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Backpropagation I: Computing Derivatives in Computational Graphs [without Backpropagation] in Exponential Time

Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.2

Why Do We Need Backpropagation?

- To perform any kind of learning, we need to compute the partial derivative of the loss function with respect to each intermediate weight.
  - Simple with single-layer architectures like the perceptron.
  - Not a simple matter with multi-layer architectures.

The Complexity of Computational Graphs

- A computational graph is a directed acyclic graph in which each node computes a function of its incoming node variables.

- A neural network is a special case of a computational graph.
  - Each node computes a combination of a linear vector multiplication and a (possibly nonlinear) activation function.

- The output is a very complicated *composition* function of each intermediate weight in the network.
  - The complex composition function might be hard to express neatly in closed form.
    - Difficult to differentiate!

Recursive Nesting is Ugly!

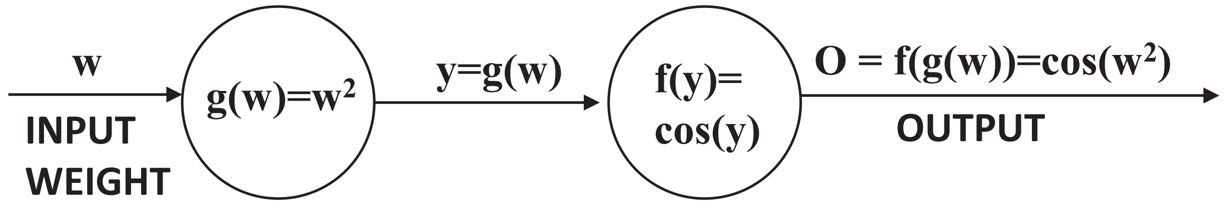
- Consider a computational graph containing two nodes in a path and input w.

- The first node computes $y = g(w)$ and the second node computes the output $o = f(y)$.
  - Overall composition function is $f(g(w))$.
  - Setting $f()$ and $g()$ to the sigmoid function results in the following:

$$f(g(w)) = \frac{1}{1 + \exp\left[-\frac{1}{1+\exp(-w)}\right]} \tag{1}$$

  - Increasing path length increases recursive nesting.

Backpropagation along Single Path (Univariate Chain Rule)



- Consider a two-node path with $f(g(w)) = \cos(w^2)$

- In the univariate chain rule, we compute product of *local* derivatives.

$$\frac{\partial f(g(w))}{\partial w} = \underbrace{\frac{\partial f(y)}{\partial y}}_{-sin(y)} \cdot \underbrace{\frac{\partial g(w)}{\partial w}}_{2w} = -2w \cdot \sin(y) = -2w \cdot \sin(w^2)$$

- Local derivatives are easy to compute because they care about their own input and output.

Backpropagation along Multiple Paths (Multivariate Chain Rule)

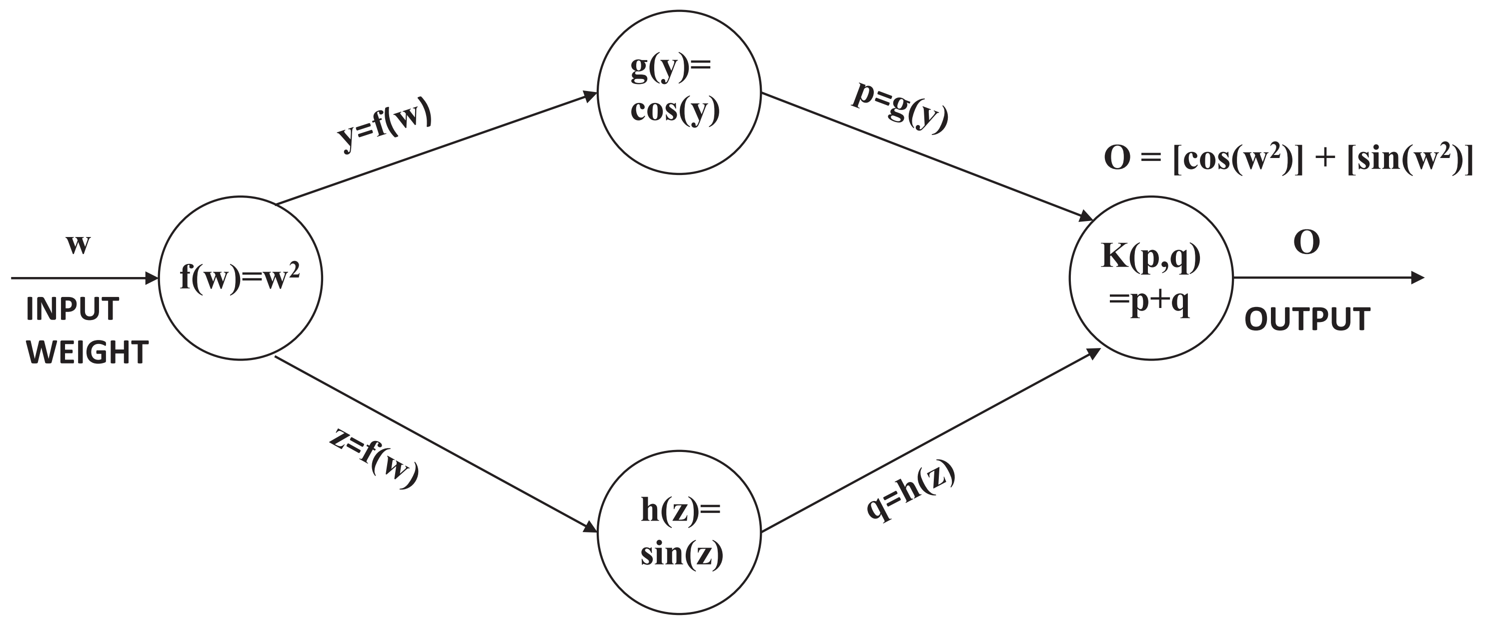
- Neural networks contain multiple nodes in each layer.

- Consider the function $f(g_1(w), \ldots g_k(w))$, in which a unit computing the *multivariate* function $f(\cdot)$ gets its inputs from k units computing $g_1(w) \ldots g_k(w)$.

- The *multivariable chain rule* needs to be used:

$$\frac{\partial f(g_1(w), \ldots g_k(w))}{\partial w} = \sum_{i=1}^{k} \frac{\partial f(g_1(w), \ldots g_k(w))}{\partial g_i(w)} \cdot \frac{\partial g_i(w)}{\partial w} \tag{2}$$

Example of Multivariable Chain Rule



$$\begin{aligned}\frac{\partial o}{\partial w} &= \underbrace{\frac{\partial K(p,q)}{\partial p}}_{1} \cdot \underbrace{g'(y)}_{\text{-sin}(y)} \cdot \underbrace{f'(w)}_{2w} + \underbrace{\frac{\partial K(p,q)}{\partial q}}_{1} \cdot \underbrace{h'(z)}_{\cos(z)} \cdot \underbrace{f'(w)}_{2w} \\ &= -2w \cdot \sin(y) + 2w \cdot \cos(z) \\ &= -2w \cdot \sin(w^2) + 2w \cdot \cos(w^2)\end{aligned}$$

- Product of local derivatives along *all* paths from w to o.

Pathwise Aggregation Lemma

- Let a non-null set $\mathcal{P}$ of paths exist from a variable w in the computational graph to output o.
  - Local gradient of node with variable $y(j)$ with respect to variable $y(i)$ for directed edge (i, j) is $z(i, j) = \frac{\partial y(j)}{\partial y(i)}$

- The value of $\frac{\partial o}{\partial w}$ is given by computing the product of the local gradients along each path in $\mathcal{P}$, and summing these products over all paths.

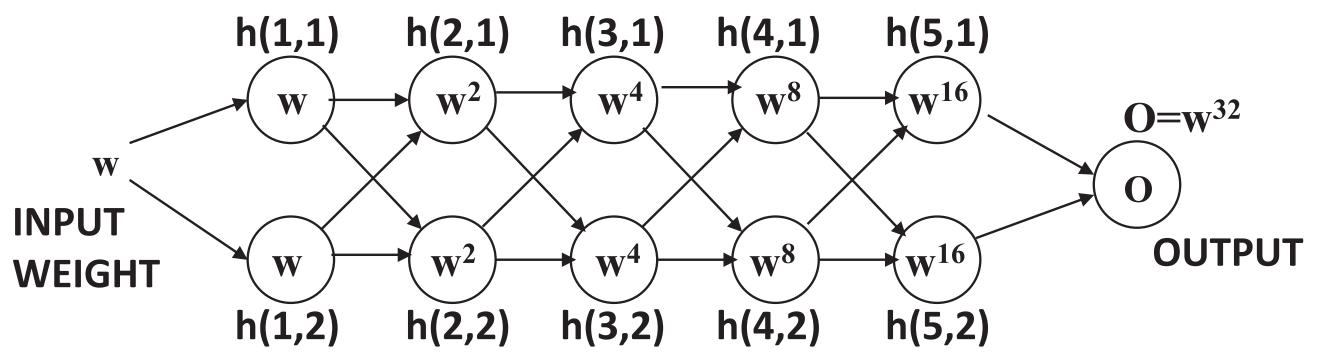
$$\frac{\partial o}{\partial w} = \sum_{P \in \mathcal{P}} \prod_{(i,j) \in P} z(i, j) \tag{3}$$

- Observation: Each $z(i, j)$ easy to compute.

An Exponential Time Algorithm for Computing Partial Derivatives

- The path aggregation lemma provides a simple way to compute the derivative with respect to intermediate variable w
  - Use computational graph to compute each value $y(i)$ of nodes i in a forward phase.
  - Compute local derivative $z(i, j) = \frac{\partial y(j)}{\partial y(i)}$ on each edge (i, j) in the network.
  - Identify the set $\mathcal{P}$ of all paths from the node with variable w to the output o.
  - For each path $P \in \mathcal{P}$ compute the product $M(P) = \prod_{(i,j)\in P} z(i, j)$ of the local derivatives on that path.
  - Add up these values over all paths $P \in \mathcal{P}$.

