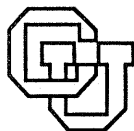


**SKELETONIZATION:
A TECHNIQUE FOR TRIMMING THE FAT FROM
A NETWORK VIA RELEVANCE ASSESSMENT**

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CU-CS-421-89



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Skeletonization: A Technique for Trimming the Fat from a Network via Relevance Assessment

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Abstract: This paper proposes a means of using the knowledge in a network to determine the functionality or *relevance* of individual units, both for the purpose of understanding the network's behavior and improving its performance. The basic idea is to iteratively train the network to a certain performance criterion, compute a measure of relevance that identifies which input or hidden units are most critical to performance, and automatically trim the least relevant units. This *skeletonization* technique can be used to simplify networks by eliminating units that convey redundant information; to improve learning performance by first learning with spare hidden units and then trimming the unnecessary ones away, thereby constraining generalization; and to understand the behavior of networks in terms of minimal "rules."

One thing that connectionist networks have in common with brains is that if you open them up and peer inside, all you can see is a big pile of goo. Internal organization is obscured by the sheer number of units and connections. Although techniques such as hierarchical cluster analysis (Sejnowski & Rosenberg, 1987) have been suggested as a step in understanding network behavior, one would like a better handle on the role that individual units play. This paper proposes one means of using the knowledge in a network to determine the functionality or *relevance* of individual units. Given a measure of relevance for each unit, the least relevant units can be automatically trimmed from the network to construct a *skeleton* version of the network.

Skeleton networks have several potential applications:

- *Constraining generalization.* By eliminating input and hidden units that serve no purpose, the number of parameters in the network is reduced and generalization will be constrained (and hopefully improved).
- *Speeding up learning.* Learning is fast with many hidden units, but a large number of hidden units allows for many possible generalizations. Learning is slower with few hidden units, but generalization tends to be better. One idea for speeding up learning is to train a network with many hidden units and then eliminate the irrelevant ones. This may lead to a rapid learning of the training set, and then gradually, an improvement in generalization performance.

- *Understanding the behavior of a network in terms of "rules"*. One often wishes to get a handle on the behavior of a network by analyzing the network in terms of a small number of rules instead of an enormous number of parameters. In such situations, one may prefer a simple network that performed correctly on 95% of the cases over a complex network that performed correctly on 100%. The skeletonization process can discover such a simplified network.

Several researchers (Chauvin, 1989; Hanson & Pratt, 1989; David Rumelhart, personal communication, 1988) have studied techniques for the closely related problem of reducing the number of free parameters in back propagation networks. Their approach involves adding extra cost terms to the usual error function that cause nonessential weights and units to decay away. We have opted for a different approach — the all-or-none removal of units — which is not a gradient descent procedure. The motivation for our approach was twofold. First, our initial interest was in designing a procedure that could serve to focus "attention" on the most important units, hence an explicit relevance metric was needed. Second, our impression is that it is a tricky matter to balance a primary and secondary error term against one another. One must determine the relative weighting of these terms, weightings that may have to be adjusted over the course of learning. In our experience, it is often impossible to avoid local minima — compromise solutions that partially satisfy each of the error terms. This conclusion is supported by the experiments of Hanson and Pratt (1989).

Determining the Relevance of a Unit

Consider a multi-layer feedforward network. How might we determine whether a given unit serves an important function in the network? One obvious source of information is its outgoing connections. If a unit in layer l has many large-weighted connections, then one might expect its activity to have a big impact on higher layers. However, this need not be. The effects of these connections may cancel each other out; even a large input to units in layer $l+1$ will have little influence if these units are near saturation; outgoing connections from the innervated units in $l+1$ may be small; and the unit in l may have a more-or-less constant activity, in which case it could be replaced by a bias on units in $l+1$. Thus, a more accurate measure of the relevance of a unit is needed.

