Calculus

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Outline

- Motivation
- Derivatives
- Optimization
- Neural network training
- Universal approximation
- References

Motivation

Optimization And Approximation

 Neural network training is an optimization problem that we solve using calculus (math highlights listed, obviously others also present)

Forward propagation

- linear algebra

Error calculation

- probability*

Backward propagation

- calculus

Weight update

- calculus

- Neural networks are universal approximators
 - General tool for solving feature extraction and prediction problems
 - A constructive proof provides some feel for how problem complexity and network design are related

^{*} Though in this lecture probability is not explicitly used, it will be covered later

Derivatives

- Scalar functions of a single variable: y = f(x)
 - f: $R \rightarrow R$

Definition of the derivative

$$df/dx = \lim_{\Delta x \to 0} (f(x + \Delta x) - f(x)) / \Delta x$$

- Interpretation
 - The derivative is a linear operator that maps functions to function
 - Intuition of sensitivity of function f to changes in input x

- Differentiable functions
 - At values of x where the limit exists f is differentiable
- Non differentiable functions
 - At values of x where the limit does not exists f is not differentiable
 - If there are a countable number of non differentiable values then it's potentially possible to approximate the derivative of f at a value where it's not differentiable via the derivative just to the left or right (or any derivative in this range)

- Example: sigmoid
 - $f(x) = 1/(1 + e^{-x})$
 - df/dx = f(x)(1 f(x))
- Example: tanh
 - $f(x) = (e^x e^{-x}) / (e^x + e^{-x})$
 - $df/dx = 1 f^2(x)$
- Example: ReLU
 - f(x) = max(0, x)
 - $df/dx = 0, x \le 0$ note that at $x = 0, df/dx \in [0, 1]$ = 1, x > 0

Product rule

- h(x) = f(x) g(x)• dh/dx = (df/dx) g(x) + f(x) (dg/dx)
- Quotient rule

```
• h(x) = f(x) / g(x)

• dh/dx = ((df/dx) g(x) - f(x) (dg/dx)) / g^{2}(x) general case

= - (dg/dx) / g^{2}(x) f(x) = 1 case
```

Chain rule

```
• h(x) = f(g(x)) and define u = g(x)
• dh/dx = (df/du) (du/dx)
```

- Scalar function of multiple variables: y = f(x)
 - f: $R^K \rightarrow R$
 - $\mathbf{x} = [x_0 \ x_1 \ ... \ x_{K-1}]^T$

- Partial derivative
 - Let **e**_k be coordinate direction k
 - $\partial f/\partial x_k = \lim_{\Delta \to 0} (f(\mathbf{x} + \Delta \mathbf{e}_k) f(\mathbf{x})) / \Delta$
- Interpretation
 - View all variables x_n where $n \neq k$ as constants
 - Take derivative of f at x with respect to x_k
 - Result is slope of the function f at point x in coordinate direction e_k

Gradient

- K x 1 vector of partial derivatives with respect to each variable
- $\nabla f(\mathbf{x}) = [(\partial f/\partial x_0) (\partial f/\partial x_1) \dots (\partial f/\partial x_{K-1})]^T$

Interpretation

- Same shape and dimension as x (note this is choosing denominator layout)
- Points in direction of maximum change of f at x
- When doing iterative error minimization we're typically going to figure out the
 gradient of the error with respect to the parameters (i.e., the sensitivity of the error
 to changes in the parameters) and adjust the parameters in the opposite direction
 of the gradient to reduce the error
- Directional derivative in unit vector direction \mathbf{u} can be found from $(\nabla f(\mathbf{x}))^T \mathbf{u}$

- Examples
 - Linear algebra
 - Vector vector multiplication

•
$$f(x)$$
 = $a^T x = x^T a$
• $\partial f/\partial x$ = a

• Vector matrix vector multiplication

```
• f(x) = x^T A x

• \partial f/\partial x = (A + A^T) x General case

= 2 A x Symmetric A case
```

- Examples (continued)
 - Error calculation
 - x* is ideal value
 - Mean square error

