Machine Learning II

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Definition. For any finite, non-empty set S, called a set of **samples**, any $X \neq \emptyset$, called an **feature space** and any $x : S \to X$, the tuple (S, X, x) is called **unlabeled data**.

For any $y: S \to \{0, 1\}$, given in addition and called a **labeling**, the tuple (S, X, x, y) is called **labeled data**.

The **supervised learning problem** is an optimization problem. It consists in finding, in a family of functions, one function that minimizes a weighted sum of two objectives:

- 1. It deviates little from given labeled data, as quantified by a loss function
- 2. It has low complexity, as quantified by a regularizer.

Definition. For any labeled data T = (S, X, x, y), any $\Theta \neq \emptyset$ and $f : \Theta \to \mathbb{R}^X$, any $R : \Theta \to \mathbb{R}_0^+$, called a **regularizer**, any $L : \mathbb{R} \times \{0, 1\} \to \mathbb{R}_0^+$, called a **loss function**, and any $\lambda \in \mathbb{R}_0^+$, the instance of the **supervised learning problem** has the form

$$\inf_{\theta \in \Theta} \quad \underbrace{\lambda R(\theta) + \sum_{s \in S} L(f_{\theta}(x_s), y_s)}_{=:\varphi(\theta)} \tag{1}$$

Example. l_2 -regularized logistic regression: Given a finite index set $J \neq \emptyset$ and $\Theta := \mathbb{R}^J$, let

$$R(\theta) := \|\theta\|_2^2$$

 $L(r, y') := -y'r + \log_2(1+2^r)$

Algorithm. Steepest descent with parameters $\eta, \epsilon \in \mathbb{R}^+_0$ and initialization $\theta \in \mathbb{R}^J$:

 $\begin{aligned} & \mathsf{repeat} \\ & d := (\nabla_\theta \varphi)(\theta) \\ & \theta := \theta - \eta d \\ & \mathsf{if} \; \|d\| < \epsilon \\ & \mathsf{return} \; \theta \end{aligned}$

Definition. For any unlabeled data T = (S, X, x), any $\hat{f} : X \to \mathbb{R}$ and any $L : \mathbb{R} \times \{0, 1\} \to \mathbb{R}_0^+$, the instance of the **inference problem** wrt. T, \hat{f} and L is defined as

$$\min_{y \in \{0,1\}^S} \sum_{s \in S} L(\hat{f}(x_s), y_s)$$
(2)

Lemma. The solutions to the inference problem are the $y: S \to \{0, 1\}$ such that

$$\forall s \in S: \quad y_s \in \underset{\hat{y} \in \{0,1\}}{\operatorname{argmin}} L(\hat{f}(x_s), \hat{y}) \quad . \tag{3}$$

Consider a real feature space $X := \mathbb{R}^K$ with finite $K \neq \emptyset$.

What functions $f_{\theta} \colon X \to \mathbb{R}$ do we wish to learn?

• Linear functions f_{θ} , i.e. $\Theta := \mathbb{R}^{K}$ and $\forall x' \in X \colon f_{\theta}(x') = \langle \theta, x' \rangle$

Functions f_{θ} defined by a **compute graph**, i.e. a deep (artificial netural) network.

Notation. Let G = (V, E) a digraph.

• For any $v \in V$, let

 $P_{v} = \{u \in V \mid (u, v) \in E\}$ the set of parents of v (4) $C_{v} = \{w \in V \mid (v, w) \in E\}$ the set of children of v. (5)

For any $u, v \in V$, let $\mathcal{P}(u, v)$ denote the set of all uv-paths of G. (Any path is a subgraph. For any node u, the uu-path ($\{u\}, \emptyset$) exists.)

Let G be acyclic.

For any $v \in V$, let

 $A_{v} = \{u \in V \mid \mathcal{P}(u, v) \neq \varnothing\} \setminus \{v\}$ the set of ancestors of v (6) $D_{v} = \{w \in V \mid \mathcal{P}(v, w) \neq \varnothing\} \setminus \{v\}$ the set of descendants of v. (7)

Definition. A tuple $(V, D, D', E, \Theta, \{g_{v\theta} : \mathbb{R}^{P_v} \to \mathbb{R}\}_{v \in (D \cup D') \setminus V, \theta \in \Theta})$ is called a **compute graph**, iff the following conditions hold:

- $G = (V \cup D \cup D', E)$ is an acyclic digraph.
- For any $v \in V$, called an **input node**, $P_v = \emptyset$.
- For any $v \in D'$, called an **output node**, $C_v = \emptyset$.
- For any $v \in D$, called a hidden node, $P_v \neq \emptyset$ and $C_v \neq \emptyset$.

Definition. For any compute graph

 $\begin{array}{l} (V,D,D',E,\Theta,\{g_{v\theta}\colon \mathbb{R}^{P_v}\to \mathbb{R}\}_{v\in (D\cup D')\setminus V,\theta\in\Theta})\text{, any }v\in V\cup D\cup D'\text{ and any }\theta\in\Theta\text{, let }\alpha_{v\theta}\colon \mathbb{R}^V\to \mathbb{R}\text{ such that for all }\hat{x}\in \mathbb{R}^V \text{:} \end{array}$

$$\alpha_{v\theta}(\hat{x}) = \begin{cases} \hat{x}_v & \text{if } v \in V\\ g_{v\theta}(\alpha_{P_v\theta}(\hat{x})) & \text{otherwise} \end{cases}$$
(8)

For any $\theta \in \Theta$ let $f_{\theta} : \mathbb{R}^{V} \to \mathbb{R}^{D'}$ such that $f_{\theta} = \alpha_{D'\theta}$. We call $\alpha_{v\theta}(\hat{x})$ the **activation** of v for **input** \hat{x} and **parameters** θ . We call $f_{\theta}(\hat{x})$ the **output** of the compute graph for input \hat{x} and parameters θ .

Example. Consider $V = \{v_0, v_1, v_2\}$, $D = \{v_3\}$, $D' = \{v_4\}$ and the edge set E of the digraph depicted below.



Consider, in addition, $\Theta = \{\theta_0, \theta_1\}$ and

$$g_{v_3\theta} \colon \mathbb{R}^{\{v_0, v_1\}} \to \mathbb{R} \colon x \mapsto x_{v_0} + \theta_0 x_{v_1} \tag{9}$$

$$g_{v_4\theta}: \quad \mathbb{R}^{\{v_2, v_3\}} \to \mathbb{R}: \quad x \mapsto x_{v_2} + x_{v_3}^{\theta_1} \quad . \tag{10}$$

The compute graph $(V,D,D',E,\Theta,\{g_{v_{3}\theta},g_{v_{4}\theta}\})$ defines the function

$$f_{\theta}: \quad \mathbb{R}^{V} \to \mathbb{R}^{D'}: \quad x \mapsto x_{v_{2}} + (x_{v_{0}} + \theta_{0} x_{v_{1}})^{\theta_{1}} \quad . \tag{11}$$

Summary.

- ► The supervised deep learning problem is a supervised learning problem (e.g. the l_2 -regularized logistic regression problem) with respect to a family of functions f_{θ} defined by a compute graph (i.e. a deep network).
- In order to apply the steepest descent algorithm to this problem, we need to repeatedly calculate ∇_θφ and thus ∇_θf. This can be done, e.g., by the forward propagation algorithm or the backward propagation algorithm, which are discussed in the course Machine Learning I.