What one really wants to know is, what will happen to the performance of the network when a unit is removed? That is, how well does the network do *with* the unit versus *without* it? For unit i , then, a straightforward measure of the relevance, ρ_i , is

$$\rho_i = E_{\text{without unit } i} - E_{\text{with unit } i},$$

where E is the error of the network on the training set. The problem with this measure is that to compute the error with a given unit removed, a complete pass must be made through the training set. Thus, the cost of computing ρ is $O(np)$ stimulus presentations, where n is the number of units in the network and p is the number of patterns in the training set. Further, if the training set is not fixed or is not known to the experimenter, additional difficulties arise in computing ρ .

We therefore set out to find a good approximation to ρ . Before presenting this approximation, it is first necessary to introduce an additional bit of notation. Suppose that associated with each unit i is a coefficient α_i which represents the *attentional strength* of the unit (see Figure 1). This coefficient can be thought of as gating the flow of activity from the unit:

$$o_j = f\left(\sum_i w_{ji} \alpha_i o_i\right),$$

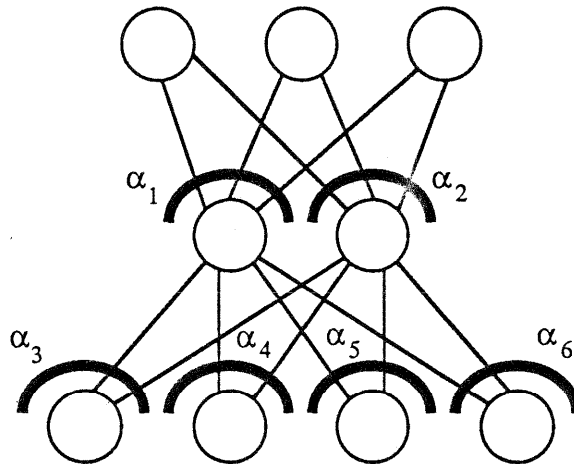


Figure 1. A 4-2-3 network with attentional coefficients on the input and hidden units.

where o_j is the activity of unit j , w_{ji} the connection strength to j from i , and f the sigmoid squashing function. If $\alpha_i = 0$, unit i has no influence on the rest of the network; if $\alpha_i = 1$, unit i is a conventional unit. In terms of α , the relevance of unit i can then be rewritten as

$$\rho_i = E_{\alpha_i=0} - E_{\alpha_i=1}.$$

We can approximate ρ_i using the derivative of the error with respect to α :

$$\lim_{\gamma \rightarrow 1} \frac{E_{\alpha_i=\gamma} - E_{\alpha_i=1}}{\gamma - 1} = \left. \frac{\partial E}{\partial \alpha_i} \right|_{\alpha_i=1}$$

Assuming that this equality holds approximately for $\gamma = 0$:

$$\frac{E_{\alpha_i=0} - E_{\alpha_i=1}}{-1} \approx \left. \frac{\partial E}{\partial \alpha_i} \right|_{\alpha_i=1}$$

or

$$-\rho_i \approx \left. \frac{\partial E}{\partial \alpha_i} \right|_{\alpha_i=1}$$

Our approximation for ρ_i is then

$$\hat{\rho}_i = - \left. \frac{\partial E}{\partial \alpha_i} \right|_{\alpha_i=1}.$$

This derivative can be computed using an error propagation procedure very similar to that used in adjusting the weights with back propagation. Additionally, note that because the approximation assumes that α_i is 1, the α_i never need be changed. Thus, the α_i are not actual parameters of the system, just a bit of notational convenience used in estimating relevance.

In practice, we have found that $\partial E / \partial \alpha$ fluctuates strongly in time and a more stable estimate that yields better results is an exponentially-decaying time average of the derivative. In the simulations reported below, we use the following measure:

$$\hat{\rho}_i(t+1) = .8\hat{\rho}_i(t) + .2 \frac{\partial E(t)}{\partial \alpha_i}$$

Relevance Computation is Based on a Linear Error Function

One problem with the proposed relevance measure is that the quadratic error function ordinarily used in back propagation networks is not suitable for estimating relevance. This error function,

$$E^q = \sum_p \sum_j (t_{pj} - o_{pj})^2$$

(where p is an index over patterns, j over output units; t_{pj} is the target output, o_{pj} the actual output), has the serious drawback that its derivative goes to zero as the total error decreases, and consequently, if $\hat{\rho}_i = -\partial E^q / \partial \alpha_i$, the relevance of all units will tend to zero as the error decreases. This certainly violates intuitions as to how the relevance measure should behave.

