CSC421/2516 Lecture 3: Automatic Differentiation & Distributed Representations

Jimmy Ba

Autodiff

- Lecture 2 covered the algebraic view of backprop.
- Here, we'll see how to implement an automatic differentiation library:
  - build the computation graph
  - vector-Jacobian products (VJP) for primitive ops
  - the backwards pass
- We'll use Autograd, a lightweight autodiff tool, as an example. The implementations of PyTorch, TensorFlow, Jax, etc. are very similar.
  - You will probably never have to implement autodiff yourself but it is good to know its inner workings.

Confusing Terminology

- Automatic differentiation (autodiff) refers to a general way of taking a program which computes a value, and automatically constructing a procedure for computing derivatives of that value.
- Backpropagation is the special case of autodiff applied to neural nets
  - But in machine learning, we often use backprop synonymously with autodiff
- Autograd is the name of a particular autodiff library we will cover in this lecture. There are many others, e.g. PyTorch, TensorFlow.

What is Autodiff

- An autodiff system will convert the program into a sequence of primitive operations (ops) which have specified routines for computing derivatives.
- In this representation, backprop can be done in a completely mechanical way.

Original program:

$$z = wx + b$$
$$y = \frac{1}{1 + \exp(-z)}$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

Sequence of primitive operations:

$$t_1 = wx$$
$$z = t_1 + b$$
$$t_3 = -z$$
$$t_4 = \exp(t_3)$$
$$t_5 = 1 + t_4$$
$$y = 1/t_5$$
$$t_6 = y - t$$
$$t_7 = t_6^2$$
$$\mathcal{L} = t_7/2$$

What is Autodiff

```
import autograd.numpy as np
from autograd import grad

def sigmoid(x):
    return 0.5*(np.tanh(x) + 1)

def logistic_predictions(weights, inputs):
    # Outputs probability of a label being true according to logistic model.
    return sigmoid(np.dot(inputs, weights))

def training_loss(weights):
    # Training loss is the negative log-likelihood of the training labels.
    preds = logistic_predictions(weights, inputs)
    label_probabilities = preds * targets + (1 - preds) * (1 - targets)
    return -np.sum(np.log(label_probabilities))
```

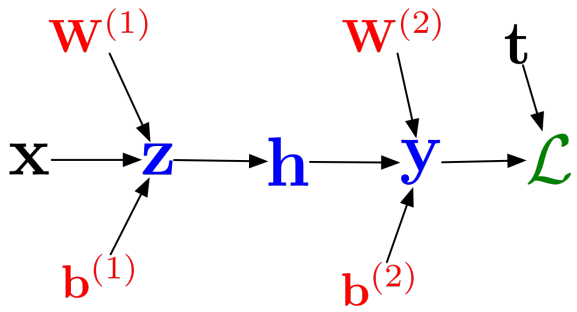
very sneaky!

… (load the data) …

```
# Define a function that returns gradients of training loss using Autograd.
training_gradient_fun = grad(training_loss)

# Optimize weights using gradient descent.
weights = np.array([0.0, 0.0, 0.0])
print "Initial loss:", training_loss(weights)
for i in xrange(100):
    weights -= training_gradient_fun(weights) * 0.01

print  "Trained loss:", training_loss(weights)
```

Autograd constructs a function for computing derivatives

Building the Computation Graph

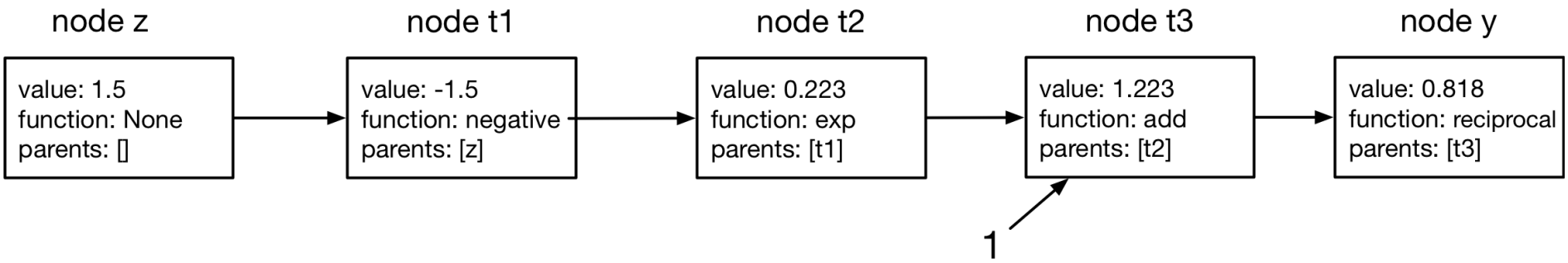


- Most autodiff systems, including Autograd, explicitly construct the computation graph.
  - Some frameworks like TensorFlow provide mini-languages for building computation graphs directly. Disadvantage: need to learn a totally new API.
  - Autograd instead builds them by tracing the forward pass computation, allowing for an interface nearly indistinguishable from NumPy.
- The `Node` class (defined in `tracer.py`) represents a node of the computation graph. It has attributes:
  - `value`, the actual value computed on a particular set of inputs
  - `fun`, the primitive operation defining the node
  - `args` and `kwargs`, the arguments the op was called with
  - `parents`, the parent `Node`s

Building the Computation Graph

- Autograd's fake NumPy module provides primitive ops which look and feel like NumPy functions, but secretly build the computation graph.
- Example:

```
def logistic(z):
    return 1. / (1. + np.exp(-z))

# that is equivalent to:
def logistic2(z):
    return np.reciprocal(np.add(1, np.exp(np.negative(z))))

z = 1.5
y = logistic(z)
```



Vector-Jacobian Products

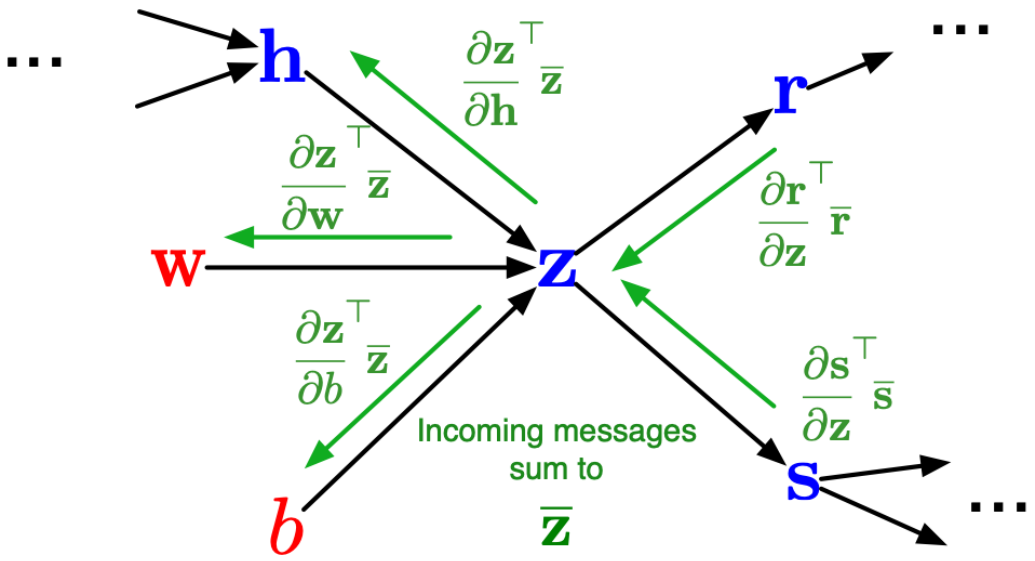
- For each primitive operation, we must specify VJPs for *each* of its arguments. Consider $y = \exp(x)$.
- This is a function which takes in the output gradient (i.e. $\bar{y}$), the answer (y), and the arguments (x), and returns the input gradient ($\bar{x}$)
- `defvjp` (defined in `core.py`) is a convenience routine for registering VJPs. It just adds them to a dict.
- Examples from `numpy/numpy_vjps.py`

```
defvjp(negative, lambda g, ans, x: -g)
defvjp(exp,      lambda g, ans, x: ans * g)
defvjp(log,      lambda g, ans, x: g / x)

defvjp(add,          lambda g, ans, x, y : g,
                     lambda g, ans, x, y : g)
defvjp(multiply,     lambda g, ans, x, y : y * g,
                     lambda g, ans, x, y : x * g)
defvjp(subtract,     lambda g, ans, x, y : g,
                     lambda g, ans, x, y : -g)
```

Backprop as Message Passing

Backprop as message passing:

- Each node receives a bunch of messages from its children, which it aggregates to get its error signal. It then passes messages to its parents.



