Università degli Studi di Pavia

Deep Learning

03- Flow Graphs & Automatic Differentiation

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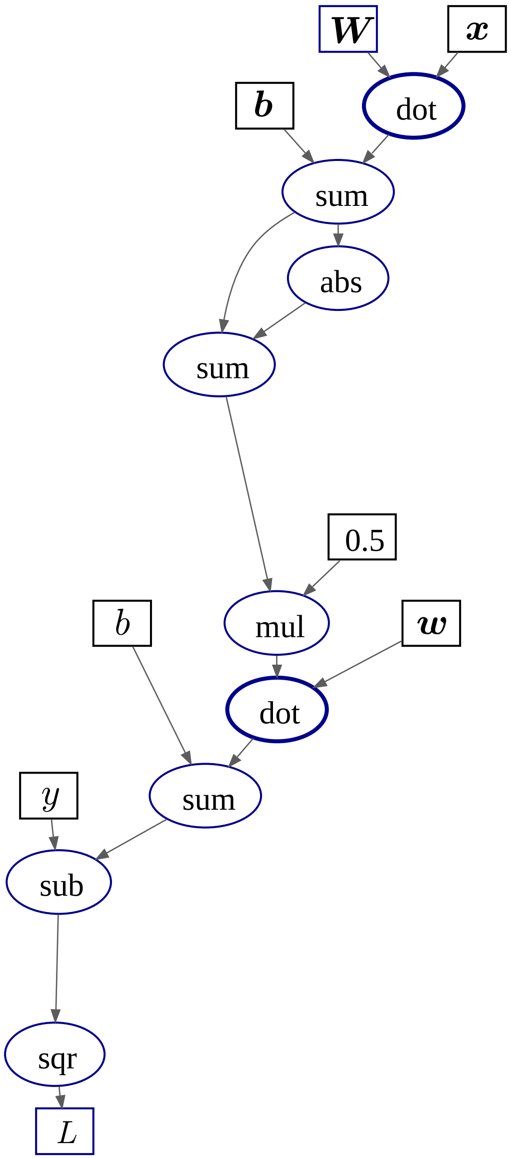
(*) Dipartimento di Matematica F. Casorati

This presentation can be downloaded at:
http://vision.unipv.it/DL

Flow Graphs

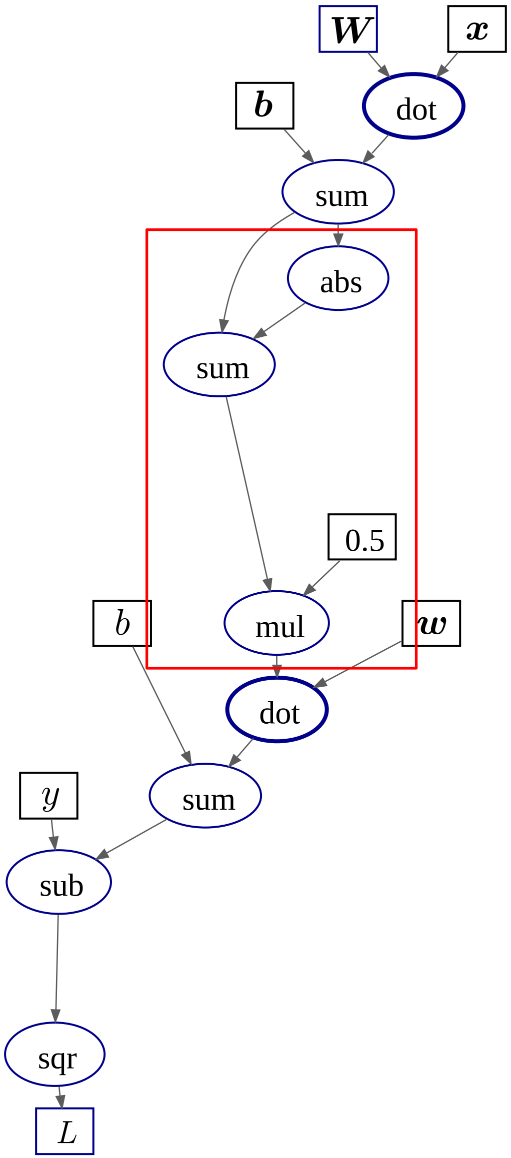
An aside: Flow Graph



$$L(\tilde{y}, y) = (\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

Item-wise loss function, with ReLU as non-linearity

An aside: Flow Graph



$$L(\tilde{y}, y) = (\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

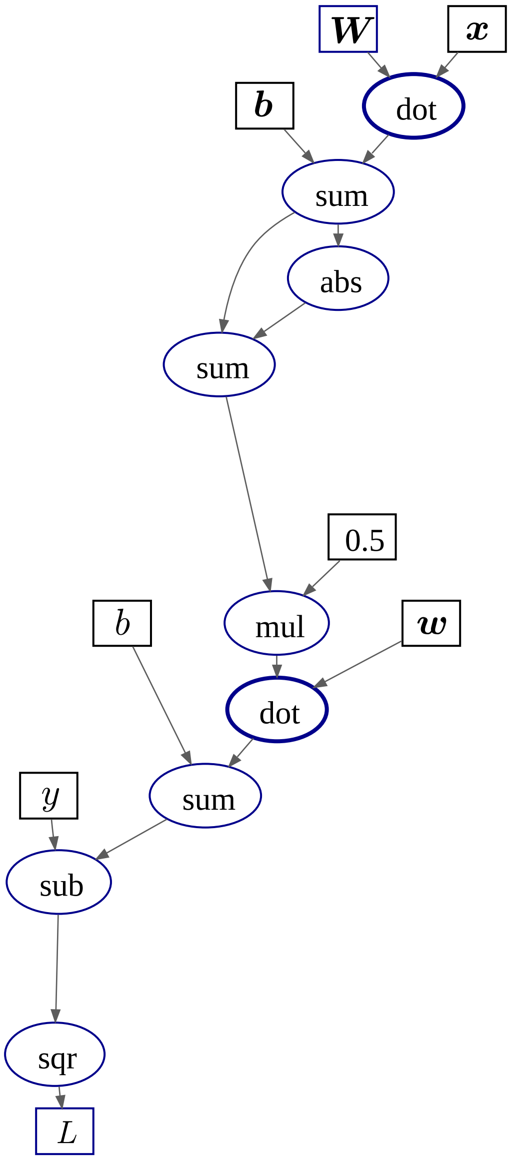
Item-wise loss function, with ReLU as non-linearity

$$\mathrm{ReLU}(x) := \max(0, x)$$

$$\mathrm{ReLU}(x) = \frac{1}{2}(x + |x|)$$

(equivalent expression)

An aside: Flow Graph



- ***Computing the Flow Graph***

$$L(\tilde{y}, y) = (\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

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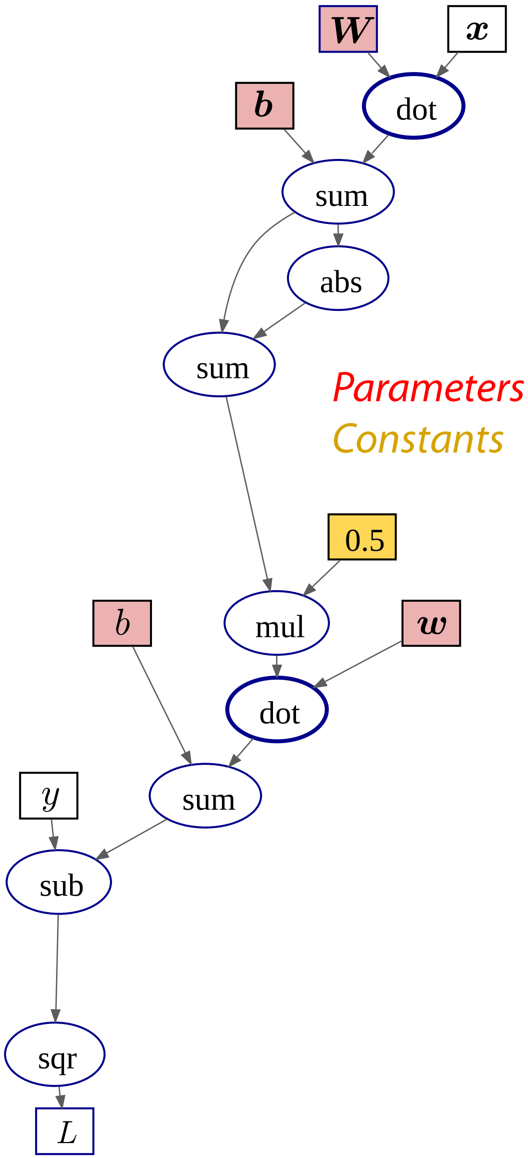

Parameters
Constants

- **Computing the Flow Graph**

$$L(\tilde{y}, y) = (\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

Item-wise loss, with ReLU as non-linearity

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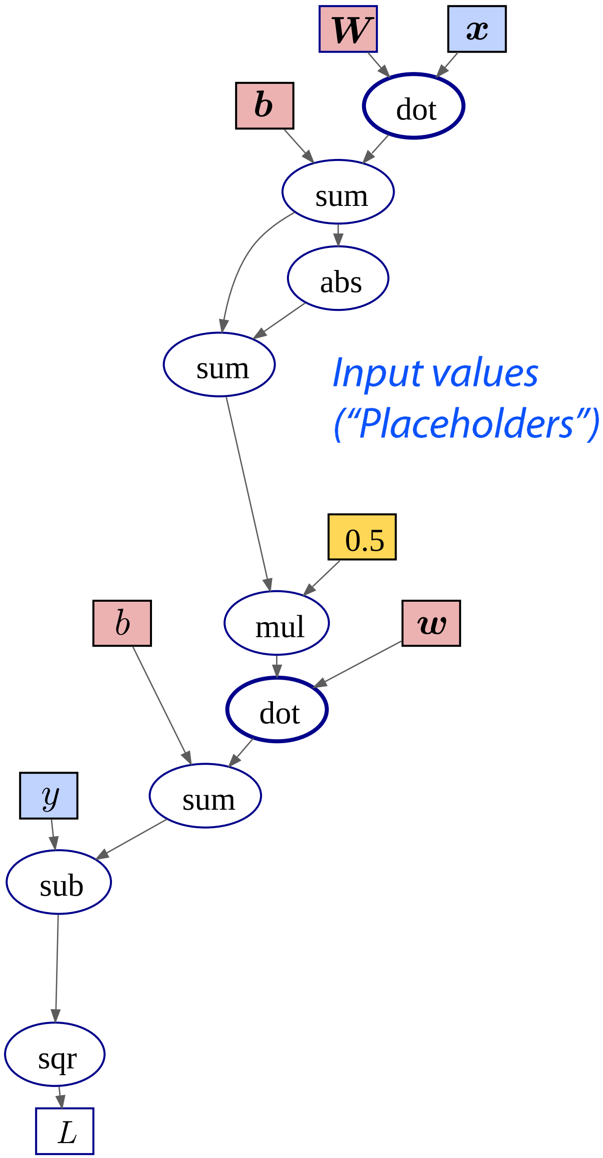

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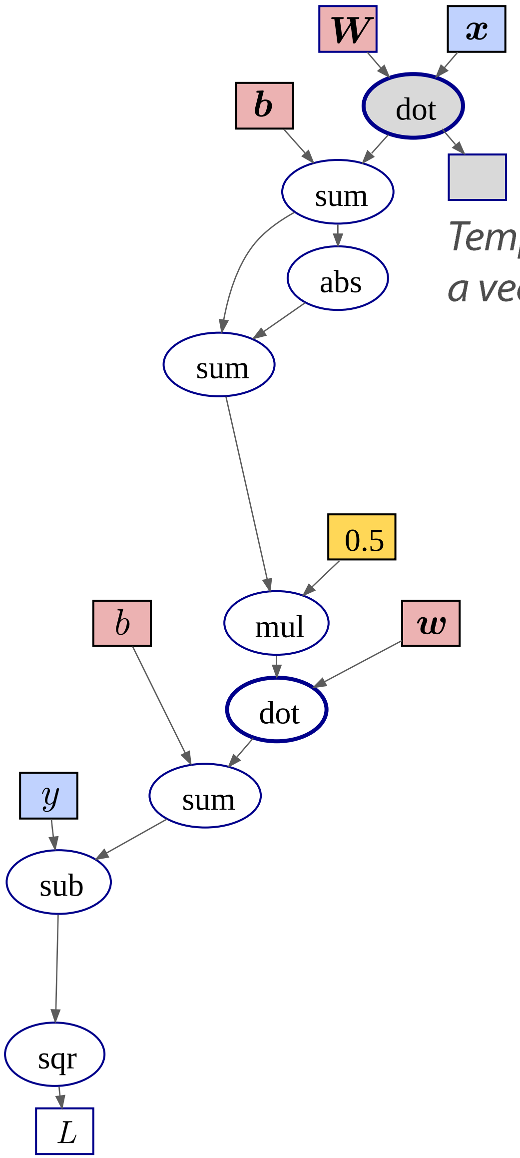

