Mathematical techniques in data science

Lecture 5: Neural networks

Reminders

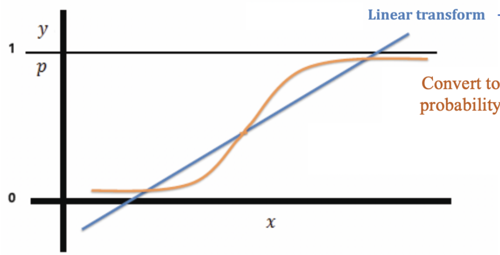
- Office hours (starting from the 2nd week):
  - Tuesdays 5:00pm-6:00pm, via Zoom
  - Wednesdays 3:30pm-4:30pm, Ewing Hall 312
  - Thursday 2pm-3pm, Ewing Hall 107A
  - By appointments
- Homework 1: due 03/03
- Sign up for group projects by the end of Week 4

Logistic regression

- Data point $(\mathbf{x}, y)$ where
  - $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ is a vector with d features
  - y is the label (0 or 1)
- Logistic regression models $P[y = 1 | X = \mathbf{x}]$

Logistic regression

$$\boldsymbol{x} \xrightarrow{\text{Linear transform}} \boldsymbol{w}^T\boldsymbol{x} + b \xrightarrow{\text{Convert to probability}} \frac{1}{1 + e^{-\boldsymbol{w}^T\boldsymbol{x} - b}}$$



Linear transform $\longrightarrow \boldsymbol{w}^T\boldsymbol{x} + b$

Convert to probability $\longrightarrow \frac{1}{1 + e^{-\boldsymbol{w}^T\boldsymbol{x} - b}}$

Logistic regression with more than 2 classes

- Suppose now the response can take any of $\{1, \ldots, K\}$ values
- We use the categorical distribution instead of the Bernoulli distribution

$$P[Y = k | X = \mathbf{x}] = p_k(\mathbf{x}), \quad \sum_{k=1}^{K} p_k(\mathbf{x}) = 1.$$

- Model

$$p_k(\mathbf{x}) = \frac{e^{w_k^T \mathbf{x}_k + b_k}}{\sum_{k=1}^{K} e^{w_k^T \mathbf{x}_k + b_k}}$$

Softmax function

$$\begin{bmatrix} 1.3 \\ 5.1 \\ 2.2 \\ 0.7 \\ 1.1 \end{bmatrix} \longrightarrow \boxed{\dfrac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}} \longrightarrow \begin{bmatrix} 0.02 \\ 0.90 \\ 0.05 \\ 0.01 \\ 0.02 \end{bmatrix}$$

Logistic regression: pros and cons

Pros:

- Simple algorithm
- Prediction is fast
- Easy to implement
- The forward map has a closed-form formula of the derivatives

$$\frac{\partial \ell}{\partial \beta_j}(\beta) = \sum_{i=1}^{n} \left[y_i x_{ij} - x_{ij} \frac{e^{x_i^T \beta}}{1 + e^{x_i^T \beta}} \right].$$

Cons:

- Linear model

How to make logistic regression better?

We want a model that

- computes the derivatives (of the objective function, with respect to the parameters) easily
- can capture complex relationships

This is difficult because complex models often have high numbers of parameters and don't have closed-form derivatives, and computations of

$$\frac{\partial \ell}{\partial \beta_i}(\beta, x) \approx \frac{\ell(\beta + \epsilon_i, x) - \ell(\beta, x)}{\epsilon_i}$$

are costly (and unstable)

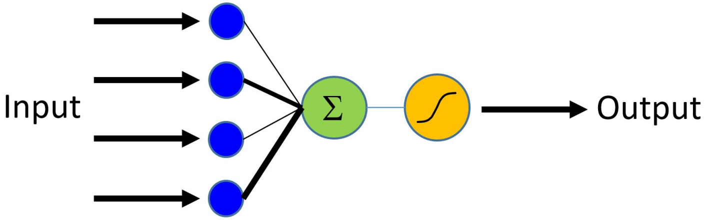
Ideas

- Automatic differentiation and back-propagation
- Ideas:
  - Organizing information using graphs (networks)
  - Chain rule

