

INF 5860 Machine learning for image classification Summary June 5, 2018





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Progress

- TensorFlow
- Convolutional neural networks
- Generalization
- Recurrent neural networks
- Deep reinforcement learning

Why do we need Deep learning frameworks?

- Speed:
 - Fast GPU/CPU implementation of matrix multiplication, convolutions and backpropagation

Automatic differentiations:

- Pre-implementation of the most common functions and it's gradients.

• Reuse:

- Easy to reuse other people's models

• Less error prone:

- The more code you write yourself, the more errors

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TensorFlow

- TensorFlow graphs
- TensorFlow session
- TensorFlow constants
- TensorFlow variables
- TensorFlow feeding data to the graph
- Tensorboard
- TensorFlow save/restore models
- TensorFlow example



Graphs



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Defining a tensor in TensorFlow

- The main types of tensors are:
 - tf.Variable / tf.get_variable
 - tf.constant
 - tf.placeholder
- Attributes (some of them):
 - Shape
 - dtype
 - name

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Example of a tensors

In [4]: import tensorflow as tf

In [5]: a = tf.constant(value=3, name='myConstant', dtype=tf.float32, shape=())
print(a)

Tensor("myConstant_1:0", shape=(), dtype=float32)

In [17]: a = tf.Variable(initial_value=3, trainable=True, name='myVariable', dtype=tf.float32)
print(a)

<tf.Variable 'myVariable_2:0' shape=() dtype=float32_ref>

In [124]: a = tf.placeholder(name='myPlaceholder', dtype=tf.float32, shape=())
print(a)

Tensor("myPlaceholder:0", shape=(), dtype=float32)

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The graph

- The TensorFlow graph is a definition, not any computation.
- The computational graph is a series of TensorFlow operations arranged into a graph. The graph is composed of two types of objects:
 - Operation: Nodes in the graph
 - Tensors: The edges in the graph



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Executing the tf.Graph: tf.Session

- We have seen that variables and constants are handles to elements in the computational graph only.
- We execute the graph using a tf.Session

```
In [50]: c = tf.add(3.0, 5.0)
sess = tf.Session()
c_val = sess.run(c)
sess.close()
print(c)
print(c_val)
Tensor("Add:0", shape=(), dtype=float32)
8.0
```

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Creating variables

We can define variables two ways:

create variables with tf.Variable
s = tf.Variable(3.0, name="scalar")

create variables with tf.get_variable
s = tf.get_variable("scalar", initializer=tf.constant(3.0))

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preferred

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Initializing variables

- The variables to be used in the graph have to be either:
 - Initialized
 - Restored

```
tf.reset_default_graph()
x = tf.Variable(initial_value=tf.ones(4), name="array")
with tf.Session() as sess:
    sess.run(x.initializer)
    x_val = sess.run(x)
    print(x_val)
```

[1. 1. 1. 1.]

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tf.placeholder

```
# create a placeholder for a vector of 2 elements, type tf.float32
x = tf.placeholder(dtype=tf.float32, shape=[2], name='p')
y = tf.constant(value=[1, 2], dtype=tf.float32, name='c')
z = x + y
with tf.Session() as sess:
    z_val = sess.run(z, feed_dict={x: [3, 4]})
    print(z_val)
```

[4.6.]



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Tensorboard: Visualizing learning



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tf.train.saver.save()

• How to save our model every 1000 iteration.

```
saver = tf.train.Saver()
global_step = tf.Variable(0, dtype=tf.int32, trainable=False, name='global_step')
with tf.Session() as sess:
    for step in range(number_of_training_steps):
        # do training of the network
        #Save the modeL every 1000 training step
        if (step + 1) % 1000==0:
            saver.save(sess, 'checkpoint_directory/model_name', global_step=global_step)
```

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Convolutional layer



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Convolutional layer



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Convolutional layer

• If we filter the input volume 6 times using a 5x5x3 filter, we get a output volume with 6 channels (depth)