•
$$f(x^*, x) = (1/K) (x - x^*)^T (x - x^*)$$

• $\partial f/\partial x = (2/K) (x - x^*)$

- Cross entropy
 - Assume log base e for convenience so no extra scale values

```
• f(\mathbf{x}^*, \mathbf{x}) = -\sum_k \mathbf{x}^*(k) \log(\mathbf{x}(k)) we'll talk about this in the probability lecture \mathbf{x}^* has a 1 at position \mathbf{k}^* and 0s elsewhere 

• \partial f/\partial \mathbf{x} = -1/(\mathbf{x}(\mathbf{k}^*)) at \mathbf{k} = \mathbf{k}^* at \mathbf{k} \neq \mathbf{k}^*
```

• The $\partial f/\partial x$ vector only having 1 non 0 element will allow the product of the derivative of the softmax function and cross entropy function to have a very nice form

- Vector functions of multiple variables: y = f(x)
 - f: $R^K \rightarrow R^M$

- Jacobian
 - M x K matrix with entry (m, k) corresponding to the partial derivative of output f_m with respect to input variable x_k

$$J_{f}(\mathbf{x}) = \begin{bmatrix} \partial f_{0} / \partial x_{0} & \cdots & \partial f_{0} / \partial x_{K-1} \\ \vdots & & \vdots \\ \partial f_{M-1} / \partial x_{0} & \cdots & \partial f_{M-1} / \partial x_{K-1} \end{bmatrix}$$

- Interpretation
 - Above definition in numerator layout to match common calculus convention
 - All other derivatives used in this presentation not on this specific slide will be in denominator layout
 - Will use to reflect error gradients through layers
 - Optimal linear approximation of a vector valued function near a point a

$$f(x) \approx f(a) + J_f(a)(x - a)$$

(note: $f^T(H, x) = x^T H^T$, $\partial f^T / \partial H^T = x$, $\partial f / \partial H = x^T$)

Vector Functions Of Multiple Variables

- Examples with parameters
 - Linear transformations
 - Matrix vector multiplication

```
• f(H, x) = H x
• \partial f/\partial x = H^T
```

•
$$\partial f/\partial H = \mathbf{x}^T$$

Matrix matrix multiplication

•
$$f(H, X) = H X$$

- Via matrix vector multiplication with vectorized X and block diagonal H
- CNN style 2D convolution

```
• f(HNoxNixFrxFc, XNixLrxLc) = HNoxNixFrxFc * XNixLrxLc
```

Via CNN style 2D convolution decomposed into using a sum of 1x1 filters leading to a sum
of matrix matrix mults

- Examples with parameters (continued)
 - Elementwise operations
 - Elementwise addition

```
• f(H, X) = X + H
• \partial f/\partial X = I
```

Elementwise multiplication

```
• f(H, X) = H \odot X
```

•
$$\partial f/\partial X = H^T$$

•
$$\partial f/\partial H = X^T$$

- Examples without parameters
 - Note: since there are no parameters only $\partial f/\partial x$ needs to be computed
 - Pointwise operations
 - Fixed scale
 - $f(X) = \alpha X$
 - $\partial f/\partial X = \alpha I$
 - ReLU, sigmoid, tanh
 - Conceptually a pointwise application of scalar derivative rules forms a diagonal matrix
 - Though in practice for efficiency only the diagonal values are generated

To do: add specific equations; currently just lists rules that will be used in back propagation

- Examples without parameters (continued)
 - Pooling
 - Average
 - Divide the gradient at the output equally to form the gradient at all the inputs
 - Max
 - Send gradient at output to the max input that created it
 - Requires saving the max index from the forward path for each output
 - Structural operations
 - Split
 - Add all gradients at the output to form the gradient at the input

To do: get better formatting for the matrix

- Examples without parameters (continued)
 - Error calculation
 - Softmax
 - No parameters so only $\partial f/\partial x$ needs to be computed

```
• f(\mathbf{x}) = (1/(\Sigma_k e^{x(k)})) [e^{x(0)} e^{x(1)} ... e^{x(K-1)}]^T
```

```
• \partial f/\partial x = [f(0)(1-f(0)) -f(1)f(0) ... -f(K-1)f(0)]

[-f(0)f(1) f(1)(1-f(1)) -f(K-1)f(1)]

[... -f(0)f(K-1) -f(1)f(K-1) f(K-1)]
```