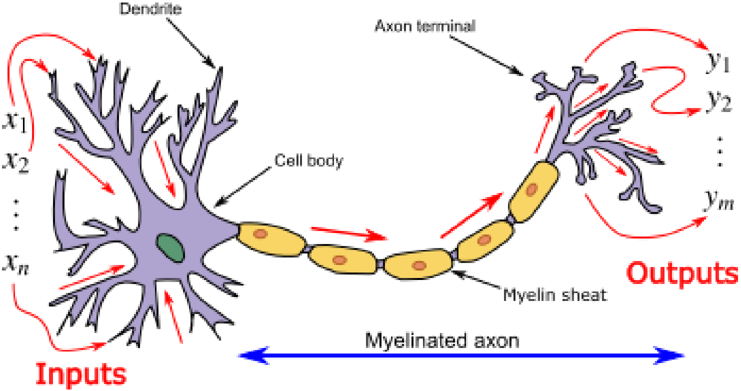
$$(f \circ g)'(x) = f'(g(x))g'(x)$$

Neural networks

Logistic neuron

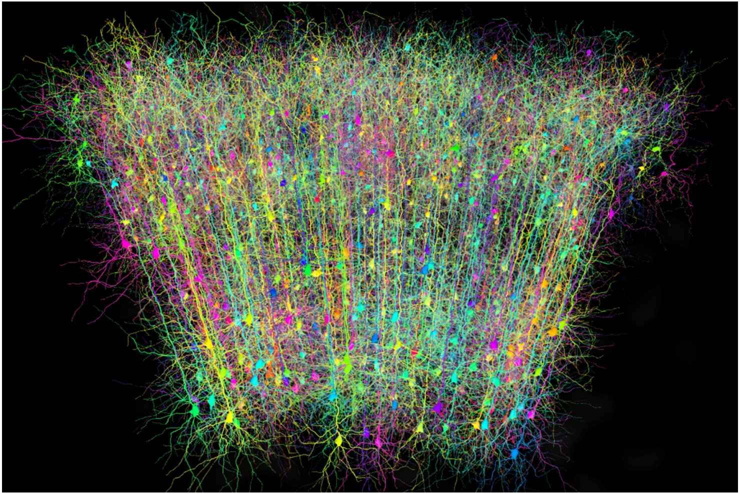


Why neuron?

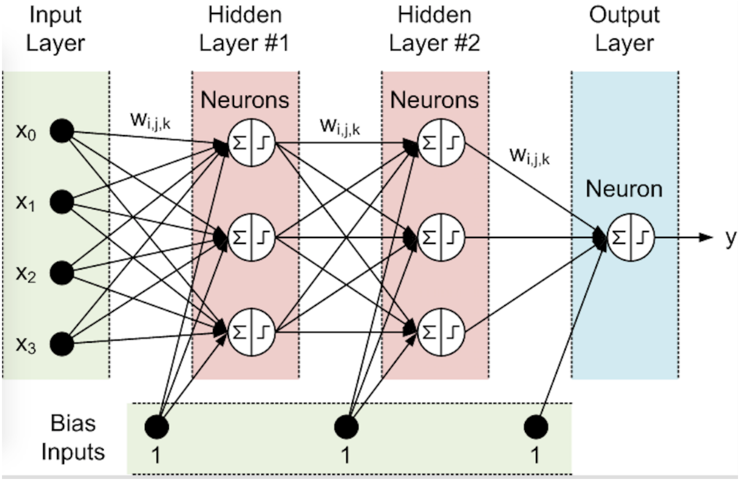


Dendrite
Axon terminal
x_1
x_2
$\vdots$
x_n
Cell body
y_1
y_2
$\vdots$
y_m
Outputs
Myelin sheat
Myelinated axon
Inputs