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Activations

• We use an activation function separately on all elements of the output volume



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Stride

- Stride is the spatial step length in the convolution operation.
- Example: Input volume 7x7x1, kernel (filter) size 3x3x1
- The stride is an important parameter for determining the spatial size of the output volume



Padding

- The output volume can get a lower spatial resolution compared to the input volume. We can solve this by padding the input volume. Common to use zero padding
- Abbreviations: Stride (*S*), filter size (*F*), input size (N^0) , output size (N^1) and padding (*P*)
- For S = 1, we can achieve $N^0 = N^1$ selecting *P* equal to:

$$P = \frac{(F-1)}{2}$$

• Calculation of the spatial output size:

$$N^{1} = \frac{N^{0} - F + 2P}{S} + 1$$

0	0	0	0	0	0		
0							
0							
0							
0							

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How large area influence the end result?

- With a convolutional network the receptive field increase with each layer
 - 3 inputs influence each node in the first hidden layer ^{Hidden} Layer ^{Hidden} Layer ^{Hidden} Layer ^{Output} ^{Output} ^{Output} ^{Output}}}</sup></sup></sup></sup></sup></sup></sup></sup></sup></sup>

Input

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How large area influence the end result?

- With a convolutional network the receptive field increase with each layer
- 3 inputs influence each node in the first hidden layer
- 5 influence the next



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How large area influence the end result?

- With a convolutional network the receptive field increase with each layer
- 3 inputs influence each node in the first hidden layer
- 5 influence the next
- 7 influence the next



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The effect of strided convolutions

- We still cover the whole input
- We have increased the receptive field from $5 \rightarrow 7$ in hidden layer 2



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With strides, spatial dimensions will become smaller

• Usually some of the of the network capacity is preserved through an increasing number of channels



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Dilated convolutions

- Skipping values in the kernel
- Same as filling the kernel with every other value as zero
- Still cover all inputs
- Larger kernel with no extra parameters



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Visualizing and Understanding deeper layers

- Looking at the filer coefficient directly at deeper layer is not meaningful.
- Visualization with Deconvnet



Zeiler M.D., Fergus R. (2014) Visualizing and Understanding Convolutional Networks

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Hierarchical learning

- A convolution neural network is built up as a hierarchy were the complexity (abstraction) is increased by depth.
- A hierarchical structure is parameter efficient



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Notation

- Formalization supervised learning:
 - Input: *x*
 - Output: *y*
 - Target function: $f : X \rightarrow Y$
 - Data: $(x_1, y_1), (x_2, y_2) \cdots, (x_N, y_N)$
 - $\downarrow \quad \downarrow \quad \downarrow$
 - Hypothesis: $h: \mathcal{X} \rightarrow \mathcal{Y}$

Example:

- Hypothesis set: $y = w_1 x + w_0$
- A hypothesis: y = 2x + 1

More notation

- **In-sample** (colored): Training data available to find your solution.
- **Out-of-sample** (gray): Data from the real world, the hypothesis will be used for.
- Final hypothesis:
- Target hypothesis: —
- **Generalization:** Difference between the in-sample error and the out-of-sample error



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What is the expected out-of-sample error?

- For a randomly selected hypothesis
- The closest error approximation is the **in-sample** error



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What is training?

- A general view of training:
 - Training is a search through possible hypothesis
 - Use in-sample data to find the best hypothesis



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What is the effect of choosing the best hypothesis?

- Smaller **in-sample** error
- Increasing the probability that the result is a coincidence
- The expected **out-of-sample** error is greater or equal to the **in-sample** error

$ h_1$
ı ₂

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Capacity of the model (hypothesis set)

- The model restrict the number of hypothesis you can find
- Model capacity is a reference to how many possible hypothesis you have
- A linear model has a set of all linear functions as its hypothesis

$$\widehat{y} = sign(\mathbf{w}^T \mathbf{x} + b)$$

$$\widehat{y} = \mathbf{x}^T W \mathbf{x} + \mathbf{w}^T x + b$$


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Measuring capacity

- Vapnik-Chervonenkis (VC) dimension
 - Denoted: $d_{VC}(\mathcal{H})$
 - Definition:
 - The maximum number of points that can be arrange such that ${\mathcal H}$ can shatter them.

