MathDNN - A deep mathematical understanding of DNNs

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Abstract

Frameworks such as TensorFlow or PyTorch make deep learning developments easy. They have made this field wide spread for every enthusiast. Implementations only needs an instinctive understanding of deep learning. The proper math aspect is little by little forgotten. Topology, Normalized vector space, Limit plus continuity, Taylor series expansion, Matrix, Finite dimensional linear algebra and Linear application matrix theories are supposed known. The objective is to do a collection of the important propositions explaining dense neural network (DNN) theories. These propositions will be mathematically proven. The subject used as reference is a multi-class classification problem with – dense layers, andactivation layers, Categorical cross-entropy loss and Stochastic gradient descent optimizer. But all the elements below can be easily re-used or re-defined to cover regressions.

Keywords: Dense neural network, Equation, Asumption, Proof

1 Fundamentals and notations

1.1 Matrices

Notation 1. Let $a_{i,j} \in \mathbb{R}$ for $i \in [\![1, n]\!]$ and $j \in [\![1, m]\!]$. Then a real matrix of dimension $n * m$ will noted as

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,m} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & \cdots & a_{n,m} \end{bmatrix}$$

The following notations are also considered

$$\forall i \in [\![1,n]\!], \forall j \in [\![1,m]\!], A_{i,j} = a_{i,j}$$

$$\forall j \in [\![1,m]\!], A_{:,j} = \begin{bmatrix} a_{1,j} \\ \vdots \\ a_{n,j} \end{bmatrix}$$

$$\forall i \in [\![1,n]\!], j \in [\![1,m]\!], A_{i,j} = \begin{bmatrix} a_{i,1} & \cdots & a_{i,n} \end{bmatrix}$$

The notation $\mathscr{M}_{n,m}$ means the matrix set of dimension $n \times m$ with coefficients in $\mathbb{R}$.

The notation $\mathscr{M}_{n,m}(E)$ means the matrix set of dimension $n \times m$ with coefficients in $E \subseteq \mathbb{R}$.

Convention 1. A vector is a matrix with only one row. Thus, the real vector set $\mathbb{R}^n$ is equivalent to $\mathscr{M}_{1,n}$.

Notation 2. Let $A \in \mathscr{M}_{n,m}$ and $B \in \mathscr{M}_{m,p}$. Let the product noted $A * B$ be

$$C = A * B$$

where $C \in \mathscr{M}_{n,p}$ with

$$\forall i \in [\![1,n]\!], \forall j \in [\![1,p]\!], C_{i,j} = \sum_{k=1}^{n} A_{i,k} * B_{k,j}$$

Notation 3. The matrix transpose operation will be noted as A^T.

Notation 4. Let $a \in \mathbb{R}^n$. The eucliean norm on $\mathbb{R}^n$ will be noted as $\|a\|_n$.

$$\|a\|_n = \sqrt{a * a^T}$$

1.2 Differential calculus

Convention 2. All sets considered are not empty.

Notation 5. Let $E \subseteq \mathbb{R}^n$ and $F \subseteq \mathbb{R}^m$.

The notation $\mathring{E}$ means the set with only the interior point of E.

The notation $f : E \longrightarrow F$ means the application from E to F.

The notation $\mathscr{C}(E,F)$ means the set of continuous applications from E to F.

The notation $\mathscr{L}(E,F)$ means the set of linear applications from E to F.

Definition 1.1. Let $E \subseteq \mathbb{R}^n$ and $F \subseteq \mathbb{R}^m$. Then f differentiable on E is equivalent to

$$\begin{gathered} \forall a \in \mathring{E}, \exists \frac{\partial f}{\partial \cdot}(a) \in \mathscr{L}(\mathbb{R}^n, \mathbb{R}^m), \\ \forall h \in \mathbb{R}^n, f(a+h) = f(a) + \frac{\partial f}{\partial h}(a) + \underset{h \to 0}{o}(\|h\|_n) \end{gathered} \tag{1}$$

$\frac{\partial f}{\partial \cdot}(a)$ is named differential of f on a.

The notation $\mathscr{D}(E,F)$ means the set of differentiable applications from E to F.

