CS-568 Deep Learning

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Training Multilayer Perceptrons: Forward Propagation

Pre-requisites

- Before looking at how a multilayer perceptron can be trained, one must study
  1. Loss functions for machine learning
  2. Gradient computation
  3. Gradient descent
  4. Smooth activation functions

Loss Functions for Machine Learning

Notation:

- Let $x \in \mathbb{R}$ denote a *univariate* input.
- Let $\mathbf{x} \in \mathbb{R}^D$ denote a *multivariate* input.
- Same for targets $t \in \mathbb{R}$ and $\mathbf{t} \in \mathbb{R}^K$.
- Same for outputs $y \in \mathbb{R}$ and $\mathbf{y} \in \mathbb{R}^K$.
- Let θ denote the set of *all* learnable parameters of a machine learning model.

Loss Functions for Machine Learning

Regression

- Univariate

$$L(\theta) = \frac{1}{2}\sum_{n=1}^{N}(y_n - t_n)^2$$

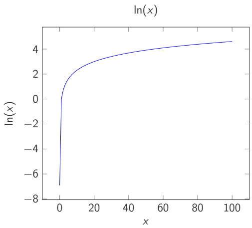
- Multivariate

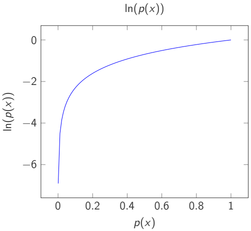
$$L(\theta) = \frac{1}{2}\sum_{n=1}^{N}\|\mathbf{y}_n - \mathbf{t}_n\|^2$$

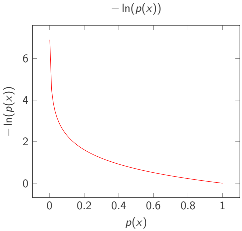
- Known as half-sum-squared-error (SSE) or ℓ_2-loss.
- *Verify that both losses are 0 when outputs match targets for all n. Otherwise, both losses are greater than 0.*

Background
Probability and Negative of Natural Logarithm

- Logarithm is a monotonically increasing function.
- Probability lies between 0 and 1.
- Between 0 and 1, logarithm is negative.
- So $-\ln(p(x))$ approaches ∞ for $p(x) = 0$ and 0 for $p(x) = 1$.
- Can be used as a loss function.







Loss Functions for Machine Learning
Binary Classification

- For *two-class classification*, targets can be binary.
  - $t_n = 0$ if $\mathbf{x}_n$ belongs to class $\mathcal{C}_0$.
  - $t_n = 1$ if $\mathbf{x}_n$ belongs to class $\mathcal{C}_1$.
- If output y_n can be restricted to lie between 0 and 1, we can *treat* it as probability of $\mathbf{x}_n$ belonging to class $\mathcal{C}_1$. That is, $y_n = P(\mathcal{C}_1|\mathbf{x}_n)$.
- Then $1 - y_n = P(\mathcal{C}_0|\mathbf{x}_n)$.
- Ideally,
  - y_n should be 1 if $\mathbf{x}_n \in \mathcal{C}_1$, and
  - $1 - y_n$ should be 1 if $\mathbf{x}_n \in \mathcal{C}_0$.
- Equivalently,
  - $-\ln y_n$ should be 0 if $x_n \in \mathcal{C}_1$, and
  - $-\ln(1 - y_n)$ should be 0 if $x_n \in \mathcal{C}_0$.
- So depending upon t_n, either $-\ln y_n$ or $-\ln(1 - y_n)$ should be considered as loss.

Loss Functions for Machine Learning
Binary Classification

- Using t_n to *pick* the relevant loss, we can write total loss as

$$L(\theta) = -\sum_{n=1}^{N} t_n \ln y_n + (1 - t_n) \ln(1 - y_n)$$

- Known as *binary cross-entropy (BCE) loss*.
- *Verify that BCE loss is 0 when outputs match targets for all n. Otherwise, loss is greater than 0.*

Loss Functions for Machine Learning
Multiclass Classification

- For *multiclass classification*, targets can be represented using *1-of-K coding*. Also known as *1-hot vectors*.
  - 1-hot vector: only one component is 1. All the rest are 0.
  - If $t_{n3} = 1$, then $\mathbf{x}_n$ belongs to class 3.
- If outputs of K output neurons can be restricted to
  1. $0 \leq y_{nk} \leq 1$, and
  2. $\sum_{k=1}^{K} y_{nk} = 1$,

  then we can *treat* outputs as probabilities.
- Later, we shall see activation functions that produce per-class probability values.

