Chapter ML:IV (continued)

IV. Neural Networks

- Perceptron Learning
- Multilayer Perceptron Basics
- Multilayer Perceptron with Two Layers
- Multilayer Perceptron at Arbitrary Depth
- Advanced MLPs
- Automatic Gradient Computation
Advanced MLPs
Output Normalization: Softmax

For two classes ($k = 2$), the scalar sigmoid output $\sigma(z)$ determines both class probabilities for $x$: $p(1 \mid x) := \sigma(z)$ and $p(0 \mid x) := 1 - \sigma(z)$.

$z$ is the dot product of the final layer’s weights with the previous layer’s output. I.e., for networks with one active layer $z = w^T x$; for $d$ active layers $z = w_d^T y^{h_{d-1}}$. 
Advanced MLPs
Output Normalization: Softmax (continued)

For two classes \((k = 2)\), the scalar sigmoid output \(\sigma(z)\) determines both class probabilities for \(x\): 
\[
p(1 \mid x) := \sigma(z) \quad \text{and} \quad p(0 \mid x) := 1 - \sigma(z)
\]

\(z\) is the dot product of the final layer’s weights with the previous layer’s output. I.e., for networks with one active layer \(z = w^T x\); for \(d\) active layers \(z = w_d^T y^{h_{d-1}}\).
Advanced MLPs
Output Normalization: Softmax (continued)

For two classes ($k = 2$), the scalar sigmoid output $\sigma(z)$ determines both class probabilities for $x$: $p(1 \mid x) := \sigma(z)$ and $p(0 \mid x) := 1 - \sigma(z)$.

$z$ is the dot product of the final layer’s weights with the previous layer’s output. I.e., for networks with one active layer $z = w^T x$; for $d$ active layers $z = w_d^T y_{h_{d-1}}$. 
Advanced MLPs
Output Normalization: Softmax (continued)

For two classes ($k = 2$), the scalar sigmoid output $\sigma(z)$ determines both class probabilities for $x$: $p(1 \mid x) := \sigma(z)$ and $p(0 \mid x) := 1 - \sigma(z)$.

$z$ is the dot product of the final layer’s weights with the previous layer’s output. I.e., for networks with one active layer $z = w^T x$; for $d$ active layers $z = w_d^T y^{h_{d-1}}$.

The softmax function $\sigma_1 : \mathbb{R}^k \rightarrow \Delta^{k-1}$, $\Delta^{k-1} \subset \mathbb{R}^k$, generalizes the logistic (sigmoid) function to $k$ dimensions (to $k$ exclusive classes) [Wikipedia]:

$$\sigma_1(z)_i = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{z_j}}$$
Advanced MLPs
Output Normalization: Softmax (continued)

The class probabilities for the two-class setting can be represented as an equivalent softmax vector:

$$
\mathbf{x} \rightarrow \begin{bmatrix} p(0 \mid \mathbf{x}) \\ p(1 \mid \mathbf{x}) \end{bmatrix} = \begin{bmatrix} 1 - \sigma(z) \\ \sigma(z) \end{bmatrix} = \begin{bmatrix} \sigma(-z) \\ \frac{1}{1+e^{-z}} \end{bmatrix} = \begin{bmatrix} \frac{e^0}{e^0 + e^z} \\ \frac{e^z}{e^0 + e^z} \end{bmatrix} = \sigma_1 \left( \binom{0}{z} \right)
$$
Advanced MLPs
Output Normalization: Softmax (continued)

The class probabilities for the two-class setting can be represented as an equivalent softmax vector:

\[
x \rightarrow \begin{bmatrix} p(0 \mid x) \\ p(1 \mid x) \end{bmatrix} = \begin{bmatrix} 1 - \sigma(z) \\ \sigma(z) \end{bmatrix} = \begin{bmatrix} \frac{1}{1 + e^{-z}} \\ \frac{e^{-z}}{1 + e^{-z}} \end{bmatrix} = \begin{bmatrix} \frac{e^0}{e^0 + e^z} \\ \frac{e^z}{e^0 + e^z} \end{bmatrix} = \sigma_1 \left( \begin{pmatrix} 0 \\ z \end{pmatrix} \right)
\]

General case for \( k \) classes:

\[
y^h \rightarrow \begin{bmatrix} e^{y_1} \\ \vdots \\ e^{y_k} \end{bmatrix} = \frac{e^{y_1}}{\sum_{j=1}^{k} e^{y_j}} \\ \vdots \\ \frac{e^{y_k}}{\sum_{j=1}^{k} e^{y_j}}
\]

Softmax \( k \) probabilities (learned distribution \( Q \))

[Cross-entropy loss]
Advanced MLPs

Output Normalization: Softmax (continued)

The class probabilities for the two-class setting can be represented as an equivalent softmax vector:

\[
\begin{pmatrix}
p(0 | x) \\
p(1 | x)
\end{pmatrix} = \begin{pmatrix} 1 - \sigma(z) \\ \sigma(z) \end{pmatrix} = \begin{pmatrix} \frac{1}{1+e^{-z}} \\ \frac{e^z}{1+e^z} \end{pmatrix} = \begin{pmatrix} \frac{e^0}{e^0+e^z} \\ \frac{e^z}{e^0+e^z} \end{pmatrix} = \sigma_1(\begin{pmatrix} 0 \\ z \end{pmatrix})
\]

General case for \( k \) classes:

... → y\(^{h_1}\) → \( \sum \) → y\(^{h_{d-1}}\) → ... → Softmax → y\(_1\) → \( \frac{e^{y_1}}{\sum_{j=1}^{k} e^{y_j}} \) → ... → y\(_k\) → \( \frac{e^{y_k}}{\sum_{j=1}^{k} e^{y_j}} \) → ... → k probabilities

