Feature learning, neural networks and backpropagation

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Slides based on Lecture 12a from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

CDS, NYU

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Today's lecture

- Neural networks: huge empirical success but poor theoretical understanding
- Key idea: representation learning
- Optimization: backpropagation + SGD

Feature engineering

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- Note that this model is not linear in the inputs x — we represent the inputs differently, and the new representation is amenable to linear modeling
- For example, we can use a feature map that defines a kernel, e.g., polynomials in x

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- Example: predicting how popular a restaurant is

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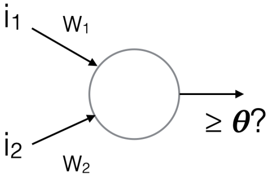
- A final *linear* predictor uses the **intermediate features** computed by the h_i's:

$$w_1 \cdot \text{food quality} + w_2 \cdot \text{walkable} + w_3 \cdot \text{noisy}$$

Perceptrons as logical gates

- Suppose that our input features indicate light at a two points in space (0 = no light; 1 = light)



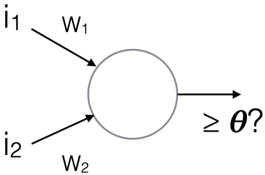
- How can we build a perceptron that detects when there is light in both locations?

$$w_1 = 1, w_2 = 1, \theta = 2$$

i_1	i_2	$w_1 i_1 + w_2 i_2$
0	0	0
0	1	1
1	0	1
1	1	2

Limitations of a perceptrons as logical gates

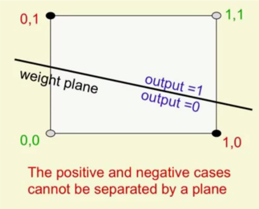
- Can we build a perceptron that fires when the two pixels have the same value ($i_1 = i_2$)?



Positive: (1, 1) (0, 0)

$$w_1 + w_2 \geq \theta, \quad 0 \geq \theta$$
$$w_1 < \theta, \quad w_2 < \theta$$

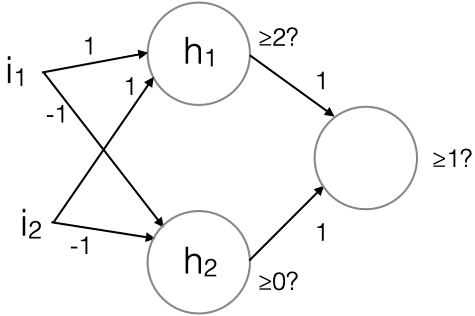
Negative: (1, 0) (0, 1)



If θ is negative, the sum of two numbers that are both less than θ cannot be greater than θ

Multilayer perceptron

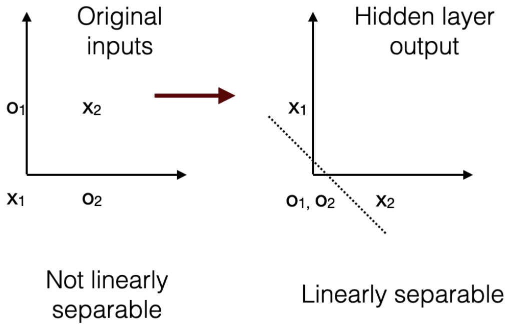
- Fire when the two pixels have the same value ($i_1 = i_2$)



			Hidden layer input		Hidden layer output		
	i_1	i_2	h_1	h_2	h_1	h_2	o
x_1	0	0	0	0	0	1	1
o_1	0	1	1	-1	0	0	0
o_2	1	0	1	-1	0	0	0
x_2	1	1	2	-2	1	0	1

(for x_1 and x_2 the correct output is 1;
for o_1 and o_2 the correct output is 0)

