Deep Neural Networks - Lecture 4

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April 4, 2018

Gradient Descent

Overfitting

Saturation

Batch Normalization

Plan

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Gradient Descent - Recap

(Batch) Gradient Descent works by making steps in direction of the gradient of the loss function, e.g.

$$L(W, B) = \frac{1}{n} \sum_i L_i(W, B),$$

where $L_i(W, B)$ is the loss on the i-th example, and depends on W and B.

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where $L_i(W, B)$ is the loss on the i-th example, and depends on W and B.

Computing the gradient requires going over the whole dataset and is very expensive, especially nowadays when often dealing with massive datasets.

Stochastic Gradient Descent

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This is very fast, but also the gradients are very noisy. In practice, with small enough η this has all the good properties of GD and works faster.

Also allows for online-learning, in particular no need to keep train set in memory.

Mini-batch SGD

Mini-batch Gradient Descent is a mix of both approaches. Split the data into mini-batches of fixed size s. For each mini-batch S compute the gradient of $\frac{1}{s}\sum_{i\in S} L_i(W, B)$ and use this as an estimate of the gradient $\nabla L(W, B)$.

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This estimate is less noisy, but takes longer to compute.

Important: Computing the gradient for a batch of size 100 is not 100 times slower than computing the single example gradient, it is much faster than that! But the larger the batch size the more linear this behaviour is.

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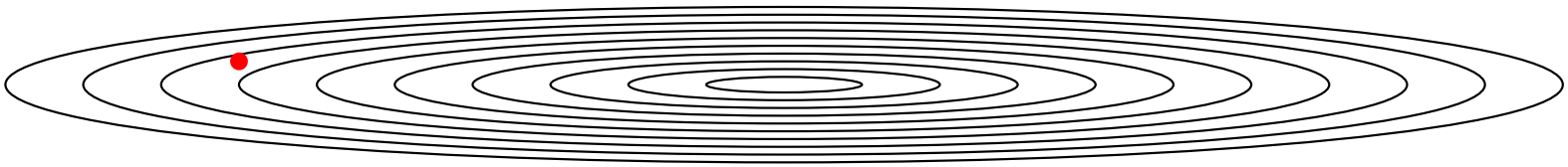
- Before each run through the whole dataset (*epoch*), you want to shuffle the dataset (could be expensive).
- If possible, you want all classes to be equally represented in batches. This is tricky if batches are small, or if classes are very unbalanced.
- The batch size does influence the learning rate, the nature of this relationship is not entirely clear, but experiments suggests that l.r. should be scaled linearly with batch size (up to a certain point, and perhaps not in the initial epochs).

Problems with GD



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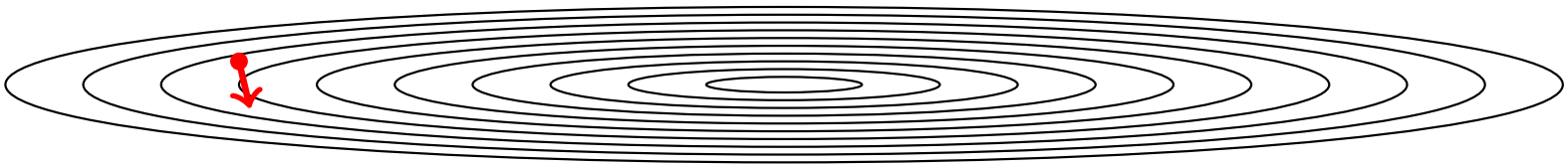

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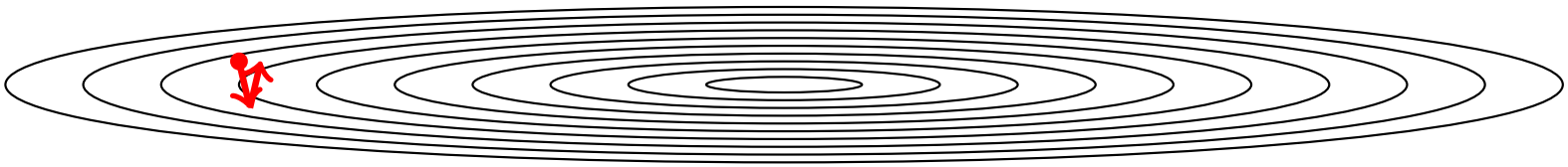