Temp value: a vector

Computing the Flow Graph

$$L(\tilde{y}, y) = (\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

Item-wise loss, with ReLU as non-linearity

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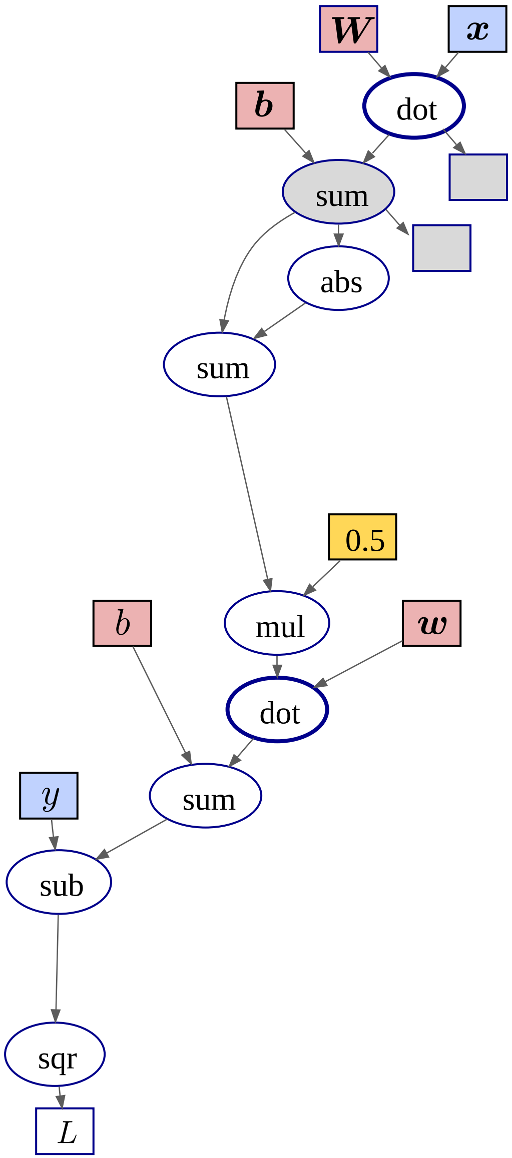

This is no longer necessary

- **Computing the Flow Graph**

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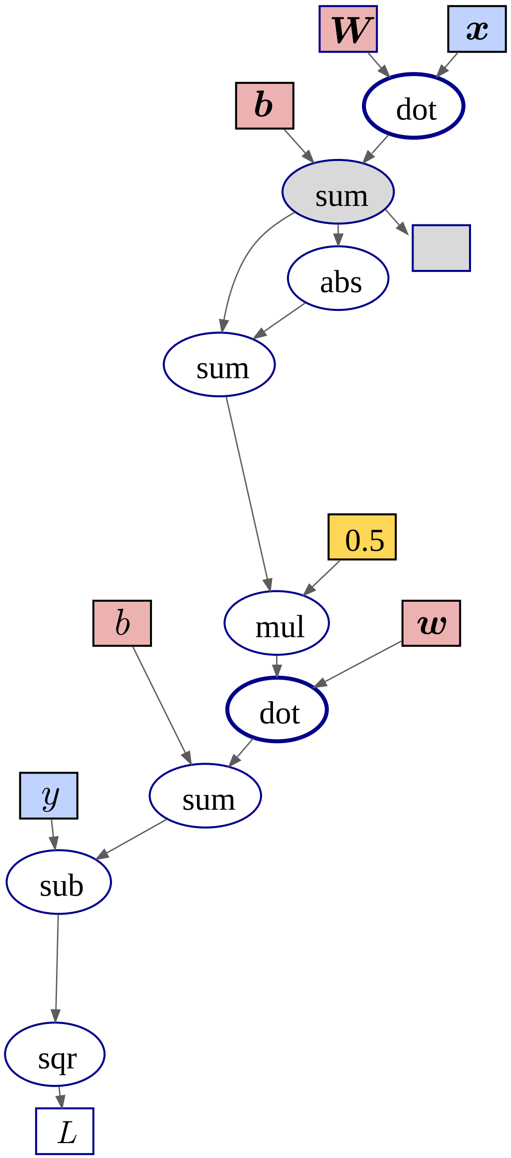

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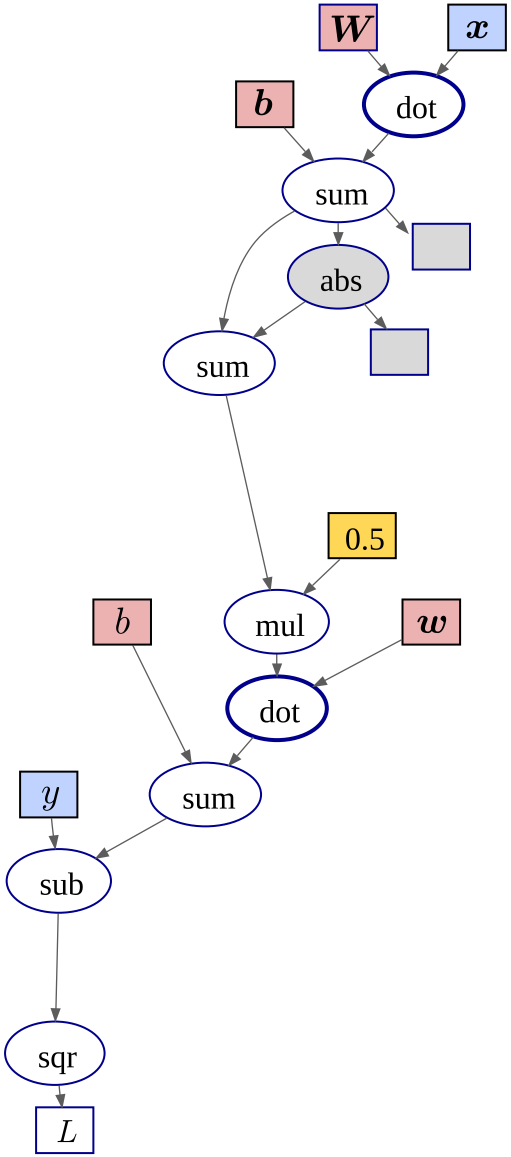

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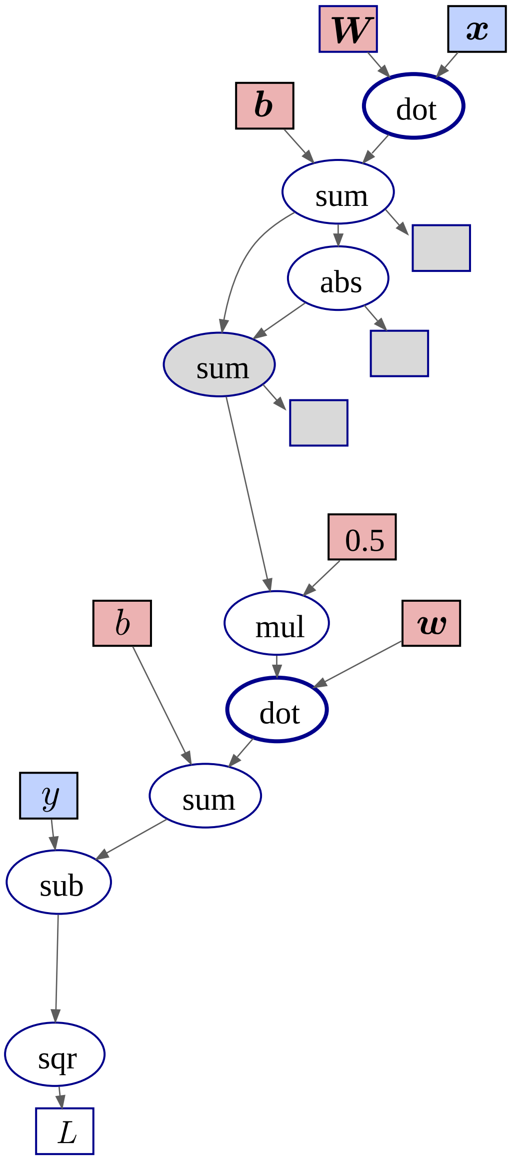

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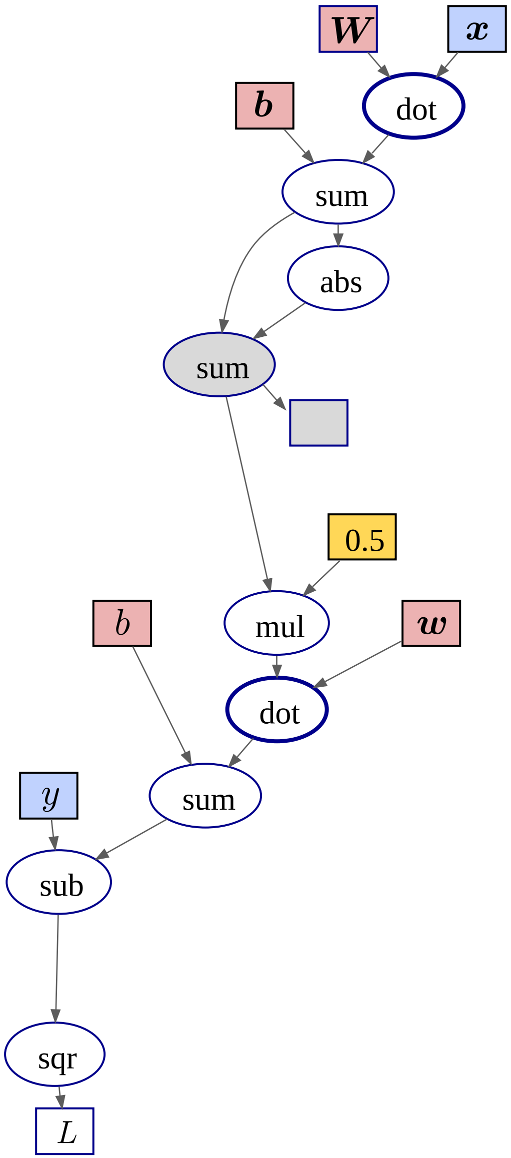

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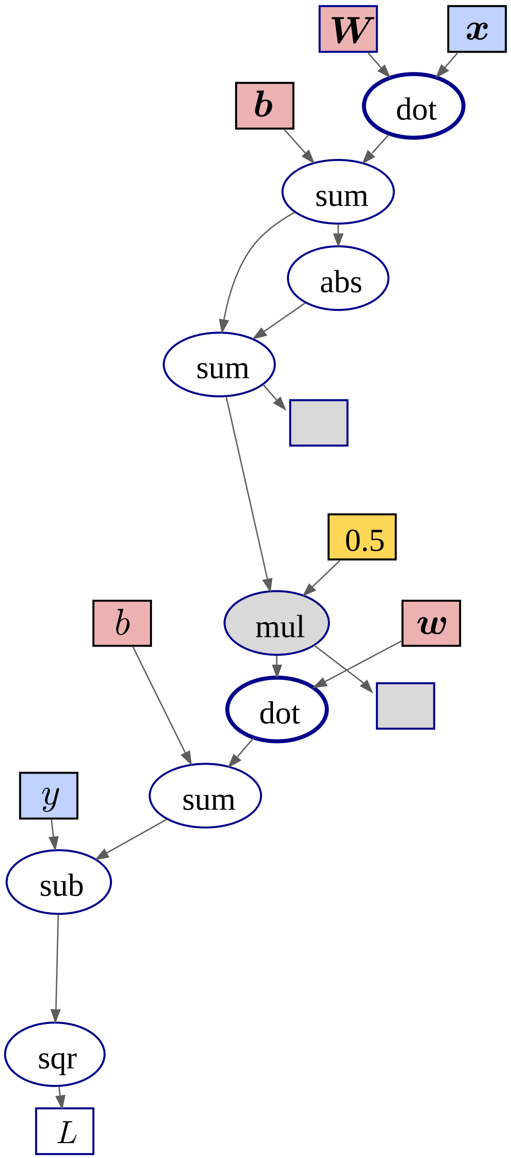

