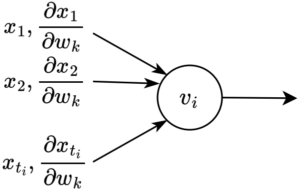
Automatic Differentiation

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

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

Reverse mode

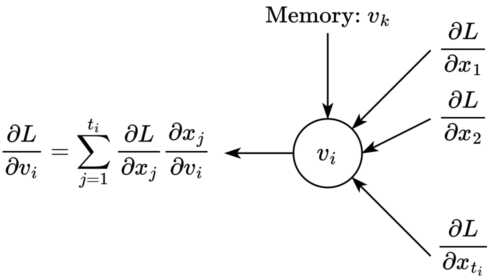


Figure 2: Illustration of reverse chain rule to calculate the derivative of the function L with respect to the node v_i.

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

Toy example

Example

$$f(x_1, x_2) = x_1 * x_2 + \sin x_1$$

Let's calculate the derivatives $\dfrac{\partial f}{\partial x_i}$ using forward and reverse modes.

Toy example

Example

$$f(x_1, x_2) = x_1 * x_2 + \sin x_1$$

Let's calculate the derivatives $\dfrac{\partial f}{\partial x_i}$ using forward and reverse modes.

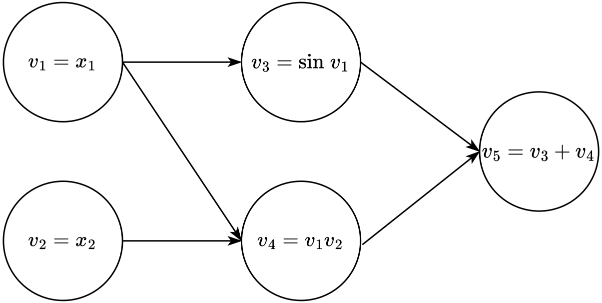


Figure 3: Illustration of computation graph of $f(x_1, x_2)$.

Automatic Differentiation with JAX

Example №1

$$f(X) = tr(AX^{-1}B)$$

$$\nabla f = -X^{-T}A^TB^TX^{-T}$$

Automatic Differentiation with JAX

Example №1

$$f(X) = tr(AX^{-1}B)$$

$$\nabla f = -X^{-T}A^TB^TX^{-T}$$

Example №2

$$g(x) = 1/3 \cdot ||x||_2^3$$

$$\nabla^2 g = ||x||_2^{-1} xx^T + ||x||_2 I_n$$

Automatic Differentiation with JAX

Example №1

$$f(X) = tr(AX^{-1}B)$$

$$\nabla f = -X^{-T}A^TB^TX^{-T}$$

Example №2

$$g(x) = 1/3 \cdot ||x||_2^3$$

$$\nabla^2 g = ||x||_2^{-1}xx^T + ||x||_2 I_n$$

Let's calculate the gradients and hessians of f and g in python

Problem 1

Question

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

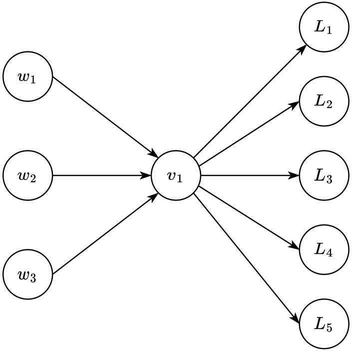


Figure 4: Which mode would you choose for calculating gradients there?

Problem 2

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 $x = A^{-1}b$.

Question

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

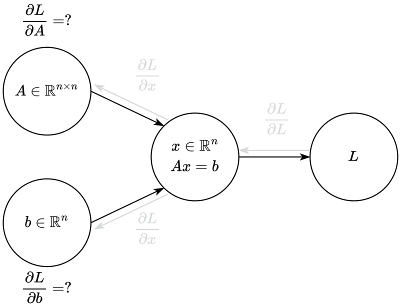


Figure 5: x could be found as a solution of linear system

Problem 3

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

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

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

Question

Find the derivative $\dfrac{\partial R}{\partial W}$.

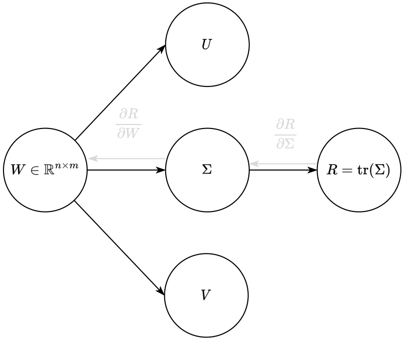


Figure 6: Computation graph for singular regularizer

Computation experiment with JAX

Let's make sure numerically that we have correctly calculated the derivatives in problems 2-3

Feedforward Architecture

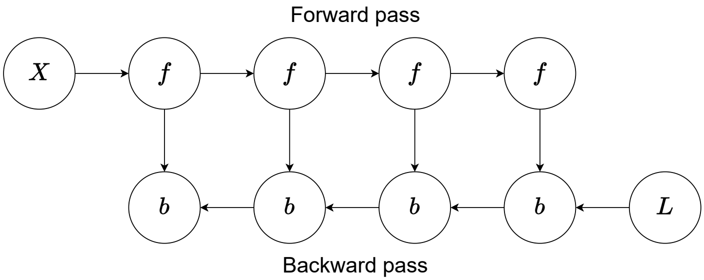


Figure 7: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The activations marked with an f. The gradient of the loss with respect to the activations and parameters marked with b.