- Chain rule
 - h(x) = f(g(x)) and define u = g(x)
 - $\partial h/\partial x = (\partial u/\partial x) (\partial f/\partial u)$

Note denominator layout ordering

- Example: softmax cross entropy error gradient for classification
 - p* has a 1 at position k* and 0s elsewhere

```
• \mathbf{p} = softmax(\mathbf{x}), Like \mathbf{u} = \mathbf{g}(\mathbf{x})
• \mathbf{f}(\mathbf{p}) = \mathbf{H}_{CF}(\mathbf{p}^*, \mathbf{p}), Like \mathbf{f}(\mathbf{u})
```

•
$$e(x) = H_{CE}(p^*, softmax(x)),$$
 Like $h(x) = f(g(x))$

•
$$\partial e/\partial x = (\partial p/\partial x) (\partial f/\partial p)$$

= $[p(0) ... p(k*-1) (p(k*)-1) p(k*+1) ... p(K-1)]^T$

Optimization

Setup

- Optimization problem
 - Minimize $f_0(\mathbf{x})$
 - Subject to $f_c(\mathbf{x}) \le b_c$, c = 1, ..., C

Objective function

Constraint functions

- Solution
 - x* is the optimal solution if it has the smallest objective value out of all vectors that satisfy the constraints
- A few special classes of optimization problems
 - Convex: $f_i(\alpha \mathbf{x}_0 + \beta \mathbf{x}_1) \le \alpha f_i(\mathbf{x}_0) + \beta f_i(\mathbf{x}_1)$, i = 0, 1, ..., C, $\alpha + \beta = 1$, $\alpha \ge 0$, $\beta \ge 0$
 - Linear: $f_i(\alpha \mathbf{x}_0 + \beta \mathbf{x}_1) = \alpha f_i(\mathbf{x}_0) + \beta f_i(\mathbf{x}_1)$, i = 0, 1, ..., C

Setup

Critical points

- For a scalar function of multiple variables a critical point is a value x at which all partial derivatives of f(x) are 0
- Local extrema of f(x) occur at critical points (Fermat's theorem)
 - Minimum (in all directions)
 - Maximum (in all directions)
 - Saddle (minimum in some directions, maximum in some directions)

Potential notational confusion

- In optimization literature it's common to optimize over parameters x
- In xNNs we have inputs **x** and optimize over parameters **h** (or some other variable)
- So in the optimization section our goal is to find the optimal **x**, and in the xNN training section it's to find the optimal **h** (or other parameter variable)

Closed Form Methods

- Example: least squares solution to a linear systems of equations
 - Minimize $f(x) = (A x y)^T (A x y)$
 - Multiply out, take partial derivatives, set to 0 and solve

 For xNN training we usually don't have a simple closed form solution for finding optimal parameters (sadness)

Iterative Methods

- Gradient descent.
 - Find x that minimizes f(x)
 - Basic strategy (many many variations exist)
 - Initialization
 - Let n = 0
 - Initial guess x₀
 - Iteration
 - Compute the gradient $\nabla f(\mathbf{x}_n)$
 - Select a step size α_n
 - Take a step in the opposite direction of the gradient: $\mathbf{x}_{n+1} = \mathbf{x}_n \alpha_n \nabla f(\mathbf{x}_n)$
 - Let n = n + 1

Iterative Methods

- Repeating the closed form example using gradient descent for ease of understanding
- Example: least squares solution to a linear systems of equations
 - Minimize $f(\mathbf{x}) = (\mathbf{A} \mathbf{x} \mathbf{y})^T (\mathbf{A} \mathbf{x} \mathbf{y})$ • $f(\mathbf{x}) = \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - \mathbf{x}^T \mathbf{A}^T \mathbf{y} - \mathbf{y}^T \mathbf{A} \mathbf{x} + \mathbf{y}^T \mathbf{y}$ = $\mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - 2 \mathbf{y}^T \mathbf{A} \mathbf{x} + \mathbf{y}^T \mathbf{y}$ • $\nabla f(\mathbf{x}) = 2 \mathbf{A}^T \mathbf{A} \mathbf{x} - 2 \mathbf{A}^T \mathbf{y}$ = $2 \mathbf{A}^T (\mathbf{A} \mathbf{x} - \mathbf{y})$ • $\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \nabla f(\mathbf{x}_n)$ = $\mathbf{x}_n - \alpha_n 2 \mathbf{A}^T (\mathbf{A} \mathbf{x}_n - \mathbf{y})$