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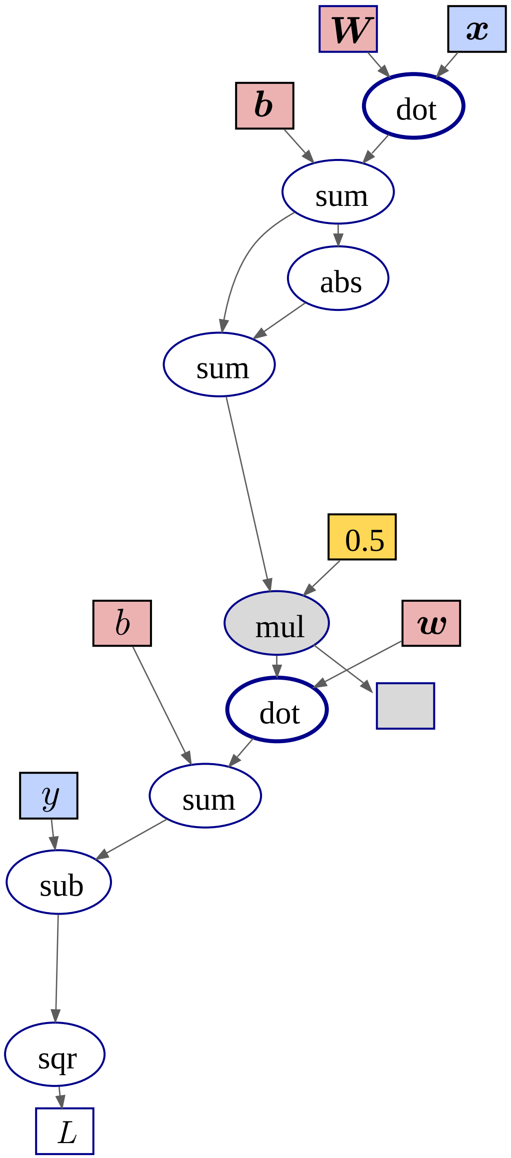

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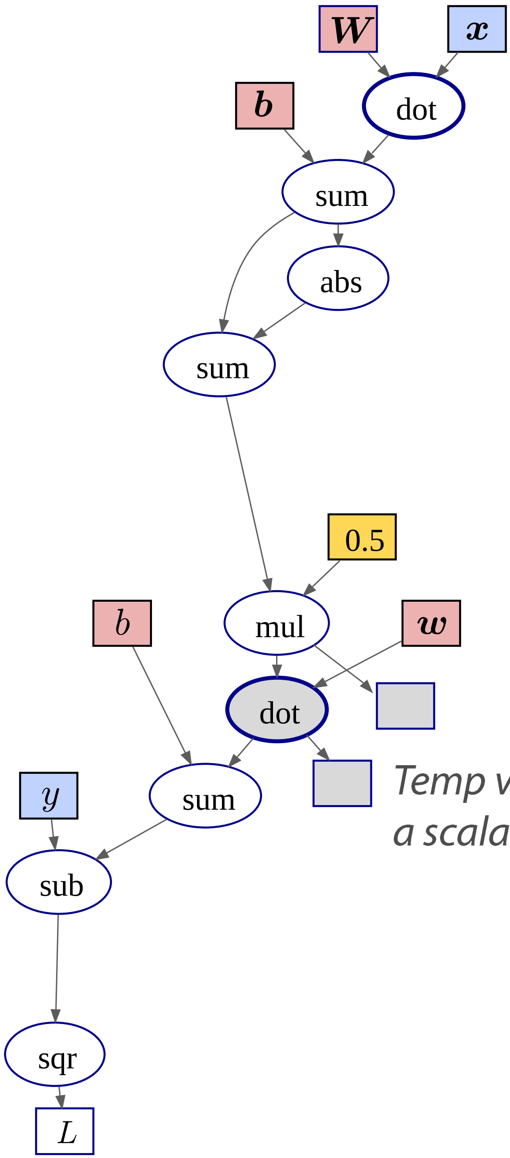

Temp value: a scalar

- ***Computing the Flow Graph***

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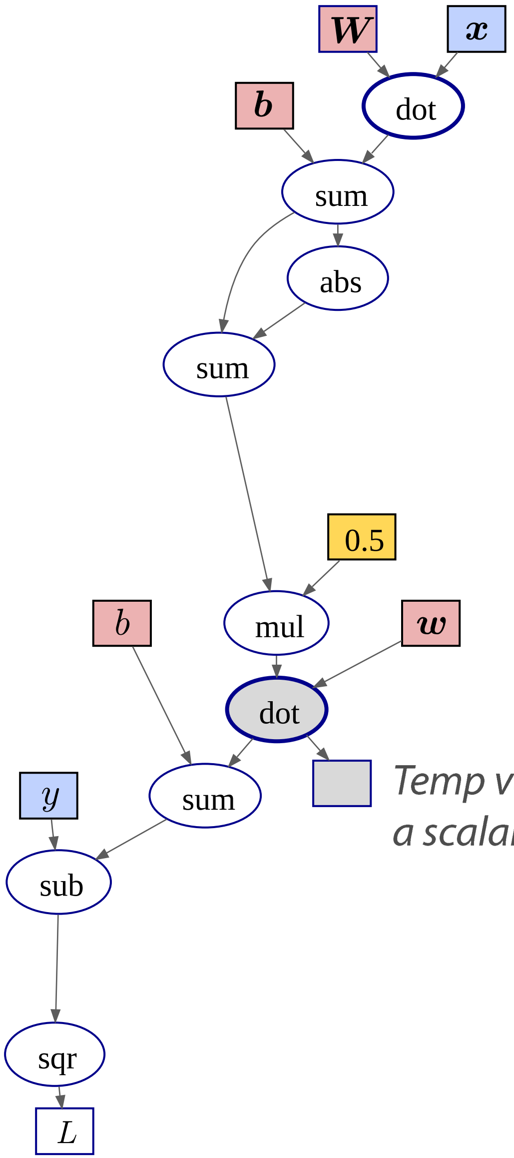

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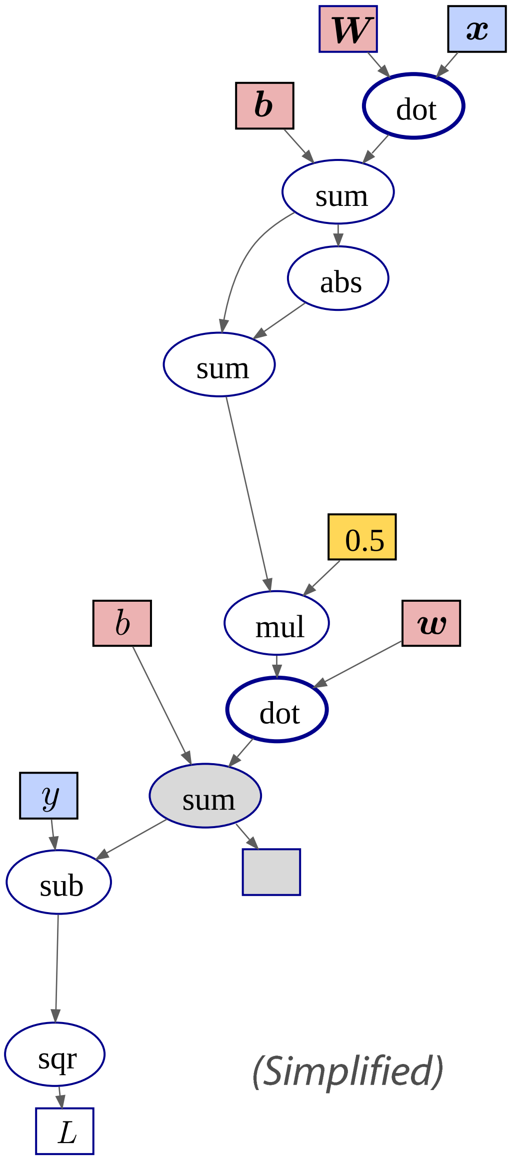

(Simplified)

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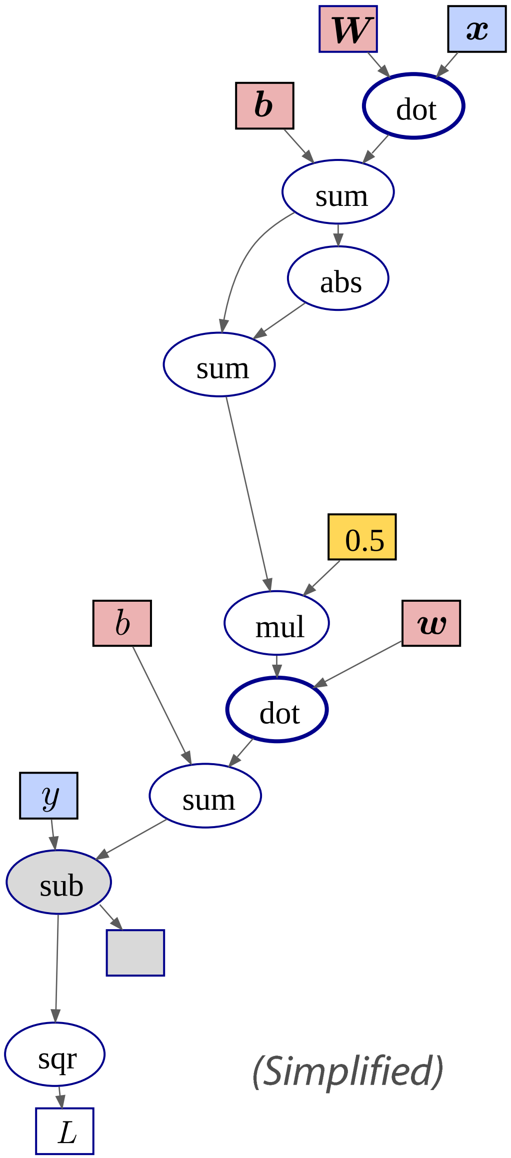

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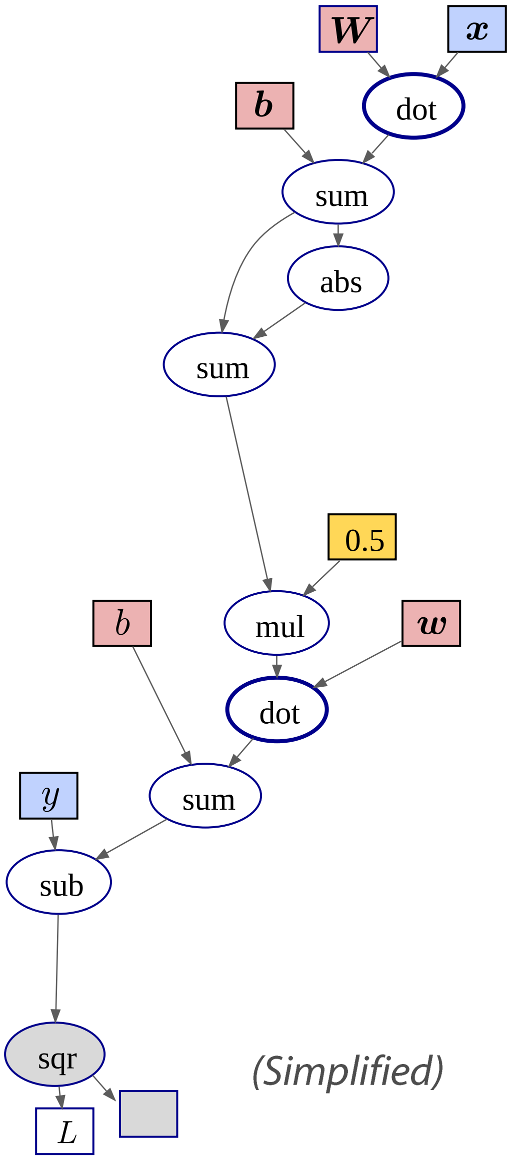

