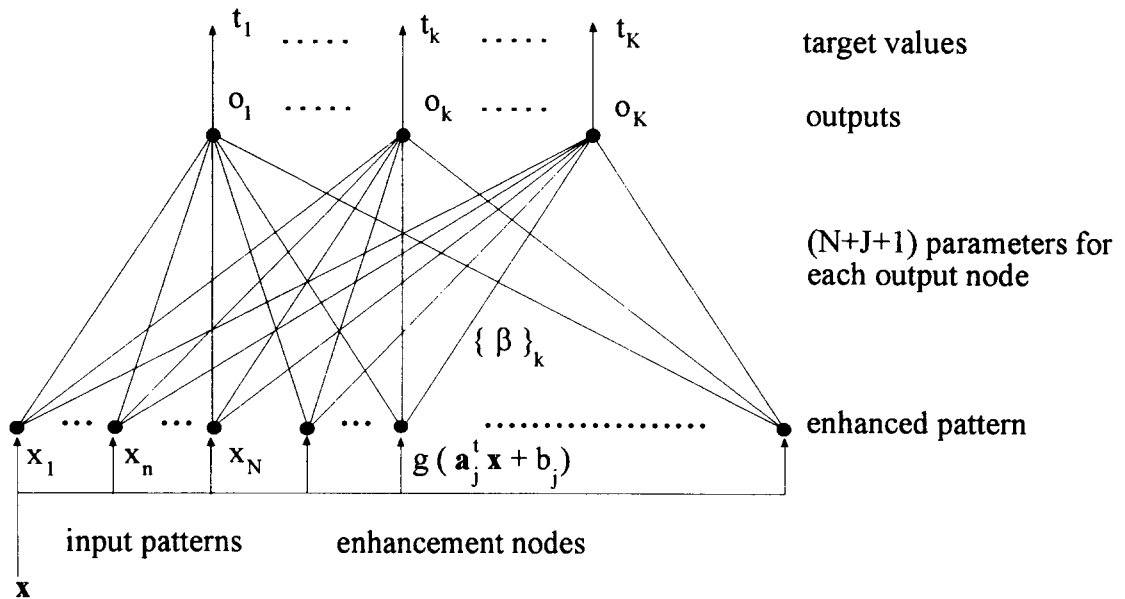
The random-vector FL network shown in *Fig. 1(b)* performs a nonlinear transformation of the input pattern before it is fed to the input layer of the network. The essential action is, therefore, the generation of an enhanced pattern to be used in place of the original. Experience indicates that supervised learning can be achieved readily using a *flat* net (one that has no hidden layers), and that the delta rule can be used in place of the generalized delta rule (GDR) if this enhancement is done correctly.

The random-vector FL net is but one specific mode of realization of the general Functional-link net idea. Other modes of instantiations of that approach have been described and discussed by us elsewhere in previous publications [4–7], but the random-vector version is attractive because it is susceptible to rigorous mathematical proof [14] and also because it is easy to use. In connection with the latter comment, we note that even though a large number of enhancement nodes might be generated initially, usually a large fraction of those candidate enhancement nodes can be pruned away if they, individually, do not contribute to the net input of the output nodes, or sometimes, depending on the circumstance, if a node does not contribute to discrimination between classes.

The network connectivities shown in *Fig. 2(a)* and *(b)* are similar to those of *Fig. 1*, except for the fact that we focus on a single output and do not require a nonlinear transform at that



(a) the GDR net

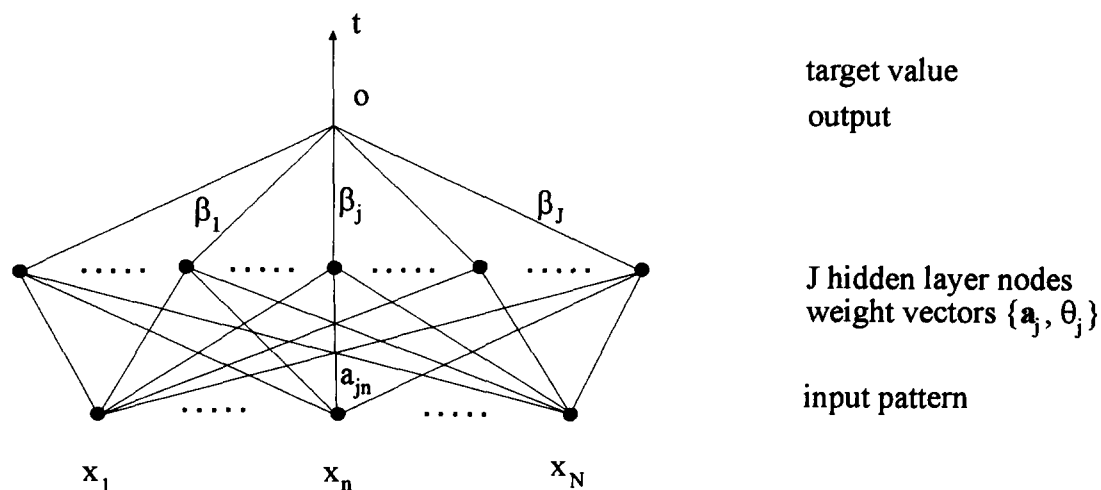


(b) the Random-Vector FL net

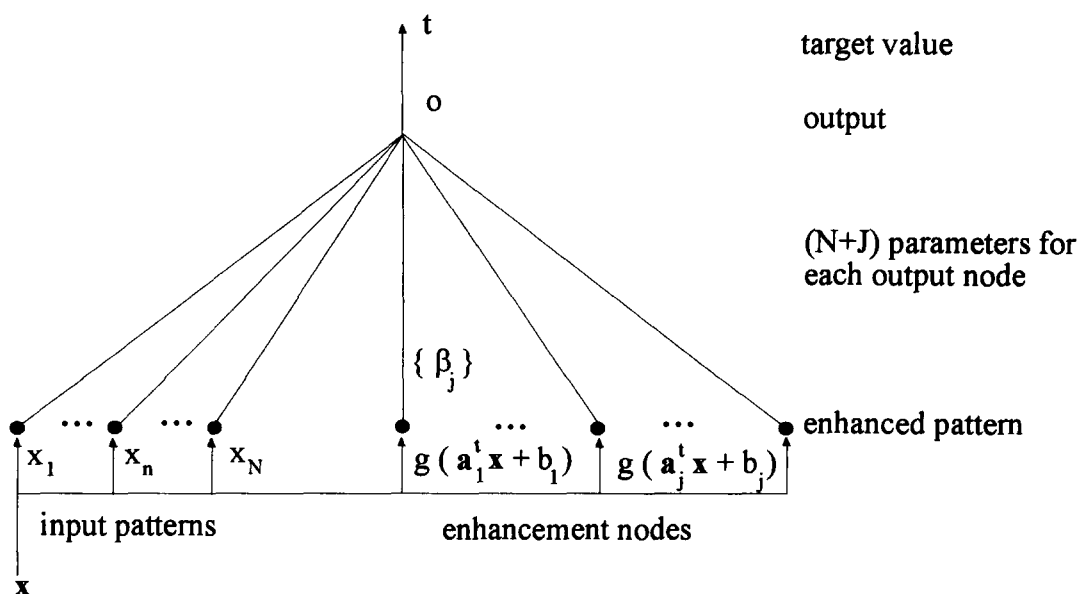
Fig. 1. Comparison of network connectivities.

final output. This allows us to illustrate explicitly some of the entities to be learned and there is no loss of generality.

