1. Why learning rates cannot be too big

To understand the role of the learning rate, it is useful to understand it in the context of the simplest possible problem first.

Suppose that we want to solve the scalar equation

$$\sigma w = y$$  \hspace{1cm} (1)

where we know that $\sigma > 0$. We proceed with an initial condition $w_0 = 0$ by using gradient descent to minimize the squared loss

$$L(w) = (y - \sigma w)^2$$  \hspace{1cm} (2)

which has a derivative with respect to the parameter $w$ of $-2\sigma(y - \sigma w)$.

Gradient descent with a learning rate of $\eta$ follows the recurrence-relation or discrete-time state evolution of:

$$w_{t+1} = w_t + 2\eta\sigma(y - \sigma w_t)$$

$$= (1 - 2\eta\sigma^2)w_t + 2\eta\sigma y.$$  \hspace{1cm} (3)

(a) For what values of learning rate $\eta > 0$ is the recurrence (3) stable?

(HINT: Remember the role of the unit circle in determining the stability or instability of such recurrences. If you keep taking higher and higher positive integer powers of a number, what does that number have to be like for this to converge?)

Solution: We can rewrite the update rule as

$$w_{t+1} - \frac{y}{\sigma} = (1 - 2\eta\sigma^2)(w_t - \frac{y}{\sigma})$$

$$w_{t+1} = \frac{y}{\sigma} + (1 - 2\eta\sigma^2)^{t+1}(w_0 - \frac{y}{\sigma})$$  \hspace{1cm} (4)

To make the recurrence (3) stable with $\eta > 0$, we need $|1 - 2\eta\sigma^2| < 1$. This gives $\eta < \frac{1}{\sigma^2}$.

(b) The previous part gives you an upper bound for the learning rate $\eta$ that depends on $\sigma$ beyond which we cannot safely go. If $\eta$ is below that upper bound, how fast does $w_t$ converge to its final solution $w^* = \frac{y}{\sigma}$? i.e. If we wanted to get within a factor $(1 - \epsilon)$ of $w^*$, how many iterations $t$ would we need?

Solution:

$$|w_T - w^*| < \epsilon|w^*|$$  \hspace{1cm} (5)

Use the derived update rule in (4). We have
\[ |w_T - \frac{y}{\sigma}| < \epsilon \frac{y}{\sigma} \]
\[ |(1 - 2\eta \sigma^2)^T| < \epsilon \]
\[ T > \frac{\log(\epsilon)}{\log(|1 - 2\eta \sigma^2|)}, \] (6)

(c) Suppose that we now have a vector problem where we have two parameters \( w[1], w[2] \). One with a large \( \sigma_\ell \) and the other with a tiny \( \sigma_s \), i.e. \( \sigma_\ell \gg \sigma_s \) and we have the vector equation we want to solve:
\[
\begin{bmatrix}
\sigma_\ell & 0 \\
0 & \sigma_s
\end{bmatrix}
\begin{bmatrix}
w[1] \\
w[2]
\end{bmatrix}
= 
\begin{bmatrix}
y[1] \\
y[2]
\end{bmatrix}.
\] (7)

We use gradient descent with a single learning rate \( \eta \) to solve this problem starting from an initial condition of \( w = 0 \).

For what learning rates \( \eta > 0 \) will we converge? Which of the two \( \sigma_i \) is limiting our learning rate?

**Solution:** Similarly, we can rewrite the loss function and update rule w.r.t the vector form.
\[
L(w) = ||y - \Sigma w||^2, \Sigma = \begin{bmatrix}
\sigma_\ell & 0 \\
0 & \sigma_s
\end{bmatrix}
\]
\[
\nabla_w L(w) = 2(\Sigma^2 w - \Sigma y)
\]
\[
w_{t+1} = (I - 2\eta \Sigma^2)w_t + 2\eta \Sigma y
\] (8)

To ensure the convergence, we need
\[
\begin{cases}
|1 - 2\eta \sigma_\ell^2| < 1 \\
|1 - 2\eta \sigma_s^2| < 1
\end{cases}
\]
\[
\eta < \min\left(\frac{1}{\sigma_\ell^2}, \frac{1}{\sigma_s^2}\right) = \frac{1}{\sigma_\ell^2}
\] (9)

(d) For the previous problem, depending on \( \eta, \sigma_\ell, \sigma_s \), which of the two dimensions is converging faster and which is converging slower?

**Solution:** We can rewrite the update rule w.r.t each dimension, this gives
\[
w[1]_t = \frac{y[1]}{\sigma_\ell} + (1 - 2\eta \sigma_\ell^2)^t\left(-\frac{y[1]}{\sigma_\ell}\right)
\]
\[
w[2]_t = \frac{y[2]}{\sigma_s} + (1 - 2\eta \sigma_s^2)^t\left(-\frac{y[2]}{\sigma_s}\right)
\]

This faster convergence dimension is \( \max(|1 - 2\eta \sigma_\ell^2|, |1 - 2\eta \sigma_s^2|) \)

(e) The speed of convergence overall will be dominated by the slower of the two. For what value of \( \eta \) will we get the fastest overall convergence to the solution?

**Solution:** \( \eta = \frac{1}{\sigma_\ell^2 + \sigma_s^2} \)
(f) Comment on what would happen if we had more parallel problems with \( \sigma_i \) that all were in between \( \sigma_\ell \) and \( \sigma_s \)? Would they influence the choice of possible learning rates or the learning rate with the fastest convergence?

(g) Using what you know about the SVD, how is the simple scalar and parallel scalar problem analysis above relevant to solving general least-squares problems of the form \( Xw \approx y \) using gradient descent?

2. ReLU with different Optimizers

Work through the notebook to explore how a simple network with ReLU non-linearities adapts to model a function using different optimizers. Training the networks takes 5-10 minutes depending on whether you run locally or the server, so you should start the training process (run through the train all layers cell) then return to the theory part of the discussion while training occurs.

Contributors:

- Anant Sahai.
- Sheng Shen.
- Kumar Krishna Agrawal.