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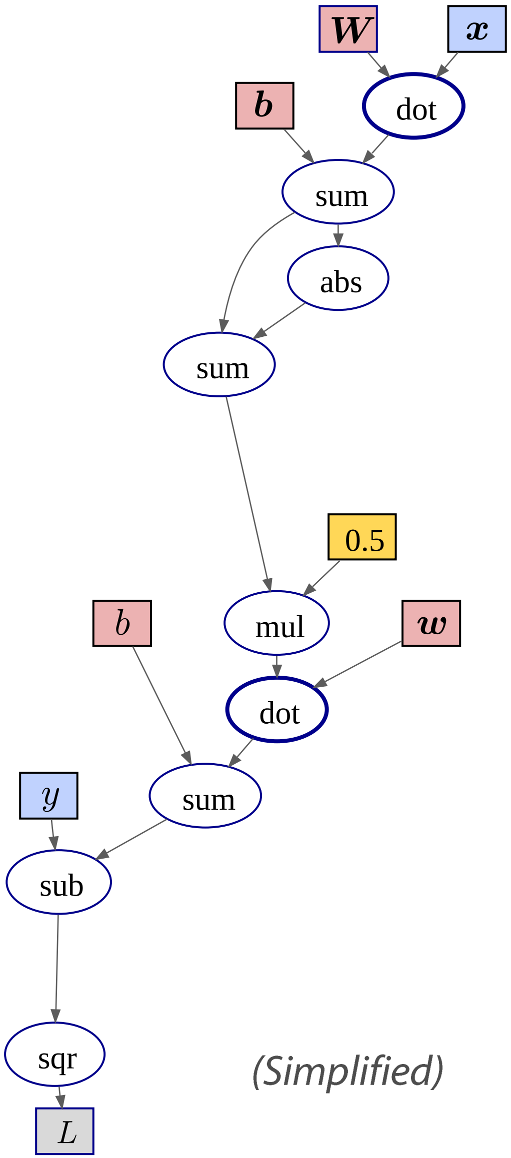

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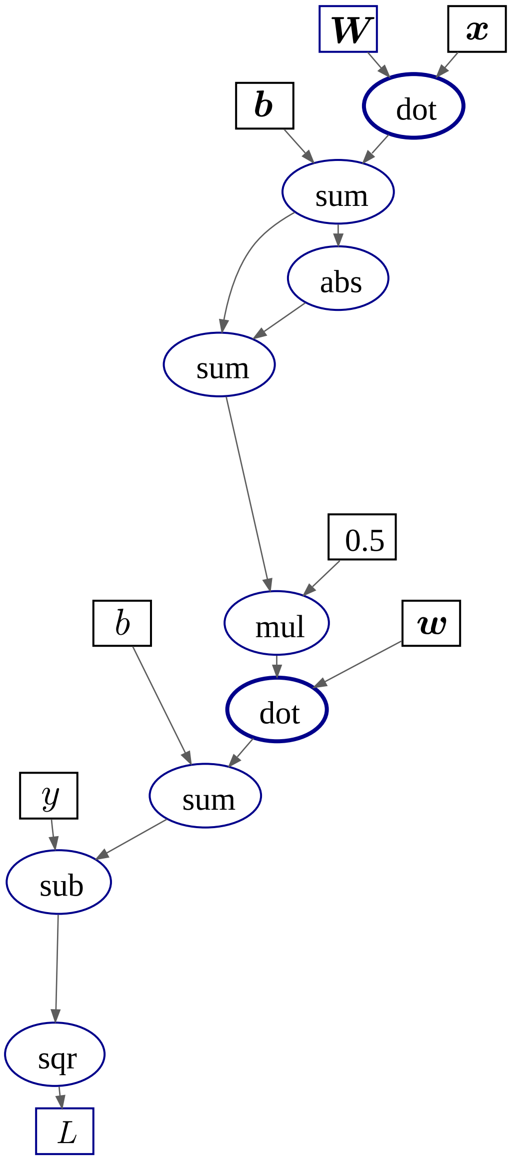
Automatic Differentiation of Flow Graphs (as Reverse Accumulation)

Computing Gradients

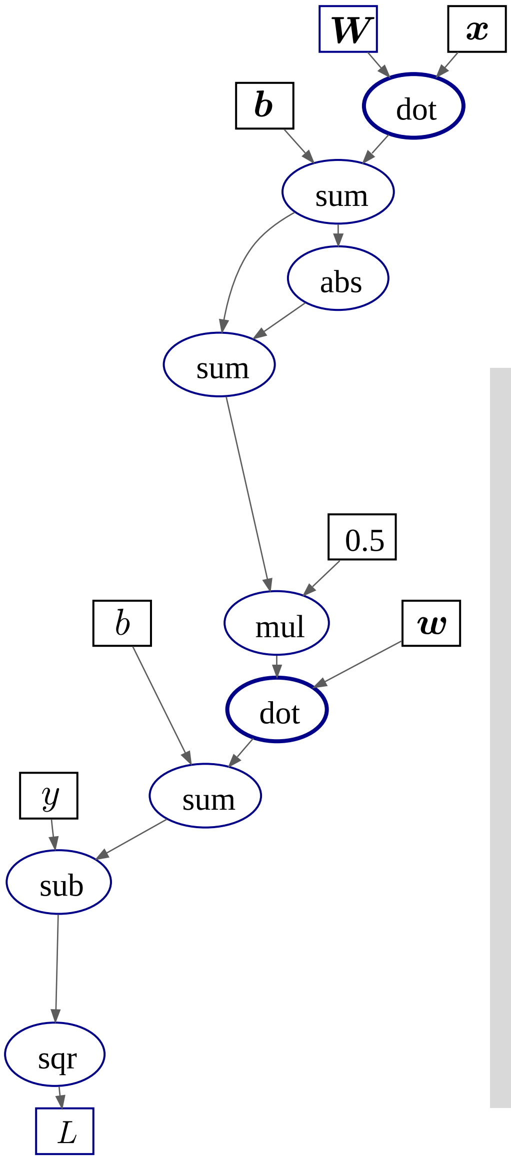


- ***Computing one gradient of the flow graph***

$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

This is the gradient we want to compute (remember this is just one of the four)

Computing Gradients



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Chain rule for derivatives (*single argument*)

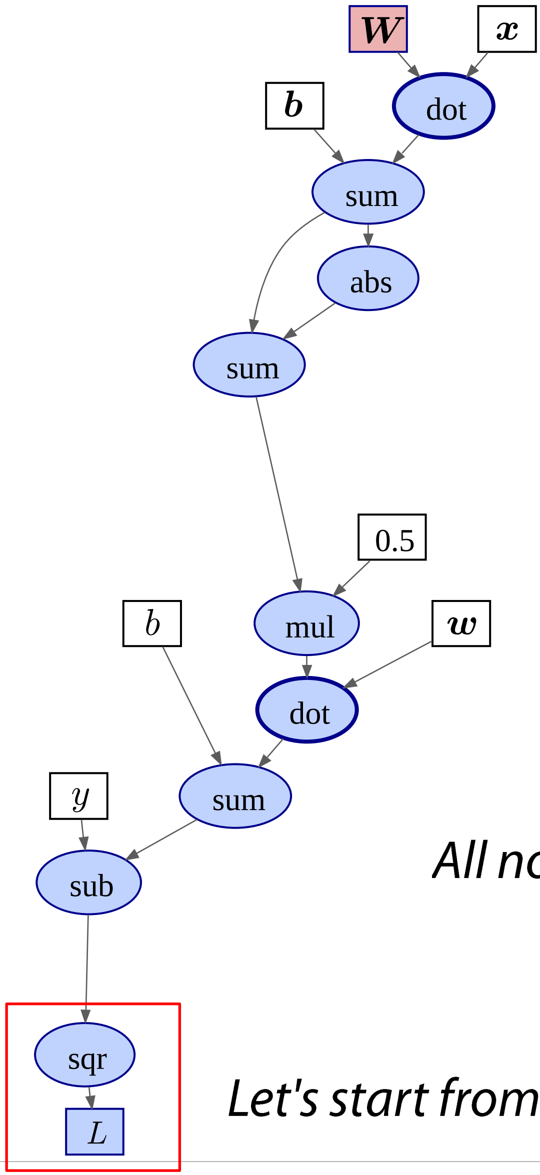
$$\frac{\partial}{\partial \boldsymbol{\vartheta}} f(g(\boldsymbol{\vartheta})) = \frac{\partial}{\partial g(\boldsymbol{\vartheta})} f(g(\boldsymbol{\vartheta})) \frac{\partial}{\partial \boldsymbol{\vartheta}} g(\boldsymbol{\vartheta})$$

Chain rule for derivatives (*multiple arguments*)

$$\frac{\partial}{\partial \boldsymbol{\vartheta}} f(g(\boldsymbol{\vartheta}), h(\boldsymbol{\vartheta})) =$$

$$\frac{\partial}{\partial g(\boldsymbol{\vartheta})} f(g(\boldsymbol{\vartheta}), h(\boldsymbol{\vartheta})) \frac{\partial}{\partial \boldsymbol{\vartheta}} g(\boldsymbol{\vartheta}) \; + \; \frac{\partial}{\partial h(\boldsymbol{\vartheta})} f(g(\boldsymbol{\vartheta}), h(\boldsymbol{\vartheta})) \frac{\partial}{\partial \boldsymbol{\vartheta}} h(\boldsymbol{\vartheta})$$

Computing Gradients

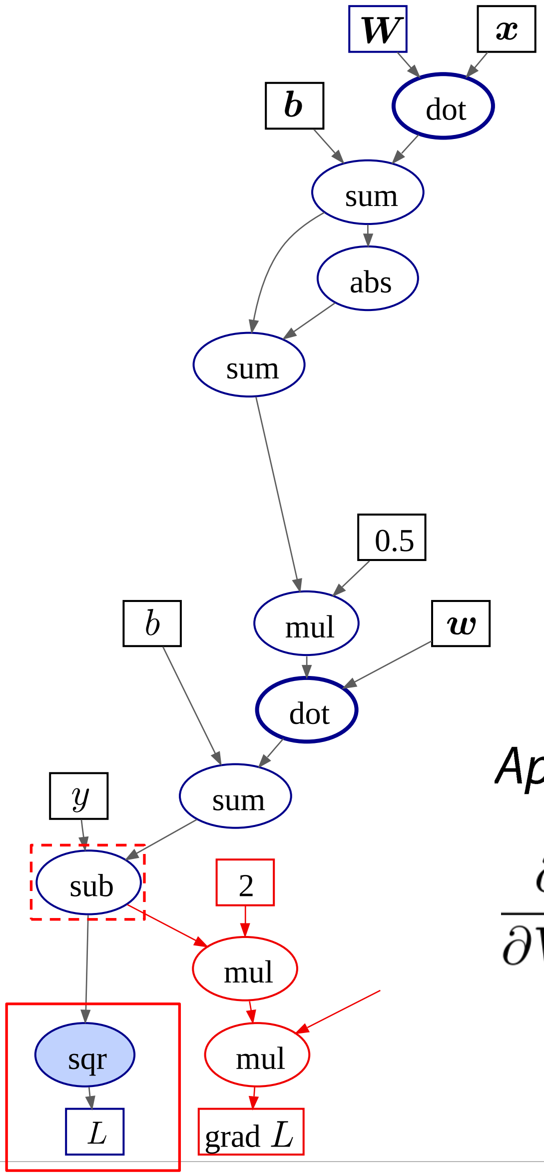


$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

All nodes depending on $\boldsymbol{W}$ are marked in blue

*Let's start from here (i.e. **backpropagation**, a.k.a. **reverse accumulation**)*

Computing Gradients



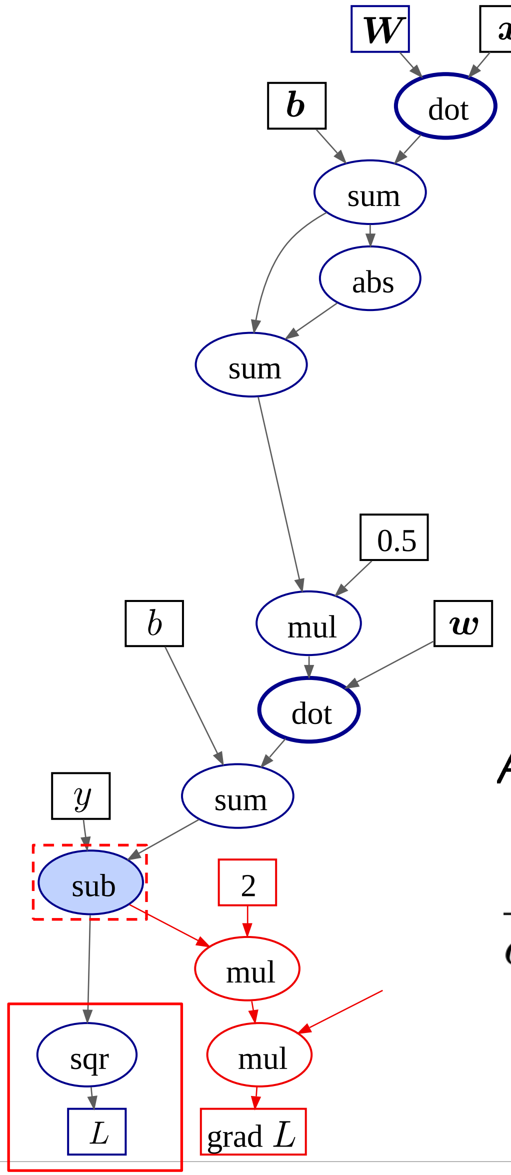
$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

