Backpropagation and the Chain Rule

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April 17, 2018

Contents

Introduction

Learning with Back-Propagation

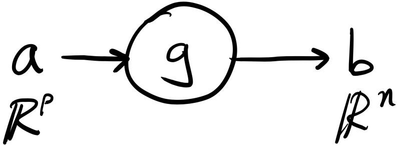
- Back-propagation is an **algorithm** for computing the gradient
- With lots of chain rule, you could also work out the gradient by hand.
- Back-propagation is
  - a clean way to organize the computation of the gradient
  - an efficient way to compute the gradient

Partial Derivatives and the Chain Rule

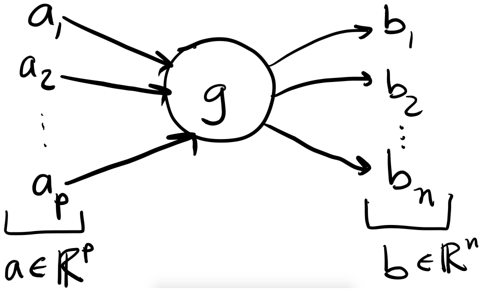
Partial Derivatives

- Consider a function $g : \mathbf{R}^p \to \mathbf{R}^n$.

  - Typical computation graph:

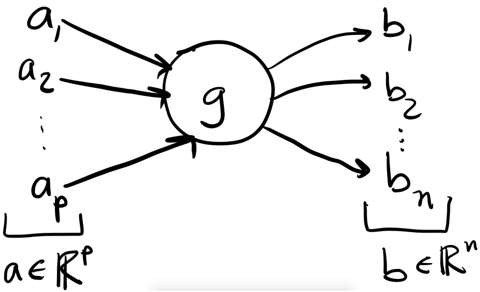


  - Broken out into components:



Partial Derivatives

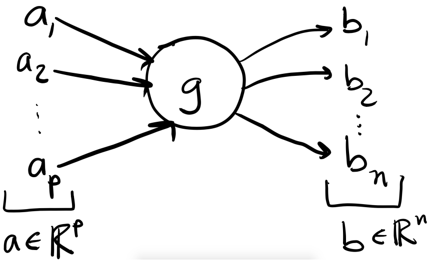
- Consider a function $g : \mathbf{R}^p \to \mathbf{R}^n$.



- Partial derivative $\frac{\partial b_i}{\partial a_j}$ is the instantaneous rate of change of b_i as we change a_j.
- If we change a_j slightly to $a_j + \delta$,
- Then (for small δ), b_i changes to approximately $b_i + \frac{\partial b_i}{\partial a_j}\delta$.

Partial Derivatives of an Affine Function

- Define the affine function $g(x) = Mx + c$, for $M \in \mathbf{R}^{n \times p}$ and $c \in \mathbf{R}$.



- If we let $b = g(a)$, then what is b_i?
- b_i depends on the ith row of M:

$$b_i = \sum_{k=1}^{p} M_{ik} a_k + c_i$$

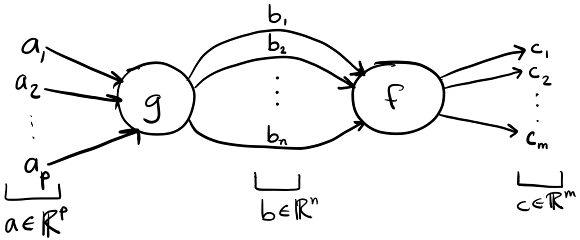
and

$$\frac{\partial b_i}{\partial a_j} = M_{ij}.$$

- So for an an affine mapping, entries of matrix M directly tell us the rates of change.

Chain Rule (in terms of partial derivatives)

- $g : \mathbf{R}^p \to \mathbf{R}^n$ and $f : \mathbf{R}^n \to \mathbf{R}^m$. Let $b = g(a)$. Let $c = f(b)$.



