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Distributed bottlenecks for improved generalization in back-propagation networks

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2. Local bottlenecks.

Insofar as bottlenecks are desirable to improve generalization, one might simply initialize the network with a small hidden layer. But such an approach is undesirable for three reasons. First, for most applications, one simply does not know, in advance, the minimal number of hidden units necessary to reach criterial error. If one initializes the network with too few units, it will not achieve sufficiently small asymptotic error. Second, even if one does know the minimal number of hidden units needed and initializes the network with that number, it is more likely that gradient-descent learning will encounter local minima or plateaux on the error surface (e.g. the XOR problem with two hidden units). Third, bottlenecks increase noise and damage sensitivity. The fewer units there are, the greater is the demand for high accuracy and precision in each unit and in the input patterns. The first two problems can be addressed by initializing the network with many hidden units, and progressively excising units as learning proceeds. One method using that approach was introduced by Kruschke [13], and improved in Kruschke and Rodriguez-Movellan [14]. In that method, hidden units compete for the right to participate in the hidden layer representation. The more similar or redundant two hidden units are. the more strongly they compete. Computations are local, using simple lateral, Hebbian connections. The result is a hidden layer in which only a few, relatively uncorrelated units remain. By linking the competition rate to the rate at which error decreases, it was also found that new hidden units could be recruited from the pool of unused units. If the error was not decreasing (i.e. learning had stalled), competition was relaxed, allowing new units to participate. When error again began to decrease, stronger competition would suppress all but a few new, dissimilar units. Other methods for excising hidden units have been independently suggested by Chauvin [15], Hanson and Pratt [5], Mozer and Smolensky [7], Rumelhart [9], and Sietsma and Dow [10]. Only one of those methods (Sietsma and Dow), is explicitly designed to excise redundant units, but it gives no method for deciding when a set of units contains sufficient redundancy for removing some units, nor a method for deciding which of the redundant units to remove. All of those methods are motivated by the goal of minimal hardware. They all create a bottleneck by de-activating units, i.e. pieces of hardware. The resulting bottleneck is localized in the few remaining units. But as more information must be passed through fewer units, each unit must make finer discriminations and carry information complementary to other units. Thus, these localized hardware bottlenecks do not address the third problem mentioned above, the increase in noise and damage sensitivity.

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Abstract: The primary goal of any adaptive system that learns by example is to generalize from the training examples to novel inputs. Empirically, back-propagation networks can sometimes generalize better when they contain a hidden layer that has significantly fewer units than previous layers. The functional properties of such hidden layer bottlenecks are described, and a method for dynamically producing them, concurrent with back-propagation learning, is explicated. The method does not remove hidden units; rather, it forms clusters of covariant units in a low-dimensional space. The result is a functional bottleneck distributed across many units. The method is a gradient descent procedure, using local

computations on simple lateral, Hebbian connections between hidden units.

1. Bottlenecks improve generalization

The primary goal of any scheme for learning by example is to generalize from the training examples to novel inputs. In particular, the back-propagation learning algorithm [1] for feedforward neural networks has enjoyed great popularity for its simplicity and for its landmark successes at generalization (e.g. NETtalk, see [2,3]). It has been observed that generalization in back-propagation networks can sometimes be improved when a hidden layer bottleneck is imposed; i.e., a layer with relatively fewer units than previous layers (see [4-12]). There may be many ways besides bottlenecks to constrain the possible types of mappings from input to output, in order to improve generalization. The point of this paper is not to argue that bottlenecks are always the best constraint. Rather, the premise is that bottlenecks are beneficial in at least some cases. This paper analyzes their functional properties, and proposes a new method for creating functional bottlenecks distributed across a large hidden layer.

3. Distributed bottlenecks

An alternative motivation is to reproduce the functional

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properties of a bottleneck without reproducing its hardware properties [13]. To do that, we must decide just what functional properties are important. Explanations as to why bottlenecks improve generalization usually reflect one of three functional properties: complexity reduction, dimensionality reduction, or reduction in the number of possible mappings from input to output.

