Google Research

Automatic differentiation

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Gradient-based learning

- Gradient-based training algorithms are the workhorse of modern machine learning.
- Deriving gradients by hand is tedious and error prone.
- This becomes quickly infeasible for complex models.
- Changes to the model require rederiving the gradient.
- Deep learning = GPU + data + autodiff

Automatic differentiation

- Evaluates the derivatives of a function at a given point.
- Not the same as numerical differentiation.
- Not the same as symbolic differentiation, which returns a "human-readable" expression.
- In a neural network context, reverse autodiff is often known as backpropagation.

Automatic differentiation

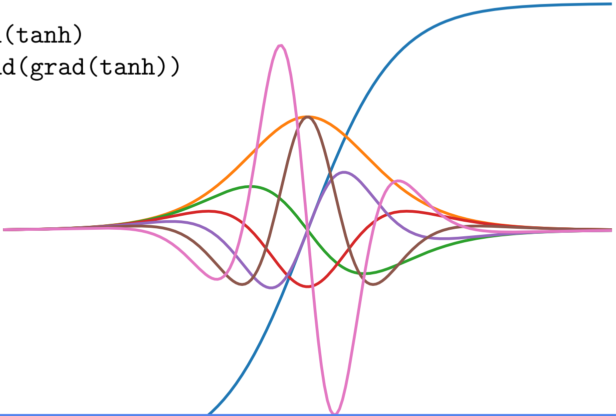
- A program is defined as the composition of primitive operations that we know how to derive.
- The user can focus on the forward computation / model.

```
import jax.numpy as jnp
from jax import grad, jit

def predict(params, inputs):
  for W, b in params:
    outputs = jnp.dot(inputs, W) + b
    inputs = jnp.tanh(outputs)
  return outputs

def logprob_fun(params, inputs, targets):
  preds = predict(params, inputs)
  return jnp.sum((preds - targets)**2)

grad_fun = jit(grad(logprob_fun))
```

Automatic differentiation

- Modern frameworks support higher-order derivatives

```
def tanh(x):
  y = jnp.exp(-2.0 * x)
  return (1.0 - y) / (1.0 + y)

fp = grad(tanh)
fpp = grad(grad(tanh))
...
```



Outline

1. **Numerical differentiation**
2. Chain compositions
3. Computational graphs
4. Implementation
5. Advanced topics
6. Conclusion

Derivatives

- Definition of derivative of $g \colon \mathbb{R} \to \mathbb{R}$

$$g'(a) = \frac{\partial g(a)}{\partial a} = \lim_{h \to 0} \frac{g(a+h) - g(a)}{h}$$

- $g'(a)$ is called Lagrange notation.
- $\frac{\partial g(a)}{\partial a}$ is called Leibniz notation.
- Interpretations: instantaneous rate of change of g, slope of the tangent of g at a.

Gradient

- The gradient of $f\colon \mathbb{R}^n \to \mathbb{R}$ is

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^n$$

  i.e., a vector that gathers the partial derivatives of f.

- Applying the definition of derivative coordinate-wise:

$$[\nabla f(\mathbf{x})]_j = \frac{\partial f}{\partial x_j}(\mathbf{x}) = \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{e}_j) - f(\mathbf{x})}{h} \quad j \in \{1, \ldots, n\}$$

  where $\mathbf{e}_j = [0, 0, \ldots, 0, \underbrace{1}_{j}, 0, \ldots, 0]^\top \in \{0, 1\}^n$ is the j^{th} standard basis vector.

Numerical gradient

- Finite difference:

$$[\nabla f(\mathbf{x})]_j = \frac{\partial f}{\partial x_j}(\mathbf{x}) \approx \frac{f(\mathbf{x} + \varepsilon \mathbf{e}_j) - f(\mathbf{x})}{\varepsilon} \quad j \in \{1, \ldots, n\}$$

  where ε is a small value (e.g., 10^{-6}).

- Central finite difference:

$$[\nabla f(\mathbf{x})]_j = \frac{\partial f}{\partial x_j}(\mathbf{x}) \approx \frac{f(\mathbf{x} + \varepsilon \mathbf{e}_j) - f(\mathbf{x} - \varepsilon \mathbf{e}_j)}{2\varepsilon} \quad j \in \{1, \ldots, n\}$$

- Computing $\nabla f(\mathbf{x})$ approximately by (central) finite difference is $n+1$ times ($2n$ times) as costly as evaluating f.

Directional derivative

- Derivative of $f\colon \mathbb{R}^n \to \mathbb{R}$ in the direction of $\mathbf{v} \in \mathbb{R}^n$

$$D_{\mathbf{v}} f(\mathbf{x}) = \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{v}) - f(\mathbf{x})}{h} \in \mathbb{R}$$

- Interpretation: rate of change of f in the direction of $\mathbf{v}$, when moving away from $\mathbf{x}$.

- $[\nabla f(\mathbf{x})]_i$ is the derivative in the direction of $\mathbf{e}_i$.

- Finite difference (and similarly for the central finite difference):

$$D_{\mathbf{v}} f(\mathbf{x}) \approx \frac{f(\mathbf{x} + \varepsilon\mathbf{v}) - f(\mathbf{x})}{\varepsilon}$$

Only 2 calls to f are needed, i.e., independent of n.

Directional derivative

- **Fact.** The directional derivative is equal to the scalar product between the gradient and $\mathbf{v}$, i.e.,

$$D_{\mathbf{v}} f(\mathbf{x}) = \nabla f(\mathbf{x}) \cdot \mathbf{v}$$

- **Proof.** Let $g(t) = f(\mathbf{x} + t\mathbf{v})$. We have

$$g'(t) = \lim_{h \to 0} \frac{f(\mathbf{x} + (t+h)\mathbf{v}) - f(\mathbf{x} + t\mathbf{v})}{h}$$

and therefore $g'(0) = D_{\mathbf{v}}(\mathbf{x})$. By the chain rule, we also have

$$g'(t) = \nabla f(\mathbf{x} + t\mathbf{v}) \cdot \mathbf{v}.$$

Hence, $g'(0) = D_{\mathbf{v}}(\mathbf{x}) = \nabla f(\mathbf{x}) \cdot \mathbf{v}$.

Jacobian

- The Jacobian of $\mathbf{f} \colon \mathbb{R}^n \to \mathbb{R}^m$

$$J_{\mathbf{f}}(\mathbf{x}) = \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

$$= \left[\frac{\partial \mathbf{f}}{\partial x_1}, \ldots, \frac{\partial \mathbf{f}}{\partial x_n} \right]$$

$$= \begin{bmatrix} \nabla f_1(\mathbf{x})^\top \\ \vdots \\ \nabla f_m(\mathbf{x})^\top \end{bmatrix}$$

- The size of the Jacobian matrix is $m \times n$.
- The gradient's transpose is thus a "wide" Jacobian ($m = 1$).