- Recode the input: the hidden layer representations are now linearly separable



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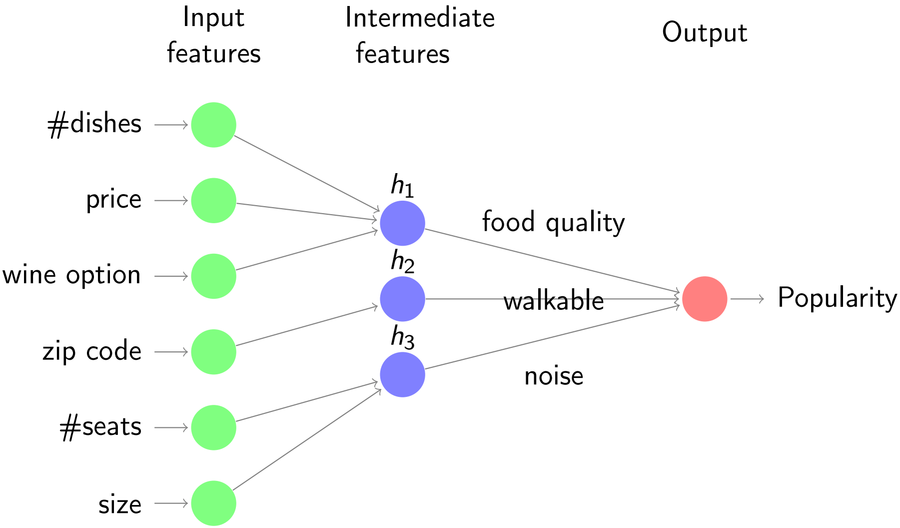
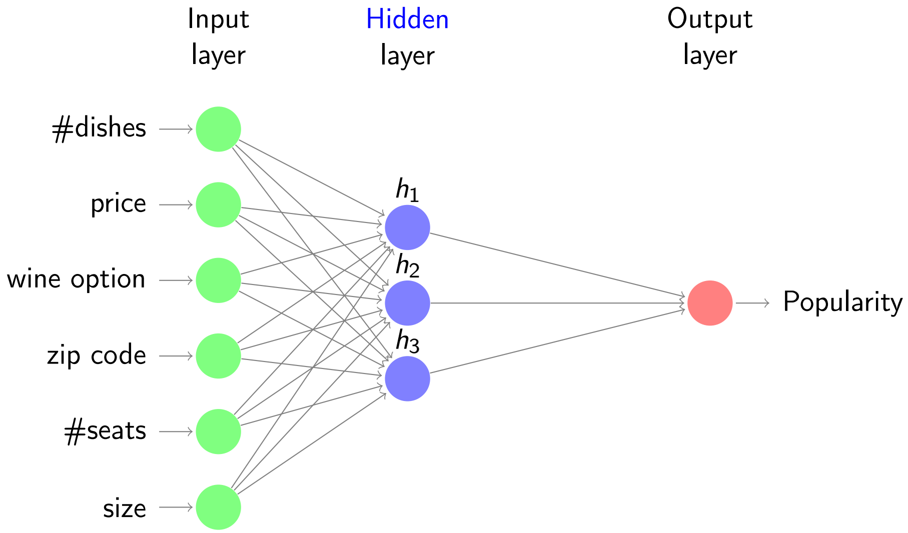
Decomposing the problem into predefined subproblems



Learned intermediate features



Neural networks

Key idea: learn the intermediate features.

Feature engineering Manually specify $\phi(x)$ based on domain knowledge and learn the weights:

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Feature learning Learn both the features (K hidden units) and the weights:

$$h(x) = [h_1(x), \ldots, h_K(x)], \tag{3}$$

$$f(x) = w^T h(x) \tag{4}$$

Activation function

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    - E.g., logistic function, hyperbolic tangent function.

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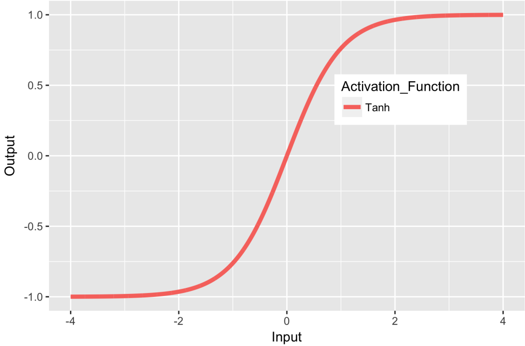
  - *Differentiable* approximations: sigmoid functions.
    - E.g., logistic function, hyperbolic tangent function.
- Two-layer neural network (one hidden layer and one output layer) with K hidden units:

$$f(x) = \sum_{k=1}^{K} w_k h_k(x) = \sum_{k=1}^{K} w_k \sigma({v_k}^T x) \tag{6}$$