Example VC dimension

- (2D) Linear model $\widehat{y} = sign(\mathbf{w}^T \mathbf{x} + b)$
- Configuration (N = 3)



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Splitting of data

- Training set (60%)
 - Used to train our model
- Validation set (20%)
 - Used to select the best hypothesis
- Test set (20%)
 - Used to get a representative **out-of-sample** error

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Important! No peeking

- Keep a dataset that you don't look at until evaluation (**test set**)
- The test set should be as different from your **training set** as you expect the real world to be



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Learning curves



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Recurrent Neural Network (RNN)

- Takes a new input
- Manipulate the state
- Reuse weights
- Gives a new output



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Recurrent Neural Network (RNN)

- Unrolled view
- x_t : The input vector:
- h_t : The hidden state of the RNN
- y_t : The output vector:



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(Vanilla) Recurrent Neural Network

- Input vector: x_t
- Hidden state vector: h_t
- Output vector: y_t
- Weight matrices: W_{hh} , W_{hx} , W_{hy}

General form:

$$h_t = f_w(h_{t-1}, x_t)$$

Vanilla RNN:

$$h_t = \tanh(W_{hh}h_{t-1} + W_{hx}x_t + b)$$
$$y_t = W_{hy}h_t$$



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RNN: Computational Graph



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RNN: Predicting the next character

- Task: Predicting the next character
- Training sequence: "hello"
- Vocabulary:
 - [h, e, l, o]
- Encoding: Onehot
- Model:
- $h_t = \tanh(W_{hh}h_{t-1} + W_{hx}x_t + b)$
- $y_t = W_{hy}h_t$



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Input-output structure of RNN's

- One-to-one
- one-to-many
- many-to-one
- Many-to-many
- many-to-many (encoder-decoder)

Vanishing gradients - "less of a problem"

- In contrast to feed-forward networks, RNNs will not stop learning in spite of vanishing gradients.
- The network gets "fresh" inputs each step, so the weights will be updated.
- The challenge is to learning long range dependencies. This can be improved using more advanced architectures.
- Outputs at time step t is mostly effected by the close previous state.



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Exploding or vanishing gradients

- tanh() solves the exploding value problem
- tanh() does NOT solve the exploding gradient problem, think of a scalar input and a scalar hidden state.

$$h_t = tanh(W_{hh}h_{t-1} + W_{hx}x_t + b)$$

$$\frac{\partial h_t}{\partial h_{t-1}} = \left[1 - \tanh^2(W_{hh}h_{t-1} + W_{hx}x_t + b)\right] \cdot W_{hh}$$

The gradient can explode/vanish exponentially in time (steps)

- If $|W_{hh}| < 1$, vanishing gradients
- If $|W_{hh}| > 1$, exploding gradients

Gated Recurrent Unit (GRU)

GRU is adding or removing to the state, not "transforming the state"

Vanilla RNN

• Cell state $h_t = tanh(W^{hx}x_t + W^{hh}h_{t-1} + b)$

GRU

With Γ^r as ones and Γ^u as zeros, GRU \rightarrow Vanilla RNN

Multi-layer Recurrent Neural Networks

- Multi-layer RNN can be used to enhance model complexity
- Similar as for feed forward neural networks, stacking layers creates higher level feature representation
- Normally, 2 or 3 layer deep, not as deep as conv nets
- More complex relationships in time



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Bidirectional recurrent neural network

- The blocks can be vanilla, LSTM and GRU recurrent units
- Real time vs post processing

$$\begin{split} \vec{h}_{t} &= f\left(\vec{W}_{hx}x_{t} + \vec{W}_{hh}\vec{h}_{t-1}\right) \\ \vec{h}_{t} &= f\left(\vec{W}_{hx}x_{t} + \vec{W}_{hh}\vec{h}_{t+1}\right) \\ y_{t} &= g\left(W_{hy}\left[\vec{h}_{t}, \vec{h}_{t}\right] + b\right) \end{split}$$



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Branches of Machine Learning



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Reinforcement learning

- Reinforcement Learning ~ Science of decision making
- In RL an agent learns from the experiences it gains by interacting with the environment.
- The goal is to maximize an accumulated reward given by the environment.
- An agent interacts with the environment via states, actions and rewards.