Jacobian vector product ("JVP")

- Right-multiply the Jacobian with a vector $\mathbf{v} \in \mathbb{R}^n$

$$
\begin{aligned}
J_{\mathbf{f}}(\mathbf{x})\mathbf{v} &= \begin{bmatrix} \nabla f_1(\mathbf{x})^\top \\ \vdots \\ \nabla f_m(\mathbf{x})^\top \end{bmatrix} \mathbf{v} \\
&= \begin{bmatrix} \nabla f_1(\mathbf{x}) \cdot \mathbf{v} \\ \vdots \\ \nabla f_m(\mathbf{x}) \cdot \mathbf{v} \end{bmatrix} \\
&= \lim_{h \to 0} \frac{\mathbf{f}(\mathbf{x} + h\mathbf{v}) - \mathbf{f}(\mathbf{x} + h\mathbf{v})}{h}
\end{aligned}
$$

- Finite difference (and similarly for the central finite difference):

$$
J_{\mathbf{f}}(\mathbf{x})\mathbf{v} \approx \frac{\mathbf{f}(\mathbf{x} + \varepsilon\mathbf{v}) - \mathbf{f}(\mathbf{x})}{\varepsilon}
$$

- Computing the JVP approximately by (central) finite difference requires only 2 calls to $\mathbf{f}$.

Vector Jacobian Product ("VJP")

- Left-multiply the Jacobian with a vector $\mathbf{u} \in \mathbb{R}^m$

$$\mathbf{u}^\top J_{\mathbf{f}}(\mathbf{x}) = \mathbf{u}^\top \left[\frac{\partial \mathbf{f}}{\partial x_1}, \ldots, \frac{\partial \mathbf{f}}{\partial x_n}\right] = \left[\mathbf{u} \cdot \frac{\partial \mathbf{f}}{\partial x_1}, \ldots, \mathbf{u} \cdot \frac{\partial \mathbf{f}}{\partial x_n}\right]$$

- Finite difference (and similarly for the central finite difference):

$$\frac{\partial \mathbf{f}}{\partial x_i} \approx \frac{\mathbf{f}(\mathbf{x} + \varepsilon \mathbf{e}_i) - \mathbf{f}(\mathbf{x})}{\varepsilon}$$

- Computing the VJP approximately by (central) finite difference requires $n+1$ calls ($2n$ calls) to $\mathbf{f}$.

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2 **Chain compositions**

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Chain rule

- Let $F(x) = f(g(x)) = f \circ g(x)$, where $f, g\colon \mathbb{R} \to \mathbb{R}$. Then,

$$F'(x) = f'(g(x))g'(x)$$

- Alternatively, let $y = g(x)$ and $z = f(y)$, then

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial z}{\partial y}\Big|_{y=g(x)} \frac{\partial y}{\partial x}\Big|_{x=x}$$

- Let $f(\mathbf{x}) = h(\mathbf{g}(\mathbf{x}))$, where $\mathbf{g}\colon \mathbb{R}^n \to \mathbb{R}^d$ and $h\colon \mathbb{R}^d \to \mathbb{R}$. Then,

$$\underbrace{\nabla f(\mathbf{x})}_{n\times 1} = (\underbrace{\nabla h(\mathbf{g}(\mathbf{x}))^\top}_{1\times d} \underbrace{J_{\mathbf{g}}(\mathbf{x})}_{d\times n})^\top = \underbrace{J_{\mathbf{g}}(\mathbf{x})^\top}_{n\times d} \underbrace{\nabla h(\mathbf{g}(\mathbf{x}))}_{d\times 1}$$

- and similarly using Leibniz notation

Chain compositions

$$\mathbf{x} = \mathbf{x}_1 \rightarrow \mathbf{f}_1 \rightarrow \mathbf{f}_2 \rightarrow \mathbf{f}_3 \rightarrow \mathbf{f}_4 \rightarrow \mathbf{o}$$

- Assume $\mathbf{f} \colon \mathbb{R}^n \rightarrow \mathbb{R}^m$ decomposes as follows:

$$\begin{aligned} \mathbf{o} &= \mathbf{f}(\mathbf{x}) \\ &= \mathbf{f}_4 \circ \mathbf{f}_3 \circ \mathbf{f}_2 \circ \mathbf{f}_1(\mathbf{x}) \\ &= \mathbf{f}_4(\mathbf{f}_3(\mathbf{f}_2(\mathbf{f}_1(\mathbf{x})))) \end{aligned}$$

  where $\mathbf{f}_1 : \mathbb{R}^n \rightarrow \mathbb{R}^{m_1}$, $\mathbf{f}_2 : \mathbb{R}^{m_1} \rightarrow \mathbb{R}^{m_2}$, ..., $\mathbf{f}_4 : \mathbb{R}^{m_3} \rightarrow \mathbb{R}^m$.

- How to compute the Jacobian $J_\mathbf{f}(\mathbf{x}) = \frac{\partial \mathbf{o}}{\partial \mathbf{x}} \in \mathbb{R}^{m \times n}$ efficiently?

Chain rule

$$\mathbf{x} = \mathbf{x}_1 \longrightarrow \boxed{\mathbf{f}_1} \xrightarrow[\mathbf{x}_2]{} \boxed{\mathbf{f}_2} \xrightarrow[\mathbf{x}_3]{} \boxed{\mathbf{f}_3} \xrightarrow[\mathbf{x}_4]{} \boxed{\mathbf{f}_4} \longrightarrow \mathbf{o}$$

- Sequence of operations

$$\begin{aligned}
\mathbf{x}_1 &= \mathbf{x} \\
\mathbf{x}_2 &= \mathbf{f}_1(\mathbf{x}_1) \\
\mathbf{x}_3 &= \mathbf{f}_2(\mathbf{x}_2) \\
\mathbf{x}_4 &= \mathbf{f}_3(\mathbf{x}_3) \\
\mathbf{o} &= \mathbf{f}_4(\mathbf{x}_4)
\end{aligned}$$