Activation Functions

- The **hyperbolic tangent** is a common activation function:

$$\sigma(x) = \tanh(x).$$

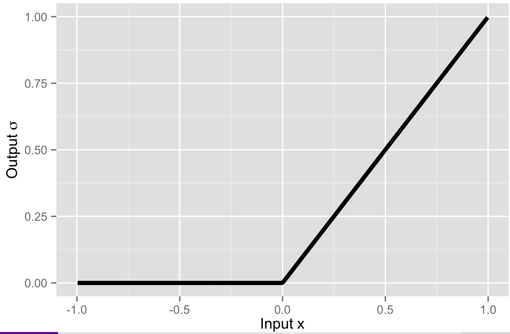


Activation Functions

- More recently, the **rectified linear (ReLU)** function has been very popular:

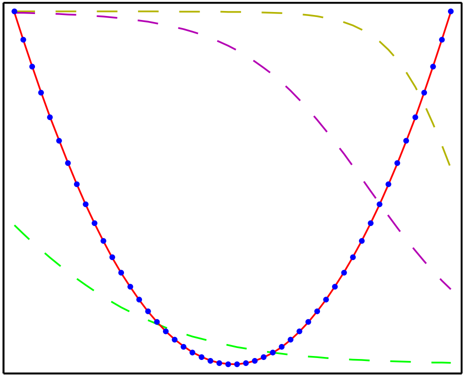
$$\sigma(x) = \max(0, x).$$

- Faster to calculate this function and its derivatives
- Often more effective in practice



Approximation Ability: $f(x) = x^2$

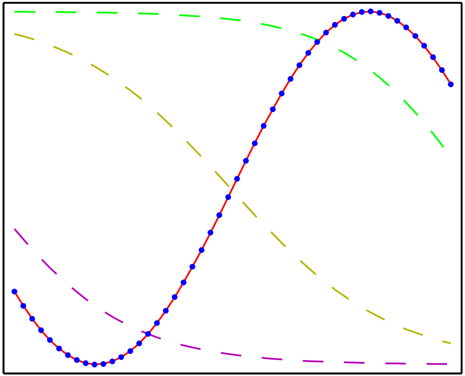
- 3 hidden units; tanh activation functions
- Blue dots are training points; dashed lines are hidden unit outputs; final output in red.



From Bishop's *Pattern Recognition and Machine Learning*, Fig 5.3

Approximation Ability: $f(x) = \sin(x)$

- 3 hidden units; logistic activation function
- Blue dots are training points; dashed lines are hidden unit outputs; final output in red.



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Approximation Ability: $f(x) = |x|$

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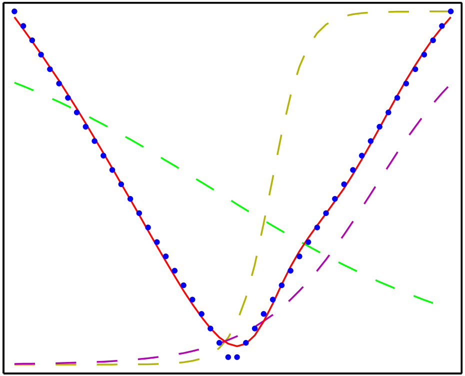

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Universal approximation theorem

Theorem (Universal approximation theorem)

A neural network with one possibly huge hidden layer $\hat{F}(x)$ can approximate any continuous function $F(x)$ on a closed and bounded subset of $\mathbb{R}^d$ under mild assumptions on the activation function, i.e. $\forall \epsilon > 0$, there exists an integer N s.t.

$$\hat{F}(x) = \sum_{i=1}^{N} w_i \sigma(v_i^T x + b_i) \tag{7}$$

satisfies $|\hat{F}(x) - F(x)| < \epsilon$.

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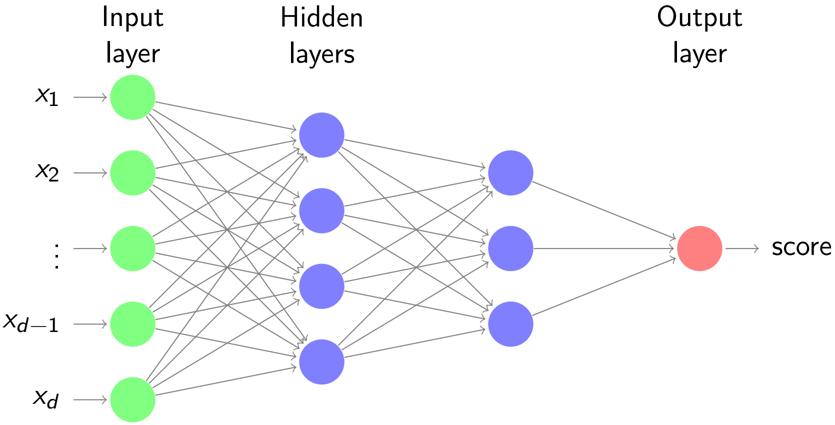
- The theorem doesn't tell us how to find the parameters of this network
- It doesn't explain why practical neural networks work, or tell us how to build them

Deep neural networks

- Wider: more hidden units (as in the approximation theorem).
- Deeper: more hidden layers.