Example: Deep Computational Graph with Product Nodes



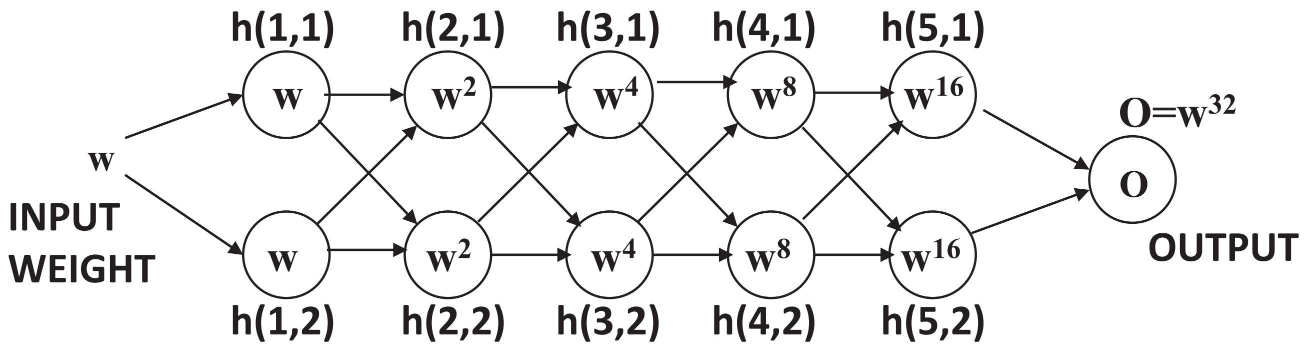
EACH NODE COMPUTES THE PRODUCT OF ITS INPUTS

- Each node computes product of its inputs $\Rightarrow$ Partial derivative of xy with respect to one input x is the other input y.

- Computing product of partial derivatives along a path is equivalent to computing product of values along the only other node disjoint path.

- Aggregative product of partial derivatives (only in this case) equals aggregating products of values.

Example of Increasing Complexity with Depth



EACH NODE COMPUTES THE PRODUCT OF ITS INPUTS

$$\frac{\partial O}{\partial w} = \sum_{j_1,j_2,j_3,j_4,j_5 \in \{1,2\}^5} \underbrace{\prod h(1,j_1)}_{w} \underbrace{h(2,j_2)}_{w^2} \underbrace{h(3,j_3)}_{w^4} \underbrace{h(4,j_4)}_{w^8} \underbrace{h(5,j_5)}_{w^{16}}$$

$$= \sum_{\text{All 32 paths}} w^{31} = 32w^{31}$$

- Impractical with increasing depth.

Observations on Exponential Time Algorithm

- Not very practical approach $\Rightarrow$ Million paths for a network with 100 nodes in each layer and three layers.

- *This is the approach of traditional machine learning with complex objective functions in closed form*.
  - For a composition function in closed form, manual differentiation explicitly traverses all paths with chain rule.
  - The algebraic expression of the derivative of a complex function might not fit the paper you write on.
  - Explains why most of traditional machine learning is a shallow neural model.

- The beautiful *dynamic programming* idea of backpropagation rescues us from complexity.

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Backpropagation II: Using Dynamic Programming [Backpropagation] to Compute Derivatives in Polynomial Time

Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.2

Differentiating Composition Functions

- Neural networks compute composition functions with a lot of *repetitiveness* caused by a node appearing in multiple paths.

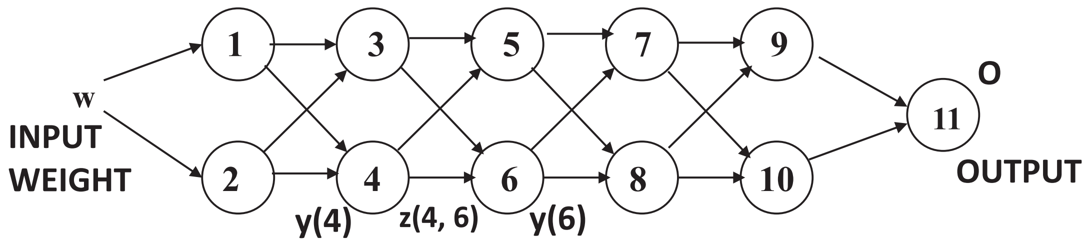
- The most natural and intuitive way to differentiate such a composition function is not the most *efficient* way to do it.

- Natural approach: Top down

$$f(w) = \sin(w^2) + \cos(w^2)$$

- We should not have to differentiate w^2 twice!

- Dynamic programming collapses repetitive computations to reduce exponential complexity into polynomial complexity!



EACH NODE i CONTAINS y(i) AND EACH EDGE BETWEEN i AND j CONTAINS z(i, j)
EXAMPLE: z(4, 6)= PARTIAL DERIVATIVE OF y(6) WITH RESPECT TO y(4)

- We want to compute the derivative of the output with respect to variable w.

- We can easily compute $z(i, j) = \frac{\partial y(j)}{\partial y(i)}$.

- Naive approach computes $S(w, o) = \frac{\partial o}{\partial w} = \sum_{P \in \mathcal{P}} \prod_{(i,j) \in P} z(i, j)$ by explicit aggregation over all paths in $\mathcal{P}$.

Dynamic Programming and Directed Acyclic Graphs

- Dynamic programming used extensively in directed acyclic graphs.
  - **Typical:** Exponentially aggregative path-centric functions between source-sink pairs.
  - **Example:** Polynomial solution to longest path problem in directed acyclic graphs (NP-hard in general).
  - **General approach:** Starts at either the source or sink and *recursively* computes the relevant function over paths of increasing length by reusing intermediate computations.
- Our path-centric function: $S(w, o) = \sum_{P \in \mathcal{P}} \prod_{(i,j) \in P} z(i, j)$.
  - Backwards direction makes more sense here because we have to compute derivative of output (sink) with respect to all variables in early layers.

Dynamic Programming Update

- Let $A(i)$ be the set of nodes at the ends of outgoing edges from node i.

- Let $S(i, o)$ be the *intermediate* variable indicating the same path aggregative function from i to o.

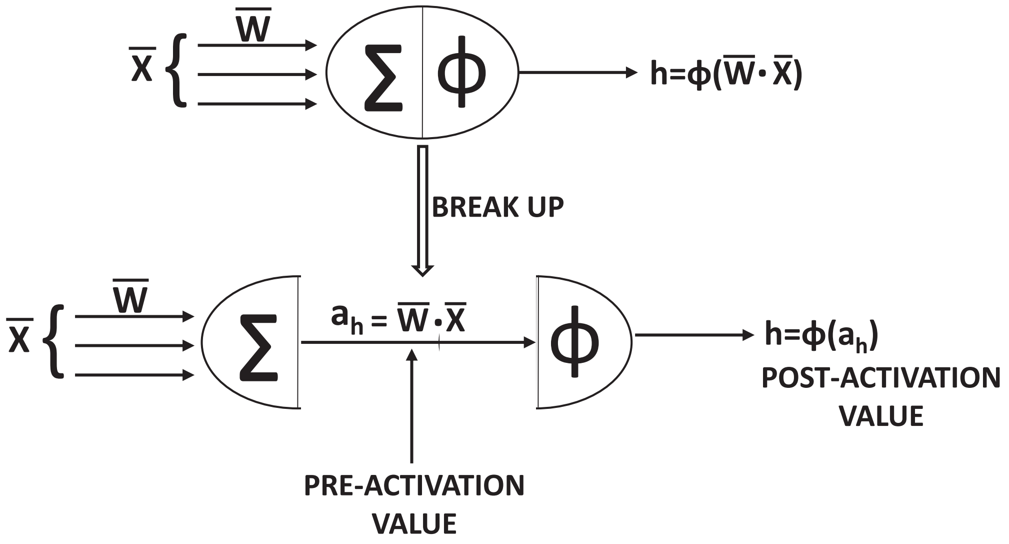
$$S(i, o) \Leftarrow \sum_{j \in A(i)} S(j, o) \cdot z(i, j) \tag{4}$$

- Initialize $S(o, o)$ to 1 and compute backwards to reach $S(w, o)$.
  - Intermediate computations like $S(i, o)$ are also useful for computing derivatives in other layers.

- Do you recognize the multivariate chain rule in Equation 4?

$$\frac{\partial o}{\partial y(i)} = \sum_{j \in A(i)} \frac{\partial o}{\partial y(j)} \cdot \frac{\partial y(j)}{\partial y(i)}$$

How Does it Apply to Neural Networks?



- A neural network is a special case of a computational graph.
  - We can define the computational graph in multiple ways.
  - Pre-activation variables or post-activation variables or both as the node variables of the computation graph?
  - The three lead to different updates but the end result is equivalent.

Pre-Activation Variables to Create Computational Graph

- Compute derivative $\delta(i,o)$ of loss L at o with respect to pre-activation variable at node i.

- We always compute loss derivatives $\delta(i,o)$ with respect to activations in *nodes* during dynamic programming rather than *weights*.
  - Loss derivative with respect to weight w_{ij} from node i to node j is given by the product of $\delta(j,o)$ and hidden variable at i (why?)

- Key points: $z(i,j) = w_{ij} \cdot \Phi'_i$, Initialize $S(o,o) = \delta(o,o) = \frac{\partial L}{\partial o}\Phi'_o$

$$\delta(i,o) = S(i,o) = \Phi'_i \sum_{j \in A(i)} w_{ij} S(j,o) = \Phi'_i \sum_{j \in A(i)} w_{ij}\delta(j,o) \tag{5}$$

Post-Activation Variables to Create Computation Graph

- The variables in the computation graph are hidden values *after* activation function application.

- Compute derivative $\Delta(i, o)$ of loss L at o with respect to post-activation variable at node i.

- Key points: $z(i, j) = w_{ij} \cdot \Phi'_j$, Initialize $S(o, o) = \Delta(o, o) = \frac{\partial L}{\partial o}$

$$\Delta(i, o) = S(i, o) = \sum_{j \in A(i)} w_{ij} S(j, o) \Phi'_j = \sum_{j \in A(i)} w_{ij} \Delta(j, o) \Phi'_j \tag{6}$$

  – Compare with pre-activation approach $\delta(i, o) = \Phi'_i \sum_{j \in A(i)} w_{ij} \delta(j, o)$

  – Pre-activation approach more common in textbooks.

Variables for Both Pre-Activation and Post-Activation Values

- Nice way of decoupling the linear multiplication and activation operations.

- Simplified approach in which each layer is treated as a single node with a vector variable.

  - Update can be computed in vector and matrix multiplications.

- Topic of discussion in next part of the backpropagation series.

Losses at Arbitrary Nodes

- We assume that the loss is incurred at a single output node.

- In case of multiple output nodes, one only has to add up the contributions of different outputs in the backwards phase.

- In some cases, penalties may be applied to hidden nodes.

- For a hidden node i, we add an "initialization value" to $S(i, o)$ just after it has been computed during dynamic programming, which is based on its penalty.

  – Similar treatment as the initialization of an output node, except that we *add* the contribution to existing value of $S(i, o)$.

Handling Shared Weights

- You saw an example in autoencoders where encoder and decoder weights are shared.

- Also happens in specialized architectures like recurrent or convolutional neural networks.

- Can be addressed with a simple application of the chain rule.

- Let $w_1 \dots w_r$ be r copies of the same weight w in the neural network.

$$\frac{\partial L}{\partial w} = \sum_{i=1}^{r} \frac{\partial L}{\partial w_i} \cdot \frac{\partial w_i}{\partial w} = \sum_{i=1}^{r} \frac{\partial L}{\partial w_i} \tag{7}$$

- Pretend all weights are different and just add!