Apply the chain rule to the sqr *node*

$$\frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})^2 = \frac{\partial}{\partial f(\boldsymbol{W})} f(\boldsymbol{W})^2 \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

$$= 2 \cdot f(\boldsymbol{W}) \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

Computing Gradients



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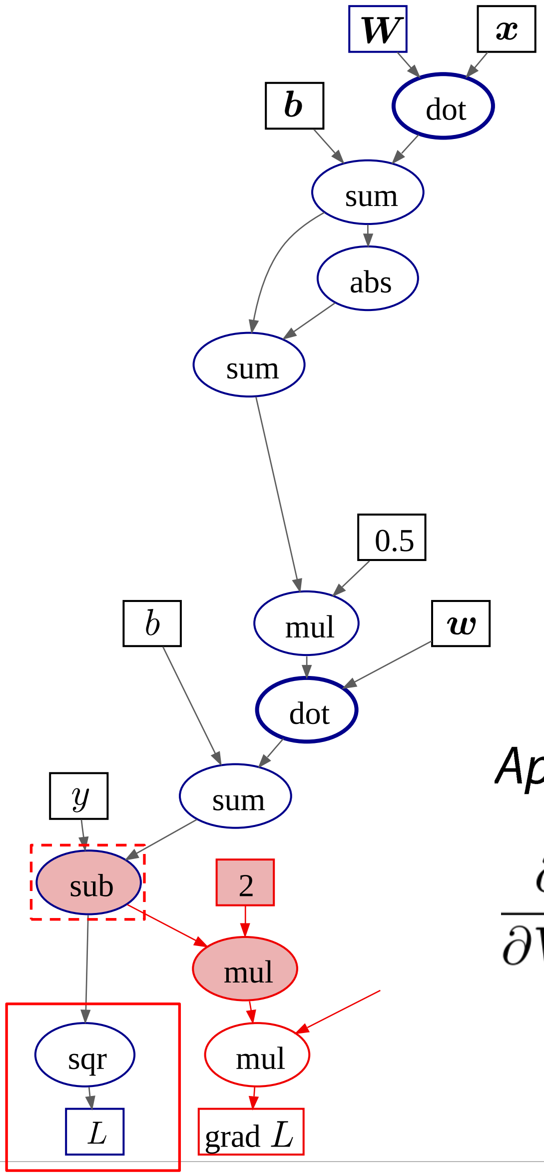
Computing Gradients



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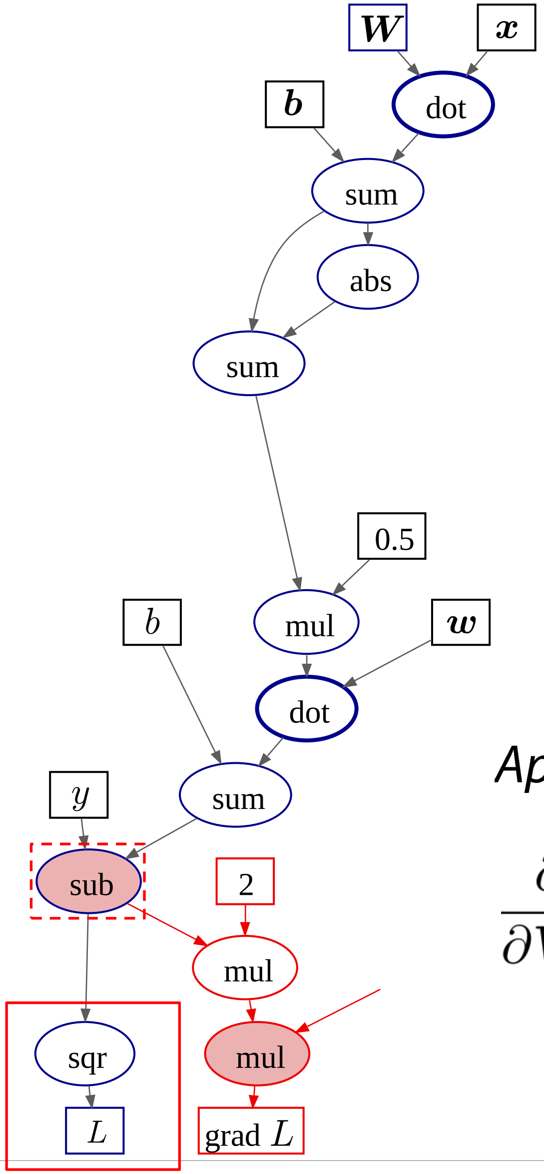
Computing Gradients



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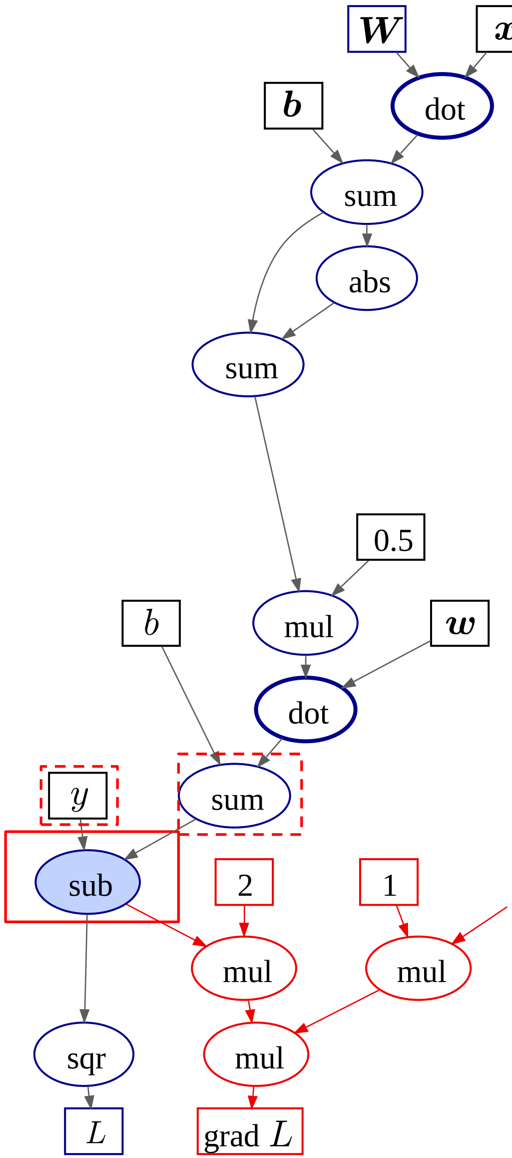
Computing Gradients

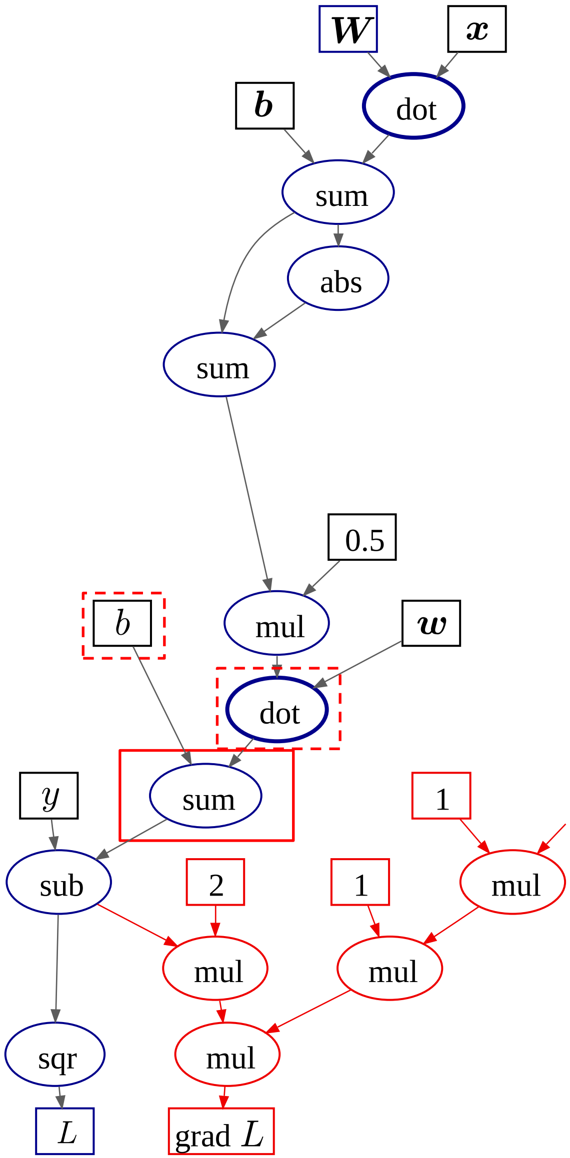


$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

$$\frac{\partial}{\partial \boldsymbol{W}}(f(\boldsymbol{W}) - y) = \frac{\partial}{\partial f(\boldsymbol{W})}(f(\boldsymbol{W}) - y)\frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

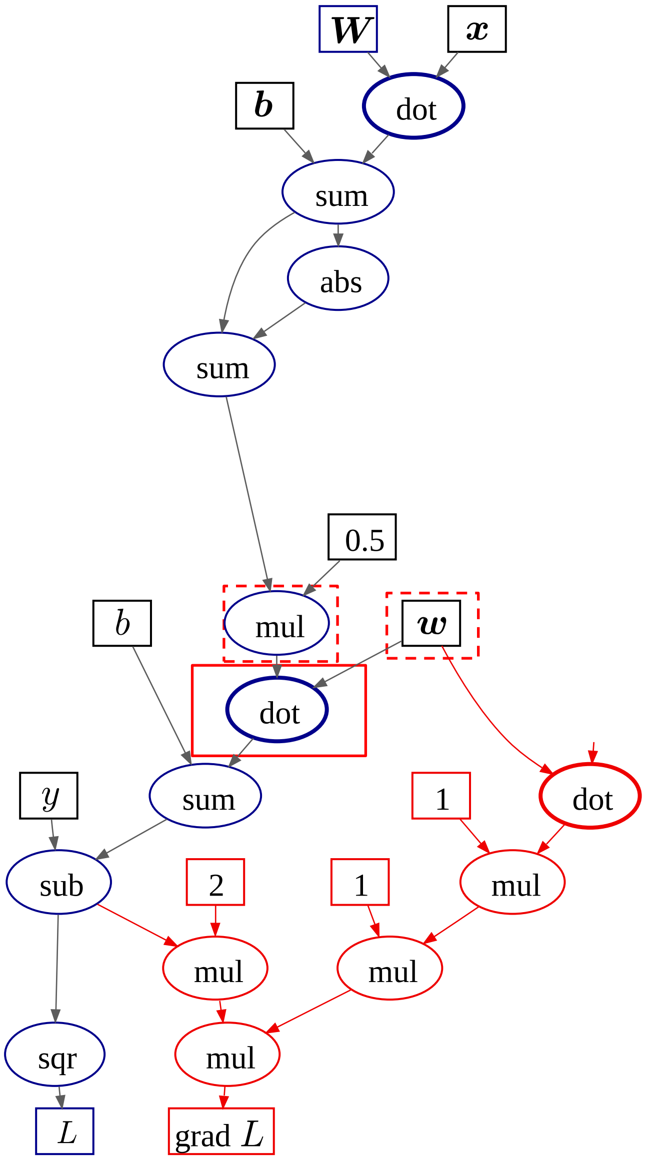
$$= 1 \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