Multilayer Perceptron (MLP): formal definition

- **Input space**: $\mathcal{X} = \mathrm{R}^d$ **Action space** $\mathcal{A} = \mathrm{R}^k$ (for k-class classification).
- Let $\sigma : \mathrm{R} \to \mathrm{R}$ be an activation function (e.g. tanh or ReLU).
- Let's consider an MLP of L hidden layers, each having m hidden units.
- First hidden layer is given by

$$h^{(1)}(x) = \sigma\left(W^{(1)}x + b^{(1)}\right),$$

for parameters $W^{(1)} \in \mathrm{R}^{m \times d}$ and $b \in \mathrm{R}^m$, and where $\sigma(\cdot)$ is applied to each entry of its argument.

Multilayer Perceptron (MLP): formal definition

- Each subsequent hidden layer takes the *output* $o \in \mathrm{R}^m$ *of previous layer* and produces

$$h^{(j)}(o^{(j-1)}) = \sigma\left(W^{(j)}o^{(j-1)} + b^{(j)}\right), \text{ for } j = 2, \ldots, L$$

where $W^{(j)} \in \mathrm{R}^{m \times m}$, $b^{(j)} \in \mathrm{R}^m$.

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- Last layer is an *affine* mapping (no activation function):

$$a(o^{(L)}) = W^{(L+1)} o^{(L)} + b^{(L+1)},$$

  where $W^{(L+1)} \in \mathbb{R}^{k \times m}$ and $b^{(L+1)} \in \mathbb{R}^k$.

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- The full neural network function is given by the *composition* of layers:

$$f(x) = \left(a \circ h^{(L)} \circ \cdots \circ h^{(1)}\right)(x) \tag{8}$$

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- Typically, the last layer gives us a score. How do we perform classification?

What did we do in multinomial logistic regression?

- From each x, we compute a linear score function for each class:

$$x \mapsto (\langle w_1, x \rangle, \ldots, \langle w_k, \rangle) \in \mathrm{R}^k$$

- We need to map this R^k vector into a probability vector θ.

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- We need to map this R^k vector into a probability vector θ.
- The **softmax function** maps scores $s = (s_1, \ldots, s_k) \in \mathrm{R}^k$ to a categorical distribution:

$$(s_1, \ldots, s_k) \mapsto \theta = \textbf{Softmax}(s_1, \ldots, s_k) = \left(\frac{\exp(s_1)}{\sum_{i=1}^{k} \exp(s_i)}, \ldots, \frac{\exp(s_k)}{\sum_{i=1}^{k} \exp(s_i)} \right)$$

Nonlinear Generalization of Multinomial Logistic Regression

- From each x, we compute a non-linear score function for each class:

$$x \mapsto (f_1(x), \ldots, f_k(x)) \in \mathrm{R}^k$$

where f_i's are the outputs of the last hidden layer of a neural network.

- Learning: Maximize the log-likelihood of training data

$$\underset{f_1, \ldots, f_k}{\arg\max} \sum_{i=1}^{n} \log \left[\operatorname{Softmax}(f_1(x), \ldots, f_k(x))_{y_i} \right].$$

Interim discussion

- With the right representations, we can turn nonlinear problems into linear ones
- The goal of represenation learning is to automatically discover useful features from raw data
- Building blocks:

Input layer	no learnable parameters
Hidden layer(s)	affine + *nonlinear* activation function
Output layer	affine (+ softmax)

- A single, potentially huge hidden layer is sufficient to approximate any function
- In practice, it is often helpful to have multiple hidden layers

Fitting the parameters of an MLP

- **Input space**: $\mathcal{X} = \mathbb{R}$
- **Action Space / Output space**: $\mathcal{A} = \mathcal{Y} = \mathbb{R}$
- **Hypothesis space**: MLPs with a single 3-node hidden layer:

$$f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x),$$

  where

$$h_i(x) = \sigma(v_i x + b_i) \text{ for } i = 1, 2, 3,$$

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$$b_1, b_2, b_3, v_1, v_2, v_3, w_0, w_1, w_2, w_3 \in \mathrm{R}$$

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- For a training set $(x_1, y_1), \ldots, (x_n, y_n)$, our goal is to find

$$\hat{\theta} = \underset{\theta \in \mathbb{R}^{10}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left(f(x_i; \theta) - y_i \right)^2 .$$

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- Is the loss convex in θ?
  - tanh is not convex
  - Regardless of nonlinearity, the composition of convex functions is not necessarily convex
- We might converge to a local minimum.