- By the chain rule, we have

$$\begin{aligned}
\frac{\partial \mathbf{o}}{\partial \mathbf{x}} &= \frac{\partial \mathbf{o}}{\partial \mathbf{x}_4} \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3} \frac{\partial \mathbf{x}_3}{\partial \mathbf{x}_2} \frac{\partial \mathbf{x}_2}{\partial \mathbf{x}} \\
&= \frac{\partial \mathbf{f}_4(\mathbf{x}_3)}{\partial \mathbf{x}_3} \frac{\partial \mathbf{f}_3(\mathbf{x}_2)}{\partial \mathbf{x}_2} \frac{\partial \mathbf{f}_2(\mathbf{x}_1)}{\partial \mathbf{x}_1} \frac{\partial \mathbf{f}_1(\mathbf{x})}{\partial \mathbf{x}} \\
&= J_{\mathbf{f}_4}(\mathbf{x}_4) J_{\mathbf{f}_3}(\mathbf{x}_3) J_{\mathbf{f}_2}(\mathbf{x}_2) J_{\mathbf{f}_1}(\mathbf{x})
\end{aligned}$$

Forward differentiation

- Recall that $\frac{\partial \mathbf{f}}{\partial x_j} \in \mathbb{R}^m$ is the j^{th} column of $J_{\mathbf{f}}(\mathbf{x})$.
- Jacobian vector product (JVP) with $\mathbf{e}_j \in \mathbb{R}^n$ "reveals" the j^{th} column

$$
\begin{aligned}
J_{\mathbf{f}}(\mathbf{x})\mathbf{e}_1 &= \frac{\partial \mathbf{f}}{\partial x_1} \\
J_{\mathbf{f}}(\mathbf{x})\mathbf{e}_2 &= \frac{\partial \mathbf{f}}{\partial x_2} \\
&\vdots \\
J_{\mathbf{f}}(\mathbf{x})\mathbf{e}_n &= \frac{\partial \mathbf{f}}{\partial x_n}
\end{aligned}
$$

- Computing a gradient ($m = 1$) requires n JVPs with $\mathbf{e}_1, \ldots, \mathbf{e}_n$.

Forward differentiation

- Jacobian-vector product with $\mathbf{v} \in \mathbb{R}^n$

$$J_{\mathbf{f}}(\mathbf{x})\mathbf{v} = \underbrace{J_{\mathbf{f}_4}(\mathbf{x}_4)}_{m \times m_3} \underbrace{J_{\mathbf{f}_3}(\mathbf{x}_3)}_{m_3 \times m_2} \underbrace{J_{\mathbf{f}_2}(\mathbf{x}_2)}_{m_2 \times m_1} \underbrace{J_{\mathbf{f}_1}(\mathbf{x})}_{m_1 \times n} \mathbf{v}$$

  Multiplication from right to left is more efficient.

- Cost of computing n JVPs:

$$n(mm_3 + m_3m_2 + m_2m_1 + m_1n)$$

- Cost of computing a gradient ($m = 1$, $m_3 = m_2 = m_1 = n$):

$$O(n^3)$$

Forward differentiation

- $\mathbf{o} = \mathbf{f}(\mathbf{x}) = \mathbf{f}_K \circ \cdots \circ \mathbf{f}_2 \circ \mathbf{f}_1(\mathbf{x})$
- $[J_\mathbf{f}(\mathbf{x})]_{:,j} = J_{\mathbf{f}_K}(\mathbf{x}_K) \dots J_{\mathbf{f}_2}(\mathbf{x}_2) J_{\mathbf{f}_1}(\mathbf{x})\mathbf{e}_j \qquad j \in \{1, \dots, n\}$

Algorithm 1 Compute $\mathbf{o} = \mathbf{f}(\mathbf{x})$ and $J_\mathbf{f}(\mathbf{x})$ alongside

1: **Input:** $\mathbf{x} \in \mathbb{R}^n$
2: $\mathbf{x}_1 \leftarrow \mathbf{x}$
3: $\mathbf{v}_j \leftarrow \mathbf{e}_j \in \mathbb{R}^n \quad j \in \{1, \dots, n\}$
4: **for** $k = 1$ to K **do**
5: $\quad \mathbf{x}_{k+1} \leftarrow \mathbf{f}_k(\mathbf{x}_k)$
6: $\quad \mathbf{v}_j \leftarrow J_{\mathbf{f}_k}(\mathbf{x}_k)\mathbf{v}_j \quad j \in \{1, \dots, n\}$
7: **end for**
8: **Returns:** $\mathbf{o} = \mathbf{x}_{K+1}$, $[J_\mathbf{f}(\mathbf{x})]_{:,j} = \mathbf{v}_j \quad j \in \{1, \dots, n\}$

Backward differentiation

- Recall that $\nabla f_i(\mathbf{x})^\top \in \mathbb{R}^n$ is the i^{th} row of $J_\mathbf{f}(\mathbf{x})$.
- Vector Jacobian product (VJP) with $\mathbf{e}_i \in \mathbb{R}^m$ "reveals" the i^{th} row

$$\begin{aligned}
\mathbf{e}_1^\top J_\mathbf{f}(\mathbf{x}) &= \nabla f_1(\mathbf{x})^\top \\
\mathbf{e}_2^\top J_\mathbf{f}(\mathbf{x}) &= \nabla f_2(\mathbf{x})^\top \\
&\vdots \\
\mathbf{e}_m^\top J_\mathbf{f}(\mathbf{x}) &= \nabla f_m(\mathbf{x})^\top
\end{aligned}$$

- Computing a gradient ($m = 1$) requires only 1 VJP with $\mathbf{e}_1 \in \mathbb{R}^1$.

Backward differentiation

- Vector Jacobian product with $\mathbf{u} \in \mathbb{R}^m$

$$\mathbf{u}^\top \underbrace{J_{\mathbf{f}_4}(\mathbf{x}_4)}_{m \times m_3} \underbrace{J_{\mathbf{f}_3}(\mathbf{x}_3)}_{m_3 \times m_2} \underbrace{J_{\mathbf{f}_2}(\mathbf{x}_2)}_{m_2 \times m_1} \underbrace{J_{\mathbf{f}_1}(\mathbf{x})}_{m_1 \times n}$$

  Multiplication from left to right is more efficient.

