Neural Networks

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Machine Learning

Need for Neural Networks

Perceptron

- Can only model *linear* functions

Kernel Machines

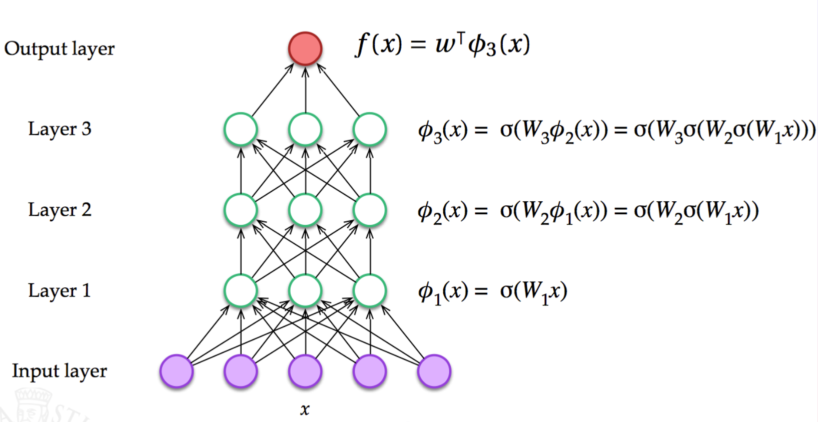
- Non-linearity provided by kernels
- Need to *design* appropriate kernels (possibly selecting from a set, i.e. kernel learning)
- Solution is *linear combination of kernels*

Need for Neural Networks

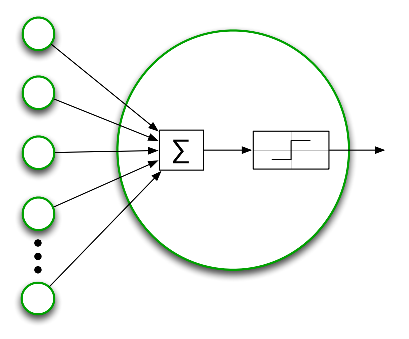
Multilayer Perceptron (MLP)

- Network of interconnected neurons
- *layered* architecture: neurons from one layer send outputs to the following layer
- Input layer at the bottom (input features)
- One or more hidden layers in the middle (learned features)
- Output layer on top (predictions)

Multilayer Perceptron (MLP)



Activation Function

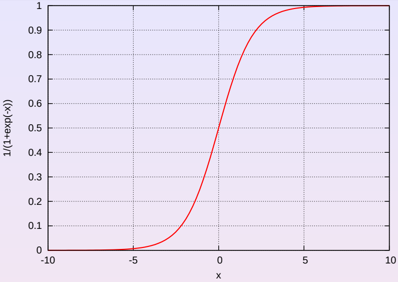


Perceptron: threshold activation

$$f(x) = sign(\boldsymbol{w}^T \boldsymbol{x})$$

- Derivative is zero everywhere apart from zero (where it's not differentiable)
- Impossible to run gradient-based optimization

Activation Function



Sigmoid

$$f(\boldsymbol{x}) = \sigma(\boldsymbol{w}^T \boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T \boldsymbol{x})}$$

- Smooth version of threshold
- approximately linear around zero
- saturates for large and small values

Output Layer

Binary classification

- One output neuron $o(\boldsymbol{x})$
- Sigmoid activation function:

$$f(\boldsymbol{x}) = \sigma(o(\boldsymbol{x})) = \frac{1}{1 + \exp\left(-o(\boldsymbol{x})\right)}$$

- Decision threshold at 0.5

$$y^* = \mathrm{sign}(f(\boldsymbol{x}) - 0.5)$$

Output Layer

Multiclass classification

- One output neuron per class (called *logits* layer):

$$[o_1(\boldsymbol{x}), \ldots, o_c(\boldsymbol{x})]$$

- Softmax activation function:

$$f_i(x) = \frac{\exp o_i(\boldsymbol{x})}{\sum_{j=1}^{c} \exp o_j(\boldsymbol{x})}$$