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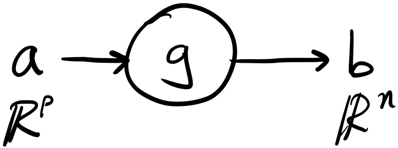
- Back-propagation computes gradients for neural networks (and other models) in a systematic and efficient way
- We can visualize the process using *computation graphs*, which expose the structure of the computation (modularity and dependency)

Functions as nodes in a graph

- We represent each component of the network as a *node* that takes in a set of *inputs* and produces a set of *outputs*.
- Example: $g : \mathrm{R}^p \to \mathrm{R}^n$.
    - Typical computation graph:



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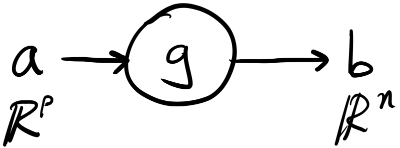
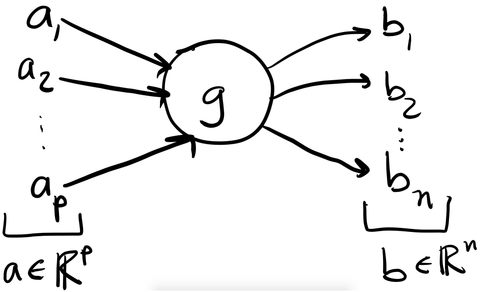
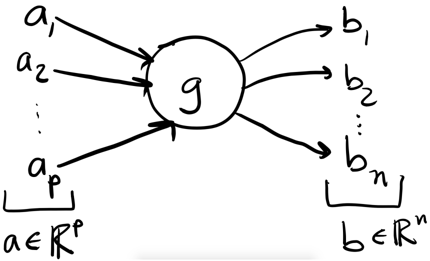


  - Broken down by component:



Partial derivatives of an affine function

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



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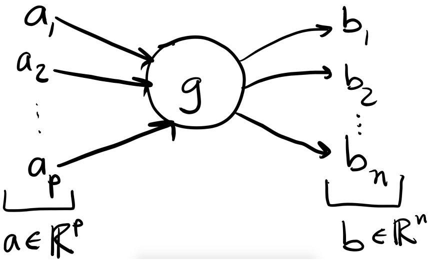

- Let $b = g(a) = Ma + c$. What is b_i?

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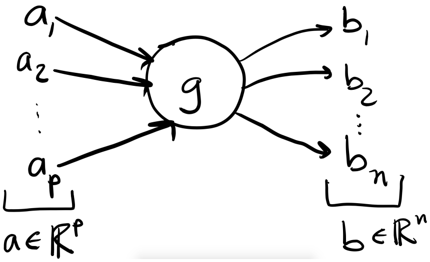

- Let $b = g(a) = Ma + c$. What is b_i?
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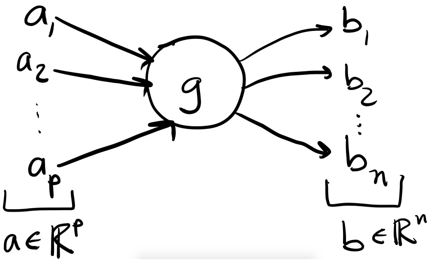

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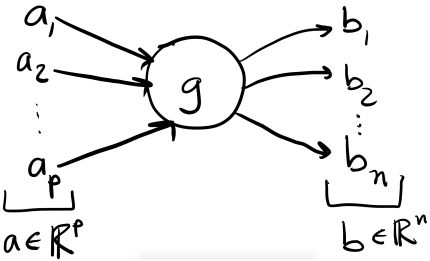

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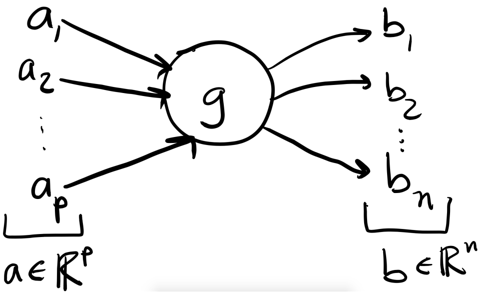
The partial derivative/gradient measures *sensitivity*: If we perturb an input a little bit, how much does the output change?

