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Deep Neural Networks - Lecture 2

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Plan

Gradient Descent

Overfitting

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Gradient Descent

Overfitting

Gradient Descent - Recap

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(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

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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.

Technical issues

Some important details:

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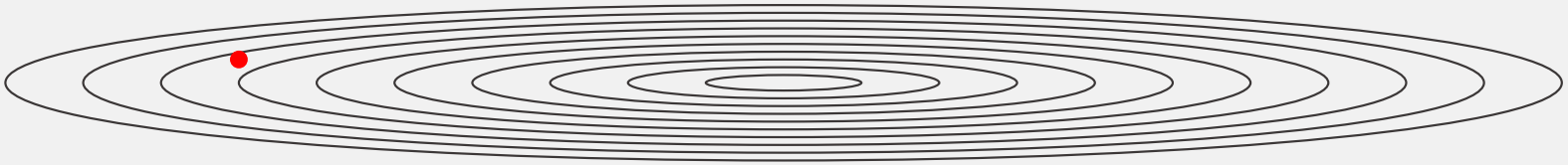
Some important details:

- 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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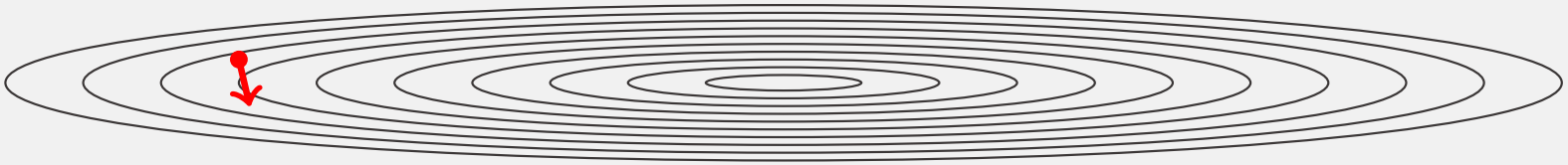

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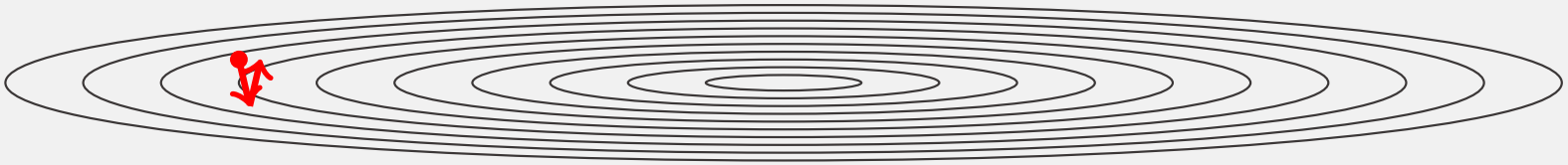

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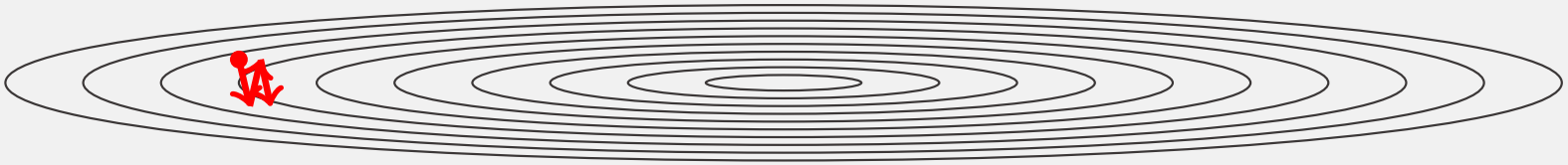

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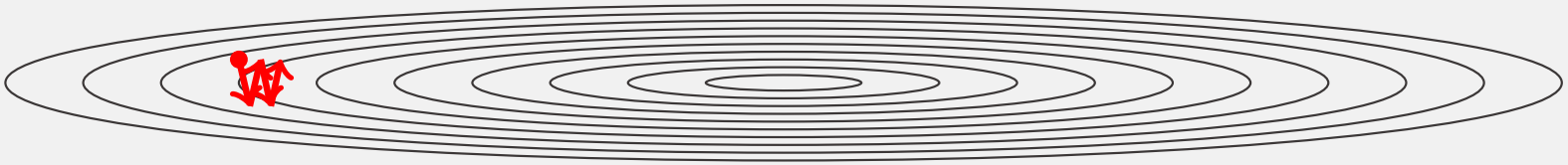