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Backpropagation III: A Decoupled View of Vector-Centric Backpropagation

Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.2

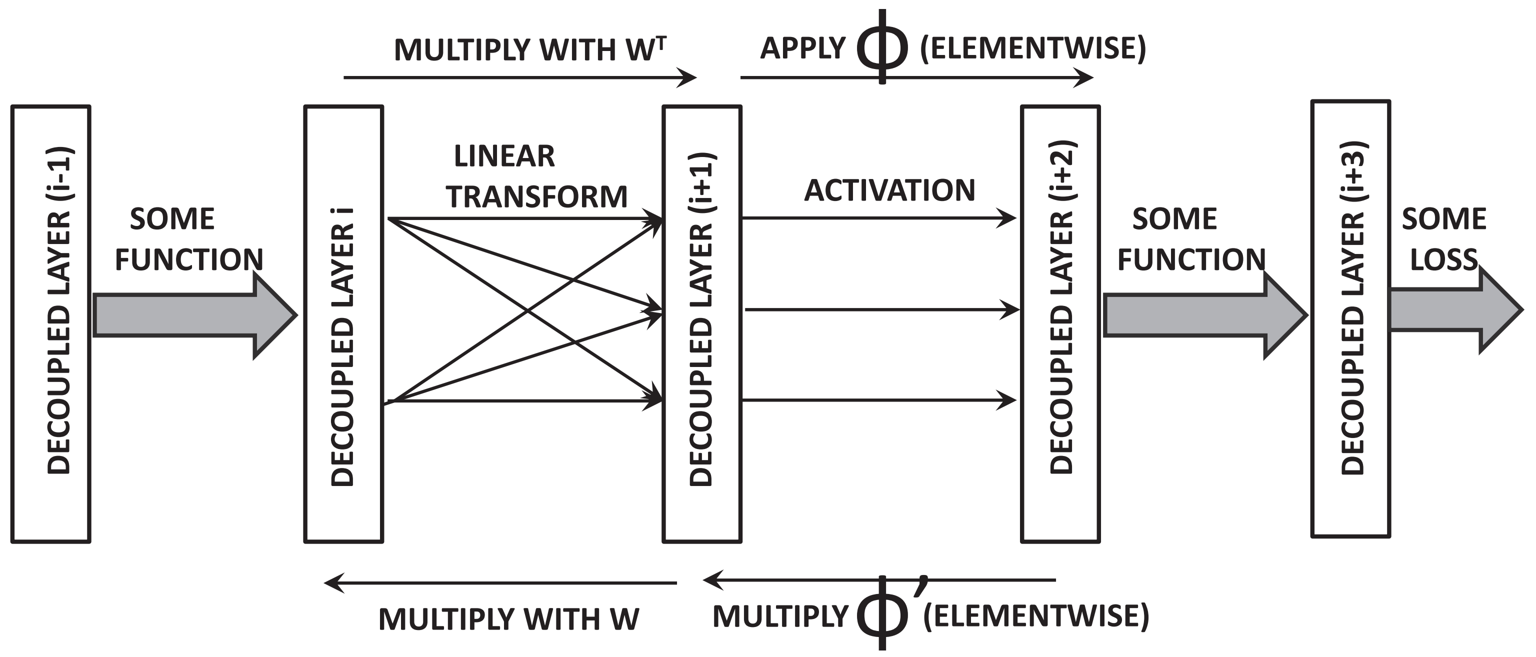
Multiple Computational Graphs from Same Neural Network

- We can create a computational graph in multiple ways from the variables in a neural network.
  - Computational graph of pre-activation variables (part II of lecture)
  - Computational graph of post-activation variables (part II of lecture)
  - Computational graph of both (this part of the lecture)
- Using both pre-activation and post-activation variables creates decoupled backpropagation updates for linear layer and for activation function.

Scalar Versus Vector Computational Graphs

- The backpropagation discussion so far uses scalar operations.
- Neural networks are constructed in layer-wise fashion.
- We can treat an entire layer as a node with a vector variable.
- We want to use layer-wise operations on vectors.
  - Most real implementations use vector and matrix multiplications.
- Want to decouple the operations of linear matrix multiplication and activation function in separate "layers."

Vector-Centric and Decoupled View of Single Layer



- Note that linear matrix multiplication and activation function are separate layers.

- Method 1 (requires knowledge of matrix calculus): You can use the vector-to-vector chain rule to backpropagate on a single path!

Converting Scalar Updates to Vector Form

- **Recap:** When the partial derivative of node q with respect to node p is $z(p,q)$, the dynamic programming update is:

$$S(p,o) = \sum_{q \in \text{Next Layer}} S(q,o) \cdot z(p,q) \tag{8}$$

- We can write the above update in vector form by creating a single column vector $\overline{g}_i$ for layer $i \Rightarrow$ Contains $S(p,o)$ for all values of p.

$$\overline{g}_i = Z\overline{g}_{i+1} \tag{9}$$

- The matrix $Z = [z(p,q)]$ is the transpose of the Jacobian!
  - We will use the notation $J = Z^T$ in further slides.

The Jacobian

- Consider layer i and layer-$(i+1)$ with activations $\overline{z}_i$ and $\overline{z}_{i+1}$.
  - The kth activation in layer-$(i+1)$ is obtained by applying an arbitrary function $f_k(\cdot)$ on the vector of activations in layer-i.

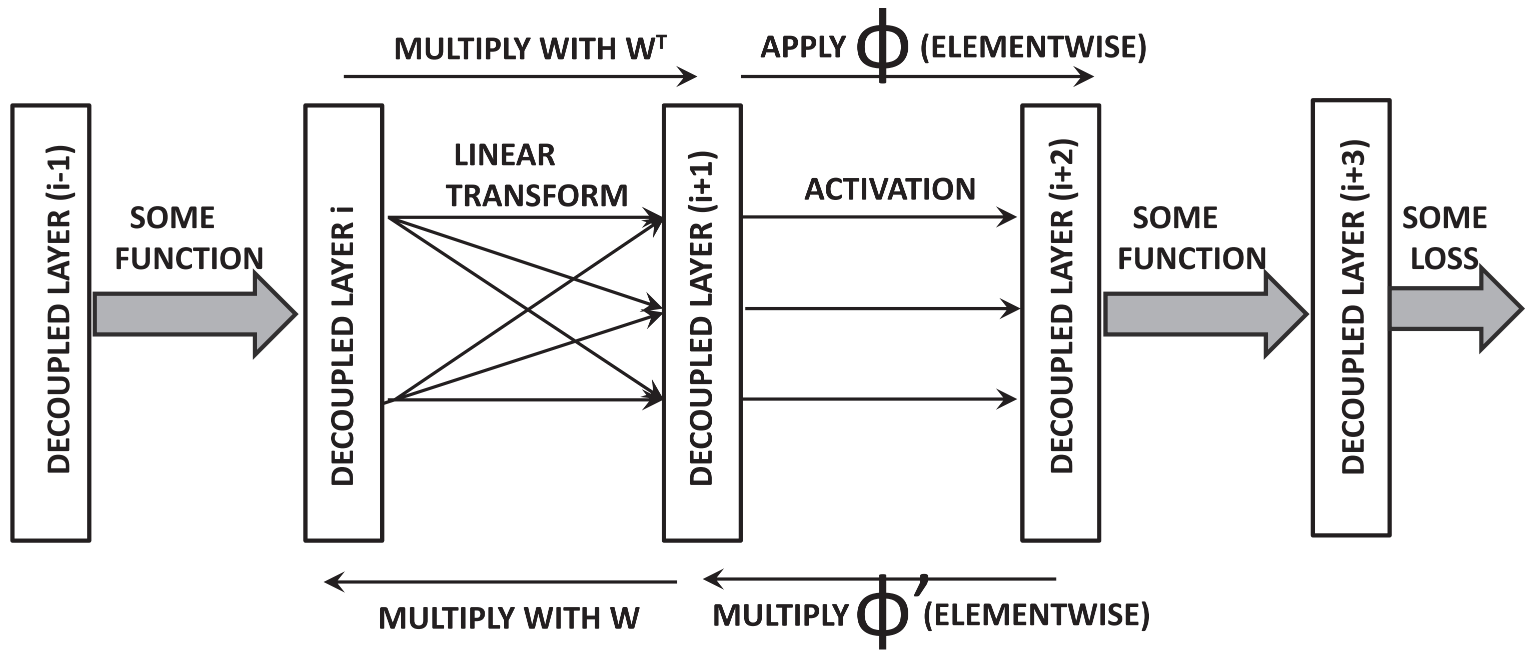
- Definition of Jacobian matrix entries:

$$J_{kr} = \frac{\partial f_k(\overline{z}_i)}{\partial \overline{z}_i^{(r)}} \tag{10}$$

- Backpropagation updates:

$$\overline{g}_i = J^T \overline{g}_{i+1} \tag{11}$$

Effect on Linear Layer and Activation Functions



- Backpropagation is multiplication with transposed weight matrix for linear layer.

- Elementwise multiplication with derivative for activation layer.

Table of Forward Propagation and Backward Propagation

Function	Forward	Backward
Linear	$\overline{z}_{i+1} = W^T \overline{z}_i$	$\overline{g}_i = W \overline{g}_{i+1}$
Sigmoid	$\overline{z}_{i+1} =$sigmoid$(\overline{z}_i)$	$\overline{g}_i = \overline{g}_{i+1} \odot \overline{z}_{i+1} \odot (1 - \overline{z}_{i+1})$
Tanh	$\overline{z}_{i+1} =$tanh$(\overline{z}_i)$	$\overline{g}_i = \overline{g}_{i+1} \odot (1 - \overline{z}_{i+1} \odot \overline{z}_{i+1})$
ReLU	$\overline{z}_{i+1} = \overline{z}_i \odot I(\overline{z}_i > 0)$	$\overline{g}_i = \overline{g}_{i+1} \odot I(\overline{z}_i > 0)$
Hard Tanh	Set to ± 1 ($\notin [-1, +1]$) Copy ($\in [-1, +1]$)	Set to 0 ($\notin [-1, +1]$) Copy ($\in [-1, +1]$)
Max	Maximum of inputs	Set to 0 (non-maximal inputs) Copy (maximal input)
Arbitrary function $f_k(\cdot)$	$\overline{z}_{i+1}^{(k)} = f_k(\overline{z}_i)$	$\overline{g}_i = J^T \overline{g}_{i+1}$ J is Jacobian (Equation 10)

- Two types of Jacobians: Linear layers are dense and activation layers are sparse.

- Maximization function used in max-pooling.

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Neural Network Training [Initialization, Preprocessing, Mini-Batching, Tuning, and Other Black Art]

Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.3

How to Check Correctness of Backpropagation

- Consider a particular weight w of a randomly selected edge in the network.

- Let $L(w)$ be the current value of the loss.

- The weight of this edge is perturbed by adding a small amount $\epsilon > 0$ to it.