Partial derivatives in general

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



- Partial derivative $\frac{\partial b_i}{\partial a_j}$ is the rate of change of b_i as we change a_j
- If we change a_j slightly to

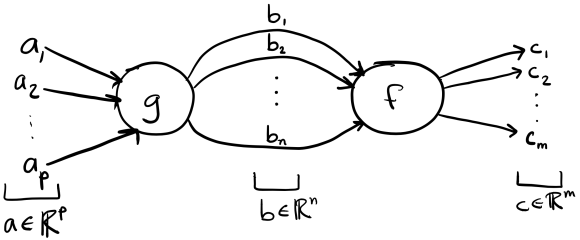
$$a_j + \delta,$$

- Then (for small δ), b_i changes to approximately

$$b_i + \frac{\partial b_i}{\partial a_j}\delta.$$

Composing multiple functions

- We have $g : \mathbb{R}^p \to \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}^m$
- $b = g(a)$, $c = f(b)$.



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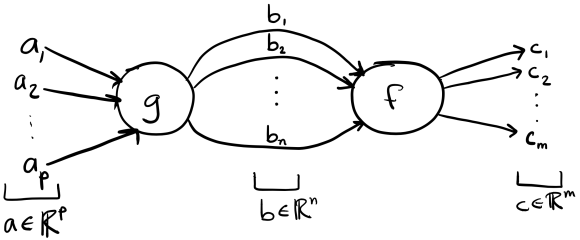

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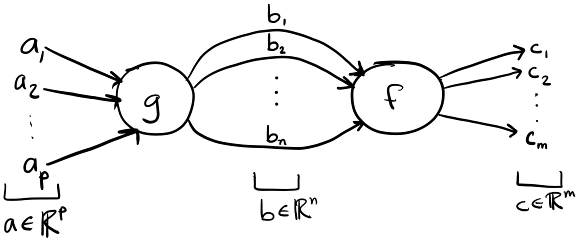

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$$\frac{\partial c_i}{\partial a_j} = \sum_{k=1}^{n} \frac{\partial c_i}{\partial b_k} \frac{\partial b_k}{\partial a_j}.$$

Example: Linear least squares

- Hypothesis space $\{f(x) = w^T x + b \mid w \in \mathbb{R}^d, b \in \mathbb{R}\}$.
- Data set $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$.
- Define
$$\ell_i(w, b) = \left[\left(w^T x_i + b\right) - y_i\right]^2.$$

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- Define
$$\ell_i(w,b) = \left[\left(w^T x_i + b\right) - y_i\right]^2.$$
- In SGD, in each round we choose a random training instance $i \in 1, \ldots, n$ 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 $\eta > 0$.
- How do we calculate these partial derivatives on a computation graph?

Computation graph and intermediate variables

- For a training point (x, y), the loss is

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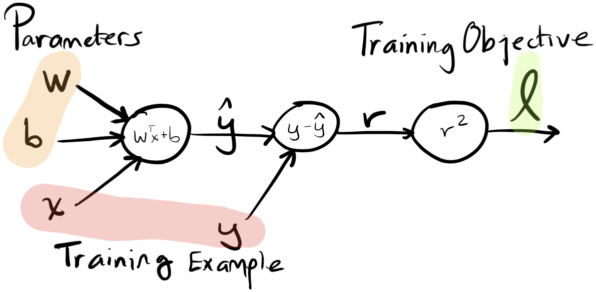
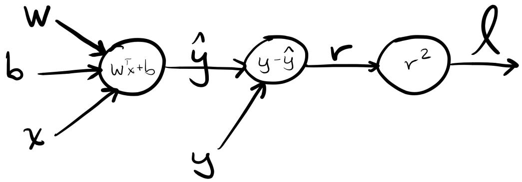


Partial derivatives on computation graph

- We'll work our way from the output ℓ back to the parameters w and b, reusing previous computations as much as possible:



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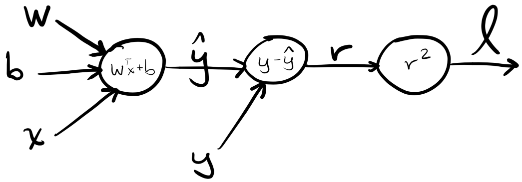