The first functional property, regarding complexity, is nicely expressed by Wieland and Leighton [11]. They suggest that 'viewing learning as curve fitting then allows us to see that generalization ... is simply the effect of a good non-linear interpolation of the data' (p.III-389). They argue that better generalization comes from smoother network mappings, and that smoother network mappings come from fewer units. Therefore, better generalization results from fewer units, to the same extent that better interpolation results from smoother data-fitting curves. Hanson and Pratt [5] corroborate: 'as a result of too many hidden units the underlying feature relations determining the output surface and category separation are arbitrary, more complex than necessary, and may result in anomalous generalizations' (italics added). The second functional property, regarding dimensionality reduction, has been mentioned by many researchers (see [6, 12, 16–19]). Each unit of a hidden layer is, potentially, an independent dimension of variation on which to represent the (transformed) input. With fewer units in a bottleneck, some dimensions of variation in the previous layer are lost; only those dimensions most important for reducing error are retained in the bottleneck layer. The third functional property, regarding the number of possible mappings from input to output, is described by Wittner *et al* [4]. They remind us that the training data usually leave the network underconstrained, and that there are usually

more possible generalizations there are. In order to train a large network to yield a particular generalization, we must either supply it with a huge training set, or reduce the number of hidden units. (Related ideas are expressed by Pavel et al [8], and by Psaltis and Neifeld [20].)

These properties can be better understood by considering two layers of a feed-forward network (see Figure 1). Suppose that layer s had N_s units, layer s-1 has N_{s-1} units, and that the $N_s \ge N_{s-1}$ weight matrix connecting them, W, has rank R. (Here we make the usual assumptions that activation flows forward from layer s-1 to layer s, that the activation of a unit is a non-linear, sigmoidal function of its net input, and that the net input of a unit is the dot product of its weight vector with the activation vector of the previous layer.) Let V be an $R \times R$ N_{S-1} matrix with rows that form a basis for the row space of W. Then there exists a $N_s \propto R$ matrix U such that W = UV. This is equivalent to supplying a 'virtual basis layer' of R linear units between layer s and layer s-1, such that the weight matrix from layer s-1 to the basis layer is V, and the weight matrix from the basis layer to layer s is U. Activation vectors in layer s all lie on an R-dimensional manifold in N_s -dimensional space. The manifold is generally not a hyperplane, because of the non-linear activation functions.

DEFINITIONS: We say layer *s* forms a bottleneck if $R < N_{s-1}$. We say layer *s* forms a local bottleneck if $N_s = R < N_{s-1}$. We say layer *s* forms a distributed bottleneck if $N_s > R < N_{s-1}$. We say layer *s* forms a distributed bottleneck if $N_s > R < N_{s-1}$. Note that we could have $N_s > N_{s-1}$, yet still have a bottleneck. The important point is that generalization is affected by both small N_s and small R, in different ways. When $R < N_{s-1}$, the (N_{s-1}) -dimensional activation vectors of *s*-1 are projected into an *R*- dimensional subspace. We then have complete generalization over the complementary $N_{s-1} - R$ dimensions, because no variation in the complementary dimensions can lead to any

a huge number of possible generalizations from a given training set. The more hidden units we supply to the network, the

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variation in the *R*-dimensional representation. In terms of curve fitting, the curve is perfectly smooth (flat) in those com-



Figure 1. The weight matrix W connecting two layers can be decomposed into two matrices of rank R. Generalization is affected in different ways by small N_s and small R. See text for details.

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plementary directions. The number of units, N_s in layer s determines the maximal complexity of regions that can be distinguished in the remaining R dimensions. In terms of curve fitting, a smaller N_s means fewer possible 'bumps' in the mapping from the R dimensions. Moreover, the maximal number of possible mappings from layer s-1 to layer s is reduced when R is small, because the weights in the mapping matrix W are constrained.