(y(x) = \sigma_1(z), [cross-entropy loss])
Remarks:

- The standard $k-1$-simplex contains all $k$-tuples with non-negative elements that sum to 1:

$$\Delta^{k-1} = \left\{ (p_1, \ldots, p_k) \in \mathbb{R}^k : \sum_{i=1}^k p_i = 1 \text{ and } p_i \geq 0 \text{ for all } i \right\}$$

- The softmax function ensures Axiom I (positivity) and Axiom II (unitarity) of Kolmogorov.
Advanced MLPs
Loss Function: Cross-Entropy

**Definition 2 (Cross Entropy)**

Let $C$ be a random variable with distribution $P$ and a finite number of realizations $C$. Let $Q$ be another distribution of $C$. Then, the cross entropy of distribution $Q$ relative to the distribution $P$, denoted as $H(P, Q)$, is defined as follows:

$$H(P, Q) = - \sum_{c \in C} P(C = c) \cdot \log (Q(C = c))$$
Definition 2 (Cross Entropy)

Let \( C \) be a random variable with distribution \( P \) and a finite number of realizations \( C \). Let \( Q \) be another distribution of \( C \). Then, the cross entropy of distribution \( Q \) relative to the distribution \( P \), denoted as \( H(P, Q) \), is defined as follows:

\[
H(P, Q) = - \sum_{c \in C} P(C=c) \cdot \log (Q(C=c))
\]

- The cross entropy \( H(P, Q) \) is the average number of total bits to represent an event \( C=c \) under the distribution \( Q \) instead of under the distribution \( P \).

- The relative entropy, also called Kullback-Leibler divergence, is the average number of additional bits to represent an event under \( Q \) instead of under \( P \).
**Definition 2 (Cross Entropy)**

Let $C$ be a random variable with distribution $P$ and a finite number of realizations $C$. Let $Q$ be another distribution of $C$. Then, the cross entropy of distribution $Q$ relative to the distribution $P$, denoted as $H(P, Q)$, is defined as follows:

$$H(P, Q) = -\sum_{c \in C} P(C=c) \cdot \log (Q(C=c))$$
Advanced MLPs

Cross-Entropy in Classification Settings

\[ H(P, Q) = - \sum_{c \in C} P(C=c) \cdot \log (Q(C=c)) \]

\[ H(p, q) = - \sum_{c \in C} p(c) \cdot \log (q(c)) \]

\[ l_\sigma(z) = -c \cdot \log (\sigma(z)) - (1-c) \cdot \log (1-\sigma(z)) \]

\[ l_{\sigma_1}(z) = - \sum_{i=1}^{k} c_i \cdot \log (\sigma_1(z)_i) \]

- Random variable C denotes a class.
- Realizations of C: \( C = \{c_1, \ldots, c_k\} \).
- \( P, Q \) define distributions of C.

- Probability functions \( p, q \) related to \( P, Q \).
- Class labels \( C = \{c_1, \ldots, c_k\} \).

- Two classes encoded as \( c, c \in \{0, 1\} \).
- Example with groundtruth \( (x, c) \in D \).
- Classifier output \( \sigma(z), z = y(x) \).

- \( k \) classes, hot-encoded as \( c^T \), \( c^T \in \{(1,0,\ldots,0), \ldots,(0,\ldots,0,1)\} \).
- Example with groundtruth \( (x, c) \in D \).
- Classifier output \( \sigma_1(z), z = y(x) \).
Advanced MLPs

Cross-Entropy in Classification Settings (continued)

[logistic loss: definition, derivation]

\[ H(P, Q) = - \sum_{c \in C} P(C=c) \cdot \log (Q(C=c)) \]

- Random variable \( C \) denotes a class.
- Realizations of \( C \): \( C = \{c_1, \ldots, c_k\} \).
- \( P, Q \) define distributions of \( C \).

\[ H(p, q) = - \sum_{c \in C} p(c) \cdot \log (q(c)) \]

- Probability functions \( p, q \) related to \( P, Q \).
- Class labels \( C = \{c_1, \ldots, c_k\} \).

\[ l_\sigma(z) = -c \cdot \log (\sigma(z)) - (1-c) \cdot \log (1-\sigma(z)) \]

- Two classes encoded as \( c, c \in \{0, 1\} \).
- Example with groundtruth \((x, c) \in D\).
- Classifier output \( \sigma(z), z = y(x) \).

\[ l_{\sigma_1}(z) = - \sum_{i=1}^{k} c_i \cdot \log (\sigma_1(z)|_i) \]

- \( k \) classes, hot-encoded as \( c^T \), \( c^T \in \{(1, 0, \ldots, 0), \ldots, (0, \ldots, 0, 1)\} \).
- Example with groundtruth \((x, c) \in D\).
- Classifier output \( \sigma_1(z), z = y(x) \).
Advanced MLPs
Cross-Entropy in Classification Settings (continued)

\[ H(P, Q) = - \sum_{c \in C} P(C=c) \cdot \log (Q(C=c)) \]

Random variable \( C \) denotes a class.

Realizations of \( C \): \( C = \{c_1, \ldots, c_k\} \).

\( P, Q \) define distributions of \( C \).

\[ H(p, q) = - \sum_{c \in C} p(c) \cdot \log (q(c)) \]

Probability functions \( p, q \) related to \( P, Q \).

Class labels \( C = \{c_1, \ldots, c_k\} \).

\[ l_{\sigma}(z) = -c \cdot \log (\sigma(z)) - (1-c) \cdot \log (1-\sigma(z)) \]

Two classes encoded as \( c, c \in \{0, 1\} \).

