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Deep Neural Networks - Lecture 3

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Plan

Saturation

Batch Normalization

Skip connections

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Motivation

Consider a single sigmoid unit trying to learn on a single example $x = 1, y = 0$. The initial weight is $w = 2.0$ and bias is $b = 2.0$ (initial prediction is $\frac{1}{1+e^{-4}} \approx 0.98$). We use a quadratic loss function. This is how loss behaves over 50 epochs.

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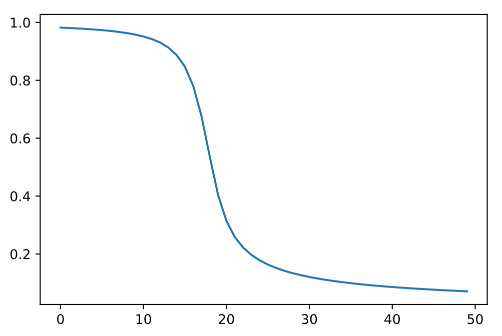

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$$\frac{\partial L(w, b)}{\partial w} = 2\sigma(w + b) \cdot \sigma(w + b) \left(1 - \sigma(w + b)\right) .$$

The second term makes this really small when prediction is close to one - very counter-intuitive.

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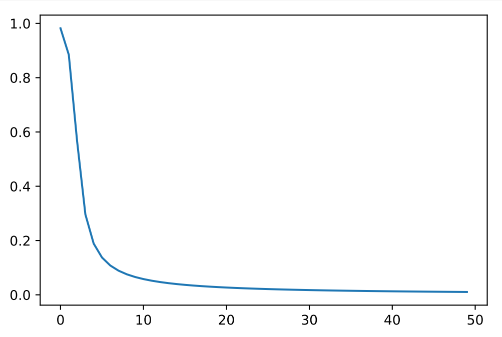

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Real message: when facing difficulties, think about what GD is really doing and figure out the problem!

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Answer: Of course it can. You can control the initial values in f^l as follows:

- Set biases to 0.
- Rescale inputs so that they are zero-centered and have unit variance.
- Set initial weights to small random values. How small?

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The same reasoning can be repeated for all layers, not only input layers. You can also use a similar reasoning for backpropagation step, and get inverse of the number of outputs (Glorot: $\sqrt{\frac{2}{m_i + m_{i+1}}}$).

Sigmoid units?

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This does not solve the problem completely - instead of saturation we get dead units etc. Reasoning like this is still very useful.

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Exercise: Why it makes less sense to normalize g^l? Give a handwaving argument.

Answer: Outputs of g^l can have rather complicated distributions. Scaling and shifting might not guarantee stable distributions. That said, recent papers actually advocate this. Apparently it often actually works better!

Implementation

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No longer clear what is really happening inside.
Instead...

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Consider a layer l and a mini-batch of size s.

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$$v_i^l = \frac{1}{s}\sum_{j=1}^{s}(f_{i,j}^l - \mu_i^l)^2.$$

This is a vector of mini-batch estimates of variances of each f_i^l.

Solution, ctd.

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This is bad since then the non-linearities will receive restricted inputs. Instead $BN^l = \gamma^l \frac{f^l - \mu^l}{\sqrt{v^l + \varepsilon}} + \beta^l$ and we activate g^l on these BN^l. Note that each node has its own γ and β - learned parameters.

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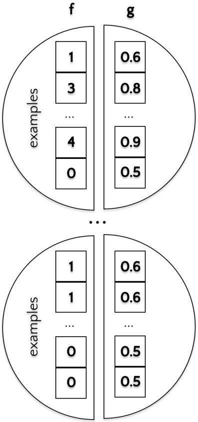
This is a significantly more complicated computation: each $BN^l_{i,j}$ depends on all $f^l_{i,j}$. But can still compute gradients of L over g^l, BN^l and f^l, and consequently over w's, b's, γ's and β's.

Batch normalization - example



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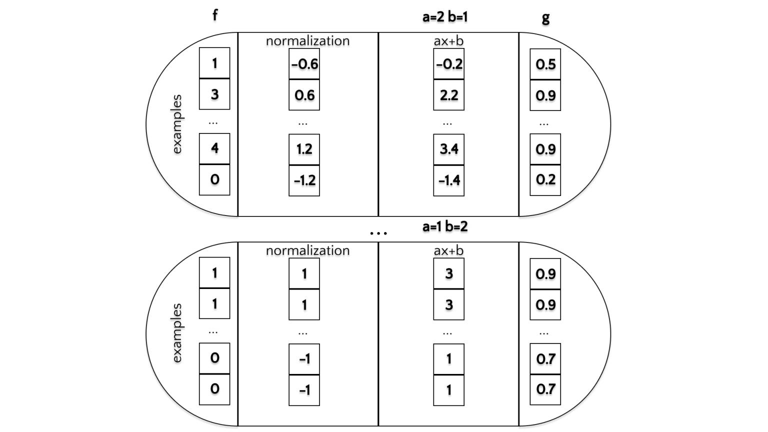

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When performing prediction, one might consider computing global mean and variance for the whole dataset (or at least better estimates than a single batch) and using them instead of batch statistics. Unfortunately this introduces a discrepancy between training and testing (same as dropout).