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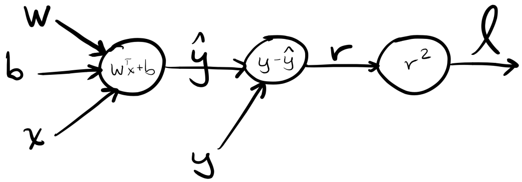

$$\frac{\partial \ell}{\partial r} = 2r$$
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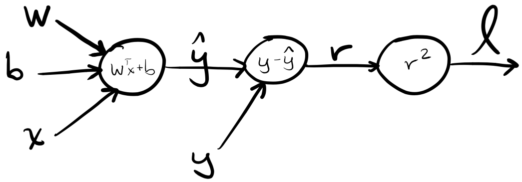

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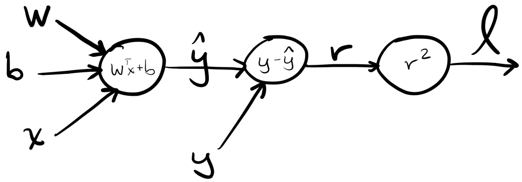

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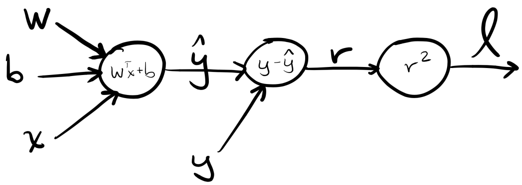

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Example: Ridge Regression

- 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:

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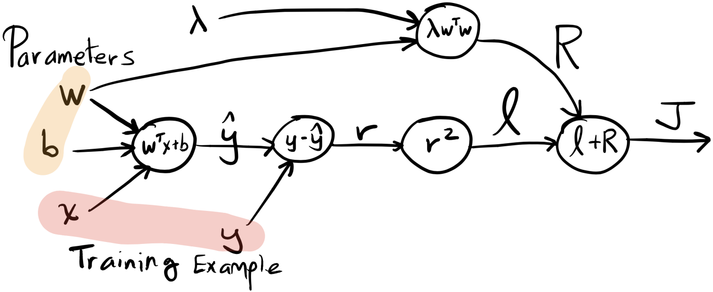

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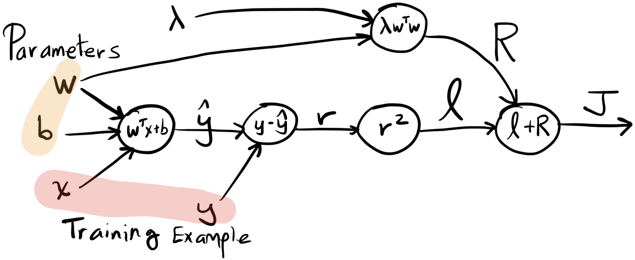

$$
\begin{aligned}
\frac{\partial J}{\partial \ell} &= \frac{\partial J}{\partial R} = 1 \\
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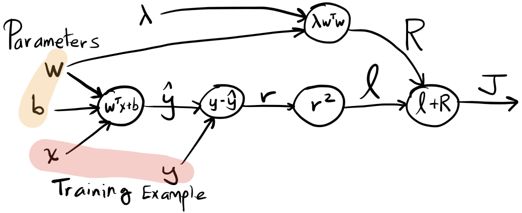
\frac{\partial J}{\partial w_j} &= \text{Exercise}
\end{aligned}
$$

Backpropagation: Overview

- **Learning**: run gradient descent to find the parameters that minimize our objective J.
- Backpropagation: we compute the gradient w.r.t. each (trainable) parameter $\frac{\partial J}{\partial \theta_i}$.



Forward pass	Compute intermediate function values, i.e. output of each node
Backward pass	Compute the partial derivative of J w.r.t. all intermediate variables and the model parameters

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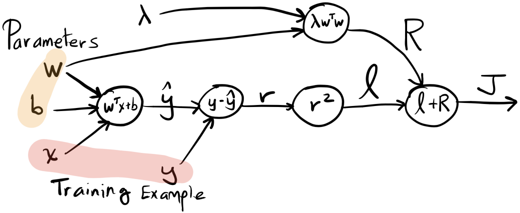

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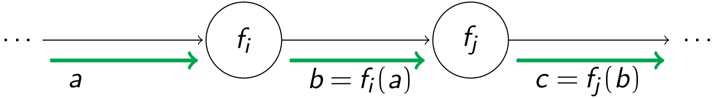
How do we minimize computation?

