Neural Networks

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Contents

Today's lecture

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

Overview

Feature engineering

- Learning non-linear models in a linear form:

$$f(x) = w^T \phi(x). \tag{1}$$

- What are possible ϕ's we have seen?
  - Feature maps that define a kernel, e.g., polynomials of x
  - Feature templates, e.g., $x_1 = 1$ AND $x_2 = 1$
  - Basis functions, e.g., (shallow) decision trees

Decompose the problem

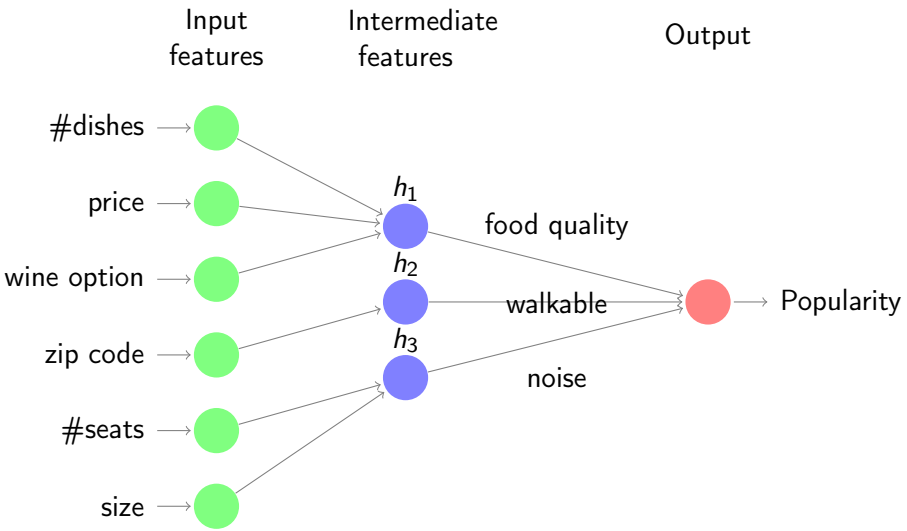
- Example:

  Task Predict popularity of restaurants.

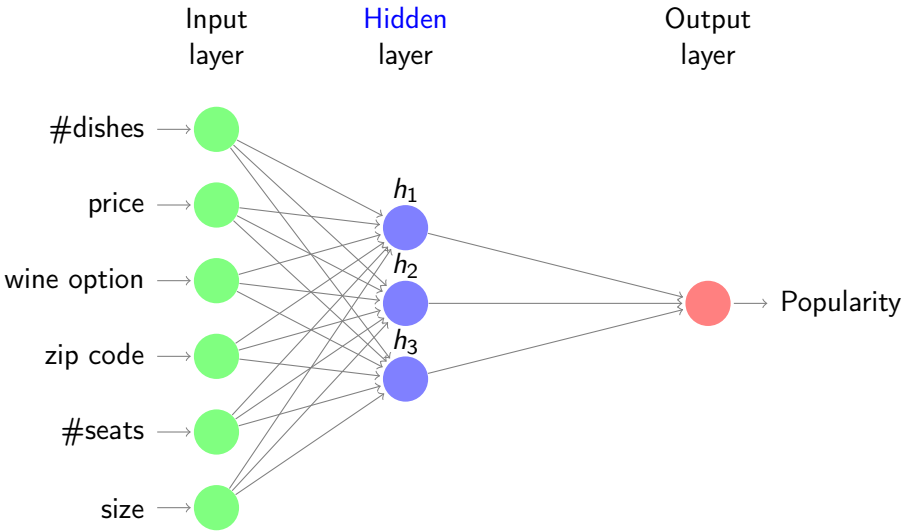
  Raw features #dishes, price, wine option, zip code, #seats, size
- Decompose into subproblems:
  - $h_1([\#\text{dishes, price, wine option}]) = \text{food quality}$
  - $h_2([\text{zip code}]) = \text{walkable}$
  - $h_3([\#\text{seats, size}]) = \text{nosie}$
- Final *linear* predictor uses **intermediate features** computed by h_i's:

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

Predefined subproblems



Learned intermediate features



Neural networks

Key idea: automatically learn the intermediate features.

