COMS 4995 Lecture 4: Optimization

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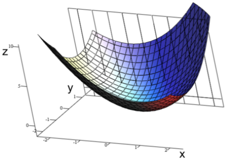
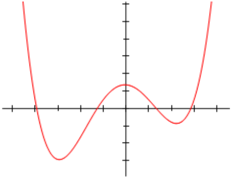
Overview

- We've talked a lot about how to compute gradients, and different neural models.
- How do we actually train those models using gradients?
- Today's lecture: various things that can go wrong in gradient descent, and what to do about them, e.g., How to tune the learning rates?
- For convenience in this part, let's group all the parameters (weights and biases) of our network into a single vector $\boldsymbol{\theta}$.

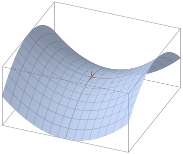
Features of the Optimization Landscape



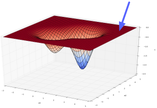
convex functions



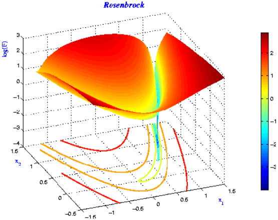
local minima



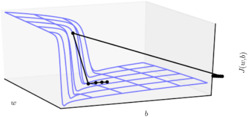
saddle points



plateaux



narrow ravines



cliffs (covered in a later lecture)

Review: Hessian Matrix

- The Hessian matrix, denoted $\mathbf{H}$, or $\nabla^2 \mathcal{J}$ is the matrix of second derivatives:

$$\mathbf{H} = \nabla^2 \mathcal{J} = \begin{pmatrix} \frac{\partial^2 \mathcal{J}}{\partial \theta_1^2} & \frac{\partial^2 \mathcal{J}}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 \mathcal{J}}{\partial \theta_1 \partial \theta_D} \\ \frac{\partial^2 \mathcal{J}}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 \mathcal{J}}{\partial \theta_2^2} & \cdots & \frac{\partial^2 \mathcal{J}}{\partial \theta_2 \partial \theta_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 \mathcal{J}}{\partial \theta_D \partial \theta_1} & \frac{\partial^2 \mathcal{J}}{\partial \theta_D \partial \theta_2} & \cdots & \frac{\partial^2 \mathcal{J}}{\partial \theta_D^2} \end{pmatrix}$$

- It's a symmetric matrix because $\frac{\partial^2 \mathcal{J}}{\partial \theta_i \partial \theta_j} = \frac{\partial^2 \mathcal{J}}{\partial \theta_j \partial \theta_i}$.

Review: Hessian Matrix

- Locally, a function can be approximated by its second-order Taylor approximation around a point $\boldsymbol{\theta}_0$:

$$\mathcal{J}(\boldsymbol{\theta}) \approx \mathcal{J}(\boldsymbol{\theta}_0) + \nabla \mathcal{J}(\boldsymbol{\theta}_0)^\top (\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{H}(\boldsymbol{\theta}_0)(\boldsymbol{\theta} - \boldsymbol{\theta}_0).$$

- A critical point is a point where the gradient is zero. In that case,

$$\mathcal{J}(\boldsymbol{\theta}) \approx \mathcal{J}(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{H}(\boldsymbol{\theta}_0)(\boldsymbol{\theta} - \boldsymbol{\theta}_0).$$

Review: Hessian Matrix

- Why the Hessian? A lot of important features of the optimization landscape can be characterized by the eigenvalues of the Hessian $\mathbf{H}$.
- Recall that a symmetric matrix (such as $\mathbf{H}$) has only real eigenvalues, and there is an orthogonal basis of eigenvectors.
- This can be expressed in terms of the spectral decomposition:

$$\mathbf{H} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\top,$$

where $\mathbf{Q}$ is an orthogonal matrix (whose columns are the eigenvectors) and $\boldsymbol{\Lambda}$ is a diagonal matrix (whose diagonal entries are the eigenvalues).