- Estimate of derivative:
$$\frac{\partial L(w)}{\partial w} \approx \frac{L(w + \epsilon) - L(w)}{\epsilon} \tag{12}$$

- When the partial derivatives do not match closely enough, it might be indicative of an incorrectness in implementation.

What Does "Closely Enough" Mean?

- Algorithm-determined derivative is G_e and the approximate derivative is G_a.

$$\rho = \frac{|G_e - G_a|}{|G_e + G_a|} \tag{13}$$

- The ratio should be less than 10^{-6}.

- If ReLU is used, the ratio should be less than 10^{-3}.

- Should perform the checks for a sample of the weights a few times during training.

Stochastic Gradient Descent

- We have always worked with *point-wise* loss functions so far.
  - Corresponds to stochastic gradient descent.
  - In practice, stochastic gradient descent is only a randomized approximation of the true loss function.

- True loss function is typically additive over points.
  - **Example:** Sum-of-squared errors in regression.
  - Computing gradient over a single point is like sampled gradient estimate.

Mini-batch Stochastic Gradient Descent

- One can improve accuracy of gradient computation by using a batch of instances.
  - Instead of holding a vector of activations, we hold a matrix of activations in each layer.
  - Matrix-to-matrix multiplications required for forward and backward propagation.
  - Increases the memory requirements.
- Typical sizes are powers of 2 like 32, 64, 128, 256

Why Does Mini-Batching Work?

- At early learning stages, the weight vectors are very poor.
  - Training data is highly redundant in terms of important patterns.
  - Small batch sizes gives the correct direction of gradient.
- At later learning stages, the gradient direction becomes less accurate.
  - But some amount of noise helps avoid overfitting anyway!
- Performance on out-of-sample data does not deteriorate!

Feature Normalization

- **Standardization:** Normalize to zero mean and unit variance.

- **Whitening:** Transform the data to a de-correlated axis system with principal component analysis (mean-centered SVD).

  – Truncate directions with extremely low variance.

  – Standardize the other directions.

- **Basic principle:** Assume that data is generated from Gaussian distribution and give equal importance to all directions.

Weight Initialization

- Initializations are surprisingly important.
  - Poor initializations can lead to bad convergence behavior.
  - Instability across different layers (vanishing and exploding gradients).
- More sophisticated initializations such as pretraining covered in later lecture.
- Even some simple rules in initialization can help in conditioning.

Symmetry Breaking

- Bad idea to initialize weights to the same value.
  - Results in weights being updated in lockstep.
  - Creates redundant features.
- Initializing weights to random values breaks symmetry.
- Average magnitude of the random variables is important for stability.

Sensitivity to Number of Inputs

- More inputs increase output sensitivity to the average weight.
  - Additive effect of multiple inputs: variance linearly increases with number of inputs r.
  - Standard deviation scales with the square-root of number of inputs r.
- Each weight is initialized from Gaussian distribution with standard deviation $\sqrt{1/r}$ ($\sqrt{2/r}$ for ReLU).
- **More sophisticated:** Use standard deviation of $\sqrt{2/(r_{in} + r_{out})}$.

Tuning Hyperparameters

- Hyperparameters represent the parameters like number of layers, nodes per layer, learning rate, and regularization parameter.

- Use separate validation set for tuning.

- Do not use same data set for backpropagation training as tuning.

Grid Search

- Perform grid search over parameter space.
  - Select set of values for each parameter in some "reasonable" range.
  - Test over all combination of values.
- Careful about parameters at borders of selected range.
- **Optimization:** Search over coarse grid first, and then drill down into region of interest with finer grids.

How to Select Values for Each Parameter

- Natural approach is to select uniformly distributed values of parameters.
  - Not the best approach in many cases! $\Rightarrow$ Log-uniform intervals.
  - Search uniformly in reasonable values of log-values and then exponentiate.
  - **Example:** Uniformly sample log-learning rate between -3 and -1, and then raise it to the power of 10.

Sampling versus Grid Search

- With a large number of parameters, grid search is still expensive.

- With 10 parameters, choosing just 3 values for each parameter leads to $3^{10} = 59049$ possibilities.

- Flexible choice is to sample over grid space.

- Used more commonly in large-scale settings with good results.

Large-Scale Settings

- Multiple threads are often run with sampled parameter settings.

- Accuracy tracked on a separate out-of-sample validation set.

- Bad runs are detected and killed after a certain number of epochs.

- New runs may also be started after killing threads (if needed).

- Only a few winners are trained to completion and the predictions combined in an ensemble.

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Gradient Ratios, Vanishing and Exploding Gradient Problems

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Chapter 3, Section 3.4

Effect of Varying Slopes in Gradient Descent

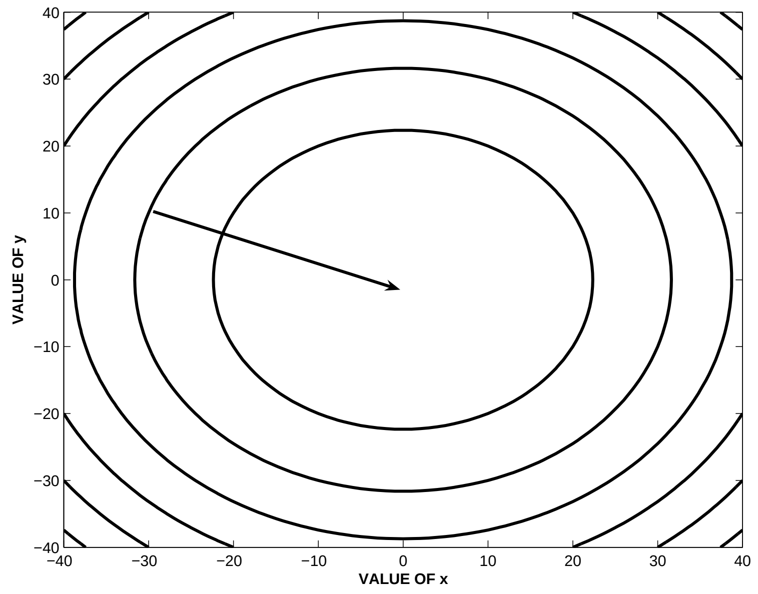
- Neural network learning is a *multivariable* optimization problem.

- Different weights have different magnitudes of partial derivatives.

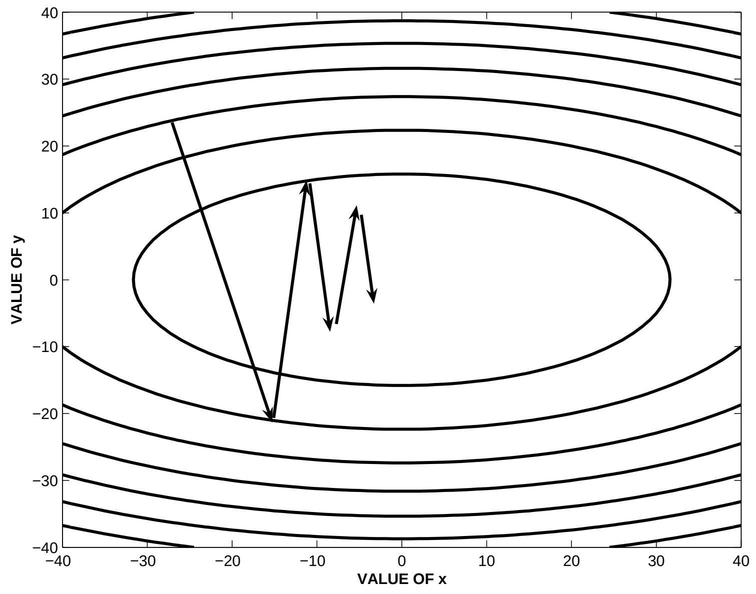
- Widely varying magnitudes of partial derivatives affect the learning.

- Gradient descent works best when the different weights have derivatives of similar magnitude.
  - *The path of steepest descent in most loss functions is only an instantaneous direction of best movement, and is not the correct direction of descent in the longer term.*

Example



(a) Loss function is circular bowl
$L = x^2 + y^2$



(b) Loss function is elliptical bowl
$L = x^2 + 4y^2$

- Loss functions with varying sensitivity to different attributes

Revisiting Feature Normalization

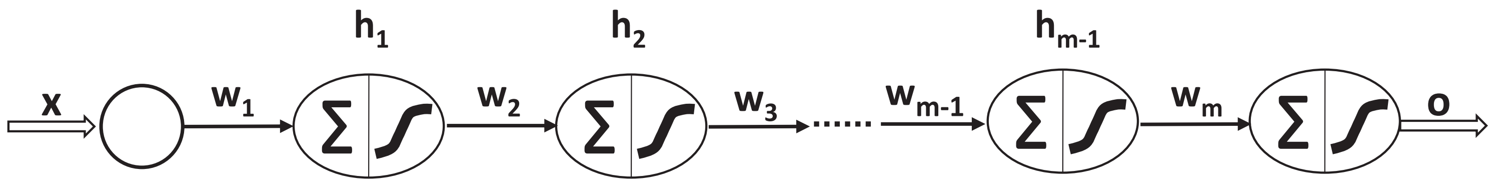
- In the previous lecture, we discussed feature normalization.
- When features have very different magnitudes, gradient ratios of different weights are likely very different.
- Feature normalization helps even out gradient ratios to some extent.
  - Exact behavior depends on target variable and loss function.

The Vanishing and Exploding Gradient Problems

- An extreme manifestation of varying sensitivity occurs in deep networks.

- The weights/activation derivatives in different layers affect the backpropagated gradient in a multiplicative way.
  - With increasing depth this effect is magnified.
  - The partial derivatives can either increase or decrease with depth.

Example



- Neural network with one node per layer.

- Forward propagation multiplicatively depends on each weight and activation function evaluation.

- Backpropagated partial derivative get multiplied by weights and activation function derivatives.

- Unless the values are exactly one, the partial derivatives will either continuously increase (explode) or decrease (vanish).

- Hard to initialize weights exactly right.