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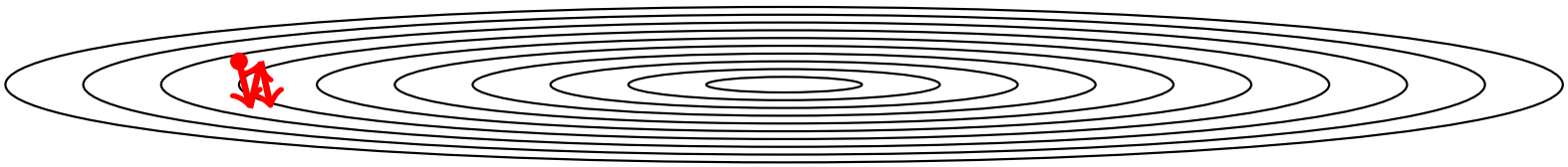

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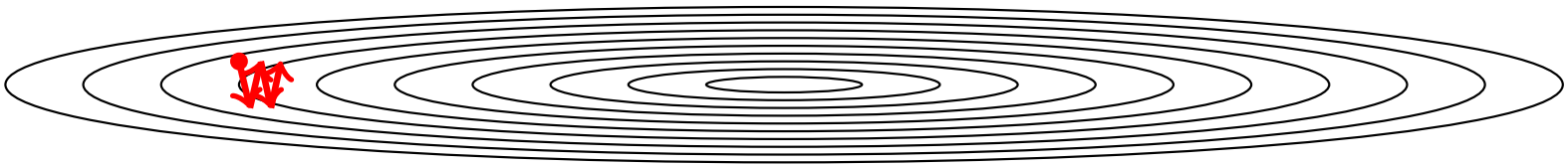

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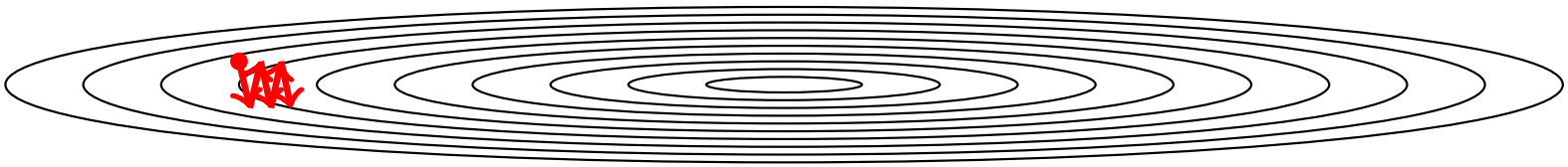

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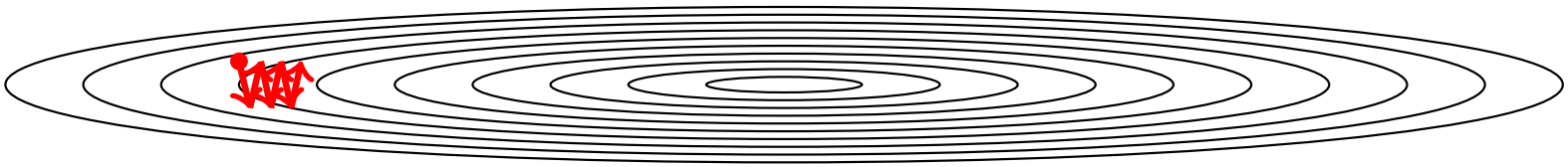

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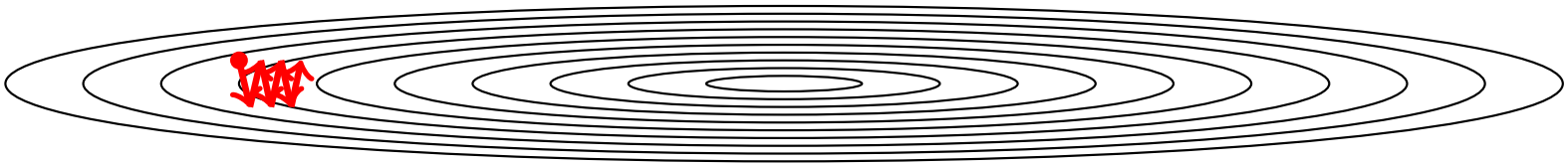

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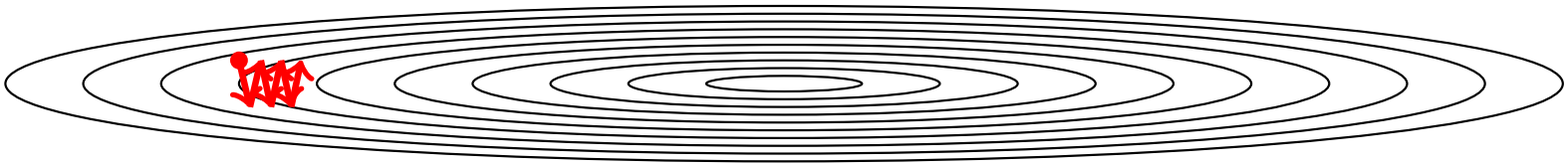

You can try to avoid this kind of scenario (later).

