Machine Learning I

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Contents. This part of the course is about a special case of supervised learning: the supervised learning of **composite functions**, aka. **supervised deep learning**.

- We define a family of (composite) functions in terms a **compute graph**.
- We describe two algorithms for computing partial derivatives (if these exist) of such functions, **forward propagation** and **backward propagation**.
- In the exercises, we compare these algorithms.

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

- For any $v \in V$, let

$$P_v = \{u \in V \mid (u, v) \in E\} \qquad \text{the set of } \textbf{parents} \text{ of } v \tag{1}$$
$$C_v = \{w \in V \mid (v, w) \in E\} \qquad \text{the set of } \textbf{children} \text{ of } v\ . \tag{2}$$

- 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

$$A_v = \{u \in V \mid \mathcal{P}(u, v) \neq \emptyset\} \setminus \{v\} \qquad \text{the set of } \textbf{ancestors} \text{ of } v \tag{3}$$
$$D_v = \{w \in V \mid \mathcal{P}(v, w) \neq \emptyset\} \setminus \{v\} \quad \text{the set of } \textbf{descendants} \text{ of } v\ . \tag{4}$$

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

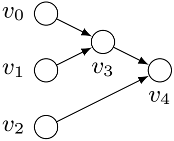
- $G = (V \cup D \cup D', E)$ is an acyclic digraph.
- For any $v \in V$, called an **input node**, $P_v = \emptyset$.
- For any $v \in D'$, called an **output node**, $C_v = \emptyset$.
- For any $v \in D$, called a **hidden node**, $P_v \neq \emptyset$ and $C_v \neq \emptyset$.

Definition. For any compute graph $(V, D, D', E, \Theta, \{g_{v\theta} \colon \mathbb{R}^{P_v} \to \mathbb{R}\}_{v \in (D \cup D') \setminus V, \theta \in \Theta})$, any $v \in V \cup D \cup D'$ and any $\theta \in \Theta$, let $\alpha_{v\theta} \colon \mathbb{R}^V \to \mathbb{R}$ such that for all $\hat{x} \in \mathbb{R}^V$:

$$\alpha_{v\theta}(\hat{x}) = \begin{cases} \hat{x}_v & \text{if } v \in V \\ g_{v\theta}(\alpha_{P_v\theta}(\hat{x})) & \text{otherwise} \end{cases} . \tag{5}$$

For any $\theta \in \Theta$ let $f_\theta \colon \mathbb{R}^V \to \mathbb{R}^{D'}$ 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

$$g_{v_3 \theta}\colon \quad \mathbb{R}^{\{v_0, v_1\}} \to \mathbb{R}\colon \quad x \mapsto x_{v_0} + \theta_0 x_{v_1} \tag{6}$$

$$g_{v_4 \theta}\colon \quad \mathbb{R}^{\{v_2, v_3\}} \to \mathbb{R}\colon \quad x \mapsto x_{v_2} + x_{v_3}^{\theta_1} \ . \tag{7}$$

The compute graph $(V, D, D', E, \Theta, \{g_{v_3 \theta}, g_{v_4 \theta}\})$ defines the function

$$f_\theta\colon \quad \mathbb{R}^V \to \mathbb{R}^{D'}\colon \quad x \mapsto x_{v_2} + \left(x_{v_0} + \theta_0 \, x_{v_1}\right)^{\theta_1} \ . \tag{8}$$

Let $(V, D, D', E, \Theta, \{g_{v\theta} \colon \mathbb{R}^{P_v} \to \mathbb{R}\}_{v \in (D \cup D') \setminus V, \theta \in \Theta})$ a compute graph with $|D'| = 1$ and $\Theta = \mathbb{R}^J$ for some finite set $J \neq \emptyset$. Let f be the family of functions defined by this compute graph. The l_2-**regularized logistic regression problem** wrt. f, labeled data $T = (S, \mathbb{R}^V, x, y)$ and $\sigma \in \mathbb{R}^+$ has the form

$$\min_{\theta \in \mathbb{R}^J} \quad \frac{1}{|S|} \sum_{s \in S} \left(-y_s f_\theta(x_s) + \log\left(1 + 2^{f_\theta(x)}\right) \right) + \frac{\log e}{2\sigma^2} \|\theta\|^2 \ . \tag{9}$$

- (9) is analogous to linear logistic regression but can be non-convex for f non-linear wrt. θ.
- If for any $j \in J$ the partial derivative of f wrt. θ_j exists, we can search for a local minimum using a steepest descent algorithm.
- To do so, we describe two techniques for computing $\nabla_\theta f$, **forward propagation** and **backward propagation**.

Lemma. Let $j \in J$. For any $v \in V$: $\frac{\partial \alpha_{v\theta}}{\partial \theta_j} = 0$. For any $v \in (D \cup D') \setminus V$:

$$\frac{\partial \alpha_{v\theta}}{\partial \theta_j} = \sum_{u \in (A_v \cup \{v\}) \setminus V} \frac{\partial g_{u\theta}}{\partial \theta_j} \Delta_{uv} \tag{10}$$

with

$$\Delta_{uv} := \sum_{(V',E') \in \mathcal{P}(u,v)} \prod_{(u',v') \in E'} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \ . \tag{11}$$

Remark. For any node u: $\Delta_{uu} = 1$. For any u, v with $\mathcal{P}(u,v) = \emptyset$: $\Delta_{uv} = 0$.