Activation Function Propensity to Vanishing Gradients

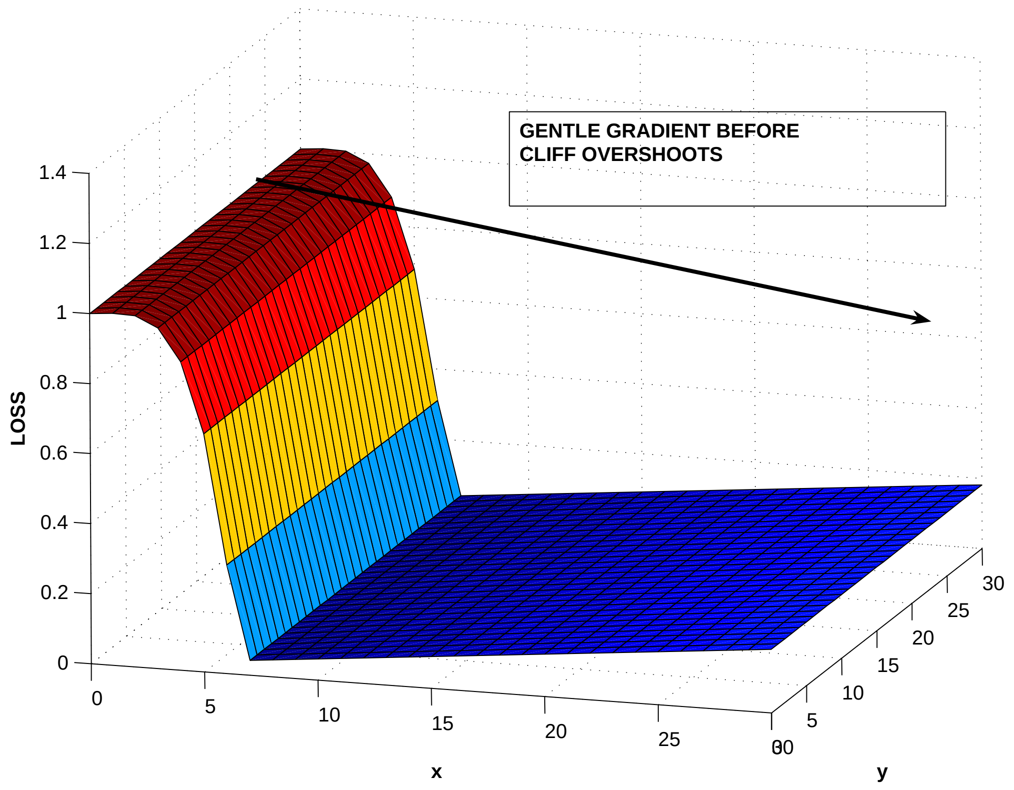
- Partial derivative of sigmoid with output $o \Rightarrow o(1 - o)$.
  - Maximum value at $o = 0.5$ of 0.25.
  - For 10 layers, the activation function alone will multiply by less than $0.25^{10} \approx 10^{-6}$.
- At extremes of output values, the partial derivative is close to 0, which is called *saturation*.
- The tanh activation function with partial derivative $(1 - o^2)$ has a maximum value of 1 at $o = 0$, but saturation will still cause problems.

Exploding Gradients

- Initializing weights to very large values to compensate for the activation functions can cause exploding gradients.

- Exploding gradients can also occur when weights across different layers are shared (e.g., recurrent neural networks).
  - The effect of a finite change in weight is extremely unpredictable across different layers.
  - Small *finite* change changes loss negligibly, but a slightly larger value might change loss drastically.

Cliffs



- Often occurs with the exploding gradient problem.

A Partial Fix to Vanishing Gradients

- The ReLU has linear activation for nonnegative values and otherwise sets outputs to 0.

- The ReLU has a partial derivative of 1 for nonnegative inputs.

- However, it can have a partial derivative of 0 in some cases and never get updated.
  - Neuron is permanently dead!

Leaky ReLU

- For negative inputs, the leaky ReLU can still propagate some gradient backwards.
  - At the reduced rate of $\alpha < 1$ times the learning case for nonnegative inputs:

$$\Phi(v) = \begin{cases} \alpha \cdot v & v \leq 0 \\ v & \text{otherwise} \end{cases} \tag{14}$$

- The value of α is a hyperparameter chosen by the user.

- The gains with the leaky ReLU are not guaranteed.

Maxout

- The activation used is $\max\{\overline{W_1}\cdot\overline{X}, \overline{W_2}\cdot\overline{X}\}$ with two coefficient vectors.

- One can view the maxout as a generalization of the ReLU.
  - The ReLU is obtained by setting one of the coefficient vectors to 0.
  - The leaky ReLU can also be simulated by setting the other coefficient vector to $\overline{W_2} = \alpha\overline{W_1}$.

- Main disadvantage is that it doubles the number of parameters.

Gradient Clipping for Exploding Gradients

- Try to make the different components of the partial derivatives more even.
  - *Value-based clipping:* All partial derivatives outside ranges are set to range boundaries.
  - *Norm-based clipping:* The entire gradient vector is normalized by the L_2-norm of the entire vector.
- One can achieve a better conditioning of the values, so that the updates from mini-batch to mini-batch are roughly similar.
- Prevents an anomalous gradient explosion during the course of training.

Other Comments on Vanishing and Exploding Gradients

- The methods discussed above are only partial fixes.

- Other fixes discussed in later lectures:
  - Stronger initializations with pretraining.
  - Second-order learning methods that make use of second-order derivatives (or *curvature* of the loss function).

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First-Order Gradient Descent Methods

Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.5

First-Order Descent

- First-order methods work with steepest-descent directions.

- Modifications to basic form of steepest-descent:
  - Need to reduce step sizes with algorithm progression.
  - Need a way of avoiding local optima.
  - Need to address widely varying slopes with respect to different weight parameters.

Learning Rate Decay

- Initial learning rates should be high but reduce over time.

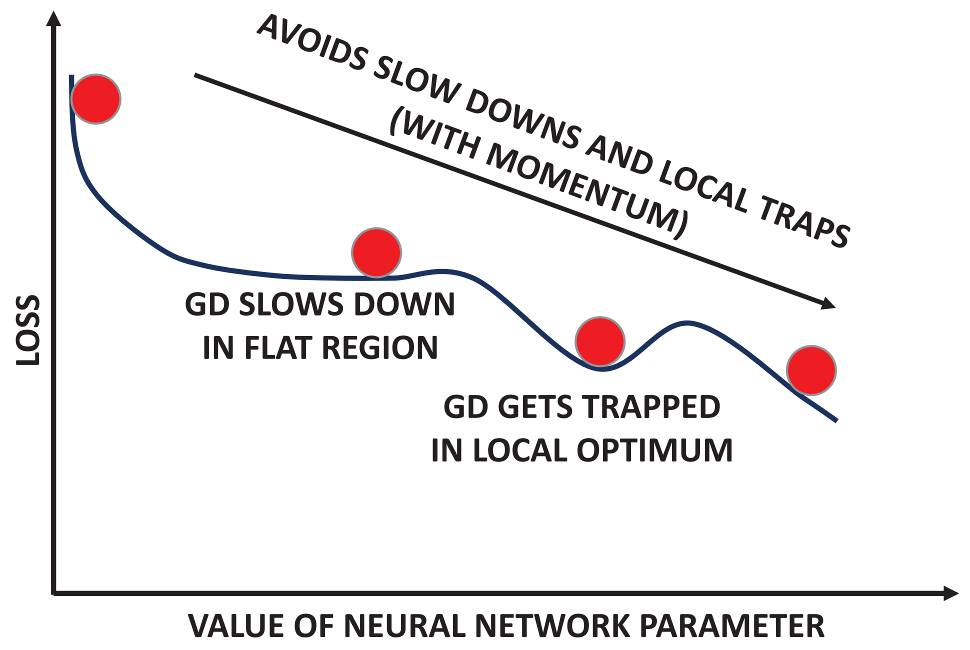
- The two most common decay functions are *exponential decay* and *inverse decay*.

- The learning rate α_t can be expressed in terms of the initial decay rate α_0 and epoch t as follows:

$$\alpha_t = \alpha_0 \exp(-k \cdot t) \quad \text{[Exponential Decay]}$$
$$\alpha_t = \frac{\alpha_0}{1 + k \cdot t} \quad \text{[Inverse Decay]}$$

  The parameter k controls the rate of the decay.

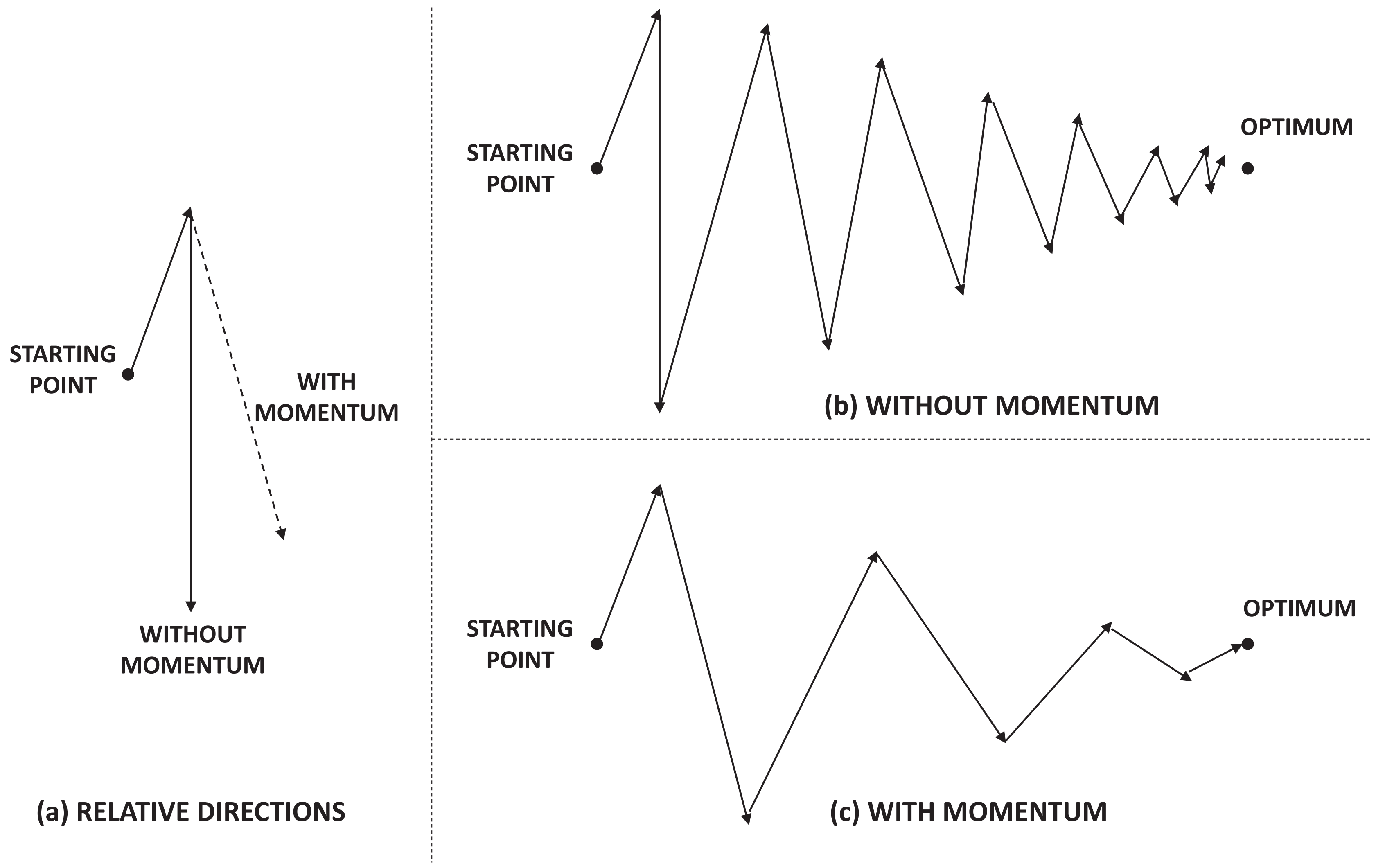
Momentum Methods: Marble Rolling Down Hill



- Use a *friction parameter* $\beta \in (0, 1)$ to gain speed in direction of movement.

$$\overline{V} \Leftarrow \beta \overline{V} - \alpha \frac{\partial L}{\partial \overline{W}}; \quad \overline{W} \Leftarrow \overline{W} + \overline{V}$$

Avoiding Zig-Zagging with Momentum



Nesterov Momentum

- Modification of the traditional momentum method in which *the gradients are computed at a point that would be reached after executing a β-discounted version of the previous step again*.