- Each of these messages is a VJP.
- This formulation provides modularity: each node needs to know how to compute its outgoing messages, i.e. the VJPs corresponding to each of its parents (arguments to the function).
- The implementation of z doesn't need to know where $\bar{z}$ came from.

Backward Pass

- The backwards pass is defined in `core.py`.
- The argument `g` is the error signal for the end node; for us this is always $\overline{\mathcal{L}} = 1$.

```
def backward_pass(g, end_node):
    outgrads = {end_node: g}
    for node in toposort(end_node):
        outgrad = outgrads.pop(node)
        fun, value, args, kwargs, argnums = node.recipe
        for argnum, parent in zip(argnums, node.parents):
            vjp = primitive_vjps[fun][argnum]
            parent_grad = vjp(outgrad, value, *args, **kwargs)
            outgrads[parent] = add_outgrads(outgrads.get(parent), parent_grad)
    return outgrad

def add_outgrads(prev_g, g):
    if prev_g is None:
        return g
    return prev_g + g
```

Put Everything Together

- `grad` (in `differential_operators.py`) is just a wrapper around `make_vjp` (in `core.py`) which builds the computation graph and feeds it to `backward_pass`.
- `grad` itself is viewed as a VJP, if we treat $\overline{\mathcal{L}}$ as the 1×1 matrix with entry 1.

$$\frac{\partial \mathcal{L}}{\partial \mathrm{w}} = \frac{\partial \mathcal{L}}{\partial \mathrm{w}} \overline{\mathcal{L}}$$

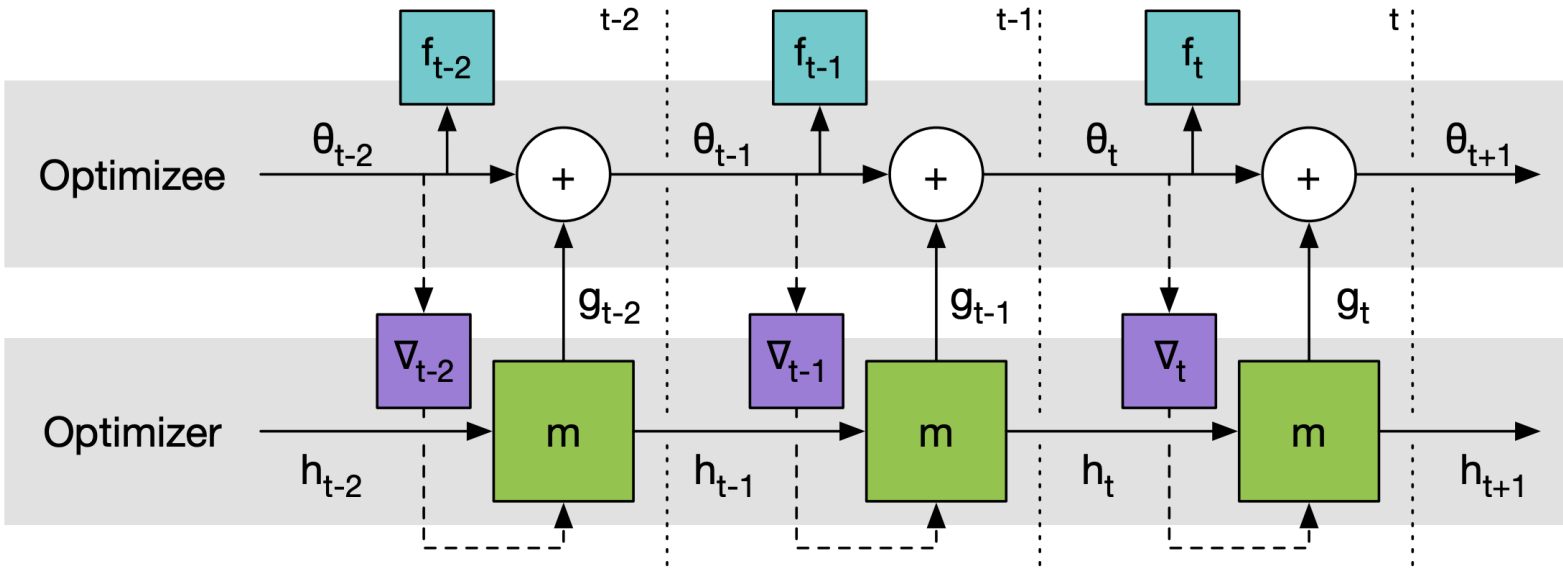
```
def make_vjp(fun, x):
    """Trace the computation to build the computation graph, and return
    a function which implements the backward pass."""
    start_node = Node.new_root()
    end_value, end_node = trace(start_node, fun, x)
    def vjp(g):
        return backward_pass(g, end_node)
    return vjp, end_value

def grad(fun, argnum=0):
    def gradfun(*args, **kwargs):
        unary_fun = lambda x: fun(*subval(args, argnum, x), **kwargs)
        vjp, ans = make_vjp(unary_fun, args[argnum])
        return vjp(np.ones_like(ans))
    return gradfun
```

Recap

- We saw three main parts to the code:
  - tracing the forward pass to build the computation graph
  - vector-Jacobian products for primitive ops
  - the backwards pass
- Building the computation graph requires fancy NumPy gymnastics, but other two items are basically what we have in the last two slides.
- You're encouraged to read the full code ($<$ 200 lines!) at:

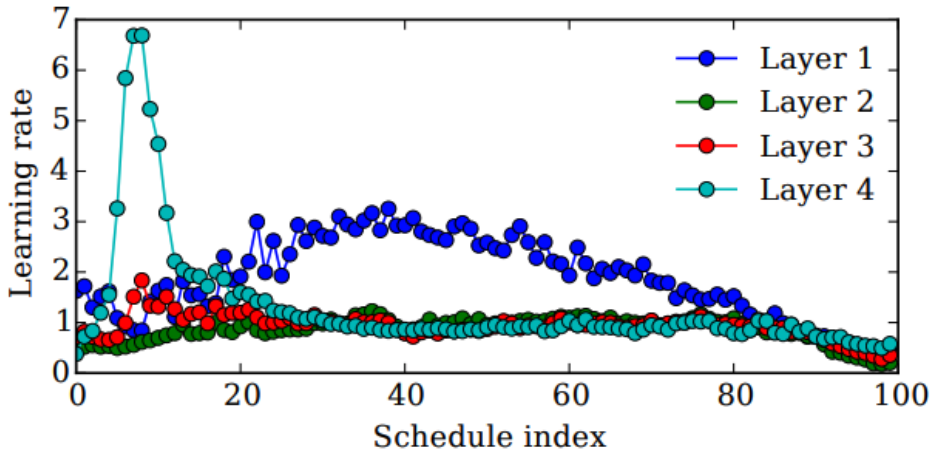
  `https://github.com/mattjj/autodidact/tree/master/autograd`

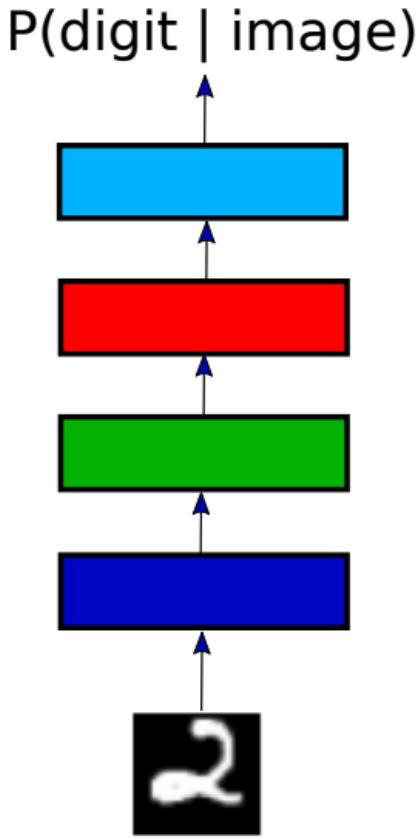
Autodiff Application: Learning to learning by gradient descent by gradient descent



https://arxiv.org/pdf/1606.04474.pdf

Autodiff Application: Gradient-Based Hyperparameter Optimization





https://arxiv.org/abs/1502.03492

After the break

After the break: **Distributed Representations**

Distributed Representations

- Let's now take a break from backpropagation and see a real example of a neural net to learn feature representations of words.
  - We'll see a lot more neural net architectures later in the course.
- We'll also introduce the models used in Programming Assignment 1.