Review: Hessian Matrix

- We often refer to **H** as the curvature of a function.
- Suppose you move along a line defined by $\boldsymbol{\theta} + t\mathbf{v}$ for some vector **v**.
- Second-order Taylor approximation:

$$\mathcal{J}(\boldsymbol{\theta} + t\mathbf{v}) \approx \mathcal{J}(\boldsymbol{\theta}) + t\nabla\mathcal{J}(\boldsymbol{\theta})^\top\mathbf{v} + \frac{t^2}{2}\mathbf{v}^\top\mathbf{H}(\boldsymbol{\theta})\mathbf{v}$$

- Hence, in a direction where $\mathbf{v}^\top\mathbf{H}\mathbf{v} > 0$, the cost function curves upwards, i.e. has positive curvature. Where $\mathbf{v}^\top\mathbf{H}\mathbf{v} < 0$, it has negative curvature.

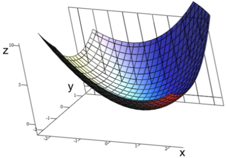
Review: Hessian Matrix

- A matrix $\mathbf{A}$ is positive definite if $\mathbf{v}^\top \mathbf{A} \mathbf{v} > 0$ for all $\mathbf{v} \neq 0$. (I.e., it curves upwards in all directions.)
  - It is positive semidefinite (PSD) if $\mathbf{v}^\top \mathbf{A} \mathbf{v} \geq 0$ for all $\mathbf{v} \neq 0$.
- Equivalently: a matrix is positive definite iff all its eigenvalues are positive. It is PSD iff all its eigenvalues are nonnegative. (Exercise: show this using the Spectral Decomposition.)
- For any critical point $\boldsymbol{\theta}_*$, if $\mathbf{H}(\boldsymbol{\theta}_*)$ exists and is positive definite, then $\boldsymbol{\theta}_*$ is a local minimum (since all directions curve upwards).

Convex Functions

- Recall: a set $\mathcal{S}$ is convex if for any $\mathbf{x}_0, \mathbf{x}_1 \in \mathcal{S}$,

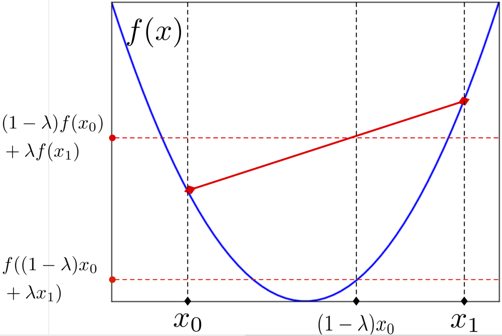
$$(1-\lambda)\mathbf{x}_0 + \lambda\mathbf{x}_1 \in \mathcal{S} \quad \text{for } 0 \leq \lambda \leq 1.$$



- A function f is convex if for any $\mathbf{x}_0, \mathbf{x}_1$,

$$f((1-\lambda)\mathbf{x}_0 + \lambda\mathbf{x}_1) \leq (1-\lambda)f(\mathbf{x}_0) + \lambda f(\mathbf{x}_1)$$

- Equivalently, the set of points lying above the graph of f is convex.
- Intuitively: the function is bowl-shaped.

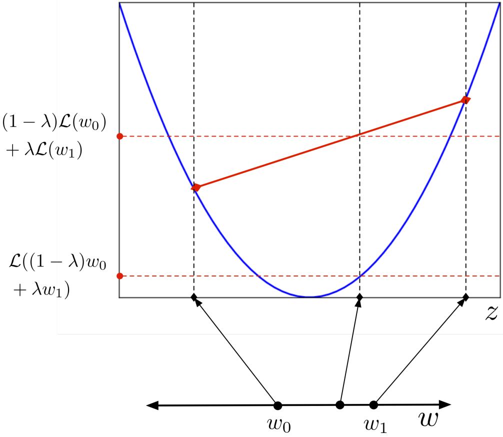


Convex Functions

- If $\mathcal{J}$ is smooth (more precisely, twice differentiable), there's an equivalent characterization in terms of $\mathbf{H}$:
  - A smooth function is convex iff its Hessian is positive semidefinite everywhere.
  - **Special case:** a univariate function is convex iff its second derivative is nonnegative everywhere.
- **Exercise:** show that squared error, logistic-cross-entropy, and softmax-cross-entropy losses are convex (as a function of the network outputs) by taking second derivatives.