Example with groundtruth \((x, c) \in D\).

Classifier output \( \sigma(z), z = y(x) \).

\[ l_{\sigma_1}(z) = - \sum_{i=1}^{k} c_i \cdot \log \left( \sigma_1(z)\right) \]

\( k \) classes, hot-encoded as \( c^T \),
\( c^T \in \{(1, 0, \ldots, 0), \ldots, (0, \ldots, 0, 1)\} \).

Example with groundtruth \((x, c) \in D\).

Classifier output \( \sigma_1(z), z = y(x) \).
Remarks:

- If not stated otherwise, log means $\log_2$.
- Synonyms: cross-entropy loss function, logarithmic loss, log loss, **logistic loss**.
Advanced MLPs

Activation Function: Rectified Linear Unit (ReLU)

[TODO]
Advanced MLPs
Regularization: Dropout

[TODO]
Advanced MLPs
Learning Rate Adaptation: Momentum

Momentum principle: a weight adaptation in iteration $t$ considers the adaptation in iteration $t-1$:

$$\Delta W^o(t) = \eta \cdot (\delta^o \otimes y^h(x)|_{1,...,l}) + \alpha \cdot \Delta W^o(t-1)$$

$$\Delta W^h(t) = \eta \cdot (\delta^h \otimes x) + \alpha \cdot \Delta W^h(t-1)$$

$$\Delta W^{hs}(t) = \eta \cdot (\delta^{hs} \otimes y^{hs-1}(x)|_{1,...,l_{s-1}}) + \alpha \cdot \Delta W^{hs}(t-1), \ s = d, d-1, \ldots, 2$$

$$\Delta W^{h1}(t) = \eta \cdot (\delta^{h1} \otimes x) + \alpha \cdot \Delta W^{h1}(t-1)$$

The term $\alpha$, $0 \leq \alpha < 1$, is called “momentum”.
Advanced MLPs
Learning Rate Adaptation: Momentum (continued)

Momentum principle: a weight adaptation in iteration $t$ considers the adaptation in iteration $t-1$:

$$
\Delta W^o(t) = \eta \cdot (\delta^o \otimes y^h(x)|_{1,...,l}) + \alpha \cdot \Delta W^o(t-1)
$$

$$
\Delta W^h(t) = \eta \cdot (\delta^h \otimes x) + \alpha \cdot \Delta W^h(t-1)
$$

$$
\Delta W^{h_s}(t) = \eta \cdot (\delta^{h_s} \otimes y^{h_{s-1}}(x)|_{1,...,l_{s-1}}) + \alpha \cdot \Delta W^{h_s}(t-1), \ s = d, d-1, \ldots, 2
$$

$$
\Delta W^{h_1}(t) = \eta \cdot (\delta^{h_1} \otimes x) + \alpha \cdot \Delta W^{h_1}(t-1)
$$

The term $\alpha$, $0 \leq \alpha < 1$, is called “momentum”.

Effects:

- Due the “adaptation inertia” local minima can be overcome.
- If the direction of the descent does not change, the adaptation increment and, as a consequence, the speed of convergence is increased.
Remarks:

- **Recap.** The symbol \( \otimes \) denotes the dyadic product, also called outer product or tensor product. The dyadic product takes two vectors and returns a second order tensor, called a dyadic in this context: \( \mathbf{v} \otimes \mathbf{w} \equiv \mathbf{vw}^T \). [Wikipedia]
IV. Neural Networks

- Perceptron Learning
- Multilayer Perceptron Basics
- Multilayer Perceptron with Two Layers
- Multilayer Perceptron at Arbitrary Depth
- Advanced MLPs
- Automatic Gradient Computation
Automatic Gradient Computation

The IGD Algorithm

Algorithm: $\text{IGD}_{\text{MLP}^*}$

IGD for the $d$-layer MLP with arbitrary model and objective functions.

Input: $D$

Multiset of examples $(x, c)$ with $x \in \mathbb{R}^p$, $c \in \{0, 1\}^k$.

$\eta, l(), R(), \lambda$

Learning rate, loss and regularization functions and parameters.

Output: $W^{h_1}, \ldots, W^{h_d}$

Weight matrices of the $d$ layers. (= hypothesis)

1. FOR $s = 1$ TO $d$ DO $\text{initialize\_random\_weights}(W^{h_s})$ ENDDO, $t = 0$
2. REPEAT
3. $t = t + 1$
4. FOREACH $(x, c) \in D$ DO
5. $\quad y^{h_1}(x) = \left(\tanh(W^{h_1}x)^1\right)$ // forward propagation; $x$ is extended by $x_0 = 1$

FOR $s = 2$ TO $d-1$ DO $\quad y^{h_s}(x) = \left(\text{ReLU}(W^{h_s}y^{h_{s-1}}(x))\right)$ ENDDO

$\quad y(x) = \sigma_1(W^{h_d}y^{h_{d-1}}(x))$

6. $\delta = c - y(x)$
7a. $\ell(w) = l(\delta) + \lambda R(w)$ // backpropagation (Steps 7a+7b)

$\quad \nabla \ell(w) = \text{autodiff}(\ell(), w)$

7b. FOR $s = 1$ TO $d$ DO $\quad \Delta W^{h_s} = \eta \cdot \nabla^{h_s} \ell(w)$ ENDDO
8. FOR $s = 1$ TO $d$ DO $\quad W^{h_s} = W^{h_s} + \Delta W^{h_s}$ ENDDO
9. ENDDO
10. UNTIL($\text{convergence}(D,y(\cdot),t))$
11. return($W^{h_1}, \ldots, W^{h_d}$)
Algorithm: IGD<sub>MLP</sub> *(IGD for the \(d\)-layer MLP with arbitrary model and objective functions.)*

Input: \(D\) Multiset of examples \((x, c)\) with \(x \in \mathbb{R}^p, c \in \{0, 1\}^k\).