- Decision is highest scoring class:

$$y^* = \arg\max_{i \in [1,c]} f_i(\boldsymbol{x})$$

Output layer

Regression

- One output neuron $o(\boldsymbol{x})$
- Linear activation function
- Decision is value of output neuron:

$$f(\boldsymbol{x}) = o(\boldsymbol{x})$$

Representational power of MLP

Representable functions

boolean functions any boolean function can be represented by some network with two layers of units

continuous functions every bounded continuous function can be approximated with arbitrary small error by a network with two layers of units (sigmoid hidden activation, linear output activation)

arbitrary functions any function can be approximated to arbitrary accuracy by a network with three layers of units (sigmoid hidden activation, linear output activation)

Shallow vs deep architectures: Boolean functions

Conjunctive normal form (CNF)

- One neuron for each clause (OR gate), with negative weights for negated literals
- One neuron at the top (AND gate)

PB: number of gates

- Some functions require an exponential number of gates!! (e.g. parity function)
- Can be expressed with linear number of gates with a *deep network* (e.g. combination of XOR gates)

Training MLP

Loss functions (common choices)

Cross entropy for binary classification ($y \in \{0, 1\}$)

$$\ell(y, f(\boldsymbol{x})) = -\left(y \log f(\boldsymbol{x}) + (1 - y) \log (1 - f(\boldsymbol{x}))\right)$$

Cross entropy for multiclass classification ($y \in [1, c]$)

$$\ell(y, f(\boldsymbol{x})) = -\log f_y(\boldsymbol{x})$$

Mean squared error for regression

$$\ell(y, f(\boldsymbol{x})) = (y - f(\boldsymbol{x}))^2$$

Note

Minimizing cross entropy corresponds to maximizing likelihood

Training MLP

Stochastic gradient descent

- Training error for example (x, y) (e.g. regression):

$$E(W) = \frac{1}{2}(y - f(x))^2$$

- Gradient update (η learning rate)

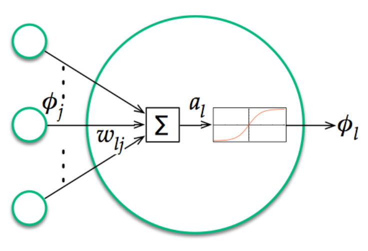
$$w_{lj} = w_{lj} - \eta \frac{\partial E(W)}{\partial w_{lj}}$$

Training MLP

Backpropagation

Use chain rule for derivation:

$$\frac{\partial E(W)}{\partial w_{lj}} = \underbrace{\frac{\partial E(W)}{\partial a_l}}_{\delta_l} \frac{\partial a_l}{\partial w_{lj}} = \delta_l \phi_j$$



Training MLP

Output units

- Delta is easy to compute on output units.
- E.g. for regression with linear outputs:

$$\delta_o = \frac{\partial E(W)}{\partial a_o} = \frac{\partial \frac{1}{2}(y - f(x))^2}{\partial a_o}$$
$$= \frac{\partial \frac{1}{2}(y - a_o)^2}{\partial a_o} = -(y - a_o)$$

Hidden units

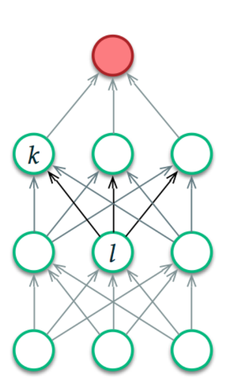
Consider contribution to error through all outer connections (sigmoid activation):

$$\delta_l = \frac{\partial E(W)}{\partial a_l} = \sum_{k \in \mathrm{ch}[l]} \frac{\partial E(W)}{\partial a_k} \frac{\partial a_k}{\partial a_l}$$

$$= \sum_{k \in \mathrm{ch}[l]} \delta_k \frac{\partial a_k}{\partial \phi_l} \frac{\partial \phi_l}{\partial a_l}$$

$$= \sum_{k \in \mathrm{ch}[l]} \delta_k w_{kl} \frac{\partial \sigma(a_l)}{\partial a_l}$$

