

CS-568 Deep Learning

Loss Functions and Activation Functions for Machine Learning

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Pre-requisites

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

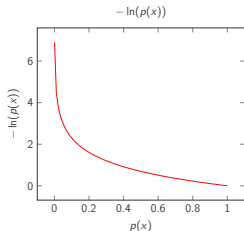
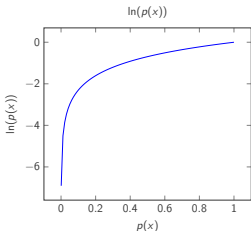
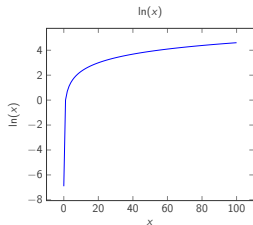
$$L(\theta) = \frac{1}{2} \sum_{n=1}^N \|\mathbf{y}_n - \mathbf{t}_n\|^2$$

- ▶ 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 $\mathbf{x}_n \in \mathcal{C}_1$, and
 - ▶ $-\ln(1 - y_n)$ should be 0 if $\mathbf{x}_n \in \mathcal{C}_0$.
- ▶ 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 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.

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

$$\mathbf{y}_n = \begin{bmatrix} P(C_1|\mathbf{x}_n) \\ P(C_2|\mathbf{x}_n) \\ P(C_3|\mathbf{x}_n) \\ P(C_4|\mathbf{x}_n) \\ P(C_5|\mathbf{x}_n) \end{bmatrix}$$

Loss Functions for Machine Learning

Multiclass Classification

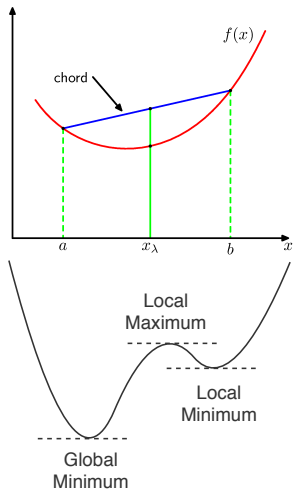
- ▶ Similar to BCE loss, we can use t_{nk} to *pick* the relevant negative log loss and write overall loss as

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

- ▶ 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 $f \in \mathbb{R}$,

$$\nabla_{\mathbf{v}} f = \frac{\partial f}{\partial \mathbf{v}} = \left[\frac{\partial f}{\partial v_1} \quad \frac{\partial f}{\partial v_2} \quad \cdots \quad \frac{\partial f}{\partial v_D} \right]$$

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

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

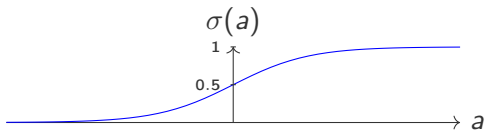
$$\nabla_{\mathbf{v}} \mathbf{f} = \begin{bmatrix} \nabla_{\mathbf{v}} f_1 \\ \nabla_{\mathbf{v}} f_2 \\ \vdots \\ \nabla_{\mathbf{v}} f_K \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial v_1} & \frac{\partial f_1}{\partial v_2} & \cdots & \frac{\partial f_1}{\partial v_D} \\ \frac{\partial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

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

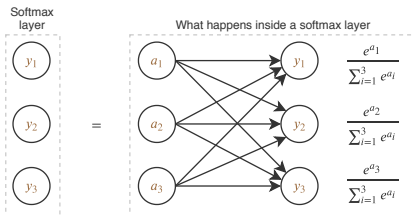
Regression

- ▶ 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, \dots, a_K , the *softmax* function is given by

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

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

Summary

- ▶ Inputs and outputs can be univariate as well multivariate.
- ▶ Regression requires SSE loss.
- ▶ Classification requires cross-entropy loss.
- ▶ Minimization corresponds to finding the point where derivate of loss is zero.
- ▶ Matrix and vector calculus makes calculations and computation cleaner and faster.
- ▶ Next lecture: Training MLPs.