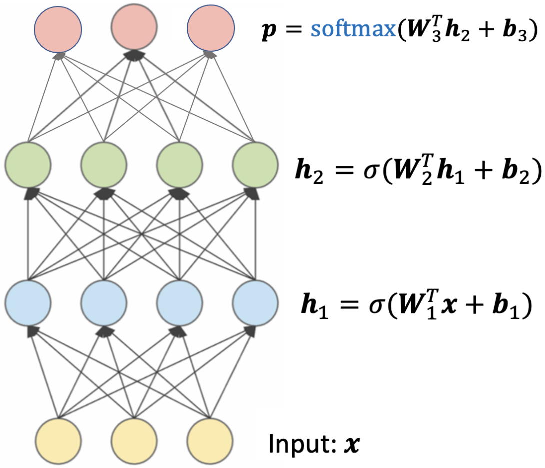
Mathematical techniques in data science

Lecture 6: Automatic differentiation and back propagation

Feed-forward neural networks (multi-class classification)



Feed-forward neural networks

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

Stochastic gradient descent

Gradient descent

Gradient Descent

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

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

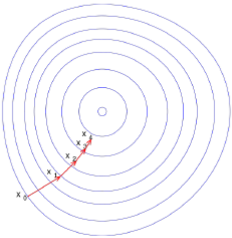


Figure: Gradient Descent. Source:
`http://en.wikipedia.org/wiki/Gradient_descent`

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 number M epochs are done

Stochastic gradient descent: teminology

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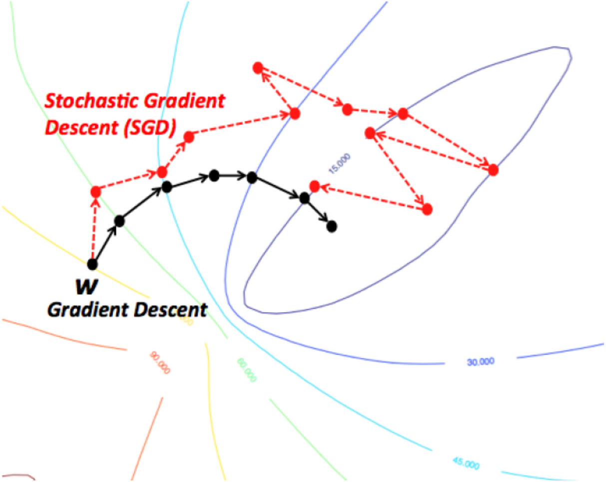
  - Repeat until an approximate minimum is obtained or a maximum numbers M epochs are done
- Terminology:
  - m: batch-size
  - ρ: learning rate
  - M: number of epochs

Stochastic gradient descent (SGD)



Automatic differentiation

Stochastic gradient descent

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

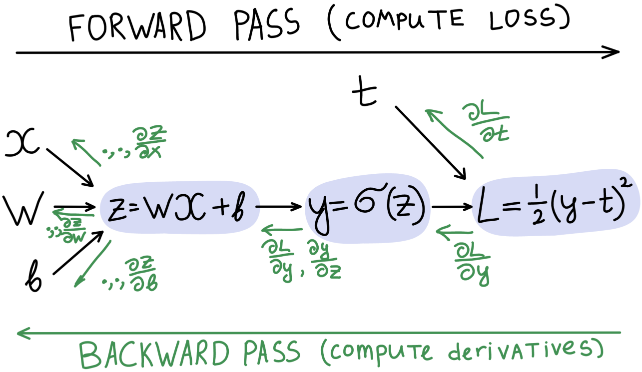
$$\frac{\partial \ell}{\partial \theta_{i,j}}$$