Or you can try to deal with it.

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Idea: Accumulate gradients from recent iterations. Update parameters like this:

$$x_{t+1} = x_t + v_{t+1}$$

with

$$v_{t+1} = \gamma v_t - \eta \nabla L(x_t),$$

where γ is a parameter (momentum), e.g $\gamma = 0.9$. Start with a zero vector v_0.

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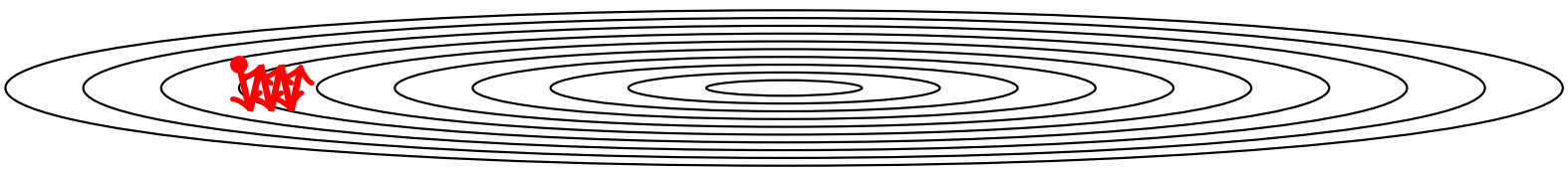

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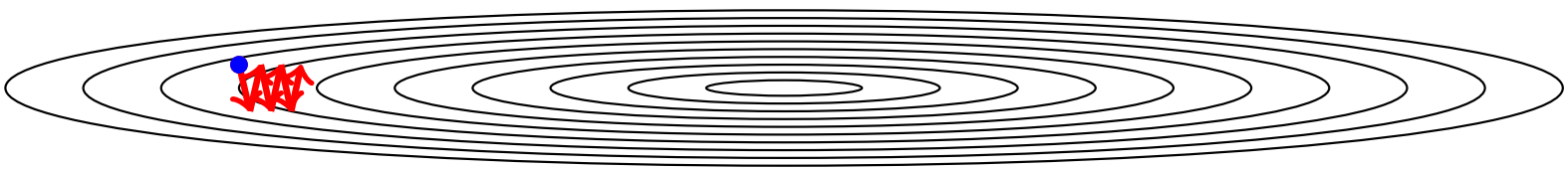

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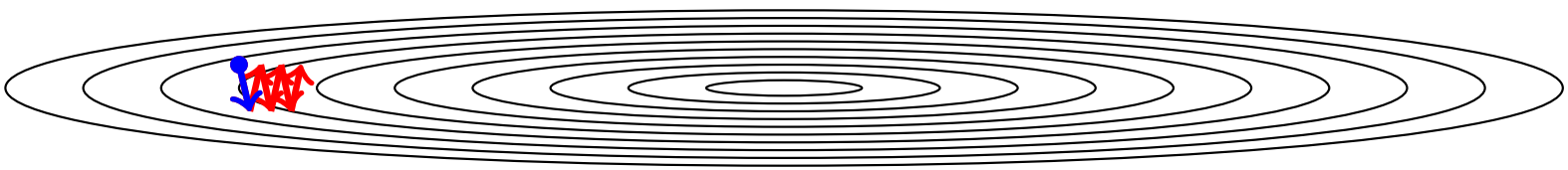