To do:

- Add how to calculate the sqrt(2) in elementary school
- Banach fixed point theorem / contraction mapping theorem

Neural Network Training

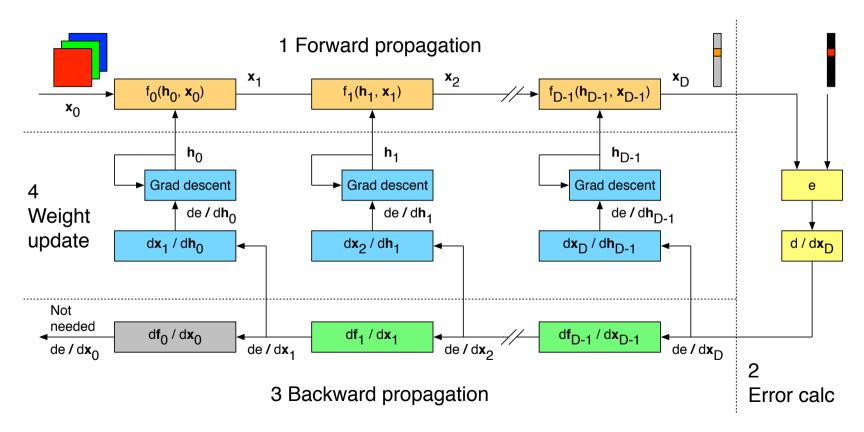
Specifically

- The basics of xNN training are described here
- Many variations to improve training will be introduced in a later lecture
 - It's ok to start a long trip with a 1st step

Strategy

- Initialization
 - Assume for now, will discuss later
- Forward propagation
- Error calculation
- Backward propagation
 - Partial derivatives and the chain rule
- Weight update
 - Gradient descent

Strategy

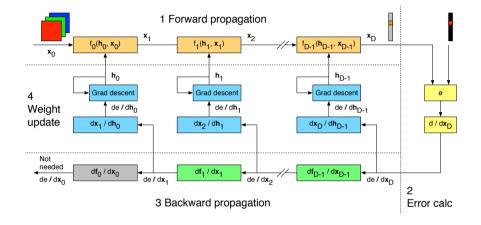


Forward Propagation

 Use the network to generate a batch of outputs from a batch of inputs

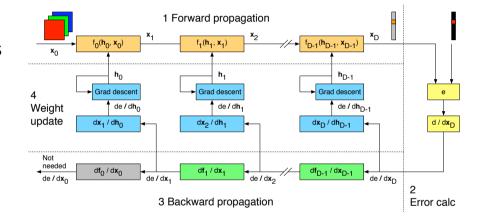
Example

- Image classification to 1 of K classes
- Network input is an image
- Network performs some calculations
 - Multiple layers
 - Some of those layers controlled are by parameters
- Network output is a K x 1 vector
 - Each element x(k) corresponds to a class
 - k* is the correct class for the image
 - Network attempts to make x(k) large for k = k* and small for k ≠ k*



Error Calculation

- How well did the network do?
 - Error calculation quantifies an answer to this question for the training input to a single number (yes, 1 number)
 - The goal of back propagation and weight update will be to adapt all the parameters in the network to minimize this error
- For the error calculation we'll assume that the ideal output is known
 - Supervised learning
- Consider errors optimized for 2 types of predictions
 - Classification
 - Regression



Error Calculation

- For classification we'll commonly use softmax cross entropy
 - Note that this is really 2 layers but for implementation reasons we'll treat together
- Error calculation
 - Network output is K x 1 vector x_D
 - $\mathbf{p} = \operatorname{softmax}(\mathbf{x}_D)$
 - p(k) is in [0, 1] and Σ_k p(k) = 1
 - Interpretation of converting the network output to probabilities
 - $e = H_{CE}(p^*, p)$
 - Ideal output p* has a 1 at position k* and 0s elsewhere
 - $e = -\sum_{k} p^{*}(k) \log(p(k)) = -\log(p(k^{*}))$
 - Interpretation of defining the error based on the converted probability for the correct class