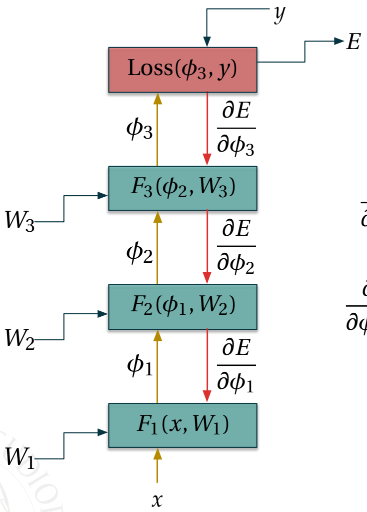
$$= \sum_{k \in \mathrm{ch}[l]} \delta_k w_{kl} \sigma(a_l)(1 - \sigma(a_l))$$



Derivative of sigmoid

$$
\begin{aligned}
\frac{\partial \sigma(x)}{\partial x} &= \frac{\partial}{\partial x}\frac{1}{1+\exp(-x)} \\
&= -(1+\exp(-x))^{-2}\frac{\partial}{\partial x}(1+\exp(-x)) \\
&= -(1+\exp(-x))^{-2} - \exp(-2x)\frac{\partial \exp(x)}{\partial x} \\
&= (1+\exp(-x))^{-2}\exp(-2x)\exp(x) \\
&= \frac{1}{1+\exp(-x)}\frac{\exp(-x)}{1+\exp(-x)} \\
&= \frac{1}{1+\exp(-x)}(1-\frac{1}{1+\exp(-x)}) \\
&= \sigma(x)(1-\sigma(x))
\end{aligned}
$$

Deep architectures: modular structure



$$\phi_j = F_j(\phi_{j-1}, W_j)$$

$$\frac{\partial E}{\partial W_j} = \frac{\partial E}{\partial \phi_j}\frac{\partial \phi_j}{\partial W_j} = \frac{\partial E}{\partial \phi_j}\frac{\partial F_j(\phi_{j-1}, W_j)}{\partial W_j}$$

$$\frac{\partial E}{\partial \phi_{j-1}} = \frac{\partial E}{\partial \phi_j}\frac{\partial \phi_j}{\partial \phi_{j-1}} = \frac{\partial E}{\partial \phi_j}\frac{\partial F_j(\phi_{j-1}, W_j)}{\partial \phi_{j-1}}$$

Remarks on backpropagation

Local minima

- The error surface of a multilayer neural network can contain several minima
- Backpropagation is only guaranteed to converge to a *local* minimum
- Heuristic attempts to address the problem:
  - use stochastic instead of true gradient descent
  - train multiple networks with different random weights and average or choose best
  - many more..

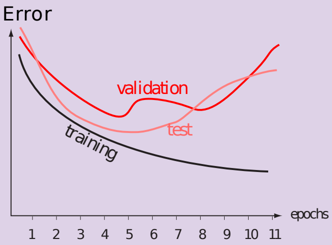
Note

- Training kernel machines requires solving *quadratic* optimization problems $\rightarrow$ global optimum guaranteed
- Deep networks are more expressive in principle, but harder to train

Stopping criterion and generalization

Stopping criterion

- How can we choose the training termination condition?
- Overtraining the network increases possibility of *overfitting* training data
- Network is initialized with small random weights ⇒ very simple decision surface
- Overfitting occurs at later iterations, when increasingly complex surfaces are being generated
- Use a separate *validation* set to estimate performance of the network and choose when to stop training



Training deep architectures

PB: Vanishing gradient

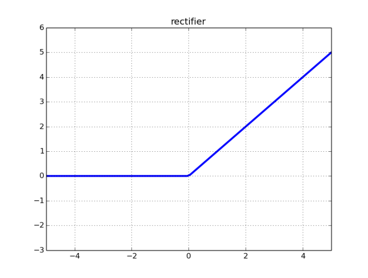
- Error gradient is backpropagated through layers
- At each step gradient is multiplied by derivative of sigmoid: very small for saturated units
- Gradient vanishes in lower layers
- Difficulty of training deep networks!!