Computing Gradients



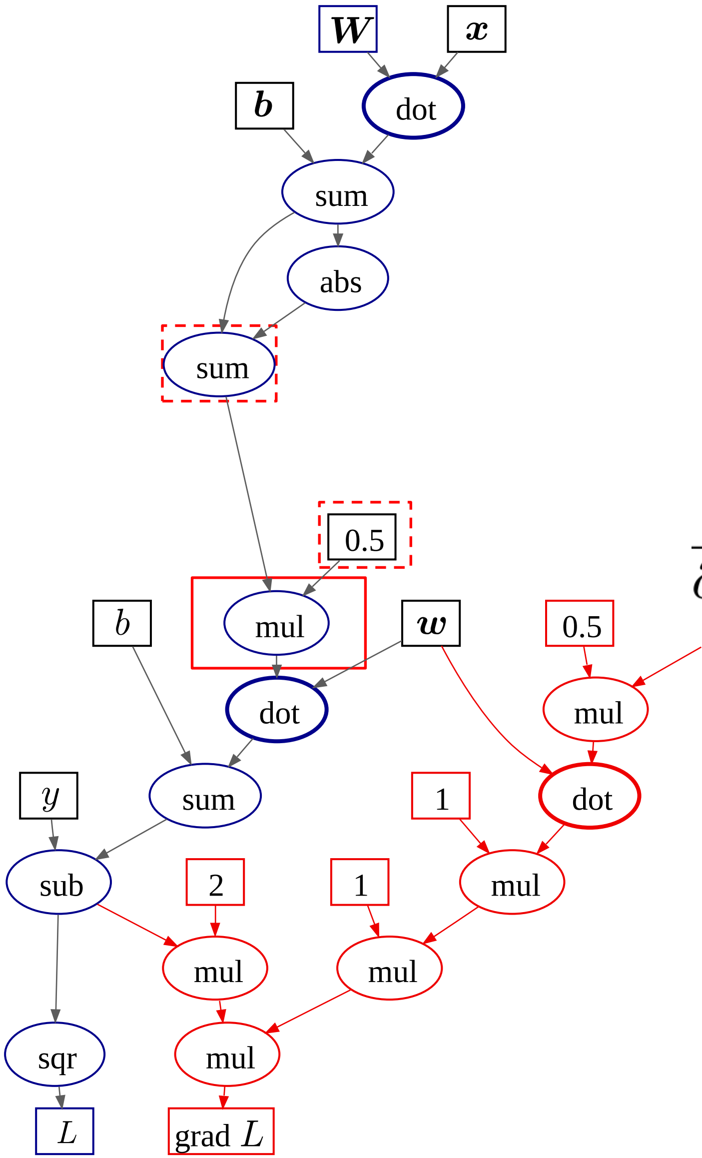
$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

$$\frac{\partial}{\partial \boldsymbol{W}}(f(\boldsymbol{W}) + b) = \frac{\partial}{\partial f(\boldsymbol{W})}(f(\boldsymbol{W}) + b)\frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$
$$= 1 \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$



$$\frac{\partial}{\partial \boldsymbol{W}} (\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

$$\begin{aligned}\frac{\partial}{\partial \boldsymbol{W}} (\boldsymbol{w} \cdot f(\boldsymbol{W})) &= \frac{\partial}{\partial f(\boldsymbol{W})} (\boldsymbol{w} \cdot f(\boldsymbol{W})) \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W}) \\ &= \boldsymbol{w} \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})\end{aligned}$$

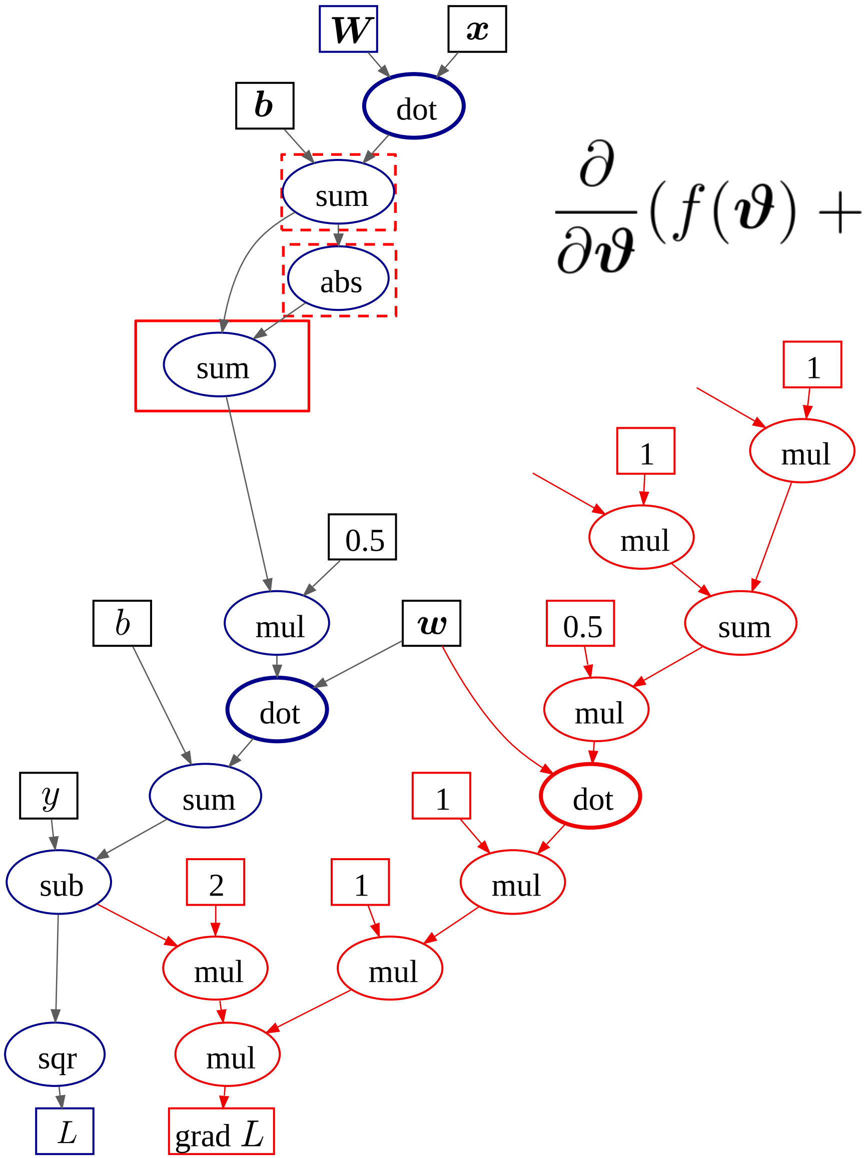


$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

$$\frac{\partial}{\partial \boldsymbol{W}}(0.5 \cdot f(\boldsymbol{W})) = \frac{\partial}{\partial f(\boldsymbol{W})}(0.5 \cdot f(\boldsymbol{W}))\frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

$$= 0.5 \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

Computing Gradients

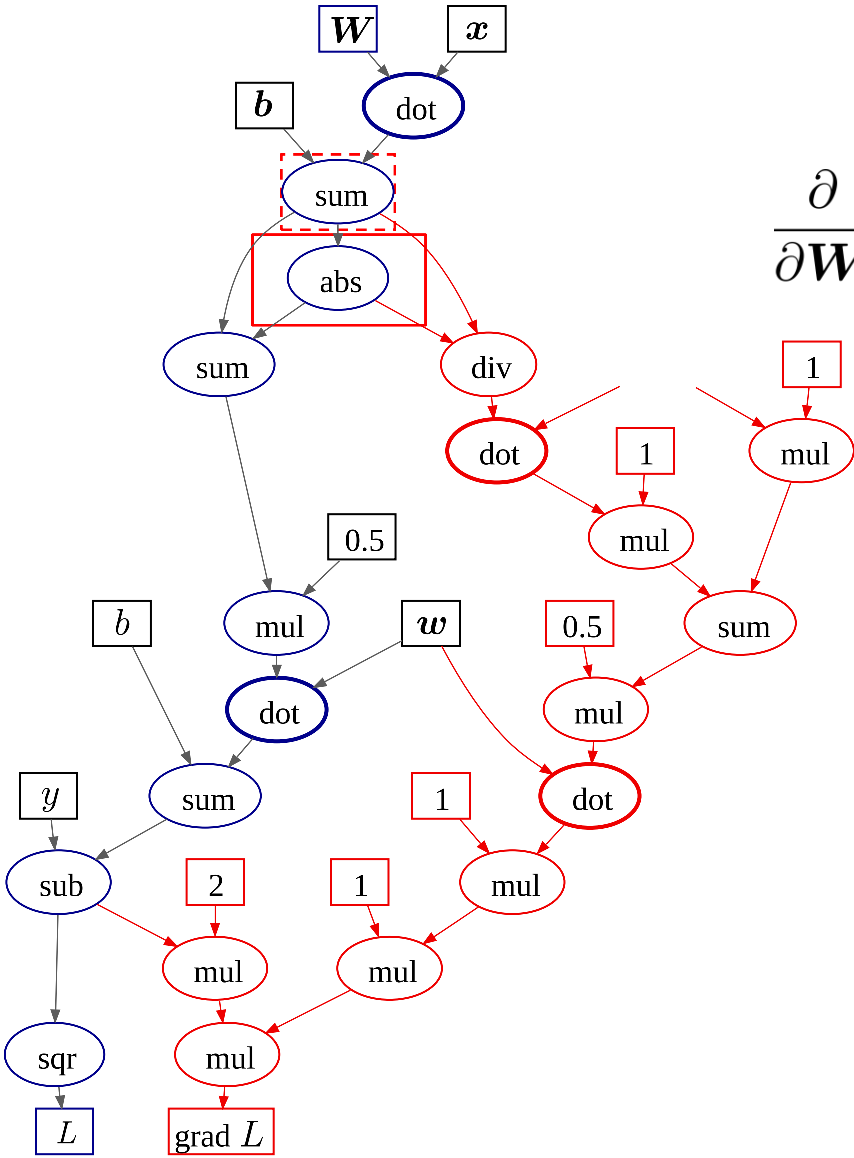


$$\frac{\partial}{\partial \boldsymbol{\vartheta}}(f(\boldsymbol{\vartheta}) + g(\boldsymbol{\vartheta})) = \frac{\partial}{\partial f(\boldsymbol{\vartheta})}(f(\boldsymbol{\vartheta}) + g(\boldsymbol{\vartheta}))\frac{\partial}{\partial \boldsymbol{\vartheta}} f(\boldsymbol{\vartheta})$$

$$+ \frac{\partial}{\partial g(\boldsymbol{\vartheta})}(f(\boldsymbol{\vartheta}) + g(\boldsymbol{\vartheta}))\frac{\partial}{\partial \boldsymbol{\vartheta}} g(\boldsymbol{\vartheta})$$

$$= 1 \cdot \frac{\partial}{\partial \boldsymbol{\vartheta}} f(\boldsymbol{\vartheta}) + 1 \cdot \frac{\partial}{\partial \boldsymbol{\vartheta}} g(\boldsymbol{\vartheta})$$

Computing Gradients



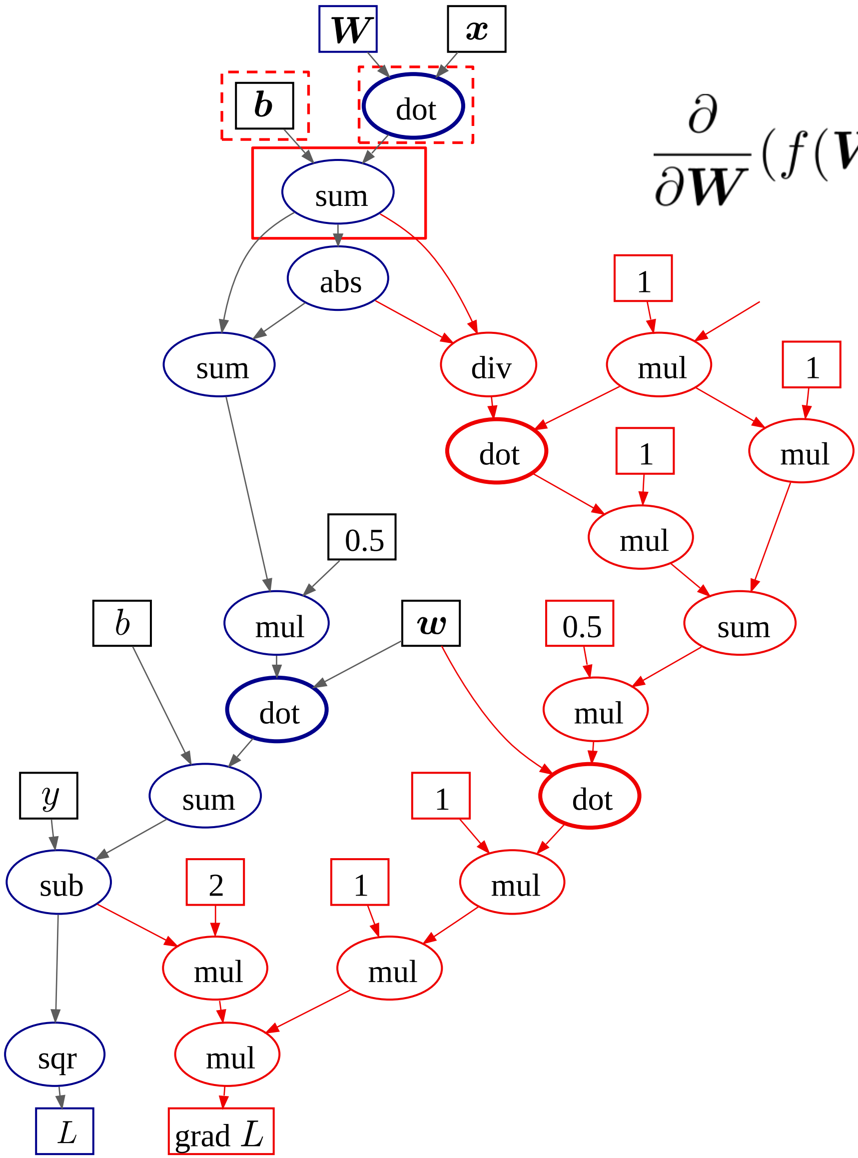
$$\frac{\partial}{\partial \boldsymbol{W}} |f(\boldsymbol{W})| = \frac{\partial}{\partial f(\boldsymbol{W})} |f(\boldsymbol{W})| \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

$$= \frac{f(\boldsymbol{W})}{|f(\boldsymbol{W})|} \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

