CS-667 Advanced Machine Learning

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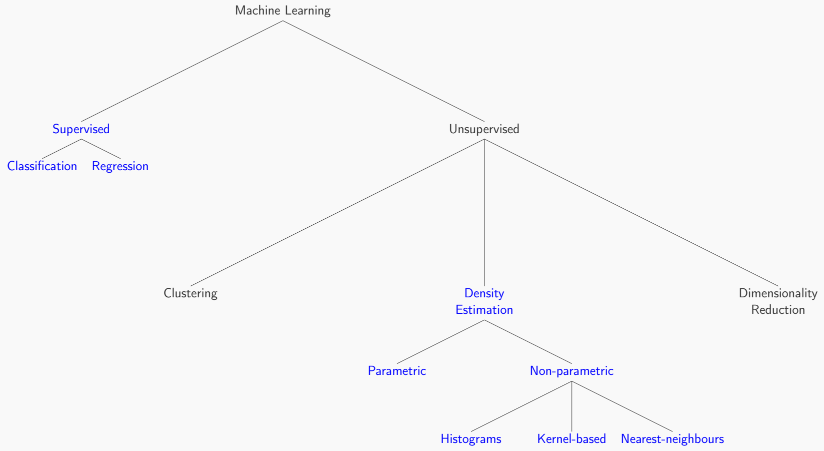
PUCIT

Neural Networks

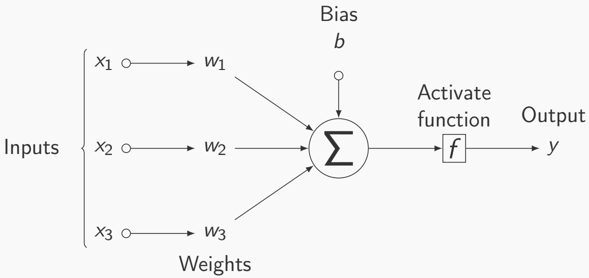
Machine Learning So Far ...



Neural Networks

- So far, we have learned $\mathbf{w}^*$ for mapping inputs $\mathbf{x} \in \mathbb{R}^D$ to targets $\mathbf{t}$.
- Often, working in a transformed space $\phi \in \mathbb{R}^M$ makes it easier to learn the mapping.
- However, not all mappings are useful for the problem at hand. Is there an optimal mapping ϕ^*?
- Neural networks learn the optimal mapping ϕ^* and also the optimal parameters $\mathbf{w}^*$.

Neural Networks
The Neuron



- The function of a biological neuron can be modelled as $y = f\left(\sum_j w_j x_j + b\right)$.

Neural Networks
The Neuron

- Model the output of the k-th neuron as
  $y_k = f(a_k) = f(\mathbf{w}_k^T\mathbf{x}) = f\left(\sum_j w_{kj}x_j\right)$ where
  - The x_j constitute values of input signals feeding into the neuron.
  - The w_{kj} are weights determining the importance given to input x_j by this neuron.
  - Dot-product $a_k = \sum_j w_{kj}x_j$ is called the *activation*.
  - $f(\cdot)$ is called the *activation function*. Determines behaviour of the neuron in response to its activation.
- The perceptron that we studied earlier is a very simple neuron model with f being the step function.

$$f(a) = \begin{cases} 1 & \text{if } a \geq 0 \\ 0 & \text{if } a < 0 \end{cases} \tag{1}$$

Neural Networks

- The linear models that we covered can be represented as

$$y_k(\mathbf{x}, \mathbf{W}) = f(\mathbf{w}_k^T \phi(\mathbf{x})) = f\left(\sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})\right)$$

  where y_k is the k-th output and index j starts from 0 to reflect bias inclusion.

$$f = \begin{cases} \text{identity} & \text{for regression} \\ \text{logistic sigmoid} & \text{for binary classification} \\ \text{softmax} & \text{for multiclass classification} \end{cases}$$