Review: Probability and Bayes' Rule

Suppose we want to build a speech recognition system.

We'd like to be able to infer a likely sentence s given the observed speech signal a. The generative approach is to build two components:

- An observation model, represented as $p(\mathrm{a} \mid \mathrm{s})$, which tells us how likely the sentence s is to lead to the acoustic signal a.
- A prior, represented as $p(\mathrm{s})$, which tells us how likely a given sentence s is. E.g., it should know that "recognize speech" is more likely that "wreck a nice beach."

Given these components, we can use Bayes' Rule to infer a posterior distribution over sentences given the speech signal:

$$p(\mathrm{s} \mid \mathrm{a}) = \frac{p(\mathrm{s})p(\mathrm{a} \mid \mathrm{s})}{\sum_{\mathrm{s}'} p(\mathrm{s}')p(\mathrm{a} \mid \mathrm{s}')}.$$

Language Modeling

From here on, we will focus on learning a good distribution $p(\mathrm{s})$ of sentences. This problem is known as language modeling.

Assume we have a corpus of sentences $\mathrm{s}^{(1)}, \ldots, \mathrm{s}^{(N)}$. The maximum likelihood criterion says we want our model to maximize the probability our model assigns to the observed sentences. We assume the sentences are independent, so that their probabilities multiply.

$$\max \prod_{i=1}^{N} p(\mathrm{s}^{(i)}).$$

Language Modeling

In maximum likelihood training, we want to maximize $\prod_{i=1}^{N} p(\mathrm{s}^{(i)})$.

The probability of generating the whole training corpus is vanishingly small — like monkeys typing all of Shakespeare.

- The log probability is something we can work with more easily. It also conveniently decomposes as a sum:

$$\log \prod_{i=1}^{N} p(\mathrm{s}^{(i)}) = \sum_{i=1}^{N} \log p(\mathrm{s}^{(i)}).$$

- This is equivalent to the cross-entropy loss.

Language Modeling

- Probability of a sentence? What does that even mean?
  - A sentence is a sequence of words $w_1, w_2, \ldots, w_T$. Using the chain rule of conditional probability, we can decompose the probability as

$$p(\text{s}) = p(w_1, \ldots, w_T) = p(w_1)p(w_2 \mid w_1) \cdots p(w_T \mid w_1, \ldots, w_{T-1}).$$

  - Therefore, the language modeling problem is equivalent to being able to predict the next word!
- We typically make a Markov assumption, i.e. that the distribution over the next word only depends on the preceding few words. I.e., if we use a context of length 3,

$$p(w_t \mid w_1, \ldots, w_{t-1}) = p(w_t \mid w_{t-3}, w_{t-2}, w_{t-1}).$$

  - Such a model is called memoryless.
  - Now it's basically a supervised prediction problem. We need to predict the conditional distribution of each word given the previous K.
  - When we decompose it into separate prediction problems this way, it's called an autoregressive model.

N-Gram Language Models

- One sort of Markov model we can learn uses a conditional probability table, i.e.

	cat	and	city	$\cdots$
the fat	0.21	0.003	0.01	
four score	0.0001	0.55	0.0001	$\cdots$
New York	0.002	0.0001	0.48	
$\vdots$		$\vdots$		

- Maybe the simplest way to estimate the probabilities is from the empirical distribution:

$$p(w_3 = \text{cat} \mid w_1 = \text{the}, w_2 = \text{fat}) = \frac{p(w_1 = \text{the}, w_2 = \text{fat}, w_3 = \text{cat})}{p(w_1 = \text{the}, w_2 = \text{fat})} \approx \frac{\text{count}(\text{the fat cat})}{\text{count}(\text{the fat})}$$

- The phrases we're counting are called n-grams (where n is the length), so this is an n-gram language model.
  - So, the above example is considered a 3-gram model.

N-Gram Language Models

- Problems with n-gram language models
  - The number of entries in the conditional probability table is exponential in the context length.
  - Data sparsity: most n-grams never appear in the corpus, even if they are possible.
- Traditional ways to deal with data sparsity

N-Gram Language Models

- Problems with n-gram language models
  - The number of entries in the conditional probability table is exponential in the context length.
  - Data sparsity: most n-grams never appear in the corpus, even if they are possible.
- Traditional ways to deal with data sparsity
  - Use a short context (but this means the model is less powerful)
  - Smooth the probabilities, e.g. by adding imaginary counts
  - Make predictions using an ensemble of n-gram models with different n

Distributed Representations

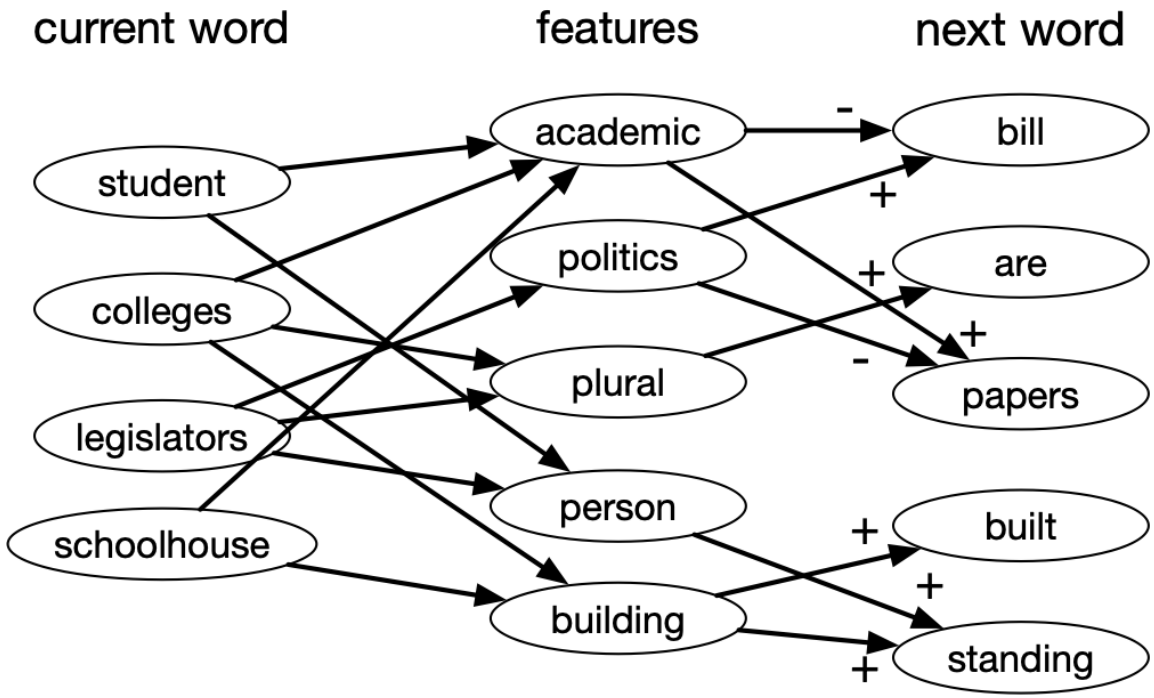
- Conditional probability tables are a kind of localist representation: all the information about a particular word is stored in one place, i.e. a column of the table.
- But different words are related, so we ought to be able to **share** information between them. For instance, consider this matrix of word attributes:

	academic	**politics**	**plural**	**person**	**building**
students	1	0	1	1	0
colleges	1	0	1	0	1
legislators	0	1	1	1	0
schoolhouse	1	0	0	0	1

- And this matrix of how each attribute influences the next word:

	bill	**is**	**are**	**papers**	**built**	**standing**
academic	$-$			$+$		
politics	$+$			$-$		
plural		$-$	$+$			
person						$+$
building					$+$	$+$

- Imagine these matrices are layers in an MLP. (One-hot representations of words, softmax over next word.)