$$\mathbf{t}_n = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{y}_n = \begin{bmatrix} P(\mathcal{C}_1|\mathbf{x}_n) \\ P(\mathcal{C}_2|\mathbf{x}_n) \\ P(\mathcal{C}_3|\mathbf{x}_n) \\ P(\mathcal{C}_4|\mathbf{x}_n) \\ P(\mathcal{C}_5|\mathbf{x}_n) \end{bmatrix}$$

Loss Functions for Machine Learning

Multiclass Classification

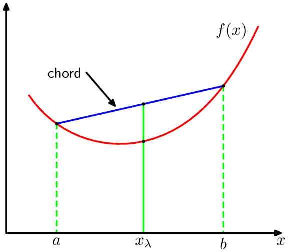
- Similary to BCE loss, we can use t_{nk} to *pick* the relevant negative log loss and write overall loss as

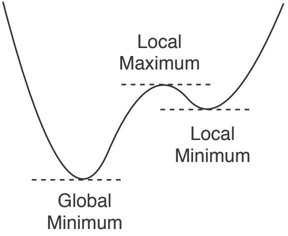
$$L(\theta) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk}$$

- Known as *multiclass cross-entropy (MCE) loss*.
- *Verify that MCE loss is 0 when outputs match targets for all n. Otherwise, loss is greater than 0.*

Convexity

- A function $f(x)$ is *convex* if *every* chord lies on or above the function.
- Can be minimized by finding stationary point. There will only be one.
- Loss functions for neural networks are *not* convex.
- They have multiple local minima and maxima.
- Can be minimized via gradient descent.





Second Derivative

- First derivative equal to zero determines stationary points.
- Second derivative distinguishes between maxima and minima.
  - At maximum, second derivative is negative.
  - At minimum, second derivative is positive.
- But all of the above applies to functions in 1-dimension.
- In higher dimensions, stationary point is still defined by $\nabla f = \mathbf{0}$.
- But there will be a second derivative in each dimension – some might be positive and some negative.
- So how can we distinguish between maxima and minima in higher dimensions?

Higher Dimensions

- In D-dimensions, maxima and minima are distinguished via a special $D \times D$ matrix of second derivatives known as the *Hessian matrix*.

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_D} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_D \partial x_1} & \frac{\partial^2 f}{\partial x_D \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_D \partial x_D} \end{bmatrix}$$

- If $\mathbf{x}^T \mathbf{H} \mathbf{x} \geq 0$ for *all* $\mathbf{x} \neq \mathbf{0}$, then $\mathbf{H}$ is *positive semi-definite*.
- This is equivalent to $\mathbf{H}$ having *non-negative eigenvalues*.

> If Hessian matrix at a stationary point $\mathbf{x}$ is positive semi-definite, then $\mathbf{x}$ is a (local) minimizer of f.

Matrix and Vector Derivatives

For scalar function $f \in \mathbb{R}$,

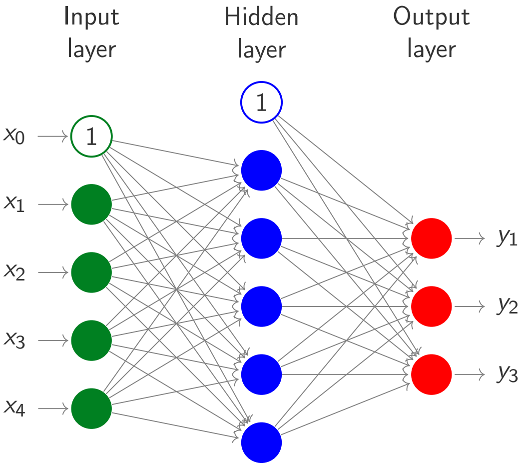
$$\nabla_{\mathbf{v}} f = \frac{\partial f}{\partial \mathbf{v}} = \begin{bmatrix} \frac{\partial f}{\partial v_1} & \frac{\partial f}{\partial v_2} & \cdots & \frac{\partial f}{\partial v_D} \end{bmatrix}$$