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

$$f(x) = w^T \phi(x). \tag{2}$$

Feature learning Automatically 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

- How should we parametrize h_i's? Can it be linear?

$$h_i(x) = \sigma(v_i^T x). \tag{5}$$

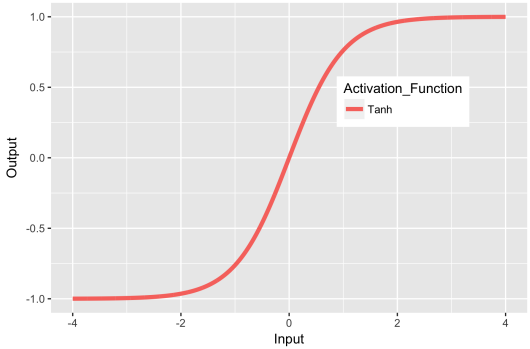
- σ is the nonlinear **activation function**.
- What might be some activation functions we want to use?
  - sign function? Non-differentiable.
  - Differentiable approximations: sigmoid functions.
    - E.g., logistic function, hyperbolic tangent function.
- Two-layer neural network (one hidden layer 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:

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

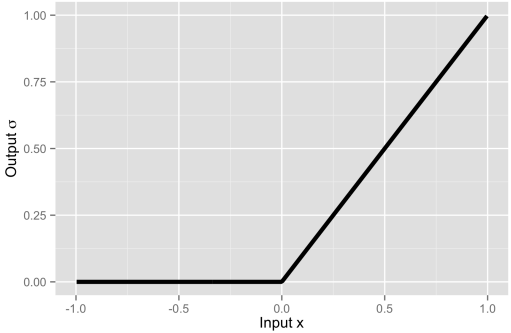


Activation Functions

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

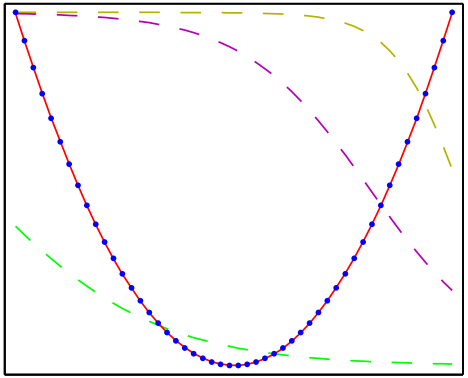
$$\sigma(x) = \max(0, x).$$

- Much faster to calculate, and to calculate its derivatives.
- Also often seems to work better.



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

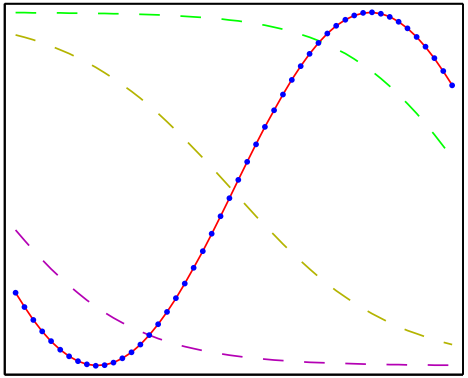
- 3 hidden units; tanh activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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

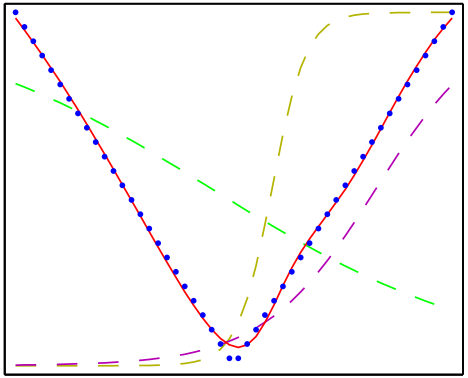
- 3 hidden units; logistic activation function
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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