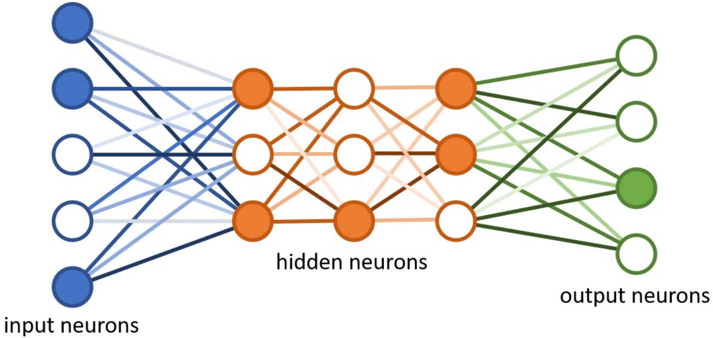
Neural circuit



Feed-forward neural networks



Feed-forward neural networks

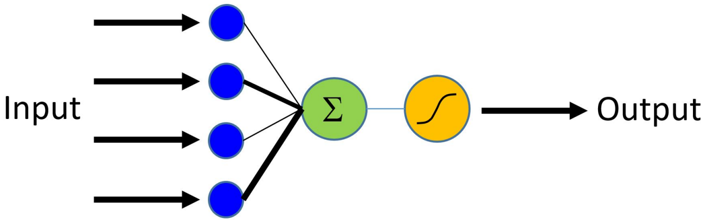


Feed-forward neural networks

- Structure:
  - Graphical representation
  - Activation functions
- Training:
  - Loss functions
  - Stochastic gradient descent
  - Back-propagation

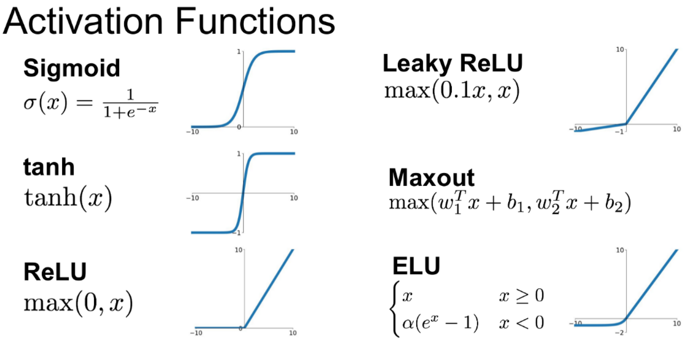
Activation functions

Activation functions



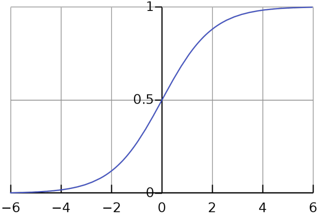
If we do not apply an activation function, then the output signal would simply be a simple linear function of the input signals

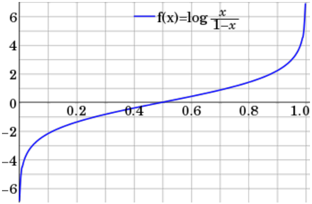
Activation functions



Logistic function (sigmoid function)