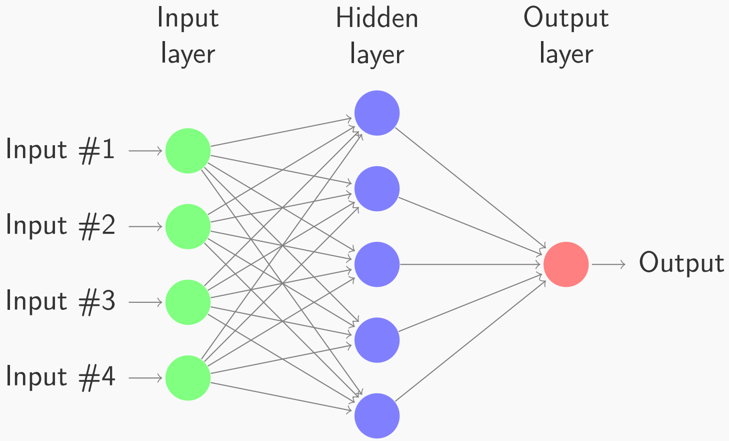
- Each $\phi_j(\mathbf{x})$ can be seen as a *basis function*.
- So far, the basis functions were fixed. Now we *adapt* them to the problem.

Neural Networks

- Model $\phi_j(\mathbf{x})$ as a non-linear function $h(a_j)$ where *activation* $a_j = \mathbf{w}_j^T\mathbf{x}$ with adjustable parameters $\mathbf{w}_j$.
- So the k-th output can be written as

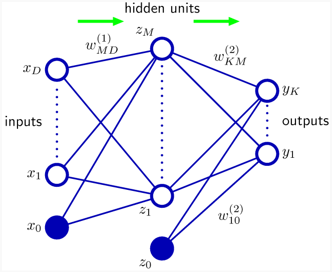
$$\begin{aligned} y_k(\mathbf{x}, \mathbf{W}) = f(a_k) = f(\mathbf{w}_k^T\phi(\mathbf{x})) &= f\left(\sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})\right) \\ &= f\left(\sum_{j=0}^{M} w_{kj} h(a_j)\right) \\ &= f\left(\sum_{j=1}^{M} w_{kj} h\left(\sum_{i=0}^{D} w_{ji}x_i\right)\right) \end{aligned}$$

Neural Networks



These computations can be visualised graphically as *forward propagation of information* through the so-called *neural network*.

Neural Networks



A two-layer neural network.

- 3 neuron types:
  - input x_i
  - hidden z_j
  - output y_k
- 2 weight layers:
  - hidden-input $w^{(1)}_{ji}$
  - output-hidden $w^{(2)}_{kj}$
- To differentiate between different layer parameters, we can write

$$y_k(\mathbf{x}, \mathbf{W}) = f\left(\sum_{j=1}^{M} w^{(2)}_{kj} h\left(\sum_{i=0}^{D} w^{(1)}_{ji} x_i\right)\right)$$

Neural Networks
As Multilayer Perceptrons

- The computation $y_k(\mathbf{x}, \mathbf{W}) = f\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right)$ can be viewed in two stages:
  1. Compute $z_j = h(\mathbf{w}_j^T \mathbf{x})$, followed by
  2. $y_k = f(\mathbf{w}_k^T \mathbf{z})$.
- Both stages resemble the perceptron model.
- Therefore, another name for such neural networks is *multilayer perceptrons* or simply *MLP*.
- However, there is a key difference:
  - Perceptron uses a non-differentiable step-function non-linearity.
  - MLP uses a differentiable sigmoidal non-linearity. So we can train via gradient based approaches.
- Therefore, despite the name, MLPs never use perceptrons!

Neural Networks
As Universal Approximators

- Neural networks are considered to be *universal approximators*.
- A two-layer network with linear outputs can uniformly approximate any continuous function on a compact input domain to arbitrary accuracy.
  - Provided that the network has a sufficiently large number of hidden units.

Neural Networks for Regression
Univariate

- In the polynomial fitting example from Chapter 1, given inputs and targets $\{\mathbf{x}_n, t_n\}$, we wanted to find the *optimal parameters* $\mathbf{w}^*$ *of the polynomial* that best fits the data.
- Assuming i.i.d data and $t_n \sim \mathcal{N}(y(\mathbf{x}_n, \mathbf{w}), \beta^{-1})$, we wrote the likelihood function whose maximisation corresponded to minimisation of the SSE function

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(y(\mathbf{x}_n, \mathbf{w}) - t_n)^2$$

- By replacing the polynomial in function $y(\mathbf{x}_n, \mathbf{w})$ by the neural network function, we can minimise $E(\mathbf{w})$ to find *optimal parameters* $\mathbf{w}^*$ *of the neural network*.

