

# Deep Learning Summer School

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# 1 Neural Networks I (Hugo Larochelle)

## 1.1 Basics

### 1.1.1 Artificial Neuron

**pre-activation**  $a(x) = w^T x + b$

**activation function**  $h(x) = g(a(x))$

### 1.1.2 Capacity of Neural Networks

combining two simple linear neurons, can create a more complex non-linear shape

**universal approximation** a single hidden layer NN can approximate any continuous function arbitrarily well (given enough neurons)

### 1.1.3 Multilayer Neural Network

we can have  $L$  hidden layers, e.g. at layer  $k$

$$a^{(k)}(x) = b^{(k)} + W^{(k)} h^{(k-1)}(x)$$

$$h^{(k)}(x) = g(a^{(k)}(x))$$

**output layer** ( $k = L + 1$ )

$$h^{(L+1)}(x) = o(a^{(L+1)}(x)) = f(x)$$

### 1.1.4 Activation Function

**sigmoid**  $\frac{1}{1+\exp(-a)}$  probability of a bernoulli

**tanh**  $\frac{\exp(a)-\exp(-a)}{\exp(a)+\exp(-a)}$  squashes between -1 and 1

**relu**  $\max(0, a)$  does not saturate

**softmax** multi-class conditional probabilities

## 1.2 Training Neural Networks

### 1.2.1 Optimization

learning as an optimization problem

**loss function**  $l(f(x; \theta), y)$  between output and true label

**regularizer**  $\Omega(\theta)$  penalize certain parameters  $\theta$

use **Stochastic Gradient Descent**

1. initialize  $\theta$

for  $N$  epochs

- for each example  $x, y$
2. calculate gradient  $\Delta = -\nabla l(\dots)$
  3. take a step  $\theta \leftarrow \theta + \alpha \Delta$

### 1.2.2 Loss Function

maximize the probability of correct class (**maximum likelihood**)  
equivalently **minimize** the negative log-probability aka **cross-entropy**

$$l(f(x), y) = - \sum_c 1(y = c) \dots$$

### 1.2.3 Backpropagation

use chain rule to compute gradients

1. compute gradient wrt pre-activation

$$\nabla_{a^{(L+1)}(x)} - \log f(x)_y \leftarrow -(e(y) - f(x))$$

for layer  $k$  from  $L + 1$  to 1

2. compute gradient of hidden layer parameter
3. compute gradient of hidden layer below
4. compute gradient of pre-activation below

reversing the flow graph representation gives us backprop for free [Section 2](#)

### 1.2.4 Initialization

- biases  $\leftarrow 0$
- weights  $\leftarrow$  random sample
  - 0 doesn't work with tanh
  - same value doesn't work
  - break symmetry, close to 0

### 1.2.5 Model Selection

search for the best hyperparameters with

- **grid search** search all possible options
- **random search** sample from distribution over hyperparams
- bayesian optimization, pbt, ...

use a **validation set** of examples to choose the best model  
stop training with **early stopping** when validation error is lowest

### 1.2.6 Tricks

- **normalize** your (real-valued) data
- **decay** your learning rate
- update your gradient on a **batch** of examples
- use exponential average of previous gradients, "gaining **momentum**"
- use adaptive learning rates: **Adagrad**, **RMSProp**, **Adam**

### 1.2.7 Gradient Checking

debug your implementation of fprop/bprop with a finite-difference approximation

$$\frac{df(x)}{dx} \approx \frac{f(x + \epsilon) - f(x - \epsilon)}{2\epsilon}$$

### 1.2.8 Debug on Small Dataset

overfit on a subset of your dataset, issues:

- units saturated before first update? initialization, regularization
- training error unstable? learning rate scheduling

## 1.3 Regularization

### 1.3.1 Unsupervised Pretraining

**unsupervised pretraining** initialize hidden layers by using unsupervised learning to represent the latent structure of data

**fine-tuning** training after initialization to adapt to data

**auto-encoder** feed-forward NN trained to reproduce its input

### 1.3.2 Dropout

**dropout** remove hidden units stochastically (usually  $p = 0.5$ )

### 1.3.3 Batch Normalization

normalize inputs to speed up training

- normalize each unit's pre-activation
- subtract mean and std deviation, calculated per minibatch
- learn a linear transformation of the normalized pre-activation
- account for it during backprop
- use global mean and std deviation at test time

## 2 Automatic Differentiation (David Duvenaud)

### 2.1 Basic Autodiff

**auto diff** programmatically finding gradients for operations

**forward mode** building the jacobian on, in the order of initial operations (expensive)

**reverse mode** keeping track of jacobian at every step and adding then in reverse

#### 2.1.1 Implementation

**static** read and generate source code (Tensorflow)

**dynamic** monitor function execution at runtime (Pytorch, autograd)

1. trace execution as composition of primitives
2. define vector-Jacobian product (VJP) operator for each primitive
3. compose VJPs backwards

fun stuff:

- we get higher order autodiff for free  
since tape-based dynamic autodiff traces execution, we automatically trace the autodifferentiation itself, and just need to follow the execution trace of the previous autodiff
- forward mode is actually just a special case of reverse mode
- VJPs are as cheap as gradients

### 2.2 Advanced Autodiff

#### 2.2.1 Higher Order Ops

higher order gradients are possible by changing vector-Jacobian for vector-Hessian etc ...