\(\eta, l(), R(), \lambda\) Learning rate, loss and regularization functions and parameters.

Output: \(W^{h_1}, \ldots, W^{h_d}\) Weight matrices of the \(d\) layers. (= hypothesis)

1. FOR \(s = 1\) TO \(d\) DO \(\text{initialize_random_weights}(W^{h_s})\) ENDDO, \(t = 0\)
2. REPEAT
3. \(t = t + 1\)
4. FOREACH \((x, c) \in D\) DO
5. \(y^{h_1}(x) = (\tanh(W^{h_1}x))^{1}\) // forward propagation; \(x\) is extended by \(x_0 = 1\)
   FOR \(s = 2\) TO \(d-1\) DO \(y^{h_s}(x) = (\text{ReLU}(W^{h_s}y^{h_{s-1}}(x)))^{1}\) ENDDO
   \(y(x) = \sigma_1(W^{h_d}y^{h_{d-1}}(x))\)
6. \(\delta = c - y(x)\)
7a. \(\ell(w) = l(\delta) + \frac{\lambda}{\eta}R(w)\) // backpropagation (Steps 7a+7b)
   \(\nabla \ell(w) = \text{autodiff}(\ell(), w)\)
7b. FOR \(s = 1\) TO \(d\) DO \(\Delta W^{h_s} = \eta \cdot \nabla^{h_s} \ell(w)\) ENDDO
8. FOR \(s = 1\) TO \(d\) DO \(W^{h_s} = W^{h_s} + \Delta W^{h_s}\) ENDDO
9. ENDDO
10. UNTIL \(\text{convergence}(D, y(\cdot), t))\)
11. return \((W^{h_1}, \ldots, W^{h_d})\)
Algorithm: IGD

IGD for the \(d\)-layer MLP with arbitrary model and objective functions.

Input:
- \(D\): Multiset of examples \((x, c)\) with \(x \in \mathbb{R}^p\), \(c \in \{0, 1\}^k\).
- \(\eta, l(), R(), \lambda\): Learning rate, loss and regularization functions and parameters.

Output:
- \(W^{h_1}, \ldots, W^{h_d}\): Weight matrices of the \(d\) layers. (= hypothesis)

1. FOR \(s = 1\) TO \(d\) DO \text{initialize\_random\_weights}(W^{h_s}) ENDDO, \(t = 0\)
2. \textbf{REPEAT}
3. \(t = t + 1\)
4. FOREACH \((x, c) \in D\) DO
5. Model function evaluation.
6. Calculation of residual vector.
7a. Calculation of derivative of the loss.
7b. Parameter vector update \(\triangleq\) one gradient step down.
8. ENDDO
9. \textbf{UNTIL}(\text{convergence}(D, y(\cdot), t))
10. \textbf{return}(W^{h_1}, \ldots, W^{h_d})

Model function evaluation.
Calculation of residual vector.
Calculation of derivative of the loss.
Parameter vector update \(\triangleq\) one gradient step down.
Reverse-mode AD corresponds to a generalized backpropagation algorithm.

Let $\mathcal{L}(w_1, \ldots, w_p)$ be the function to be differentiated.

- Consider $\mathcal{L}$ as a computational graph of elementary operations, assigning each intermediate result to a variable $v_i$ with $-p \leq i \leq m$

  (naming convention: $v_{-p...0}$ for inputs, $v_{1...m-1}$ for intermediate variables, $v_m \equiv \mathcal{L}$ for the output)
Automatic Gradient Computation
Reverse-Mode Automatic Differentiation in Computational Graphs (continued)

For each intermediate variable \( v_i \), an adjoint value \( \nabla v_i \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_i} \) is computed based on its descendants in the computation graph.

(1) \[ \nabla v_m \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_m} = \frac{\partial v_m}{\partial v_m} = 1 \]

(2) \[ \nabla v_i \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_i} = \frac{\partial \mathcal{L}}{\partial v_k} \cdot \frac{\partial v_k}{\partial v_i} = \nabla v_k \mathcal{L} \cdot \frac{\partial v_k}{\partial v_i} \]

(3) \[ \nabla v_k \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial v_k} = \frac{\partial \mathcal{L}}{\partial v_j} \cdot \frac{\partial v_j}{\partial v_k} = \nabla v_j \mathcal{L} \cdot \frac{\partial v_j}{\partial v_k} \]

\[ \nabla v_i \mathcal{L} = \nabla v_j \mathcal{L} \cdot \frac{\partial v_j}{\partial v_i} + \nabla v_k \mathcal{L} \cdot \frac{\partial v_k}{\partial v_i} \]
Remarks:

- Adjoint are computed in reverse, starting from $\nabla^{v_m} L$.
- For any step $v_j = g(\ldots, v_i, \ldots)$ in the graph, the local gradients $\frac{\partial g}{\partial v_i}$ must be computable.
Automatic Gradient Computation

Autodiff Example: Setting

Consider the RSS loss for a simple logistic regression model and a very small dataset.