- **Chain rule** says that

$$\frac{\partial c_i}{\partial a_j} = \sum_{k=1}^{n} \frac{\partial c_i}{\partial b_k} \frac{\partial b_k}{\partial a_j}.$$

- Change in a_j may change each of $b_1, \ldots, b_n$.
- Changes in $b_1, \ldots, b_n$ may each effect c_i.
- Chain rule tells us that, to first order, the net change in c_i is
  - the sum of the changes induced along each path from a_j to c_i.

Example: Least Squares Regression

Review: Linear least squares

- Hypothesis space $\left\{f(x) = w^T x + b \mid w \in \mathbf{R}^d, b \in \mathbf{R}\right\}$.
- Data set $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbf{R}^d \times \mathbf{R}$.
- Define

$$\ell_i(w,b) = \left[\left(w^T x_i + b\right) - y_i\right]^2.$$

- In SGD, in each round we'd choose a random index $i \in 1, \ldots, n$ and take a gradient step

$$\begin{aligned} w_j &\leftarrow w_j - \eta \frac{\partial \ell_i(w,b)}{\partial w_j}, \text{ for } j = 1, \ldots, d \\ b &\leftarrow b - \eta \frac{\partial \ell_i(w,b)}{\partial b}, \end{aligned}$$

  for some step size $\eta > 0$.
- Let's revisit how to calculate these partial derivatives...

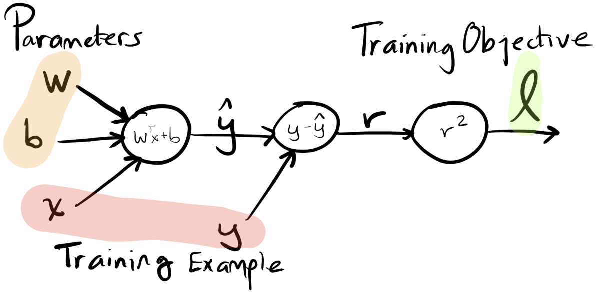
Computation Graph and Intermediate Variables

- For a generic training point (x, y), denote the loss by

$$\ell(w, b) = \left[\left(w^T x + b\right) - y\right]^2.$$

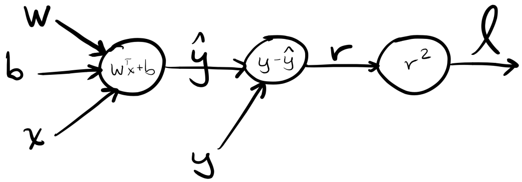
- Let's break this down into some intermediate computations:

$$\begin{aligned}
\text{(prediction) } \hat{y} &= \sum_{j=1}^{d} w_j x_j + b \\
\text{(residual) } r &= y - \hat{y} \\
\text{(loss) } \ell &= r^2
\end{aligned}$$



Partial Derivatives on Computation Graph

- We'll work our way from graph output ℓ back to the parameters w and b:



$$
\begin{aligned}
\frac{\partial \ell}{\partial r} &= 2r \\
\frac{\partial \ell}{\partial \hat{y}} &= \frac{\partial \ell}{\partial r}\frac{\partial r}{\partial \hat{y}} = (2r)(-1) = -2r \\
\frac{\partial \ell}{\partial b} &= \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial b} = (-2r)(1) = -2r \\
\frac{\partial \ell}{\partial w_j} &= \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w_j} = (-2r)x_j = -2rx_j
\end{aligned}
$$

Example: Ridge Regression

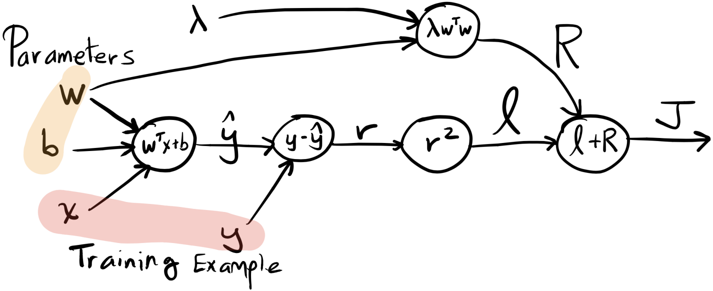
Ridge Regression: Computation Graph and Intermediate Variables