Tricks of the trade

Few simple suggestions

- Do not initialize weights to zero, but to small random values around zero
- Standardize inputs ($x' = (x - \mu_x)/\sigma_x$) to avoid saturating hidden units
- Randomly shuffle training examples before each training epoch

Tricks of the trade: activation functions

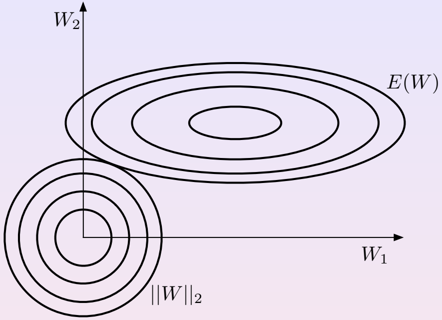


Rectifier

$$f(x) = max(0, \mathbf{w}^T \mathbf{x})$$

- Linearity is nice for learning
- Saturation (as in sigmoid) is bad for learning (gradient vanishes $\rightarrow$ no weight update)
- Neuron employing rectifier activation called rectified linear unit (ReLU)

Tricks of the trade: regularization

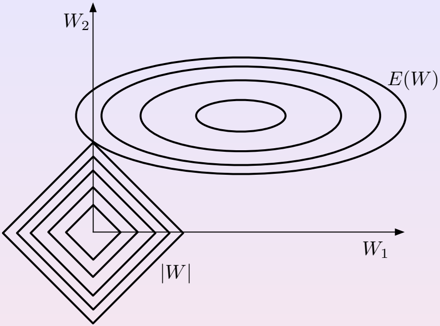


2-norm regularization

$$J(W) = E(W) + \lambda ||W||_2$$

- Penalizes weights by Euclidean norm
- Weights with less influence on error get smaller values

Tricks of the trade: regularization



1-norm regularization

$$J(W) = E(W) + \lambda|W|$$

- Penalizes weights by sum of absolute values
- Encourages less relevant weights to be exactly zero (sparsity inducing norm)

Tricks of the trade: initialization

Suggestions

- Randomly initialize weights (for breaking *symmetries* between neurons)
- Carefully set initialization range (to preserve forward and backward variance)

$$W_{ij} \sim U\left(-\frac{\sqrt{6}}{\sqrt{n+m}}, \frac{\sqrt{6}}{\sqrt{n+m}}\right)$$

  n and m number of inputs and outputs
- *Sparse* initialization: enforce a fraction of weights to be non-zero (encourages *diversity* between neurons)

Tricks of the trade: gradient descent

Batch vs Stochastic

- Batch gradient descent updates parameters after seeing all examples $\rightarrow$ too slow for large datasets
- Fully stochastic gradient descent updates parameters after seeing each example $\rightarrow$ objective too different from true one
- *Minibatch* gradient descent: update parameters after seeing a minibach of m examples (m depends on many factors, e.g. size of GPU memory)

Tricks of the trade: gradient descent

Momentum

$$
\begin{aligned}
v_{ji} &= \alpha v_{ji} - \eta \frac{\partial E(W)}{\partial w_{lj}} \\
\mathbf{w}_{ji} &= w_{ji} + v_{ji}
\end{aligned}
$$

- $0 \leq \alpha < 1$ is called **momentum**
- Tends to keep updating weights in the same direction
- Think of a ball rolling on an error surface
- Possible effects:
  - roll through small local minima without stopping
  - traverse flat surfaces instead of stopping there
  - increase step size of search in regions of constant gradient

Tricks of the trade: adaptive gradient

Decreasing learning rate

$$\eta_t = \begin{cases} (1 - \frac{t}{\tau})\eta_0 + \frac{t}{\tau}\eta_\tau & \text{if } t < \tau \\ \eta_\tau & \text{otherwise} \end{cases}$$

- Larger learning rate at the beginning for faster convergence towards attraction basin
- Smaller learning rate at the end to avoid oscillation close to the minimum

Tricks of the trade: adaptive gradient

Adagrad

$$
\begin{aligned}
r_{ji} &= r_{ji} + \left(\frac{\partial E(W)}{\partial w_{lj}}\right)^2 \\
\mathbf{w}_{ji} &= w_{ji} - \frac{\eta}{\sqrt{r_{ji}}}\frac{\partial E(W)}{\partial w_{lj}}
\end{aligned}
$$