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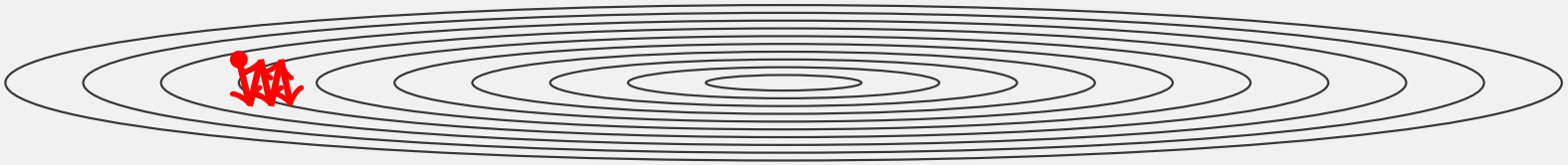

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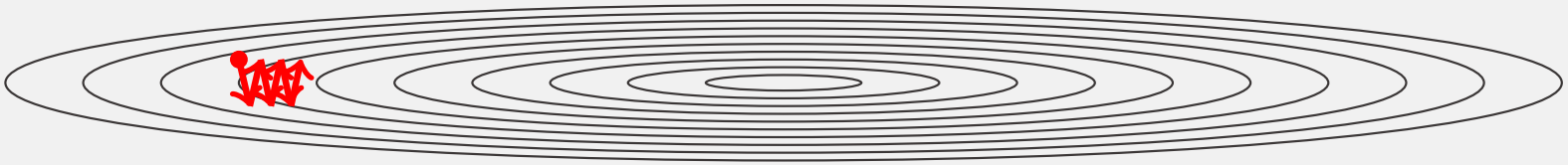

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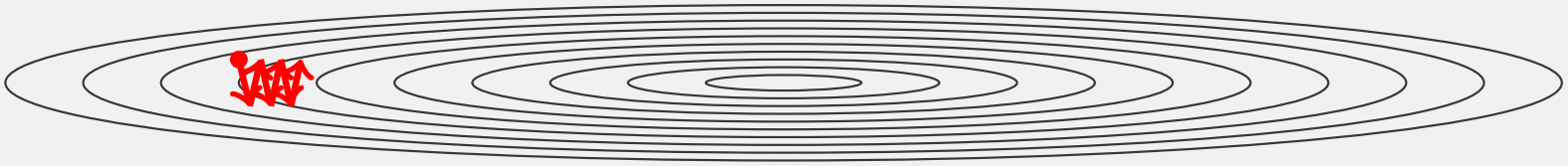

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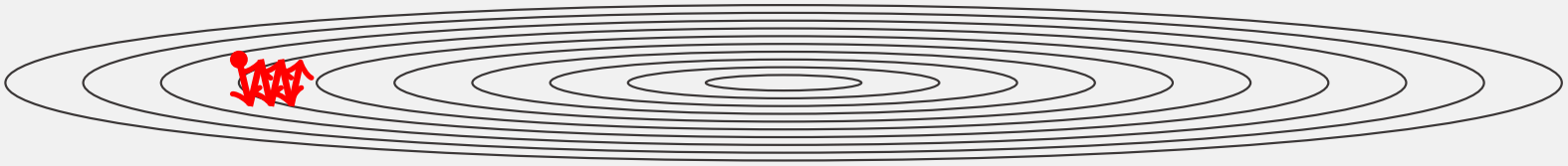

You can try to avoid this kind of scenario (later).

Or you can try to deal with it.

Momentum

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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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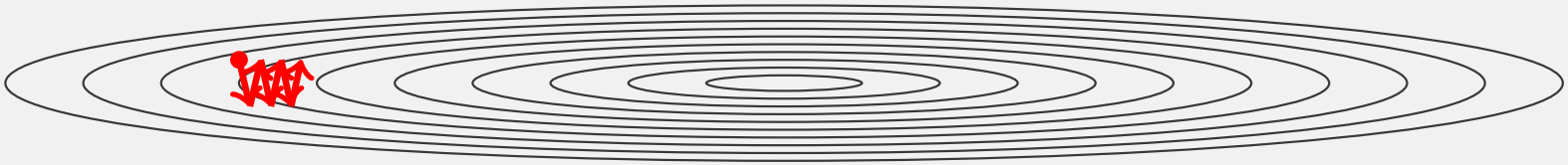

