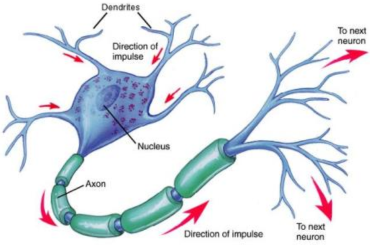
Topic 10: NEURAL NETWORKS

STAT 37710/CAAM 37710/CMSC 35400 Machine Learning

Risi Kondor, The University of Chicago

Intro to neural networks



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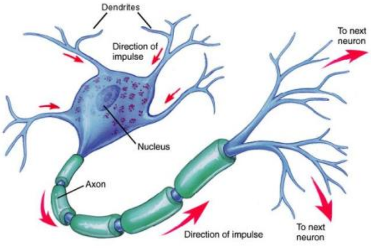

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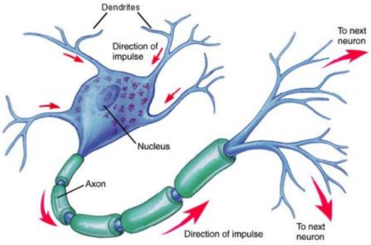

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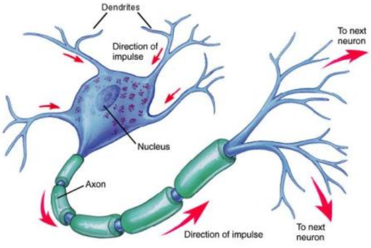

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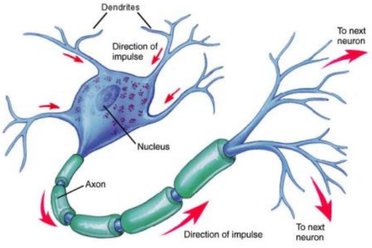

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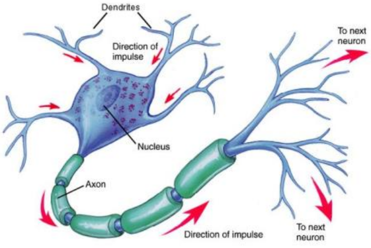

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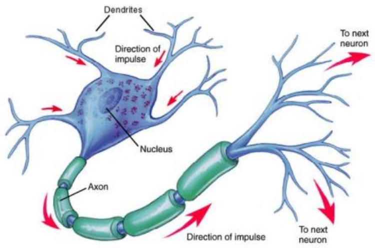

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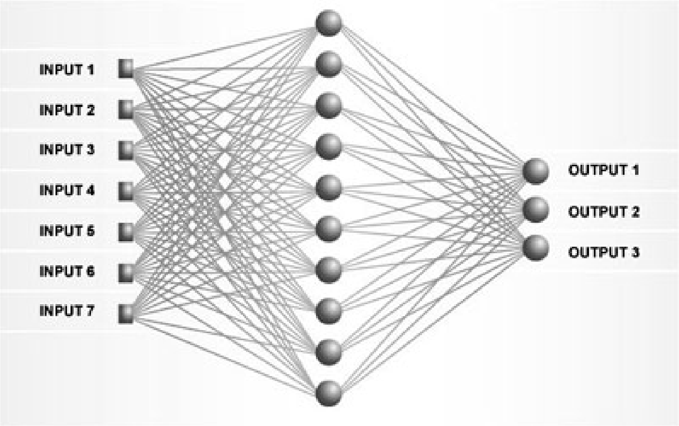
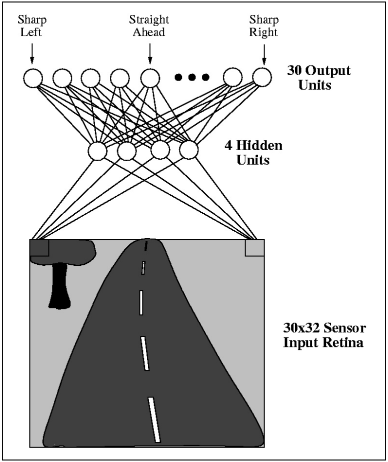
IDEA: Humans seem to be okay at learning, so why not try to replicate this in a computer? Goes back to the early days of AI, many successes and failures.

Multilayer artificial neural net



Question: But what should the individual neurons do and how should they learn?

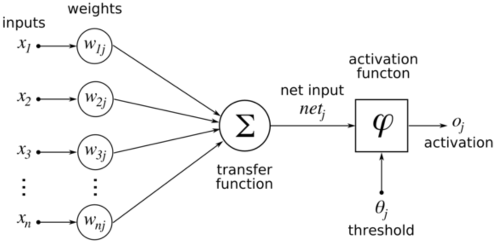
A success: ALVINN [Pomerleau ’95]



Drove unassisted from Pittsburgh to NYC on the highway.

A model neuron

$$o = \sigma\Big(\theta + \sum_p w_p x_p\Big),$$



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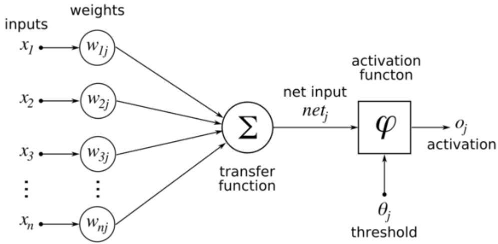

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- x_i : the i'th input

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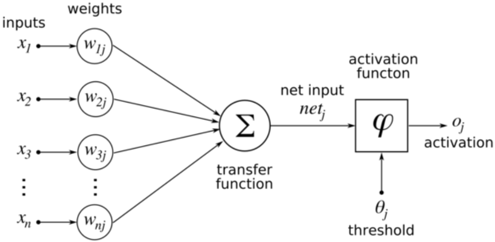

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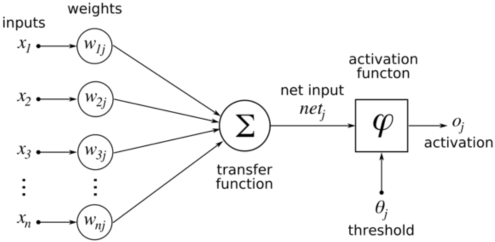

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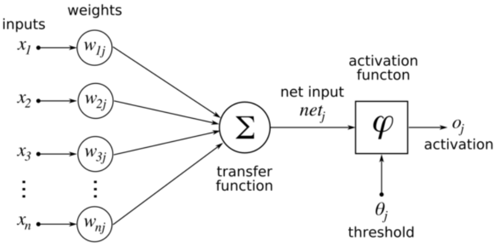