Transformation between $(-\infty, \infty)$ and $[0, 1]$

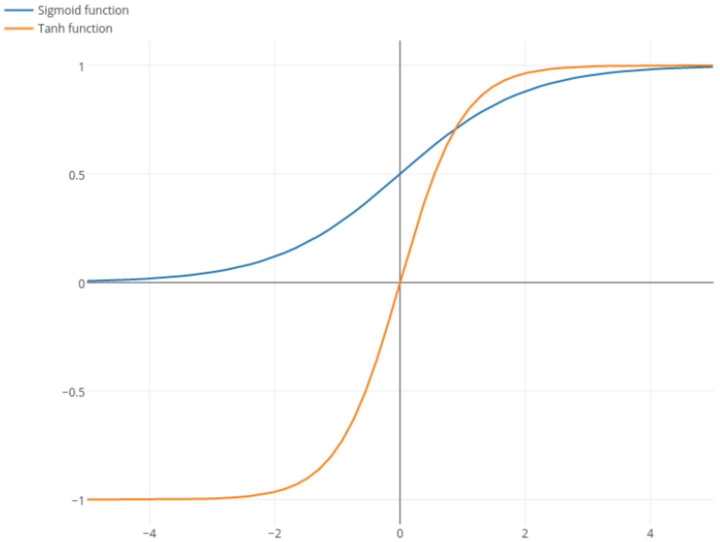




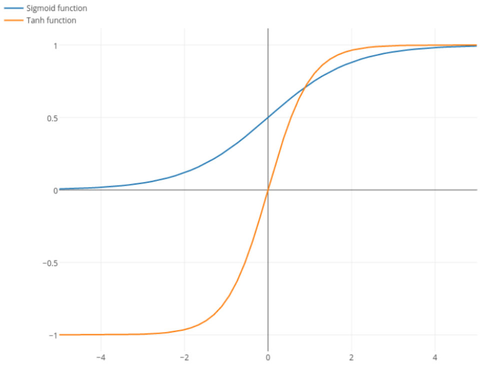
$$f(x) = \frac{e^x}{1 + e^x}$$

$$logit(p) = \log \frac{p}{1 - p}$$

Hyperbolic tangent

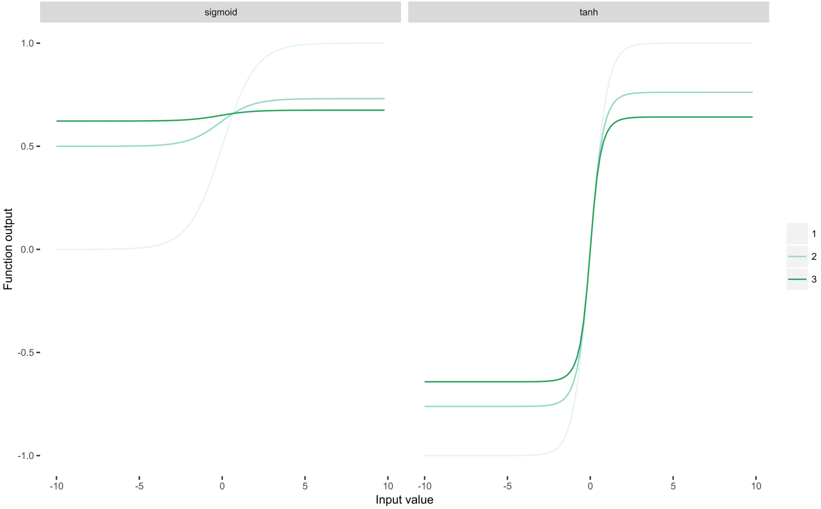


Hyperbolic tangent



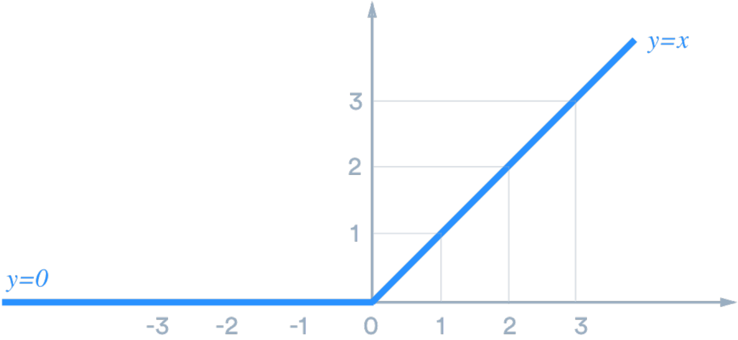
Issue: vanishing gradient problem

Hyperbolic tangent

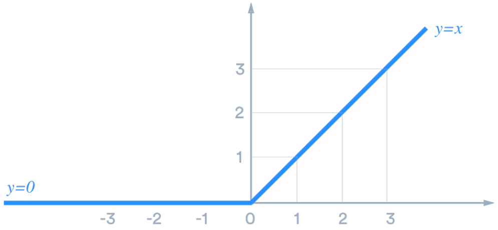


Vanishing gradient problem

Rectified linear unit (ReLU)



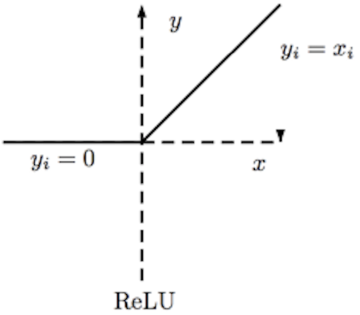
Rectified linear unit (ReLU)



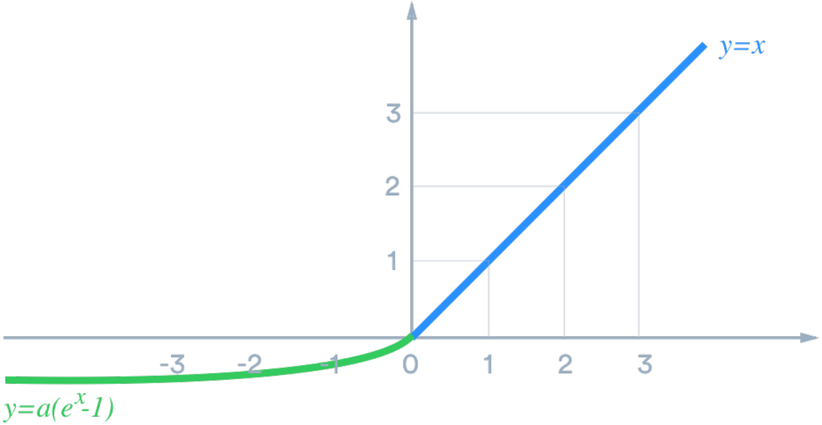
Advantage: model sparsity, cheap to compute (no complicated math), partially address the vanishing gradient problem