- Cost of computing m VJPs:

$$m(mm_3 + m_3 m_2 + m_2 m_1 + m_1 n)$$

- Cost of computing a gradient ($m = 1$, $m_3 = m_2 = m_1 = n$):

$$O(n^2)$$

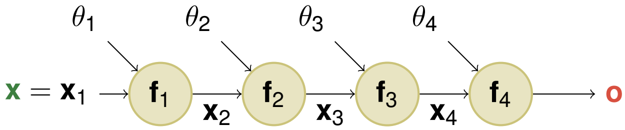
Backward differentiation

- $\mathbf{o} = \mathbf{f}(\mathbf{x}) = \mathbf{f}_K \circ \cdots \circ \mathbf{f}_2 \circ \mathbf{f}_1(\mathbf{x})$
- $[J_{\mathbf{f}}(\mathbf{x})]_{i,:} = \mathbf{e}_i^\top J_{\mathbf{f}_K}(\mathbf{x}_K) \ldots J_{\mathbf{f}_2}(\mathbf{x}_2) J_{\mathbf{f}_1}(\mathbf{x}) \qquad i \in \{1, \ldots, m\}$

Algorithm 2 Compute $\mathbf{o} = \mathbf{f}(\mathbf{x})$ and $J_{\mathbf{f}}(\mathbf{x})$

Input: $\mathbf{x} \in \mathbb{R}^n$
$\mathbf{x}_1 \leftarrow \mathbf{x}$, $\mathbf{u}_i \leftarrow \mathbf{e}_i \in \mathbb{R}^m \quad i \in \{1, \ldots, m\}$
for $k = 1$ to K **do**
    $\mathbf{x}_{k+1} \leftarrow \mathbf{f}_k(\mathbf{x}_k)$
end for
for $k = K$ to 1 **do**
    $\mathbf{u}_i \leftarrow \mathbf{u}_i^\top J_{\mathbf{f}_k}(\mathbf{x}_k) \quad i \in \{1, \ldots, m\}$
end for
Returns: $\mathbf{o} = \mathbf{x}_{K+1}$, $[J_{\mathbf{f}}(\mathbf{x})]_{i,:} = \mathbf{u}_i \quad i \in \{1, \ldots, m\}$

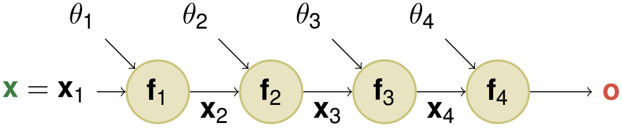
Feedforward networks



- Each function can now have two arguments: $\mathbf{f}_k(\mathbf{x}_k, \theta_k)$, where $\mathbf{x}_k$ is the previous output and θ_k are learnable parameters.
- Example one hidden layer, one output layer, squared loss

$$
\begin{aligned}
\mathbf{f} &= \mathbf{f}_4 \circ \cdots \circ \mathbf{f}_1 \\
\mathbf{x}_2 &= \mathbf{f}_1(\mathbf{x}, W_1) = W_1 \mathbf{x} && W_1 \in \mathbb{R}^{m_1 \times n} \\
\mathbf{x}_3 &= \mathbf{f}_2(\mathbf{x}_2, \emptyset) = \mathrm{relu}(\mathbf{x}_2) \\
\mathbf{x}_4 &= \mathbf{f}_3(\mathbf{x}_3, W_3) = W_3 \mathbf{x}_3 && W_3 \in \mathbb{R}^{1 \times m_3} \\
\mathbf{o} &= \mathbf{f}_4(\mathbf{x}_4, \mathbf{y}) = \frac{1}{2} \|\mathbf{x}_4 - \mathbf{y}\|^2
\end{aligned}
$$

Feedforward network example



- Applying the chain rule once again we have

$$
\begin{aligned}
&\frac{\partial \mathbf{o}}{\partial \theta_4} \\
&\frac{\partial \mathbf{o}}{\partial \theta_3} = \frac{\partial \mathbf{o}}{\partial \mathbf{x}_4} \frac{\partial \mathbf{x}_4}{\partial \theta_3} \\
&\frac{\partial \mathbf{o}}{\partial \theta_2} = \frac{\partial \mathbf{o}}{\partial \mathbf{x}_4} \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3} \frac{\partial \mathbf{x}_3}{\partial \theta_2} \\
&\vdots
\end{aligned}
$$

- Apart from the last multiplication, the Jacobians $\frac{\partial \mathbf{o}}{\partial \mathbf{x}_k}$ and $\frac{\partial \mathbf{o}}{\partial \theta_k}$ share the same computations!

Backprop for feedforward networks

Algorithm 3 Compute $\mathbf{o} = \mathbf{f}(\mathbf{x}, \theta_1, \dots, \theta_K)$ and its Jacobians.

Input: $\mathbf{x} \in \mathbb{R}^n, \theta_1, \dots, \theta_K$
$\mathbf{x}_1 \leftarrow \mathbf{x}$
$\mathbf{u}_i \leftarrow \mathbf{e}_i \in \mathbb{R}^m \quad i \in \{1, \dots, m\}$
for $k = 1$ to K **do**
    $\mathbf{x}_{k+1} \leftarrow \mathbf{f}_k(\mathbf{x}_k, \theta_k)$
end for
for $k = K$ to 1 **do**
    $\mathbf{j}_{i,k} \leftarrow \mathbf{u}_i^\top \frac{\partial \mathbf{f}_k(\mathbf{x}_k, \theta_k)}{\partial \theta_k} \quad i \in \{1, \dots, m\}$
    $\mathbf{u}_i \leftarrow \mathbf{u}_i^\top \frac{\partial \mathbf{f}_k(\mathbf{x}_k, \theta_k)}{\partial \mathbf{x}_k} \quad i \in \{1, \dots, m\}$
end for
Returns: $\mathbf{o} = \mathbf{x}_{K+1}, \left[\frac{\partial \mathbf{o}}{\partial \mathbf{x}}\right]_{i,:} = \mathbf{u}_i, \left[\frac{\partial \mathbf{o}}{\partial \theta_k}\right]_{i,:} = \mathbf{j}_{i,k} \quad i \in \{1, \dots, m\}, k \in \{1, \dots, K\}$

Examples of VJPs

Let $W \in \mathbb{R}^{a \times b}$, $u \in \mathbb{R}^a$, $x \in \mathbb{R}^b$.

- $\mathbf{f}(x) = g(x)$ (element-wise)
  - $\mathbf{f}$ maps $\mathbb{R}^b$ to $\mathbb{R}^b$
  - $J_\mathbf{f}(x) = J_\mathbf{f}(x)^\top = \operatorname{diag}(g'(x))$ maps $\mathbb{R}^b$ to $\mathbb{R}^b$, i.e., $b \times b$ matrix
  - $u^\top J_\mathbf{f}(x) = J_\mathbf{f}(x)^\top u = u * g'(x) \in \mathbb{R}^b$, where $*$ means element-wise multiplication
- $\mathbf{f}(x) = Wx$
  - $\mathbf{f}$ maps $\mathbb{R}^b$ to $\mathbb{R}^a$
  - $J_\mathbf{f}(x) = W$ maps $\mathbb{R}^b$ to $\mathbb{R}^a$, i.e., $a \times b$ matrix
  - $J_\mathbf{f}(x)^\top = W^\top$ maps $\mathbb{R}^a$ to $\mathbb{R}^b$, i.e., $b \times a$ matrix
  - $u^\top J_\mathbf{f}(x) = J_\mathbf{f}(x)^\top u = W^\top u \in \mathbb{R}^b$

Examples of VJPs

- $\mathbf{f}(W) = Wx$
  - $\mathbf{f}$ maps $\mathbb{R}^{a \times b}$ to $\mathbb{R}^a$
  - $J_{\mathbf{f}}(W)$ maps $\mathbb{R}^{a \times b}$ to $\mathbb{R}^a$, i.e., $a \times (a \times b)$ matrix
  - $J_{\mathbf{f}}(W)^\top$ maps $\mathbb{R}^a$ to $\mathbb{R}^{a \times b}$, i.e., $(a \times b) \times a$ matrix
  - $J_{\mathbf{f}}(W)^\top u = ux^\top$

VJPs make things easier when dealing with matrix or tensor inputs.