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Learning rule: Define a loss function $\ell(\mathbf{y}, \widehat{\mathbf{y}})$ for the entire network, and change the weights so as to reduce it. For example, for regression one can use

$$\ell(y, \widehat{y}) = (y - \widehat{y})^2.$$

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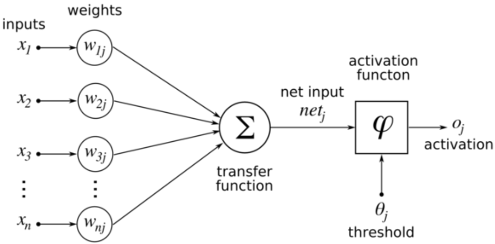

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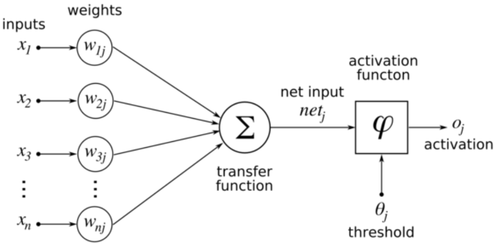

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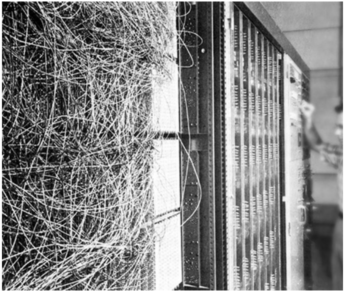
Multilayer Perceptron



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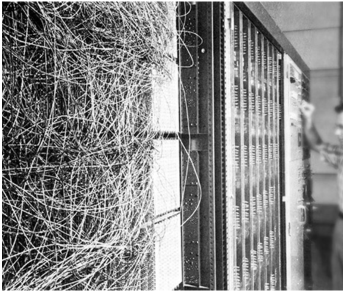

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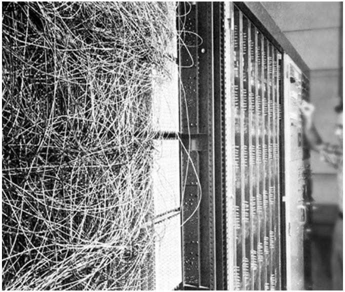

- Multilayer perceptron was thought of as universal model of the brain
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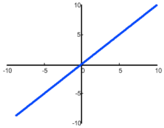
- Problem: hard to train, multilayer perceptron plagued with local minima

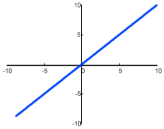
Activation functions



Linear: $\sigma(t) = t$

Question: What is the problem with this?

Activation functions



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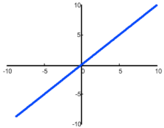

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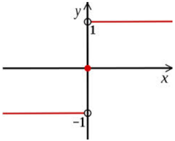

Hard threshold: $\sigma(t) = \mathrm{sgn}(t)$

"Threshold Logic Unit" [McCulloch & Pitts, 1943]

$\rightarrow$ Perceptron [Rosenblatt, 1958]

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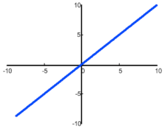

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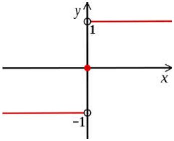

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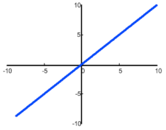

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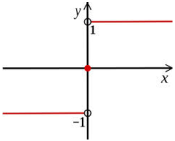

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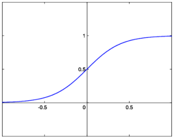

(log-)sigmoid: $\sigma(t) = 1/(1 + e^{-t})$

Also called the logistic function.

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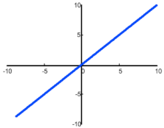

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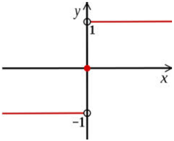

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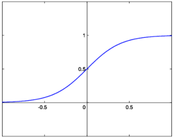

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This is what we will use.

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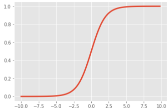

tanh: $\sigma(x) = \tanh(x) = (e^{x} - e^{-x})/(e^{x} + e^{-x})$

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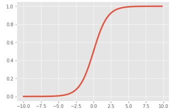

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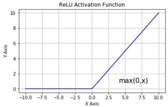

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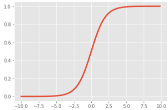

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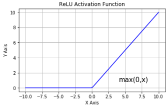

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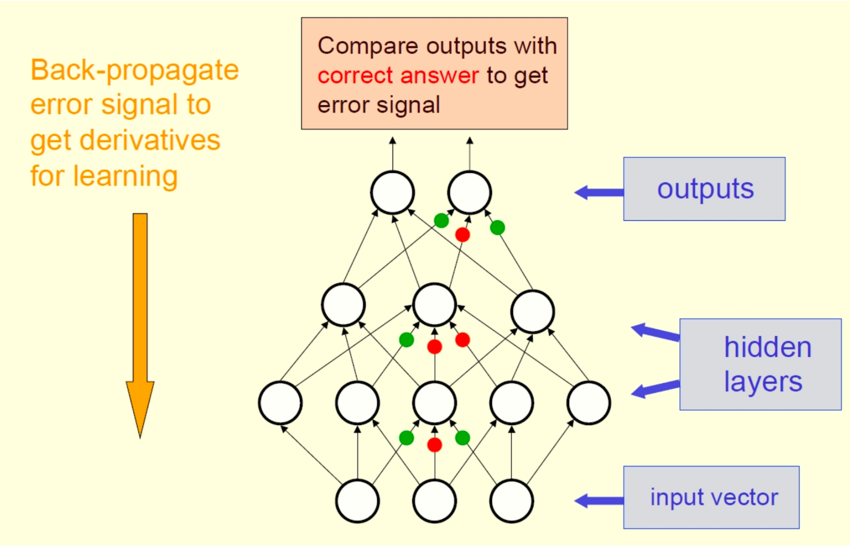

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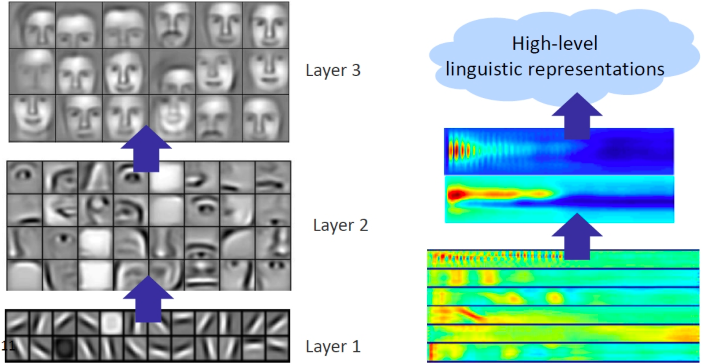
  - Modern GPU architectures make training much faster.