To be specific for the GDR net, the input to each hidden layer node is $net_j = \sum a_{jn} x_n =$



(a) the GDR net



(b) the Random-Vector FL net

Fig. 2. Illustration of network parameters.

$a_j^t x$ and the output is $g(a_j^t x + b_j)$ where b_j is the threshold parameter for the node j and $g(\cdot)$ is the sigmoid function. The net to the single (nonlinear) output is simply $\sum \beta_j g(a_j^t x + b_j)$. In the *random-vector* FL net, the functional enhancements are achieved in essentially the same

manner as in the first layer of the GDR net. The additional enhancements are $g(\mathbf{a}_j^t \mathbf{x} + b_j)$. The random-vector implementation of the FL net can be viewed as essentially the same as the GDR except for the fact that the hidden layer is moved down to serve as an enhancement of the input vector and the weights vectors $\{\mathbf{a}_j\}$ are *not* learned but are randomly generated (but appropriately¹). The random-vector implementation can also be viewed as a type of encoding comparable to the coarse-coding of patterns with linguistic symbolic feature values [10]. A mapping from N -dimensional space to K -dimensional space is represented by K independent networks and each network can be modified adaptively without entanglement with the others.

3. Learning and generalization characteristics

For the random-vector FL net, only the weights β_j need to be learned. Including the original inputs, there are $(N + J)$ components in the enhanced pattern and there are accordingly $(N + J)$ weights (or β_j values), to be determined.

Learning is by minimization of the system error defined as

$$E = \frac{1}{2P} \sum_{p=1}^P (t^{(p)} - \mathbf{B}^t \mathbf{d}^{(p)})^2$$

where \mathbf{B}^t is the vector of weight values β_j , $j = 1, 2, 3, \dots, N + J$, and \mathbf{d} is the enhanced pattern vector (not the original input pattern vector). There are P training set patterns and the subscript (p) is the pattern index.

E is quadratic with respect to the $(N + J)$ dimensional vector \mathbf{B} . This means that the unique minimum can be found in no more than $N + J$ iterations of a learning procedure such as the conjugate gradient (CG) approach [11, 12], if the explicit matrix inversion needs to be avoided. If matrix inversion with use of a pseudo-inverse is feasible, then a single step learning would suffice.

In this paper, we report on the learning and generalization characteristics of the random-vector FL net for two different circumstances, one being that of a deterministic R^1 to R^1 mapping and the other being a mapping for noisy *real-world* data.

A well-behaved continuous function might be that shown as $f_1(x)$ in Fig. 3. However, the circumstance is that the function $f_1(x)$ is known to us only through the point marked with bold dots. As we will describe in further detail in the following, the function $f_2(x)$ is another function, learned in error by the GDR net if training is terminated prematurely. As shown in Fig. 4, the FL net can achieve satisfactory learning of the training set points if 300 enhancements are used. A system error of 0.000025 is attained after 12,065 iterations. The net is a flat net, i.e. a linear net. We did not use the CG approach partly because we want the FL and GDR net results to be comparable and also because of simplicity in the straightforward gradient iterative approach.

In generalization mode the performance of the FL net is not bad, as illustrated in Fig. 5. Comparable learning is achieved by a GDR net with 20 hidden layer nodes. The accuracy

¹The vector \mathbf{a}_j^t needs to be constrained so that activation functions $g(\mathbf{a}_j^t \mathbf{x} + b_j)$ are not saturated most of the time.

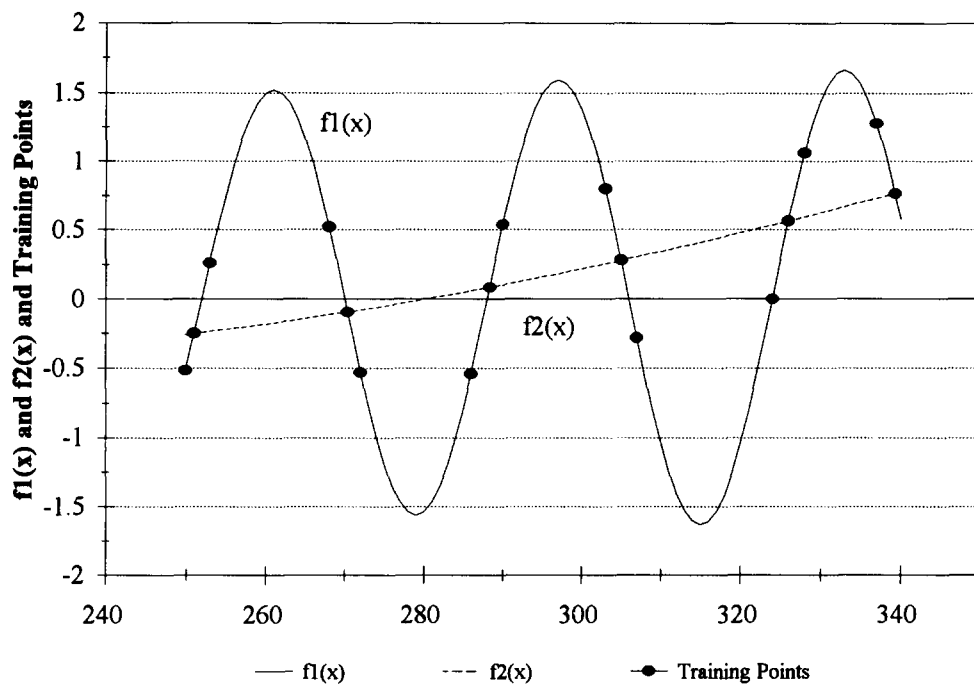


Fig. 3. The function $f_1(x)$ to be learned, the training set points and the erroneous function $f_2(x)$.