Neural Networks for Regression
Multivariate

- Similarly, for multivariate targets, assuming multivariate Gaussian density leads to the SSE function

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} ||\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n||^2$$

  where $y_k = a_k = \mathbf{w}_k^T \mathbf{x}$.

- Notice and prove that

$$\frac{\partial E_n}{\partial a_k} = \underbrace{(y_{kn} - t_{kn})}_{\text{error}_n}$$

Neural Networks for Classification
Binary

- Similarly, for binary classification, we can assume a Bernoulli distribution on targets which leads to minimisation of the *cross-entropy* function

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \left(t_n \ln y(\mathbf{x}_n, \mathbf{w}) + (1 - t_n) \ln(1 - y(\mathbf{x}_n, \mathbf{w}))\right)$$

  where $y(\mathbf{x}_n, \mathbf{w}) = P(\mathcal{C}_1|\mathbf{x}_n) = \sigma(a) = \sigma(\mathbf{w}^T\mathbf{x}_n)$.

- Notice (and prove) that

$$\frac{\partial E_n}{\partial a} = \underbrace{(y_n - t_n)}_{\text{error}_n}$$

Neural Networks for Classification
Multiclass

- For multiclass classification, we can minimise the *multiclass cross-entropy* function

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K}\left(t_{kn}\ln y_k(\mathbf{x}_n, \mathbf{w})\right)$$

where $y_k(\mathbf{x}_n, \mathbf{w}) = P(\mathcal{C}_k|\mathbf{x}_n) = \frac{e^{a_k}}{\sum_{j=1}^{K} e^{a_j}}$ and $a_k = \mathbf{w}_k^T\mathbf{x}$.

- Notice (and prove) that

$$\frac{\partial E_n}{\partial a_k} = \underbrace{(y_{kn} - t_{kn})}_{\text{error}_n}$$

- In the following we will denote the error $\frac{\partial E}{\partial a_k}$ as δ_k.

Neural Networks for Classification

- Note that we can learn classifiers via SSE minimisation also, but the cross-entropy formulations
  1. can be derived probabilistically,
  2. train faster, and
  3. generalise better.

Optimisation

- For optimisation, we notice that $\mathbf{w}^*$ must be a *stationary point* of $E(\mathbf{w})$.
  - Minimum, maximum, or saddle point.
  - A saddle point is where gradient vanishes but point is not an extremum (Example).
- The goal in neural network minimisation is to find a local minimum.
- A global minimum, even if found, cannot be verified as globally minimum.
- Due to symmetry, there are multiple equivalent local minima. Reaching any suitable local minimum is the goal of neural network optimisation.
- Since there are no analytical solutions for $\mathbf{w}^*$, we use iterative, numerical procedures.

Optimisation

- Options for iterative optimisation
  - Online methods
    - Stochastic gradient descent
    - Stochastic gradient descent using mini-batches
  - Batch methods
    - Batch gradient descent
    - Conjugate gradient descent
    - Quasi-Newton methods
- Online methods
  - converge faster since parameter updates are more frequent, and
  - have greater chance of escaping local minima because stationary point w.r.t to whole data set will generally not be a stationary point w.r.t an individual data point.
- Batch methods: Conjugate gradient descent and quasi-Newton methods
  - are more robust and faster than batch gradient descent, and
  - decrease the error function at each iteration until arriving at a minimum.

Backpropagation

- For all gradient based methods, however, we must first compute the gradient $\nabla_{\mathbf{w}} E(\mathbf{w})$.
- We have seen that many error functions of practical interest can be written as a sum of terms

$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

- So the essential gradient is $\nabla_{\mathbf{w}} E_n(\mathbf{w})$ which we write in its complete form $\nabla_{\mathbf{w}} E(\mathbf{y}(\mathbf{x}_n, \mathbf{w}))$.

Multivariate Chain Rule

- The chain rule of differentiation states

$$\frac{df(u(x))}{dx} = \frac{df}{du}\frac{du}{dx}$$

- The *multivariate* chain rule of differentiation states

$$\frac{df(u(x), v(x))}{dx} = \frac{\partial f}{\partial u}\frac{du}{dx} + \frac{\partial f}{\partial v}\frac{dv}{dx}$$

- Backpropagation is just an application of the multivariate chain rule.