Dataset: \( D = \{(1, 1.5)^T, 0\}, \{(1.5, -1)^T, 1\}\)

Model function: \( y(x) = \sigma(w^T x) \)

Loss function: \( \mathcal{L}(w) = L_2(w) = \sum_{(x, c) \in D} \left( c - y(x) \right)^2 \)

\( \mathcal{L}(w) \) is the objective function to be minimized, and hence what we want to compute the derivative of; everything except \( w \) is held constant.

Given the setting above, we can rewrite \( \mathcal{L} \) as:

\[
\begin{align*}
\mathcal{L}(w) &= (c_1 - \sigma(w^T x_1))^2 + (c_2 - \sigma(w^T x_2))^2 \\
&= (\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2
\end{align*}
\]

Using reverse-mode automatic differentiation, we’ll simultaneously evaluate the loss and its derivative at \( w = (-1, 1.5, 0.5)^T \).
Automatic Gradient Computation

Autodiff Example: Computational Graph

\[ \mathcal{L}(\mathbf{w}) = (-\sigma(w_0 + w_1 + 1.5w_2)^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2)^2) \]
Automatic Gradient Computation

Autodiff Example: Forward and Reverse Trace

\[ \mathcal{L}(w) = \left(-\sigma\left(w_0 + w_1 + 1.5w_2\right)\right)^2 + \left(1 - \sigma\left(w_0 + 1.5w_1 - w_2\right)\right)^2 \]

at \[ w = (-1, 1.5, 0.5)^T \]

<table>
<thead>
<tr>
<th>Forward primal trace</th>
<th>Reverse adjoint trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>( v_0 = w_0 )</td>
<td>( v_7 )</td>
</tr>
<tr>
<td>( v_{-1} = w_1 )</td>
<td>( v_8 )</td>
</tr>
<tr>
<td>( v_{-2} = w_2 )</td>
<td>( v_3 )</td>
</tr>
<tr>
<td>( v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2} ) = 1.25</td>
<td>( v_9 = v_7 + v_8 ) = 0.71</td>
</tr>
<tr>
<td>( v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2} ) = 0.75</td>
<td>( \mathcal{L} = v_9 ) = 0.71</td>
</tr>
</tbody>
</table>
Automatic Gradient Computation

Autodiff Example: Forward and Reverse Trace (continued)

\[
\mathcal{L}(\mathbf{w}) = \left(-\sigma\left(w_0 + w_1 + 1.5w_2\right)\right)^2 + \left(1 - \sigma\left(w_0 + 1.5w_1 - w_2\right)\right)^2
\]

at \( \mathbf{w} = (-1, 1.5, 0.5)^T \)

<table>
<thead>
<tr>
<th>Forward primal trace</th>
<th>Reverse adjoint trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>( v_0 = w_0 )</td>
<td>( = -1 )</td>
</tr>
<tr>
<td>( v_{-1} = w_1 )</td>
<td>( = 1.5 )</td>
</tr>
<tr>
<td>( v_{-2} = w_2 )</td>
<td>( = 0.5 )</td>
</tr>
<tr>
<td>( v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2} )</td>
<td>( = 1.25 )</td>
</tr>
<tr>
<td>( v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2} )</td>
<td>( = 0.75 )</td>
</tr>
<tr>
<td>( v_3 = \sigma(v_1) )</td>
<td>( = 0.78 )</td>
</tr>
<tr>
<td>( v_4 = \sigma(v_2) )</td>
<td>( = 0.68 )</td>
</tr>
<tr>
<td>( v_5 = 0 - v_3 )</td>
<td>( = -0.78 )</td>
</tr>
<tr>
<td>( v_6 = 1 - v_4 )</td>
<td>( = 0.32 )</td>
</tr>
<tr>
<td>( v_7 = v_5^2 )</td>
<td>( = 0.61 )</td>
</tr>
<tr>
<td>( v_8 = v_6^2 )</td>
<td>( = 0.1 )</td>
</tr>
<tr>
<td>( v_9 = v_7 + v_8 )</td>
<td>( = 0.71 )</td>
</tr>
</tbody>
</table>

\( \mathcal{L} = v_9 \) \( = 0.71 \)

\( \nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 \)
Automatic Gradient Computation

Autodiff Example: Forward and Reverse Trace (continued)

\[ \mathcal{L}(\mathbf{w}) = (-\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2 \]

at \( \mathbf{w} = (-1, 1.5, 0.5)^T \)

<table>
<thead>
<tr>
<th>Forward primal trace</th>
<th>Reverse adjoint trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>( v_0 = w_0 )</td>
<td>( \nabla v_8 \mathcal{L} = \nabla v_9 \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1 = 1 )</td>
</tr>
<tr>
<td>( v_{-1} = w_1 )</td>
<td>( \nabla v_7 \mathcal{L} = \nabla v_9 \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1 = 1 )</td>
</tr>
<tr>
<td>( v_{-2} = w_2 )</td>
<td>( \nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 )</td>
</tr>
<tr>
<td>( v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2} )</td>
<td>0.75</td>
</tr>
<tr>
<td>( v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2} )</td>
<td>0.78</td>
</tr>
<tr>
<td>( v_3 = \sigma(v_1) )</td>
<td>0.75</td>
</tr>
<tr>
<td>( v_4 = \sigma(v_2) )</td>
<td>0.68</td>
</tr>
<tr>
<td>( v_5 = 0 - v_3 )</td>
<td>0.61</td>
</tr>
<tr>
<td>( v_6 = 1 - v_4 )</td>
<td>0.32</td>
</tr>
<tr>
<td>( v_7 = v_5^2 )</td>
<td>0.1</td>
</tr>
<tr>
<td>( v_8 = v_6^2 )</td>
<td>0.1</td>
</tr>
<tr>
<td>( v_9 = v_7 + v_8 )</td>
<td>0.71</td>
</tr>
</tbody>
</table>

\[ \mathcal{L} = v_9 \]