$$\nabla_{\mathbf{M}} f = \frac{\partial f}{\partial \mathbf{M}} = \begin{bmatrix} \frac{\partial f}{\partial M_{11}} & \frac{\partial f}{\partial M_{12}} & \cdots & \frac{\partial f}{\partial M_{1n}} \\ \frac{\partial f}{\partial M_{21}} & \frac{\partial f}{\partial M_{22}} & \cdots & \frac{\partial f}{\partial M_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial M_{m1}} & \frac{\partial f}{\partial M_{m2}} & \cdots & \frac{\partial f}{\partial M_{mn}} \end{bmatrix}$$

For vector function $\mathbf{f} \in \mathbb{R}^K$,

$$\nabla_{\mathbf{v}} \mathbf{f} = \begin{bmatrix} \nabla_{\mathbf{v}} f_1 \\ \nabla_{\mathbf{v}} f_2 \\ \vdots \\ \nabla_{\mathbf{v}} f_K \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial v_1} & \frac{\partial f_1}{\partial v_2} & \cdots & \frac{\partial f_1}{\partial v_D} \\ \frac{\partial f_2}{\partial v_1} & \frac{\partial f_2}{\partial v_2} & \cdots & \frac{\partial f_2}{\partial v_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_K}{\partial v_1} & \frac{\partial f_K}{\partial v_2} & \cdots & \frac{\partial f_K}{\partial v_D} \end{bmatrix}$$

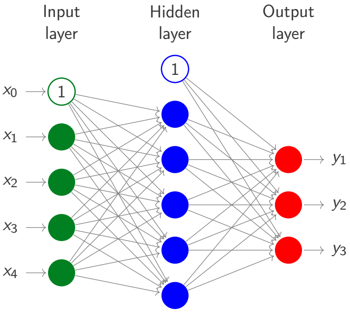
Neural Networks



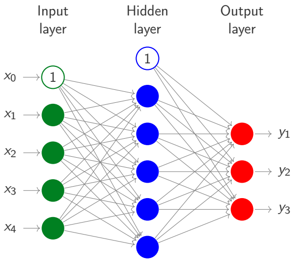
Output of a neural network can be visualised graphically as *forward propagation of information*.

Neural Networks
Notation

- Input layer neurons will be indexed by i.
- Hidden layer neurons will be indexed by j.
- Next hidden layer or output layer neurons will be indexed by k.
- Weights of j-th hidden neuron will be denoted by the vector $\mathbf{w}_j^{(1)} \in \mathbb{R}^D$.
- Weight between i-th input neuron and j-th hidden neuron is $w_{ji}^{(1)}$.
- Weights of k-th output neuron will be denoted by the vector $\mathbf{w}_k^{(2)} \in \mathbb{R}^M$.
- Weight between j-th hidden neuron and k-th output neuron is $w_{kj}^{(2)}$.



Neural Networks
Forward Propagation



- For input $\mathbf{x}$, denote output of hidden layer as the vector $\mathbf{z}(\mathbf{x}) \in \mathbb{R}^M$.
- Model $z_j(\mathbf{x})$ as a non-linear function $h(a_j)$ where *pre-activation* $a_j = \mathbf{w}_j^{(1)\,T}\mathbf{x}$ with adjustable parameters $\mathbf{w}_j^{(1)}$.
- So the k-th output can be written as

$$y_k(\mathbf{x}) = f(a_k) = f(\mathbf{w}_k^{(2)\,T}\mathbf{z}(\mathbf{x}))$$
$$= f\left(\sum_{j=1}^{M} w_{kj}^{(2)} z_j(\mathbf{x}) + w_{k0}^{(2)}\right) = f\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right) + w_{k0}^{(2)}\right)$$

where we have prepended $x_0 = 1$ to to absorb bias input and $w_{j0}^{(1)}$ and $w_{k0}^{(2)}$ represent biases.