- For training point (x, y), the ℓ_2-regularized objective function is

$$J(w,b) = \left[\left(w^T x + b\right) - y\right]^2 + \lambda w^T w.$$

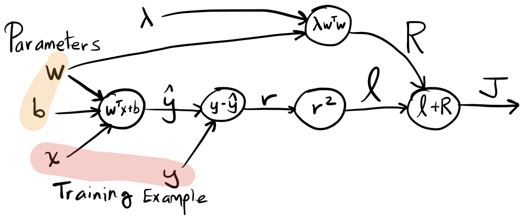
- Let's break this down into some intermediate computations:

$$\begin{aligned}
\text{(prediction) } \hat{y} &= \sum_{j=1}^{d} w_j x_j + b \\
\text{(residual) } r &= y - \hat{y} \\
\text{(loss) } \ell &= r^2 \\
\text{(regularization) } R &= \lambda w^T w \\
\text{(objective) } J &= \ell + R
\end{aligned}$$



Partial Derivatives on Computation Graph

- We'll work our way from graph output ℓ back to the parameters w and b:



$$\frac{\partial J}{\partial \ell} = \frac{\partial J}{\partial R} = 1$$

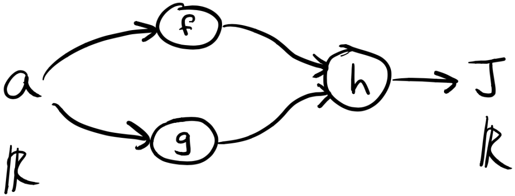
$$\frac{\partial J}{\partial \hat{y}} = \frac{\partial J}{\partial \ell}\frac{\partial \ell}{\partial r}\frac{\partial r}{\partial \hat{y}} = (1)(2r)(-1) = -2r$$

$$\frac{\partial J}{\partial b} = \frac{\partial J}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial b} = (-2r)(1) = -2r$$

$$\frac{\partial J}{\partial w_j} = ?$$

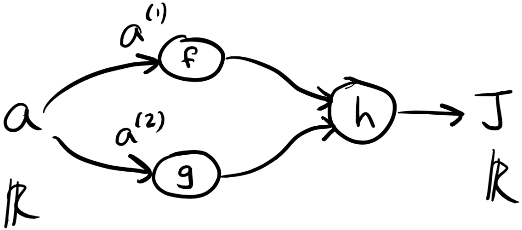
Handling Nodes with Multiple Children

- Consider $a \mapsto J = h(f(a), g(a))$.



- It's helpful to think about having two independent copies of a, call them $a^{(1)}$ and $a^{(2)}$...

Handling Nodes with Multiple Children

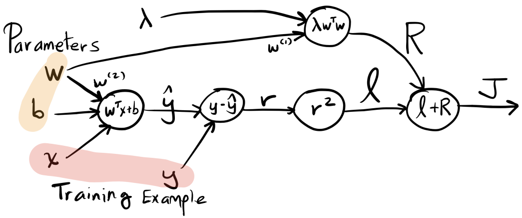


$$
\begin{aligned}
\frac{\partial J}{\partial a} &= \frac{\partial J}{\partial a^{(1)}}\frac{\partial a^{(1)}}{\partial a} + \frac{\partial J}{\partial a^{(2)}}\frac{\partial a^{(2)}}{\partial a} \\
&= \frac{\partial J}{\partial a^{(1)}} + \frac{\partial J}{\partial a^{(2)}}
\end{aligned}
$$

- Derivative w.r.t. a is the sum of derivatives w.r.t. each copy of a.