Proposition 1.1. *Let $E \subseteq \mathbb{R}^n$, $F \subseteq \mathbb{R}^m$ and $f \in \mathscr{D}(E,F)$. Then $\frac{\partial f}{\partial \cdot}(a)$ is unique and $\mathscr{D}(E,F) \subset \mathscr{C}(E,F)$.*

Proof. Suppose ϕ_1 and ϕ_2 two differentiales of f on a.

$$\forall h \in \mathbb{R}^n, \phi_2(h) - \phi_1(h) \underset{(1)}{=} \underset{h \to 0}{o}(\|h\|_n)$$

$$\underset{def}{\Longrightarrow} \forall \epsilon > 0, \exists \eta > 0, \forall h \in \mathbb{R}^n, (\|h\|_n \leq \eta \Rightarrow \left\|\phi_2(h) - \phi_1(h)\right\|_m \leq 2 * \|h\|_n * \epsilon)$$

$$\underset{\phi_2 - \phi_1 \in \mathscr{L}(\mathbb{R}^n, \mathbb{R}^m)}{\Longrightarrow} \forall \epsilon > 0, \forall h \in \mathbb{R}^n, \left\|\phi_2(h) - \phi_1(h)\right\|_m \leq 2 * \|h\|_n * \epsilon$$

$$\underset{\epsilon \to 0}{\Longrightarrow} \forall h \in \mathbb{R}^n, \phi_2(h) = \phi_1(h)$$

Let $f \in \mathscr{D}(E, F)$. and $a \in \mathring{E}$.

$$\frac{\partial f}{\partial \cdot}(a) \in \mathscr{L}(\mathbb{R}^n, \mathbb{R}^m) \implies \frac{\partial f}{\partial \cdot}(a) \in \mathscr{C}(\mathbb{R}^n, \mathbb{R}^m), \frac{\partial f}{\partial 0_{\mathbb{R}^n}}(a) = 0_{\mathbb{R}^m}$$

$$\underset{(1)}{\Longrightarrow} f(a+h) \underset{h \to 0}{\to} f(a)$$

$\square$

Definition 1.2. Let $E \subseteq \mathbb{R}^n$, $F \subseteq \mathbb{R}^m$ and $f = (f_1 \ldots f_m) \in \mathscr{D}(E, F)$. Then f_i is differentiable on E for all $i \in [\![1, m]\!]$. The jacobian is defined as

$$\begin{aligned} \mathscr{J}_f \quad : \quad \mathring{E} & \longrightarrow \mathscr{M}_{m,n} \\ a & \longmapsto \begin{bmatrix} \frac{\partial f}{\partial e_1}(a) & \cdots & \frac{\partial f}{\partial e_n}(a) \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial e_1}(a) & \cdots & \frac{\partial f_1}{\partial e_n}(a) \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial e_1}(a) & \cdots & \frac{\partial f_m}{\partial e_n}(a) \end{bmatrix} \end{aligned} \tag{2}$$

$(e_i)_{i \in [\![1,n]\!]}$ means the matrices $e_i = \begin{bmatrix} 0 & \cdots & \underset{\text{at index } 0}{1} & \cdots & 0 \end{bmatrix}$ corresponding to $\mathbb{R}^n$ standard basis.
$\frac{\partial f}{\partial e_i}$ is named the partial derivative of f according the i^{th} variable.
The jacobian is also named gradient when $m = 1$ and is noted as $\nabla_f = \mathscr{J}_f$.

Proof. Suppose $f = (f_1 \ldots f_m) \in \mathscr{D}(E, F)$. Let $i \in [\![1, m]\!]$, $a \in \mathring{E}$ and $h \in \mathbb{R}^n$.

$$\begin{aligned} f_i(a+h) &= f(a+h)_i \\ &= f(a)_i + \frac{\partial f}{\partial h}(a)_i + \underset{h \to 0}{o}(\|h\|_n)_i \\ &= f_i(a) + \frac{\partial f}{\partial h}(a)_i + \underset{h \to 0}{o}(\|h\|_n)_i \end{aligned}$$

$$\frac{\partial f}{\partial \cdot}(a)_i \in \mathscr{L}(\mathbb{R}^n, \mathbb{R}) \underset{1.1}{\Longrightarrow} \frac{\partial f_i}{\partial h}(a) = \frac{\partial f}{\partial h}(a)_i$$

$\square$