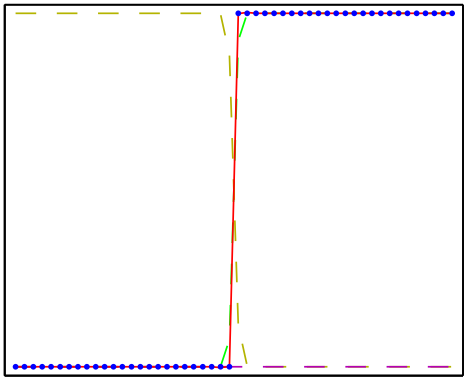
- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

Approximation Ability: $f(x) = 1(x > 0)$

- 3 hidden units; logistic activation function
- 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

Universal approximation theorems

How much expressive power do we gain from the nonlinearity?

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 R^d under mild assumptions on the activation function, i.e. $\forall \epsilon > 0$, there exists an integer N s.t.

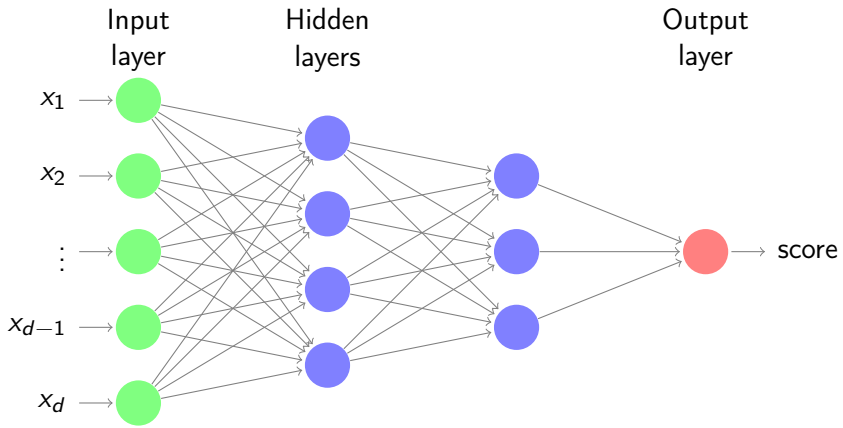
$$\hat{F}(x) = \sum_{i=1}^{N} w_i \sigma(v_i^T x + b_i) \tag{7}$$

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

- Number of hidden units needs to be exponential in d.
- Doesn't say how to learn these parameters.

Multilayer perceptron / Feed-forward neural networks

- Wider: more hidden units.
- Deeper: more hidden layers.



Multilayer Perceptron: Standard Recipe

- **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: Standard Recipe

- Each subsequent hidden layer takes the output $o \in \mathbb{R}^m$ 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 $W^{(j)} \in \mathbb{R}^{m \times m}$, $b^{(j)} \in \mathbb{R}^m$.

- 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 $b^{(L+1)} \in \mathbb{R}^k$.

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

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

- Last layer typically gives us a score. How to do classification?

Multinomial Logistic Regression

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

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

- 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:

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

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 outputs of the last hidden layer of a neural network.
- Learning: Maximize the log-likelihood of training data

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

Neural network as a feature extractor

- OverFeat is a neural network for object classification, localization, and detection.
  - Trained on the huge ImageNet dataset
  - Lots of computing resources used for training the network.
- All those hidden layers of the network are very valuable features.
  - Paper: "CNN Features off-the-shelf: an Astounding Baseline for Recognition"
  - Showed that using features from OverFeat makes it easy to achieve state-of-the-art performance on new vision tasks.

OverFeat code is at https://github.com/sermanet/OverFeat

Review

We've seen

- Key idea: automatically discover useful features from raw data—feature/representation learning.
- Building blocks:

Input layer	no learnable parameters
Hidden layer(s)	perceptron + nonlinear activation function
Output layer	affine (+ transformation)

- A single hidden layer is sufficient to approximate any function.
- In practice, often have multiple hidden layers.

Next, how to learn the parameters.