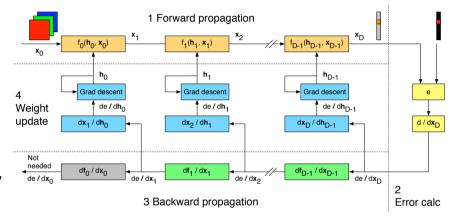
Error Calculation

- For regression we'll commonly use 0.5 MSE
 - 0.5 really isn't needed, just makes equations look more beautiful
- Error calculation
 - Network output is K x 1 vector x_D
 - e = 0.5 mse(x^* , x_D)
 - Ideal output x*
 - $e = (0.5/K) (\mathbf{x}^* \mathbf{x}_D)^T (\mathbf{x}^* \mathbf{x}_D)$
 - Interpretation of defining the error based on the 2 norm distance between the network output and the ideal value

Backward Propagation

Goal

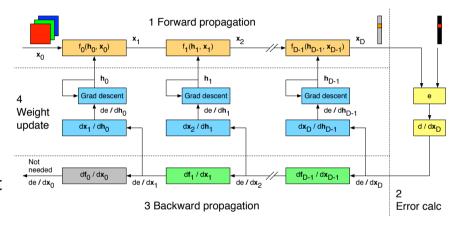
- Determine sensitivity (gradient) of the error with respect to all feature maps
- Automatic differentiation with reverse mode accumulation
 - Decompose forward propagation into a set of building blocks (practically layers, theoretically any primitive operation with a known derivative)
 - Build associated graph for back propagation ~ via reversing arrows and replacing forward propagation nodes representing layers with back propagation nodes representing layer derivatives
 - Back propagation nodes map from ∂e/∂x_d to ∂e/∂x_{d-1} via the chain rule



Backward Propagation

Cookbook

- Build backward propagation graph
- Start with $\partial e/\partial x_D$, the gradient of the error with respect to the output of the last layer
 - How to calculate this was conveniently shown on an earlier slide for softmax cross entropy and MSE errors
- Compute the gradient of the error at the input of the last layer (which is the output of the next to last layer)
 - This is found using the chain rule $\partial e/\partial \mathbf{x}_{D-1} = (\partial \mathbf{x}_D/\partial \mathbf{x}_{D-1}) (\partial e/\partial \mathbf{x}_D) = (\partial \mathbf{f}_{D-1}/\partial \mathbf{x}_{D-1}) (\partial e/\partial \mathbf{x}_D)$
 - $\partial e/\partial x_D$ is given
 - $\partial \mathbf{f}_{D-1}/\partial \mathbf{x}_{D-1}$ for many common layers was conveniently shown on an earlier slide
- Compute the gradient of the error at the input of the next to last layer ... (and repeat)



Weight Update

Goal

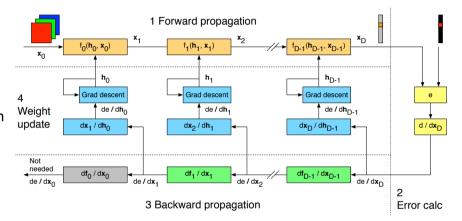
• Update weights to reduce the error

Strategy

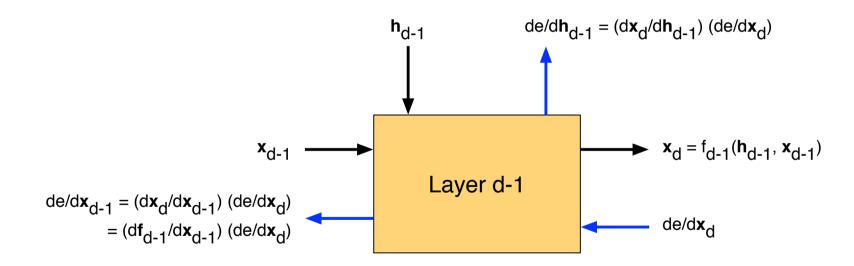
- Use the error gradient with respect to the feature map output for the current layer provided via back propagation
- With the derivative of the forward node output with respect to the parameters
- To determine the error gradient with respect to the parameters (1)
- Then use gradient descent to adapt the parameters to reduce the error (2)