#### 2.2.2 Meta-Optimization

can optimize through the whole network to learn the learning rate for the training

#### 2.2.3 Implicit Function Theorem

## 3 Neural Networks II Hugo Larochelle

### 3.1 Types

**supervised** examples have labels

**unsupervised** examples don't have labels

**semi-supervised** some examples have labels

**multi-task** multiple labels per example

**transfer** multiple labels but test on a specific label

**structured** labels have arbitrary structure

**domain adaptation** training and testing distributions are different

**zero-shot** examples are completely novel

### 3.2 Intriguing Properties

- there are powerful small changes that create visual adversarial examples
- bad local optima are unlikely (for high dimensional loss surface like NNs)
- NNs are strangely non-convex
- flat minima are better than sharp minima (probably?)
- NNs can easily memorize
- knowledge can be distilled
- catastrophic forgetting is a real issue with SGD

## 4 Intro to Convolutional Neural Networks Jon Shlens

### 4.1 Convolutional Neural Networks

images are different from other data

- fully connected layers would use too many parameters to input an image
- convolutions provide translational invariance

convolutional neural networks

- learn filters that pass over the image
- use fewer parameters
- use more computations

### 4.2 Modern Developments

- normalization stabilizes activations and is important for training  
Group Normalization (Wu and He 2018)
- vanishing gradients motivate deeper, better architectures
- architectures transfer across tasks
- learned architecture searches find even better models  
NAS (Zoph 2016), DARTS (Liu et al 2018)



## 4.3 Understanding CNNs

how to approach what CNNs understand at each layer?

- find images/pixels that elicit largest activation
- reconstruct image from network activations
- distort pixels to amplify activations (deep dream)
- change lower level activations while maintaining high-level (neural style transfer)

## 5 Deep Computer Vision Sanja Fidler

### 5.1 Segmentation

**semantic** assign each pixel a category based on the object it belongs to

**unsupervised** group pixels

**co-segmentation** same objects from different images

**instance** semantic but differentiate instances (e.g. car 1, car 2)

**panoptic**

convert classification network to segmentation network by pre-training and converting fully connected to fully convolutional layers

**CRF** conditional random field (unary, pairwise, and optional global term)

**dense CRF** all pixels are connected pairwise

### 5.2 3D Semantic Segmentation

**fusion** late fusion of CNNs over depth and image

**multi-view** CNN over every viewpoint

**VoxNet** 3D convolution over point cloud

**OctNet** exploit sparsity in 3D representation using octree

**PointNet** represent point clouds directly

**3D Graph NN** point cloud graph

## 6 Generative Models II

### 6.1 Data Prediction

#### 6.1.1 Conditional Generative Models

challenges

1. output is high-dimensional, structured
2. uncertainty in mapping, distribution of possibilities

two methods

1. model  $p(x, \cdot)$  and use inference to get  $p(x|y)$
2. directly model  $p(x|y)$

**GAN**

- a generator  $G$  creates fake images
- a discriminator  $D$  tries to discern between the fake image and a real image

**conditional GAN**

- add class  $y$  as extra input to both  $G$  and  $D$
- 

#### 6.1.2 Structured Prediction

want to model whole joint

- a GAN with sufficient capacity samples from full joint at equilibrium
- needs sufficient capacity and a lot of data

**conditional VAE**

- condition on observation  $x$
- $z$  learns to encode difference between  $x$  and  $y$

### 6.2 Domain Mapping

**domain mapping** given two un-paired datasets  $x, y$ , lets us translate an input  $x$  to  $y$

**cycleGAN** map from  $x \rightarrow \hat{y} \rightarrow \hat{x}$  and minimize reconstruction

- why do we get correct mapping? **simplicity hypothesis**
- minimizing cycle loss in turn minimizes condition entropy

**domain adaption** given classifier in one domain, map it to another domain

## 6.3 Representation Learning

Generative models learn good representations

- generative models must learn to model the data distribution
- good models should learn to model the semantics of the data
- learned semantics should correspond to the same stuff we care about

Representation Learning with Contrastive Predictive Coding (van der Oord et al 2018)

- encode sequence with RNN
- predict future latent states
- modelling new states is now easier since you have predictions about what they should be before you see them

## 6.4 Model-based Intelligence

Yann Lecun's cake

- cake: understanding and modelling the world around us well
- cherry on top: planning and reasoning using that representation

deep visual foresight (Finn and Levine 2017)

1. model to predict future frame given action
2. specify target future frame
3. select best action for that

world models (Ha and Schmidhuber 2018)

1. simulate video game with RNN
2. train a policy on the simulation (latent space)
3. policy works on the real game

incentivizing exploration in RL with deep predictive models (Stadie et al 2015)

1. model to predict next state given action and previous state
2. reward agent for visiting "surprising" states

## 7 Interpretability Been Kim

### 7.1 Why Interpretability

there is **no one-size-fits-all** method for interpretability

- decision trees can't explain the most important factor
- rule lists can be too long to be understandable

the goal is use machine learning more **responsibly**

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the issue is **underspecification** of what we truly want

- neither more data nor better algorithms can solve it

### 7.2 Interpretability Methods

before training: **exploratory data analysis**

- visualize data by features, splits
- find examples that are outliers in their class

during training: building a model

- rule-based methods as a model (e.g. rule lists)
- fit a simpler function for each feature
- choose representative examples to cluster
- train on sparse features
- learn a monotonic function (always increasing)
- distill your model

after training: investigate the model

- **ablation** train without certain features to see their effect
- test **input-feature importance** by sensitivity analysis (e.g. saliency maps)
- concept activation vector **CAV** separates activations of true class and rest

### 7.3 Evaluating Methods

- testing with humans
- ground truth experiments