- Here, the information about a given word is distributed throughout the representation. We call this a distributed representation.
- In general, when we train an MLP with backprop, the hidden units won't have intuitive meanings like in this cartoon. But this is a useful intuition pump for what MLPs can represent.

Distributed Representations

- We would like to be able to share information between related words. E.g., suppose we've seen the sentence
  The cat got squashed in the garden on Friday.
- This should help us predict the previously unseen words
  The dog got flattened in the yard on Monday.
- An n-gram model can't generalize this way, but a distributed representation might let us do so.

Neural Language Model

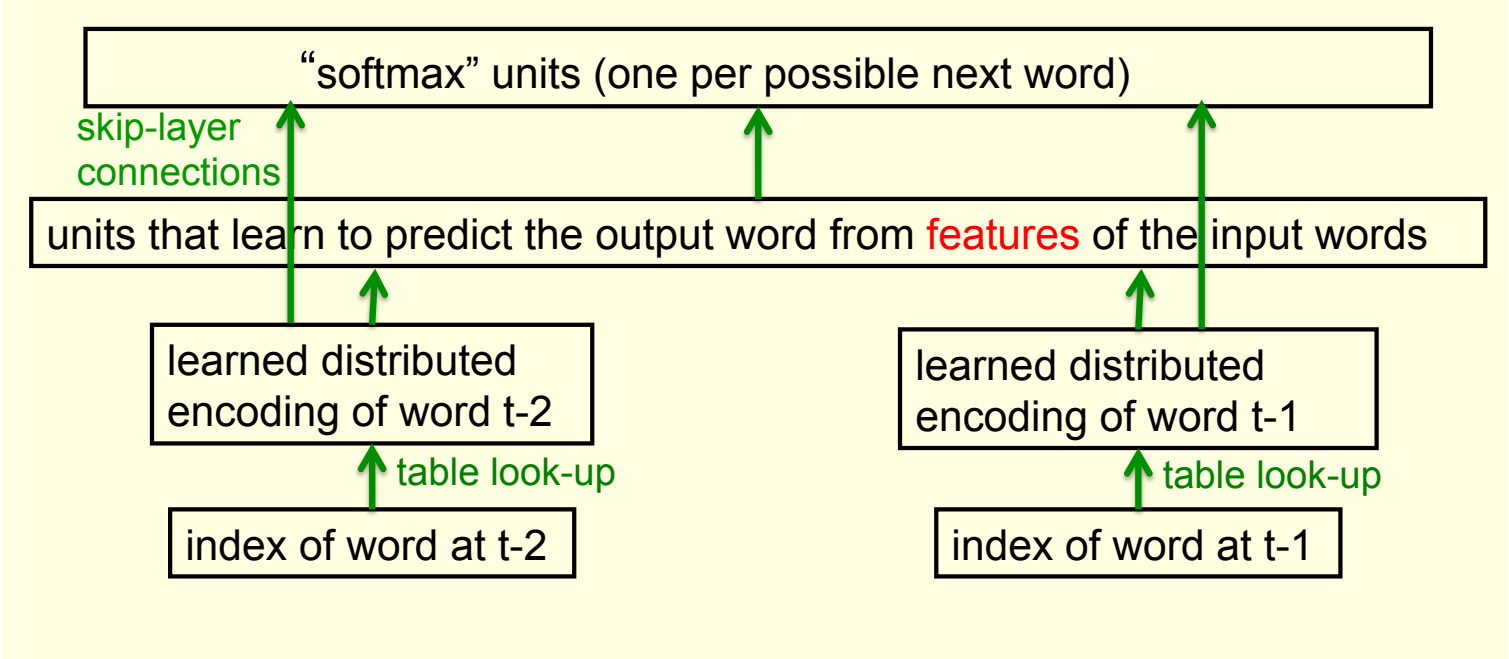
- Predicting the distribution of the next word given the previous K is just a multiway classification problem.
- **Inputs:** previous K words
- **Target:** next word
- **Loss:** cross-entropy. Recall that this is equivalent to maximum likelihood:

$$\begin{aligned} -\log p(\mathrm{s}) &= -\log \prod_{t=1}^{T} p(w_t \mid w_1, \ldots, w_{t-1}) \\ &= -\sum_{t=1}^{T} \log p(w_t \mid w_1, \ldots, w_{t-1}) \\ &= -\sum_{t=1}^{T} \sum_{v=1}^{V} t_{tv} \log y_{tv}, \end{aligned}$$

where t_{iv} is the one-hot encoding for the ith word and y_{iv} is the predicted probability for the ith word being index v.

Bengio's Neural Language Model

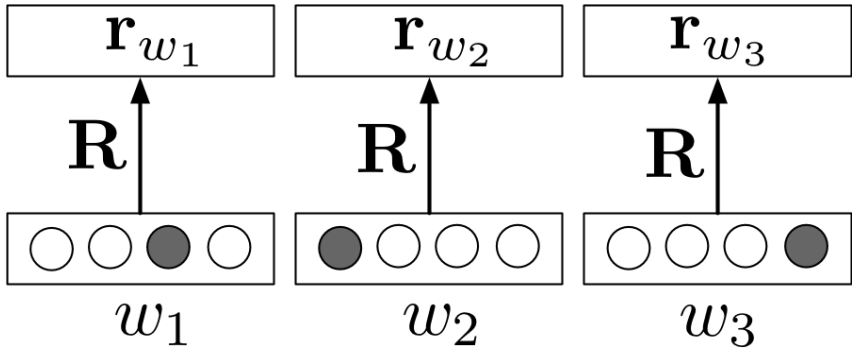
- Here is a classic neural probabilistic language model, or just neural language model:



http://www.jmlr.org/papers/volume3/bengio03a/bengio03a.pdf

Neural Language Model

- If we use a 1-of-K encoding for the words, the first layer can be thought of as a linear layer with tied weights.



- The weight matrix basically acts like a lookup table. Each column is the representation of a word, also called an embedding, feature vector, or encoding.
  - "Embedding" emphasizes that it's a location in a high-dimensonal space; words that are closer together are more semantically similar
  - "Feature vector" emphasizes that it's a vector that can be used for making predictions, just like other feature mappigns we've looked at (e.g. polynomials)

Neural Language Model

- What do these word embeddings look like?
- The following 2-D embeddings are done with an algorithm called tSNE which tries to make distnaces in the 2-D embedding match the original 30-D distances as closely as possible.

Neural Language Model

Neural Language Model

- Thinking about high-dimensional embeddings
  - Most vectors are nearly orthogonal (i.e. dot product is close to 0)
  - Most points are far away from each other
  - "In a 30-dimensional grocery store, anchovies can be next to fish and next to pizza toppings." – Geoff Hinton
- The 2-D embeddings might be fairly misleading, since they can't preserve the distance relationships from a higher-dimensional embedding. (I.e., unrelated words might be close together in 2-D, but far apart in 30-D.)

GloVe: Neural Language Model as Matrix Factorization

- Fitting language models is really hard.
- Maybe this is overkill if all you want is word representations.
- Global Vector (GloVe) embeddings are a simpler and faster approach based on a matrix factorization similar to principal component analysis (PCA).

GloVe: Neural Language Model as Matrix Factorization

- Distributional hypothesis again: words with similar distributions have similar meanings ("judge a word by the company it keeps")
- Consider a co-occurrence matrix X, which counts the number of times two words appear nearby (say, less than 5 positions apart)
- This is a $V \times V$ matrix, where V is the vocabulary size (very large)
- **Intuition pump:** suppose we fit a rank-K approximation $\mathsf{X} \approx \mathsf{R}\tilde{\mathsf{R}}^\top$, where R and $\tilde{\mathsf{R}}$ are $V \times K$ matrices.
  - Each row r_i of R is the K-dimensional representation of a word
  - Each entry is approximated as $x_{ij} \approx \mathsf{r}_i^\top \tilde{\mathsf{r}}_j$
  - Hence, more similar words are more likely to co-occur
  - **Minimizing the squared Frobenius norm** $\|\mathsf{X} - \mathsf{R}\tilde{\mathsf{R}}^\top\|_F^2 = \sum_{i,j}(x_{ij} - \mathsf{r}_i^\top \tilde{\mathsf{r}}_j)^2$ is basically PCA.

