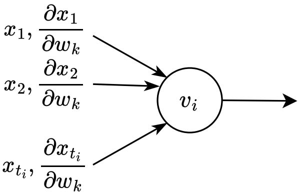
# Automatic Differentiation

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

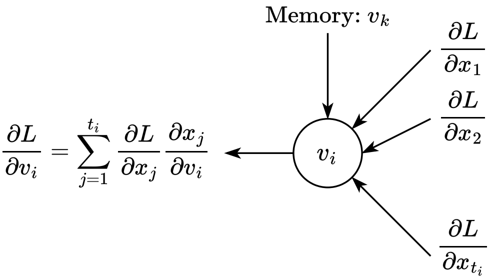



Figure 2: Illustration of reverse chain rule to calculate the derivative of the function $L$ with respect to the node $v_i$.

- 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.

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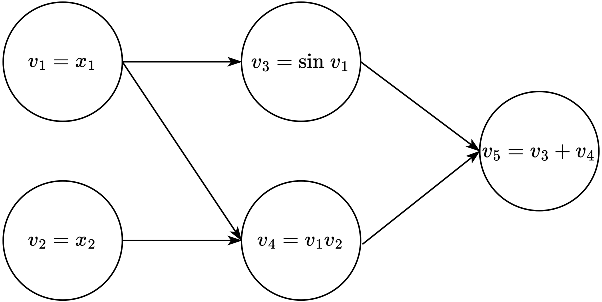


Figure 3: Illustration of computation graph of $f(x_1, x_2)$.

# Automatic Differentiation with JAX

**Example №1**

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

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

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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?

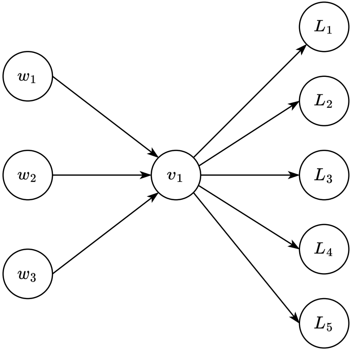



Figure 4: Which mode would you choose for calculating gradients there?

# 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 $\dfrac{\partial L}{\partial A}, \dfrac{\partial L}{\partial b}$.