Convex Functions

- For a linear model, $z = \mathbf{w}^\top \mathbf{x} + b$ is a linear function of $\mathbf{w}$ and b. If the loss function is convex as a function of z, then it is convex as a function of $\mathbf{w}$ and b.
- Hence, linear regression, logistic regression, and softmax regression are convex.

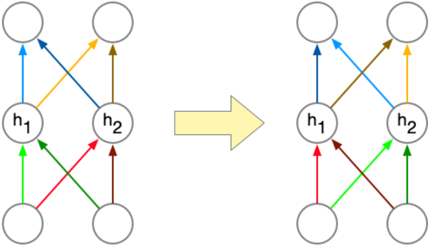


Local Minima

- If a function is convex, it has no spurious local minima, i.e. any local minimum is also a global minimum.
- This is very convenient for optimization since if we keep going downhill, we'll eventually reach a global minimum.

Local Minima

- If a function is convex, it has no spurious local minima, i.e. any local minimum is also a global minimum.
- This is very convenient for optimization since if we keep going downhill, we'll eventually reach a global minimum.
- Unfortunately, training a network with hidden units cannot be convex because of permutation symmetries.
  - I.e., we can re-order the hidden units in a way that preserves the function computed by the network.



Local Minima

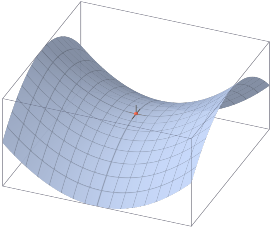
Special case: a univariate function is convex iff its second derivative is nonnegative everywhere.

- By definition, if a function $\mathcal{J}$ is convex, then for any set of points $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_N$ in its domain,

$$\mathcal{J}(\lambda_1 \boldsymbol{\theta}_1 + \cdots + \lambda_N \boldsymbol{\theta}_N) \leq \lambda_1 \mathcal{J}(\boldsymbol{\theta}_1) + \cdots + \lambda_N \mathcal{J}(\boldsymbol{\theta}_N) \quad \text{for } \lambda_i \geq 0, \sum_i \lambda_i = 1.$$

- Because of permutation symmetry, there are $K!$ permutations of the hidden units in a given layer which all compute the same function.
- Suppose we average the parameters for all $K!$ permutations. Then we get a degenerate network where all the hidden units are identical.
- If the cost function were convex, this solution would have to be better than the original one, which is ridiculous!
- Hence, training multilayer neural nets is non-convex.

Saddle points

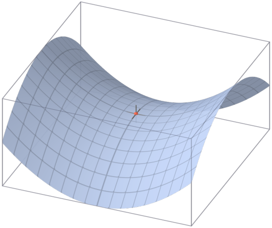


A saddle point is a point where:

- $\nabla \mathcal{J}(\boldsymbol{\theta}) = \mathbf{0}$
- $\mathbf{H}(\boldsymbol{\theta})$ has some positive and some negative eigenvalues, i.e. some directions with positive curvature and some with negative curvature.

When would saddle points be a problem?

Saddle points



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- $\mathbf{H}(\boldsymbol{\theta})$ has some positive and some negative eigenvalues, i.e. some directions with positive curvature and some with negative curvature.

When would saddle points be a problem?

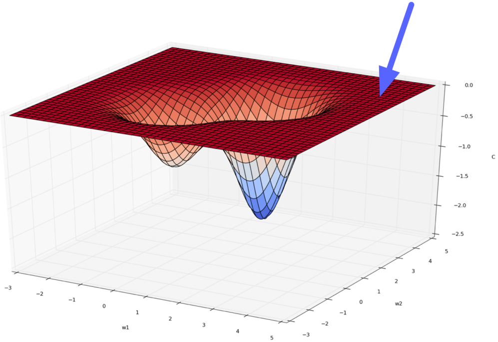
- If we're exactly on the saddle point, then we're stuck.
- If we're slightly to the side, then we can get unstuck.

Saddle points

- Suppose you have two hidden units with identical incoming and outgoing weights.
- After a gradient descent update, they will still have identical weights. By induction, they'll always remain identical.
- But if you perturbed them slightly, they can start to move apart.
- Important special case: don't initialize all your weights to zero!
  - Instead, break the symmetry by using small random values.