Multilayer Representations



For vision tasks in particular, representing complex scenes in terms of a hierarchy of features makes sense.

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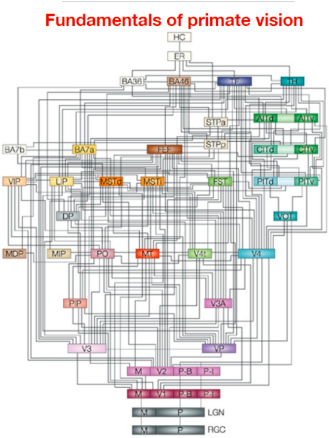

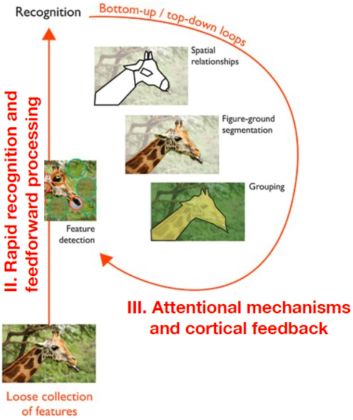

Feed-forward NN for regression

For regression $f : \mathbb{R}^n \to \mathbb{R}^m$:

- n neurons in input layer (layer 0)

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where $a_{\tau(i)}$ is the output of the i 'th neuron in the output layer.

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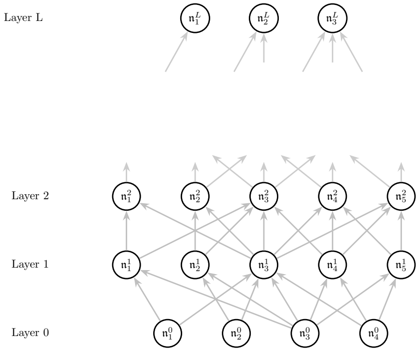
- Each neuron may be connected to all the neurons in the previous layer or just a subset of them.



Feed-forward NN for classification

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where $a_{\tau(i)}$ is the output of the i'th neuron in the output layer.

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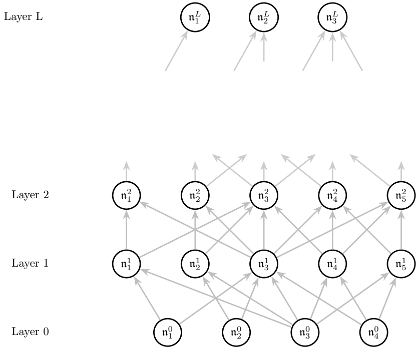
  where $a_{\tau(i)}$ is the output of the i'th neuron in the output layer.
- Each neuron may be connected to all the neurons in the previous layer or just a subset of them.



Training NNs with backpropagation

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- Adjust each weight of each neuron in each layer by gradient descent

$$w_{s \to t} \leftarrow w_{s \to t} - \eta \, \frac{\partial \mathcal{E}}{\partial w_{s \to t}},$$

  where η is a parameter called the **learning rate**.

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$$a_t = \sigma\underbrace{\Bigg(\sum_{s\in\mathcal{I}(t)} w_{s\to t}\, a_s + b_t\Bigg)}_{z_t} = \sigma(z_t),$$

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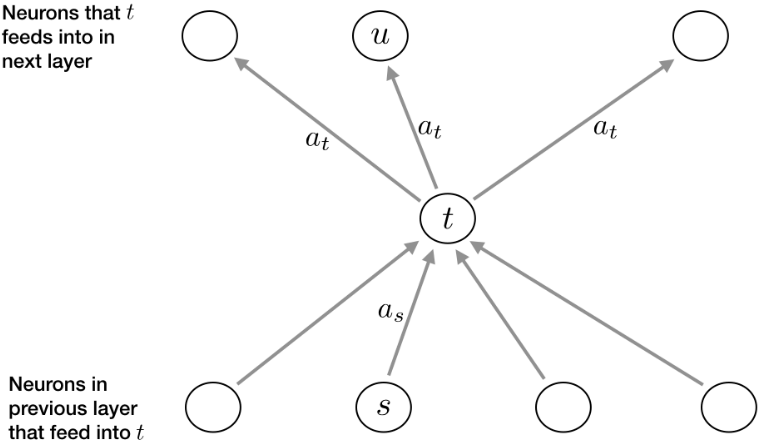
- Similarly, $\mathcal{O}_t$ is the set of neurons in the next layer that t feeds into.
- The "pre-activation" z_t plays an important role in the following.


Neurons that t feeds into in next layer
u
a_t
a_t
a_t
t
a_s
Neurons in previous layer that feed into t
s

Backpropagation

Problem: how to compute the $\frac{\partial \mathcal{E}}{\partial w_{s \to t}}$ derivatives efficiently for all the weights in the neural network?

- Define the **error** (slight misnomer)

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- Using the chain rule, we then have the very simple relations

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So now the question becomes: how do we compute δ_t for all neurons in the network simultaneously?

Backpropagation

Assume that δ_u errrors have been computed for for all neurons in layer $\ell + 1$. Then for any neuron t in layer ℓ,

$$\delta_t = \frac{\partial \mathcal{E}}{\partial z_t} = \sum_{u \in \mathcal{O}_t} \underbrace{\frac{\partial \mathcal{E}}{\partial z_u}}_{\delta_t} \frac{\partial z_u}{\partial z_t}.$$

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So we have the simple backpropagation formula

$$\delta_t = \sum_{u \in \mathcal{O}_t} w_{t \to u}\, \sigma'(z_t)\, \delta_u.$$

In the last layer, δ_t is computed directly from the loss.

Forward pass

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- Read off $\widehat{\mathbf{y}}$ from the last layer, and compute the loss $\mathcal{E}(\widehat{\mathbf{y}}, \mathbf{y})$.