GloVe

- **Problem 1:** X is extremely large, so fitting the above factorization uisng least squares is infeasible.
  - **Solution:** Reweight the entries so that only nonzero counts matter
- **Problem 2:** Word counts are a heavy-tailed distribution, so the most common words will dominate the cost function.
  - **Solution:** Approximate $\log x_{ij}$ instead of x_{ij}.
- Global Vector (GloVe) embedding cost function:

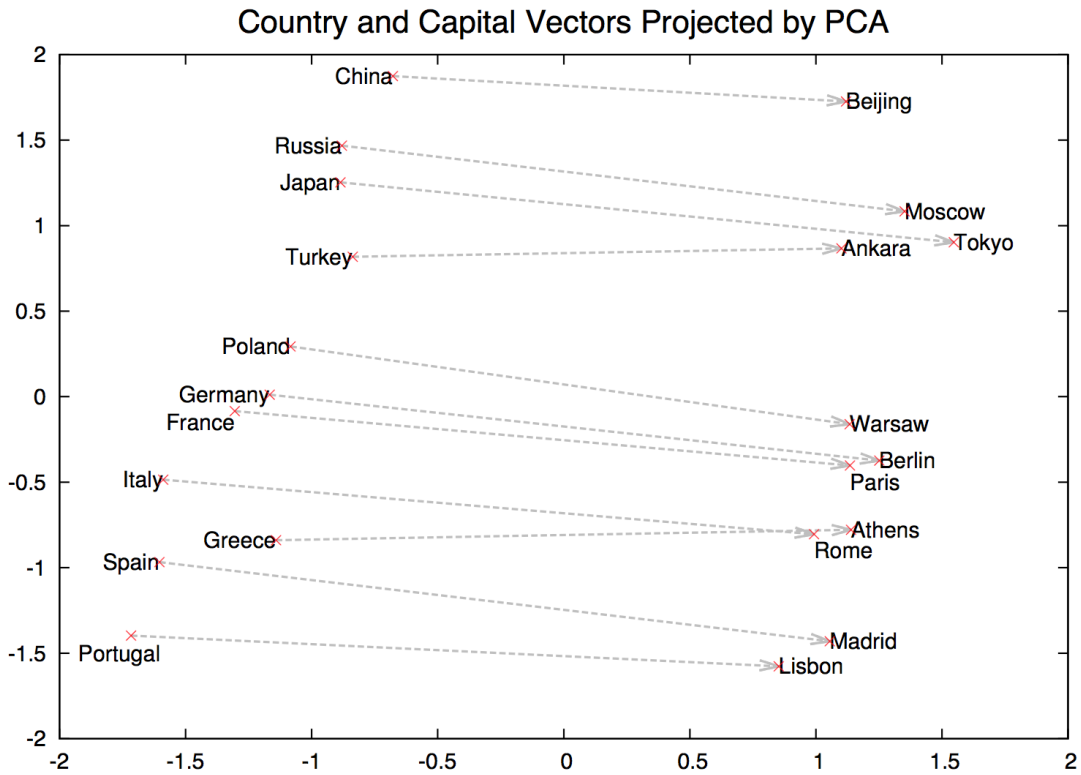
$$\mathcal{J}(\mathrm{R}) = \sum_{i,j} f(x_{ij})(\mathrm{r}_i^\top \tilde{\mathrm{r}}_j + b_i + \tilde{b}_j - \log x_{ij})^2$$

$$f(x_{ij}) = \begin{cases} \left(\frac{x_{ij}}{100}\right)^{3/4} & \text{if } x_{ij} < 100 \\ 1 & \text{if } x_{ij} \geq 100 \end{cases}$$

- b_i and $\tilde{b}_j$ are bias parameters.
- We can avoid computing $\log 0$ since $f(0) = 0$.
- We only need to consider the nonzero entries of X. This gives a big computational savings since X is extremely sparse!

Word Analogies

- Here's a linear projection of word representations for cities and capitals into 2 dimensions.
- The mapping $\text{city} \rightarrow \text{capital}$ corresponds roughly to a single direction in the vector space:



- Note: this figure actually comes from skip-grams, a predecessor to GloVe.

Word Analogies

- In other words,
  $\text{vector}(\text{Paris}) - \text{vector}(\text{France}) \approx \text{vector}(\text{London}) - \text{vector}(\text{England})$
- This means we can analogies by doing arithmetic on word vectors:
  - e.g. "Paris is to France as London is to _____"
  - Find the word whose vector is closest to
    $\text{vector}(\text{France}) - \text{vector}(\text{Paris}) + \text{vector}(\text{London})$
- Example analogies:

Relationship	Example 1	Example 2	Example 3
France - Paris	Italy: Rome	Japan: Tokyo	Florida: Tallahassee
big - bigger	small: larger	cold: colder	quick: quicker
Miami - Florida	Baltimore: Maryland	Dallas: Texas	Kona: Hawaii
Einstein - scientist	Messi: midfielder	Mozart: violinist	Picasso: painter
Sarkozy - France	Berlusconi: Italy	Merkel: Germany	Koizumi: Japan
copper - Cu	zinc: Zn	gold: Au	uranium: plutonium
Berlusconi - Silvio	Sarkozy: Nicolas	Putin: Medvedev	Obama: Barack
Microsoft - Windows	Google: Android	IBM: Linux	Apple: iPhone
Microsoft - Ballmer	Google: Yahoo	IBM: McNealy	Apple: Jobs
Japan - sushi	Germany: bratwurst	France: tapas	USA: pizza

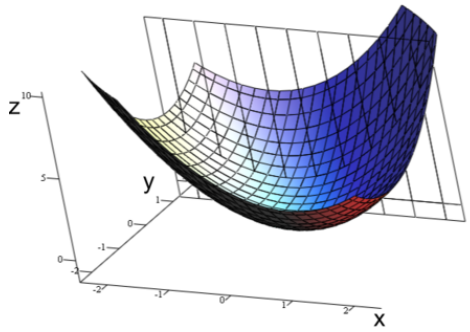
After the break

After the break: **Optimization**

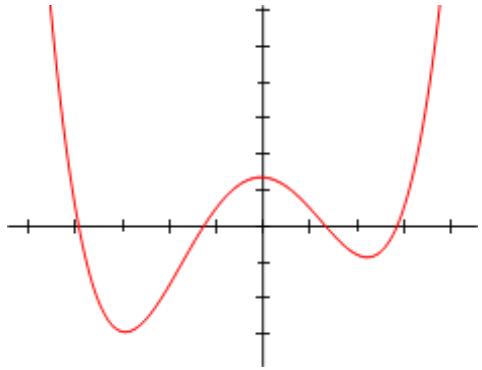
Optimization

- So far, we've talked a lot about computing gradients and different neural models.
- How do we actually train those models using gradients?
- There are various things that can go wrong in gradient descent, we will learn 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 θ.