Back-propagation

A brief history of artificial neural networks

early 1940s–late 1960s

- Initial idea from neuroscience: create a computational model of neural networks.
- Development: perceptron [Rosenblatt, 1958], networks with many layers.
- Optimization: automatic differentiation [Linnainmaa, 1970].

late 1960s–late 1980s

- Computers didn't have enough processing power [Minsky and Papert, 1969].
- Back-propagation invented [Werbos, 1975] (but still hard to train).
- AI research focused on expert systems and symbolic systems.

late 1980s–early 2000s

- SVMs and linear models dominated ML.
- Continual developments in ANN: Schmidhuber, Hinton, Yann etc.

Example: MLP Regression

- **Input space**: $\mathcal{X} = \mathrm{R}$
- **Action Space / Output space**: $\mathcal{A} = \mathcal{Y} = \mathrm{R}$
- **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

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

for some fixed activation function $\sigma : \mathrm{R} \to \mathrm{R}$.

- What are the parameters we need to fit?

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

How to choose the best hypothesis?

- As usual, choose our prediction function using empirical risk minimization.
- Our hypothesis space is parameterized by

$$\theta = (b_1, b_2, b_3, v_1, v_2, v_3, w_0, w_1, w_2, w_3) \in \Theta = \mathrm{R}^{10}$$

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

$$\hat{\theta} = \arg\min_{\theta \in \mathrm{R}^{10}} \frac{1}{n} \sum_{i=1}^{n} (f(x_i; \theta) - y_i)^2 .$$

- Gradient descent:
  - Is it differentiable w.r.t. θ? $f(x) = w_0 + \sum_{i=1}^{3} w_i \tanh(v_i x + b_i)$.
  - Is it convex in θ? Might converge to a local minimum.

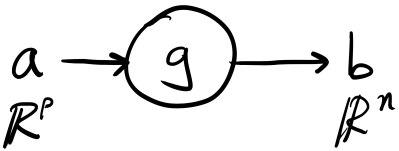
Gradient descent for (large) neural networks

- Mathematically, it's just partial derivatives, which you can compute by hand using the chain rule.
  - In practice, this could be time-consuming and error-prone.
- How do we compute gradients in a systematic and efficient way?
  - Back-propagation (a special case of automatic differentiation).
  - Not limited to neural networks.
- Visualize with computation graphs.
  - Avoid long equations.
  - Structure of the computation (modularity and dependency), which allows for modern computation frameworks such as Tensorflow/Pytorch/MXNet/etc.

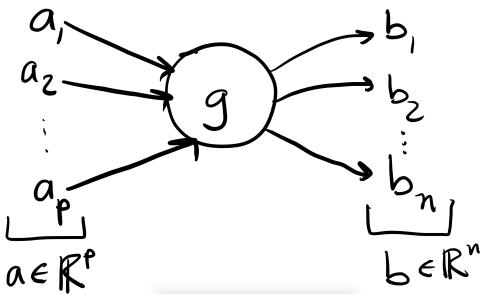
Function as a graph

- Function 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:

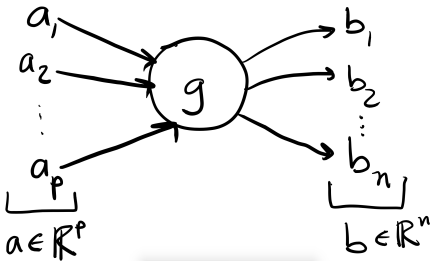


- Broken out into components:



Partial Derivatives of an affine function

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



- Let $b = g(a) = Ma + c$. What is b_i?
- b_i depends on the ith row of M:

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

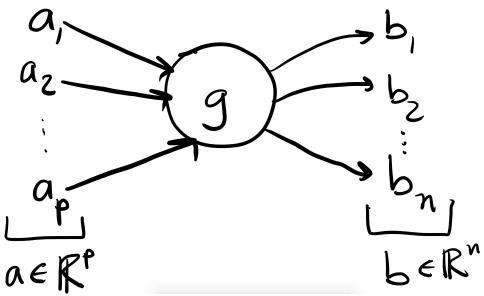
- If $a_j \leftarrow a_j + \delta$, what is b_i?