So, to improve generalization by creating a functional bottleneck, we want to do two things: (1) decrease the functional dimensionality R of the weight matrix W; and (2) decrease the functional number of units in layer s. These goals do not necessarily imply excising units, as done by the methods for creating local bottlenecks described earlier. Rather, the goals imply that we should (1) dynamically compress the weight vectors (rows of W) into a low dimensional space and (2) cluster the vectors within that low dimensional space. There are potentially many ways of achieving those goals. I have worked under two constraints on the choice of method: it should be describable as gradient descent on some objective function, and it should be locally computable in a network.

A slight variant of equation (1) was applied directly, in conjunction with back-propagation learning, by Kruschke [13]. While the results were encouraging, the method was unsatisfactory for two reasons: It was not explicitly gradient descent, so its stability was questionable, and it was not locally computable (although some parts of it were), so its network implementation was doubtful. Those two problems are resolved presently.

While Shepard never explicitly described his algorithm as gradient descent on the variance of the distances, he might have had in mind something like the following. Let



4. Shepard's method.

A method for compressing the dimensionality of a set of vectors, and simultaneously clustering them, was described by Shepard [21]. He motivated his algorithm by arguing that '... the way to flatten a configuration into a space of smaller dimensionality is to increase the variance of the distances by further stretching those distances that are already large and by further shrinking those distances that are already where

$$d_{ij} \equiv ||\mathbf{w}_i - \mathbf{w}_j||$$
 and $\overline{d} \equiv \frac{1}{B^2} \sum_{k,l}^{B,B} d_{kl}$.

(Here $\|\mathbf{x}\| = \sqrt{\sum_{n} x_{n}^{2}}$ denotes the Euclidean norm of x.) Then

$$\Delta \mathbf{w}_{I} \propto -\frac{\partial D}{\partial \mathbf{w}_{I}} = \sum_{j}^{B} (d_{Ij} - \overline{d}) \frac{(\mathbf{w}_{I} - \mathbf{w}_{j})}{d_{Ij}}.$$
 (3)

(See the Appendix for notes on the derivation.) Equations (1) and (3) are, of course, the same. Maximal variance techniques are further discussed in Cunningham & Shepard [22]. Even though we have been able to re-express Shepard's method as a gradient descent procedure, it remains unclear how to compute it in a network. The algorithm demands computing the global mean distance, d, and some way of multiplying corresponding d_{IJ} and $w_{In} - w_{jn}$. We seek something like Shepard's method that not only is nicely expressed as gradient descent, but also is locally computable in a network. To achieve that goal it is helpful to abstract the essential properties of the method, so that they might be realized other ways. The key property of the algorithm is that it increases the variance of the separations of the vectors. The vectors are then re-centered and re-scaled so that they do not explode. We should retain those essentials, but we are then free to define the separation of vectors any way that is sensible, and free to keep the vectors from exploding in any reasonable way.

small' (p. 131). Let $\mathbf{w}_{i}^{s} = [w_{i1}^{s}, ..., w_{iN}^{s}]^{T}$ be the column vector of fan-in weights connecting the N units of layer s-1 to the ith unit of layer s. (While the typographical difference between \mathbf{w}_{i}^{s} and \mathbf{w}_{ij}^{s} is slight, it is important. The first denotes a vector of fan-in weights; the second denotes the jth component of that vector.) Denote the distance between vectors by $d_{ij}^{s} = |\mathbf{w}_{i}^{s} - \mathbf{w}_{j}^{s}||$. The mean distance is denoted \overline{d}^{s} . Then for each vector \mathbf{w}_{i}^{s} , we shift it by an amount

$$\Delta \mathbf{w}_i \propto \sum_{j}^{B} (d_{ij} - \overline{d}) \frac{(\mathbf{w}_i - \mathbf{w}_j)}{d_{ij}}.$$
 (1)

(Here and throughout the remainder of this paper, the superscript denoting the layer will be suppressed whenever possible. Layer s is assumed unless otherwise marked.) Thus if $d_{ij} > \overline{d}$, then w_i tends to be shifted away from w_j , and if $d_{ij} < \overline{d}$, then w_i tends to be shifted toward w_j . After each shift, the vectors are re-centered so that their centroid is zero, and they are re-scaled so that their mean separation, \overline{d} , is a predefined constant. Without re-scaling, the vectors will 'explode', i.e. become infinitely long.