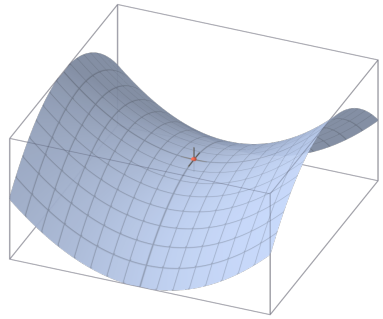
Features of the Optimization Landscape



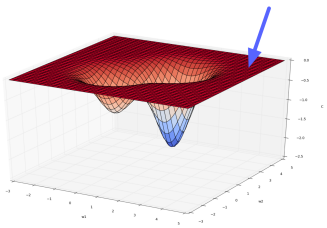
convex functions



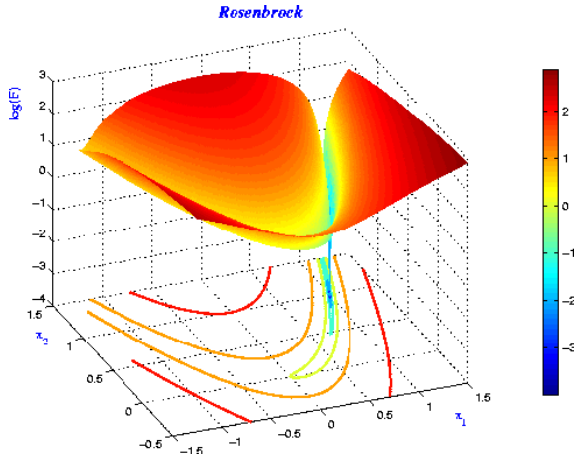
local minima



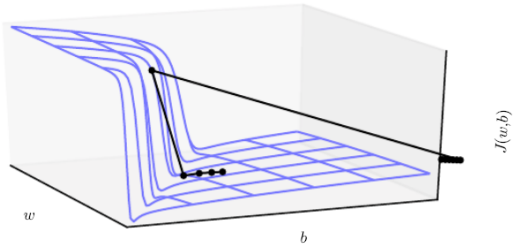
saddle points



plateaux



narrow ravines



cliffs (covered in a later lecture)

Review: Hessian Matrix

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

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

- 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 $\boldsymbol{\theta}_0$:

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

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

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

Review: Hessian Matrix

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

$$H = Q \Lambda Q^\top,$$

where Q is an orthogonal matrix (whose columns are the eigenvectors) and Λ 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 $\boldsymbol{\theta} + t\mathrm{v}$ for some vector v.
- Second-order Taylor approximation:

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

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

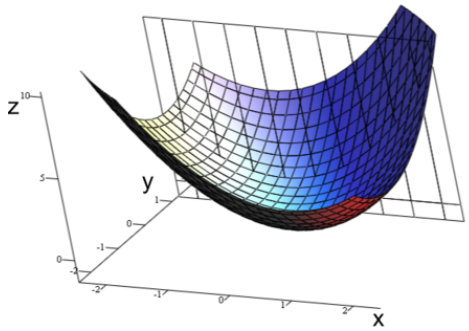
Review: Hessian Matrix

- A matrix A is positive definite if $v^\top Av > 0$ for all $v \neq 0$. (I.e., it curves upwards in all directions.)
  - It is positive semidefinite (PSD) if $v^\top Av \geq 0$ for all $v \neq 0$.
- 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 $H(\boldsymbol{\theta}_*)$ exists and is positive definite, then $\boldsymbol{\theta}_*$ is a local minimum (since all directions curve upwards).

Review: Convex Functions

- Recall: a set $\mathcal{S}$ is convex if for any $x_0, x_1 \in \mathcal{S}$,

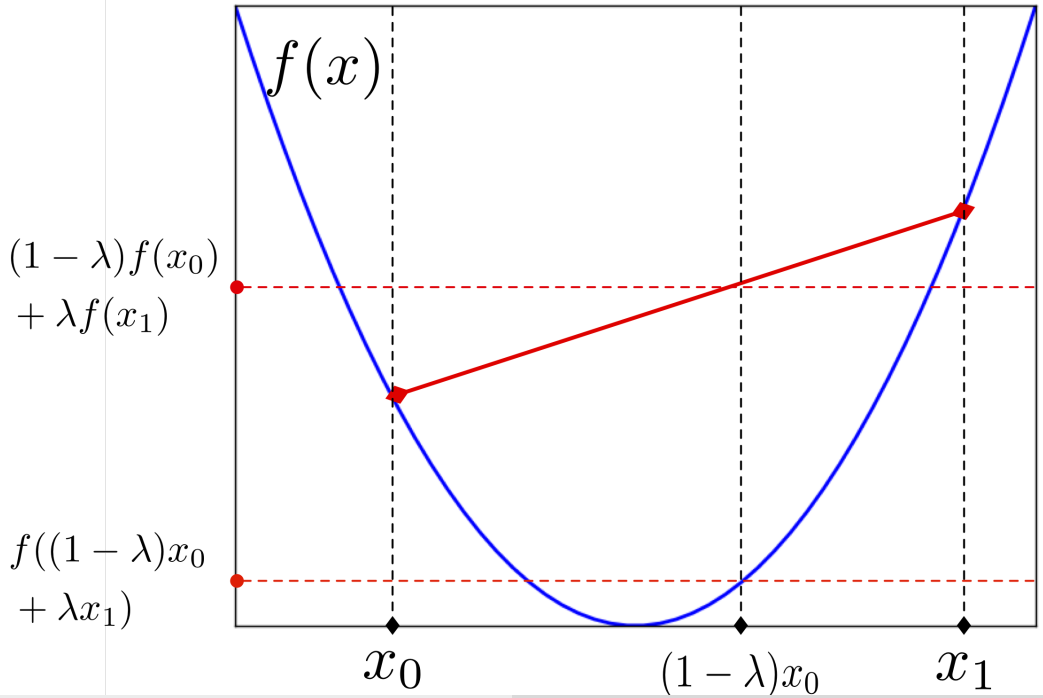
$$(1-\lambda)x_0 + \lambda x_1 \in \mathcal{S} \quad \text{for } 0 \leq \lambda \leq 1.$$



- A function f is convex if for any x_0, x_1,

$$f((1-\lambda)x_0 + \lambda x_1) \leq (1-\lambda)f(x_0) + \lambda f(x_1)$$

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

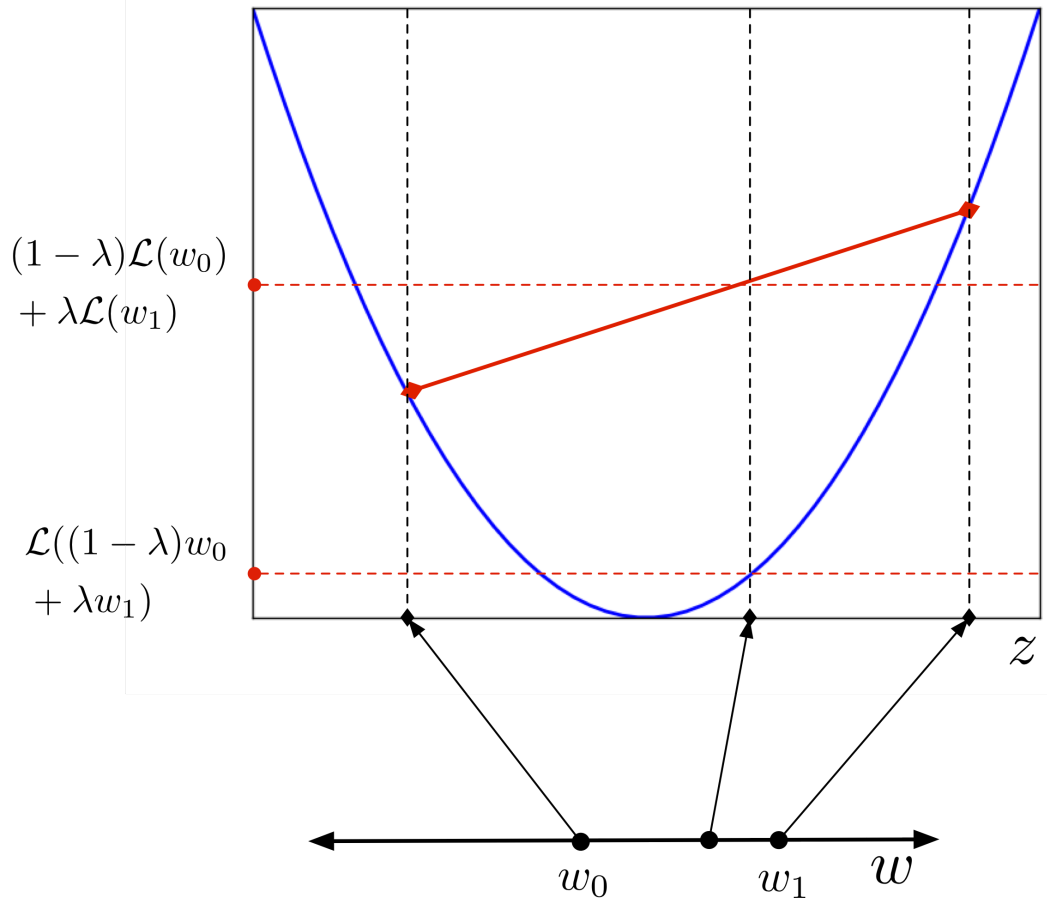


Review: Convex Functions

- If $\mathcal{J}$ is smooth (more precisely, twice differentiable), there's an equivalent characterization in terms of H:
  - A smooth function is convex iff its Hessian is positive semidefinite 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.