- Reduce learning rate in steep directions
- Increase learning rate in gentler directions

Problem

- Square gradient accumulated over all iterations
- For non-convex problems, learning rate reduction can be excessive/premature

Tricks of the trade: adaptive gradient

RMSProp

$$
\begin{aligned}
r_{ji} &= \rho r_{ji} + (1-\rho)\left(\frac{\partial E(W)}{\partial w_{lj}}\right)^2 \\
\mathbf{w}_{ji} &= w_{ji} - \frac{\eta}{\sqrt{r_{ji}}}\frac{\partial E(W)}{\partial w_{lj}}
\end{aligned}
$$

- Exponentially decaying accumulation of squared gradient ($0 < \rho < 1$)
- Avoids premature reduction of Adagrad
- Adagrad-like behaviour when reaching convex bowl

Tricks of the trade: batch normalization

Covariate shift problem

- Covariate shift problem is when the input distribution to your model changes over time (and the model does not adapt to the change)
- In (very) deep networks, *internal* covariate shift takes place among layers when they get updated by backpropagation

Tricks of the trade: batch normalization

Solution (sketch)

- Normalize each node activation (input to activation function) by its batch statistics

$$\hat{x}_i = \frac{x_i - \mu_B}{\sigma_B}$$

  where:
  - x is the activation of an arbitrary node in an arbitrary layer
  - $\mathcal{B} = \{x_1, \ldots, x_m\}$, is a batch of values for that activation
  - μ_B, σ_B^2 are batch mean and variance

- Scale and shift each activation with adjustable parameters (γ and β become part of the network parameters)

$$y_i = \gamma \hat{x}_i + \beta$$

Tricks of the trade: batch normalization

Advantages

- More robustness to parameter initialization
- Allows for faster learning rates without divergence
- Keeps activations in non-saturated region even for saturating activation functions
- Regularizes the model

Tricks of the trade: pre-training

Approaches

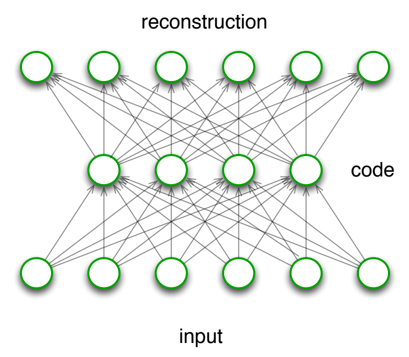
- Layerwise pre-training: layerwise training with actual labels
- Transfer learning: train network on similar task, discard last layers and retrain on target task
- Multi-level supervision: auxhiliary output nodes at intermediate layers to speed up learning

Popular deep architectures

Many different architectures

- *autoenconders* for unsupervised representation learning
- *convolutional networks* for exploiting local correlations (e.g. for images)
- *recurrent networks* for sequential predictions (e.g. sequence labelling)
- *generative adversarial networks* to generate new instances as a *game between discriminator and generator*
- *transformer* models exploiting attention to perform sequence prediction
- *graph neural networks* to process networked data

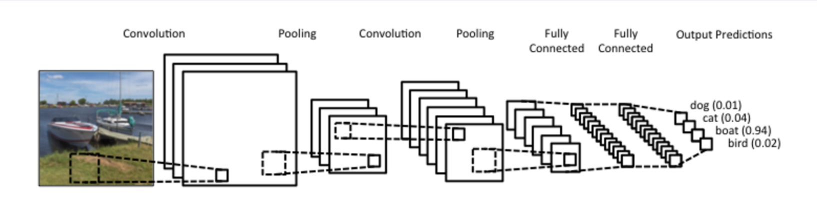
Autoencoders



Unsupervised representation learning

- train network to *reproduce* input in the output
- learns to map inputs into a sensible hidden representation (*representation learning*)
- can be done with unlabelled examples (*unsupervised learning*)

Convolutional networks (CNN)