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- Avoids saturation for sigmoid and tanh units and dying ReLU units. This makes training deeper networks possible.
- No careful initialization required.

Recent research I

Laarhoven [2017] argues that:

- If using batch normalization, using L2 regularization as well might be crucial for convergence, BUT
- The L2 regularization coefficient only influences effective learning rate!

Recent research II

Later, Santurkar et al. [2018] argue that:

- Batch normalization helping with internal covariate shift is a myth.
- What batch normalization really does: it smoothens the loss funcion and its gradient.

Recent research III

In a more recent research paper, Brock et al. [2021] manage to obtain SOTA results on ImageNet recognition without batch normalization (they use clipping instead), and almost 10x faster.

Is this a beginning of a revolution? Does not seem so thus far.

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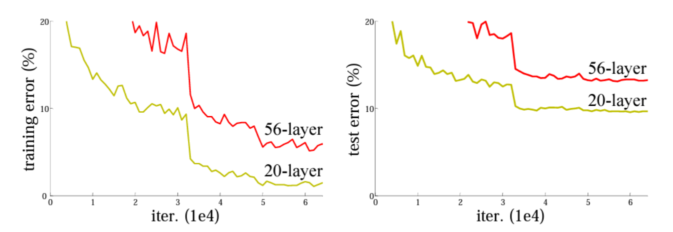
- Deeper networks do work better on both train and test in practice (using BN). To a point...



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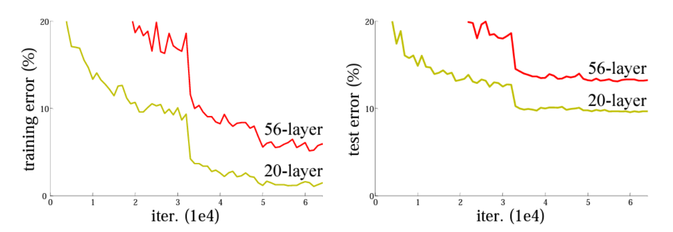


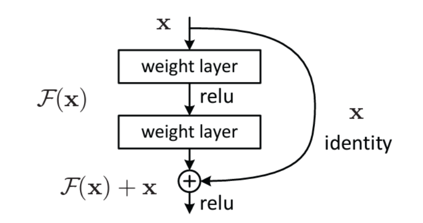
What seems to be the problem?

Identity seems to be a rather difficult mapping to learn!

Residual connections

Solution: residual connection.

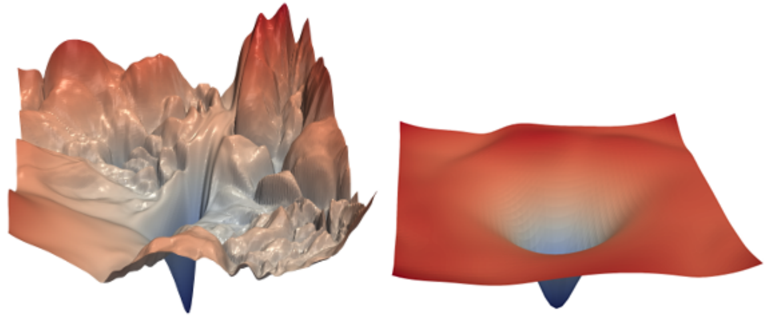
- Signal is copied several layers forward.
- It is ADDED to layers' output, so it learns the RESIDUAL.
- To go deeper we learn the 0 mapping, not identity - easier.
- Dimension needs to agree.
- No new parameters!



Does it work?

Spectacular success stories, e.g. ResNet (next lecture) or transformers.

Today: a suggestive image (for ResNet).



(a) without skip connections (b) with skip connections

Concatenation

Sometimes it makes more sense to use a skip connection to APPEND an early layer to deeper layer.

Useful for “annotating the input” style problems with dense outputs, like image segmentation, etc. (see U-Net in next lecture). Even for shallow networks

Typically these are called “skip connections” (vs “residual connections”), but not always!

Extra reading

Original batch norm paper

Batch norm with L2 regularization

Exploration of what batch norm does

Original ResNet paper

Visualization of skip connection landscape

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