5. A new method

Define the 'distance' between two weight vectors \mathbf{w}_i^s and \mathbf{w}_j^s









(4)

(2)

where net $\sum_{i \in p}^{s}$ is the net input to unit *i* on pattern *p*, and the sum is taken over all training patterns in an epoch. It is convenient to express the net input as the inner product of the unit's fan-in weight vector with the activation vector of the layer below, net $_{ip}^{s} = \langle \mathbf{w}_{i}^{s}, \mathbf{a}_{p}^{s-1} \rangle$, where $\mathbf{a}_{p}^{s-1} = [a_{1p}^{s-1}, ..., a_{Np}^{s-1}]^{T}$ is the column vector of activations of the units of layer s-1 for pattern p. The newly defined d_{ij} , essentially the covariance of the net inputs, does not satisfy all the distance axioms. It is symmetric, but it is not positive definite and does not satisfy the triangle inequality. However, it does describe the similarity of the units. We define D as in equation (2), where the sum is taken over all units in the bottleneck layer. Then (see the Appendix for notes on derivation)

The average fan-out weight is locally computable, since each unit has direct access to all its fan-out weights. By equation (7), each weight tends toward a value that makes the average fan-out weight closer to zero. If we do very rapid gradient descent, using a proportionality constant of 1, we get to zero in one update (since trajectories are linear in this case). With $\overline{d} = 0$, equation (5) becomes the following simple expression for weight change due to dimensional compression:

$$\Delta_D \mathbf{w}_I \propto \sum_p \left(\sum_{j}^B d_{Ij} \operatorname{net}_{jp} \right) \mathbf{a}_p^{s-1}.$$
(8)

$$\frac{\partial D}{\partial \mathbf{w}_I} = -\sum_{j}^{B} \left(d_{Ij} - \overline{d} \right) \sum_{p} \operatorname{net}_{jp} \mathbf{a}_p^{s-1}.$$
 (5)

That is a bit of an improvement over equation (3), but we still must compute the global mean convariance \overline{d} . However, if we can force \overline{d} to be zero, then the expression is significantly simplified. (It makes no sense to force the average *distance* between vectors to be zero, for then all the weight vectors would have zero length. But with the new definition of d_{ij} as covariance in equation (4), some 'distances' are negative, so forcing \overline{d} to be zero is quite acceptable.)

As a step toward the goal of forcing the global mean distance to zero, note that if

$$\overline{\mathbf{w}} \equiv \frac{1}{B} \sum_{i}^{B} \mathbf{w}_{i} = \mathbf{0},$$

Now that requires only simple lateral connections between units with the value d_{I_i} as their connection strength (see Figure 2). The value of d_{li} is obtained by simple Hebbian learning during an epoch, as in equation (4). The lateral connections do not participate in the forward propagation of activation, nor in the backward propagation of error.

Like the back-propagation learning rule, the weight change rule in equation (8) conforms to the 'principle of minimal disturbance' [23]. Weight vectors are changed only parallel to the current activation vector. If two units have positive covariance, then their weight vectors tend to move in the same direction (both parallel or antiparallel to a_{p}^{s-1}). If two units have negative covariance, then their weight vectors tend to move in opposite directions (one parallel, the other antiparallel, to a_p^{s-1}).

We have only one more step. So far, the value of D can be made infinitely negative by increasing the magnitudes of the weights infinitely. We can prevent that by including standard

then $\overline{d} = 0$, as follows:

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$$\overline{d} \equiv \frac{1}{B^2} \sum_{k,l}^{B,B} \sum_p \langle \mathbf{w}_k, \mathbf{a}_p^{s-1} \rangle \langle \mathbf{w}_l, \mathbf{a}_p^{s-1} \rangle$$
$$= \sum_p \langle \overline{\mathbf{w}}, \mathbf{a}_p^{s-1} \rangle^2$$
$$= 0.$$