Summary: Forward vs. Backward

- Forward
  - Uses Jacobian vector products (JVPs)
  - Each JVP call builds one column of the Jacobian
  - Efficient for tall Jacobians ($m \geq n$)
  - Need not store intermediate computations
- Backward
  - Uses vector Jacobian products (VJPs)
  - Each VJP call builds one row of the Jacobian
  - Efficient for wide matrices ($m \leq n$)
  - Needs to store intermediate computations

Machine learning use case

- Most objectives in machine learning can be written in the form

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) = \sum_{i=1}^{N} \ell_i(f_i(\mathbf{x}))$$

  where $f \colon \mathbb{R}^n \to \mathbb{R}^M$ and $\ell_i \colon \mathbb{R}^M \to \mathbb{R}$.

- The minimization needs to be w.r.t. a scalar valued loss.
- This corresponds to the $m = 1$ setting, for which backward differentiation is more efficient.
- This explains the immense success of reverse autodiff in machine learning.

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2 Chain compositions

3 **Computational graphs**

4 Implementation

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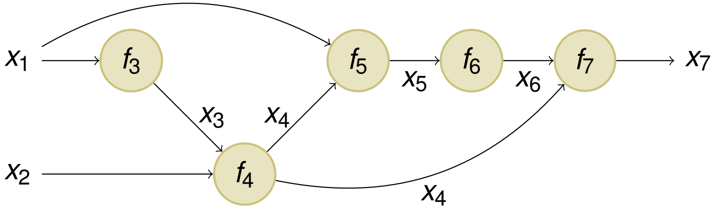
Computational graph

$$f(x_1, x_2) = x_2 e^{x_1} \sqrt{x_1 + x_2 e^{x_1}}$$

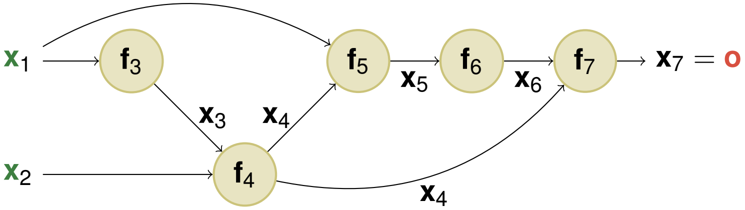
- Operations in topological order

$$\begin{aligned}
x_3 &= f_3(x_1) = e^{x_1} \\
x_4 &= f_4(x_2, x_3) = x_2 x_3 \\
x_5 &= f_5(x_1, x_4) = x_1 + x_4 \\
x_6 &= f_6(x_5) = \sqrt{x_5} \\
x_7 &= f_7(x_4, x_6) = x_4 x_6
\end{aligned}$$

- Directed acyclic graph traversal



Forward differentiation example



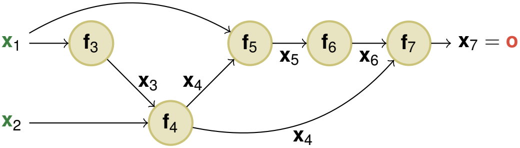
- $\mathbf{x}_4$ is influenced by $\mathbf{x}_3$ and $\mathbf{x}_2$, therefore

$$\frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_1} = \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3}\frac{\partial \mathbf{x}_3}{\partial \mathbf{x}_1} + \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_2}\frac{\partial \mathbf{x}_2}{\partial \mathbf{x}_1}$$

- $\mathbf{x}_7$ is influenced by $\mathbf{x}_4$ and $\mathbf{x}_6$, therefore

$$\frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_1} = \frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_4}\frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_1} + \frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_6}\frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_1}$$

Forward differentiation example

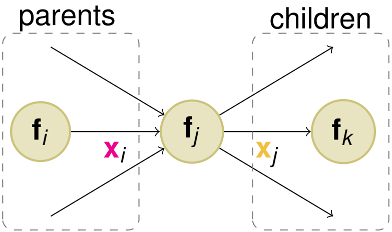


- Recurse in topological order

$$\frac{\partial \mathbf{x}_1}{\partial \mathbf{x}_1} = \mathrm{Id}_n$$
$$\frac{\partial \mathbf{x}_2}{\partial \mathbf{x}_2} = \mathrm{Id}_n$$
$$\frac{\partial \mathbf{x}_3}{\partial \mathbf{x}_1} = \frac{\partial \mathbf{x}_3}{\partial \mathbf{x}_1}\frac{\partial \mathbf{x}_1}{\partial \mathbf{x}_1}$$
$$\frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_1} = \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3}\frac{\partial \mathbf{x}_3}{\partial \mathbf{x}_1} + \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_2}\frac{\partial \mathbf{x}_2}{\partial \mathbf{x}_1}$$
$$\vdots$$

- Everything can be computed in terms of JVPs

Forward differentiation



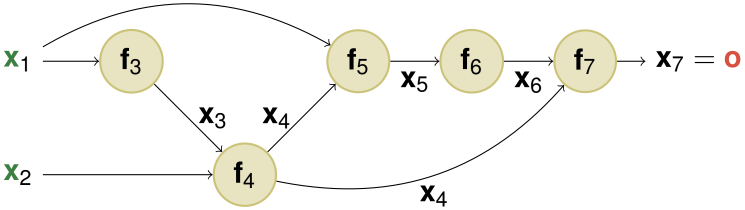
- In the general case, we have

$$\frac{\partial \mathbf{x}_j}{\partial \mathbf{x}_1} = \sum_{i \in \text{Parents}(j)} \frac{\partial \mathbf{x}_j}{\partial \mathbf{x}_i} \frac{\partial \mathbf{x}_i}{\partial \mathbf{x}_1}$$

- $\frac{\partial \mathbf{x}_j}{\partial \mathbf{x}_i}$ is easy to compute as f_j is a direct function of $\mathbf{x}_i$.