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

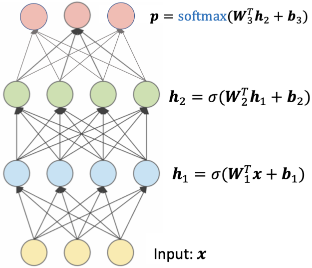
Automatic differentiation

- 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



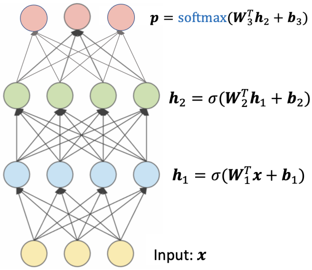
Back-propagation



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

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

Back-propagation



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

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

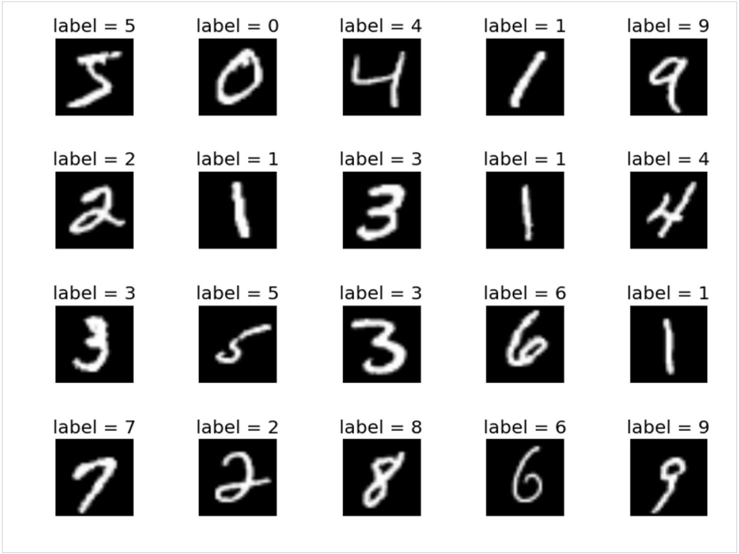
Some intros to computer vision

Computer vision

A field that enables computers and systems to derive meaningful information from digital images, videos and other visual inputs

- Image classification/object recognition
- Object detection
- Image segmentation
- Image generation
- Image style transfer

Image classification



Object detection

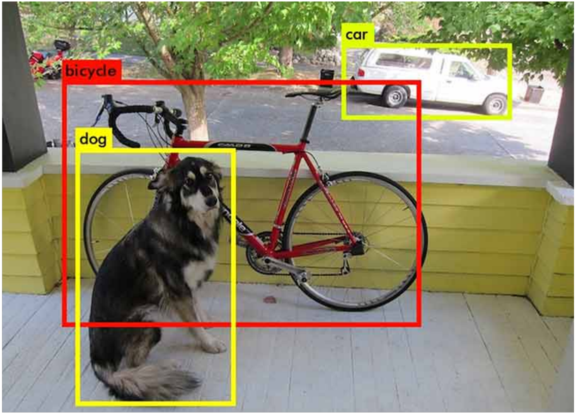


Image segmentation

Image generation

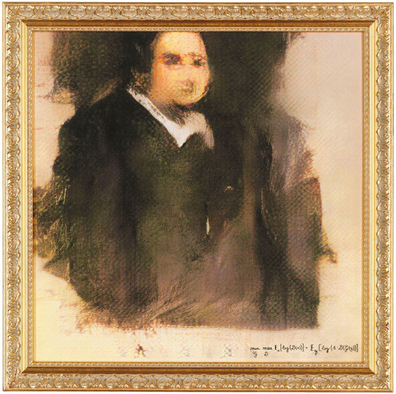
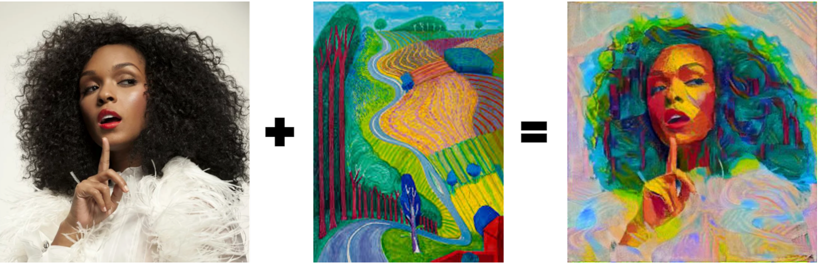
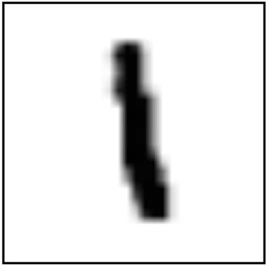