So now the goal is to make $\overline{w} = 0$, and that is easy. Simply do very fast gradient descent on

$$M \equiv \left\| \overline{\mathbf{w}} \right\|^2. \tag{6}$$

The change in the weight w_{IJ} due to gradient descent on M is proportional to the negative of the average fan-out weight from unit J in layer s-1:

weight decay. But we have already included a component of weight decay, the term M, in equations (6) and (7). M makes the mean weight vector tend toward zero. We must now also put a cost on the remaining component of weight magnitude, the variance of the weight vectors, V. The decomposition of weight decay is made explicit in the following formula:



Gradient descent on V is also locally computable:

$$\Delta_V w_{IJ} \propto -\frac{\partial V}{\partial w_{IJ}} \propto \frac{1}{B} \sum_k^B w_{kJ} - w_{IJ}.$$
(10)



Each weight is pushed toward the average fan-out weight, which in this case is zero because we have done fast descent on M. Note that by adding equations (7) and (10) we get $\Delta w_{IJ} \propto w_{IJ}$, the standard form of weight decay.

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That recursive formula for β_{Ip}^{s} is exactly the same formula used for back propagating the error gradient in back-propagation learning. Therefore all we must do to back propagate $\partial D/\partial$ net is inject β into the error signal at the bottleneck layer, and then standard backward error propagation automatically carries it to lower layers. We determined the value of β at the bottleneck layer in equation (8), $\beta_{Ip} = \sum_{j} d_{Ij} \operatorname{net}_{jp}$. The modified error signal at the bottleneck layer is simply $\sum_{p} (\delta_{Ip} + \beta_{Ip})$, where δ_{Ip} is the error computed by standard back propagation for unit *I* on pattern *p*.

Thus the gradient of D can be back propagated through lower layers using exactly the same machinery as back-propagation of error. No lateral connections are needed in any layer other than the bottleneck layer, and the lower layer units do not need to compute any values other than those used in standard backward error propagation.

Figure 2. Lateral Hebbian connections between bottleneck units permit local computation of $\Sigma_j d_{Ij}$ net_{jp} in equation 8. See text for details.

6. Multiple layers.

The function D is defined for the particular layer we have designated as the bottleneck layer. In the previous section we computed the gradient of D with respect to weights fanning into the bottleneck layer (equation 8). But because the covariances which constitute D are defined in terms of activations of lower layers, we can also compute the gradient of D with respect to weights in lower layers.

Let $\operatorname{net}_{p}^{s} \equiv [\operatorname{net}_{1p}^{s}, ..., \operatorname{net}_{Bp}^{s}]^{T}$ be the column vector of net input values in layer s for pattern p. Let the activation of a unit be given by $\operatorname{a}_{ip}^{s} = f(\operatorname{net}_{ip}^{s})$. For purposes of the following derivation, let s denote any layer below the bottleneck layer. Define $\beta_{ip}^{s} \equiv \partial D/\partial \operatorname{net}_{ip}^{s}$. By chain rule:

7. Summary and discussion.

Bottlenecks in hidden layers of back-propagation networks have been found to improve the generalization capabilities of the network, in at least some applications. It is desirable to reproduce the functional properties of a bottleneck without incurring the noise and damage sensitivity of localized hardware bottlenecks. Two important functional properties of a bottleneck are the dimensionality of its weight vectors and the number of dissimilar units it has. To decrease the dimensionality of the weight vectors and cluster them within those dimensions, we do gradient descent on three terms, D, V, and M, with respect to connection weights. The D term is a measure of dimensionality and clustering. It is the (negative of the) variance of the separations of the vectors, with separation defined as covariance of net input values (equation 4). The V and M terms are orthogonal components of weight decay. Fast descent on the M term causes the mean weight vector to be zero, and consequently greatly simplifies the expression for gradient descent on D. The V term causes the variance of the weight vectors not to grow too large, thereby preventing the weight vectors from 'exploding' under the influence of the D term. All that is needed to make gradient descent on D strictly local is the inclusion of lateral connections which have connection strengths given by simple Hebbian learning over an epoch. The lateral connections do not participate in propagating activation or error. The decomposition of standard weight decay into two orthogonal components has not been previously noted (see, e.g. Kruschke [24]. In the present application the mean component, M, is decreased much more rapidly than the variance component, V. However, it is possible that this decomposition alone, without the dimensionality term D, could be useful for generalization, if we do slow descent on the mean and more rapid descent on the variance. The result would be a cluster of weight vectors around the non-zero mean weight vector. Most likely, however, the training examples could not very easily be learned by a single cluster of weight vectors.