Backward pass

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- For each neuron in each layer compute the partial derivatives that we ultimately need

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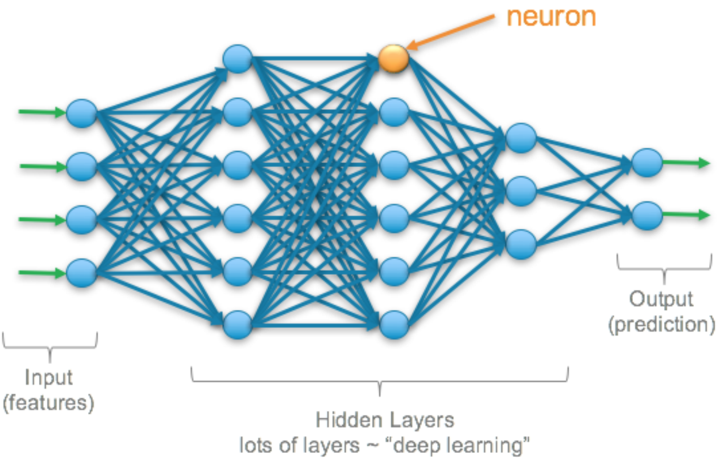
- Update the weights and biases by the SGD rule.

The multi-layer perceptron



A feed-forward network where is layer is fully connected is called a multi-layer perceptron.

Forward pass

For a MLP, the forward iteration can be expressed as

$$\boldsymbol{a}_\ell = \sigma(\underbrace{W_\ell\, \boldsymbol{a}_{\ell-1}}_{\boldsymbol{z}_\ell} + \boldsymbol{b}_\ell),$$

where

- $\boldsymbol{a}_\ell$ is the vector activations in layer ℓ,
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The forward pass consists of just computing $\mathbf{x} \mapsto \boldsymbol{a}_1 \mapsto \boldsymbol{a}_2 \mapsto \ldots \mapsto \boldsymbol{a}_L \mapsto \widehat{y} \mapsto \mathcal{E}$.

Backward pass

Setting $\boldsymbol{\delta}_\ell$ as the vector of errors in layer ℓ, the backward iteration is

$$\boldsymbol{\delta}_\ell = \sigma'(\boldsymbol{z}_t) \odot (W_\ell^\top \boldsymbol{\delta}_{\ell+1}),$$

where $\odot$ is the elementwise product of two vectors.

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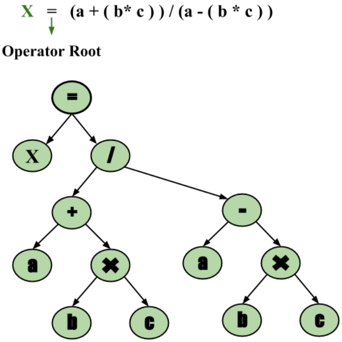
The individual $\partial \mathcal{E} / \partial w_{s \to t}$ and $\partial \mathcal{E} / \partial b_t$ derivatives are computed as before.

Differentiable computing

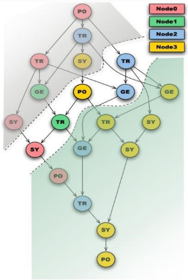
Computation graphs

It is an old idea in compilers to use a directed acyclic graph (DAG) as an intermediate representation (IR).



Similarly, in high performance computing (HPC) large DAGs are used to depict the interdependencies between parts of a massive compute job.

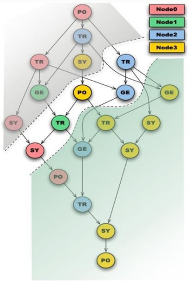
Computation graphs



The DAG can be used to

- Optimize the order in which computations are performed.

Computation graphs



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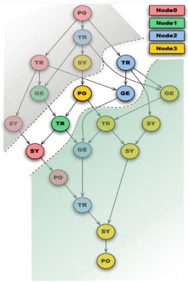
- Optimize the way in which parts of the computation are allocated to processors/nodes.

Computation graphs



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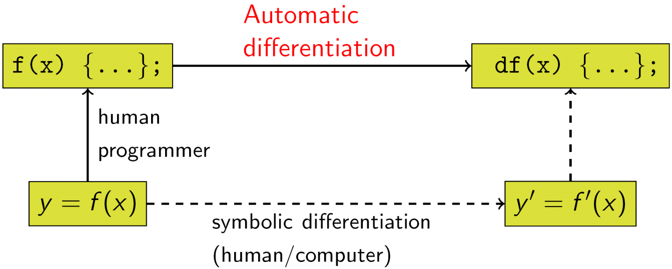
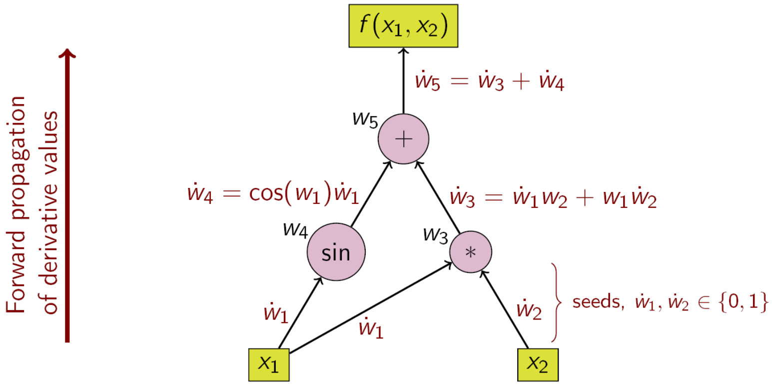
All this can be done statically (ahead of time) or dynamically (at runtime).

Automatic differentation

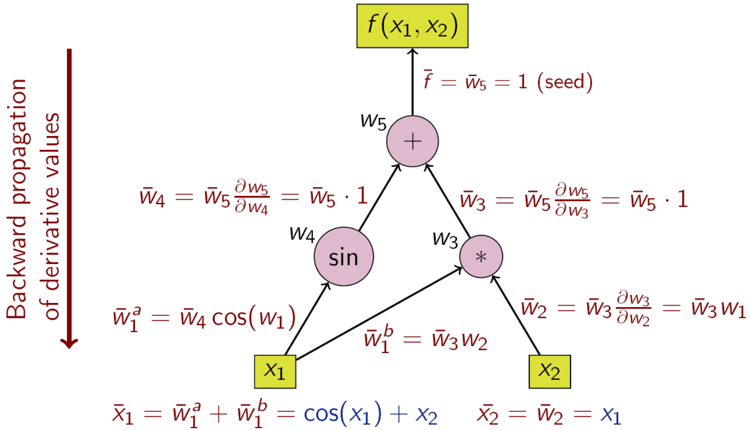
Another interesting field deals with writing compilers that can compute the derivative of any user defined (differentiable) function.