- Compute at a point reached using only the momentum portion of the current update:

$$\overline{V} \Leftarrow \underbrace{\beta\overline{V}}_{\text{Momentum}} - \alpha\frac{\partial L(\overline{W} + \beta\overline{V})}{\partial\overline{W}}; \quad \overline{W} \Leftarrow \overline{W} + \overline{V}$$

- Put on the brakes as the marble reaches near bottom of hill.

- Nesterov momentum should always be used with mini-batch SGD (rather than SGD).

AdaGrad

- *Aggregate* squared magnitude of ith partial derivative in A_i.

- The square-root of A_i is proportional to the root-mean-square slope.

  – The absolute value will increase over time.

$$A_i \Leftarrow A_i + \left(\frac{\partial L}{\partial w_i}\right)^2 \quad \forall i \tag{15}$$

- The update for the ith parameter w_i is as follows:

$$w_i \Leftarrow w_i - \frac{\alpha}{\sqrt{A_i}}\left(\frac{\partial L}{\partial w_i}\right); \quad \forall i \tag{16}$$

- Use $\sqrt{A_i + \epsilon}$ in the denominator to avoid ill-conditioning.

AdaGrad Intuition

- Scaling the derivative inversely with $\sqrt{A_i}$ encourages faster *relative* movements along gently sloping directions.
  - Absolute movements tend to slow down prematurely.
  - Scaling parameters use stale values.

RMSProp

- The RMSProp algorithm uses *exponential smoothing* with parameter $\rho \in (0, 1)$ in the relative estimations of the gradients.
  - Absolute magnitudes of scaling factors do not grow with time.
  - Problem of staleness is ameliorated.

$$A_i \Leftarrow \rho A_i + (1-\rho)\left(\frac{\partial L}{\partial w_i}\right)^2 \quad \forall i \tag{17}$$

$$w_i \Leftarrow w_i - \frac{\alpha}{\sqrt{A_i}}\left(\frac{\partial L}{\partial w_i}\right); \quad \forall i$$

- Use $\sqrt{A_i + \epsilon}$ to avoid ill-conditioning.

RMSProp with Nesterov Momentum

- Possible to combine RMSProp with Nesterov Momentum

$$v_i \Leftarrow \beta v_i - \frac{\alpha}{\sqrt{A_i}} \left(\frac{\partial L(\overline{W} + \beta \overline{V})}{\partial w_i} \right); \quad w_i \Leftarrow w_i + v_i \quad \forall i$$

- Maintenance of A_i is done with shifted gradients as well.

$$A_i \Leftarrow \rho A_i + (1-\rho) \left(\frac{\partial L(\overline{W} + \beta \overline{V})}{\partial w_i} \right)^2 \quad \forall i \tag{18}$$

AdaDelta and Adam

- Both methods derive intuition from RMSProp
  - AdaDelta track of an exponentially smoothed value of the *incremental changes* of weights Δw_i in previous iterations to decide parameter-specific learning rate.
  - Adam keeps track of exponentially smoothed gradients from previous iterations (in addition to normalizing like RMSProp).
- Adam is extremely popular method.

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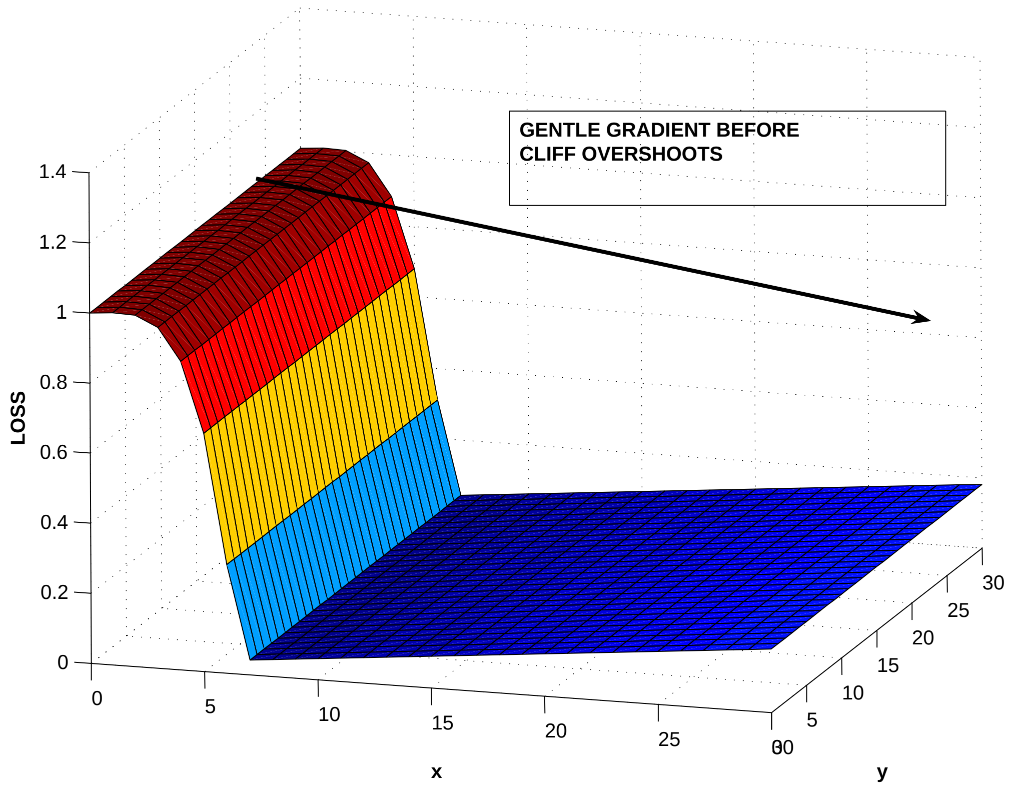
Second-Order Gradient Descent Methods

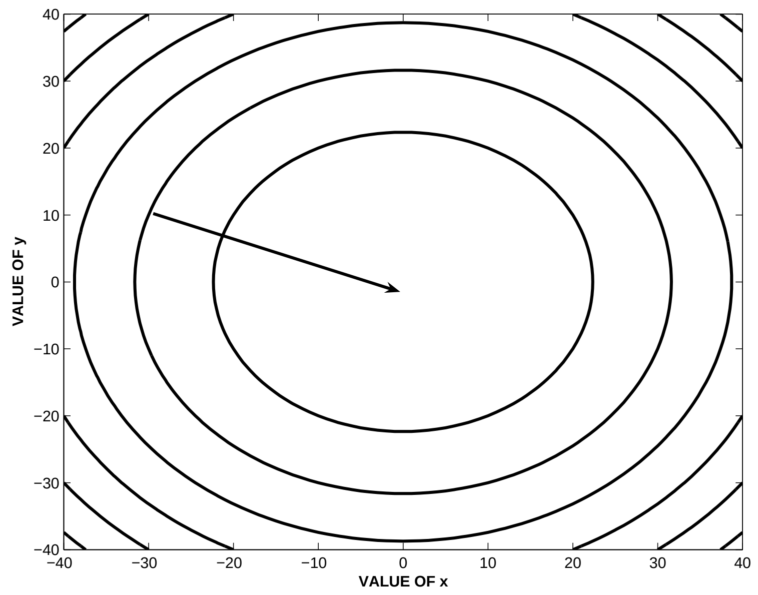
Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.5.5

Why Second-Order Methods?

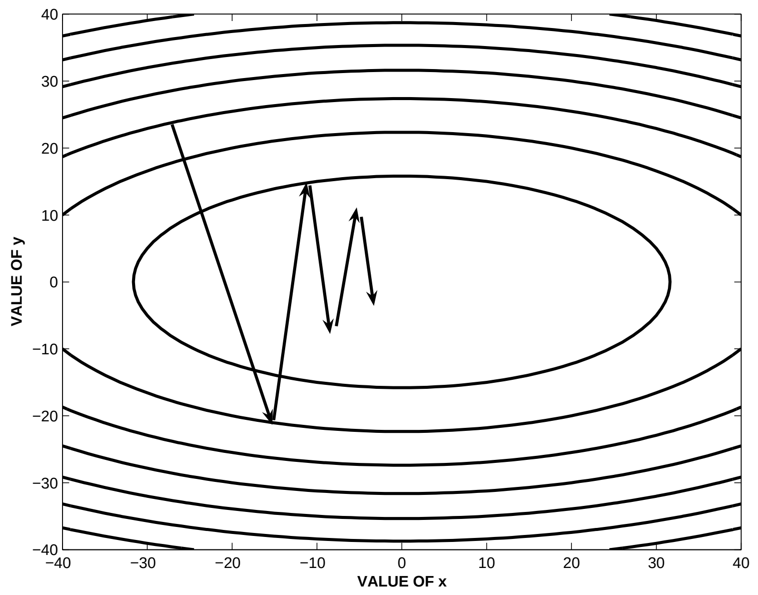


- First-order methods are not enough when there is curvature.