Issue: Dying ReLU

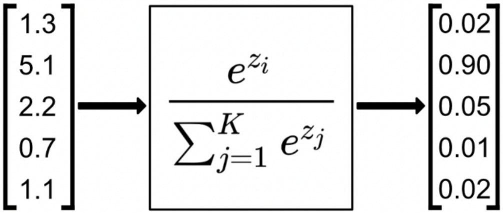
Leaky relu



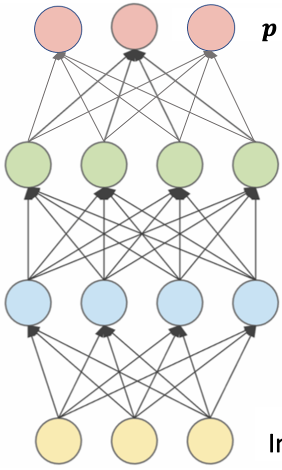
Exponential Linear Unit (ELU, SELU)



Softmax function



Feed-forward neural networks (multi-class classification)



$\boldsymbol{p} = \text{softmax}(\boldsymbol{W}_3^T \boldsymbol{h}_2 + \boldsymbol{b}_3)$

$\boldsymbol{h}_2 = \sigma(\boldsymbol{W}_2^T \boldsymbol{h}_1 + \boldsymbol{b}_2)$

$\boldsymbol{h}_1 = \sigma(\boldsymbol{W}_1^T \boldsymbol{x} + \boldsymbol{b}_1)$

Input: $\boldsymbol{x}$

Feed-forward neural networks

- Structure:
  - Graphical representation
  - Activation functions
- Training:
  - Loss functions
  - Stochastic gradient descent
  - Back-propagation

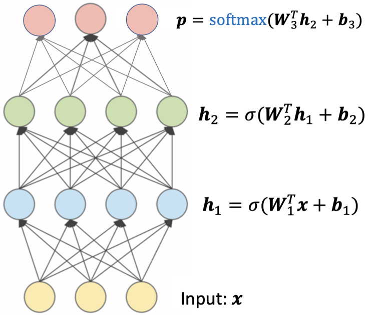
Train feed-forward neural networks

Settings

- Data:
  $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$
- Model parameters:

  $$\theta = (W_1, b_1, W_2, b_2, \ldots, W_L, b_L)$$

- Training: Find the best value of θ that fits the data



Maximum-likelihood method

- Average log-likelihood

$$\mathcal{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \log P(y = y_i | \mathbf{x}_i, \theta)$$

- Model parameters:

$$\theta = (W_1, b_1, W_2, b_2, \ldots, W_L, b_L)$$

- Training: Maximize $\mathcal{L}(\theta)$

Cross-entropy loss (log loss)

- Cross-entropy loss = negative log-likelihood:

$$\ell(\theta) = -\mathcal{L}(\theta)$$

- Goal: Minimize $\ell(\theta)$

One-hot encoding

id	color
1	red
2	blue
3	green
4	blue

One Hot Encoding →

id	color_red	color_blue	color_green
1	1	0	0
2	0	1	0
3	0	0	1
4	0	1	0

Convert a categorical value into a binary vector with exactly one "1" element, and the rest are 0

Loss function for classification: cross-entropy

Code

```
def CrossEntropy(yHat, y):
    if y == 1:
      return -log(yHat)
    else:
      return -log(1 - yHat)
```

Math

In binary classification, where the number of classes M equals 2, cross-entropy can be calculated as:

$$-(y\log(p) + (1-y)\log(1-p))$$

If $M > 2$ (i.e. multiclass classification), we calculate a separate loss for each class label per observation and sum the result.

$$-\sum_{c=1}^{M} y_{o,c}\log(p_{o,c})$$

Note: Here $y_{o,:}$ is the one-hot encoding of the label and $p_{o,c}$ is the predicted probability for the observation o is of class c, respectively

Stochastic gradient descent

Gradient descent

Gradient Descent

Minimize a function by moving in the opposite direction of the gradient.

