Lecture 6. Training neural networks II

Disclaimer: This note was modified from cs231n lecture notes by Prof. Li Fei-Fei at Stanford University.

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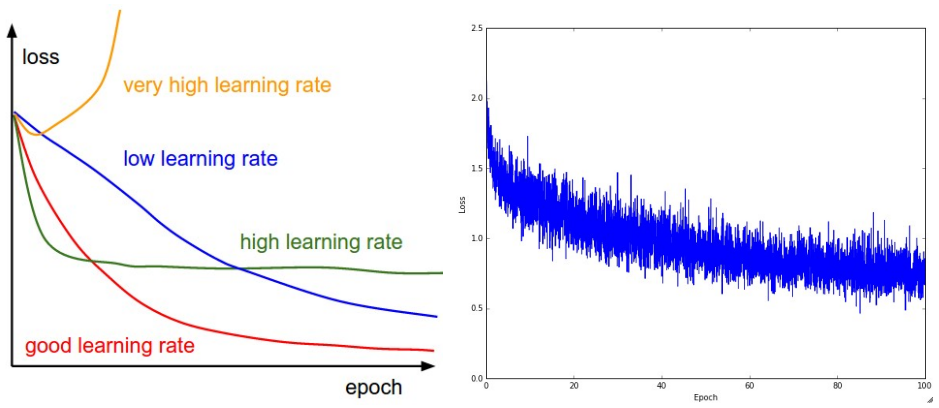
Babysitting the Learning Process

There are multiple useful quantities you should monitor during training of a neural network. These plots are the window into the training process and should be utilized to get intuitions about different hyperparameter settings and how they should be changed for more efficient learning.

The x-axis of the plots below are always in units of epochs, which measure how many times every example has been seen during training in expectation (e.g. one epoch means that every example has been seen once). It is preferable to track epochs rather than iterations since the number of iterations depends on the arbitrary setting of batch size.

Loss function

The first quantity that is useful to track during training is the loss, as it is evaluated on the individual batches during the forward pass. Below is a cartoon diagram showing the loss over time, and especially what the shape might tell you about the learning rate:



Left: A cartoon depicting the effects of different learning rates. With low learning rates the improvements will be linear. With high learning rates they will start to look more exponential. Higher learning rates will decay the loss faster, but they get stuck at worse values of loss (green line). This is because there is too much "energy" in the optimization and the parameters are bouncing around chaotically, unable to settle in a nice spot in the optimization landscape. **Right:** An example of a typical loss function over time, while training a small network on CIFAR-10 dataset. This loss function looks reasonable (it might indicate a slightly too small learning rate based on its speed of decay, but it's hard to say), and also indicates that the batch size might be a little too low (since the cost is a little too noisy).

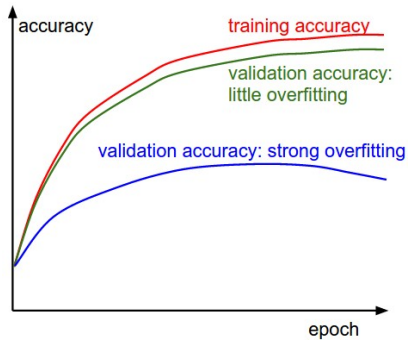
The amount of "wiggle" in the loss is related to the batch size. When the batch size is 1, the wiggle will be relatively high. When the batch size is the full dataset, the wiggle will be minimal because every gradient update should be improving the loss function monotonically (unless the learning rate is set too high).

Some people prefer to plot their loss functions in the log domain. Since learning progress generally takes an exponential form shape, the plot appears as a slightly more interpretable straight line, rather than a hockey stick. Additionally, if multiple cross-validated models are plotted on the same loss graph, the differences between them become more apparent.

Sometimes loss functions can look funny lossfunctions.tumblr.com.

Train/Val accuracy

The second important quantity to track while training a classifier is the validation/training accuracy. This plot can give you valuable insights into the amount of overfitting in your model:



The gap between the training and validation accuracy indicates the amount of overfitting. Two possible cases are shown in the diagram on the left. The blue validation error curve shows very small validation accuracy compared to the training accuracy, indicating strong overfitting (note, it's possible for the validation accuracy to even start to go down after some point). When you see this in practice you probably want to increase regularization (stronger L2 weight penalty, more dropout, etc.) or collect more data. The other possible case is when the validation accuracy tracks the training accuracy fairly well. This case indicates that your model capacity is not high enough: make the model larger by increasing the number of parameters.