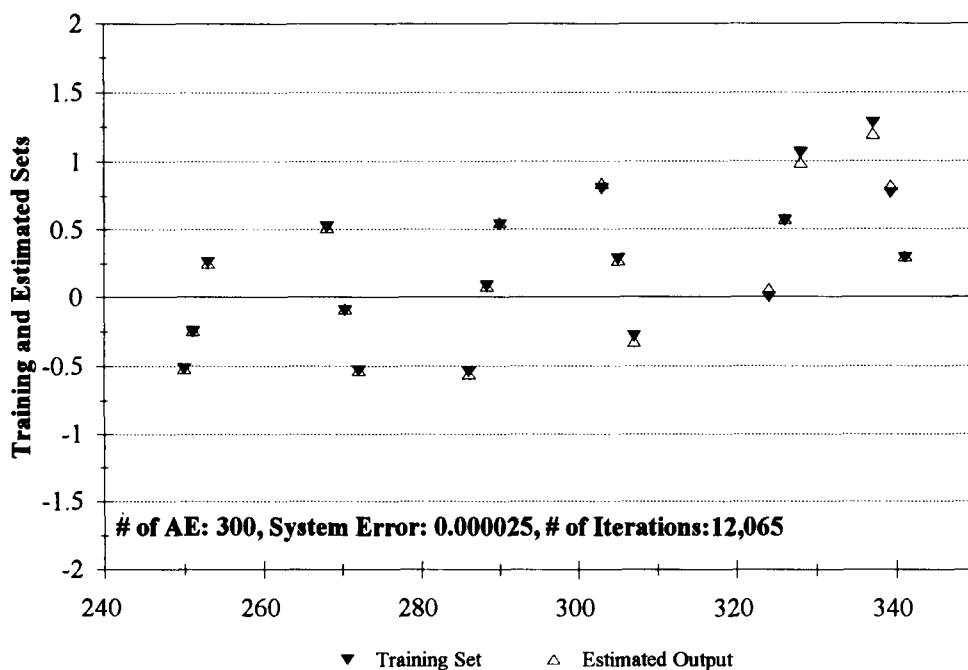


Fig. 4. Learning achieved by FL net for training set points.

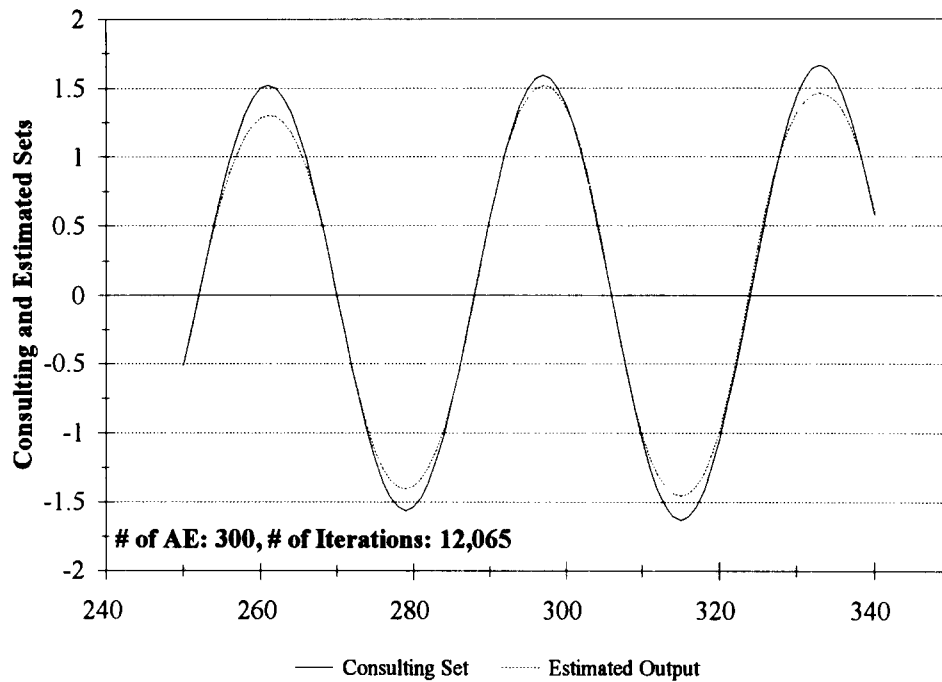


Fig. 5. Comparison of actual and estimated function values for FL net in generalization mode.

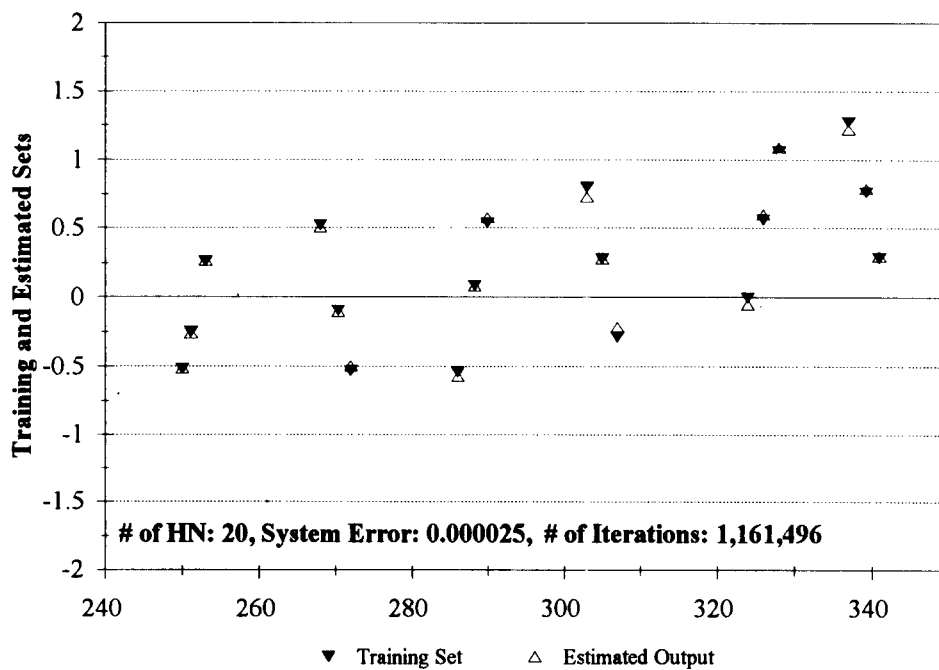


Fig. 6. Learning achieved by GDR net for training set points.

of the learning achieved by the GDR net for the training set points is illustrated in *Fig. 6*, but this was achieved only after 1,161,496 iterations. In generalization mode the performance of the GDR net is not bad either, as illustrated in *Fig. 7*. It is interesting to note that if GDR learning were stopped at 200,000 iterations, the function learned is $f_2(x)$ and not $f_1(x)$. This is shown for the training set points and for the generalization mode in *Fig. 8* and *Fig. 9* respectively.