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Reinforcement learning

- What makes reinforcement learning different from other machine learning paradigms?
 - There is no supervisor, only a reward signal
 - Feedback is delayed, not instantaneous
 - Time really matters (sequential, non i.i.d data)
 - Agent's actions affect the subsequent data it receives

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Mountain Car

- Objective:
 - Get to the goal
- State variables:
 - Position and velocity
- Actions:
 - Motor: Left, Neutral, right
- Reward:
 - (-1) for each time step





History (trajectory) and State

- History / trajectory :
 - $\quad H_t = \tau_t = \ O_1, A_1, R_1, \ O_2, A_2, R_2, \dots, \ O_t, A_t, R_t$
- Full observatory:
 - Agent direct observe the environment state.
 - $\quad O_t = S_t^e = S_t^a$
- State:
 - The state is a summary (of the actions and observations) that determines what happens next given an action.
 - $S_t = f(H_t)$

• Partially observability:

- The agent indirectly observes the environment.
- Robot with a camera



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Markov Property

- Definition:
 - A state S_t is Markov if and only if: $\mathbb{P}[S_{t+1}|S_t] = \mathbb{P}[S_{t+1} | S_1, S_2, \dots, S_t]$
- The state capture all relevant information from the history
- The state is sufficient to describe the statistics of the future.



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Reward and Return

- The **reward**, R_t , is a scalar value the agent receives for each step t.
- The **return**, G_t , is the total discounted accumulated reward form a given time-step t.

$$- \quad G_t = R_t + \gamma R_{t+1} + \dots = \sum_{k=0}^{\infty} \gamma^k R_{t+k}$$

- Discount factor:
 - − We can apply a discord factor, $\gamma \in [0,1]$, to weight how we evaluate return.
- The agent's goal is to maximize the **return**



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Markov Decision Process (MDP)

- The mathematical formulation of the reinforcement learning (RL) problem.
- A **Markov Decision Process** is a tuple, $\mathcal{M} = \langle S, A, P, R, \gamma \rangle$, where every state has the Markov property.
 - S: A finite set of states
 - A: A finite set of actions
 - *P*: The transition probability matrix $P_{s_t s_{t+1}}^a = \mathbb{P}[S_{t+1} = s_{t+1} | S_t = s_t, A_t = a_t]$
 - R: Reward function:

 $R_s^a = \mathbb{E}[S_t = s_t, A_t = a_t]$

 γ : is a discount factor $\gamma \in [0,1]$

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Objective

• Our goal is it find the policy which maximize the accumulated reward:

 $G_t = R_t + \gamma R_{t+1} + \dots = \sum_{k=0}^{\infty} \gamma^k R_{t+k}$

• Due to the randomness of the transition probability and the reward function, we use the expected value in the definition of the optimal policy.

$$\pi_* = \arg\max_{\pi} \mathbb{E}\left[G_t\right]$$



Bellman (optimality) equation

• Lets define the optimal Q-value (*action-value*) function, *Q*_{*}, to be the maximum expected reward given an state, action pair.

$$Q_*(s_t, a_t) = \max_{\pi} \mathbb{E}_{\pi}[G_t | A_t = a_t, S_t = s_t]$$

• The optimal Q-value function, Q_* , satisfy the following form of the bellman equation:

$$Q_*(s_t, a_t) = \mathbb{E}\left[R_t + \gamma \max_{a_{t+1}} Q_*(s_{t+1}, a_{t+1}) \mid A_t = a_t, S_t = s_t\right]$$

- Note: The optimal policy, π_* , is achieved by taking the action with the highest Q-value.
- Note: We still need the expectation, as the randomness of the environment is unknown.