Clearly, this term is not defined for any $W_{ij} = 0$

(Typically, this is a *protected* *division* $\frac{x}{0} := 1$ *)*

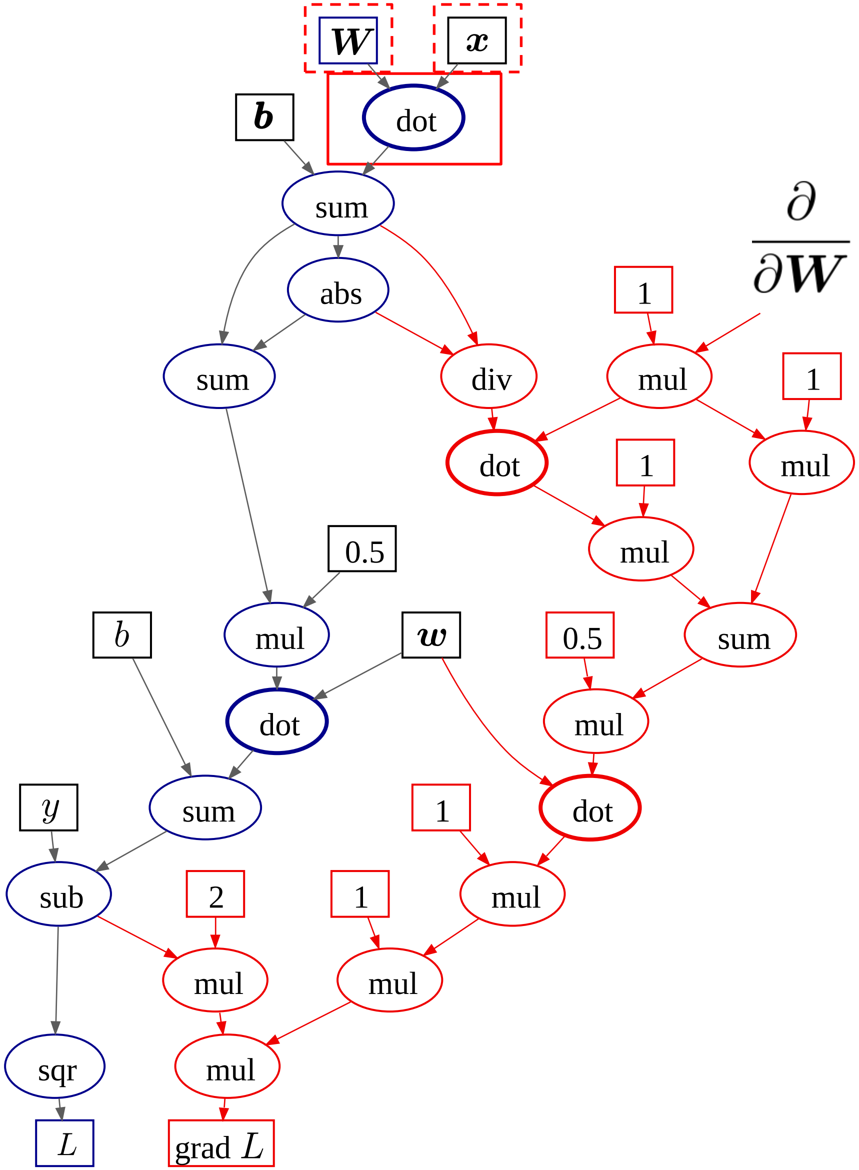
Computing Gradients



$$\frac{\partial}{\partial \boldsymbol{W}}(f(\boldsymbol{W}) + \boldsymbol{b}) = \frac{\partial}{\partial f(\boldsymbol{W})}(f(\boldsymbol{W}) + \boldsymbol{b}) \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

$$= 1 \cdot \frac{\partial}{\partial \boldsymbol{W}} f(\boldsymbol{W})$$

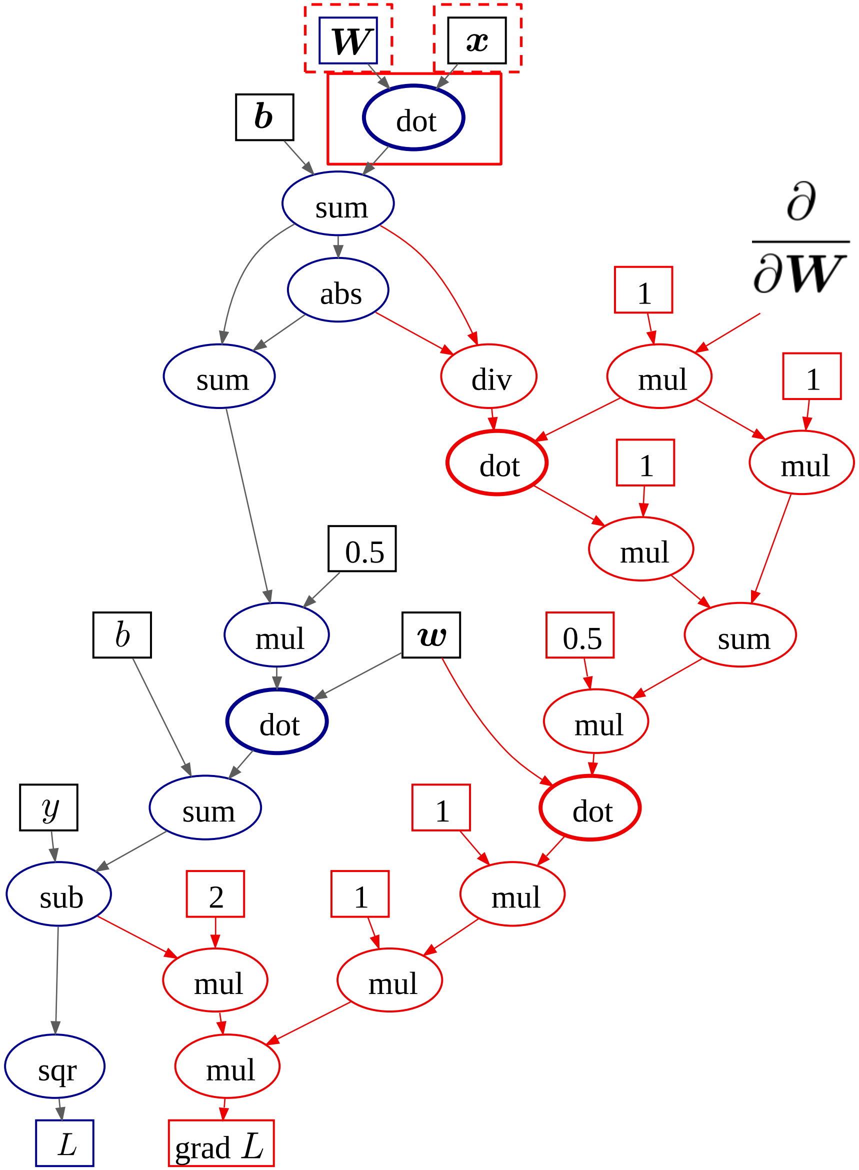
Computing Gradients



$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{W} \cdot \boldsymbol{x})$$

Well, this is tricky….

Computing Gradients



$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{W} \cdot \boldsymbol{x})$$

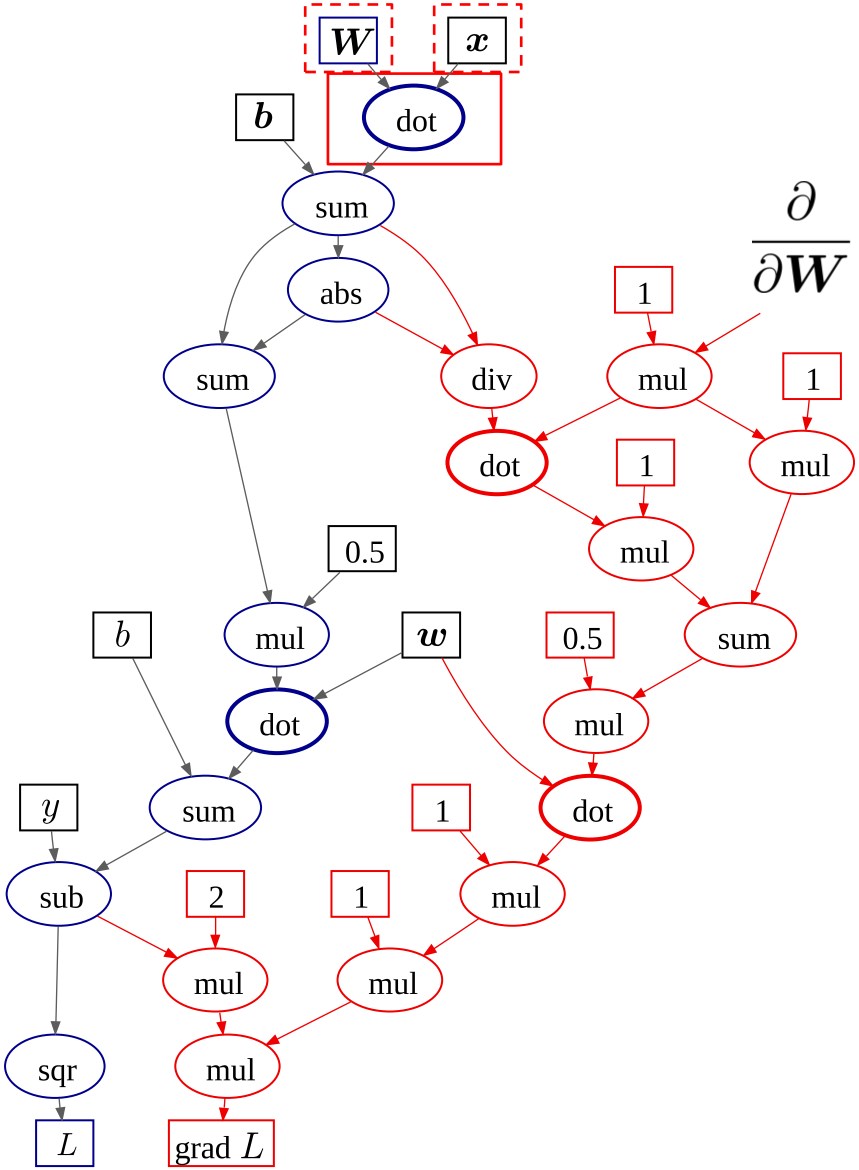
This is a third-order tensor

$$\left(\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{W} \cdot \boldsymbol{x})\right)_{ijk} = \frac{\partial}{\partial W_{kj}}(\boldsymbol{W} \cdot \boldsymbol{x})_i$$