Location invariance + compositionality

- *convolution filters* extracting local features
- *pooling* to provide invariance to local variations
- *hierarchy of filters* to compose complex features from simpler ones (e.g. pixels to edges to shapes)
- *fully connected layers* for final classification

Long Short-Term Memory Networks (LSMT)

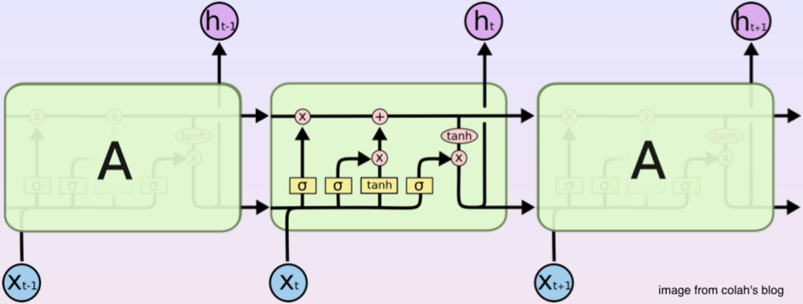
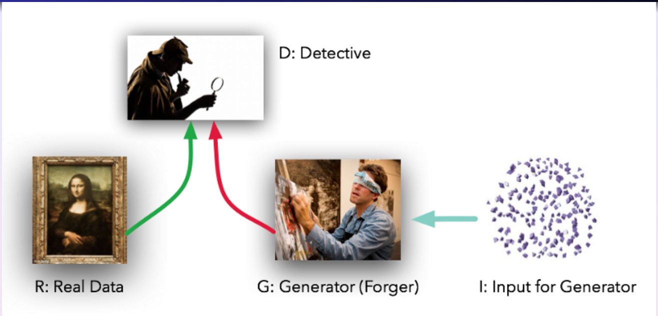


image from colah's blog

Recurrent computation with selective memory

- *Cell state* propagated along chain
- *Forget gate* selectively forgets parts of the cell state
- *Input gate* selectively chooses parts of the candidate for cell update
- *Output gate* selectively chooses parts of the cell state for output

Generative Adversarial Networks (GAN)



Generative learning as an adversarial game

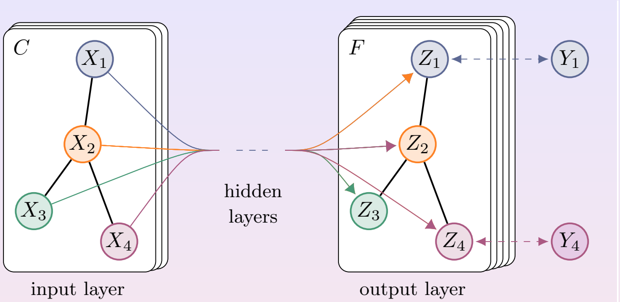
- A *generator* network learns to generate items (e.g. images) from random noise
- A *discriminator* network learns to distinguish between real items and generated ones
- The two networks are jointly learned (adversarial game)
- No human supervision needed!!

Transformers

Attention is all you need

- Use attention mechanism to learn input word encodings that depend on other words in the sentence
- Use attention mechanism to learn output word encodings that depend on input word encodings and previously generated output words
- Predict output words sequentially stopping when the "word" end-of-sentence is predicted

Graph Neural Networks



Learning with graph "convolution"

- Allow to *learn* feature representations for nodes
- Allow to propagate information between neighbouring nodes
- Allow for efficient training (wrt to e.g. graph kernels)

References

Libraries

- TensorFlow (https://www.tensorflow.org/)
- PyTorch (http://pytorch.org/)
- Microsoft Cognitive Toolkit (https://cntk.ai/)
- Deep Learning for Java (https://deeplearning4j.org/)
- MXNet (https://mxnet.apache.org/)

Literature

- Ian Goodfellow, Yoshua Bengio and Aaron Courville, *Deep Learning*, MIT Press, 2016 [https://www.deeplearningbook.org/]
- Eli Stevens, Luca Antiga, Thomas Viehmann, *Deep Learning with PyTorch*, Manning, 2020 [https://pytorch.org/assets/deep-learning/Deep-Learning-with-PyTorch.pdf]
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