Backpropagation

- For the output layer weights

$$\frac{\partial E(y_k(a_k(w_{kj})))}{\partial w_{kj}} = \frac{\partial E}{\partial a_k}\frac{\partial a_k}{\partial w_{kj}} = \delta_k z_j$$

- For the hidden layer weights, using the multivariate chain rule

$$\frac{\partial}{\partial w_{ji}} E(y_1(a_1(z_j(a_j(w_{ji})))), y_2(a_2(z_j(a_j(w_{ji})))), \dots, y_k(a_k(z_j(a_j(w_{ji}))))$$

$$= \frac{\partial E}{\partial a_j}\frac{\partial a_j}{\partial w_{ji}} = \underbrace{\sum_{k=1}^{K} \underbrace{\frac{\partial E}{\partial a_k}}_{\delta_k} \underbrace{\frac{\partial a_k}{\partial z_j}}_{w_{kj}} \underbrace{\frac{\partial z_j}{\partial a_j}}_{h'(a_j)}}_{\delta_j} \underbrace{\frac{\partial a_j}{\partial w_{ji}}}_{x_i} = \delta_j x_i$$

- For each layer, notice the familiar form

$$\text{gradient} = \text{error} \times \text{input}$$

Backpropagation

- It is important to note that

$$\delta_j = h'(a_j) \sum_{k=1}^{K} \delta_k w_{kj}$$

  yields the error δ_j at hidden neuron j by *backpropagating* the errors δ_k from all output neurons that use the output of neuron j.
- More generally, compute error δ_j at a layer by *backpropagating* the errors δ_k from next layer.
- Hence the names *error backpropagation*, *backpropagation*, or simply *backprop*.
- Very useful machine learning technique that is not limited to neural networks.

Backpropagation

$$\delta_j^{(1)} = h'(a_j) \sum_{k=1}^{K} \delta_k^{(2)} w_{kj}$$

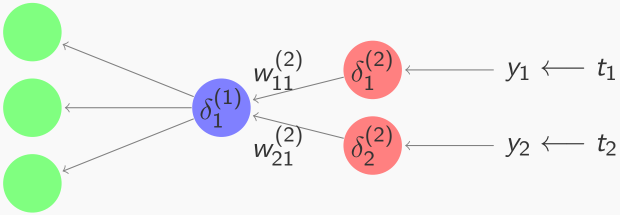


Figure: Visual representation of backpropagation of delta values of layer $l+1$ to compute delta values of layer l.

Backpropagation
Learning Algorithm

1. Forward propagate the input vector $\mathbf{x}_n$ to compute activations and outputs of every neuron in every layer.
2. Evaluate δ_k for every neuron in output layer.
3. Evaluate δ_j for every neuron in <u>every</u> hidden layer via backpropagation.
4. Compute derivative of each weight $\frac{\partial E}{\partial w}$ via $\delta \times$input.
5. Update each weight via gradient descent $w^{\tau+1} = w^{\tau} - \eta \frac{\partial E}{\partial w}$.

Background Math

A $(-1, 1)$ sigmoidal function

- Since range of logistic sigmoid $\sigma(a)$ is $(0, 1)$, we can obtain a function with $(-1, 1)$ range as $2\sigma(a) - 1$.
- Another related function with $(-1, 1)$ range is the tanh function.

$$\tanh(a) = 2\sigma(2a) - 1 = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$

  where σ is applied on $2a$.
- Preferred over logistic sigmoid as activation function $h(a)$ of hidden neurons. (Read Yann LeCun's "Efficient Backprop" paper to understand why.)
- Just like the logistic sigmoid, derivative of $\tanh(a)$ is simple: $1 - \tanh^2(a)$. (Prove it.)

Backpropagation
A Simple Example

- Two-layer MLP for multivariate regression from $\mathbb{R}^D \longrightarrow \mathbb{R}^K$.
- Linear outputs $y_k = a_k$ with SSE $E_n = \frac{1}{2}\sum_{k=1}^{K}(y_k - t_k)^2$.
- M hidden neurons with $\tanh(\cdot)$ activation functions.

Forward propagation

$$a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i$$

$$z_j = \tanh(a_j)$$

$$y_k = \sum_{j=0}^{M} w_{kj}^{(2)} z_j$$

$$\delta_k = y_k - t_k$$

Backpropagate

$$\delta_j = (1 - z_j^2) \sum_{k=1}^{K} w_{kj}^{(2)} \delta_k$$

- Compute derivatives $\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \delta_j x_i$ and $\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \delta_k z_j$.