Revisiting the Bowl



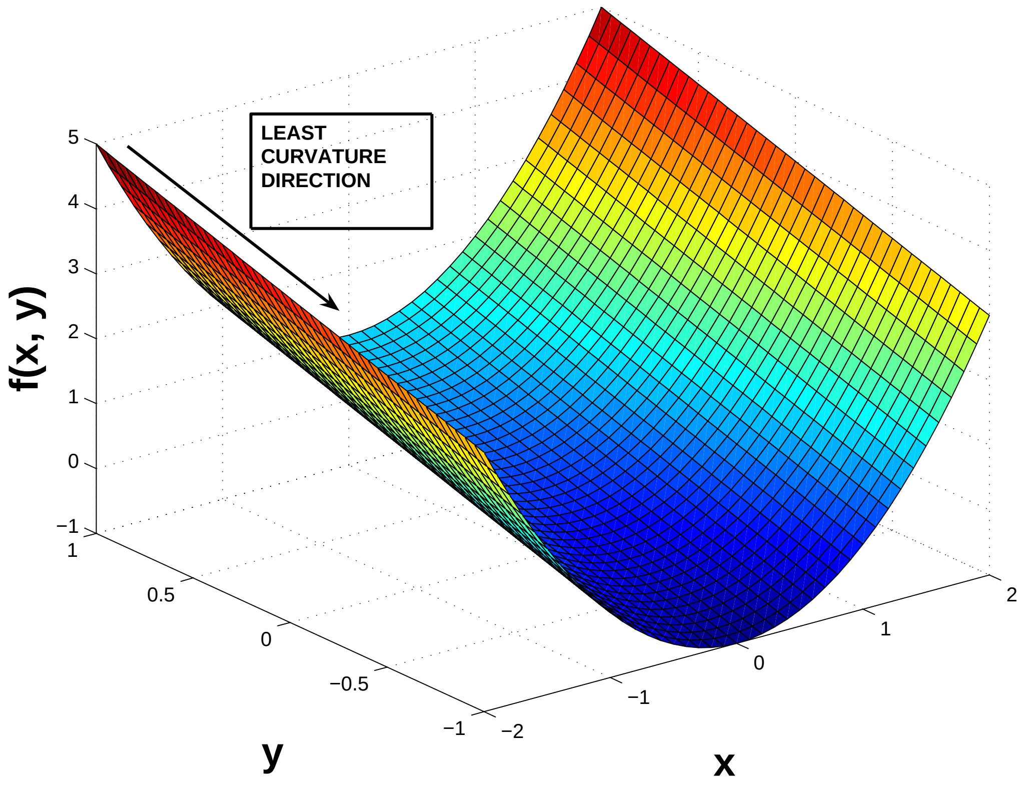
(a) Loss function is circular bowl $L = x^2 + y^2$



(b) Loss function is elliptical bowl $L = x^2 + 4y^2$

- High curvature directions cause bouncing in spite of higher gradient $\Rightarrow$ Need second-derivative for more information.

A Valley



- Gently sloping directions are better with less curvature!

The Hessian

- The second-order derivatives of the loss function $L(\overline{W})$ are of the following form:

$$H_{ij} = \frac{\partial^2 L(\overline{W})}{\partial w_i \partial w_j}$$

- The partial derivatives use all pairwise parameters in the denominator.

- For a neural network with d parameters, we have a $d \times d$ *Hessian matrix* H, for which the (i, j)th entry is H_{ij}.

Quadratic Approximation of Loss Function

- One can write a quadratic approximation of the loss function with Taylor expansion about $\overline{W_0}$:

$$L(\overline{W}) \approx L(\overline{W}_0)+(\overline{W}-\overline{W}_0)^T[\nabla L(\overline{W}_0)]+\frac{1}{2}(\overline{W}-\overline{W}_0)^T H(\overline{W}-\overline{W}_0) \tag{19}$$

- One can derive a single-step optimality condition from initial point $\overline{W_0}$ by setting the gradient to 0.

Newton's Update

- Can solve quadratic approximation in one step from initial point $\overline{W}_0$.

  $\nabla L(\overline{W}) = 0$ [Gradient of Loss Function]
  $\nabla L(\overline{W}_0) + H(\overline{W} - \overline{W}_0) = 0$ [Gradient of Taylor approximation]

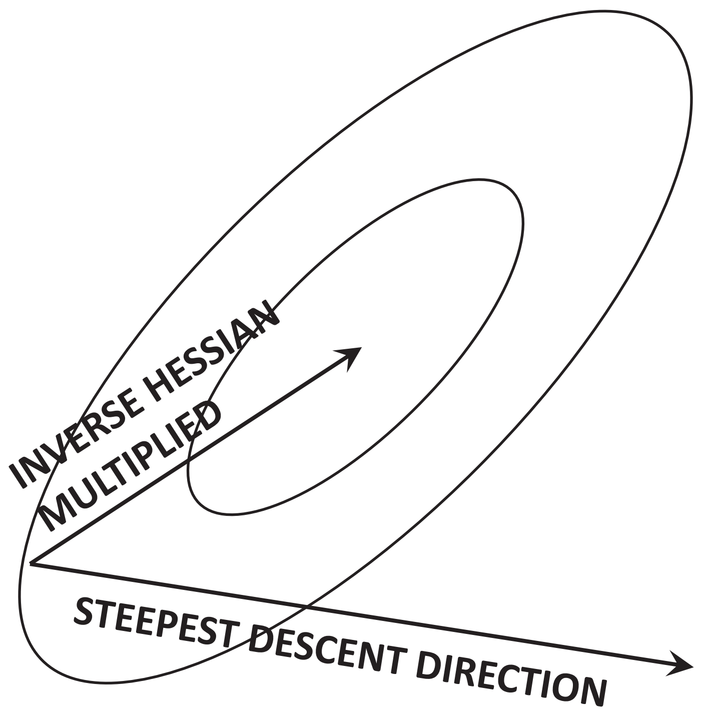
- Rearrange optimality condition to obtain Newton update:

$$\overline{W}^* \Leftarrow \overline{W}_0 - H^{-1}[\nabla L(\overline{W}_0)] \tag{20}$$

- Note the ratio of first-order to second-order $\Rightarrow$ Trade-off between speed and curvature

- Step-size not needed!

Why Second-Order Methods?



- Pre-multiplying with the inverse Hessian finds a trade-off between speed of descent and curvature.

Basic Second-Order Algorithm and Approximations

- Keep making Newton's updates to convergence (single step needed for quadratic function)
  - Even computing the Hessian is difficult!
  - Inverting it is even more difficult
- Solutions:
  - Approximate the Hessian.
  - Find an algorithm that works with projection $H\overline{v}$ for some direction $\overline{v}$.

Conjugate Gradient Method

- Get to optimal in d steps (instead of single Newton step) where d is number of parameters.

- Use optimal step-sizes to get best point along a direction.

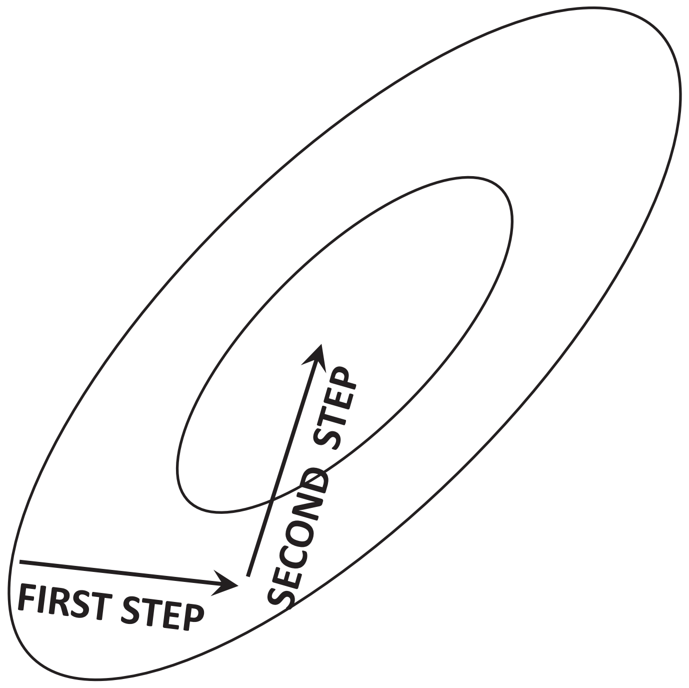
- *Thou shalt not worsen with respect to previous directions!*

- **Conjugate direction:** The gradient of the loss function on *any* point on an update direction is always orthogonal to the previous update directions.

$$\overline{q}_{t+1} = -\nabla L(\overline{W}_{t+1}) + \left(\frac{\overline{q}_t^T H [\nabla L(\overline{W}_{t+1})]}{\overline{q}_t^T H \overline{q}_t} \right) \overline{q}_t \tag{21}$$

- For quadratic function, it requires d updates instead of single update of Newton method.

Conjugate Gradients on 2-Dimensional Quadratic



- Two conjugate directions are required to reach optimality

Conjugate Gradient Algorithm

- For quadratic functions only.
  - Update $\overline{W}_{t+1} \Leftarrow \overline{W}_t + \alpha_t \overline{q}_t$. Here, the step size α_t is computed using line search.
  - Set $\overline{q}_{t+1} = -\nabla L(\overline{W}_{t+1}) + \left(\frac{\overline{q}_t^T H[\nabla L(\overline{W}_{t+1})]}{\overline{q}_t^T H \overline{q}_t}\right) \overline{q}_t$. Increment t by 1.

- For non-quadratic functions approximate loss function with Taylor expansion and perform $\ll d$ of the above steps. Then repeat.

Efficiently Computing Projection of Hessian

- The update requires computation of the *projection* of the Hessian rather than inversion of Hessian.

$$\overline{q}_{t+1} = -\nabla L(\overline{W}_{t+1}) + \left(\frac{\overline{q}_t^T H[\nabla L(\overline{W}_{t+1})]}{\overline{q}_t^T H \overline{q}_t}\right) \overline{q}_t \tag{22}$$

- Easy to perform numerically!

$$H\overline{v} \approx \frac{\nabla L(\overline{W}_0 + \delta \overline{v}) - \nabla L(\overline{W}_0)}{\delta} \tag{23}$$

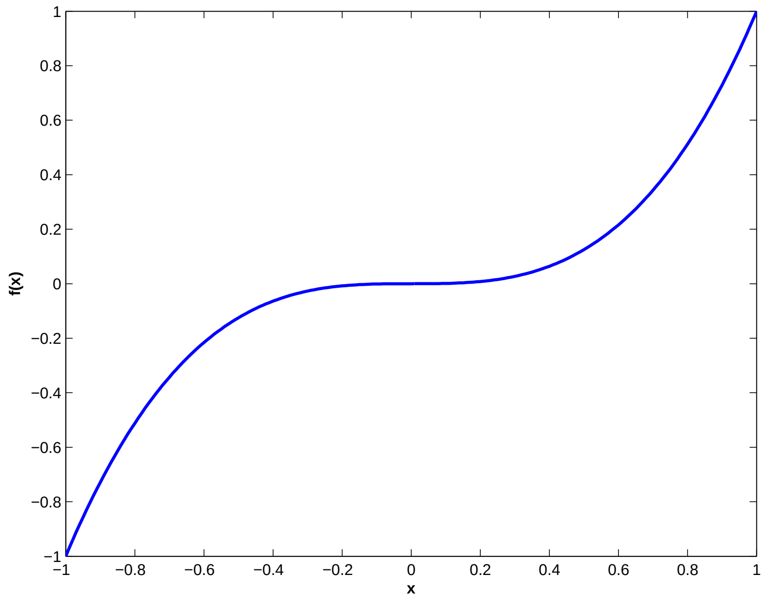
Other Second-Order Methods

- *Quasi-Newton Method:* A sequence of increasingly accurate approximations of the inverse Hessian matrix are used in various steps.