$$\theta_i := \theta_i - \rho \frac{\partial J}{\partial \theta_i}$$

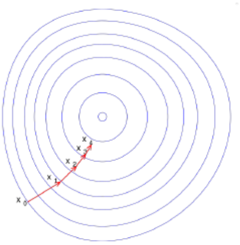
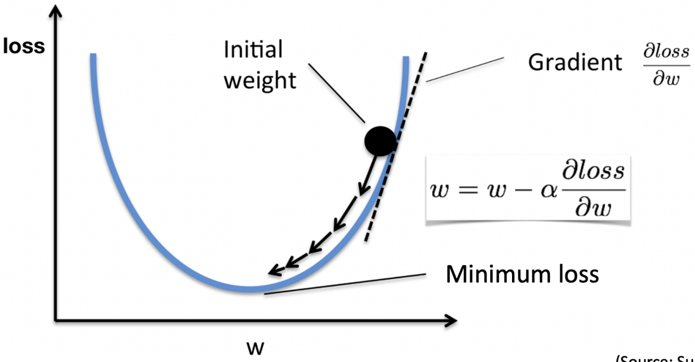


Figure: Gradient Descent. Source: `http://en.wikipedia.org/wiki/Gradient_descent`

Gradient descent



(Source: Sung Kim)

Stochastic gradient descent

- Recall that our objective function has the form

$$\ell(\theta) = \frac{1}{n}\sum_{i=1}^{n} L(\theta, x_i, y_i)$$

- Mini-batch stochastic gradient descent
  - randomly shuffle examples in the training set, divide them into k mini-batches of data of size m
  - for each batch I_i (i=1, ..., k), approximate the empirical risk by

$$\hat{\ell}(\theta) = \frac{1}{m}\sum_{j \in I_i} L(\theta, x_j, y_j)$$

    and update θ

$$\theta \leftarrow \theta - \rho \nabla \hat{\ell}(\theta)$$

  - Repeat until an approximate minimum is obtained or a maximum numbers M epochs are done

Stochastic gradient descent: teminology

- Mini-batch stochastic gradient descent
  - randomly shuffle examples in the training set, divide them into k mini-batches of data of size m
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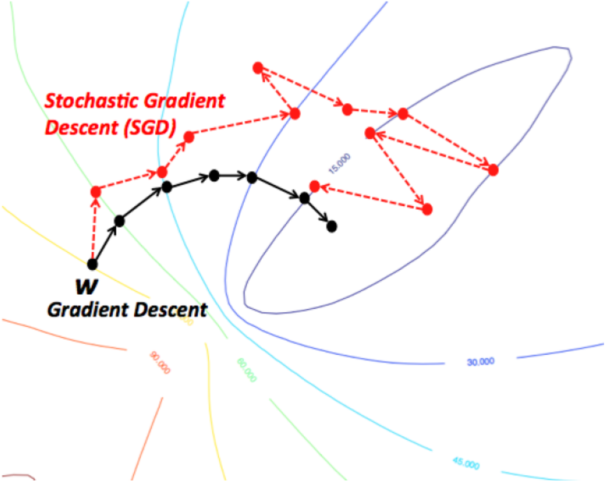
    and update θ

$$\theta \leftarrow \theta - \rho \nabla \hat{\ell}(\theta)$$

  - Repeat until an approximate minimum is obtained or a maximum numbers M epochs are done
- Terminology:
  - m: batch-size
  - ρ: learning rate
  - M: number of epochs

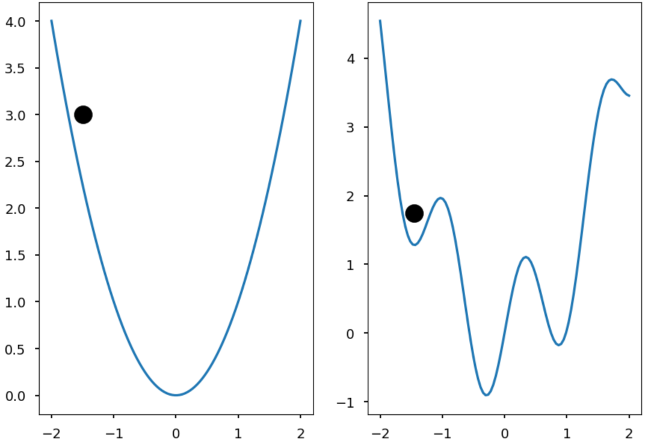
Stochastic gradient descent (SGD)