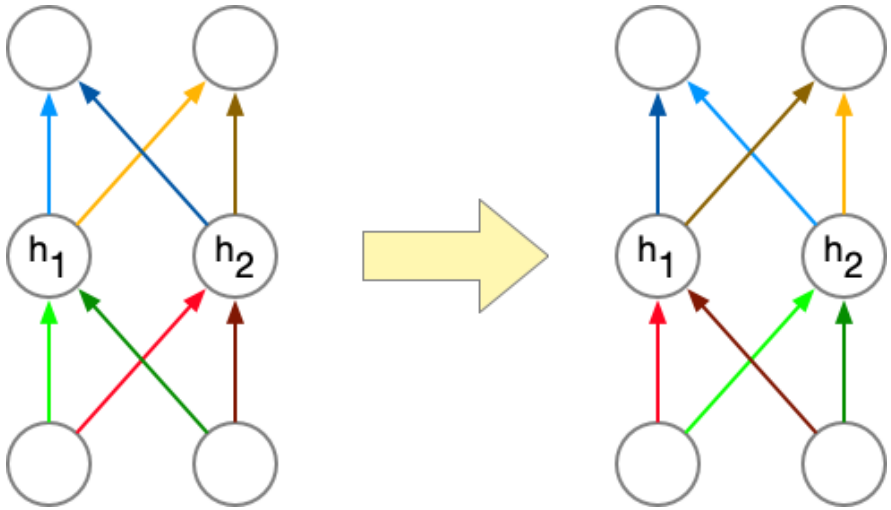
Review: Convex Functions

- 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.
- 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

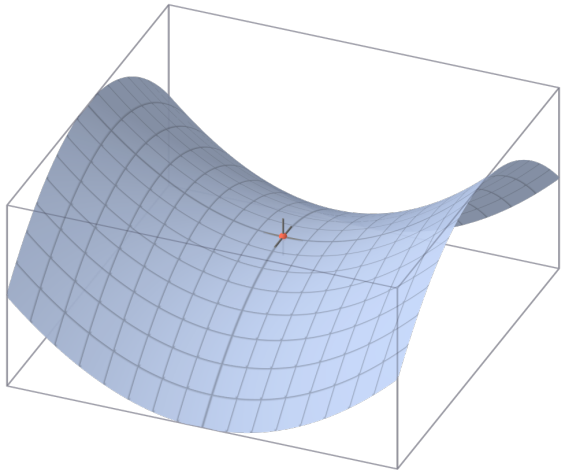
Special case: a univariate function is convex iff its second derivative is nonnegative everywhere.

- 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:

- $\nabla \mathcal{J}(\boldsymbol{\theta}) = 0$
- $\mathrm{H}(\boldsymbol{\theta})$ 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?

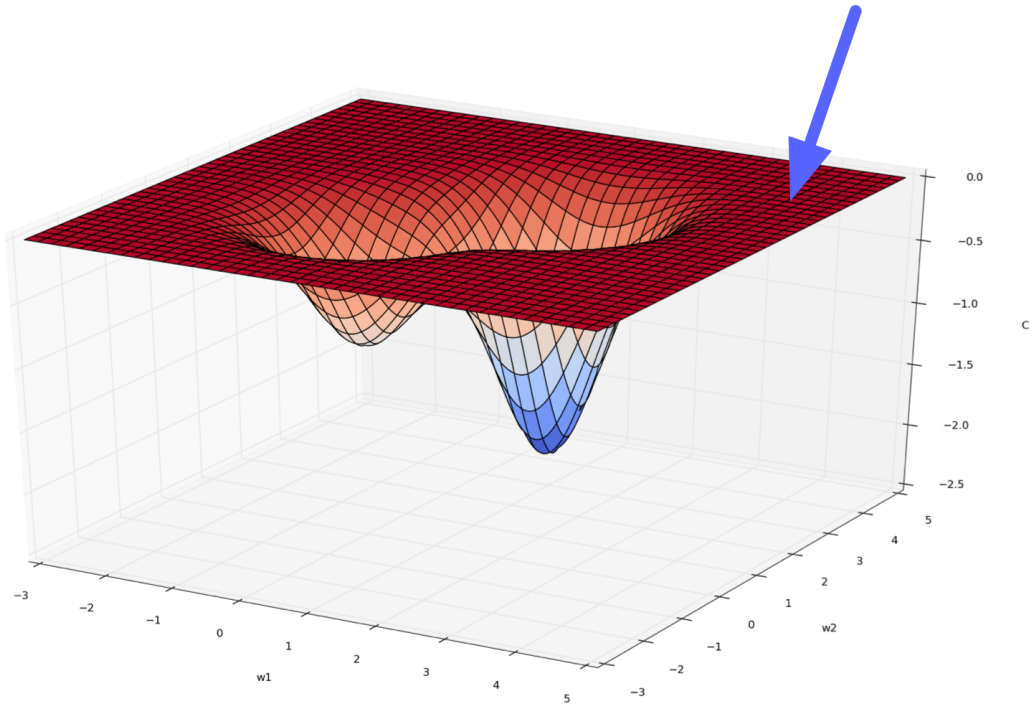
- If we're exactly on the saddle point, then we're stuck.
- If we're slightly to the side, then we can get unstuck.

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)



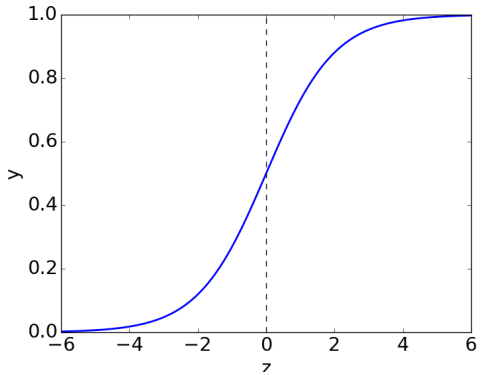
Examples of plateaux:

- 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:

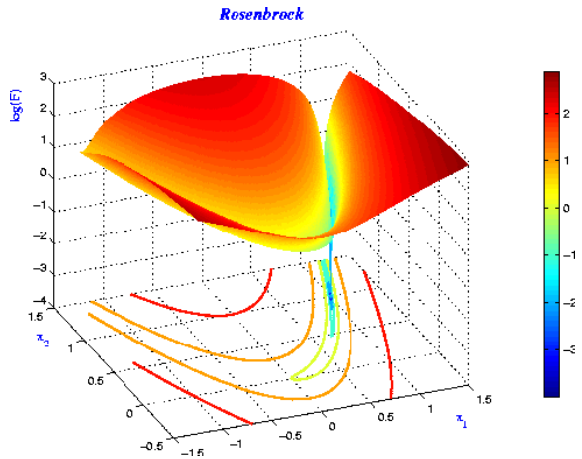
$$\overline{z_i} = \overline{h_i}\,\phi'(z)$$
$$\overline{w_{ij}} = \overline{z_i}\,x_j$$

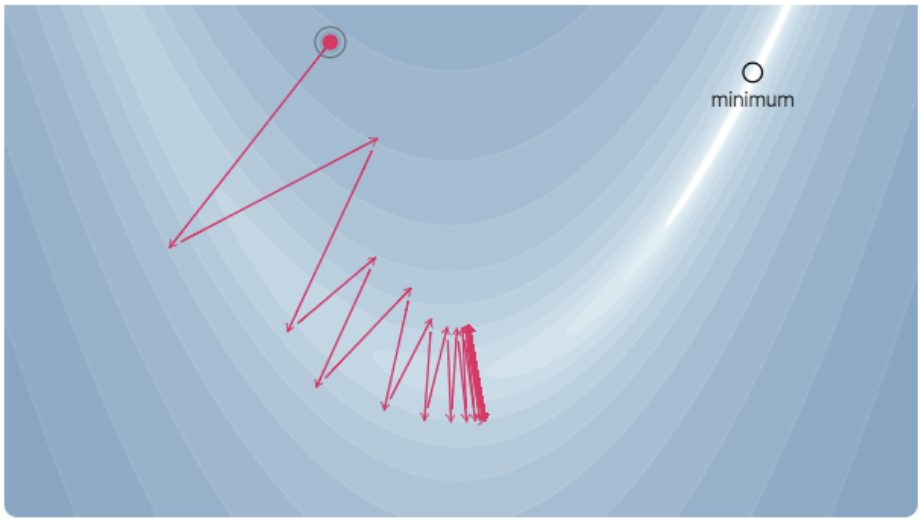


- If $\phi'(z_i)$ is always close to zero, then the weights will get stuck.
- If there is a ReLU unit whose input z_i is always negative, the weight derivatives will be *exactly* 0. We call this a dead unit.