- $\frac{\partial \mathbf{x}_i}{\partial \mathbf{x}_1}$ is obtained from the previous iterations in topological order.

Backward differentiation example



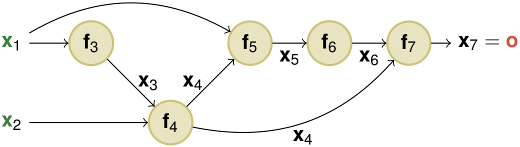
- $\mathbf{x}_5$ influences only $\mathbf{x}_6$, therefore

$$\frac{\partial \mathbf{o}}{\partial \mathbf{x}_5} = \frac{\partial \mathbf{o}}{\partial \mathbf{x}_6} \frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5}$$

- $\mathbf{x}_4$ influences $\mathbf{x}_5$ and $\mathbf{x}_7$, therefore

$$\frac{\partial \mathbf{o}}{\partial \mathbf{x}_4} = \frac{\partial \mathbf{o}}{\partial \mathbf{x}_5} \frac{\partial \mathbf{x}_5}{\partial \mathbf{x}_4} + \frac{\partial \mathbf{o}}{\partial \mathbf{x}_7} \frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_4}$$

Backward differentiation example

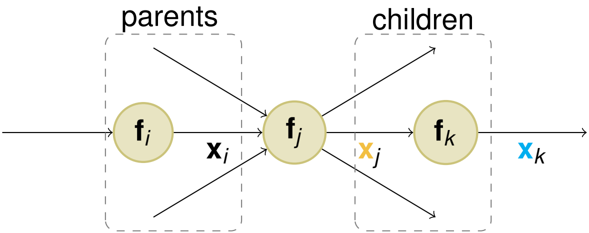


- Recurse in reverse topological order

$$
\begin{aligned}
\frac{\partial \mathbf{o}}{\partial \mathbf{x}_7} &= \frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_7} = \mathrm{Id}_m \\
\frac{\partial \mathbf{o}}{\partial \mathbf{x}_6} &= \frac{\partial \mathbf{o}}{\partial \mathbf{x}_7} \frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_6} \\
\frac{\partial \mathbf{o}}{\partial \mathbf{x}_5} &= \frac{\partial \mathbf{o}}{\partial \mathbf{x}_6} \frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5} \\
\frac{\partial \mathbf{o}}{\partial \mathbf{x}_4} &= \frac{\partial \mathbf{o}}{\partial \mathbf{x}_5} \frac{\partial \mathbf{x}_5}{\partial \mathbf{x}_4} + \frac{\partial \mathbf{o}}{\partial \mathbf{x}_7} \frac{\partial \mathbf{x}_7}{\partial \mathbf{x}_4} \\
&\vdots
\end{aligned}
$$

- Everything can be computed in terms of VJPs

Backward differentiation



- In the general case, we have

$$\frac{\partial \mathbf{o}}{\partial \mathbf{x}_j} = \sum_{k \in \text{Children}(j)} \frac{\partial \mathbf{o}}{\partial \mathbf{x}_k} \frac{\partial \mathbf{x}_k}{\partial \mathbf{x}_j}$$

- $\frac{\partial \mathbf{o}}{\partial \mathbf{x}_k}$ is obtained from previous iterations (reverse topological order) and is known as “adjoint”.
- $\frac{\partial \mathbf{x}_k}{\partial \mathbf{x}_j}$ is easy to compute as f_k is a direct function of $\mathbf{x}_j$.

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Obtaining the computational graph

- Ahead of time
  - Read from source or abstract syntax tree (AST). Ex: Tangent.
  - API for composing primitive operations (the graph is fully built before the program is evaluated). Ex: Tensorflow.
- Just in time
  - Tracing: monitor the program execution (the graph is built while the program is being executed). Ex: Tensorflow Eager, JAX, PyTorch.

```python
import jax.numpy as jnp
from jax import grad

def add(a, b):
  return a + b

a = jnp.array([1, 2, 3])
b = jnp.array([4, 5, 6])
print(grad(add)(a, b))
```

Key components of an implementation

- VJP for all primitive operations
- Node class
- Topological sort
- Forward pass
- Backward pass

We will now briefly review each component using a rudimentary implementation (mine ;-)).

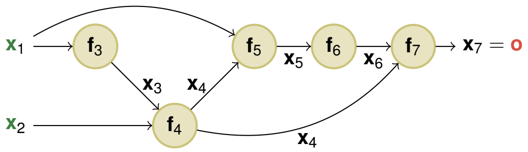
VJPs for primitive operations

```
def dot(x, W):
  return np.dot(W, x)

def dot_make_vjp(x, W):
  def vjp(u):
    return W.T.dot(u), np.outer(u, x)
  return vjp

dot.make_vjp = dot_make_vjp

def add(a, b):
  return a + b

def add_make_vjp(a, b):
  gprime = np.ones(len(a))

  def vjp(u):
    return u * gprime, u * gprime

  return vjp

add.make_vjp = add_make_vjp
```

Node class

```
class Node(object):

  def __init__(self, value=None, func=None, parents=None, name=""):
    # Value stored in the node.
    self.value = value
    # Function producing the node.
    self.func = func
    # Inputs to the function.
    self.parents = [] if parents is None else parents
    # Unique name of the node (for debugging and hashing).
    self.name = name
    # Gradient / Jacobian.
    self.grad = 0
    if not name:
      raise ValueError("Each node must have a unique name.")

  def __hash__(self):
    return hash(self.name)

  def __repr__(self):
    return "Node(%s)" % self.name
```

DAG




```python
def create_dag(x):
  x1 = Node(value=np.array([x[0]]), name="x1")
  x2 = Node(value=np.array([x[1]]), name="x2")
  x3 = Node(func=exp, parents=[x1], name="x3")
  x4 = Node(func=mul, parents=[x2, x3], name="x4")
  x5 = Node(func=add, parents=[x1, x4], name="x5")
  x6 = Node(func=sqrt, parents=[x5], name="x6")
  x7 = Node(func=mul, parents=[x4, x6], name="x7")
  return x7
```

A good implementation would support tracing, instead of building the DAG manually.