Ratio of weights:updates

The last quantity you might want to track is the ratio of the update magnitudes to the value magnitudes. Note: *updates*, not the raw gradients (e.g. in vanilla sgd this would be the gradient multiplied by the learning rate). You might want to evaluate and track this ratio for every set of parameters independently. A rough heuristic is that this ratio should be somewhere around 1e-3. If it is lower than this then the learning rate might be too low. If it is higher then the learning rate is likely too high. Here is a specific example:

```
# assume parameter vector W and its gradient vector dW
param_scale = np.linalg.norm(W.ravel())
update = -learning_rate*dW # simple SGD update
update_scale = np.linalg.norm(update.ravel())
W += update # the actual update
print update_scale / param_scale # want ~1e-3
```

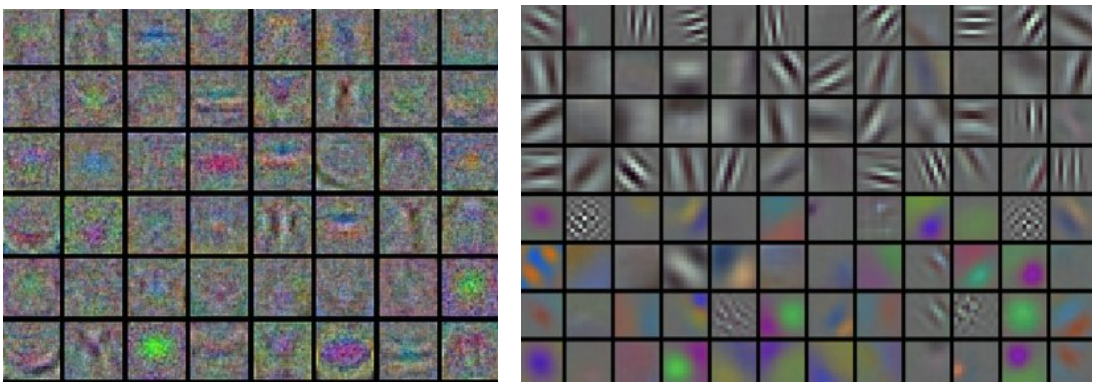
Instead of tracking the min or the max, some people prefer to compute and track the norm of the gradients and their updates instead. These metrics are usually correlated and often give approximately the same results.

Activation / Gradient distributions per layer

An incorrect initialization can slow down or even completely stall the learning process. Luckily, this issue can be diagnosed relatively easily. One way to do so is to plot activation/gradient histograms for all layers of the network. Intuitively, it is not a good sign to see any strange distributions - e.g. with tanh neurons we would like to see a distribution of neuron activations between the full range of [-1,1], instead of seeing all neurons outputting zero, or all neurons being completely saturated at either -1 or 1.

First-layer Visualizations

Lastly, when one is working with image pixels it can be helpful and satisfying to plot the first-layer features visually:



Examples of visualized weights for the first layer of a neural network. **Left**: Noisy features indicate could be a symptom: Unconverged network, improperly set learning rate, very low weight regularization penalty. **Right:** Nice, smooth, clean and diverse features are a good indication that the training is proceeding well.

Regularization

There are several ways of controlling the capacity of Neural Networks to prevent overfitting:

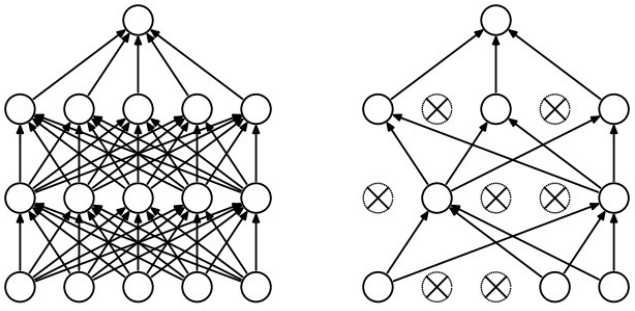
L2 regularization is perhaps the most common form of regularization. It can be implemented by penalizing the squared magnitude of all parameters directly in the objective. That is, for every weight w in the network, we add the term $\frac{1}{2}\lambda w^2$ to the objective, where λ is the regularization strength. It is common to see the factor of $\frac{1}{2}$ in front because then the gradient of this term with respect to the parameter w is simply λw instead of $2\lambda w$. The L2 regularization has the intuitive interpretation of heavily penalizing peaky weight vectors and preferring diffuse weight vectors. As we discussed in the Linear Classification section, due to multiplicative interactions between weights and inputs this has the appealing property of encouraging the network to use all of its inputs a little rather than some of its inputs a lot. Lastly, notice that during gradient descent parameter update, using the L2 regularization ultimately means that every weight is decayed linearly: `W += -lambda * W` towards zero.

