CS-453 Machine Learning

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Loss Functions for Machine Learning

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

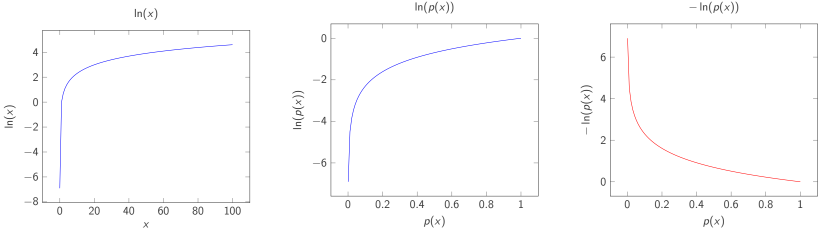
$$L(\theta) = \frac{1}{2}\sum_{n=1}^{N}\|\mathrm{y}_n - \mathrm{t}_n\|^2$$

- 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 x_n belongs to class $\mathcal{C}_0$.
  - $t_n = 1$ if 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 x_n belonging to class $\mathcal{C}_1$. That is, $y_n = P(\mathcal{C}_1|\mathrm{x}_n)$.
- Then $1 - y_n = P(\mathcal{C}_0|\mathrm{x}_n)$.
- Ideally,
  - y_n should be 1 if $\mathrm{x}_n \in \mathcal{C}_1$, and
  - $1 - y_n$ should be 1 if $\mathrm{x}_n \in \mathcal{C}_0$.
- Equivalently,
  - $-\ln y_n$ should be 0 if $\mathrm{x}_n \in \mathcal{C}_1$, and
  - $-\ln(1 - y_n)$ should be 0 if $\mathrm{x}_n \in \mathcal{C}_0$.
- 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.

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

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

Loss Functions for Machine Learning

Multiclass Classification

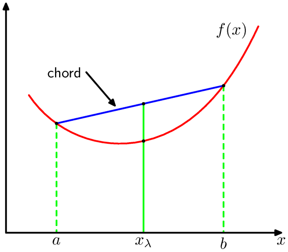
- Similar to BCE loss, we can use t_{nk} to *pick* the relevant negative log loss and write overall loss as

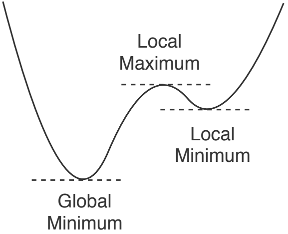
$$L(\theta) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk}$$

- 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 $\nabla f = 0$.
- 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*.

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

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

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

Matrix and Vector Derivatives

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

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

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

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

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