Plateaux

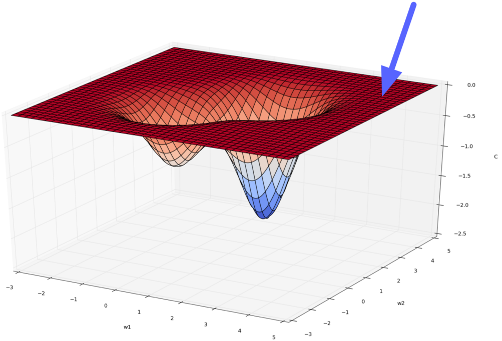
A flat region is called a plateau. (Plural: plateaux)



Can you think of examples?

Plateaux

A flat region is called a plateau. (Plural: plateaux)



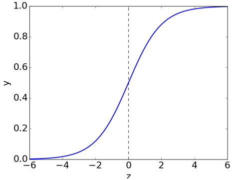
Can you think of examples?

- 0–1 loss
- hard threshold activations
- logistic activations & least squares

Plateaux

- An important example of a plateau is a saturated unit. This is when it is in the flat region of its activation function. Recall the backprop equation for the weight derivative:

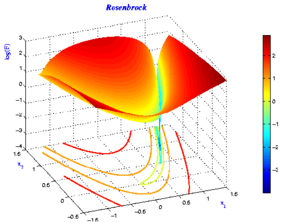
$$\begin{aligned} \overline{z_i} &= \overline{h_i}\,\phi'(z) \\ \overline{w_{ij}} &= \overline{z_i}\,x_j \end{aligned}$$

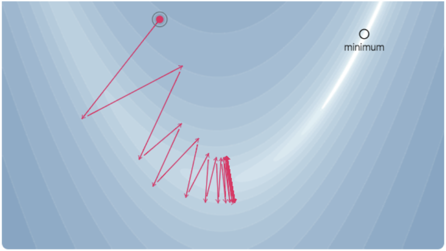


- If $\phi'(z_i)$ is always close to zero, then the weights will get stuck.
- If there is a ReLU unit whose input z_i is always negative, the weight derivatives will be *exactly* 0. We call this a dead unit.

Ill-conditioned curvature

Long, narrow ravines:





- Suppose **H** has some large positive eigenvalues (i.e. high-curvature directions) and some eigenvalues close to 0 (i.e. low-curvature directions).
- Gradient descent bounces back and forth in high curvature directions and makes slow progress in low curvature directions.
  - To interpret this visually: the gradient is perpendicular to the contours.
- This is known as ill-conditioned curvature. It's very common in neural net training.

Ill-conditioned curvature: gradient descent dynamics

- To understand why ill-conditioned curvature is a problem, consider a convex quadratic objective

  $$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\theta}^\top \mathbf{A}\boldsymbol{\theta},$$

  where **A** is PSD.
- Gradient descent update:

  $$\begin{aligned}\boldsymbol{\theta}_{k+1} &\leftarrow \boldsymbol{\theta}_k - \alpha \nabla \mathcal{J}(\boldsymbol{\theta}_k) \\ &= \boldsymbol{\theta}_k - \alpha \mathbf{A}\boldsymbol{\theta}_k \\ &= (\mathbf{I} - \alpha \mathbf{A})\boldsymbol{\theta}_k\end{aligned}$$

- Solving the recurrence,

  $$\boldsymbol{\theta}_k = (\mathbf{I} - \alpha \mathbf{A})^k \boldsymbol{\theta}_0$$

Ill-conditioned curvature: gradient descent dynamics

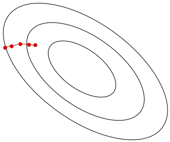
- We can analyze matrix powers such as $(\mathbf{I} - \alpha \mathbf{A})^k \boldsymbol{\theta}_0$ using the spectral decomposition.
- Let $\mathbf{A} = \mathbf{Q} \boldsymbol{\Lambda} \mathbf{Q}^\top$ be the spectral decomposition of $\mathbf{A}$.