$$b_i \leftarrow b_i + M_{ij}\delta.$$

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

Partial Derivatives in general

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



- 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

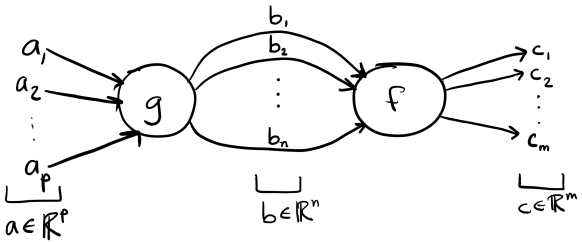
$$a_j + \delta,$$

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

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

Compose multiple functions

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



- How does change in a_j affect c_i?
- Visualize **chain rule**:
  - Sum changes induced on all paths from a_j to c_i.
  - Changes on one path is the product of changes on each edge along the path.

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

.

Example: Linear least squares

- Hypothesis space $\left\{ f(x) = w^T x + b \mid w \in \mathrm{R}^d, b \in \mathrm{R} \right\}$.
- Data set $(x_1, y_1), \ldots, (x_n, y_n) \in \mathrm{R}^d \times \mathrm{R}$.
- 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 see how to calculate these partial derivatives on a computation graph.

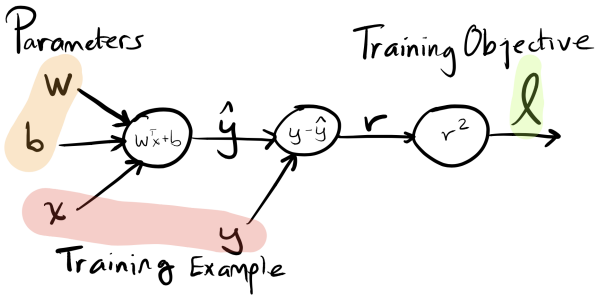
Computation Graph and Intermediate Variables

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

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

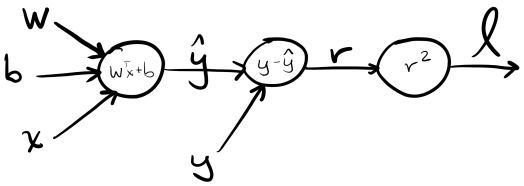
- Let's break this down into some intermediate computations:

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



Partial Derivatives on Computation Graph

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



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

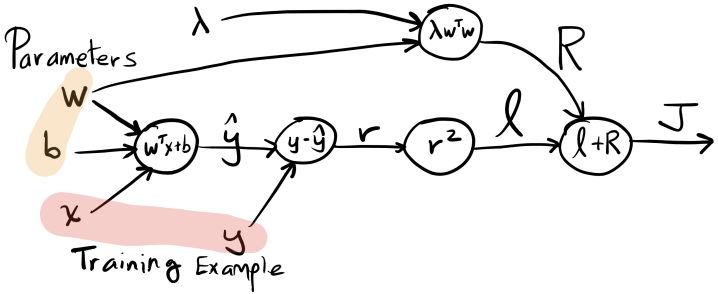
Example: Ridge Regression

- 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:

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



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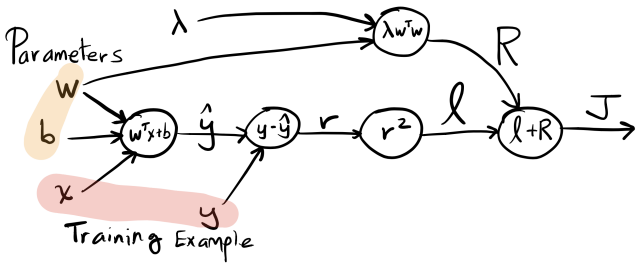


$$\frac{\partial J}{\partial \ell} = \frac{\partial J}{\partial R} = 1$$

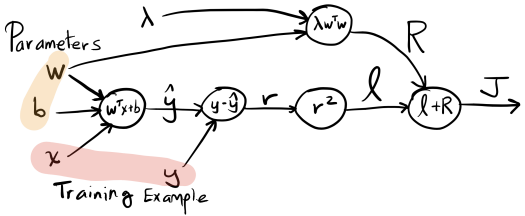
$$\frac{\partial J}{\partial \hat{y}} = \frac{\partial J}{\partial \ell}\frac{\partial \ell}{\partial r}\frac{\partial r}{\partial \hat{y}} = (1)(2r)(-1) = -2r$$