In math

- d-1 is the layer, n is the current time
- 1: $\partial e/\partial \mathbf{h}_{d-1} = (\partial \mathbf{x}_d/\partial \mathbf{h}_{d-1}) (\partial e/\partial \mathbf{x}_d) = (\partial \mathbf{f}_{d-1}/\partial \mathbf{h}_{d-1}) (\partial e/\partial \mathbf{x}_d)$
- 2: $\mathbf{h}_{n+1, d-1} = \mathbf{h}_{n, d-1} \alpha_n \partial e / \partial \mathbf{h}_{n, d-1}$



Summary For 1 Layer



Summary For 1 Layer

- Example: matrix vector multiplication
 - $\mathbf{x}_{d} = f_{d-1}(\mathbf{H}_{d-1}, \mathbf{x}_{d-1}) = \mathbf{H}_{d-1} \mathbf{x}_{d-1}$
 - Dimensions (M x 1) = (M x K) (K x 1)
- Error gradient with respect to the feature map
 - Given: $\partial e/\partial x_d$
 - Compute: $\partial e/\partial \mathbf{x}_{d-1} = (\partial \mathbf{x}_d/\partial \mathbf{x}_{d-1}) (\partial e/\partial \mathbf{x}_d) = (\partial \mathbf{f}_{d-1}/\partial \mathbf{x}_{d-1}) (\partial e/\partial \mathbf{x}_d) = (\mathbf{H}_{d-1})^T (\partial e/\partial \mathbf{x}_d)$
 - Dimensions (K x 1) = (K x M) (M x 1)
- Error gradient with respect to the filter coefficients
 - Given: $\partial e/\partial x_d$
 - Compute: $\partial e/\partial \mathbf{H}_{d-1} = (\partial \mathbf{x}_d/\partial \mathbf{H}_{d-1}) (\partial e/\partial \mathbf{x}_d) = (\partial e/\partial \mathbf{x}_d) (\partial \mathbf{f}_{d-1}/\partial \mathbf{H}_{d-1}) = (\partial e/\partial \mathbf{x}_d) (\mathbf{x}_{d-1})^T$
 - Dimensions (M x K) = (M x 1) (1 x K)
 - Note the reversing of order as a consequence of the transpose for this case (to see match terms with previous case)
 - Note that this implies saving \mathbf{x}_{d-1} from the forward pass
- Weight update
 - Compute: $\mathbf{H}_{n+1, d-1} = \mathbf{H}_{n+1, d-1} \alpha_n \partial e / \partial \mathbf{H}_{n, d-1}$
 - Time n to time n + 1

Training Vs Standard Optimization

- There are a number of differences between xNN training and optimization
 - Optimize an error function with the training data to perform well on testing data
 - Typically thought of as optimizing for empirical vs true distribution
 - The concept of an input distribution is used as there's typically not a practical deterministic model for the input
 - Use a surrogate error function vs actual error function
 - E.g., softmax + cross entropy vs arg max
 - Also don't use the actual top 1 for all training data at 1x
 - Only use a fraction or batch of it at a time
- These differences highlight the need for generalization
 - Want to train xNNs on training data with a surrogate error function such that they will generalize well to new data with high levels of accuracy
 - In a later lecture will look at various regularization methods to improve generalization

Universal Approximation

Will Save For The Next Lecture

References

List

- Convolutional neural networks: theory, implementation and application
 - Chapter 4 calculus
 - https://github.com/arthurredfern/UT-Dallas-CS-6301-CNNs/blob/master/References/ConvolutionalNeuralNetworks.pdf
- Calculus
 - http://mathonline.wikidot.com/calculus
- Convex optimization
 - https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf
- Automatic differentiation in machine learning: a survey
 - https://arxiv.org/abs/1502.05767