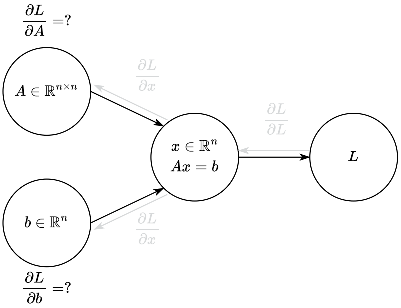



Figure 5: $x$ could be found as a solution of linear system

# Problem 3

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

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

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

**Question**

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

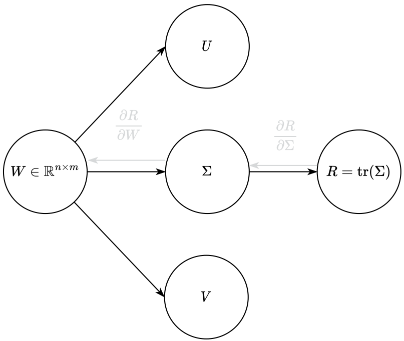



Figure 6: Computation graph for singular regularizer

# Computation experiment with JAX

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

# Feedforward Architecture

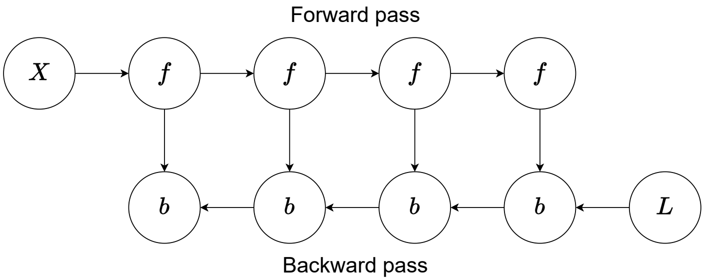
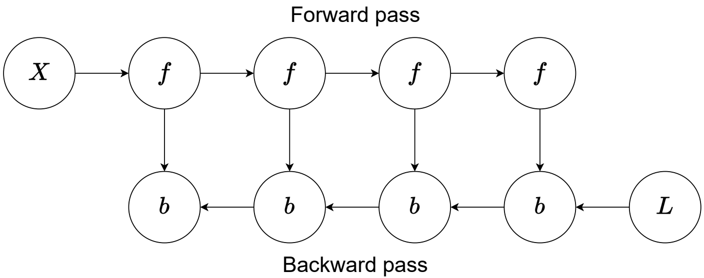



Figure 7: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The activations marked with an $f$. The gradient of the loss with respect to the activations and parameters marked with $b$.

# Feedforward Architecture

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**! Important**

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

# Vanilla backpropagation

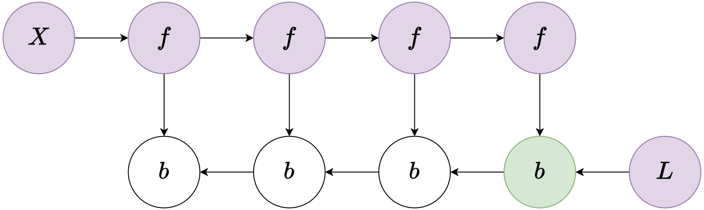


Figure 8: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

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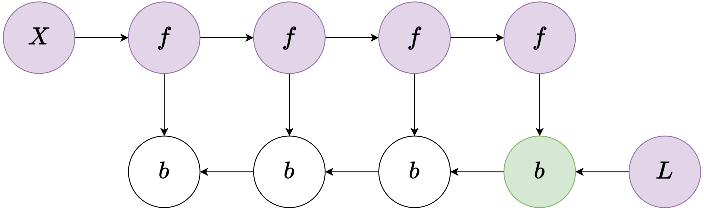


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- All activations $f$ are kept in memory after the forward pass.

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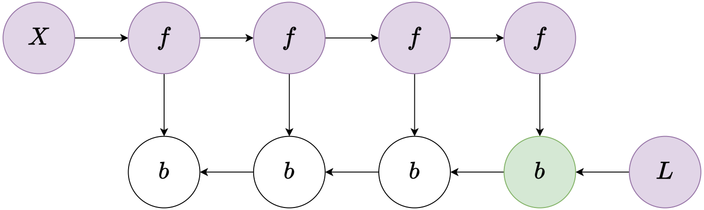


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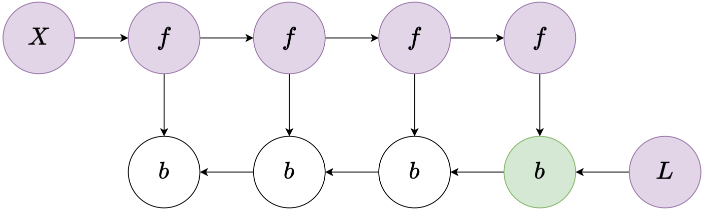


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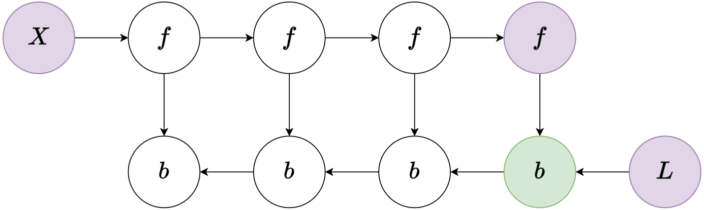
- Optimal in terms of computation: it only computes each node once.