$$\begin{aligned}(\mathbf{I} - \alpha \mathbf{A})^k \boldsymbol{\theta}_0 &= (\mathbf{I} - \alpha \mathbf{Q} \boldsymbol{\Lambda} \mathbf{Q}^\top)^k \boldsymbol{\theta}_0 \\ &= [\mathbf{Q}(\mathbf{I} - \alpha \boldsymbol{\Lambda}) \mathbf{Q}^\top]^k \boldsymbol{\theta}_0 \\ &= \mathbf{Q}(\mathbf{I} - \alpha \boldsymbol{\Lambda})^k \mathbf{Q}^\top \boldsymbol{\theta}_0\end{aligned}$$

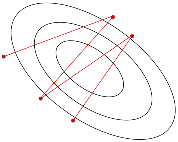
- Hence, in the $\mathbf{Q}$ basis, each coordinate gets multiplied by $(1 - \alpha \lambda_i)^k$, where the λ_i are the eigenvalues of $\mathbf{A}$.
- Cases:
  - $0 < \alpha \lambda_i \leq 1$: decays to 0 at a rate that depends on $\alpha \lambda_i$
  - $1 < \alpha \lambda_i \leq 2$: oscillates
  - $\alpha \lambda_i > 2$: unstable (diverges)

Learning Rate

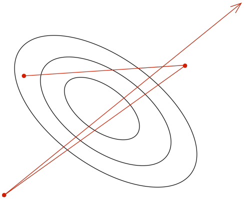
- How can spectral decomposition help?
- The learning rate α is a hyperparameter we need to tune. Here are the things that can go wrong in batch mode:



α too small: slow progress



α too large: oscillations



α much too large: instability

Ill-conditioned curvature: gradient descent dynamics

- Just showed
  - $0 < \alpha\lambda_i \leq 1$: decays to 0 at a rate that depends on $\alpha\lambda_i$
  - $1 < \alpha\lambda_i \leq 2$: oscillates
  - $\alpha\lambda_i > 2$: unstable (diverges)
- Hence, we need to set the learning rate $\alpha < 2/\lambda_{\max}$ to prevent instability, where $\lambda_{\max}$ is the largest eigenvalue, i.e. maximum curvature.
- This bounds the rate of progress in another direction:

$$\alpha\lambda_i < \frac{2\lambda_i}{\lambda_{\max}}.$$

- The quantity $\lambda_{\max}/\lambda_{\min}$ is known as the condition number of **A**. Larger condition numbers imply slower convergence of gradient descent.

Ill-conditioned curvature: gradient descent dynamics

- The analysis we just did was for a quadratic toy problem

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\theta}^\top \mathbf{A}\boldsymbol{\theta}.$$

- It can be easily generalized to a quadratic not centered at zero, since the gradient descent dynamics are invariant to translation.

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\theta}^\top \mathbf{A}\boldsymbol{\theta} + \mathbf{b}^\top \boldsymbol{\theta} + c$$

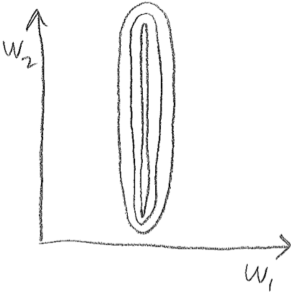
- Since a smooth cost function is well approximated by a convex quadratic (i.e. second-order Taylor approximation) in the vicinity of a (local) optimum, this analysis is a good description of the behavior of gradient descent near a (local) optimum.
- If the Hessian is ill-conditioned, then gradient descent makes slow progress towards the optimum.

Ill-conditioned curvature: normalization

- Suppose we have the following dataset for linear regression.

x_1	x_2	t
114.8	0.00323	5.1
338.1	0.00183	3.2
98.8	0.00279	4.1
⋮	⋮	⋮

$$\overline{w_i} = \overline{y}\, x_i$$

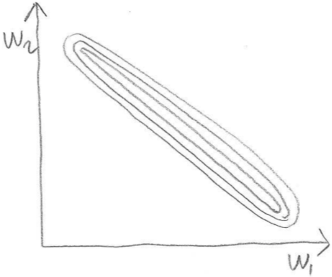


- Which weight, w_1 or w_2, will receive a larger gradient descent update?
- Which one do you want to receive a larger update?
- Note: the figure vastly *understates* the narrowness of the ravine!