To see the problem more clearly, consider the simple situation of estimating the relevance of an output unit whose target activity level is 1. Treating α as a gating coefficient on the unit's activity, o , the error will be

$$E^q = (1 - \alpha o)^2$$

and the relevance of the output unit using this error function will be

$$\begin{aligned} \hat{\rho}^q &= - \left. \frac{\partial E^q}{\partial \alpha} \right|_{\alpha=1} \\ &= 2o(1-o) \end{aligned}$$

As o approaches the target value of 1, the relevance will go to zero. Thus, $\hat{\rho}^q$ grossly underestimates relevance of outputs that are close to the target. Figure 2 depicts the situation graphically. The solid curve is the "true" relevance, ρ , as a function of the activity of the output unit. Note that if the activity is close to zero, so is the relevance because suppressing the unit by setting α to zero will not alter its activity much; if the activity is close to 1, setting α to zero will have maximal effect. The short-dashed curve is $\hat{\rho}^q$, rescaled by a multiplicative constant to best fit the ρ curve. This approximation is reasonably good only when the activity of the unit is less than .5. As the activity of the output unit approaches 1, $\hat{\rho}^q$ decreases whereas ρ increases.

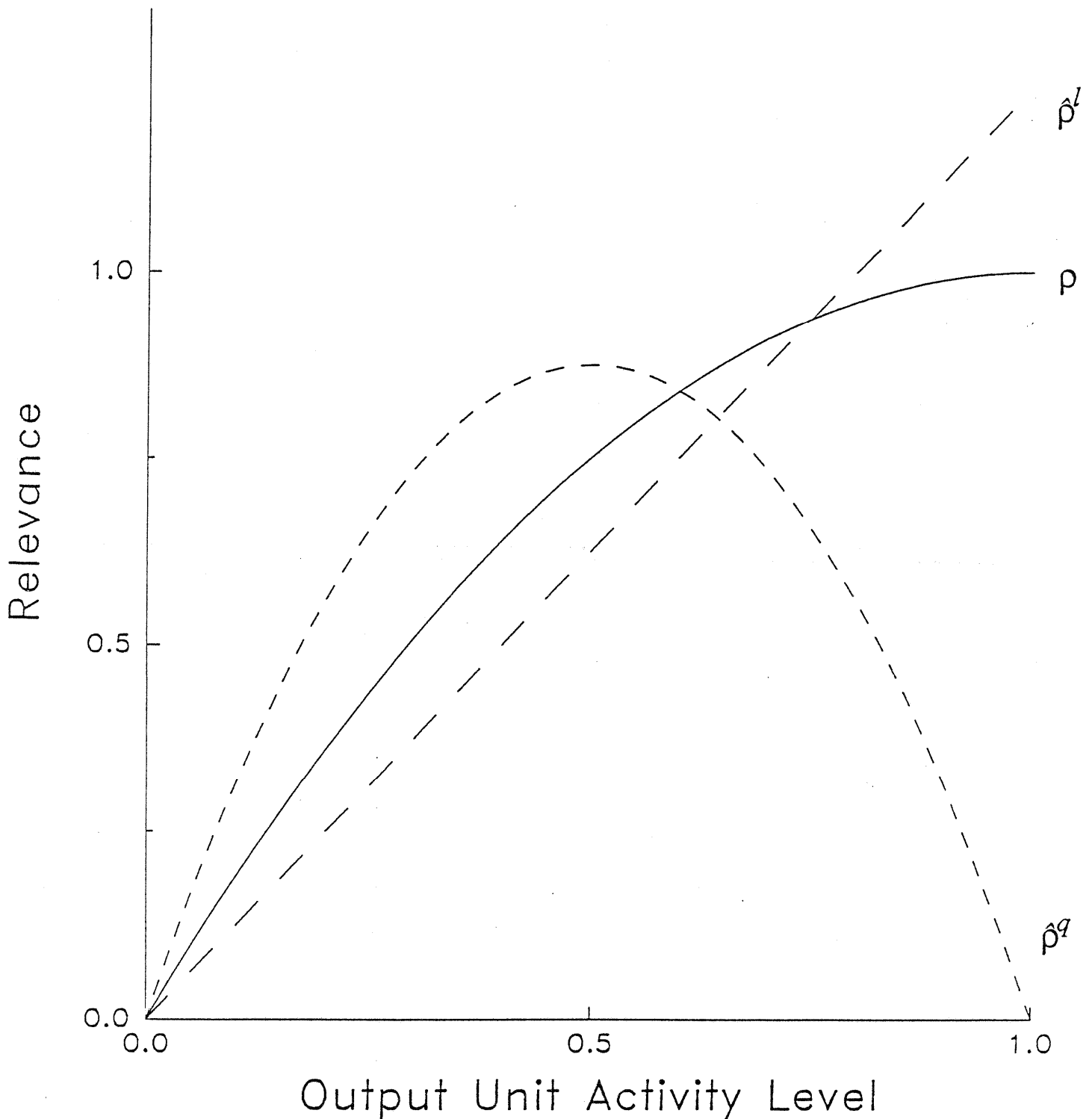


Figure 2. Three measures of the relevance of an output unit whose target activity is 1, as a function of the unit's activity level. The solid curve labeled ρ is the true relevance, $E_{z=0} - E_{z=1}$; the short-dashed curve is the approximation to ρ using the derivative of E^q ; and the long-dashed line is the approximation using the derivative of E^I . The two approximations have been rescaled by a multiplicative constant to best fit the ρ curve.

One possibility is to make use of the relevance measure only for ranges of output values where the approximation is good. In practice, this turns out to be quite difficult. Instead, we have opted for a different solution: to use a *linear* error function,

$$E^l = \sum_p \sum_j |t_{pj} - o_{pj}|$$

in computing the relevance. The derivative of E^l does not depend on how close the output activity is to the target, and thus does not go to zero as the error decreases. Figure 2 shows an estimate of relevance, $\hat{\rho}^l$, computed from derivative of E^l . Unlike $\hat{\rho}^q$, $\hat{\rho}^l$ is monotonically increasing and appears to be a reasonable approximation for all values of the output unit activity. Monotonicity is particularly important because the skeletonization procedure we will present uses $\hat{\rho}$ primarily to rank-order the units by relevance.

