Smaller Standard Deviation for Initial Weights Improves Neural Networks Performance: A Theoretical Explanation of Unexpected Simulation Results

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1. Selecting Initial Weights Is Important

- In deep learning, a neural network that classifies into c classes starts with the inputs x_1, \ldots, x_v .
- On each layer, input signals s_1, \ldots, s_m to this layer get transformed into outputs $s'_i = \max\left(\sum_{j=1}^m w_{ij} \cdot s_j, 0\right)$.
- These outputs serve as inputs to the next layer.
- We do this until we reach the last layer, where we use softmax.
- Namely, based on c neural outputs z_j , we compute the probability p_i of being in a i-th class as

$$p_i = \frac{\exp(\beta \cdot z_i)}{\sum\limits_{j=1}^{c} \exp(\beta \cdot z_j)}$$
 for some $\beta > 0$.



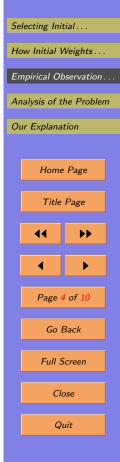
2. Selecting Initial Weights Is Important

- Training a neural network means selecting the weights w_{ij} for which:
 - for the training set,
 - the outputs are the closest to the desired ones.
- We start with some initial weights, and then iteratively update them until we get a good match.
- How fast the network learns depends on how well we selected the initial weights.
- If the initial weights are too far from the actual ones, training takes much longer.



3. How Initial Weights Are Selected Now

- Weights are selected layer-by-layer, starting with the input layer.
- For each neuron i in the currently considered layer, we start with weights $w_{ij} \sim U([-Z, Z])$.
- This means that w_{ij} are uniformly distributed on some interval [-Z, Z].
- Then, we apply Gram-Schmidt orthonormalization to the vectors $w_i = (w_{i1}, \ldots, w_{in})$.
- Then, for each neuron i, we select a small sample of K patterns, get outputs $y_i^{(1)}, \ldots, y_i^{(K)}$.
- We then multiply all the weights w_{ij} by some constant $C: w_{ij} \to C \cdot w_{ij}$.
- The constant is selected so that so that the standard deviation of the K values $y^{(k)}$ become equal to $\sigma_0 = 1$.



4. How Initial Weights Are Selected Now

- Then we freeze these weights and go to the next layer.
- To select the weights from the last (linear) layer, we match with the desired outputs.



5. Empirical Observation That Needs Explaining

- One of us (DA) tried to use $\sigma_0 < 1$ in the above algorithm.
- He got much better results than for $\sigma_0 = 1$.
- Moreover, the smaller σ_0 , the better results.
- In this talk, we provide a theoretical explanation for this unexpected result.



6. Analysis of the Problem

- If we use $\sigma_0 < 1$, then on the first layer, instead of the original weights w_{ij} , we get new weights $w'_{ij} = \sigma_0 \cdot w_{ij}$.
- Then, with the same weights on other layers, we get standard deviation σ_0 on each of them.
- After L layers, we get new signals $z'_i = \sigma_0 \cdot z_i$.



7. Our Explanation

- Until we get to the last layer, we do not use the actual output.
- So we do now know the actual probabilities q_1, \ldots, q_c of different classes.
- It is therefore reasonable to select the initial weights so that:
 - the resulting probabilities p_i
 - are, on average, as close to the actual (unknown) probabilities q_i as possible.



8. Our Explanation (cont-d)

- The closeness can be described:
 - either by the Euclidean distance

$$||p - q||^2 = \sum_{i} (p_i - q_i)^2 \to \min,$$

- or by any other strictly convex function C(p,q) of p, e.g., by relative entropy.
- So, we minimize the expected value $\int C(p,q) \cdot \rho(q) dq$.
- At this stage, we do not have any information about the probabilities of different classes.
- So, it is reasonable to assume that this criterion does not change if we simply re-order the classes.
- Since the function C(p,q) is convex, there is only one p for which this minimum is attained.



9. Our Explanation (cont-d)

- Thus, the optimal tuple p should also be invariant under such re-ordering, i.e., $p_i = p_j$ for all i and j.
- Hence, in the optimal case, we get $p_i = 1/c$ for all i.
- The use of $\sigma_0 < 1$ places all z_i closer to 0.
- Thus, the corresponding softmax values p_i are closer to the optimal values 1/c.
- This explains why the results of using $\sigma_0 < 1$ are better.
- There is a minor difference between z_i and 0 and thus, between p_i and the optimal values 1/c.
- The smaller σ_0 , the smaller this difference.
- This explains why the smaller σ_0 , the better the results.

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