Ill-conditioned curvature: normalization

- Or consider the following dataset:

x_1	x_2	t
1003.2	1005.1	3.3
1001.1	1008.2	4.8
998.3	1003.4	2.9
⋮	⋮	⋮



Ill-conditioned curvature: normalization

- To avoid these problems, it's a good idea to center your inputs to zero mean and unit variance, especially when they're in arbitrary units (feet, seconds, etc.).

$$\tilde{x}_j = \frac{x_j - \mu_j}{\sigma_j}$$

- Hidden units may have non-centered activations, and this is harder to deal with.
  - One trick: replace logistic units (which range from 0 to 1) with tanh units (which range from -1 to 1)
  - A recent method called batch normalization explicitly centers each hidden activation. It often speeds up training by 1.5-2x, and it's available in all the major neural net frameworks.

Momentum

- Unfortunately, even with these normalization tricks, ill-conditioned curvature is a fact of life. We need algorithms that are able to deal with it.
- Momentum is a simple and highly effective method. Imagine a hockey puck on a frictionless surface (representing the cost function). It will accumulate momentum in the downhill direction:

$$\mathbf{p} \leftarrow \mu \mathbf{p} - \alpha \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mathbf{p}$$

- α is the learning rate, just like in gradient descent.
- μ is a damping parameter. It should be slightly less than 1 (e.g. 0.9 or 0.99). Why not exactly 1?

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- α is the learning rate, just like in gradient descent.
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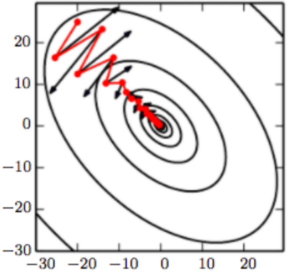
  - If $\mu = 1$, conservation of energy implies it will never settle down.

Momentum



- In the high curvature directions, the gradients cancel each other out, so momentum dampens the oscillations.
- In the low curvature directions, the gradients point in the same direction, allowing the parameters to pick up speed.
- If the gradient is constant (i.e. the cost surface is a plane), the parameters will reach a terminal velocity of

$$-\frac{\alpha}{1-\mu} \cdot \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}$$

  This suggests if you increase μ, you should lower α to compensate.
- Momentum sometimes helps a lot, and almost never hurts.

Ravines

- Even with momentum and normalization tricks, narrow ravines are still one of the biggest obstacles in optimizing neural networks.
- Empirically, the curvature can be many orders of magnitude larger in some directions than others!
- An area of research known as second-order optimization develops algorithms which explicitly use curvature information (second derivatives), but these are complicated and difficult to scale to large neural nets and large datasets.
- There is an optimization procedure called Adam which uses just a little bit of curvature information and often works much better than gradient descent. It's available in all the major neural net frameworks.

RMSprop and Adam

- Recall: SGD takes large steps in directions of high curvature and small steps in directions of low curvature.
- RMSprop is a variant of SGD which rescales each coordinate of the gradient to have norm 1 on average. It does this by keeping an exponential moving average s_j of the squared gradients.
- The following update is applied to each coordinate j independently:

$$
\begin{aligned}
s_j &\leftarrow (1-\gamma)s_j + \gamma[\tfrac{\partial \mathcal{J}}{\partial \theta_j}]^2 \\
\theta_j &\leftarrow \theta_j - \frac{\alpha}{\sqrt{s_j + \epsilon}} \frac{\partial \mathcal{J}}{\partial \theta_j}
\end{aligned}
$$

- If the eigenvectors of the Hessian are axis-aligned (dubious assumption), then RMSprop can correct for the curvature. In practice, it typically works slightly better than SGD.
- Adam = RMSprop + momentum
- Both optimizers are included in TensorFlow, Pytorch, etc.

Recap

- We've seen how to analyze the typical phenomena in optimization:
  - Local minima: neural nets are not convex.
  - Saddle points: Hessian has both positive and negative eigenvalues. Occurs when there are weight symmetries upon initialization.
  - Plateaux: Jacobian close to zero, e.g., dead neurons.
  - Ill-conditioned cuvature (ravines): Hessian has extremely large and very small positive eigenvalues. Affects the largest possible learning rate before divergence.
- You will likely encounter some of these problems when training neural nets.
- This lecture helps understanding the causes of these phenomena. We will discuss the workarounds in a future lecture.