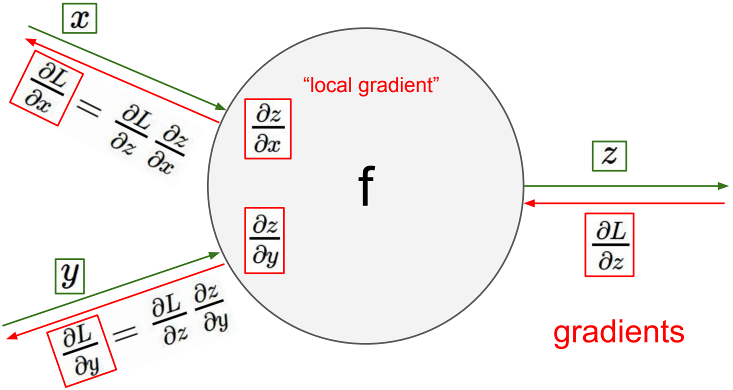
Automatic differentiation



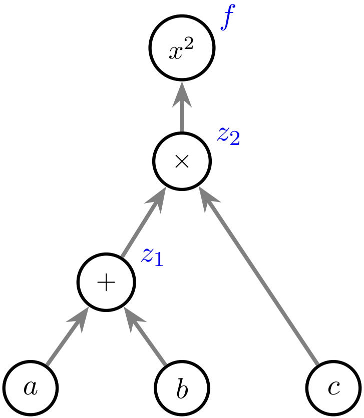
Automatic differentiation



Modern deep learning frameworks combine this idea with DAG-based runtimes.

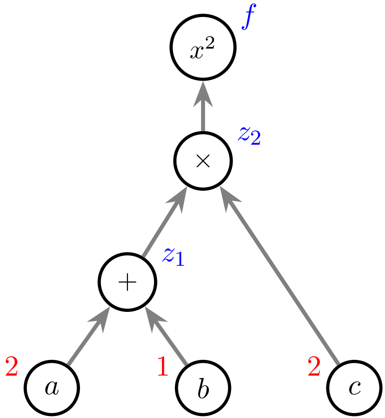

x
y
z
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
$\frac{\partial L}{\partial z}$
gradients
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$

Forward and backward computations

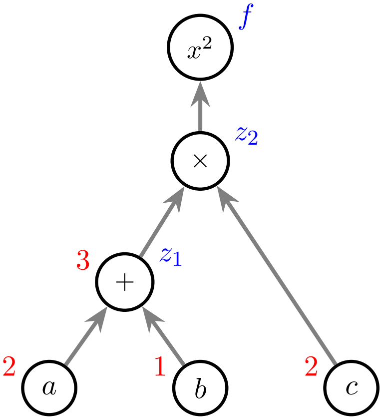


$$f(a, b, c) = ((a + b)c)^2$$

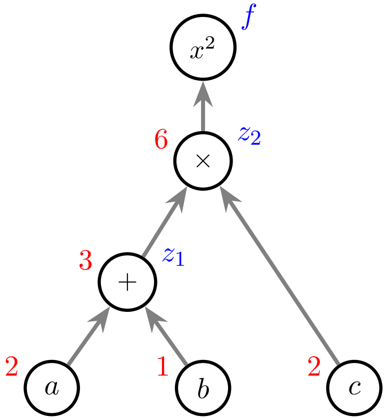
Forward



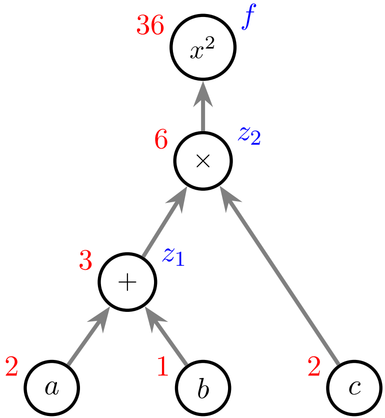
Forward



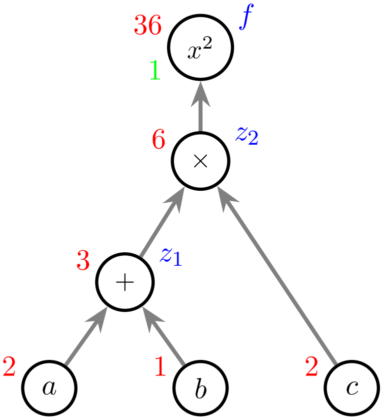
Forward



Forward

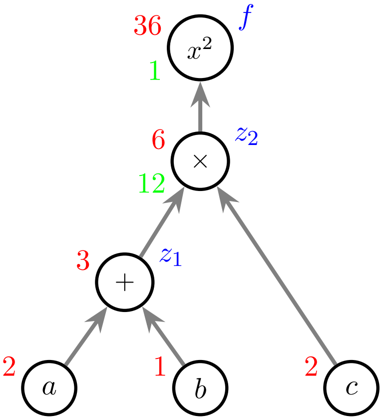


Backward



$$\frac{\partial f}{\partial f} = 1$$

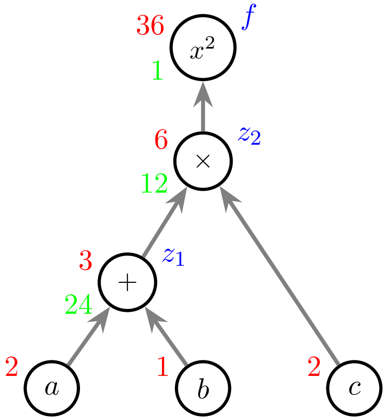
Backward



$$f = z_2^2$$

$$\frac{\partial f}{\partial z_2} = \underbrace{\frac{\partial f}{\partial f}}_{1} \underbrace{\frac{\partial f}{\partial z_2}}_{2z_2=12} = 12$$

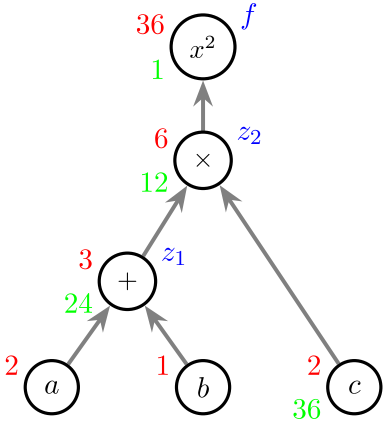
Backward



$$z_2 = z_1 \cdot c$$

$$\frac{\partial f}{\partial z_1} = \underbrace{\frac{\partial f}{\partial z_2}}_{12} \underbrace{\frac{\partial z_2}{\partial z_1}}_{c} = 24$$