Partial Derivatives on Computation Graph

- We'll work our way from graph output ℓ back to the parameters w and b:



$$
\begin{aligned}
\frac{\partial J}{\partial \hat{y}} &= \frac{\partial J}{\partial \ell}\frac{\partial \ell}{\partial r}\frac{\partial r}{\partial \hat{y}} = (1)(2r)(-1) = -2r \\
\frac{\partial J}{\partial w_j^{(2)}} &= \frac{\partial J}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w_j^{(2)}} = \frac{\partial J}{\partial \hat{y}} x_j \\
\frac{\partial J}{\partial w_j^{(1)}} &= \frac{\partial J}{\partial R}\frac{\partial R}{\partial w_j^{(1)}} = (1)\left(2\lambda w_j^{(1)}\right) \\
\frac{\partial J}{\partial w_j} &= \frac{\partial J}{\partial w_j^{(1)}} + \frac{\partial J}{\partial w_j^{(2)}}
\end{aligned}
$$

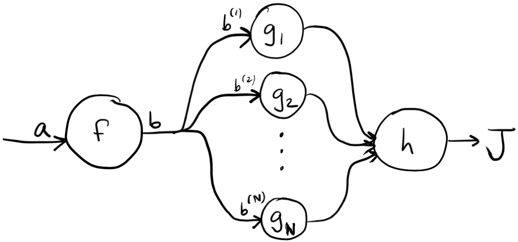
General Backpropagation

Backpropagation: Overview

- Backpropagation is a specific way to evaluate the partial derivatives of a computation graph output J w.r.t. the inputs and outputs of all nodes.
- Backpropagation works node-by-node.
- To run a "backward" step at a node f, we assume
  - we've already run "backward" for all of f's children.
- **Backward** at node $f : a \mapsto b$ returns
  - Partial of objective value J w.r.t. f's output: $\frac{\partial J}{\partial b}$
  - Partial of objective value J w.r.t f's input: $\frac{\partial J}{\partial a}$

Backpropagation: Simple Case

- Simple case: all nodes take a single scalar as input and have a single scalar output.



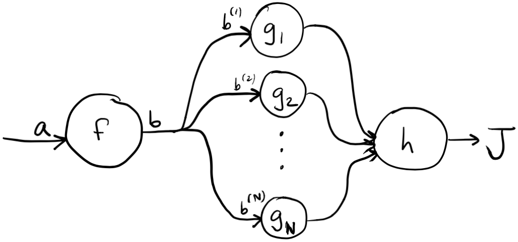
- Backprop for node f:
- **Input**: $\frac{\partial J}{\partial b^{(1)}}, \ldots, \frac{\partial J}{\partial b^{(N)}}$
  (Partials w.r.t. inputs to all children)
- **Output**:

$$\frac{\partial J}{\partial b} = \sum_{k=1}^{N} \frac{\partial J}{\partial b^{(k)}}$$

$$\frac{\partial J}{\partial a} = \frac{\partial J}{\partial b} \frac{\partial b}{\partial a}$$

Backpropagation (General case)

- More generally, consider $f : \mathbf{R}^d \to \mathbf{R}^n$.



- **Input**: $\frac{\partial J}{\partial b_j^{(i)}}$, $i = 1, \ldots, N$, $j = 1, \ldots, n$
- **Output**:

$$\frac{\partial J}{\partial b_j} = \sum_{k=1}^{N} \frac{\partial J}{\partial b_j^{(k)}}$$

$$\frac{\partial J}{\partial a_i} = \sum_{j=1}^{n} \frac{\partial J}{\partial b_j} \frac{\partial b_j}{\partial a_i}$$

Running Backpropagation

- If we run "backward" on every node in our graph,
  - we'll have the gradients of J w.r.t. all our parameters.
- To run backward on a particular node,
  - we assumed we already ran it on all children.
- A **topological sort** of the nodes in a directed [acyclic] graph
  - is an ordering which every node appears before its children.
- So we'll evaluate backward on nodes in a **reverse topological ordering**.