0.71
Automatic Gradient Computation

Autodiff Example: Forward and Reverse Trace (continued)

\[ \mathcal{L}(\mathbf{w}) = ( -\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2 \]

at \[ \mathbf{w} = (-1, 1.5, 0.5)^T \]

<table>
<thead>
<tr>
<th>Forward primal trace</th>
<th>Reverse adjoint trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ v_0 = w_0 ]</td>
<td>[ \nabla v_3 \mathcal{L} = \nabla v_5 \mathcal{L} \cdot (-1) = 1.55 ]</td>
</tr>
<tr>
<td>[ v_{-1} = w_1 ]</td>
<td>[ \nabla v_4 \mathcal{L} = \nabla v_6 \mathcal{L} \cdot (-1) = -0.64 ]</td>
</tr>
<tr>
<td>[ v_{-2} = w_2 ]</td>
<td>[ \nabla v_7 \mathcal{L} = \nabla v_7 \mathcal{L} \cdot \frac{\partial \mathcal{L}}{\partial v_7} = \nabla v_7 \mathcal{L} \cdot 2v_5 = -1.55 ]</td>
</tr>
<tr>
<td>[ v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2} = 1.25 ]</td>
<td>[ \nabla v_8 \mathcal{L} = \nabla v_8 \mathcal{L} \cdot \frac{\partial \mathcal{L}}{\partial v_8} = \nabla v_8 \mathcal{L} \cdot 2v_6 = 0.64 ]</td>
</tr>
<tr>
<td>[ v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2} = 0.75 ]</td>
<td>[ \nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 ]</td>
</tr>
<tr>
<td>[ v_3 = \sigma(v_1) = 0.78 ]</td>
<td>[ \nabla v_3 \mathcal{L} = \nabla v_5 \mathcal{L} \cdot (-1) = 1.55 ]</td>
</tr>
<tr>
<td>[ v_4 = \sigma(v_2) = 0.68 ]</td>
<td>[ \nabla v_4 \mathcal{L} = \nabla v_6 \mathcal{L} \cdot (-1) = -0.64 ]</td>
</tr>
<tr>
<td>[ v_5 = 0 - v_3 = -0.78 ]</td>
<td>[ \nabla v_7 \mathcal{L} = \nabla v_7 \mathcal{L} \cdot \frac{\partial \mathcal{L}}{\partial v_7} = \nabla v_7 \mathcal{L} \cdot 2v_5 = -1.55 ]</td>
</tr>
<tr>
<td>[ v_6 = 1 - v_4 = 0.32 ]</td>
<td>[ \nabla v_8 \mathcal{L} = \nabla v_8 \mathcal{L} \cdot \frac{\partial \mathcal{L}}{\partial v_8} = \nabla v_8 \mathcal{L} \cdot 2v_6 = 0.64 ]</td>
</tr>
<tr>
<td>[ v_7 = v_5^2 = 0.61 ]</td>
<td>[ \nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 ]</td>
</tr>
<tr>
<td>[ v_8 = v_6^2 = 0.1 ]</td>
<td>[ \nabla v_7 \mathcal{L} = \nabla v_9 \mathcal{L} \cdot \frac{\partial \mathcal{L}}{\partial v_7} = 1 \cdot 1 = 1 ]</td>
</tr>
<tr>
<td>[ v_9 = v_7 + v_8 = 0.71 ]</td>
<td>[ \nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 ]</td>
</tr>
<tr>
<td>[ \mathcal{L} = v_9 = 0.71 ]</td>
<td>[ \nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 ]</td>
</tr>
</tbody>
</table>
## Automatic Gradient Computation

### Autodiff Example: Forward and Reverse Trace (continued)

\[
\mathcal{L}(\mathbf{w}) = (-\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2
\]

at \quad \mathbf{w} = (-1, 1.5, 0.5)^T

<table>
<thead>
<tr>
<th>Forward primal trace</th>
<th>Reverse adjoint trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>(v_0 = w_0)</td>
<td>(\nabla v_1 \mathcal{L} = \nabla v_3 \mathcal{L} \cdot \sigma(v_1) \cdot (1 - \sigma(v_1)) = 0.27)</td>
</tr>
<tr>
<td>(v_{-1} = w_1)</td>
<td>(\nabla v_2 \mathcal{L} = \nabla v_4 \mathcal{L} \cdot \sigma(v_2) \cdot (1 - \sigma(v_2)) = -0.14)</td>
</tr>
<tr>
<td>(v_{-2} = w_2)</td>
<td>(\nabla v_3 \mathcal{L} = \nabla v_5 \mathcal{L} \cdot (-1) = 1.55)</td>
</tr>
<tr>
<td>(v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2})</td>
<td>(\nabla v_4 \mathcal{L} = \nabla v_6 \mathcal{L} \cdot (-1) = -0.64)</td>
</tr>
<tr>
<td>(v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2})</td>
<td>(\nabla v_5 \mathcal{L} = \nabla v_7 \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5} = \nabla v_7 \mathcal{L} \cdot 2v_5 = -1.55)</td>
</tr>
<tr>
<td>(v_3 = \sigma(v_1))</td>
<td>(\nabla v_6 \mathcal{L} = \nabla v_8 \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6} = \nabla v_8 \mathcal{L} \cdot 2v_6 = 0.64)</td>
</tr>
<tr>
<td>(v_4 = \sigma(v_2))</td>
<td>(\nabla v_7 \mathcal{L} = \nabla v_9 \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7} = 1 \cdot 1 = 1)</td>
</tr>
<tr>
<td>(v_5 = 0 - v_3)</td>
<td>(\nabla v_8 \mathcal{L} = \nabla v_9 \mathcal{L} \cdot \frac{\partial v_9}{\partial v_8} = 1 \cdot 1 = 1)</td>
</tr>
<tr>
<td>(v_6 = 1 - v_4)</td>
<td>(\nabla v_9 \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1)</td>
</tr>
<tr>
<td>(v_7 = v_5^2)</td>
<td></td>
</tr>
<tr>
<td>(v_8 = v_6^2)</td>
<td></td>
</tr>
<tr>
<td>(v_9 = v_7 + v_8)</td>
<td></td>
</tr>
<tr>
<td>(\mathcal{L} = v_9)</td>
<td></td>
</tr>
</tbody>
</table>