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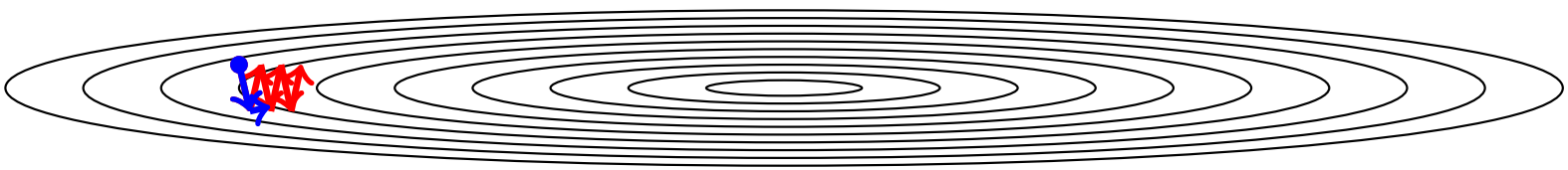

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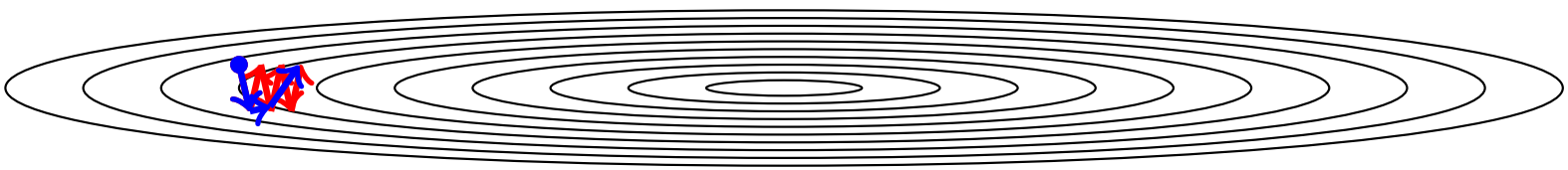

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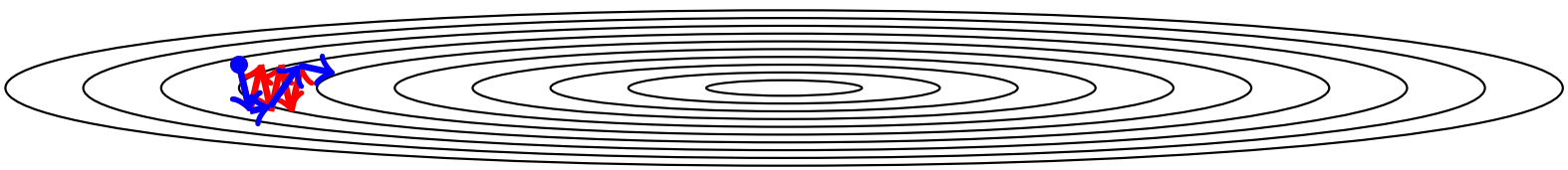

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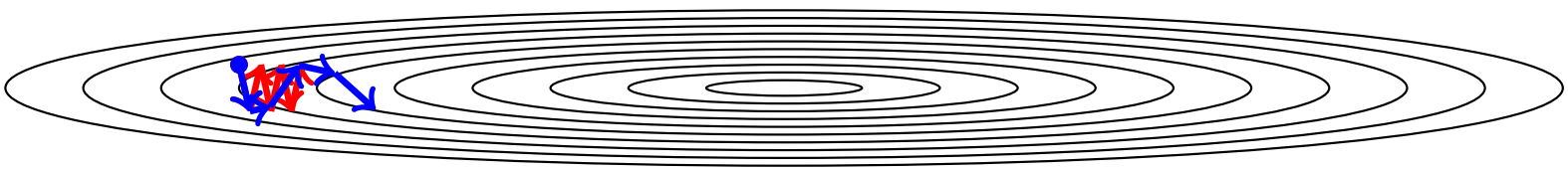

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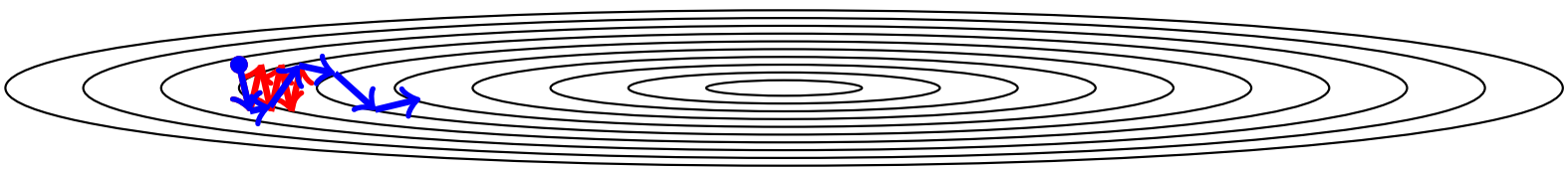