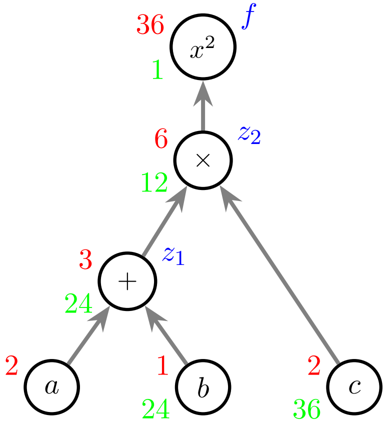
Backward



$$z_2 = z_1 \cdot c$$

$$\frac{\partial f}{\partial c} = \underbrace{\frac{\partial f}{\partial z_2}}_{12} \underbrace{\frac{\partial z_2}{\partial c}}_{z_1} = 36$$

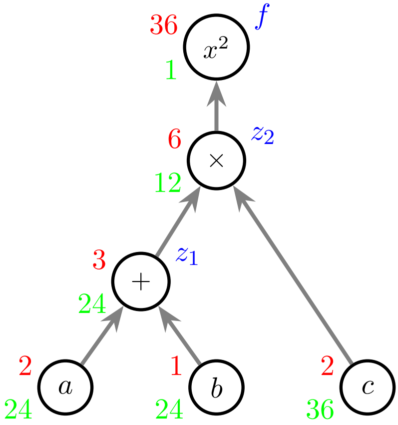
Backward



$$z_1 = a + b$$

$$\frac{\partial f}{\partial b} = \underbrace{\frac{\partial f}{\partial z_1}}_{24} \underbrace{\frac{\partial z_1}{\partial b}}_{1} = 24$$

Backward

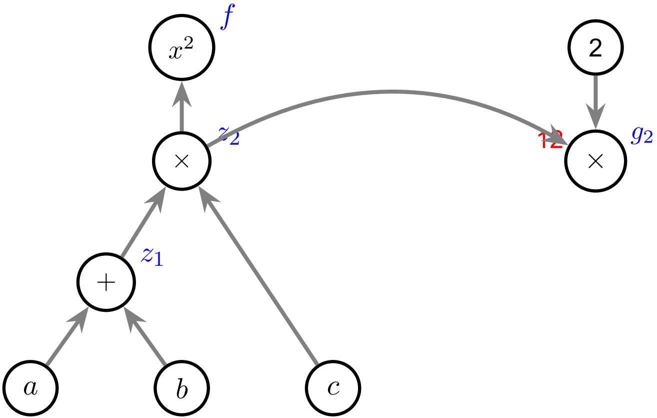


$$z_1 = a + b$$

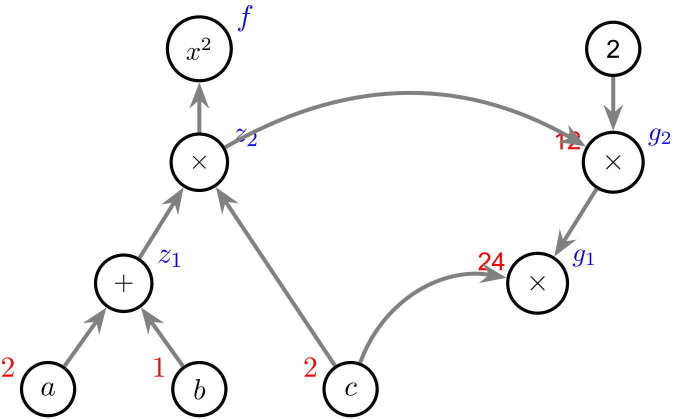
$$\frac{\partial f}{\partial a} = \underbrace{\frac{\partial f}{\partial z_1}}_{24} \underbrace{\frac{\partial z_1}{\partial a}}_{1} = 24$$

Symbolic differentiation

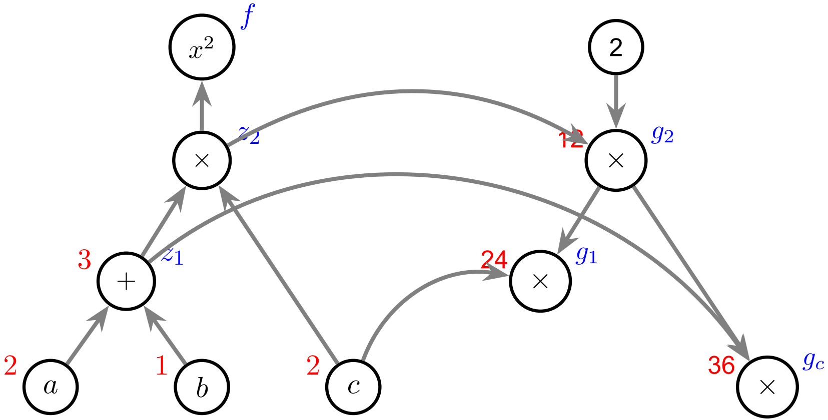
$$g_2 = \frac{\partial f}{\partial z_2} = 2 \cdot z_2$$



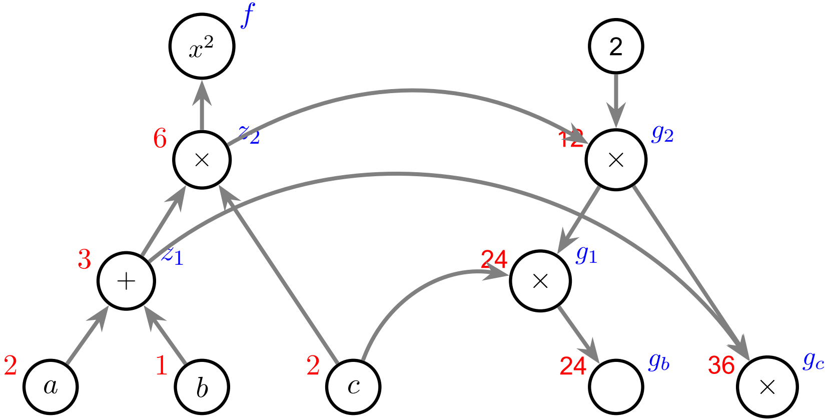
$$g_1 = \frac{\partial f}{\partial z_1} = \frac{\partial f}{\partial z_2} \underbrace{\frac{\partial z_2}{\partial z_1}}_{c}$$