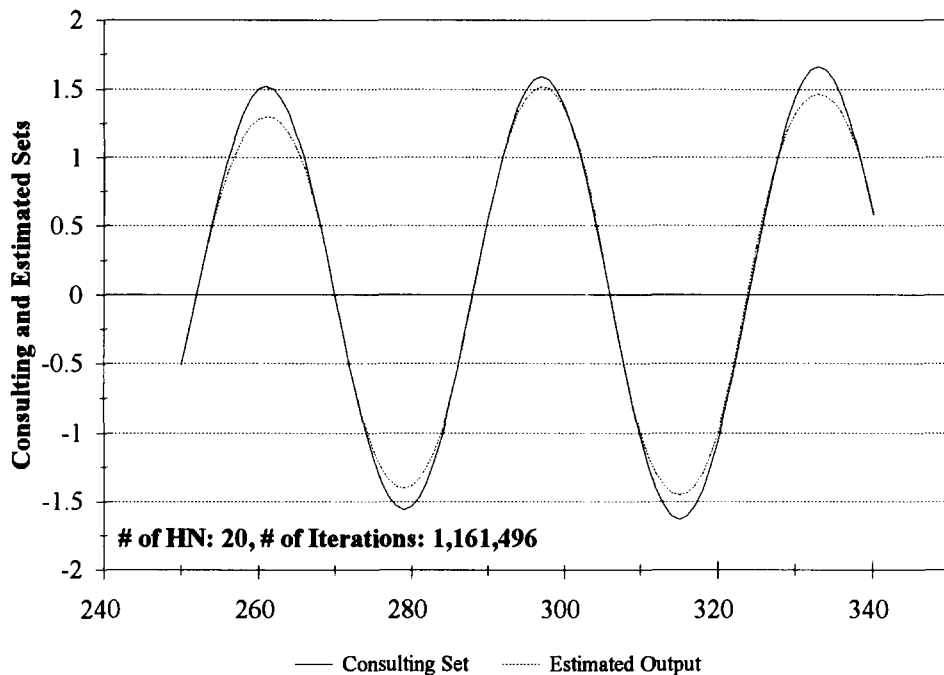


Fig. 7. Comparison of actual and estimated function values for GDR net in consulting mode.

The random vector version of the FL net is characterized by the need for a relatively large number of *auto-enhancement*, i.e. the additional enhancement nodes. This is not objectionable because the number needed does not seem to grow much with the dimension of the patterns involved.

Figure 10 shows that the number of iterations required to achieve a system error 0.000025 decreases rapidly with the increase in the number of auto-enhancements. The difference between the performances achievable with the training and test set is well illustrated by *Figs. 11* and *12*. From the curves shown in *Fig. 11*, we see that after about 20,000 iterations there is no further significant improvement in the performance of the FL net in so far as generalization is concerned. In this case, it is probably not quite accurate to say that such a net is *overtrained*, but additional improvement is marginal. Similar behavior is shown in *Fig. 12* for the GDR net.

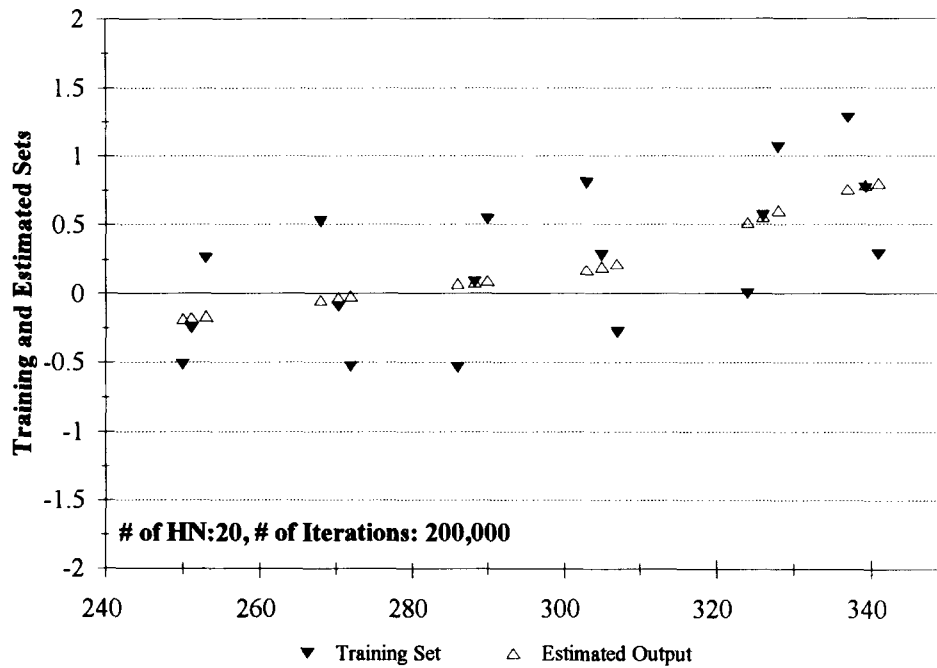


Fig. 8. Failure of the GDR net to learn the training set points if training is stopped at 200,000 iterations.

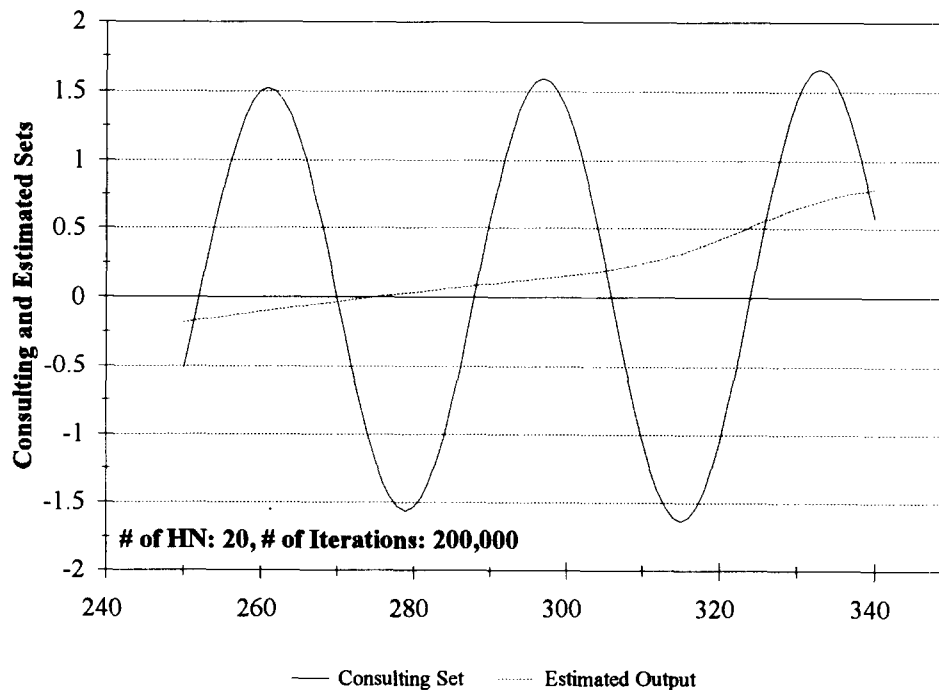


Fig. 9. Failure of 'undertrained' GDR net to generalize adequately in consulting mode.