Neural Networks
Forward Propagation

- The computation $y_k(\mathbf{x}, \mathbf{W}) = f\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right) + w_{k0}^{(2)}\right)$ can be viewed in two stages:
  1. $z_j = h(\mathbf{w}_j^{(1)T}\mathbf{x})$ for $j = 1, \ldots, M$.
  2. $y_k = f(\mathbf{w}_k^{(2)T}\mathbf{z})$.
- If we define the matrices

$$\mathbf{W}^{(1)} = \underbrace{\begin{bmatrix} \longleftarrow & \mathbf{w}_1^{(1)T} & \longrightarrow \\ \longleftarrow & \mathbf{w}_2^{(1)T} & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{w}_M^{(1)T} & \longrightarrow \end{bmatrix}}_{M\times(D+1)} \text{ and } \mathbf{W}^{(2)} = \underbrace{\begin{bmatrix} \longleftarrow & \mathbf{w}_1^{(2)T} & \longrightarrow \\ \longleftarrow & \mathbf{w}_2^{(2)T} & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{w}_K^{(2)T} & \longrightarrow \end{bmatrix}}_{K\times(M+1)}$$

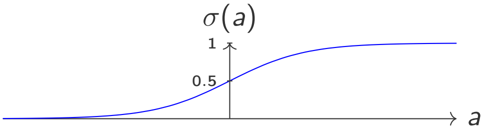
  then forward propagation constitutes
  1. $\mathbf{z} = h(\mathbf{W}^{(1)}\mathbf{x})$.
  2. Prepend 1 to $\mathbf{z}$.
  3. $\mathbf{y} = f(\mathbf{W}^{(2)}\mathbf{z})$.

Activation Functions

- Recall that a perceptron has a non-differentiable activation function, i.e., step function.
  - Zero-derivative everywhere except at 0 where it is non-differentiable.
- Prevents gradient descent.
- Can we use a smooth activation function that behaves similar to a step function?
- Perceptron with a smooth activation function is called a *neuron*.
- Neural networks are also called multilayer perceptrons (MLP) even though they do not contain any perceptron.

Logistic Sigmoid Function

- For $a \in \mathbb{R}$, the *logistic sigmoid* function is given by $\sigma(a) = \frac{1}{1+e^{-a}}$
- *Sigmoid* means S-shaped.
- Maps $-\infty \leq a \leq \infty$ to the range $0 \leq \sigma \leq 1$. Also called *squashing* function.
- **Can be treated as a probability value**.
- Symmetry $\sigma(-a) = 1 - \sigma(a)$. **Prove it.**
- Easy derivative $\sigma' = \sigma(1 - \sigma)$. **Prove it.**



Activation Functions

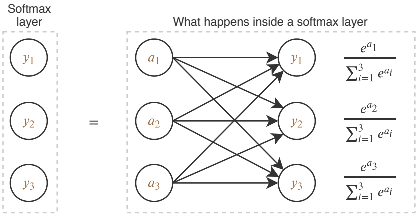
Regression

- Univariate: use 1 output neuron with identity activation function $y(a) = a$.
- Multivariate: use K output neurons with identity activation functions $y(a_k) = a_k$.

Classification

- Binary: use 1 output neuron with logistic sigmoid $y(a) = \sigma(a)$.
- Multiclass: use K output neurons with *softmax* activation function.

Softmax Activation Function



- For real numbers $a_1, \ldots, a_K$, the *softmax* function is given by

$$y(a_k; a_1, a_2, \ldots, a_K) = \frac{e^{a_k}}{\sum_{i=1}^{K} e^{a_i}}$$

- Output of k-th neuron depends on activations of *all neurons in the same layer*.
- Softmax is ≈ 1 when $a_k >> a_j \; \forall j \neq k$ and ≈ 0 otherwise.

Softmax Activation Function

- Provides a smooth (differentiable) approximation to finding the *index of the maximum element.*
  - Compute softmax for $1, 10, 100$.
  - Does not work everytime.
    - Compute softmax for $1, 2, 3$. Solution: multiply by 100.
    - Compute softmax for $1, 10, 1000$. Solution: subtract maximum before computing softmax.
- Also called the *normalized exponential* function.
- Since $0 \leq y_k \leq 1$ and $\sum_{k=1}^{K} y_k = 1$, *softmax outputs can be treated as probability values.*
- Take-home Quiz 2: Show that $\frac{\partial y_k}{\partial a_j} = y_k(\delta_{jk} - y_j)$ where $\delta_{jk} = 1$ if $j = k$ and 0 otherwise.