To summarize, in the results reported below, while E^q is used as the error metric in training the weights via conventional back propagation, $\hat{\rho}$ is measured using E^l . This involves separate back propagation phases for computing the weight updates and the relevance measures.

In the next two sections, we discuss sample applications of relevance assessment. We then discuss how to use relevance assessment for the construction of skeleton networks.

A Simple Example: The Cue Saliency Problem

Consider a network with four inputs labeled A-D, one hidden unit, and one output. We generated ten training patterns such that the correlations between each input unit and the output are as shown in the first row of Table 1. (In this particular task, a hidden layer is not necessary. The inclusion of the hidden unit does not affect any of the reported results, and in fact increases the difficulty of relevance assessment. It simply allowed us to use a standard three-layer architecture for all tasks.)

In this and subsequent simulations, unit activities range from -1 to 1, input and target output patterns are binary (-1 or 1) vectors. Training continues until all output activities are within some acceptable range of the target value. Additional details of the training procedure and network parameters are described in the Appendix.

To perform perfectly, the network need only attend to input A. This is not what the input-hidden connections do, however; their weights have the same qualitative profile as the correlations (second row of Table 1).¹ In contrast, the relevance values for the input units show A to be highly relevant while B-D have negligible relevance. Additionally, the qualitative picture presented by the profile of $\hat{\rho}_i$'s is identical to that

Table 1

	Input Unit			
	A	B	C	D
Correlation with Output Unit	1.0	0.6	0.2	0.0
Input-Hidden Connection Strengths	3.15	1.23	.83	-.01
ρ_i	5.36	0.07	0.06	0.00
$\hat{\rho}_i$	0.46	-0.03	0.01	-0.02

¹ The values reported in Table 1 are an average over 100 replications of the simulation with different initial random weights. Before averaging, however, the signs of the weights were flipped if the hidden-output connection was negative.

of the ρ_i s. Thus, while the weights merely reflect the statistics of the training set, $\hat{\rho}_i$ indicates the *functionality* of the units.