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

$$\frac{\partial J}{\partial w_j} = \text{Exercise}$$

Backpropagation overview

- **Learning**: run gradient descent to find the parameters that minimize our objective J.
- Backpropagation: compute 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

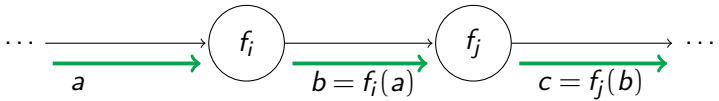
Backward pass: Compute the partial derivative of J w.r.t. all intermediate variables and the model parameters

How to save computation?

- Path sharing: each node needs to cache the intermediate results.
- Think dynamic programming.

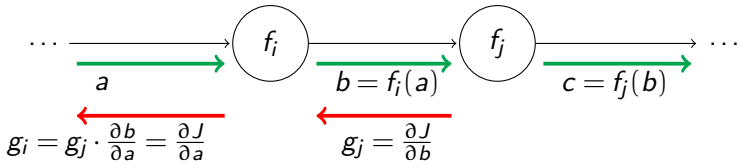
Forward pass

- 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:



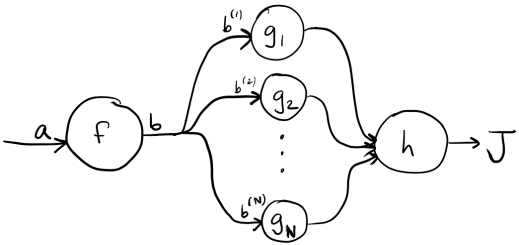
Backward pass

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



Multiple children

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



- 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 in practice

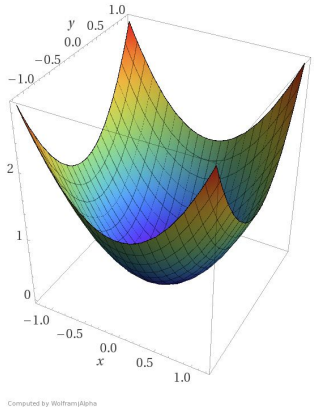
- Inputs and outputs of nodes are generally vectorized (efficient to compute on GPUs).
- Computation graphs can be composed from a set of basic operation nodes, e.g., addition/multiplication, dot product, logistic function etc.
- Programming paradigms:

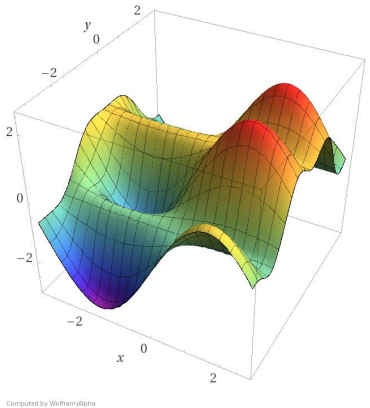
  Symbolic Specify all computation before data—efficient, e.g., Tensorflow.

  Imperative Specify the computation step by step—flexible/easier to write, e.g., Pytorch.

  Hybrid Can use either paradigm for computation subgraphs, e.g., MXNet.

Non-convex optimization



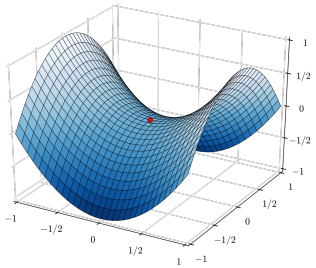


- Left: convex loss function. Right: non-convex loss function.

Non-convex optimization: challenges

Optimization of neural networks is generally hard.