Exploration vs Exploitation

- "The "*max*" property while sampling new episodes can lead to suboptimal policy"
- Exploitation:
 - By selecting the action with the highest q-value while sampling new episodes, we can refine our policy efficiently from an already promising region in the state action space.
- Exploration:
 - To find a new and maybe more promising region within the state action space, we do not want to limit our search in the state action space.
 - We introduce a randomness while sampling new episodes.
 - With a probability of ϵ lets choose a random action:

$$\pi(a|s) = \begin{cases} a_* = \underset{a \in A}{\operatorname{argmax}} Q(s,a), & \text{with probability } 1 - \epsilon \\ \text{random action,} & \text{with probability } \epsilon \end{cases}$$

Function approximation

- In the Gridworld example, we stored the state-values for each state. What if the state-action space is too large to be stored e.g. continuous?
- We approximate the Q-value using a parameterized function e.g. neural network.

 $\hat{Q}(s,a,\theta) \approx Q(s,a)$

- We want the function to generalize:
 - Similar states should get similar action-values, $\hat{Q}(s, a, \theta)$ can also generalize to unseen states. A table version would just require to much data.
- In supervised learning:
 - Building a function approximation vs memorizing all images (table).

Solving for the optimal policy: Q-learning

- **Goal**: Find a Q-function satisfying the Bellman (optimality) equation.
- **Idea**: The Q-value at the last time step is bounded by the true Q-value, the correctness of the Q-value estimates increase with time-steps.
- **Init:** Initialize the weights in the neural network e.g. randomly.

$$Q_*(s_t, a_t, \theta_i) = \mathbb{E}\left[R_t + \gamma \max_{a_{t+1}} Q_*(s_{t+1}, a_{t+1}, \theta_{i-1}) \mid A_t = a_t, S_t = s_t\right]$$

• Reference:

$$y_{i} = \mathbb{E}\left[R_{t} + \gamma \max_{a_{t+1}} Q(s_{t+1}, a_{t+1}, \theta_{i-1}) \mid A_{t} = a_{t}, S_{t} = s_{t}\right]$$

• Loss:

$$L_i(\theta_i) = \mathbb{E}_{s_t, s_{t+1}, a_t, r_t \sim D_i} \left[\left(y_i - Q(s_t, a_t, \theta_i) \right)^2 \right]$$

 D_i is your dataset with state action pairs s_t , s_{t+1} , a_t , r_t

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Policy based methods

- Value function based methods:
 - Learning the expected future reward for a given action.
 - The policy was to act greedily or epsilon-greedily on the estimated values.
- Policy based methods:
 - Learning the probability that an action is good directly.
- Advantage of Policy based methods:
 - We might need a less complex function for approximating the best action compared to estimate the final reward.
 - Example: Think of Pong

Policy based methods

- Goal:
 - The goal is to use experience/samples to try to make a policy better.
- Idea:
 - If a trajectory achieves a high reward, the actions were good
 - If a trajectory achieves a low reward, the actions were bad
 - We will use gradients to enforce more of the good actions and less of the bad actions. Hence the method is called Policy Gradients.

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Playing games of Pong

- Examples of games/episodes
- You play a lot of actions and receive an reward at the end
- You get a result, WIN! Great, but how do you know which action, caused the victory?
 - Well... you don't



Which action caused the final results?

- In a winning series there may be many non-optimal actions
- In a losing series there may be good actions
- The true effect is found by averaging out the noise, as winnings series tend to have more good action and visa versa





Policy gradients: High variance



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Policy gradients: High variance



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Variance - all choices get the reward





Variance - other possible paths





Variance - high probability to chose some other path



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Variance - same actions for same state: now negative



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