Stochastic gradient descent

- Gradient descent converges to the local minimum, and the fluctuation is small
- SGD's fluctuation is large, but enables jumping to new/better local minima

Escaping local minima



Automatic diffierentiation

Stochastic gradient descent

- The most computationally heavy part in the training of a neural net is to compute

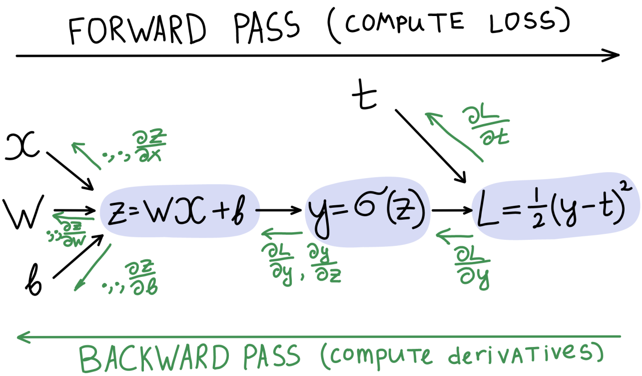
$$\frac{\partial \ell}{\partial \theta_{i,j}}$$

- Numerical differentiation is not realistic, and symbolic differentiation is impossible

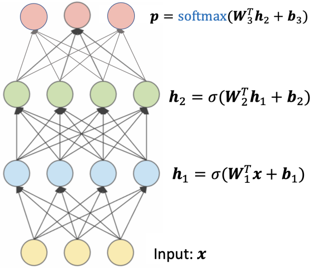
Automatic differentiation

- Assume that
$$y = f(g(h(x)))$$
- Denote $x = u_0$, $h(u_0) = u_1$, $g(u_1) = u_2$, $f(u_2) = u_3 = y$, then
$$\frac{dy}{du_i} = \frac{dy}{du_{i+1}} \frac{du_{i+1}}{du_i}$$

Back-propagation



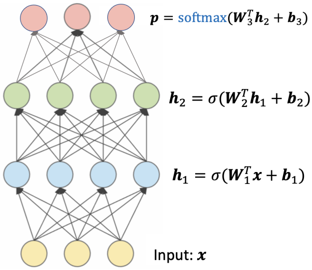
Back-propagation



Use chain rule to compute $\nabla \ell(\theta)$

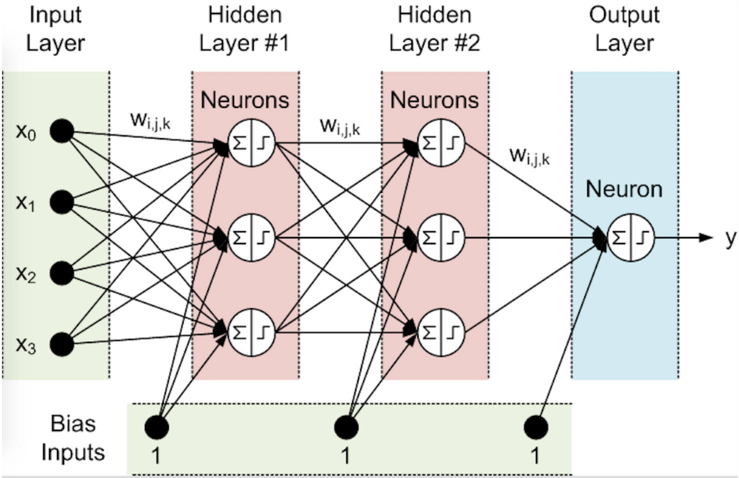
$$\frac{\partial \ell}{\partial b_1} = \frac{\partial \ell}{\partial p}(p) \cdot \frac{\partial p}{\partial h_2}(h_2, W_3, b_3) \cdot \frac{\partial h_2}{\partial h_1}(h_1, W_2, b_2) \cdot \frac{\partial h_1}{\partial b_1}(x, W_1, b_1)$$

Back-propagation



- One forward pass to evaluate h_1, h_2, p, ℓ
- One backward pass to compute $\nabla \ell(\theta)$

Feed-forward neural networks



Back-propagation

- Advantage: The cost to compute the partial derivatives with respect to all parameters are just twice the cost of a forward evaluations
- Drawback: The functions used to describe the network (activation functions and loss functions) needs to belong to the class of functions supported by the computational platform