\(v_0 = -1\), \(v_1 = 1.5\), \(v_2 = 0.5\)
### Automatic Gradient Computation

#### Autodiff Example: Forward and Reverse Trace (continued)

The loss function is given by:

\[
\mathcal{L}(\mathbf{w}) = (-\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2
\]

At \(\mathbf{w} = (-1, 1.5, 0.5)^T\)

#### Forward primal trace

<table>
<thead>
<tr>
<th>Term</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(v_0 = w_0)</td>
<td>-1</td>
</tr>
<tr>
<td>(v_{-1} = w_1)</td>
<td>1.5</td>
</tr>
<tr>
<td>(v_{-2} = w_2)</td>
<td>0.5</td>
</tr>
<tr>
<td>(v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2})</td>
<td>1.25</td>
</tr>
<tr>
<td>(v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2})</td>
<td>0.75</td>
</tr>
<tr>
<td>(v_3 = \sigma(v_1))</td>
<td>0.78</td>
</tr>
<tr>
<td>(v_4 = \sigma(v_2))</td>
<td>0.68</td>
</tr>
<tr>
<td>(v_5 = 0 - v_3)</td>
<td>-0.78</td>
</tr>
<tr>
<td>(v_6 = 1 - v_4)</td>
<td>0.32</td>
</tr>
<tr>
<td>(v_7 = v_5^2)</td>
<td>0.61</td>
</tr>
<tr>
<td>(v_8 = v_6^2)</td>
<td>0.1</td>
</tr>
<tr>
<td>(v_9 = v_7 + v_8)</td>
<td>0.71</td>
</tr>
</tbody>
</table>

#### Reverse adjoint trace

<table>
<thead>
<tr>
<th>Term</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\nabla^{v_2} \mathcal{L} = \nabla^{v_2} \mathcal{L} + \nabla^{v_1} \mathcal{L} \cdot 1.5)</td>
<td>0.54</td>
</tr>
<tr>
<td>(\nabla^{v_1} \mathcal{L} = \nabla^{v_1} \mathcal{L} + \nabla^{v_1} \mathcal{L})</td>
<td>0.06</td>
</tr>
<tr>
<td>(\nabla^{v_0} \mathcal{L} = \nabla^{v_0} \mathcal{L} + \nabla^{v_1} \mathcal{L})</td>
<td>0.13</td>
</tr>
<tr>
<td>(\nabla^{v_2} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot (-1))</td>
<td>0.14</td>
</tr>
<tr>
<td>(\nabla^{v_1} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot 1.5)</td>
<td>-0.28</td>
</tr>
<tr>
<td>(\nabla^{v_0} \mathcal{L} = \nabla^{v_2} \mathcal{L})</td>
<td>-0.14</td>
</tr>
<tr>
<td>(\nabla^{v_1} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot \sigma(v_1) \cdot (1 - \sigma(v_1)))</td>
<td>0.27</td>
</tr>
<tr>
<td>(\nabla^{v_2} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot \sigma(v_2) \cdot (1 - \sigma(v_2)))</td>
<td>-0.14</td>
</tr>
<tr>
<td>(\nabla^{v_0} \mathcal{L} = \nabla^{v_5} \mathcal{L} \cdot (-1))</td>
<td>1.55</td>
</tr>
<tr>
<td>(\nabla^{v_1} \mathcal{L} = \nabla^{v_6} \mathcal{L} \cdot (-1))</td>
<td>-0.64</td>
</tr>
<tr>
<td>(\nabla^{v_5} \mathcal{L} = \nabla^{v_7} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5})</td>
<td>-1.55</td>
</tr>
<tr>
<td>(\nabla^{v_6} \mathcal{L} = \nabla^{v_8} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6})</td>
<td>0.64</td>
</tr>
<tr>
<td>(\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_9}{\partial v_7})</td>
<td>1</td>
</tr>
<tr>
<td>(\nabla^{v_8} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_9})</td>
<td>1</td>
</tr>
<tr>
<td>(\nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_9})</td>
<td>1</td>
</tr>
</tbody>
</table>

\(\mathcal{L} = v_9\)  \(= 0.71\)
**Automatic Gradient Computation**

**Autodiff Example: Forward and Reverse Trace** (continued)

\[
\mathcal{L}(\mathbf{w}) = (-\sigma(w_0 + w_1 + 1.5w_2))^2 + (1 - \sigma(w_0 + 1.5w_1 - w_2))^2
\]

at \( \mathbf{w} = (-1, 1.5, 0.5)^T \)