Image style transfer

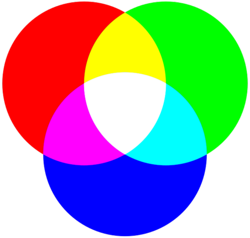


Grayscale image representation



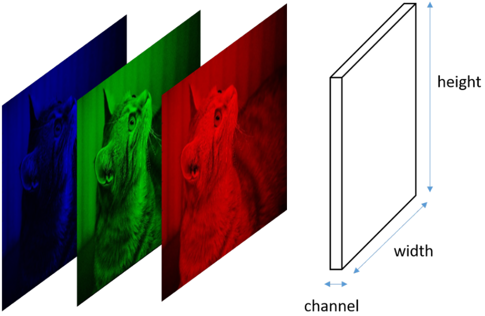
$$
\simeq
\begin{bmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&.6&.8&0&0&0&0&0&0\\
0&0&0&0&0&0&.7&1&0&0&0&0&0&0\\
0&0&0&0&0&0&.7&1&0&0&0&0&0&0\\
0&0&0&0&0&0&.5&1&.4&0&0&0&0&0\\
0&0&0&0&0&0&0&1&.4&0&0&0&0&0\\
0&0&0&0&0&0&0&1&.4&0&0&0&0&0\\
0&0&0&0&0&0&0&1&.7&0&0&0&0&0\\
0&0&0&0&0&0&0&1&1&0&0&0&0&0\\
0&0&0&0&0&0&0&.9&1&.1&0&0&0&0\\
0&0&0&0&0&0&0&.3&1&.1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix}
$$

Color image representation



- Use RGB color mode
- Represent a color by 3 values: R (Red) G (Green) B (Blue)
- There are other color modes

Image representation



- An image is an H x W x C matrix: H (height), W (width), C (depth or number of channels)
- Grayscale image: C = 1
- RGB image: C = 3

Demo: train an MLP using Keras

sklearn.neural_network.MLPClassifier

class sklearn.neural_network.MLPClassifier(*hidden_layer_sizes=(100,), activation='relu', *, solver='adam', alpha=0.0001, batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True, random_state=None, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000*) [source]

Multi-layer Perceptron classifier.

This model optimizes the log-loss function using LBFGS or stochastic gradient descent.

New in version 0.18.

Parameters:

hidden_layer_sizes : *tuple, length = n_layers - 2, default=(100,)*

The ith element represents the number of neurons in the ith hidden layer.

activation : *{'identity', 'logistic', 'tanh', 'relu'}, default='relu'*

Activation function for the hidden layer.

- 'identity', no-op activation, useful to implement linear bottleneck, returns f(x) = x
- 'logistic', the logistic sigmoid function, returns f(x) = 1 / (1 + exp(-x)).
- 'tanh', the hyperbolic tan function, returns f(x) = tanh(x).
- 'relu', the rectified linear unit function, returns f(x) = max(0, x)

- High level API for deep learning
- More flexible to define network architecture than sklearn

Define network architecture (1)

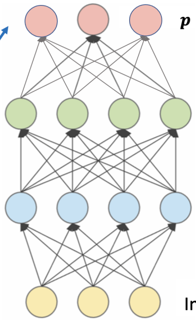
- Define a network as a Sequential object
- Add layers to it one-by-one

```
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense

model = Sequential()
model.add(Dense(50, activation='relu'))
model.add(Dense(50, activation='relu'))
model.add(Dense(10, activation='softmax'))
```

Define network architecture (2)

Dense /
Fully connected layer



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

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

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

Input: $\boldsymbol{x}$

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

Labels in Keras are usually encoded as one-hot vectors