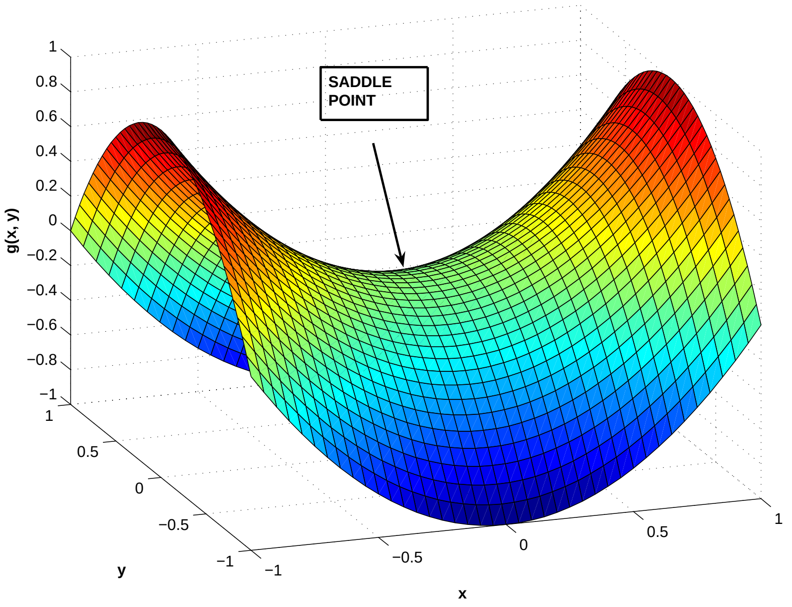
- Many variations of this approach.

- Commonly-used update is BFGS, which stands for the Broyden–Fletcher–Goldfarb–Shanno algorithm and its limited memory variant L-BFGS.

Problems with Second-Order Methods



(a) $f(x) = x^3$
Degenerate



(b) $f(x) = x^2 - y^2$
Stationary

- Saddle points: Whether it is maximum or minimum depends on which direction we approach it from.

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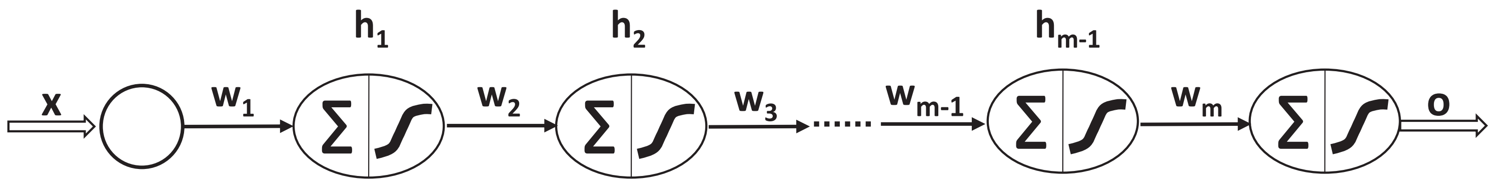
Batch Normalization

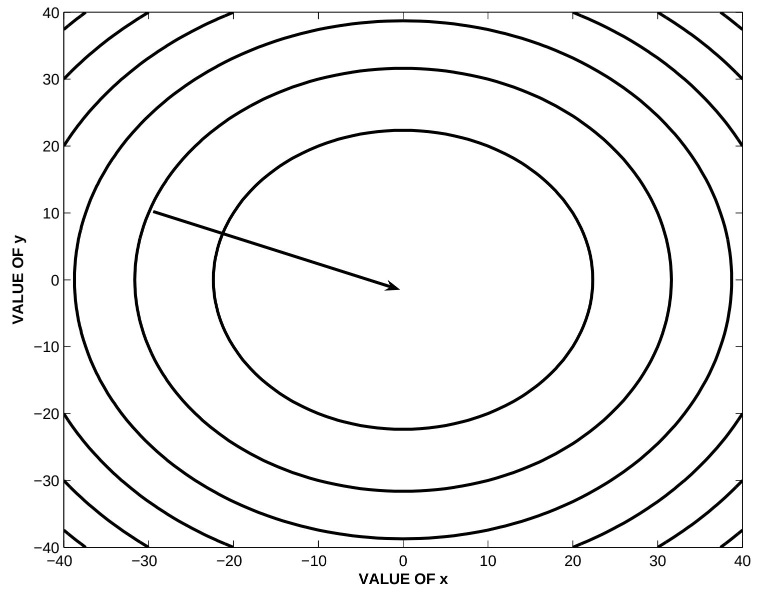
Neural Networks and Deep Learning, Springer, 2018
Chapter 3, Section 3.6

Revisiting the Vanishing and Exploding Gradient Problems

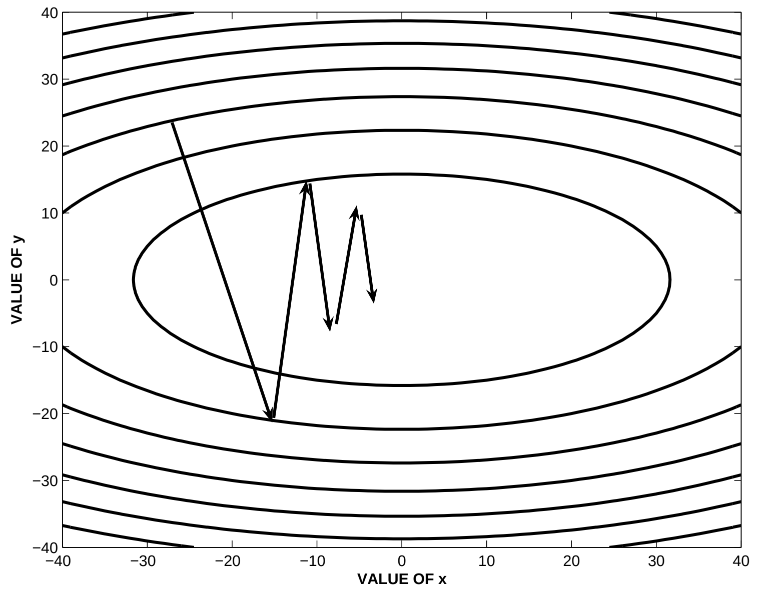


- Neural network with one node per layer.
- Forward propagation multiplicatively depends on each weight and activation function evaluation.
- Backpropagated partial derivative get multiplied by weights and activation function derivatives.
- Unless the values are exactly one, the partial derivatives will either continuously increase (explode) or decrease (vanish).
- Hard to initialize weights exactly right.

Revisiting the Bowl



(a) Loss function is circular bowl $L = x^2 + y^2$



(b) Loss function is elliptical bowl $L = x^2 + 4y^2$

- Varying scale of different parameters will cause bouncing
- Varying scale of features causes varying scale of parameters

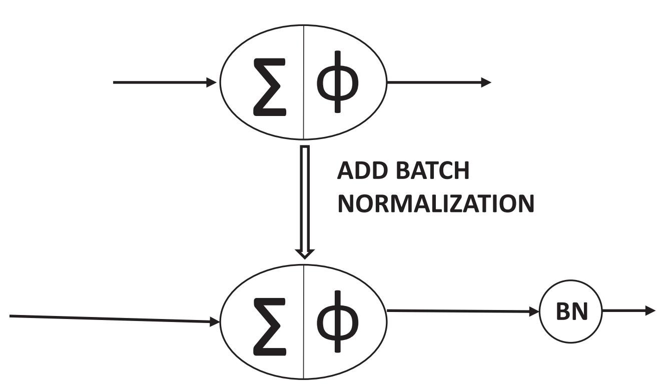
Input Shift

- One can view the input to each layer as a shifting data set of hidden activations during training.

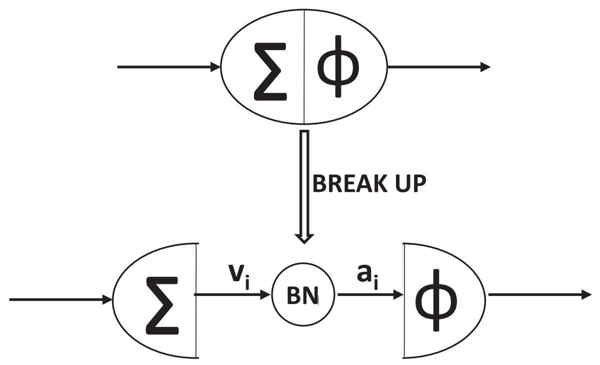
- A shifting input causes problems during learning.
  - Convergence becomes slower.
  - Final result may not generalize well because of unstable inputs.

- Batch normalization ensures (somewhat) more stable inputs to each layer.

Solution: Batch Normalization



(a) Post-activation normalization



(b) Pre-activation normalization

- Add an additional layer than normalizes in *batch-wise* fashion.

- Additional learnable parameters to ensure that optimal level of nonlinearity is used.

- Pre-activation normalization more common than post-activation normalization.

Batch Normalization Node

- The ith unit contains two parameters β_i and γ_i that need to be learned.

- Normalize over *batch* of m instances for ith unit.

$$\mu_i = \frac{\sum_{r=1}^{m} v_i^{(r)}}{m} \quad \forall i \qquad \text{[Batch Mean]}$$

$$\sigma_i^2 = \frac{\sum_{r=1}^{m} (v_i^{(r)} - \mu_i)^2}{m} + \epsilon \quad \forall i \qquad \text{[Batch Variance]}$$

$$\hat{v}_i^{(r)} = \frac{v_i^{(r)} - \mu_i}{\sigma_i} \quad \forall i, r \qquad \text{[Normalize Batch Instances]}$$

$$a_i^{(r)} = \gamma_i \cdot \hat{v}_i^{(r)} + \beta_i \quad \forall i, r \qquad \text{[Scale with Learnable Parameters]}$$

- Why do we need β_i and γ_i?
  - Most activations will be near zero (near-linear regime).

Changes to Backpropagation

- We need to backpropagate through the newly added layer of normalization nodes.
  - The BN node can be treated like any other node.
- We want to optimize the parameters β_i and γ_i.
  - The gradients with respect to these parameters are computed during backpropagation.
- Detailed derivations in book.

Issues in Inference

- The transformation parameters μ_i and σ_i depend on the batch.

- How should one compute them during testing when a *single* test instance is available?

- The values of μ_i and σ_i are computed up front using the *entire* population (of training data), and then treated as constants during testing time.

  – One can also maintain exponentially weighted averages during training.

- The normalization is a simple linear transformation during inference.

Batch Normalization as Regularizer

- Batch normalization also acts as a regularizer.
- Same data point can cause somewhat different updates depending on which batch it is included in.
- One can view this effect as a kind of noise added to the update process.
- Regularization is can be shown to be equivalent to adding a small amount of noise to the training data.
- The regularization is relatively mild.