$$\frac{\partial D}{\partial \mathbf{w}_{I}^{s}} = \frac{\partial D}{\partial \operatorname{net}_{p}^{s+1}} \frac{\partial \operatorname{net}_{p}^{s+1}}{\partial a_{Ip}^{s}} \frac{\partial a_{Ip}^{s}}{\partial \operatorname{net}_{Ip}^{s}} \frac{\partial \operatorname{net}_{Ip}^{s}}{\partial \mathbf{w}_{I}^{s}}$$

Expanding each partial derivative yields:



In particular, the first three terms indicate that



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Gradient descent on D can also be computed for lower layers. The gradient of D is simply injected into the error gradient at the bottleneck layer, and is propagated back to lower layers using exactly the same machinery as backward error propagation. No lateral connections are needed in any layer but the bottleneck layer, and no new values need to be computed by lower layer units. Gradient descent on the V and M terms is carried out only in the bottleneck layer.

It is important to note that the computations in the bottleneck layer itself do not depend on back-propagation, and that it is not necessary to propagate the gradient of D to lower layers. Therefore, this algorithm for creating distributed bottlenecks can be used in conjunction with any iterative learning algorithm (e.g. Boltzmann machine learning), not just backward error propagation. The procedure is the same in any case. With every update of the bottleneck connection weights due to learning, we also make an adjustment due to gradient descent on D, M, and V. The process of concurrently performing dimensional compression and clustering with learning allows the selection of as many dimensions and clusters as needed. Of course, if the descent rate on D is too fast relative to the learning rate, then too few dimensions and clusters will be formed to reach criterial error on the training patterns. That can be avoided by dynamically adjusting the descent rate on D so that it is linked to the actual progress of learning (error reduction). Linking of descent rates to error reduction was successfully used by Kruschke and Rodriguez-Movellan [14] to create localized hardware bottlenecks. The linking operates as follows: if error reduction is slow, then the rate of dimensional compression and clustering is automatically reduced or even reversed (made negative), so that a new trajectory through weight space can be found, and error again begins to decrease. When gradient descent on D is reversed, there is a pressure on the units to uncluster themselves. Unclustering of units was used by Sandon and Uhr [25] to escape local minima. They tried several different heuristic formulae for unclustering, all of which helped escape local minima to varying degrees. The method described here goes beyond their attempts by doing explicit gradient descent on a measure of clustering and dimensionality, D. A clustering technique for back-propagation networks was proposed by Psaltis and Neifeld [20], with the goal of improving generalization. Their technique required the user to specify in advance the number of clusters to be formed, unlike the method proposed here, which dynamically forms as few clusters as possible during learning. Additionally, it is not at all clear how their technique might be implemented by local computations in the network, unlike the method proposed here, which requires only simple lateral, Hebbian connections in the bottleneck layer. The main point of this paper is that if one desires to impose a bottleneck in a network, then one should consider creating a distributed bottleneck rather than a localized bottleneck. One method for creating distributed bottlenecks was described. The important issue of deciding which applications would benefit from bottlenecks is not addressed here, and is a topic for future research.

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Appendix.

The derivation of $\partial D/\partial w_I$ is greatly simplified if it is first noticed that



The first line is just the chain rule. In going from the first line to the second, we use the fact that $\partial \overline{d}/\partial w_I$ is independent of the indices *i* and *j*. The transition from the second to third lines uses simply the definition of *d* in terms of d_{ij} . The derivation is true regardless of the definition of d_{ij} in terms of weights.

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