Matrix Derivatives. Automatic Differentiation

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

Theory recap. Differential

- Differential $df(x)[\cdot] : U \to V$ in point $x \in U$ for $f(\cdot) : U \to V$:

$$f(x+h) - f(x) = \underbrace{df(x)[h]}_{\text{differential}} + \bar{o}(||h||)$$

- Canonical form of the differential:

$U \to V$	$\mathbb{R}$	$\mathbb{R}^n$	$\mathbb{R}^{n \times m}$
$\mathbb{R}$	$f'(x)dx$	$\nabla f(x)dx$	$\nabla f(x)dx$
$\mathbb{R}^n$	$\nabla f(x)^T dx$	$J(x)dx$	—
$\mathbb{R}^{n \times m}$	$tr(\nabla f(X)^T dX)$	—	—

Theory recap. Differentiation Rules

- Useful differentiation rules and standard derivatives:

Differentiation Rules	Standard Derivatives
$dA = 0$	$d(\langle A, X\rangle) = \langle A, dX\rangle$
$d(\alpha X) = \alpha(dX)$	$d(\langle Ax, x\rangle) = \langle (A + A^T)x, dx\rangle$
$d(AXB) = A(dX)B$	$d(Det(X)) = Det(X)\langle X^{-T}, dX\rangle$
$d(X + Y) = dX + dY$	$d(X^{-1}) = -X^{-1}(dX)X^{-1}$
$d(X^T) = (dX)^T$	
$d(XY) = (dX)Y + X(dY)$	
$d(\langle X, Y\rangle) = \langle dX, Y\rangle + \langle X, dY\rangle$	
$d\left(\frac{X}{\phi}\right) = \frac{\phi dX - (d\phi)X}{\phi^2}$	

Matrix Calculus. Problem 1

Example

Find $\nabla f(x)$, if $f(x) = \frac{1}{2}x^T Ax + b^T x + c$.

Matrix Calculus. Problem 2

Example

Find $\nabla f(X)$, if $f(X) = tr(AX^{-1}B)$

- $h(x) = f(g(x)) \Rightarrow dh(x_0)[dx] = df(g(x_0))[dg(x_0)[dx]]$

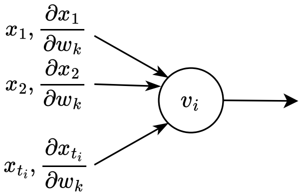
Matrix Calculus. Problem 3

Example

Find the gradient $\nabla f(x)$ and hessian $\nabla^2 f(x)$, if $f(x) = \frac{1}{3}\|x\|_2^3$

- $d^2 f(x)[h_1, h_2] = d\left(df(x)[\underbrace{h_1}_{\text{fixed when take outer } d(\cdot)}]\right)[h_2]$
- Canonic form for $f : \mathbb{R}^n \to \mathbb{R}$: $d^2 f(x)[h_1, h_2] = h_1^T \underbrace{\nabla^2 f(x)}_{\text{hessian}} h_2$

Automatic Differentiation. Forward mode



$$v_i = v_i(x_1, \ldots, x_{t_i})$$

$$\frac{\partial v_i}{\partial w_k} = \sum_{j=1}^{t_i} \frac{\partial v_i}{\partial x_j} \frac{\partial x_j}{\partial w_k}$$

Figure 1: Illustration of forward chain rule to calculate the derivative of the function v_i with respect to w_k.

- Uses the forward chain rule
- Has complexity $d \times \mathcal{O}(T)$ operations

Automatic Differentiation. Reverse mode

$$\frac{\partial L}{\partial v_i} = \sum_{j=1}^{t_i} \frac{\partial L}{\partial x_j} \frac{\partial x_j}{\partial v_i}$$

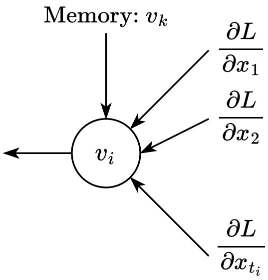


Figure 2: Illustration of reverse chain rule to calculate the derivative of the function L with respect to the node v_i.

- Uses the backward chain rule
- Stores the information from the forward pass
- Has complexity $\mathcal{O}(T)$ operations

Automatic Differentiation. Problem 1

Example

Which of the AD modes would you choose (forward/ reverse) for the following computational graph of primitive arithmetic operations?

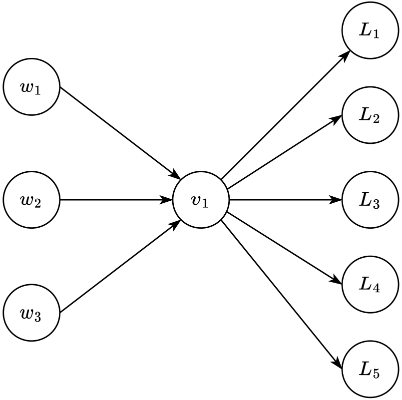


Figure 3: Which mode would you choose for calculating gradients there?

Automatic Differentiation. Problem 2

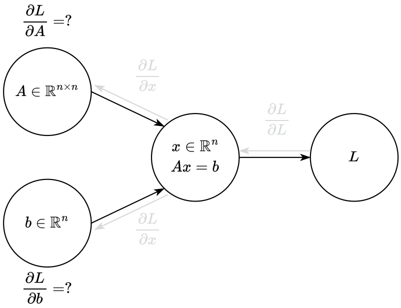


Figure 4: x could be found as a solution of linear system

Suppose, we have an invertible matrix A and a vector b, the vector x is the solution of the linear system $Ax = b$, namely one can write down an analytical solution $x = A^{-1}b$.

Find the derivatives $\dfrac{\partial L}{\partial A}, \dfrac{\partial L}{\partial b}$.

Automatic Differentiation. Problem 3

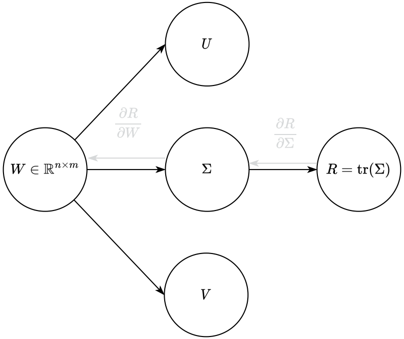


Figure 5: Computation graph for singular regularizer

Suppose, we have the rectangular matrix $W \in \mathbb{R}^{m \times n}$, which has a singular value decomposition:

$$W = U \Sigma V^T, \quad U^T U = I, \quad V^T V = I, \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_{\min(m,n)})$$

The regularizer $R(W) = \text{tr}(\Sigma)$ in any loss function encourages low rank solutions. Find the derivative $\dfrac{\partial R}{\partial W}$.

Computation experiment with JAX

- JAX docs: https://jax.readthedocs.io/en/latest/notebooks/quickstart.html