Feedforward Architecture

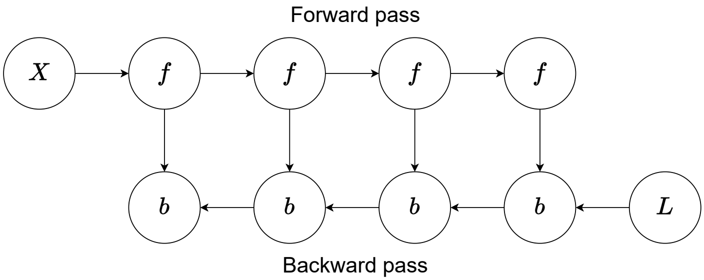


Figure 7: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The activations marked with an f. The gradient of the loss with respect to the activations and parameters marked with b.

! Important

The results obtained for the f nodes are needed to compute the b nodes.

Vanilla backpropagation

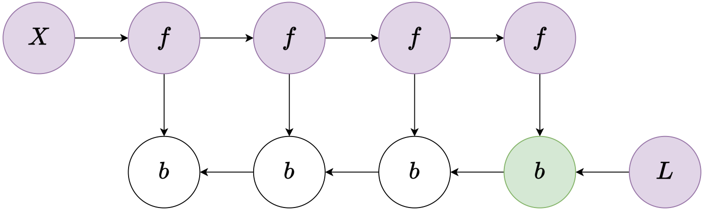


Figure 8: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Vanilla backpropagation

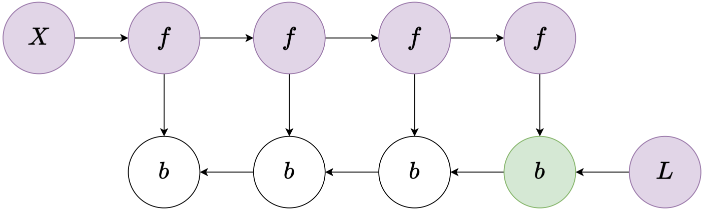


Figure 8: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- All activations f are kept in memory after the forward pass.

Vanilla backpropagation

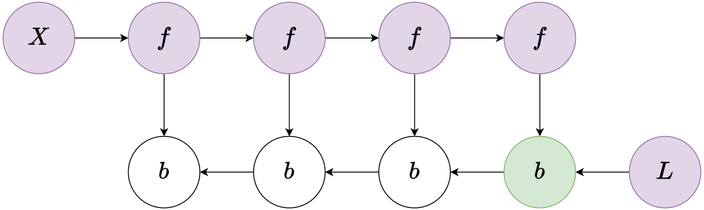


Figure 8: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- All activations f are kept in memory after the forward pass.

- Optimal in terms of computation: it only computes each node once.

Vanilla backpropagation

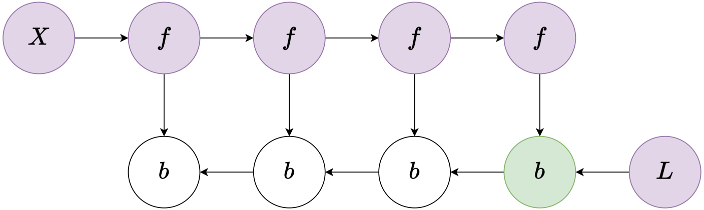


Figure 8: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- All activations f are kept in memory after the forward pass.

- Optimal in terms of computation: it only computes each node once.

- High memory usage. The memory usage grows linearly with the number of layers in the neural network.

Memory poor backpropagation

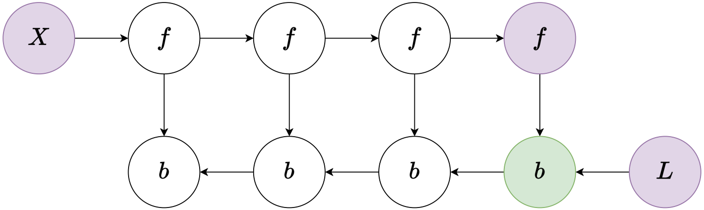


Figure 9: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Memory poor backpropagation

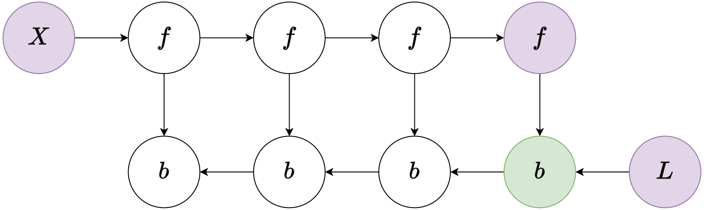


Figure 9: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Each activation f is recalculated as needed.