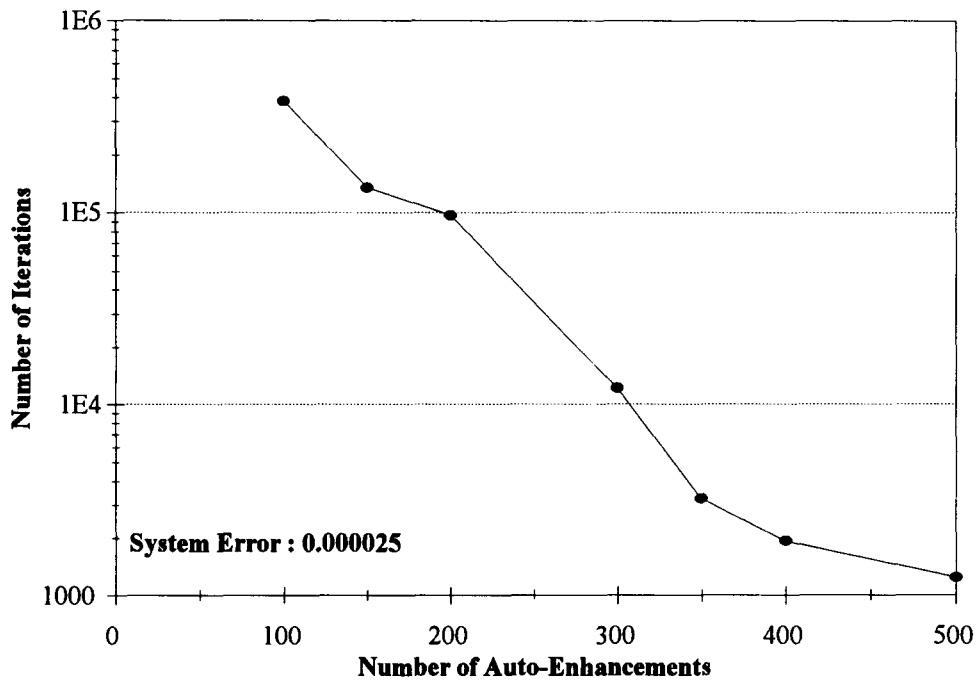


Fig. 10. Variation of number of iterations needed for training with number of auto-enhancements (for FL net).

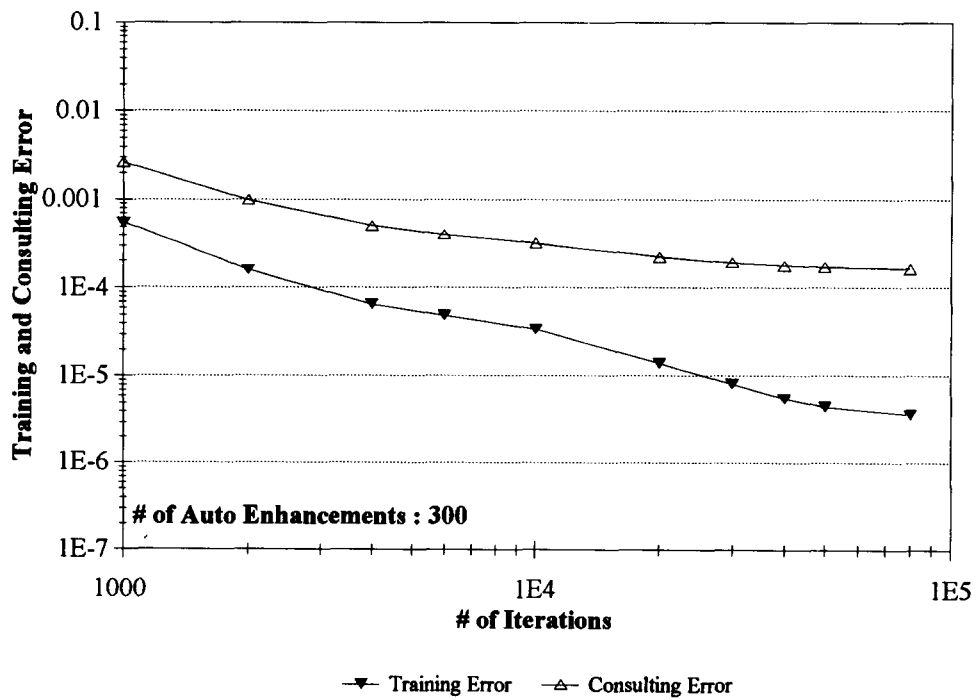


Fig. 11. Saturation of training for the FL net.