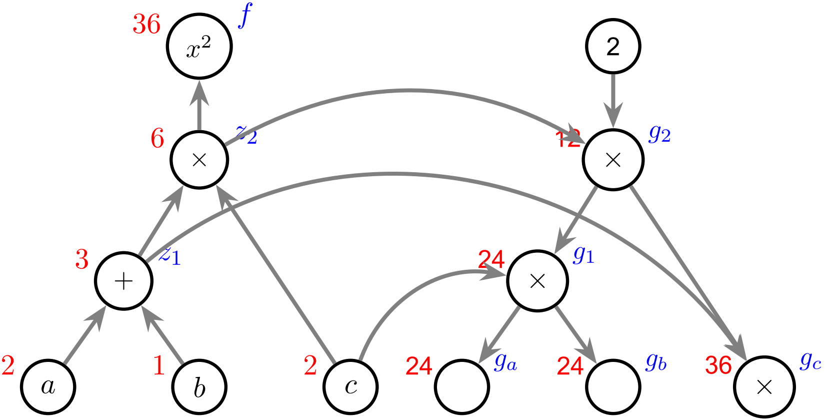
$$g_c = \frac{\partial f}{\partial c} = \frac{\partial f}{\partial z_2} \underbrace{\frac{\partial z_2}{\partial c}}_{z_1}$$



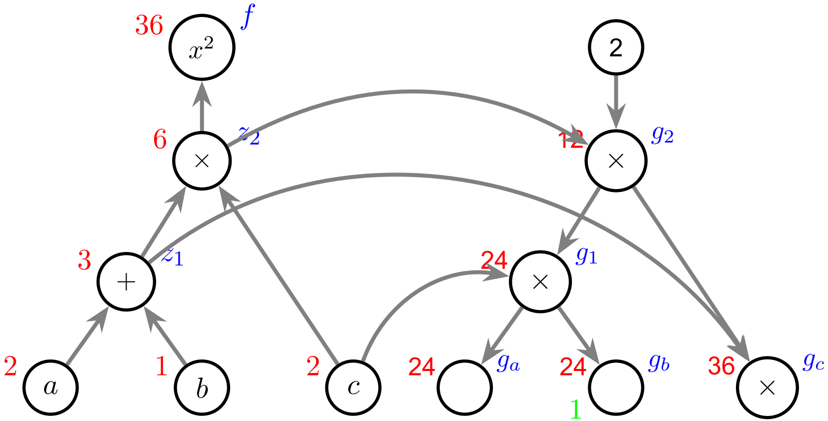
$$g_b = \frac{\partial f}{\partial b} = \frac{\partial f}{\partial z_1} \underbrace{\frac{\partial z_1}{\partial b}}_{1}$$



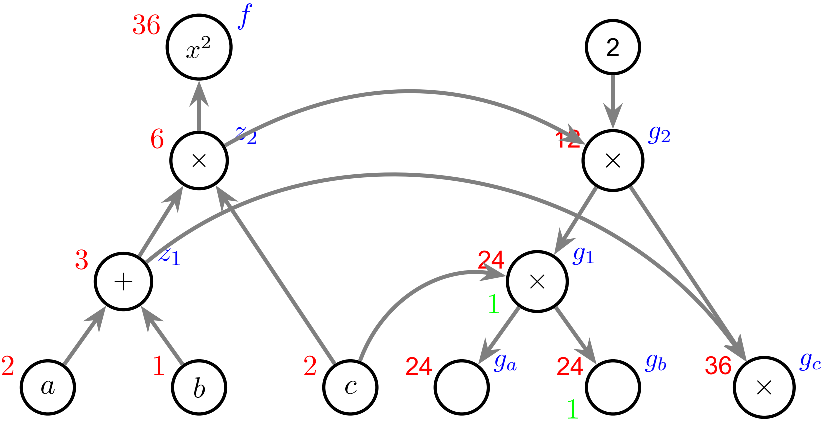
$$g_a = \frac{\partial f}{\partial a} = \frac{\partial f}{\partial z_1} \underbrace{\frac{\partial z_1}{\partial a}}_{1}$$



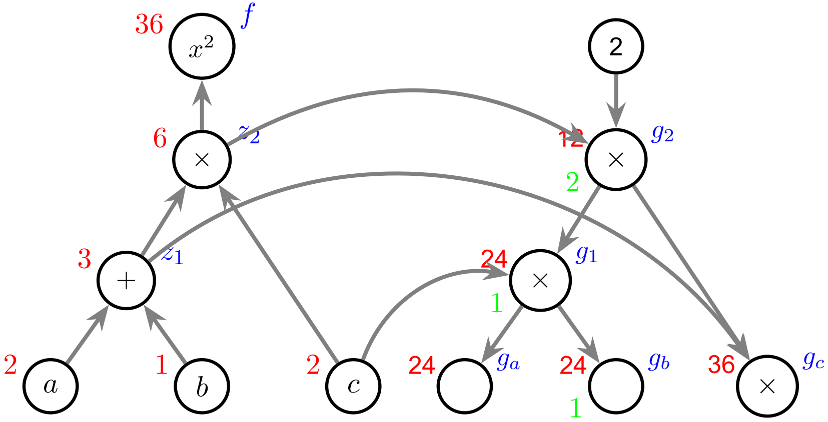
$$\frac{\partial g_b}{\partial g_b} = 1$$



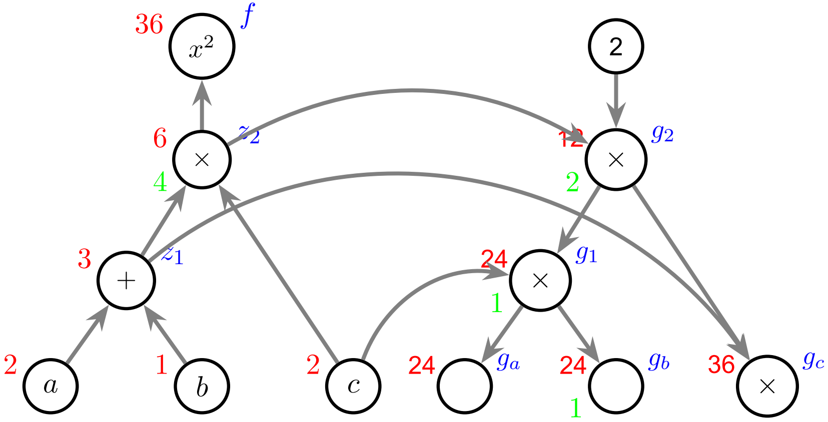
$$\frac{\partial g_b}{\partial g_1} = \frac{\partial g_b}{\partial g_b} = 1$$