Its ijk-th component

Note the inversion of indices

Computing Gradients



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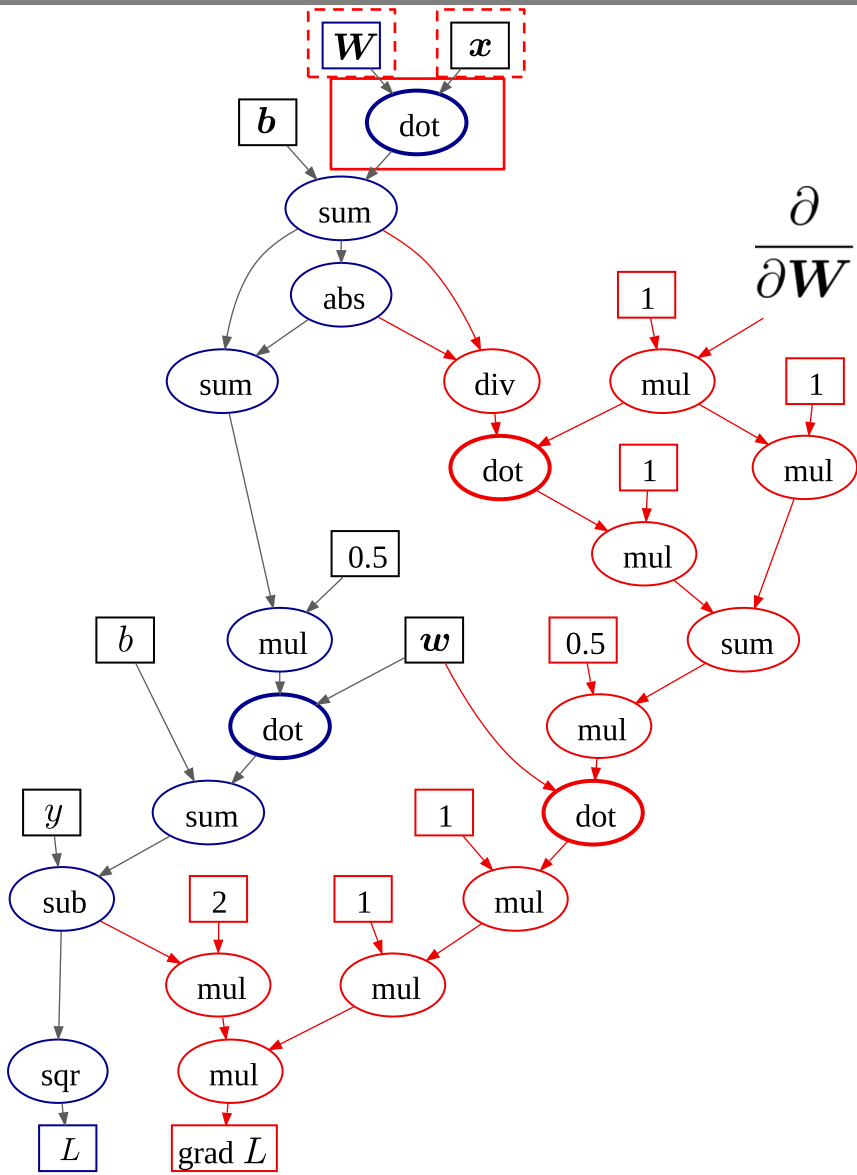
Its ijk-th component

Note the inversion of indices

$$= \frac{\partial}{\partial W_{kj}}(\boldsymbol{W}_{i,:} \cdot \boldsymbol{x})$$

The i-th line in the matrix

$$= \begin{cases} 0 & k \neq i \\ x_j & k = i \end{cases}$$

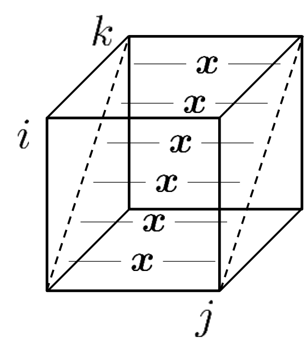


$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{W} \cdot \boldsymbol{x})$$

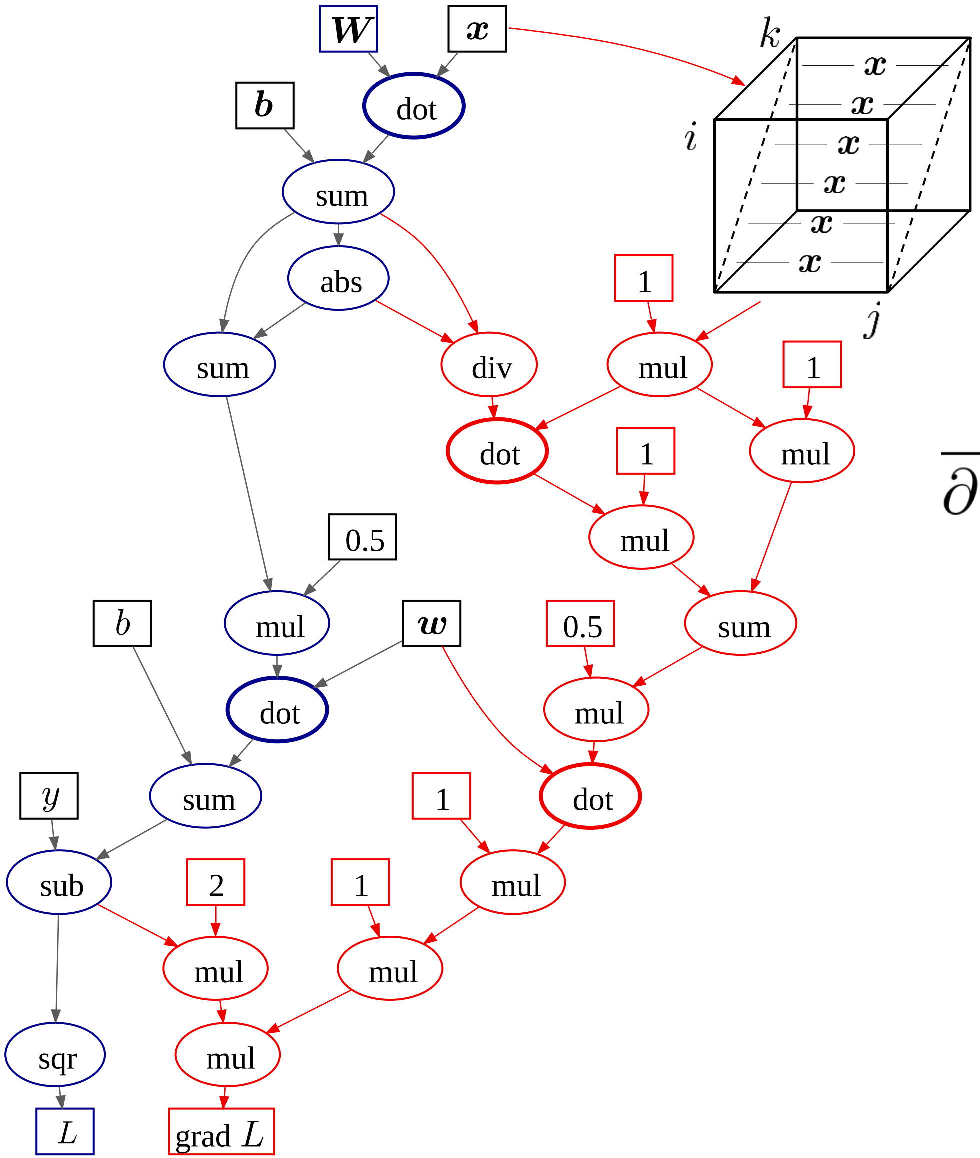
Putting it all together…

$$\left(\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{W} \cdot \boldsymbol{x})\right)_{ijk} = \begin{cases} 0 & k \neq i \\ x_j & k = i \end{cases}$$

This 'thing' is a cube having copies of $\boldsymbol{x}$ *on one diagonal 'plane' and zeros elsewhere*



Computing Gradients



$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \mathrm{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

(Mini) Batches in Matrix Form

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N}\sum_{D}((\boldsymbol{w}\cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)}+\boldsymbol{b})+b)-y^{(i)})^2$$

Let's focus first on $\boldsymbol{W}\boldsymbol{x}$

by defining

$$\boldsymbol{X} := \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$$

*input data in matrix form (**item index first**)*

Then we can write

$$\boldsymbol{W}\boldsymbol{X}^T = \begin{bmatrix} | & & | \\ \boldsymbol{W}\boldsymbol{x}^{(1)} & \dots & \boldsymbol{W}\boldsymbol{x}^{(N)} \\ | & & | \end{bmatrix}$$

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N}\sum_{D}((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Consider then $(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$

by defining

$$\hat{\boldsymbol{X}} := \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} & 1 \end{bmatrix} \qquad \hat{\boldsymbol{W}} := \begin{bmatrix} & & | \\ & \boldsymbol{W} & \boldsymbol{b} \\ & & | \end{bmatrix}$$

Then we could write

$$\hat{\boldsymbol{W}}\hat{\boldsymbol{X}}^T = \begin{bmatrix} | & & | \\ \boldsymbol{W}\boldsymbol{x}^{(1)} + \boldsymbol{b} & \dots & \boldsymbol{W}\boldsymbol{x}^{(N)} + \boldsymbol{b} \\ | & & | \end{bmatrix}$$

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N}\sum_{D}((\boldsymbol{w}\cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Consider then $(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$

and keep the definition

$$\boldsymbol{X} := \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$$

It could be convenient to redefine the operator $+$ such that is interpreted as

$$\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b} := \begin{bmatrix} | & & | \\ \boldsymbol{W}\boldsymbol{x}^{(1)} & \dots & \boldsymbol{W}\boldsymbol{x}^{(N)} \\ | & & | \end{bmatrix} + \underbrace{\begin{bmatrix} | & & | \\ \boldsymbol{b} & \dots & \boldsymbol{b} \\ | & & | \end{bmatrix}}_{N \text{ times}}$$

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N} \sum_{D} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Consider then $(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$

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$$\boldsymbol{X} := \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$$

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*This is called **broadcasting***

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N} \sum_{D} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

where

$$\boldsymbol{X} := \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix} \qquad \boldsymbol{y} := \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{bmatrix}$$

More on Matrix Forms

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$$L(D) = \frac{1}{N} \sum_{D} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N}((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

This is a matrix $g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) \in \mathbb{R}^{h \times N}$

(Note the ***broadcast*** *with* $+$ *)*

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N}\sum_{D}((\boldsymbol{w}\cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N}((\boldsymbol{w}\cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

*This is a **row** vector*

$$\boldsymbol{w}\cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) = \boldsymbol{w}^T g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) \in \mathbb{R}^N$$

*(The 'dot' operator **transposes** vectors automatically, as required)*

More on Matrix Forms

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$$L(D) = \frac{1}{N}\sum_{D}((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N}((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

*This is also a **row** vector* $\in \mathbb{R}^N$, *after a **broadcast** on* b

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N}\sum_{D}((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N}((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

*… whereas this is a **column** vector $\in \mathbb{R}^N$*

*This is also a **row** vector $\in \mathbb{R}^N$, after a **broadcast** on b*

More on Matrix Forms

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Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N}((\boldsymbol{w}\cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

*This is also a **row** vector $\in \mathbb{R}^N$, after a **broadcast** on b*

*… whereas this is a **column** vector $\in \mathbb{R}^N$*

*(Also the $-$ operator **transposes** vectors automatically, as required)*

More on Matrix Forms

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We may want to get rid of the summation when computing the loss function

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*… whereas this is a **column** vector $\in \mathbb{R}^N$*

*This is also a **row** vector $\in \mathbb{R}^N$, after a **broadcast** on b*

*(Also the $-$ operator **transposes** vectors automatically, as required)*

A similar behavior of operators is standard in NumPy TensorFlow

More on Matrix Forms

Say it with matrices…

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$$L(D) = \frac{1}{N} \sum_{D} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{X}^T + \boldsymbol{b}) + b) - \boldsymbol{y})^2$$

This is a matrix $\boldsymbol{W}\boldsymbol{X}^T \in \mathbb{R}^{h \times N}$

Ouch! No ***item index first*** *…*

More on Matrix Forms

Say it with matrices…

We may want to get rid of the summation when computing the loss function

$$L(D) = \frac{1}{N} \sum_{D} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

Using broadcasting operators, we can express the above as

$$L(D) = \frac{1}{N} ((g(\boldsymbol{X}\boldsymbol{W}^T + \boldsymbol{b}) \cdot \boldsymbol{w} + b) - \boldsymbol{y})^2$$

This is a matrix $\boldsymbol{X}\boldsymbol{W}^T \in \mathbb{R}^{N \times h}$

Item index first!

More on Matrix Forms

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$$L(D) = \frac{1}{N} \sum_{D} ((\boldsymbol{w} \cdot g(\boldsymbol{W}\boldsymbol{x}^{(i)} + \boldsymbol{b}) + b) - y^{(i)})^2$$

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*This is a **column** vector* $\in \mathbb{R}^h$
(it will be transposed automatically)

This is a matrix $\boldsymbol{X}\boldsymbol{W}^T \in \mathbb{R}^{N \times h}$

Item index first!