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

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

  where A is PSD.

- Gradient descent update:

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

- Solving the recurrence,

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

Ill-conditioned curvature: gradient descent dynamics

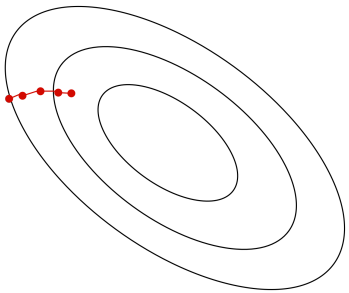
- We can analyze matrix powers such as $(I - \alpha A)^k \boldsymbol{\theta}_0$ using the spectral decomposition.
- Let $A = Q \Lambda Q^\top$ be the spectral decomposition of A.

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

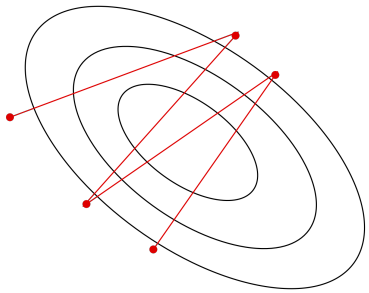
- Hence, in the Q basis, each coordinate gets multiplied by $(1 - \alpha \lambda_i)^k$, where the λ_i are the eigenvalues of A.
- Cases:
  - $0 < \alpha \lambda_i \leq 1$: decays to 0 at a rate that depends on $\alpha \lambda_i$
  - $1 < \alpha \lambda_i \leq 2$: oscillates
  - $\alpha \lambda_i > 2$: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

Tuning Learning Rate

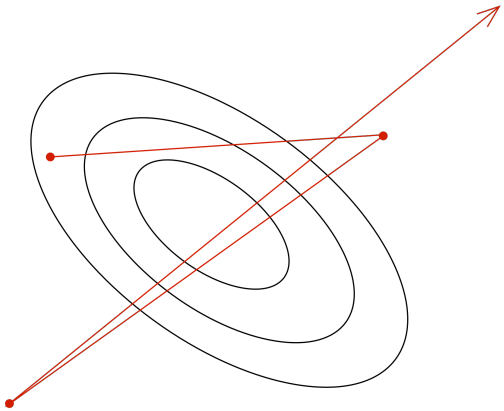
- How can spectral decomposition help?
- The learning rate α is a hyperparameter we need to tune. Here are the things that can go wrong:



α too small:
slow progress



α too large:
oscillations



α much too large:
instability (diverges)

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)
- **Ill-conditioned curvature bounds the maximum learning rate choice**. 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

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

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

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

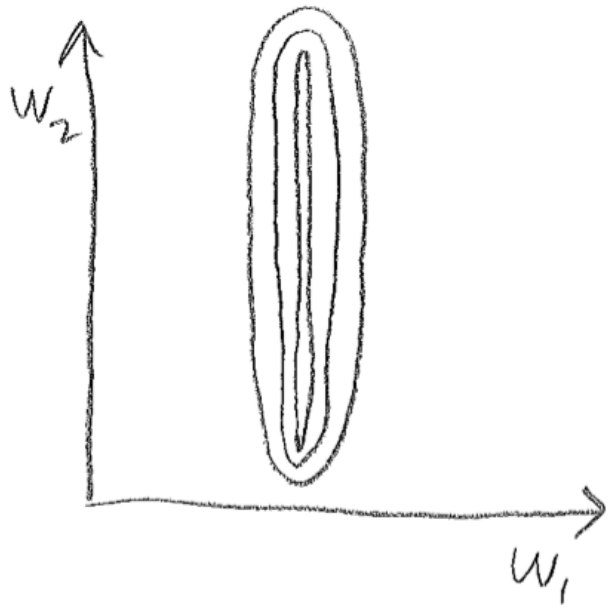
- Since a smooth cost function is well approximated by a convex quadratic (i.e. second-order Taylor approximation) in the vicinity of a (local) optimum, this analysis is a good description of the behavior of gradient descent near a (local) optimum.
- If the Hessian is ill-conditioned, then gradient descent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

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

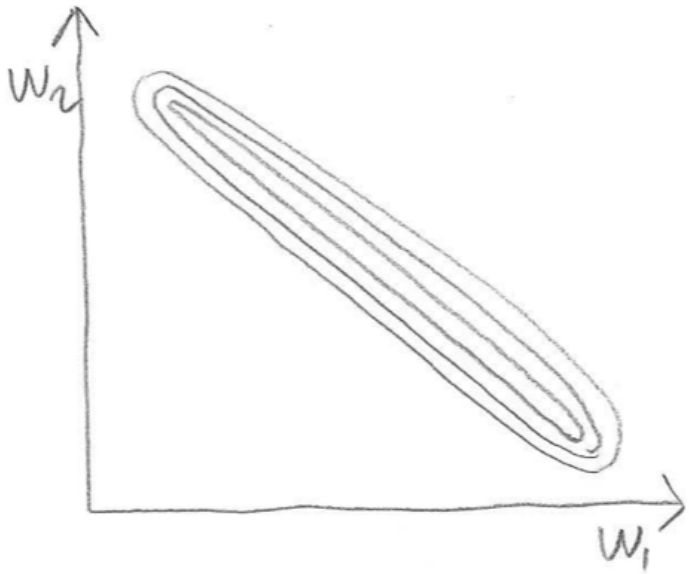


- Which weight, w_1 or w_2, will receive a larger gradient descent update?
- Which one do you want to receive a larger update?
- Note: the figure vastly *understates* the narrowness of the ravine!

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:

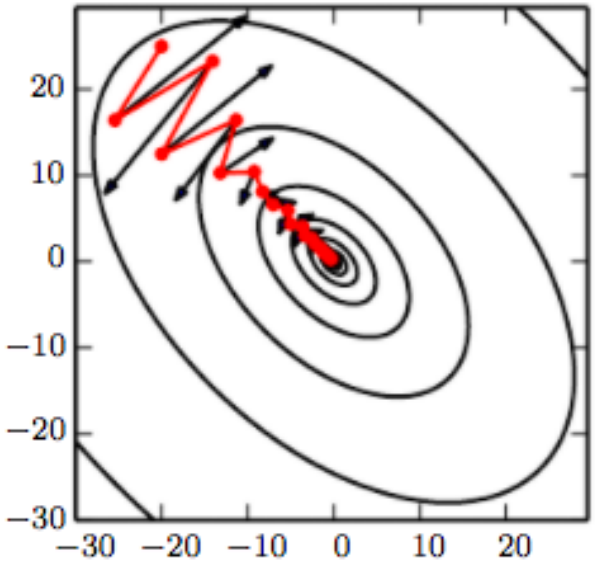
$$\mathsf{p} \leftarrow \mu \mathsf{p} - \alpha \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}$$

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

- 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?
  - 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: Gradient descent takes large steps in directions of high curvature and small steps in directions of low curvature.
- RMSprop is a variant of GD 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:

$$s_j \leftarrow (1-\gamma)s_j + \gamma[\frac{\partial \mathcal{J}}{\partial \theta_j}]^2$$

$$\theta_j \leftarrow \theta_j - \frac{\alpha}{\sqrt{s_j + \epsilon}} \frac{\partial \mathcal{J}}{\partial \theta_j}$$

- 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. Affect 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.