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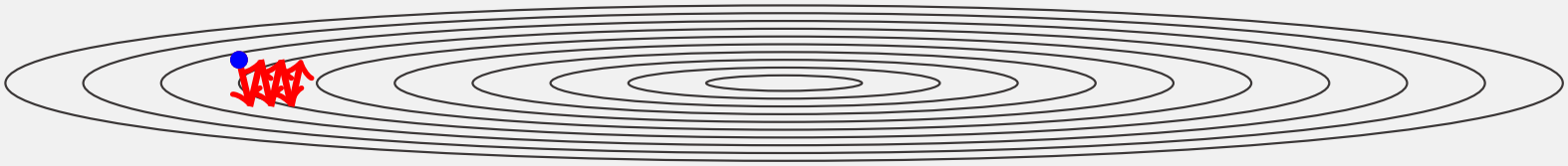

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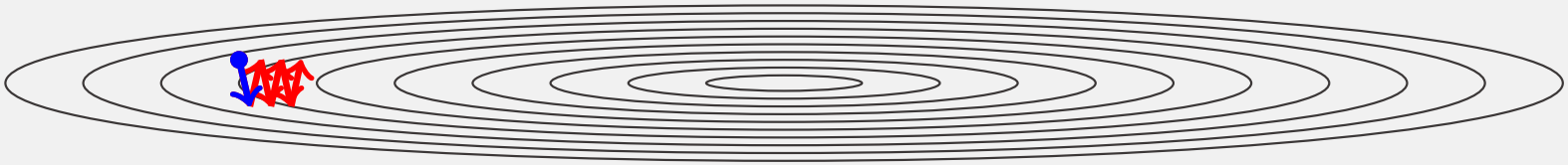

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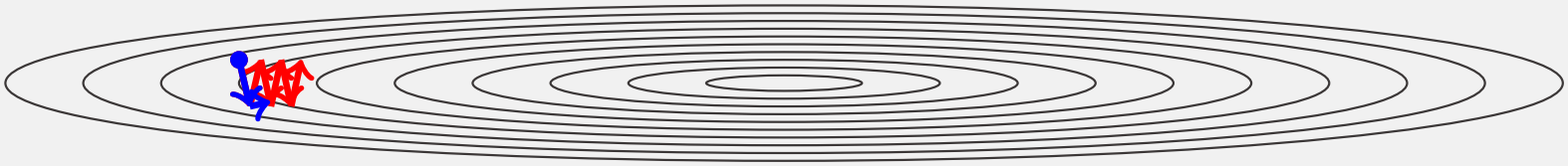

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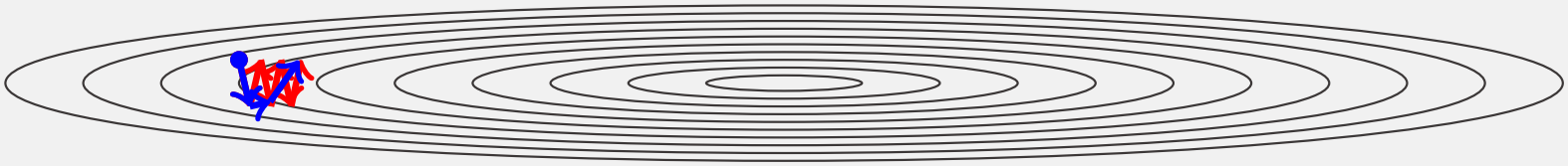

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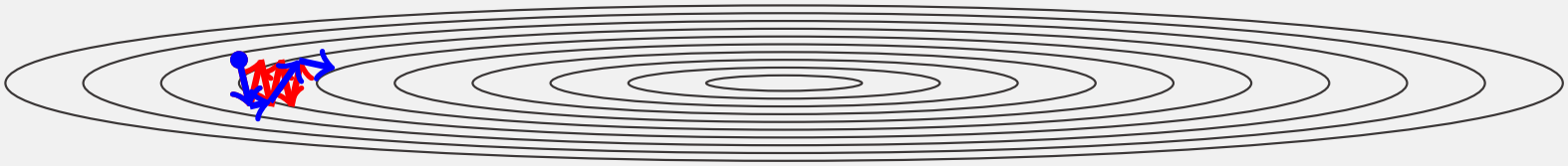