- Path sharing: each node *caches intermediate results*: we don't need to compute them over and over again
- An example of dynamic programming

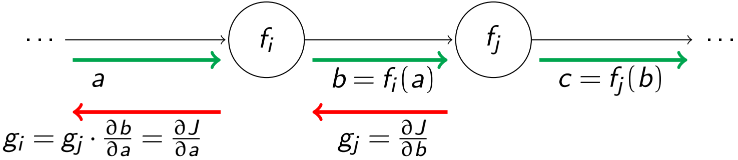
Forward pass

- Order nodes by **topological sort** (every node appears before its children)
- For each node, compute the output given the input (output of its parents).
- Forward at intermediate node f_i and f_j:



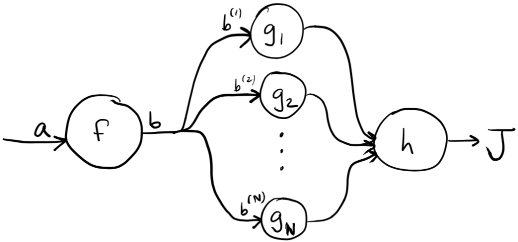
Backward pass

- Order nodes in **reverse topological order** (every node appears after its children)
- For each node, compute the partial derivative of its output w.r.t. its input, multiplied by the partial derivative of its children (chain rule)
- Backward pass at intermediate node f_i:



Multiple children

- First sum partial derivatives from all children, then multiply.



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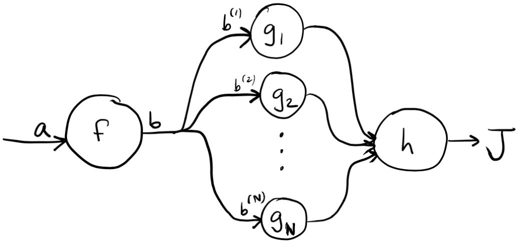
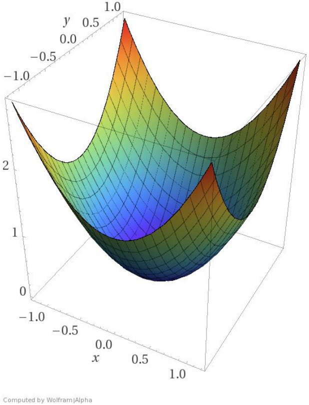


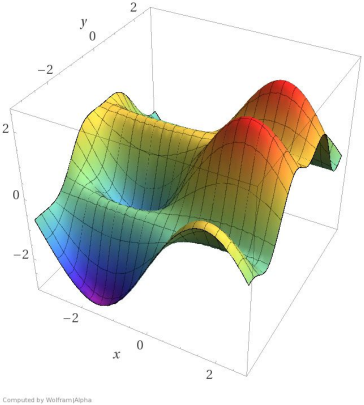
- Backprop for node f:
- **Input**: $\frac{\partial J}{\partial b^{(1)}}, \ldots, \frac{\partial J}{\partial b^{(N)}}$
  (Partials w.r.t. inputs to all children)
- **Output**:

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

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

Non-convex optimization

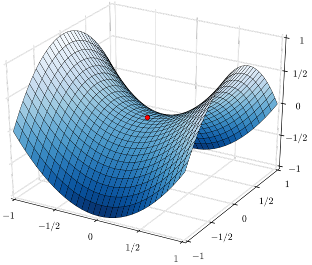




- Left: convex loss function. Right: non-convex loss function.

Non-convex optimization: challenges

- What if we converge to a bad local minimum?
  - Rerun with a different initialization
- Hit a saddle point
  - Doesn't often happen with SGD
  - Second partial derivative test
- Flat region: low gradient magnitude
  - Possible solution: use ReLU instead of sigmoid
- High curvature: large gradient magnitude
  - Possible solutions: Gradient clipping, adaptive step sizes



Reference: Chris De Sa's slides (CS6787 Lecture 7).

Review

- Backpropagation is an algorithm for computing the gradient (partial derivatives + chain rule) efficiently
- It is used in gradient descent optimization for neural networks
- Key idea: function composition and dynamic programming
- In practice, we can use existing software packages, e.g. PyTorch (backpropagation, neural network building blocks, optimization algorithms etc.)