The Rule-Plus-Exception Problem

Consider a network with four binary inputs labeled A-D and one binary output. The task is to learn the function $AB + \overline{ABCD}$; the output unit should be on whenever both A and B are on, or in the special case that all inputs are off. With two hidden units, back propagation arrives at a solution in which one unit responds to AB — the rule — and the other to \overline{ABCD} — the exception (Figure 3). Clearly, the AB unit is more relevant to the solution; it accounts for fifteen cases whereas the \overline{ABCD} unit accounts for only one. This fact is reflected in the $\hat{\rho}_i$: in 100 replications of the simulation, the mean value of $\hat{\rho}_{AB}$ was 1.49 whereas $\hat{\rho}_{\overline{ABCD}}$ was only .17. These values are extremely reliable; the standard errors are .003 and .005, respectively.

Relevance was also measured using the quadratic error function. With this metric, the AB unit is incorrectly judged as being *less* relevant than the \overline{ABCD} unit: $\hat{\rho}_{AB}^q$ is .029 and $\hat{\rho}_{\overline{ABCD}}^q$ is .033. As explained above, the basis of the failure of the quadratic error function is that $\hat{\rho}^q$ grossly underestimates the true relevance as the output error goes to zero. Because the one exception pattern is invariably the last to be learned, the output error for the fifteen non-exception patterns is significantly lower, and consequently, the relevance values derived from the non-exception patterns are much smaller than that derived from the one exception pattern. This results in the relevance assessment based on the exception pattern dominating the overall relevance measure, and in the incorrect relevance assignments described above. However, this problem can be avoided by assessing relevance using the linear error function.

If we attempted to "trim" the rule-plus-exception network by eliminating hidden units, the logical first candidate would be the less relevant \overline{ABCD} unit. This trimming process would leave us with a simpler network — a skeleton network — whose behavior is easily characterized in terms of a simple rule, but which could only account for 15 of the 16 input cases.

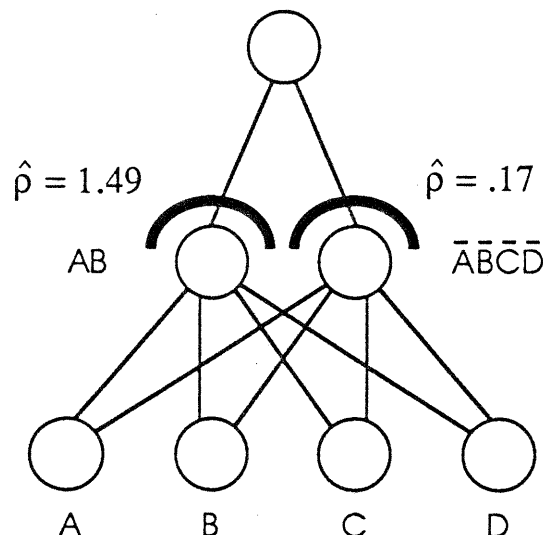


Figure 3. A 4-2-1 network used to learn the rule-plus-exception problem. One hidden unit learns to respond to AB — the rule — and the other to \overline{ABCD} — the exception.

Constructing Skeleton Networks

In the remaining examples we construct skeleton networks using the relevance metric. The procedure is as follows: (1) train the network until all output unit activities are within some specified range of the target value (see Appendix); (2) compute β for each unit; (3) remove the unit with the smallest β ; and (4) repeat steps 1-3 a specified number of times. In the examples below, we have chosen to trim either the input units or the hidden units, not both simultaneously, but there is no reason why this could not be done.

We have not yet addressed the crucial question of how much to trim away from the network. At present, we specify in advance when to stop trimming. However, the procedure described above makes use only of the ordinal values of the β . One untapped source of information that may be quite informative is the magnitudes of the β . A large increase in the minimum β value as trimming progresses may indicate that further trimming will seriously disrupt performance in the network.