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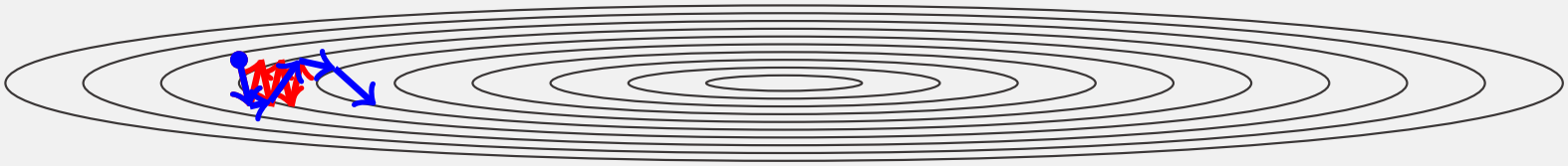

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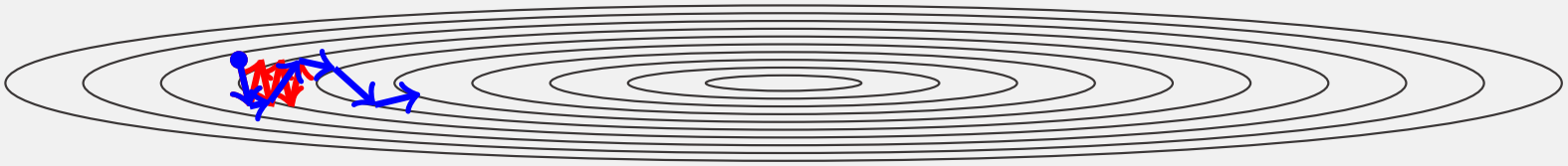

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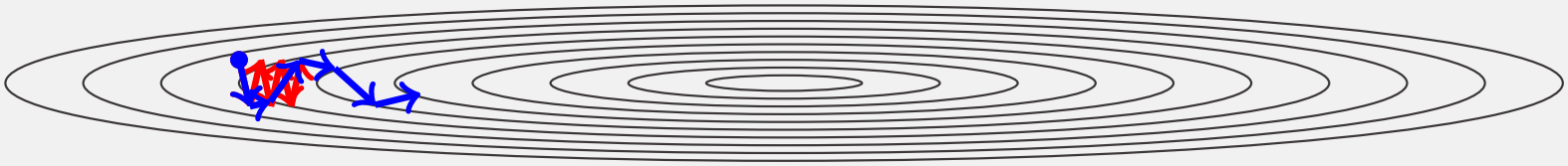

Note: With momentum you might get different kind of oscillation, usually not a big problem.

Nesterov's momentum

This is the update vector again:

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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.

Adam variants

Due to Adam's overwhelming success, many variants have been proposed - fixing deficiencies and offering specialized versions:

- AdamW - fixing L_2-regularization behaviour (see next slide)
- NAdam - Nesterov's momentum + Adam
- RAdam - *rectified* Adam, incorporates a kind of warm up schedule into Adam (fixing large variance in adaptive learning rates)

and many, many more...

AdamW

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Existing research seems to support the claim that this outperforms standard Adam, especially in terms of generalization.

See *Decoupled Weight Decay Regularization* Ilya Loshchilov, Frank Hutter

Which algorithm?

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Vanilla GD and momentum methods require choosing the learning rate and learning rate decay. They also tend to give slower convergence, especially for sparse data.

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Adagrad based methods often work with less tuning, and in general better, but not always.

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Goal: We want our network to generalize - learn to recognize 6s and 9s and not *overfit* to the exact 6s and 9s from the training data.

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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.

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

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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:

$$L(W, B) = \frac{1}{n} \sum L_i(W, B) + R_2(W, B)$$

where

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How to implement this in GD?

L2 regularization - gradient

The gradient of the regularization part over the weights is independent from the mini-batch data and equals

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

L1 regularization

Another idea - use L1 norm instead:

$$L(W, B) = \frac{1}{n} \sum L_i(W, B) + R_1(W, B)$$

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$$R_1(W, B) = \lambda \sum_{w \in W} |w| .$$

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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.

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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?

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- "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.

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