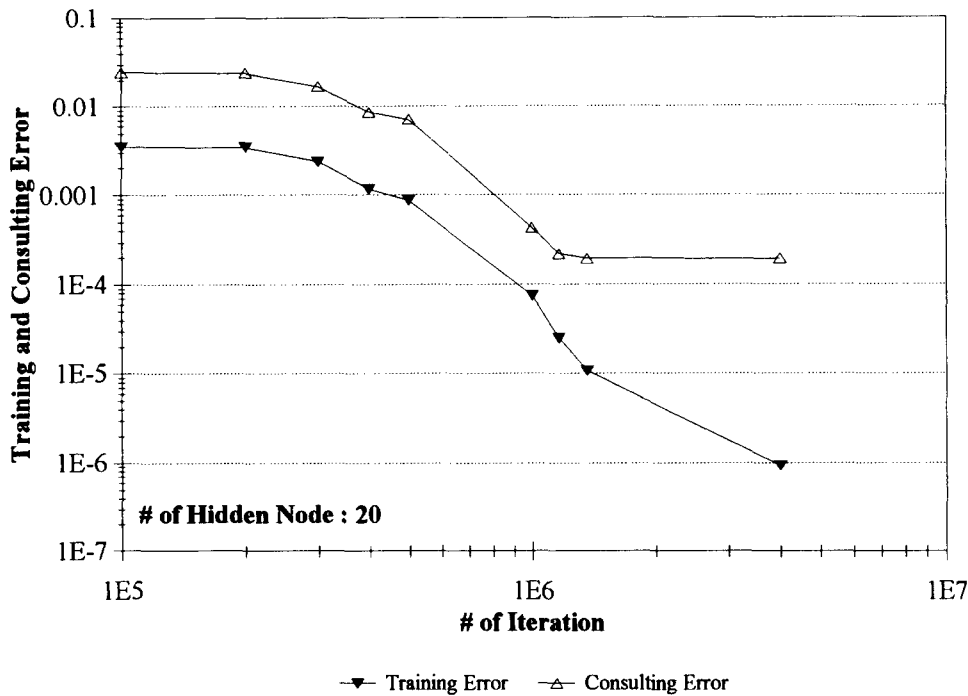


Fig. 12. Saturation of training for the GDR net.

In the preceeding discussion, we have endeavored to present a picture of the learning and generalization capabilities of the random-vector FL net as compared with those of the GDR net for a single well-behaved function which exists and is known to us, even though not known to the nets. Under such circumstances, we do not have the phenomenon of *overtraining* but only that of saturation of training. The magnitude of estimation errors in generalization mode cannot be reduced further without improving the quality of the training set.

The situation is different for *real-world* data where the functional mapping to be learned is stochastic. For those cases we can have *overtraining* and actually worsen the accuracy of estimated values as we increase the degree of training.

We illustrate some aspects of such situations with use of one instance of a real-world learning task. For that real-world task, one aspect of the overall training task could be viewed as learning a mapping from R^4 to R^1 . The training set consisted of 28 input patterns with corresponding outputs. These are listed in *Table 1*. The test set of 10 patterns is also described in *Table 1*.

The training and generalization capabilities achieved by the GDR and FL nets are illustrated in *Figs. 13* and *14* respectively. In *Fig. 13*, we see that for the FL net, there is not much point in going beyond about 500 iterations. There is indeed a slight deterioration in consulting capability as we overtrain but the deterioration is minor.

In the case of the GDR net, it is encouraging to note that training should probably be stopped after 1000 iterations, at which point the generalization quality is about twice as good as that of the FL net. But if this is not monitored, then the performance of the generalization mode deteriorates due to overtraining and the performance becomes about only half as good as that of the FL net.

Table 1. Training and consulting sets (patterns are obtained from practical chemical data).

Training Set					
#	X1	X2	X3	X4	Y
1	1.25	1	1.25	1.25	23.2
2	2	1.75	3	1.75	17.4
3	2	1.75	5.16	1.75	13.7
4	2	1.75	0.84	1.75	24.5
5	2	1.75	3	3.05	22.7
6	2	1.75	3	0.45	7.8
7	2	3.05	3	1.75	16.5
8	2	1.75	3	1.75	17.3
9	2	1	1.75	2.5	22.6
10	2	1	3.75	1	11.7
11	2	2.5	1.75	1	15.4
12	2	2.5	1.75	2.5	22.7
13	2	2.5	3.75	2.5	18.3
14	2	2.5	3.75	1	10.7
15	2	0.45	3	1.75	16.2
16	2	1.75	3	1.75	16.2
17	1.75	2	2.75	2	18.5
18	1.75	1	2.75	1	15
19	0.75	2	2.75	1	17.7
20	0.75	1	2.75	2	25.5
21	1.25	1.5	2	1.5	20
22	2.25	1.5	2	1.5	16.6
23	0.25	1.5	2	1.5	33.8
24	1.25	0.5	2	1.5	23.5
25	1.25	1.5	2	2.5	25.1
26	1.25	1.5	0.5	1.5	23.8
27	1.25	1.5	3.5	1.5	16.1
28	1.25	1.5	2	1.5	19.5

Consulting Set					
#	X1	X2	X3	X4	Y
1	2	1.75	3	1.75	16.7
2	2	1	1.75	1	15.8
3	2	1	3.75	2.5	19.2
4	1.25	1	1.25	1.25	22.2
5	1.75	2	1.25	2	22.2
6	1.75	1	1.25	1	19.2
7	0.75	2	1.25	1	23.7
8	0.75	1	1.25	2	32.8
9	1.25	2.5	2	1.5	19.7
10	1.25	1.5	2	0.5	13

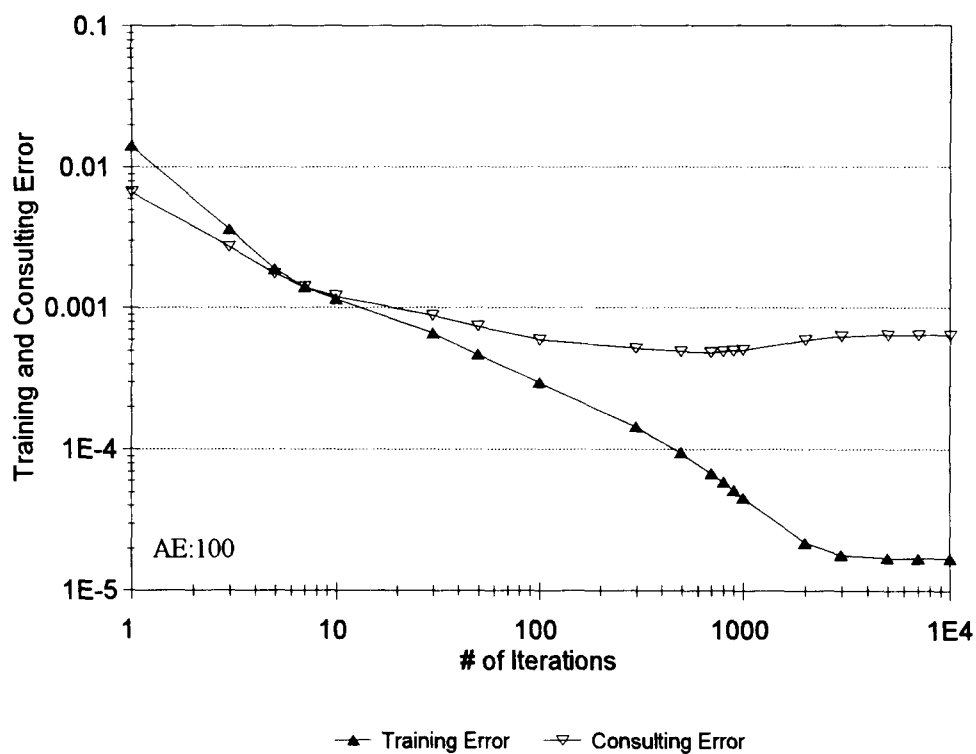


Fig. 13. Overtraining of the FL net from chemical compounding data (real-world data).