The Train Problem

Consider the task of determining a rule that discriminates the "east" trains from the "west" trains in Figure 4. There are two simple rules — simple in the sense that the rules require a minimal number of input features: East trains have *a long car and triangle load in car* or *an open car* or *white wheels on car*. Thus, of the seven features that describe each train, only two are essential for making the east/west discrimination.

A 7-1-1 network trained on this task using back propagation learns quickly, but the final solution takes into consideration nearly all the inputs because 6 of the 7 features are partially correlated with the east/west discrimination. When the skeletonization procedure is applied to trim the number of inputs from 7 to 2, however, the network is successfully trimmed to the minimal set of input features — either *long car* and *triangle load*, or *open car* and *white wheels on car* — on each of 100 replications of the simulation we ran.

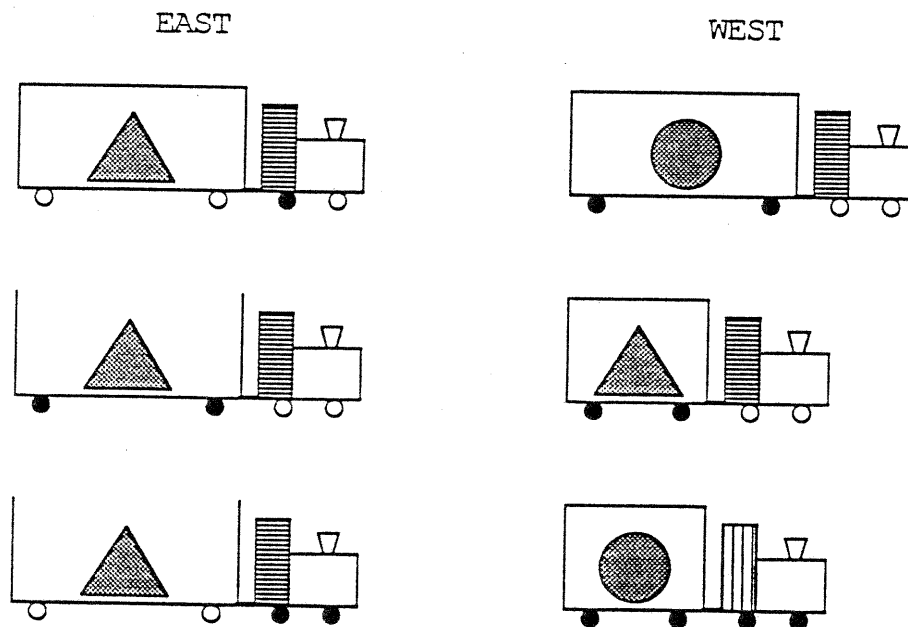


Figure 4. The train problem. Adapted from Medin, Wattenmaker, & Michalski, 1987.

The trimming task is far from trivial. The expected success rate with random removal of the inputs is only 9.5%. Other skeletonization procedures we experimented with resulted in success rates of 50%-90%.

The Four-Bit Multiplexor Problem

Consider a network that learns to behave as a four-bit multiplexor. The task is, given 6 binary inputs labeled A-D, M_1 , and M_2 , and one binary output, to map one of the inputs A-D to the output contingent on the values of M_1 and M_2 . The logical function being computed is $\overline{M_1}\overline{M_2}A + \overline{M_1}M_2B + M_1\overline{M_2}C + M_1M_2D$.

A standard 4-hidden unit back propagation network was tested against a skeletonized network that began with 8 hidden units initially and was trimmed to 4 (an 8→4 *skeleton network*). If the network did not reach the performance criterion within 1000 training epochs, we assumed that the network was stuck in a local minimum and counted the run as a failure.