<table>
<thead>
<tr>
<th>Forward primal trace</th>
<th>Reverse adjoint trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>( v_0 = w_0 )</td>
<td>( \nabla^{w_0} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial w_0} = \nabla^{v_0} \mathcal{L} = 0.13 )</td>
</tr>
<tr>
<td>( v_{-1} = w_1 )</td>
<td>( \nabla^{w_1} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial w_1} = \nabla^{v_{-1}} \mathcal{L} = 0.06 )</td>
</tr>
<tr>
<td>( v_{-2} = w_2 )</td>
<td>( \nabla^{w_2} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial w_2} = \nabla^{v_{-2}} \mathcal{L} = 0.54 )</td>
</tr>
<tr>
<td>( v_1 = v_0 + v_{-1} + 1.5 \cdot v_{-2} )</td>
<td>( \nabla^{v_{-2}} \mathcal{L} = \nabla^{v_{-2}} \mathcal{L} + \nabla^{v_1} \mathcal{L} \cdot 1.5 = 0.54 )</td>
</tr>
<tr>
<td>( v_2 = v_0 + 1.5 \cdot v_{-1} - v_{-2} )</td>
<td>( \nabla^{v_{-1}} \mathcal{L} = \nabla^{v_2} \mathcal{L} \cdot (-1) = 0.14 )</td>
</tr>
<tr>
<td>( v_3 = \sigma(v_1) )</td>
<td>( \nabla^{v_3} \mathcal{L} = \nabla^{v_3} \mathcal{L} \cdot \sigma(v_1) = 0.78 )</td>
</tr>
<tr>
<td>( v_4 = \sigma(v_2) )</td>
<td>( \nabla^{v_4} \mathcal{L} = \nabla^{v_4} \mathcal{L} \cdot \sigma(v_2) = 0.68 )</td>
</tr>
<tr>
<td>( v_5 = 0 - v_3 )</td>
<td>( \nabla^{v_5} \mathcal{L} = \nabla^{v_5} \mathcal{L} \cdot (-1) = 0.32 )</td>
</tr>
<tr>
<td>( v_6 = 1 - v_4 )</td>
<td>( \nabla^{v_6} \mathcal{L} = \nabla^{v_6} \mathcal{L} \cdot (-1) = 0.61 )</td>
</tr>
<tr>
<td>( v_7 = v_5^2 )</td>
<td>( \nabla^{v_5} \mathcal{L} = \nabla^{v_7} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_5} = 0.1 )</td>
</tr>
<tr>
<td>( v_8 = v_6^2 )</td>
<td>( \nabla^{v_6} \mathcal{L} = \nabla^{v_8} \mathcal{L} \cdot \frac{\partial v_8}{\partial v_6} = 1.1 )</td>
</tr>
<tr>
<td>( v_9 = v_7 + v_8 )</td>
<td>( \nabla^{v_7} \mathcal{L} = \nabla^{v_9} \mathcal{L} \cdot \frac{\partial v_7}{\partial v_9} = 1.1 )</td>
</tr>
<tr>
<td>( \mathcal{L} = v_9 )</td>
<td>( \nabla^{v_9} \mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_9} = 1 )</td>
</tr>
</tbody>
</table>
Remarks:

- For brevity, in the example, we assumed that the derivative $\frac{\partial}{\partial z} \sigma(z) = \sigma(z) \cdot (1 - \sigma(z))$ is already known. We could also have decomposed $\sigma(z) = \frac{1}{1 + \exp(-z)}$ into e.g., $v_1 = -z$, $v_2 = \exp(v_1)$, $v_3 = 1 + v_2$, $v_4 = \frac{1}{v_3}$. In this case, only the four atomic derivatives would need to be known.

- The function to be automatically differentiated need not have a closed-form representation; it only has to be composed of computable and differentiable atomic steps. Thus, AD can also compute derivatives for various algorithms that may take different branches depending on the input.
Automatic Gradient Computation
Reverse-mode Autodiff Algorithm for Scalar-valued Functions

Algorithm: autodiff
Reverse-mode automatic differentiation

Input:
\[ f : \mathbb{R}^p \to \mathbb{R} \]
Function to differentiate.
\[(w_1, \ldots, w_p)^T\]
Point at which the gradient should be evaluated

Output:
\[(\bar{w}_1, \ldots, \bar{w}_p)^T\]
Gradient of \(f\) at the point \((w_1, \ldots, w_p)^T\).

1. \(\bar{w}_i = 0\) for \(i\) in \(1 \ldots p\) \hspace{1cm} \// \text{initialize gradients}
2. \(v_1, \ldots, v_k = \text{operands}(f)\)
3. \(\frac{\partial f}{\partial v_1}, \ldots, \frac{\partial f}{\partial v_k} = \text{gradients}(f)\) \hspace{1cm} \// \text{gradient of } f \text{ wrt. its immediate operands}
4. FOREACH \(j = 1, \ldots, k\) DO
5. IF \(v_j \in \{w_1, \ldots, w_p\}\) THEN
6. \(\bar{v}_j += \frac{\partial f}{\partial v_j}\)
7. ELSE
8. \((\bar{w}_1, \ldots, \bar{w}_p)^T += \frac{\partial f}{\partial v_j} \cdot \text{autodiff}(v_j, (w_1, \ldots, w_p)^T)\)
9. RETURN \((\bar{w}_1, \ldots, \bar{w}_p)^T\)
Remarks:

- There exists also a forward mode of automatic differentiation. One key difference is in the runtime complexity; for a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, to compute all $n \cdot m$ partial derivatives in the Jacobian matrix requires $O(n)$ iterations in forward mode and $O(m)$ iterations in reverse mode. Reverse mode is usually preferred in machine learning, where we typically have $m = 1$ (a scalar loss), and $n$ arbitrarily large (e.g., billions of parameters of a deep neural network).

See also [Baydin et al., 2018].