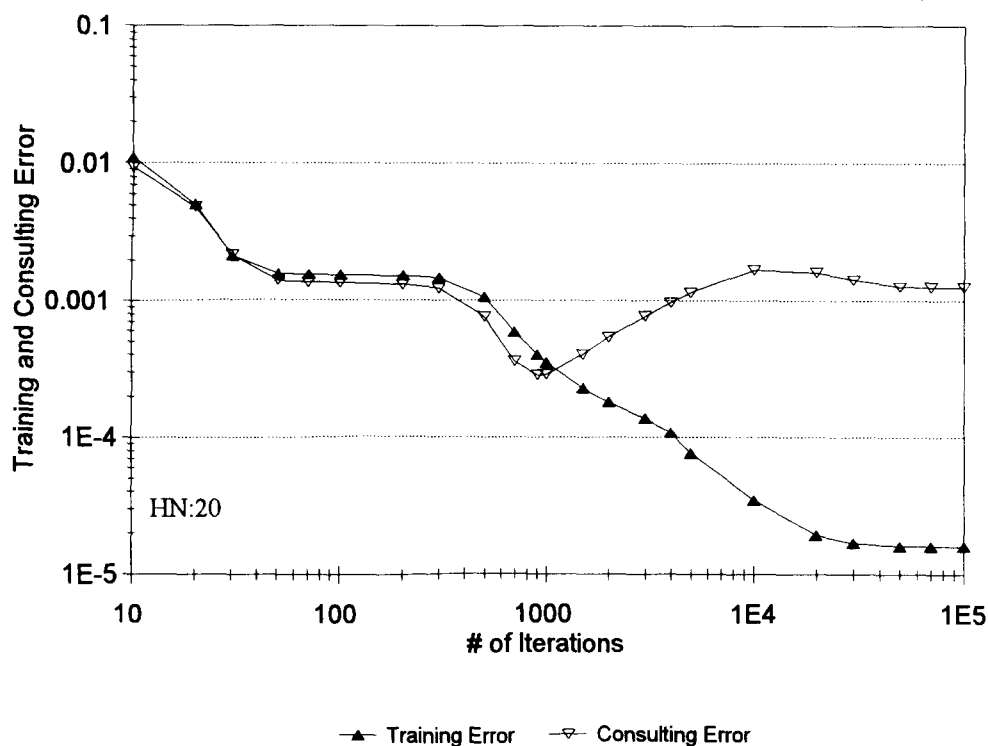


Fig. 14. Overtraining of GDR net from chemical compounding data (real-world data).

4. Concluding remarks

The objective of this paper is to promote increased understanding of some related matters in the general topic area of learning and generalization. Some of these are listed in the following:

- (1) Adequacy of the feedforward net architecture does not imply that the GDR approach must be used in training. Other variations exist.
- (2) Even in the absence of noise, estimation errors in generalization mode are generally not as small as those attained for the training set.
- (3) In the absence of noise, generalization errors are due to inadequacy by interpolation or extrapolation and cannot be reduced by further training. They can be reduced by increase in the quality of the training set, such as making the exemplars more representative of the behavior of the function to be learned.
- (4) For real-world data with usually a stochastic element in the function, overtraining can occur. Overtraining is aggravated through increase in the number of parameters made available or through use of excessive number of adaptive iterations in training.
- (5) The random-vector FL net trains simply and rapidly and is guaranteed to converge to the optimal solution in a known number of iterative steps.

Postscript

Rigorous justification of the random-vector functional-link approach has since been obtained by B. Igel'nik and Yoh-Han Pao. Part of that justification is presented in "Additional perspectives on feedforward neural-nets and the Functional-link", by B. Igel'nik and Yoh-Han Pao, IJCNN'93, Nagoya, Japan (Oct. 1993) [14] with additional material in [15] and [16].

Appendix 1. Observations on rapid convergence attainable with the random vector FL net

A typical RV Functional-link net is depicted in *Fig. 2(b)* of text. It is useful and important to note that the output of an augmentation node is a scalar, but that scalar is a function of the entire input pattern vector. In a function mapping $R^n \rightarrow R$, the output is $o = \sum \beta_j g(\mathbf{a}_j^t \mathbf{x} + b_j)$.

In practice, we have the original vector components as well as the augmentation nodes. In the interest of simplicity in representation we do not distinguish between the two different types of input nodes in the following formalism. That is, all the weights are denoted β_j , each one of which weights the output of the corresponding node j and all of the weighted values are summed to yield the output.

The scalar output o is computed as $o = \mathbf{B}^t \mathbf{d}$, where

$$\mathbf{B} = [\beta_1 \ \beta_2 \ \dots \ \beta_{N+J}]^t, \quad \text{and}$$

$$\mathbf{d} = [\delta_1 \ \delta_2 \ \dots \ \delta_{N+J}]^t.$$

The symbol J denotes the total number of augmentation nodes and N denotes the number of components of the original input vector.

For the augmentation nodes, $\delta_m = g(\text{net}_m)$ for $m = N + 1, \dots, N + J$ where $\text{net}_m = a_{m1}x_1 + \dots + a_{mN}x_N + b_m = \mathbf{a}_m^t \mathbf{x} + b_m$,

$$\mathbf{a}_m^t = [a_{m1}, a_{m2}, \dots, a_{mN}]^t, \quad \text{and}$$

$$\mathbf{x} = [x_1, x_2, x_3, \dots, x_N]^T.$$

The \mathbf{a}_m , b_m parameters are selected at random but are scaled to avoid saturation of $g(\cdot)$. For pattern $\mathbf{x}^{(p)}$ we get $\text{net}_m^{(p)} = \mathbf{a}_m^t \mathbf{x}^{(p)} + b_m$, $\delta_m^{(p)} = g(\text{net}_m^{(p)})$ and $o^{(p)} = \mathbf{B}^t \mathbf{d}^{(p)}$.

For a given set of input and target data pairs $\{\mathbf{x}^{(p)}, t^{(p)}\}$, $p = 1, 2, \dots, P$, the task is to determine (learn) unknown β parameters. The learning process can be posed as an optimization problem, where the criterion function E defined as

$$E = \frac{1}{2P} \sum_{p=1}^P (t^{(p)} - \mathbf{B}^t \mathbf{d}^{(p)})^2$$

is to be minimized.