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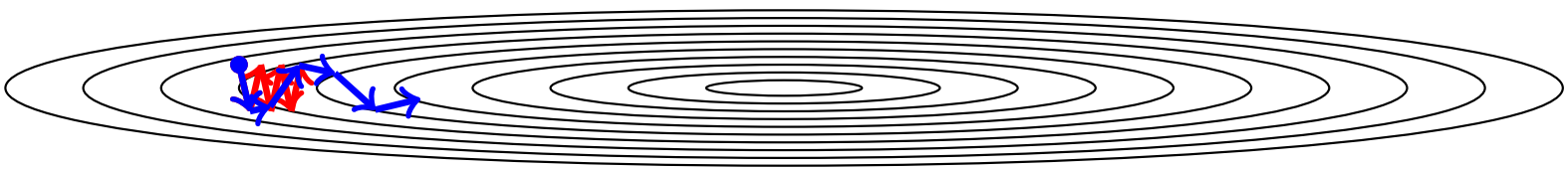

Note: With momentum you might get different kind of oscillation, usually not a big problem.

Nesterov's momentum

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Here is a different approach (*Nesterov's momentum*)

$$v_{t+1} = \gamma v_t - \eta \nabla L(x_t + \gamma v_t).$$

We move first to see what is there!

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Often works better.

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Other options: polynomial schedule, stages, cyclic learning rate. Additional parameters to tune.

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We do it for all parameters, by keeping G matrices and vectors on top of weight and bias matrices.

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One problem: Sometimes the learning rates die to quickly.

RMSProp

RMSProp uses an exponential moving average of squares of past updates to help this.

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Very efficient implementation of GD in practice.

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It also uses special correction terms to fight initial bias towards zero of the EMAs.

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Interestingly, in many top research papers, plain SGD or momentum is used.

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Motivation

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Exercise: Consider data with $N = 1000$ different examples in $x^i \in \{-1, 1\}^m$ and binary outputs $y^i \in \{0, 1\}$. Argue that a perceptron network with a single hidden layer of size N can learn to discriminate perfectly. Is this useful?

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Solution: The i-th perceptron in the hidden layer triggers only for x_i, by setting $w = x^i$ and $b = m$.

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You can simulate any perceptron network this way. Bad, because you can achieve "this and nothing else" behaviour.

Motivation II

Another point of view on generalization: general concepts (6 vs a specific 6 from the input data) are resistant to noise.

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How to create a network that does not change much when fed noisy data?

Use small weights!

L2 regularization

Standard way to avoid large weights is to include a penalty term in the objective function:

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How to implement this in GD?

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This is sometimes called *weight decay* for obvious reasons.

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Exercise: Note that this does not really penalize large weights, but only their total! What is the effect on the learned weights?

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Another idea - use L1 norm instead:

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How to implement this in GD?

L1 regularization - GD

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For $w = 0$ the penalty term is not differentiable, makes sense to not touch the weight. One might argue that weights w with $|w| < \lambda$ should be just set to zero.

Augmentation

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Exercise: Propose ways to create synthetic data for MNIST.

Answer: There are many reasonable ideas: tiny rotations, shifts.

Dropout

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A generalization of this idea is to drop connections, not nodes - we will not discuss details.

Why dropout works?

- "This prevents complex co-adaptations in which a feature detector is only helpful in the context of several other specific feature detectors. Instead, each neuron learns to detect a feature that is generally helpful for producing the correct answer given the combinatorially large variety of internal contexts in which it must operate." – G. Hinton

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- Dropout introduces noise, so features train to be more resistant to this kind of noise.
- Problem can have an obvious plateau of an easy solution. Dropout (especially on the input layer) can force the network to look beyond that.

Plan

Gradient Descent

Overfitting

Saturation

Batch Normalization

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 $\frac{1}{1+e^{-5}} \approx 0.99$). We use a quadratic loss function. This is how loss behaves over 50 epochs.