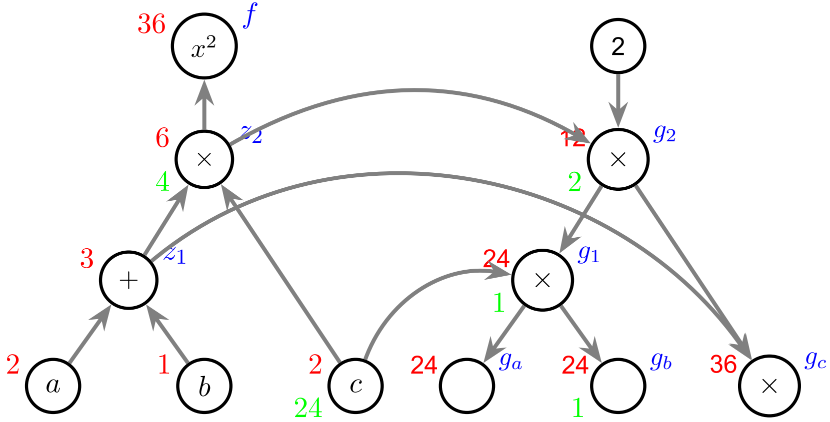
$$\frac{\partial g_b}{\partial g_2} = \underbrace{\frac{\partial g_b}{\partial g_1}}_{1} \underbrace{\frac{\partial g_1}{\partial g_2}}_{c} = 2$$



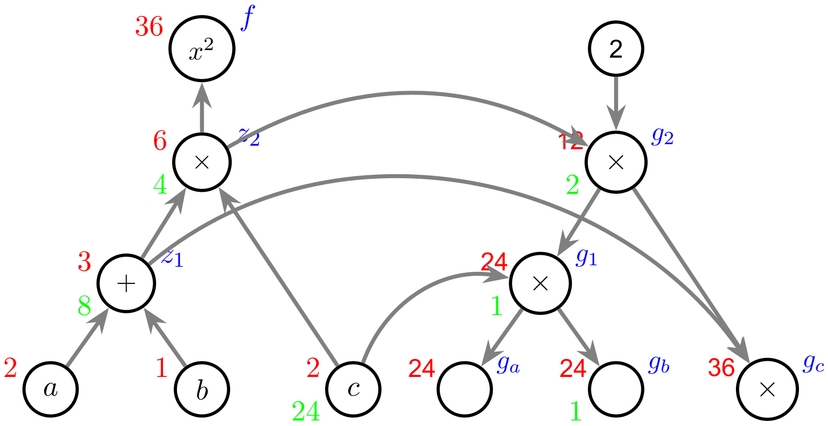
$$\frac{\partial g_b}{\partial z_2} = \underbrace{\frac{\partial g_b}{\partial g_2}}_{2} \underbrace{\frac{\partial g_2}{\partial z_2}}_{2} = 4$$



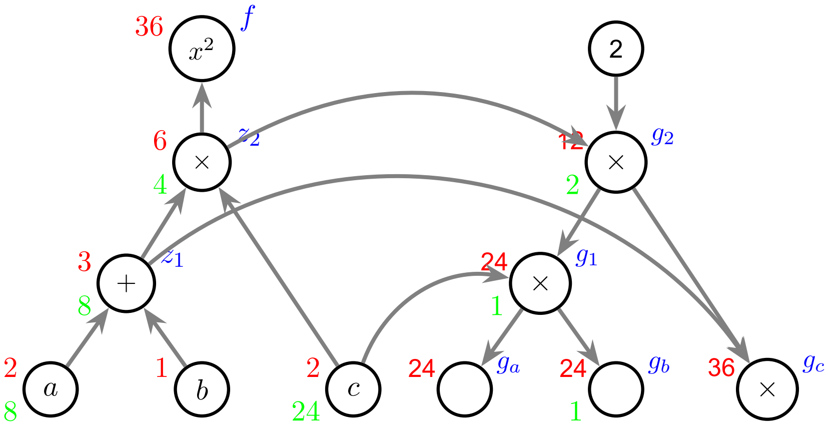
$$\frac{\partial g_b}{\partial c} = \underbrace{\frac{\partial g_b}{\partial z_2}}_{4}\underbrace{\frac{\partial z_2}{\partial c}}_{z_1} + \underbrace{\frac{\partial g_b}{\partial g_1}}_{1}\underbrace{\frac{\partial g_1}{\partial c}}_{g_2} = 4{\cdot}3+1{\cdot}12 = 24$$



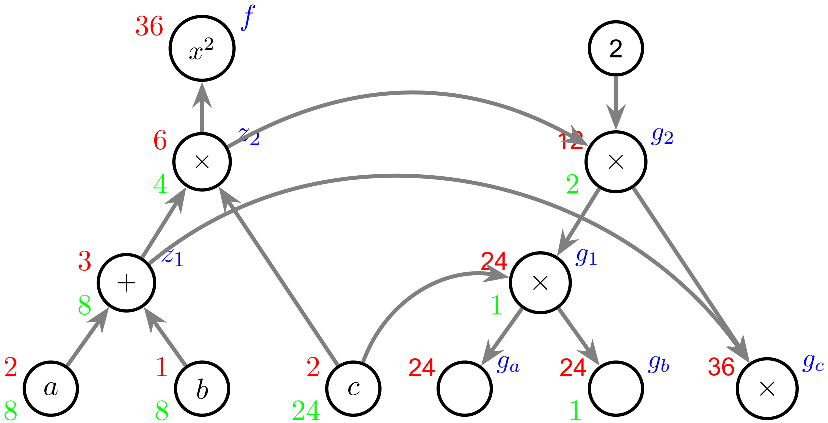
$$\frac{\partial g_b}{\partial z_1} = \underbrace{\frac{\partial g_b}{\partial z_2}}_{4} \underbrace{\frac{\partial z_2}{\partial z_1}}_{c} = 8$$



$$\frac{\partial g_b}{\partial a} = \underbrace{\frac{\partial g_b}{\partial z_1}}_{8} \underbrace{\frac{\partial z_1}{\partial a}}_{1} = 8$$



$$\frac{\partial g_b}{\partial b} = \underbrace{\frac{\partial g_b}{\partial z_1}}_{8} \underbrace{\frac{\partial z_1}{\partial b}}_{1} = 8$$



Verification

$$f = ((a+b)c)^2$$

$$\frac{\partial f}{\partial b} = 2(a+b)c^2$$

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$$\frac{\partial f}{\partial b} = 2(a+b)c^2$$

$$\frac{\partial f}{\partial a \partial b} = 2c^2 = 8$$

$$\frac{\partial f}{\partial a \partial c} = 2(a+b)c = 12$$