L1 regularization is another relatively common form of regularization, where for each weight w we add the term $\lambda \mid w \mid$ to the objective. It is possible to combine the L1 regularization with the L2 regularization: $\lambda_1 \mid w \mid + \lambda_2 w^2$ (this is called Elastic net regularization). The L1 regularization has the intriguing property that it leads the weight vectors to become sparse during optimization (i.e. very close to exactly zero). In other words, neurons with L1 regularization end up using only a sparse subset of their most important inputs and become nearly invariant to the "noisy" inputs. In comparison, final weight vectors from L2 regularization are usually diffuse, small numbers. In practice, if you are not concerned with explicit feature selection, L2 regularization can be expected to give superior performance over L1.

Max norm constraints. Another form of regularization is to enforce an absolute upper bound on the magnitude of the weight vector for every neuron and use projected gradient descent to enforce the constraint. In practice, this corresponds to performing the parameter update as normal, and then enforcing the constraint by clamping

the weight vector $\vec{w}$ of every neuron to satisfy $||\vec{w}||_2 < c$. Typical values of c are on orders of 3 or 4. Some people report improvements when using this form of regularization. One of its appealing properties is that network cannot "explode" even when the learning rates are set too high because the updates are always bounded.

Dropout is an extremely effective, simple and recently introduced regularization technique by Srivastava et al. in Dropout: A Simple Way to Prevent Neural Networks from Overfitting (pdf) that complements the other methods (L1, L2, maxnorm). While training, dropout is implemented by only keeping a neuron active with some probability p (a hyperparameter), or setting it to zero otherwise.



(a) Standard Neural Net (b) After applying dropout.

Figure taken from the Dropout paper that illustrates the idea. During training, Dropout can be interpreted as sampling a Neural Network within the full Neural Network, and only updating the parameters of the sampled network based on the input data. (However, the exponential number of possible sampled networks are not independent because they share the parameters.) During testing there is no dropout applied, with the interpretation of evaluating an averaged prediction across the exponentially-sized ensemble of all sub-networks (more about ensembles in the next section).

Vanilla dropout in an example 3-layer Neural Network would be implemented as follows:

```
""" Vanilla Dropout: Not recommended implementation (see notes below) """

p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

In the code above, inside the `train_step` function we have performed dropout twice: on the first hidden layer and on the second hidden layer. It is also possible to perform dropout right on the input layer, in which case we

would also create a binary mask for the input `X`. The backward pass remains unchanged, but of course has to take into account the generated masks `U1,U2`.

Crucially, note that in the `predict` function we are not dropping anymore, but we are performing a scaling of both hidden layer outputs by p. This is important because at test time all neurons see all their inputs, so we want the outputs of neurons at test time to be identical to their expected outputs at training time. For example, in case of $p = 0.5$, the neurons must halve their outputs at test time to have the same output as they had during training time (in expectation). To see this, consider an output of a neuron x (before dropout). With dropout, the expected output from this neuron will become $px + (1 - p)0$, because the neuron's output will be set to zero with probability $1 - p$. At test time, when we keep the neuron always active, we must adjust $x \rightarrow px$ to keep the same expected output. It can also be shown that performing this attenuation at test time can be related to the process of iterating over all the possible binary masks (and therefore all the exponentially many sub-networks) and computing their ensemble prediction.

The undesirable property of the scheme presented above is that we must scale the activations by p at test time. Since test-time performance is so critical, it is always preferable to use **inverted dropout**, which performs the scaling at train time, leaving the forward pass at test time untouched. Additionally, this has the appealing property that the prediction code can remain untouched when you decide to tweak where you apply dropout, or if at all. Inverted dropout looks as follows:

```
"""
Inverted Dropout: Recommended implementation example.
We drop and scale at train time and don't do anything at test time.
"""