Memory poor backpropagation

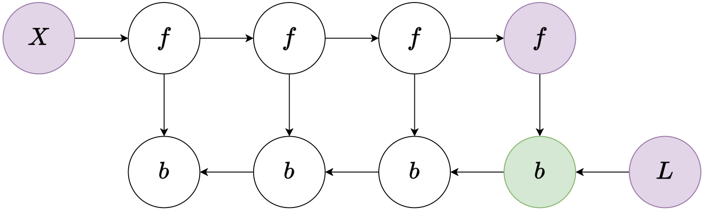


Figure 9: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Each activation f is recalculated as needed.

- Optimal in terms of memory: there is no need to store all activations in memory.

Memory poor backpropagation

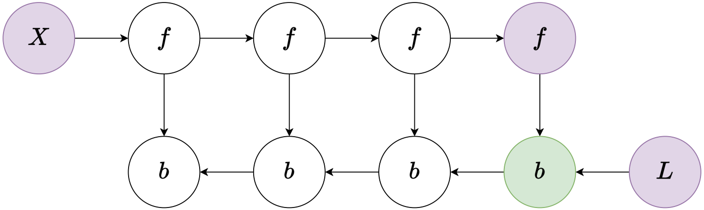


Figure 9: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Each activation f is recalculated as needed.

- Optimal in terms of memory: there is no need to store all activations in memory.

- Computationally inefficient. The number of node evaluations scales with n^2, whereas it vanilla backprop scaled as n: each of the n nodes is recomputed on the order of n times.

Checkpointed backpropagation

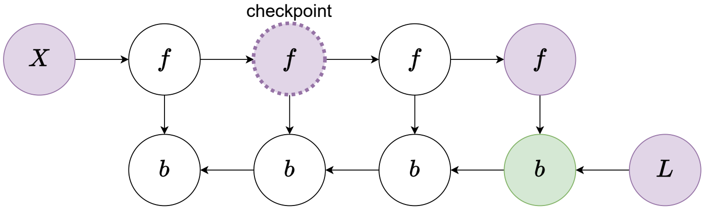


Figure 10: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Checkpointed backpropagation

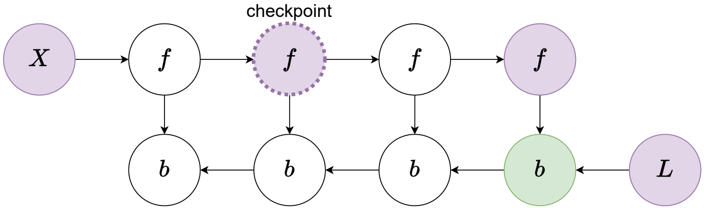


Figure 10: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Trade-off between the **vanilla** and **memory poor** approaches. The strategy is to mark a subset of the neural net activations as checkpoint nodes, that will be stored in memory.

Checkpointed backpropagation

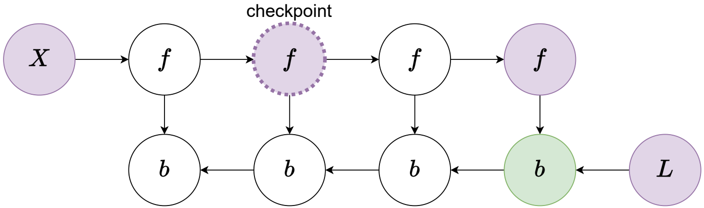


Figure 10: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Trade-off between the **vanilla** and **memory poor** approaches. The strategy is to mark a subset of the neural net activations as checkpoint nodes, that will be stored in memory.

- Faster recalculation of activations f. We only need to recompute the nodes between a b node and the last checkpoint preceding it when computing that b node during backprop.

Checkpointed backpropagation

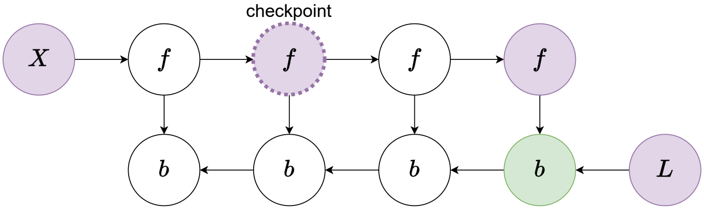


Figure 10: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Trade-off between the **vanilla** and **memory poor** approaches. The strategy is to mark a subset of the neural net activations as checkpoint nodes, that will be stored in memory.

- Faster recalculation of activations f. We only need to recompute the nodes between a b node and the last checkpoint preceding it when computing that b node during backprop.

- Memory consumption depends on the number of checkpoints. More effective then **vanilla** approach.

Gradient checkpointing visualization

The animated visualization of the above approaches

An example of using a gradient checkpointing