Proof (idea).

$$\begin{aligned}
\frac{\partial \alpha_{v\theta}}{\partial \theta_j} &= \frac{\partial g_{v\theta}}{\partial \theta_j} + \sum_{u \in P_v} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \frac{\partial \alpha_{u\theta}}{\partial \theta_j} \qquad (12) \\
&= \frac{\partial g_{v\theta}}{\partial \theta_j} + \sum_{u \in P_v} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \frac{\partial g_{u\theta}}{\partial \theta_j} + \sum_{u \in P_v} \sum_{u' \in P_u} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \frac{\partial g_{u\theta}}{\partial \alpha_{u'\theta}} \frac{\partial \alpha_{u'\theta}}{\partial \theta_j} \\
&= \text{repeated application (12)} \\
&= \sum_{u \in (A_v \cup \{v\}) \setminus V} \frac{\partial g_{u\theta}}{\partial \theta_j} \sum_{(V',E') \in \mathcal{P}(u,v)} \prod_{(u',v') \in E'} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}}
\end{aligned}$$

Lemma (forward propagation). For all nodes $u \neq w$ such that $\mathcal{P}(u,w) \neq \emptyset$:

$$\Delta_{uw} = \sum_{v \in P_w} \frac{\partial g_{w\theta}}{\partial \alpha_{v\theta}} \, \Delta_{uv} \tag{13}$$

Proof.

$$\begin{aligned}
\Delta_{uw} &= \sum_{(V',E') \in \mathcal{P}(u,w)} \prod_{(u',v') \in E'} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \\
&= \sum_{v \in P_w} \sum_{(V'',E'') \in \mathcal{P}(u,v)} \prod_{(u',v') \in E'' \cup \{v,w\}} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \\
&= \sum_{v \in P_w} \frac{\partial g_{w\theta}}{\partial \alpha_{v\theta}} \sum_{(V'',E'') \in \mathcal{P}(u,v)} \prod_{(u',v') \in E''} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \\
&= \sum_{v \in P_w} \frac{\partial g_{w\theta}}{\partial \alpha_{v\theta}} \, \Delta_{uv}
\end{aligned}$$

$\square$

The **forward propagation algorithm** computes Δ_{uw} for one node u and all nodes w. It is defined wrt. an arbitrary partial order $<_P$ of the nodes such that

$$\forall w \in D \cup D' \quad \forall w' \in P_w\colon \quad w' <_P w \ . \tag{14}$$

Input:
Compute graph $(V, D, D', E, \Theta, \{g_{v\theta}\colon \mathbb{R}^{P_v} \to \mathbb{R}\}_{v \in (D \cup D') \setminus V, \theta \in \Theta})$
Node $u \in V \cup D \cup D'$

for w ordered by $<_P$ (14)
  if $w = u$
    $\Delta_{uw} := 1$
  else if $\mathcal{P}(u, w) = \emptyset$
    $\Delta_{uw} := 0$
  else
    $\Delta_{uw} := \sum_{v \in P_w} \frac{\partial g_{w\theta}}{\partial \alpha_{v\theta}} \Delta_{uv}$ (13)

Lemma (backward propagation). For all nodes $u \neq w$ such that $\mathcal{P}(u,w) \neq \emptyset$:

$$\Delta_{uw} = \sum_{v \in C_u} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \, \Delta_{vw} \tag{15}$$

Proof.

$$\begin{aligned}
\Delta_{uw} &= \sum_{(V',E') \in \mathcal{P}(u,w)} \prod_{(u',v') \in E'} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \\
&= \sum_{v \in C_u} \sum_{(V'',E'') \in \mathcal{P}(v,w)} \prod_{(u',v') \in E'' \cup \{(u,v)\}} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \\
&= \sum_{v \in C_u} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \sum_{(V'',E'') \in \mathcal{P}(v,w)} \prod_{(u',v') \in E''} \frac{\partial g_{v'\theta}}{\partial \alpha_{u'\theta}} \\
&= \sum_{v \in C_u} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \, \Delta_{vw}
\end{aligned}$$

$\square$

The **backward propagation algorithm** computes Δ_{uw} for one node w and all nodes u. It is defined wrt. an arbitrary partial order $<_C$ of the nodes such that

$$\forall u \in V \cup D \quad \forall v \in C_u \colon \quad v <_C u \ . \tag{16}$$

Input:
Compute graph $(V, D, D', E, \Theta, \{g_{v\theta} \colon \mathbb{R}^{P_v} \to \mathbb{R}\}_{v \in (D \cup D') \setminus V, \theta \in \Theta})$
Node $w \in V \cup D \cup D'$

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for u ordered by $<_C$ (16)
    if $u = w$
        $\Delta_{uw} := 1$
    else if $\mathcal{P}(u, w) = \emptyset$
        $\Delta_{uw} := 0$
    else
        $\Delta_{uw} := \sum_{v \in C_u} \frac{\partial g_{v\theta}}{\partial \alpha_{u\theta}} \Delta_{vw}$ (15)