p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  out = np.dot(W3, H2) + b3
```

There has a been a large amount of research after the first introduction of dropout that tries to understand the source of its power in practice, and its relation to the other regularization techniques. Recommended further reading for an interested reader includes:

- Dropout paper by Srivastava et al. 2014.
- Dropout Training as Adaptive Regularization: "we show that the dropout regularizer is first-order equivalent to an L2 regularizer applied after scaling the features by an estimate of the inverse diagonal Fisher information matrix".

Theme of noise in forward pass. Dropout falls into a more general category of methods that introduce stochastic behavior in the forward pass of the network. During testing, the noise is marginalized over *analytically* (as is the case with dropout when multiplying by p), or *numerically* (e.g. via sampling, by performing several forward passes with different random decisions and then averaging over them). An example of other research in this direction includes DropConnect, where a random set of weights is instead set to zero during forward pass. As foreshadowing, Convolutional Neural Networks also take advantage of this theme with methods such as stochastic pooling, fractional pooling, and data augmentation. We will go into details of these methods later.

Bias regularization. As we already mentioned in the Linear Classification section, it is not common to regularize the bias parameters because they do not interact with the data through multiplicative interactions, and therefore do not have the interpretation of controlling the influence of a data dimension on the final objective. However, in practical applications (and with proper data preprocessing) regularizing the bias rarely leads to significantly worse performance. This is likely because there are very few bias terms compared to all the weights, so the classifier can "afford to" use the biases if it needs them to obtain a better data loss.

Per-layer regularization. It is not very common to regularize different layers to different amounts (except perhaps the output layer). Relatively few results regarding this idea have been published in the literature.

In practice: It is most common to use a single, global L2 regularization strength that is cross-validated. It is also common to combine this with dropout applied after all layers. The value of $p = 0.5$ is a reasonable default, but this can be tuned on validation data.

Parameter Updates

Once the analytic gradient is computed with backpropagation, the gradients are used to perform a parameter update. There are several approaches for performing the update, which we discuss next.

We note that optimization for deep networks is currently a very active area of research. In this section we highlight some established and common techniques you may see in practice, briefly describe their intuition, but leave a detailed analysis outside of the scope of the class. We provide some further pointers for an interested reader.

SGD and bells and whistles

Vanilla update. The simplest form of update is to change the parameters along the negative gradient direction (since the gradient indicates the direction of increase, but we usually wish to minimize a loss function). Assuming a vector of parameters `x` and the gradient `dx`, the simplest update has the form:

```
# Vanilla update
x += - learning_rate * dx
```

where `learning_rate` is a hyperparameter - a fixed constant. When evaluated on the full dataset, and when the learning rate is low enough, this is guaranteed to make non-negative progress on the loss function.

Momentum update is another approach that almost always enjoys better converge rates on deep networks. This update can be motivated from a physical perspective of the optimization problem. In particular, the loss can be interpreted as the height of a hilly terrain (and therefore also to the potential energy since $U = mgh$ and therefore $U \propto h$). Initializing the parameters with random numbers is equivalent to setting a particle with zero initial velocity at some location. The optimization process can then be seen as equivalent to the process of simulating the parameter vector (i.e. a particle) as rolling on the landscape.

Since the force on the particle is related to the gradient of potential energy (i.e. $F = -\nabla U$), the **force** felt by the particle is precisely the (negative) **gradient** of the loss function. Moreover, $F = ma$ so the (negative) gradient is in this view proportional to the acceleration of the particle. Note that this is different from the SGD

update shown above, where the gradient directly integrates the position. Instead, the physics view suggests an update in which the gradient only directly influences the velocity, which in turn has an effect on the position:

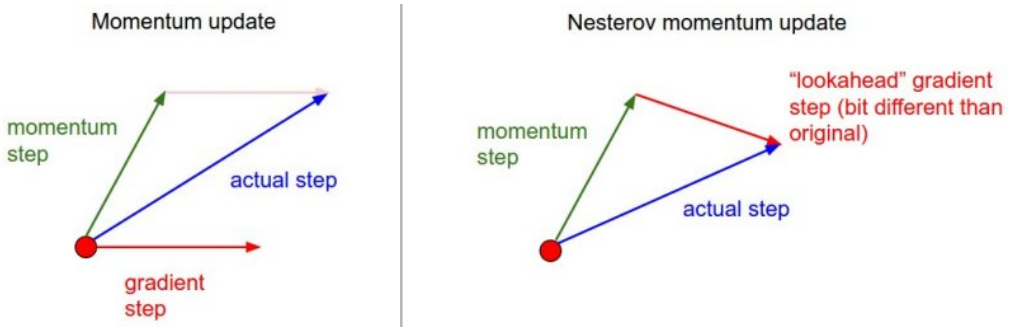
```
# Momentum update
v = mu * v - learning_rate * dx # integrate velocity
x += v # integrate position
```

Here we see an introduction of a `v` variable that is initialized at zero, and an additional hyperparameter (`mu`). As an unfortunate misnomer, this variable is in optimization referred to as *momentum* (its typical value is about 0.9), but its physical meaning is more consistent with the coefficient of friction. Effectively, this variable damps the velocity and reduces the kinetic energy of the system, or otherwise the particle would never come to a stop at the bottom of a hill. When cross-validated, this parameter is usually set to values such as [0.5, 0.9, 0.95, 0.99]. Similar to annealing schedules for learning rates (discussed later, below), optimization can sometimes benefit a little from momentum schedules, where the momentum is increased in later stages of learning. A typical setting is to start with momentum of about 0.5 and anneal it to 0.99 or so over multiple epochs.

> *With Momentum update, the parameter vector will build up velocity in any direction that has consistent gradient.*

Nesterov Momentum is a slightly different version of the momentum update that has recently been gaining popularity. It enjoys stronger theoretical converge guarantees for convex functions and in practice it also consistenly works slightly better than standard momentum.

The core idea behind Nesterov momentum is that when the current parameter vector is at some position `x`, then looking at the momentum update above, we know that the momentum term alone (i.e. ignoring the second term with the gradient) is about to nudge the parameter vector by `mu * v`. Therefore, if we are about to compute the gradient, we can treat the future approximate position `x + mu * v` as a "lookahead" - this is a point in the vicinity of where we are soon going to end up. Hence, it makes sense to compute the gradient at `x + mu * v` instead of at the "old/stale" position `x`.



Nesterov momentum. Instead of evaluating gradient at the current position (red circle), we know that our momentum is about to carry us to the tip of the green arrow. With Nesterov momentum we therefore instead evaluate the gradient at this "looked-ahead" position.

That is, in a slightly awkward notation, we would like to do the following:

```
x_ahead = x + mu * v
# evaluate dx_ahead (the gradient at x_ahead instead of at x)
v = mu * v - learning_rate * dx_ahead
x += v
```

However, in practice people prefer to express the update to look as similar to vanilla SGD or to the previous momentum update as possible. This is possible to achieve by manipulating the update above with a variable transform `x_ahead = x + mu * v`, and then expressing the update in terms of `x_ahead` instead of `x`. That

is, the parameter vector we are actually storing is always the ahead version. The equations in terms of `x_ahead` (but renaming it back to `x`) then become:

```
v_prev = v # back this up
v = mu * v - learning_rate * dx # velocity update stays the same
x += -mu * v_prev + (1 + mu) * v # position update changes form
```

We recommend this further reading to understand the source of these equations and the mathematical formulation of Nesterov's Accelerated Momentum (NAG):

- Advances in optimizing Recurrent Networks by Yoshua Bengio, Section 3.5.
- Ilya Sutskever's thesis (pdf) contains a longer exposition of the topic in section 7.2

Annealing the learning rate

In training deep networks, it is usually helpful to anneal the learning rate over time. Good intuition to have in mind is that with a high learning rate, the system contains too much kinetic energy and the parameter vector bounces around chaotically, unable to settle down into deeper, but narrower parts of the loss function. Knowing when to decay the learning rate can be tricky: Decay it slowly and you'll be wasting computation bouncing around chaotically with little improvement for a long time. But decay it too aggressively and the system will cool too quickly, unable to reach the best position it can. There are three common types of implementing the learning rate decay:

- **Step decay**: Reduce the learning rate by some factor every few epochs. Typical values might be reducing the learning rate by a half every 5 epochs, or by 0.1 every 20 epochs. These numbers depend heavily on the type of problem and the model. One heuristic you may see in practice is to watch the validation error while training with a fixed learning rate, and reduce the learning rate by a constant (e.g. 0.5) whenever the validation error stops improving.
- **Exponential decay.** has the mathematical form $\alpha = \alpha_0 e^{-kt}$, where α_0, k are hyperparameters and t is the iteration number (but you can also use units of epochs).
- **1/t decay** has the mathematical form $\alpha = \alpha_0/(1 + kt)$ where a_0, k are hyperparameters and t is the iteration number.

In practice, we find that the step decay is slightly preferable because the hyperparameters it involves (the fraction of decay and the step timings in units of epochs) are more interpretable than the hyperparameter k. Lastly, if you can afford the computational budget, err on the side of slower decay and train for a longer time.

Second order methods

A second, popular group of methods for optimization in context of deep learning is based on Newton's method, which iterates the following update:

$$x \leftarrow x - [Hf(x)]^{-1} \nabla f(x)$$

Here, $Hf(x)$ is the Hessian matrix, which is a square matrix of second-order partial derivatives of the function. The term $\nabla f(x)$ is the gradient vector, as seen in Gradient Descent. Intuitively, the Hessian describes the local curvature of the loss function, which allows us to perform a more efficient update. In particular, multiplying by the inverse Hessian leads the optimization to take more aggressive steps in directions of shallow curvature and shorter steps in directions of steep curvature. Note, crucially, the absence of any learning rate hyperparameters in the update formula, which the proponents of these methods cite this as a large advantage over first-order methods.

However, the update above is impractical for most deep learning applications because computing (and inverting) the Hessian in its explicit form is a very costly process in both space and time. For instance, a Neural Network with

one million parameters would have a Hessian matrix of size [1,000,000 x 1,000,000], occupying approximately 3725 gigabytes of RAM. Hence, a large variety of *quasi-Newton* methods have been developed that seek to approximate the inverse Hessian. Among these, the most popular is L-BFGS, which uses the information in the gradients over time to form the approximation implicitly (i.e. the full matrix is never computed).

However, even after we eliminate the memory concerns, a large downside of a naive application of L-BFGS is that it must be computed over the entire training set, which could contain millions of examples. Unlike mini-batch SGD, getting L-BFGS to work on mini-batches is more tricky and an active area of research.

In practice, it is currently not common to see L-BFGS or similar second-order methods applied to large-scale Deep Learning and Convolutional Neural Networks. Instead, SGD variants based on (Nesterov's) momentum are more standard because they are simpler and scale more easily.

Additional references:

- Large Scale Distributed Deep Networks is a paper from the Google Brain team, comparing L-BFGS and SGD variants in large-scale distributed optimization.
- SFO algorithm strives to combine the advantages of SGD with advantages of L-BFGS.

Per-parameter adaptive learning rate methods

All previous approaches we've discussed so far manipulated the learning rate globally and equally for all parameters. Tuning the learning rates is an expensive process, so much work has gone into devising methods that can adaptively tune the learning rates, and even do so per parameter. Many of these methods may still require other hyperparameter settings, but the argument is that they are well-behaved for a broader range of hyperparameter values than the raw learning rate. In this section we highlight some common adaptive methods you may encounter in practice:

Adagrad is an adaptive learning rate method originally proposed by Duchi et al..