Performance statistics for the two networks are shown in Table 2, averaged over 100 replications. The standard network fails to reach criterion on 17% of the runs, whereas the skeleton network always obtains a solution with 8 hidden units and the solution is not lost as the hidden layer is trimmed to 4 units.² The skeleton network with 8 hidden units reaches criterion in about half the number of training epochs required by the standard network. From this point, hidden units are trimmed one at a time from the skeleton network, and after each cut the network is retrained to criterion. Nonetheless, the total number of epochs required to train the initial 8 hidden unit network and then trim it down to 4 is still less than that required for the standard network with 4 units. Furthermore, as hidden units are trimmed, the performance of the skeleton network remains close to criterion, so the improvement in learning is substantial (Figure 5).

The Random Mapping Problem

The problem here is to map a set of random 20-element input vectors to random 2-element output vectors. Twenty random input-output pairs were used as the training set. Ten such training sets were generated and tested. A standard 2-hidden unit network was tested against a 6→2 skeleton network. For each training set and architecture, 100 replications of the simulation were run. If criterion was not reached within 1000 training epochs, we assumed that the network was stuck in a local minimum and counted the run as a failure.³

Table 2

architecture	failure rate	median epochs to criterion (with 8 hidden)	median epochs to criterion (with 4 hidden)
standard 4-hidden net	17%	--	52
8→4 skeleton net	0%	25	45

² Here and below we report median epochs to criterion rather than mean epochs to avoid aberrations caused by the large number of epochs consumed in failure runs.

³ To eliminate floor and ceiling effects, we rejected training sets that were either extremely simple to learn — i.e., standard network could learn in under 20 epochs — and were impossible to learn — i.e., standard network was never able to find a solution.

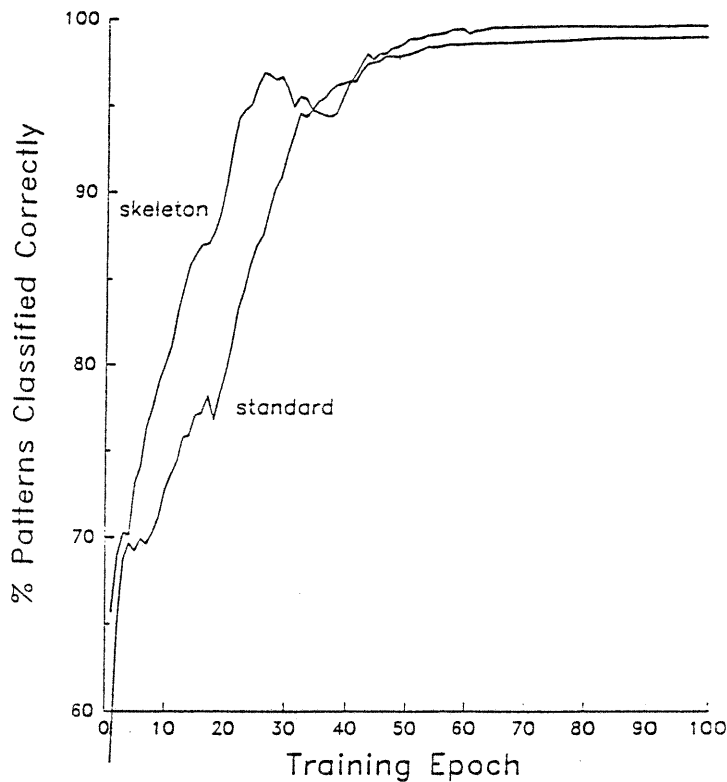


Figure 5. Average performance on the four-bit multiplexor task.

As Table 3 shows, the standard network failed to reach criterion with two hidden units on 17% of all runs, whereas the skeleton network failed with the hidden layer trimmed to two units on only 8.3% of runs. In 9 of the 10 training sets, the failure rate of the skeleton network was lower than that of the standard network. Both networks required comparable amounts of training to reach criterion with two hidden units, but the skeleton network reaches criterion much sooner with six hidden units, and its performance does not significantly decline as the network is trimmed. These results parallel those of the four-bit multiplexor.