We observe that equations $t^{(1)} = \mathbf{B}^t \mathbf{d}^{(1)} = (\mathbf{d}^{(1)})^t \mathbf{B}$, $t^{(2)} = \mathbf{B}^t \mathbf{d}^{(2)} = (\mathbf{d}^{(2)})^t \mathbf{B}$, \dots , $t^{(P)} = \mathbf{B}^t \mathbf{d}^{(P)} = (\mathbf{d}^{(P)})^t \mathbf{B}$ can be written in a compact form as $\mathbf{t} = \mathbf{V} \mathbf{B}$ where $\mathbf{t} = [t^{(1)}, t^{(2)}, \dots, t^{(P)}]^t$ and $\mathbf{V} = [(\mathbf{d}^{(1)})^t, (\mathbf{d}^{(2)})^t, \dots, (\mathbf{d}^{(P)})^t]^t$ so that criterion E can be expressed as

$$E = \frac{1}{2P} (\mathbf{t} - \mathbf{V} \mathbf{B})^t (\mathbf{t} - \mathbf{V} \mathbf{B}).$$

The gradient is accordingly

$$\mathbf{r} = \frac{\partial E}{\partial \mathbf{B}} = -\frac{1}{P} \mathbf{V}^t (\mathbf{t} - \mathbf{V} \mathbf{B})$$

and the learning process can be written as

$$\mathbf{B}^{\text{new}} = \mathbf{B}^{\text{old}} + \frac{\eta}{P} \mathbf{V}^t (\mathbf{t} - \mathbf{V} \mathbf{B}^{\text{old}}),$$

where η is used to minimize E in the \mathbf{r} direction.

Search for an optimal \mathbf{B}^* in the negative direction of the gradient of E is usually efficient for a quadratic E function but there is some waste motion due to the zig-zagging nature of the search process.

The waste motion can be eliminated with use of the Conjugate Gradient (CG) method, a first-order indirect optimization process. That method uses gradient information for finding better directions for search. In all cases of quadratic optimization the system optimum can be reached in a *finite number of iterations* but the CG method guarantees convergence in a specific predetermined number of operations.

According to the CG methodology, the parameter update is defined by

$$\mathbf{B}^{\text{new}} = \mathbf{B}^{\text{old}} + \eta \mathbf{s}.$$

Directions of search \mathbf{s} are computed at every point $\mathbf{b}^{(\cdot)}$ as

$$\begin{aligned}
\text{At } \mathbf{B}^{(0)} : \quad & \mathbf{s}^{(0)} = -\mathbf{r}^{(0)} \\
\mathbf{B}^{(1)} : \quad & \mathbf{s}^{(1)} = -\mathbf{r}^{(1)} + \gamma_1 \mathbf{s}^{(0)} \\
\mathbf{B}^{(2)} : \quad & \mathbf{s}^{(2)} = -\mathbf{r}^{(2)} + \gamma_2 \mathbf{s}^{(1)} \\
& \dots \quad \dots \dots \\
\mathbf{B}^{(N+J-1)} : \quad & \mathbf{s}^{(N+J-1)} = -\mathbf{r}^{(N+J-1)} + \gamma_{N+J-1} \mathbf{s}^{(N+J-2)} \\
\mathbf{B}^{(N+J)} : \quad & \text{True optimum reached not later than this}
\end{aligned}$$

where $M = N + J$ is the dimension of the parameter vector \mathbf{B} , and

$$\gamma_1 = \frac{\|\mathbf{r}^{(1)}\|^2}{\|\mathbf{r}^{(0)}\|^2}, \quad \gamma_2 = \frac{\|\mathbf{r}^{(2)}\|^2}{\|\mathbf{r}^{(1)}\|^2},$$

and so on.

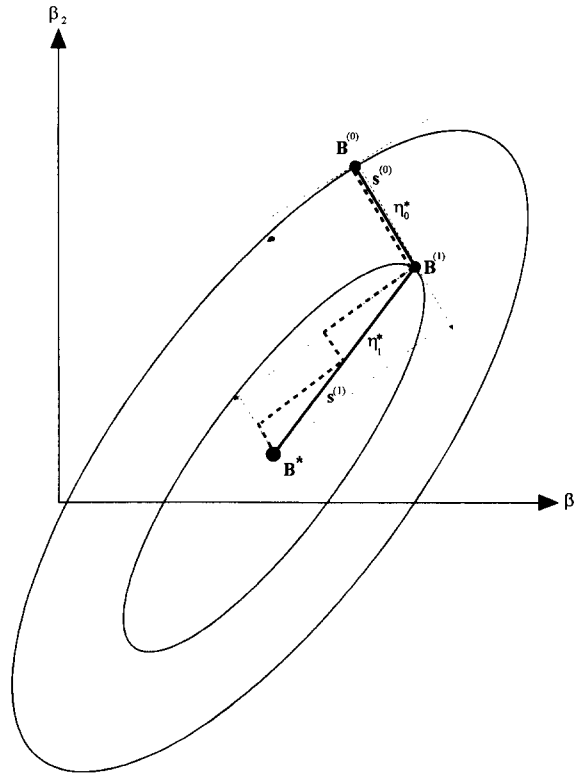


Fig. A.1. A comparison of two search strategies: --- quadratic descent minimization, — conjugate gradient method, --- lines used to establish direction for conjugate gradient method.

In general,

$$\begin{aligned}
\mathbf{B}^{(\lambda+1)} &= \mathbf{B}^{(\lambda)} + \eta \mathbf{s}^{(\lambda)} \\
\mathbf{s}^{(\lambda)} &= -\mathbf{r}^{(\lambda)} + \frac{\|\mathbf{r}^{(\lambda)}\|^2}{\|\mathbf{r}^{(\lambda-1)}\|^2} \mathbf{s}^{(\lambda-1)}
\end{aligned}$$

for $\lambda = 0$, $s^{(0)} = -r^{(0)}$

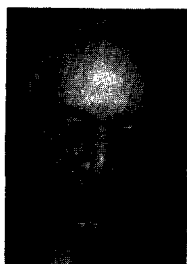
and $\lambda = K$, $B^{(K)}$ is optimum, $K \leq N + J$.

In Fig. A.1, we demonstrate graphically the difference which occurs during the minimization of a quadratic function of two variables ($M = 2$) using the directions of search

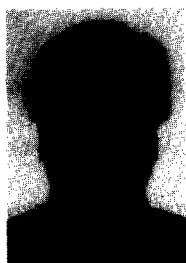
- (a) along the negative gradient of the criterion function E or
- (b) along the direction computed according to the CG methodology.

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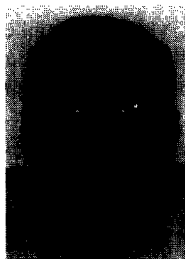
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