```
# Assume the gradient dx and parameter vector x
cache += dx**2
x += - learning_rate * dx / (np.sqrt(cache) + eps)
```

Notice that the variable `cache` has size equal to the size of the gradient, and keeps track of per-parameter sum of squared gradients. This is then used to normalize the parameter update step, element-wise. Notice that the weights that receive high gradients will have their effective learning rate reduced, while weights that receive small or infrequent updates will have their effective learning rate increased. Amusingly, the square root operation turns out to be very important and without it the algorithm performs much worse. The smoothing term `eps` (usually set somewhere in range from 1e-4 to 1e-8) avoids division by zero. A downside of Adagrad is that in case of Deep Learning, the monotonic learning rate usually proves too aggressive and stops learning too early.

RMSprop. RMSprop is a very effective, but currently unpublished adaptive learning rate method. Amusingly, everyone who uses this method in their work currently cites slide 29 of Lecture 6 of Geoff Hinton's Coursera class. The RMSProp update adjusts the Adagrad method in a very simple way in an attempt to reduce its aggressive, monotonically decreasing learning rate. In particular, it uses a moving average of squared gradients instead, giving:

```
cache = decay_rate * cache + (1 - decay_rate) * dx**2
x += - learning_rate * dx / (np.sqrt(cache) + eps)
```

Here, `decay_rate` is a hyperparameter and typical values are [0.9, 0.99, 0.999]. Notice that the `x+=` update is identical to Adagrad, but the `cache` variable is a "leaky". Hence, RMSProp still modulates the learning rate of

each weight based on the magnitudes of its gradients, which has a beneficial equalizing effect, but unlike Adagrad the updates do not get monotonically smaller.

Adam. Adam is a recently proposed update that looks a bit like RMSProp with momentum. The (simplified) update looks as follows:

```
m = beta1*m + (1-beta1)*dx
v = beta2*v + (1-beta2)*(dx**2)
x += - learning_rate * m / (np.sqrt(v) + eps)
```

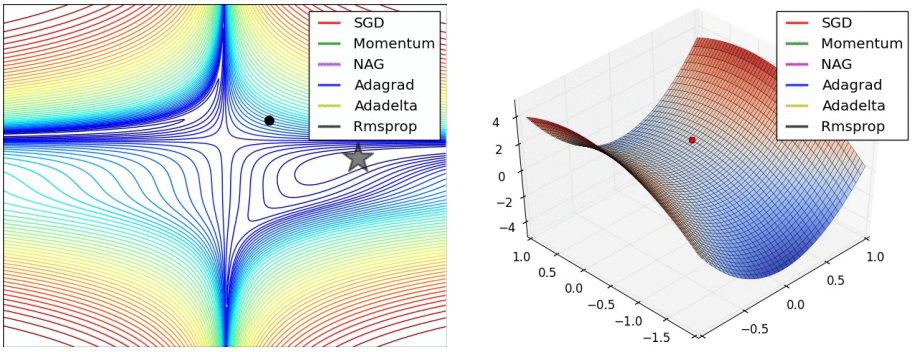
Notice that the update looks exactly as RMSProp update, except the "smooth" version of the gradient `m` is used instead of the raw (and perhaps noisy) gradient vector `dx`. Recommended values in the paper are `eps = 1e-8`, `beta1 = 0.9`, `beta2 = 0.999`. In practice Adam is currently recommended as the default algorithm to use, and often works slightly better than RMSProp. However, it is often also worth trying SGD+Nesterov Momentum as an alternative. The full Adam update also includes a *bias correction* mechanism, which compensates for the fact that in the first few time steps the vectors `m,v` are both initialized and therefore biased at zero, before they fully "warm up". With the *bias correction* mechanism, the update looks as follows:

```
# t is your iteration counter going from 1 to infinity
m = beta1*m + (1-beta1)*dx
mt = m / (1-beta1**t)
v = beta2*v + (1-beta2)*(dx**2)
vt = v / (1-beta2**t)
x += - learning_rate * mt / (np.sqrt(vt) + eps)
```

Note that the update is now a function of the iteration as well as the other parameters. We refer the reader to the paper for the details, or the course slides where this is expanded on.

Additional References:

- Unit Tests for Stochastic Optimization proposes a series of tests as a standardized benchmark for stochastic optimization.



Animations that may help your intuitions about the learning process dynamics. **Left:** Contours of a loss surface and time evolution of different optimization algorithms. Notice the "overshooting" behavior of momentum-based methods, which make the optimization look like a ball rolling down the hill. **Right:** A visualization of a saddle point in the optimization landscape, where the curvature along different dimension has different signs (one dimension curves up and another down). Notice that SGD has a very hard time breaking symmetry and gets stuck on the top. Conversely, algorithms such as RMSprop will see very low gradients in the saddle direction. Due to the denominator term in the RMSprop update, this will increase the effective learning rate along this direction, helping RMSProp proceed. Images credit: Alec Radford.

Hyperparameter Optimization

As we've seen, training Neural Networks can involve many hyperparameter settings. The most common hyperparameters in context of Neural Networks include:

- the initial learning rate
- learning rate decay schedule (such as the decay constant)
- regularization strength (L2 penalty, dropout strength)

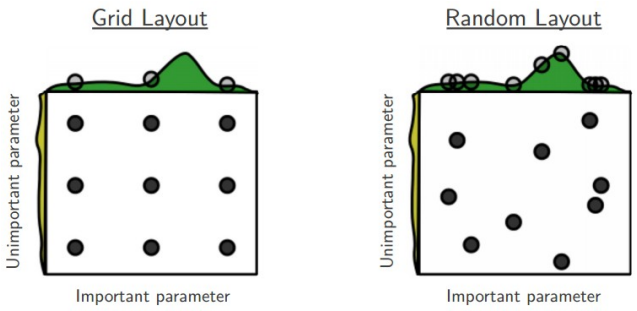
But as we saw, there are many more relatively less sensitive hyperparameters, for example in per-parameter adaptive learning methods, the setting of momentum and its schedule, etc. In this section we describe some additional tips and tricks for performing the hyperparameter search:

Implementation. Larger Neural Networks typically require a long time to train, so performing hyperparameter search can take many days/weeks. It is important to keep this in mind since it influences the design of your code base. One particular design is to have a **worker** that continuously samples random hyperparameters and performs the optimization. During the training, the worker will keep track of the validation performance after every epoch, and writes a model checkpoint (together with miscellaneous training statistics such as the loss over time) to a file, preferably on a shared file system. It is useful to include the validation performance directly in the filename, so that it is simple to inspect and sort the progress. Then there is a second program which we will call a **master**, which launches or kills workers across a computing cluster, and may additionally inspect the checkpoints written by workers and plot their training statistics, etc.

Prefer one validation fold to cross-validation. In most cases a single validation set of respectable size substantially simplifies the code base, without the need for cross-validation with multiple folds. You'll hear people say they "cross-validated" a parameter, but many times it is assumed that they still only used a single validation set.

Hyperparameter ranges. Search for hyperparameters on log scale. For example, a typical sampling of the learning rate would look as follows: `learning_rate = 10 ** uniform(-6, 1)`. That is, we are generating a random number from a uniform distribution, but then raising it to the power of 10. The same strategy should be used for the regularization strength. Intuitively, this is because learning rate and regularization strength have multiplicative effects on the training dynamics. For example, a fixed change of adding 0.01 to a learning rate has huge effects on the dynamics if the learning rate is 0.001, but nearly no effect if the learning rate when it is 10. This is because the learning rate multiplies the computed gradient in the update. Therefore, it is much more natural to consider a range of learning rate multiplied or divided by some value, than a range of learning rate added or subtracted to by some value. Some parameters (e.g. dropout) are instead usually searched in the original scale (e.g. `dropout = uniform(0,1)`).

Prefer random search to grid search. As argued by Bergstra and Bengio in Random Search for Hyper-Parameter Optimization, "randomly chosen trials are more efficient for hyper-parameter optimization than trials on a grid". As it turns out, this is also usually easier to implement.



Core illustration from Random Search for Hyper-Parameter Optimization by Bergstra and Bengio. It is very often the case that some of the hyperparameters matter much more than others (e.g. top hyperparam vs. left one in this figure). Performing random search rather than grid search allows you to much more precisely discover good values for the important ones.

Careful with best values on border. Sometimes it can happen that you're searching for a hyperparameter (e.g. learning rate) in a bad range. For example, suppose we use `learning_rate = 10 ** uniform(-6, 1)`. Once we receive the results, it is important to double check that the final learning rate is not at the edge of this interval, or otherwise you may be missing more optimal hyperparameter setting beyond the interval.

Stage your search from coarse to fine. In practice, it can be helpful to first search in coarse ranges (e.g. 10 ** [-6, 1]), and then depending on where the best results are turning up, narrow the range. Also, it can be helpful to perform the initial coarse search while only training for 1 epoch or even less, because many hyperparameter settings can lead the model to not learn at all, or immediately explode with infinite cost. The second stage could then perform a narrower search with 5 epochs, and the last stage could perform a detailed search in the final range for many more epochs (for example).

Bayesian Hyperparameter Optimization is a whole area of research devoted to coming up with algorithms that try to more efficiently navigate the space of hyperparameters. The core idea is to appropriately balance the exploration - exploitation trade-off when querying the performance at different hyperparameters. Multiple libraries have been developed based on these models as well, among some of the better known ones are Spearmint, SMAC, and Hyperopt. However, in practical settings with ConvNets it is still relatively difficult to beat random search in a carefully-chosen intervals. See some additional from-the-trenches discussion here.

Model Ensembles

In practice, one reliable approach to improving the performance of Neural Networks by a few percent is to train multiple independent models, and at test time average their predictions. As the number of models in the ensemble increases, the performance typically monotonically improves (though with diminishing returns). Moreover, the improvements are more dramatic with higher model variety in the ensemble. There are a few approaches to forming an ensemble:

- **Same model, different initializations**. Use cross-validation to determine the best hyperparameters, then train multiple models with the best set of hyperparameters but with different random initialization. The danger with this approach is that the variety is only due to initialization.
- **Top models discovered during cross-validation**. Use cross-validation to determine the best hyperparameters, then pick the top few (e.g. 10) models to form the ensemble. This improves the variety of the ensemble but has the danger of including suboptimal models. In practice, this can be easier to perform since it doesn't require additional retraining of models after cross-validation
- **Different checkpoints of a single model**. If training is very expensive, some people have had limited success in taking different checkpoints of a single network over time (for example after every epoch) and using those to form an ensemble. Clearly, this suffers from some lack of variety, but can still work reasonably well in practice. The advantage of this approach is that is very cheap.
- **Running average of parameters during training**. Related to the last point, a cheap way of almost always getting an extra percent or two of performance is to maintain a second copy of the network's weights in memory that maintains an exponentially decaying sum of previous weights during training. This way you're averaging the state of the network over last several iterations. You will find that this "smoothed" version of the weights over last few steps almost always achieves better validation error. The rough intuition to have in mind is that the objective is bowl-shaped and your network is jumping around the mode, so the average has a higher chance of being somewhere nearer the mode.

One disadvantage of model ensembles is that they take longer to evaluate on test example. An interested reader may find the recent work from Geoff Hinton on "Dark Knowledge" inspiring, where the idea is to "distill" a good ensemble back to a single model by incorporating the ensemble log likelihoods into a modified objective.