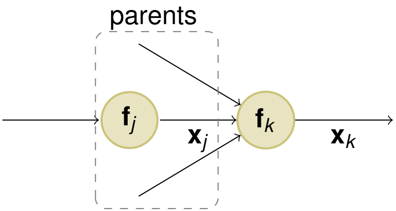
Topological sort

```
def dfs(node, visited):
  visited.add(node)
  for parent in node.parents:
    if not parent in visited:
      # Yield parent nodes first.
      yield from dfs(parent, visited)
  # And current node later.
  yield node

def topological_sort(end_node):
  visited = set()
  sorted_nodes = []

  # All non-visited nodes reachable from end_node.
  for node in dfs(end_node, visited):
    sorted_nodes.append(node)

  return sorted_nodes
```

Forward pass

```
def evaluate_dag(sorted_nodes):
  for node in sorted_nodes:
    if node.value is None:
      values = [p.value for p in node.parents]
      node.value = node.func(*values)
  return sorted_nodes[-1].value
```

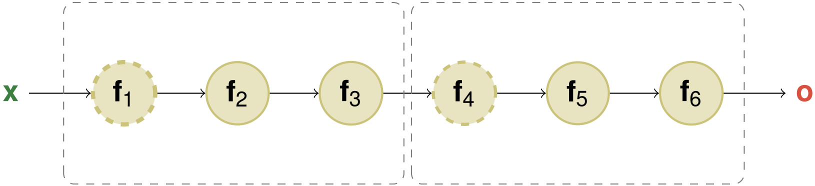
Backward pass




```
def backward_diff_dag(sorted_nodes):
  value = evaluate_dag(sorted_nodes)
  m = value.shape[0]  # Output size

  # Initialize recursion.
  sorted_nodes[-1].grad = np.eye(m)

  for node_k in reversed(sorted_nodes):
    if not node_k.parents:
      # We reached a node without parents.
      continue

    # Values of the parent nodes.
    values = [p.value for p in node_k.parents]

    # Iterate over outputs.
    for i in range(m):
      # A list of size len(values) containing the vjps.
      vjps = node_k.func.make_vjp(*values)(node_k.grad[i])

      for node_j, vjp in zip(node_k.parents, vjps):
        node_j.grad += vjp

  return sorted_nodes
```

Checkpointing

- During the forward pass, save computations at intermediate locations only (checkpoints).
- During the backward pass, recompute other locations on the fly, starting from the checkpoints.
- Tradeoff between memory and computation time.



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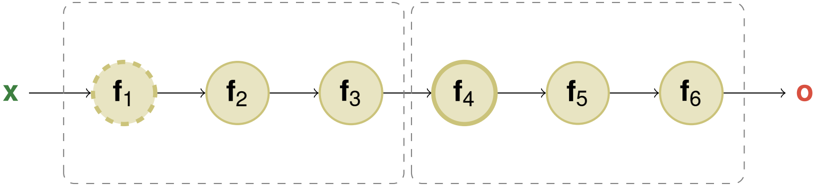

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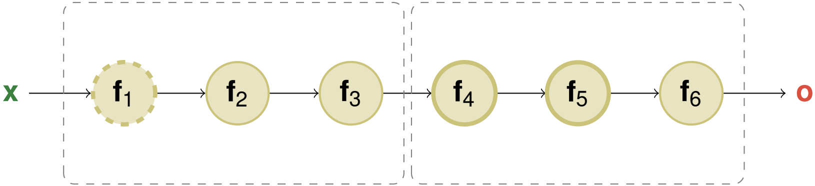

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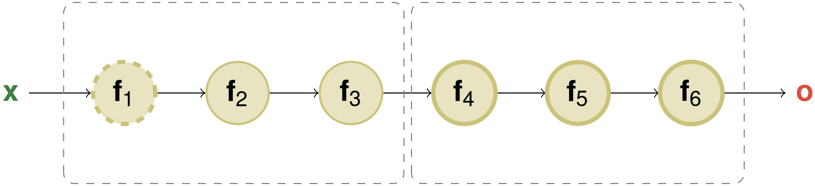

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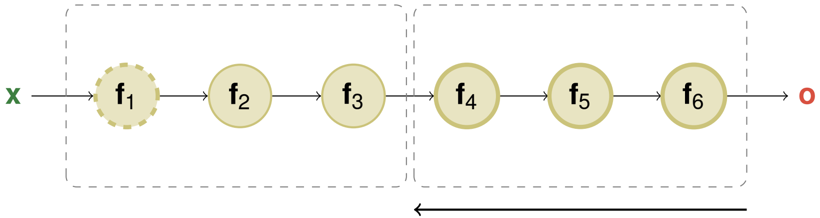

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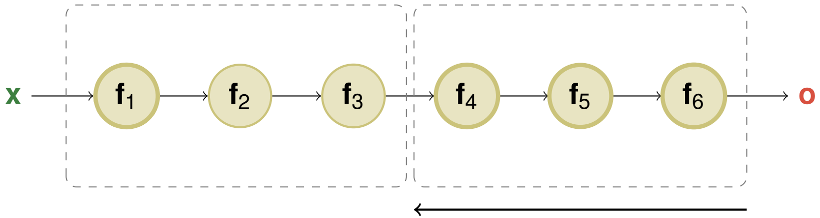

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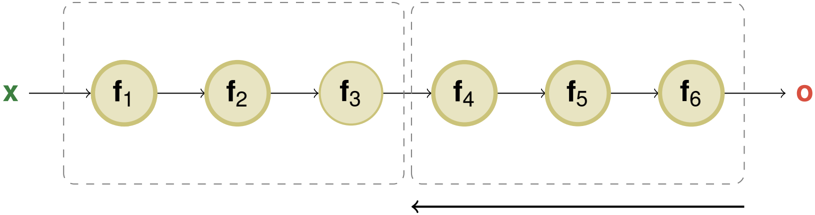

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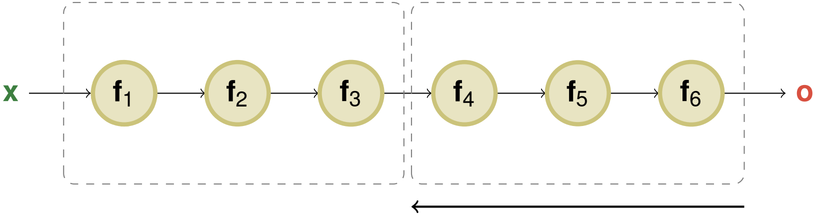

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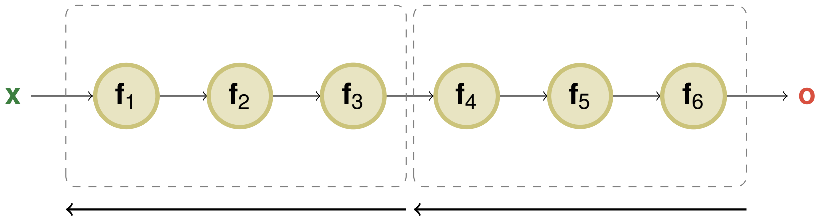

JAX

- Automatic differentiation (**grad**)
- Just-in-time compilation (**jit**)
- NumPy and SciPy compatible
- Automatic vectorization (**vmap**)
- Code transformations are composable
- Actively developed by Google
- Gaining a lot of popularity among ML and science researchers