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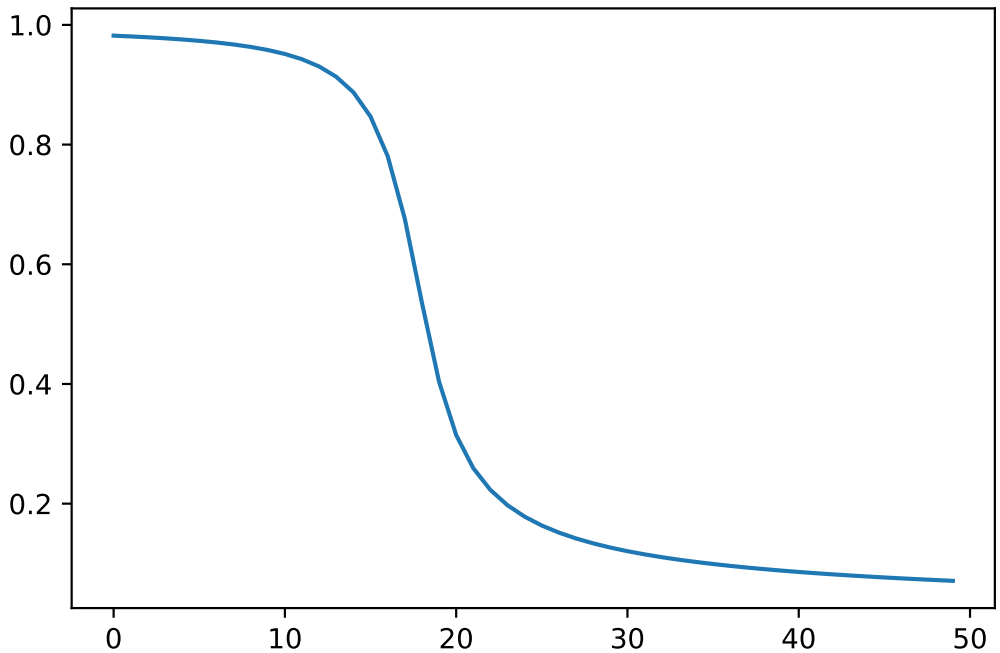

This unit is a *saturated* unit.

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

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

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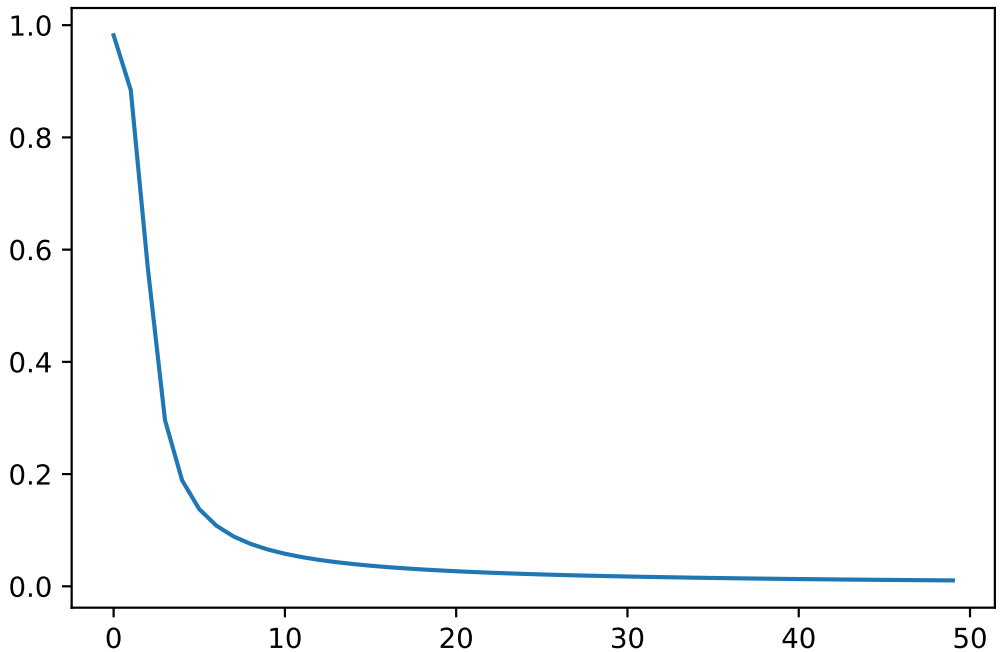
Log-loss



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

Exercise

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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?

Exercise, ctd

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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.

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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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!

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Also, one can argue that the network will learn to counteract such measures. Instead...

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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.

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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 more complicated computation graph: each $BN^l_{i,j}$ depends on all $f^l_{i,j}$, but still a DAG. Can compute gradients of L over g^l, BN^l and f^l, and consequently over w's, b's, γ's and β's (lab).

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In a recent paper, 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!

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- No careful initialization required.