Backpropagation
Verifying Correctness

- *Numerical derivatives* can be computed via finite *central differences*

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{E_n(w_{ji}+\epsilon) - E_n(w_{ji}-\epsilon)}{2\epsilon} + O(\epsilon^2)$$

- *Analytical derivatives* computed via backpropagation **must be compared** with numerical derivatives for a few examples to verify correctness.
- Any implementation of analytical derivatives (not just backpropagation) must be compared with numerical derivatives.
- Notice that we could have avoided backpropagation and computed all required derivatives numerically.
  - But cost of numerical differentiation is $O(W^2)$ while that of backpropagation is $O(W)$ where W is the total number of weights (and biases) in the network. (Why?)

Regularization in Neural Networks

- Recall that over-fitting can be lessened via regularization.
  1. Decrease model complexity.
     1.1 Penalise magnitudes of weights: $\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$.
     1.2 Separately penalise magnitudes of weights of each layer: $\tilde{E}(\mathbf{w}) = E(\mathbf{w}) + \sum_{l=1}^{L} \frac{\lambda_l}{2}\mathbf{w}^{(l)^T}\mathbf{w}^{(l)}$.
     1.3 *Dropout*: *During training*, a randomly selected subset of activations are set to zero within each layer.
     1.4 *DropConnect*: *During training*, a randomly selected subset of weights within the network are set to zero.
  2. *Early stopping* by checking $E(\mathbf{w})$ on a validation set. Stop when error on validation set starts increasing.
  3. Training with *augmented*/transformed data.
  4. Batch Normalization (to be covered in the Deep Learning lecture).
  5. Building invariance into the network structure (to be covered in the Convolutional Neural Networks lecture).

Dropout vs. DropConnect

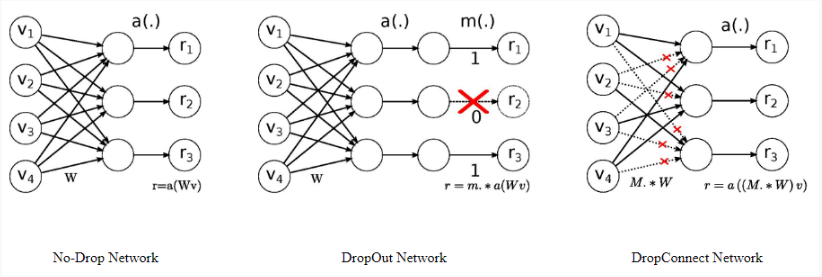


Figure: Dropout vs. DropConnect[2]. Image taken from `https://cs.nyu.edu/~wanli/dropc/`

[2] Wan et al., 'Regularization of Neural Network using DropConnect'.

Assignment 3
Backpropagation for MLPs

- Implement the backpropagation algorithm for training an MLP.
  - Code up a generic implementation.
  - Verify correctness of analytical derivatives.
  - **Part 1: Regression**
    - Understand the experiment and network used for Figure 5.3 in Bishop's book.
    - Regenerate Figure 5.3 using your implementation.
  - **Part 2: Classification**
    - Replace the Multiclass Logistic Regression module from Assignment 2 by a neural network with
      1. 1 hidden layer of 50 neurons
      2. 2 hidden layers of 50 neurons each
      3. 3 hidden layers of 50 neurons each

      and report results of each network on the same MNIST dataset.

Assignment 3

Backpropagation for MLPs

- Submit your_roll_number_MLP.zip containing
  - code,
  - generated image for Part 1,
  - accuracies and confusion matrices for Part 2,
  - report.txt/pdf explaining your results.
- Due Tuesday (March 21, 2018 before 5:30 pm) on \\printsrv.

Neural Network Tips

- Use a global structure
  - layers{l}.w, layers{l}.a, layers{l}.y
  - layers{l}.delta, layers{l}.dw
  - layers{l}.eta, layers{l}.afunc
  - ...
- Modularity
  - layers=fprop(layers,X,t)
  - layers=bprop(layers)
  - check_gradients(layers,X,t)
  - layers=update_weights(layers)
- Matrix-vector implementation will keep your code concise and readable ($\mathbf{a} = W^T \mathbf{x}$).