Table 3

training set	standard network		6→2 skeleton network		
	% failures	median epochs to criterion (2 hidden)	% failures	median epochs to criterion (6 hidden)	median epochs to criterion (2 hidden)
1	14	20	7	11	22
2	16	69	13	12	47
3	25	34	0	7	14
4	33	38	0	10	21
5	38	96	55	35	<max>
6	9	17	1	9	17
7	9	28	5	14	43
8	6	13	0	8	16
9	8	12	0	8	17
10	12	12	2	8	17

Summary and Conclusions

We proposed a method of using the knowledge in a network to determine the relevance of individual units. The relevance metric can identify which input or hidden units are most critical to the performance of the network. The least relevant units can then be trimmed to construct a skeleton version of the network.

Skeleton networks have application in two different scenarios, as our simulations demonstrated:

- Understanding the behavior of a network in terms of "rules"
 - *The cue salience problem.* The relevance metric singled out the one input that was sufficient to solve the problem. The other inputs conveyed redundant information.
 - *The rule-plus-exception problem.* The relevance metric was able to distinguish the hidden unit that was responsible for correctly handling most cases (the general rule) from the hidden unit that dealt with an exceptional case.
 - *The train problem.* The relevance metric correctly discovered the minimal set of input features required to describe a category.
- Improving learning performance
 - *The four-bit multiplexor.* Whereas a standard network was often unable to discover a solution, the skeleton network never failed. Further, the skeleton network learned the training set more quickly.
 - *The random mapping problem.* As in the multiplexor problem, the skeleton network succeeded considerably more often with comparable overall learning speed, and less training was required to reach criterion initially.

Basically, the skeletonization technique allows a network to use spare input and hidden units to learn a set of training examples rapidly, and gradually, as units are trimmed, to discover a more concise characterization of the underlying regularities of the task. In the process, local minima seem to be avoided without increasing the overall learning time.

One somewhat surprising result is the ease with which a network is able to recover when a unit is removed. Conventional wisdom has it that if, say, a network is given excess hidden units, it will memorize the training set, thereby making use of all the hidden units available to it. However, in our simulations, the network does not seem to be distributing the solution across all hidden units because even with no further training, removal of a hidden unit often does not drop performance below the criterion. In any case, there generally appears to be an easy path from the solution with many units to the solution with fewer.

Although we have presented skeletonization as a technique for trimming units from a network, there is no reason why a similar procedure could not operate on individual connections instead. Basically, an α coefficient would be required for each connection, allowing for the computation of $\partial E / \partial \alpha$. Yann le Cun (personal communication, 1989) has independently developed a procedure quite similar to our skeletonization technique which operates on individual connections.

Table 4

simulation	margin	learning rate	layer trimmed
cue salience	0.1	4.0	input
rule plus exception	0.1	3.0	hidden
train	0.1	3.0	input
4-bit multiplexor	0.9	2.0	hidden
random mapping	0.9	3.0	hidden

Appendix: Training Procedure

All simulations made use of a three-layer feedforward network with input-hidden and hidden-output connections. For several tasks, the hidden layer was not strictly necessary, but was included to keep the architecture uniform across problems. The inclusion of the hidden layer in no way affected the qualitative results. Input and target output patterns were binary (-1 or 1) vectors. Hidden and output units used the conventional logistic activity function with an activity range of -1 to 1: $f(x) = \tanh(x/2)$.

Initially, connection strengths are selected at random from a mean-zero Gaussian distribution and are rescaled such that the L_1 norm of the connection strengths feeding into a unit is 2.0. If a unit has many inputs, then, weights tend to be smaller. With the initial weights chosen in this manner, each unit has some variation in its output but tends to operate in the linear range of the sigmoid curve. Weights are updated only after a complete pass through the entire training set, and training continues until all output activities are within some acceptable range around the target value (the *margin*, see Table 4).

A fixed learning rate was determined for each simulation to optimize performance for the standard network. This learning rate was divided by the number of inputs to a unit, so that it would scale up as units were trimmed from the network. Dividing the learning rate by the fan-in is probably an overly conservative procedure and, if anything, penalizes the simulations involving skeletonization of the hidden layer due to the larger number of hidden units initially. It also allows for different learning rates in the input-hidden and hidden-output connections.

Momentum was used, with a generic momentum parameter of .5 — probably not large enough to help a lot, but not large enough to hurt either.

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