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Hessian

- The matrix gathering second-order derivatives

$$\nabla^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \, \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \, \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \, \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \, \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \, \partial x_1} & \frac{\partial^2 f}{\partial x_n \, \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

- Hessian vector product = gradient of directional derivative

$$\nabla^2 f(\mathbf{x})\mathbf{v} = \nabla(\nabla f(\mathbf{x}) \cdot \mathbf{v})$$

- JAX supports fully closed tracing: we can “trace through tracing”

Recovering JVPs from VJPs

- Suppose we already have a VJP routine for computing $\mathbf{u}^\top J_\mathbf{f}(\mathbf{x})$
- By linearity we have

$$\frac{\partial \mathbf{u}^\top J_\mathbf{f}(\mathbf{x})}{\partial \mathbf{u}} = J_\mathbf{f}(\mathbf{x})^\top$$

- and therefore

$$\mathbf{v}^\top \frac{\partial \mathbf{u}^\top J_\mathbf{f}(\mathbf{x})}{\partial \mathbf{u}} = \mathbf{v}^\top J_\mathbf{f}(\mathbf{x})^\top = (J_\mathbf{f}(\mathbf{x})\mathbf{v})^\top$$

- The VJP w.r.t. $\mathbf{u}$ of the VJP w.r.t. $\mathbf{x}$ is equal to the transopose of the JVP w.r.t. $\mathbf{x}$.
- The trick does not work in the other direction!

Differentiating min problems

- Consider the function

$$f(\theta) = \min_x E(x, \theta) = E(x^\star(\theta), \theta)$$

- From Danskin's theorem (a.k.a. envelope theorem)

$$\nabla f(\theta) = \nabla_2 E(x^\star(\theta), \theta)$$

  where ∇_2 indicates the gradient w.r.t. the second argument.

- Informally, the theorem says that we can treat $x^\star(\theta)$ as if it did not depend on θ.

Differentiating argmin problems

- Now, consider the function

$$x^\star(\theta) = \operatorname*{argmin}_x E(x, \theta)$$
$$f(\theta) = L(x^\star(\theta), \theta)$$

- By the chain rule, we have

$$\nabla f(\theta) = (J\, x^\star(\theta))^\top \nabla_1 L(x^\star(\theta), \theta) + \nabla_2 L(x^\star(\theta), \theta)$$

- How to compute $J\, x^\star(\theta) = \frac{\partial x^\star(\theta)}{\partial \theta}$?

Fixed points

- Consider the following fixed point iteration

$$x^\star(\theta) = g(x^\star(\theta), \theta) \Leftrightarrow h(x^\star(\theta), \theta) = 0$$

where $h(x, \theta) = x - g(x, \theta)$

- By the implicit function theorem

$$J\, x^\star(\theta) = -(J_1 h(x^\star(\theta), \theta))^{-1} J_2 h(x^\star(\theta), \theta)$$

where J_1 and J_2 are the Jacobians w.r.t. the 1st and 2nd variables

Differentiating argmin problems

- Recall that

$$x^\star(\theta) = \operatorname*{argmin}_x E(x, \theta)$$

- We have the fixed point iteration (gradient descent)

$$x^\star(\theta) = x^\star(\theta) - \nabla_1 E(x^\star(\theta), \theta)$$

- Choosing $h(x, \theta) = \nabla_1 E(x, \theta)$, we get

$$\begin{aligned} J\, x^\star(\theta) &= -(J_1 \nabla_1 E(x^\star(\theta), \theta))^{-1} J_2 \nabla_1 E(x^\star(\theta), \theta) \\ &= -(\nabla_1^2 E(x^\star(\theta), \theta))^{-1} J_2 \nabla_1 E(x^\star(\theta), \theta) \end{aligned}$$

- In practice, we need to replace $x^\star(\theta)$ by an approximate solution.

Differentiating argmin problems

- Example: hyper-parameter optimization for ridge regression

$$
\begin{aligned}
E(x, \theta) &= \frac{1}{2}\|Ax - b\|^2 + \frac{\theta}{2}\|x\|^2 \in \mathbb{R} \\
\nabla_1 E(x, \theta) &= A^\top(Ax - b) + \theta x \in \mathbb{R}^d \\
\nabla_1^2 E(x, \theta) &= A^\top A + \theta I \in \mathbb{R}^{d \times d} \\
J_2 \nabla_1 E(x, \theta) &= x \in \mathbb{R}^{d \times 1} \\
x^\star(\theta) &= (A^\top A + \theta I)^{-1} A^\top b
\end{aligned}
$$

- $J\, x^\star(\theta)$ is therefore obtained by solving the following linear system

$$
(A^\top A + \theta I)[J\, x^\star(\theta)] = -x^\star(\theta)
$$

Differentiating argmin problems

- An alternative idea to obtain $J\,x^\star(\theta)$ is to to backpropagate through gradient descent:

$$x^{t+1}(\theta) = x^t(\theta) - \eta_t \nabla_1 E(x^t(\theta), \theta)$$

- No longer needs to solve a linear system...
- ...but needs to store intermediate iterates $x^t(\theta)$ or checkpoints
- Possibility to use truncated backpropagation
- Possibility to use reversible dynamics in some cases

Inference in graphical models

- Gibbs distribution

$$\mathbb{P}(Y = y; \theta) \propto \exp(y \cdot \theta)$$

  where $y \in \mathcal{Y} \subset \{0, 1\}^n$

- Log-partition function

$$f(\theta) = \log \sum_{y \in \mathcal{Y}} \exp(y \cdot \theta)$$

- **Fact.**

$$(\mathbb{P}(Y_i = 1; \theta))_{i=1}^n = \mathbb{E}[Y] = \nabla f(\theta)$$

- If we know how to compute $f(\theta)$, we can get expectations / marginal probabilities by autodiff! Recovers forward-backward algorithms as special case. For a proof, see e.g. this paper.

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Summary

- Automatic differentiation is one of the keys that enabled the deep learnnig “revolution”.
- Backward / reverse differentiation is more efficient when the function has more inputs than outputs.
- Which is the de-facto setting in machine learning!
- Even if you use Tensorflow / JAX / PyTorch, implementing a rudimentary autodiff library is a very good exercise.

References

The following tutorials have been a great inspiration:

- Automatic Differentiation, Matthew Johnson, Deep Learning Summer School Montreal, 2017.
- Differential programming, Gabriel Peyré, Mathematical Coffees, 2018.

Two minimalist implementations of autodiff:

- Autodidact, by Matthew Johnson.
- Micrograd, by Andrej Karpathy.