- Converge to a bad local minimum.
  - Try different initialization and rerun.
- Saddle point.
  - Doesn't often happen with SGD.
  - Second partial derivative test.
- "Flat" region: low gradient magnitude
  - Use ReLU instead of sigmoid as activation functions.
- High curvature: high gradient magnitude
  - Gradient clipping.
  - Adaptive step sizes.



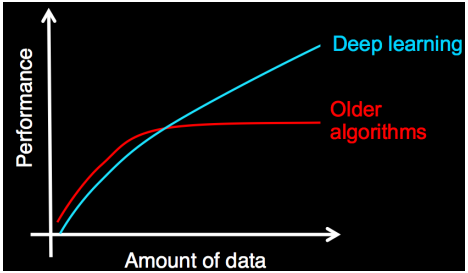
Reference: Chris De Sa's slides (CS6787 Lecture 7).

Review

- Backpropagation is an algorithm to compute gradient (partial derivatives + chain rule) efficiently.
- It is used in gradient descent optimization with neural networks.
- Key idea: function composition and dynamic programming
- In practice, efficient software exists (backpropagation, neural network building blocks, optimization algorithms etc.).

Advantages of Neural Networks

Neural Networks Benefit from Big Data



- Empirical observation: performance of deep neural networks has not plateaued with increasing amount of data.
- Higher data throughput compared to other nonlinear methods.
- Recent trends in system for ML: how to run (training/inference) large neural networks efficiently.

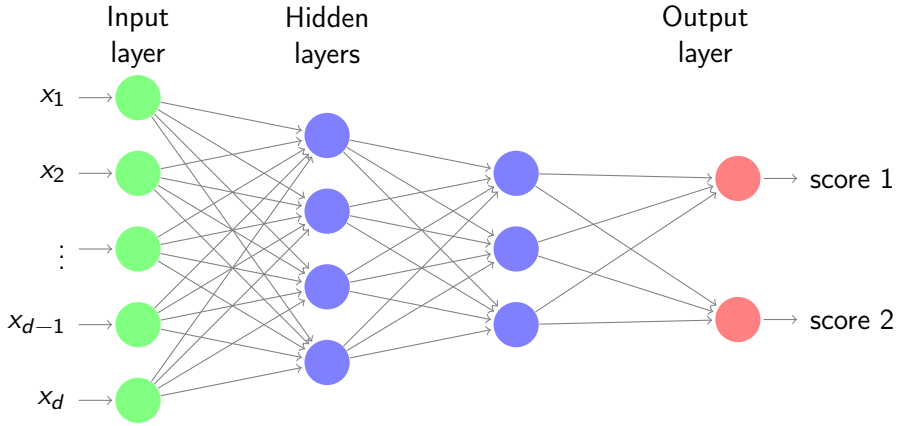
From Andrew Ng's CS229 Deep Learning slides (http://cs229.stanford.edu/materials/CS229-DeepLearning.pdf)

Versatile architectures

- Easy to incorporate inductive bias for different tasks.
- Examples:
  - Translation invariance in image recognition—convolution.
  - Dependence on past observations in time series—recurrence.
  - Alignment between input and (structured) output—attention.
- Many building blocks than can be composed together.

Representation sharing

- "Classifiers" are task-specific but representation/features can be shared.



Multitask Learning and transfer learning

Multitask learning:

- Learn related tasks together, e.g.,
  - Object classification: cat or dog?
  - Object localization: location of the objects?
- Basic features (e.g., edges, texture) can be shared by tasks.
  - Different output layers for each task; the rest is shared.
  - Objective function combines losses from both predictions, e.g. by averaging.

Transfer learning:

- Self-supervised **pre-training** to learn generic features.
  - General idea: denoising, i.e. perturbed input $\rightarrow$ original input.
- On downstream tasks: **fine-tune** pre-trained models (reuse representation).

Summary

- Powerful use of features: representation learning
- Fast and scalable with data given the right system support.
- Hard to train: non-convex optimization
  - Easier in practice with released code and libraries.
- Gap exists between theory and practice: when and why does it work?