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

# Memory poor backpropagation

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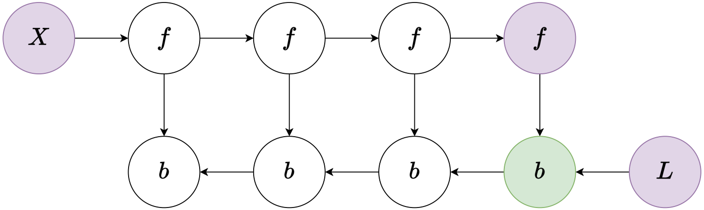


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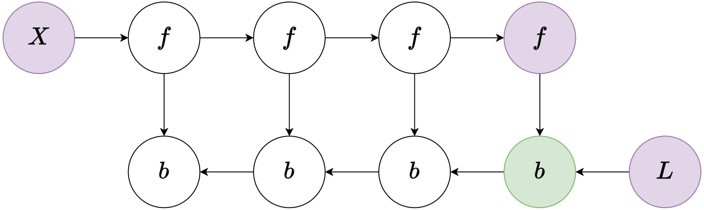


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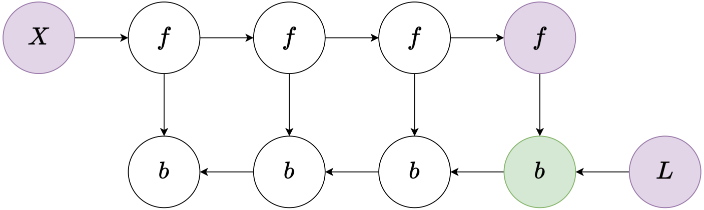


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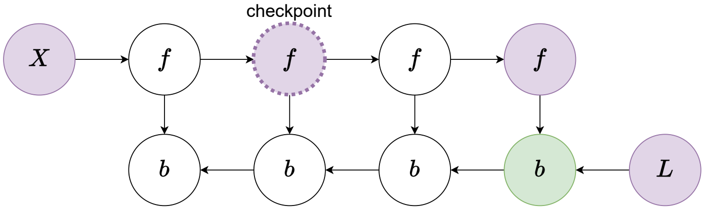
- Computationally inefficient. The number of node evaluations scales with $n^2$, whereas it vanilla backprop scaled as $n$: each of the n nodes is recomputed on the order of $n$ times.

# Checkpointed backpropagation

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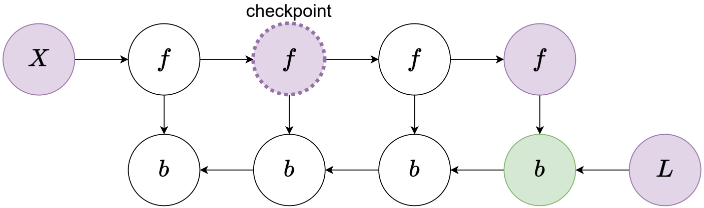


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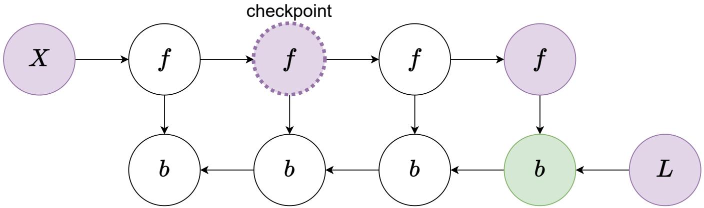


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- Faster recalculation of activations $f$. We only need to recompute the nodes between a $b$ node and the last checkpoint preceding it when computing that $b$ node during backprop.

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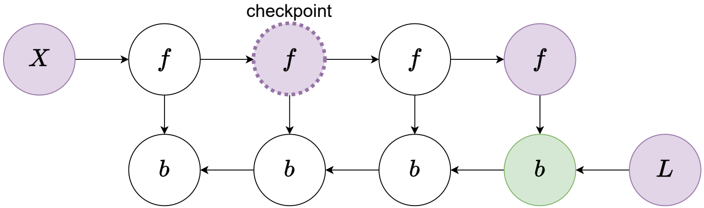


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- Faster recalculation of activations $f$. We only need to recompute the nodes between a $b$ node and the last checkpoint preceding it when computing that $b$ node during backprop.

- 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