

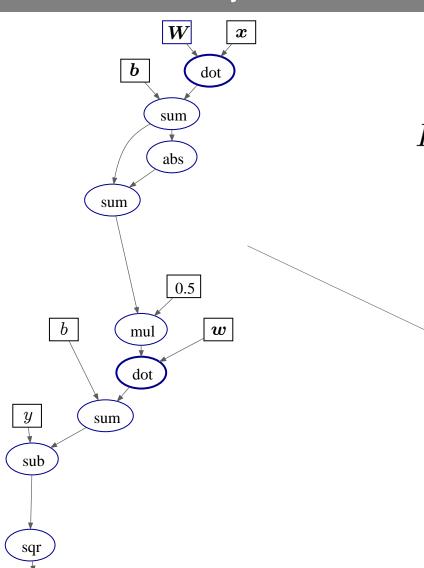
Deep Learning

03-Flow Graphs & Automatic Differentiation

Marco Piastra

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

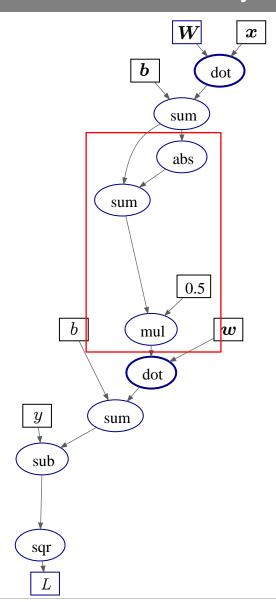
Flow Graphs



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

Item-wise loss function, FF neural network with ReLU as non-linearity

The above expression translates into this flow graph



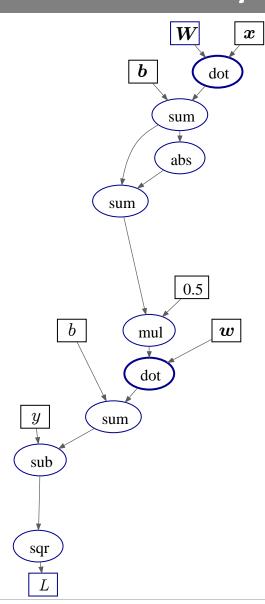
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Item-wise loss function, FF neural network with ReLU as non-linearity

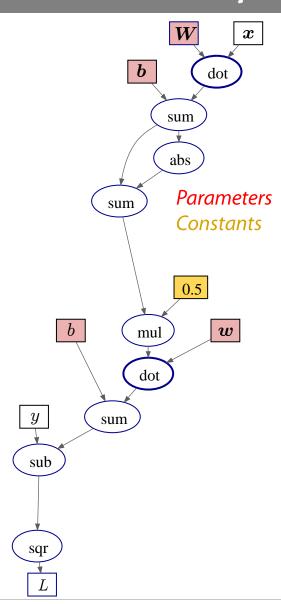
$$ReLU(x) := max(0, x)$$

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

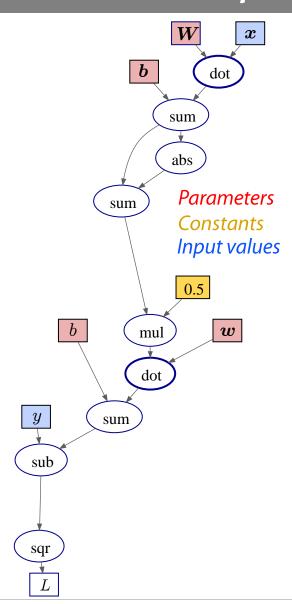
(equivalent expression)



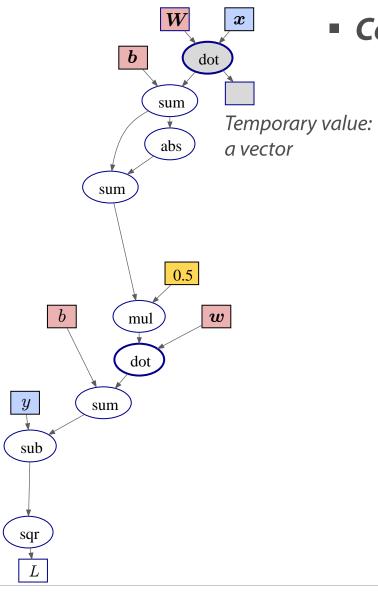
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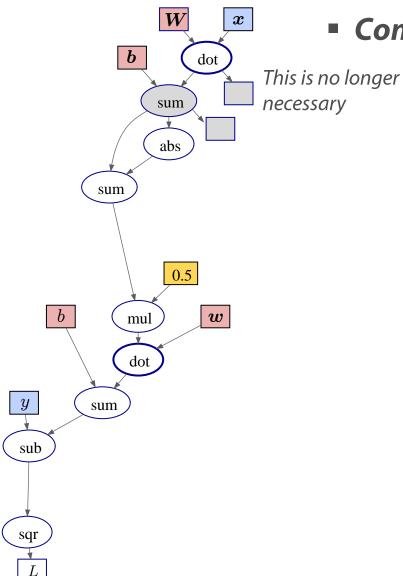


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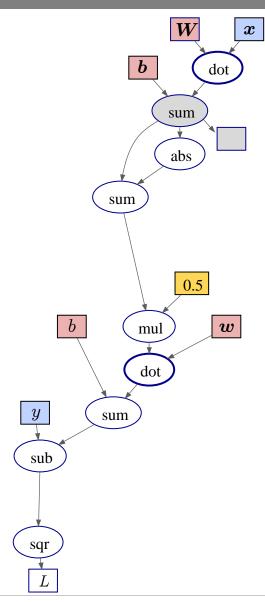
Computing the Flow Graph

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



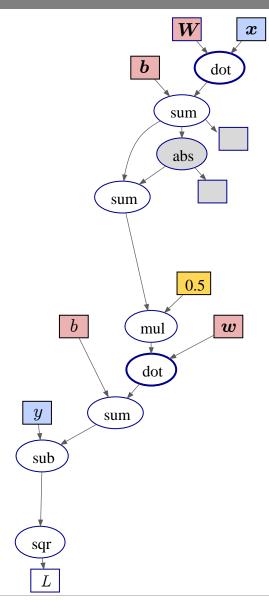
Computing the Flow Graph

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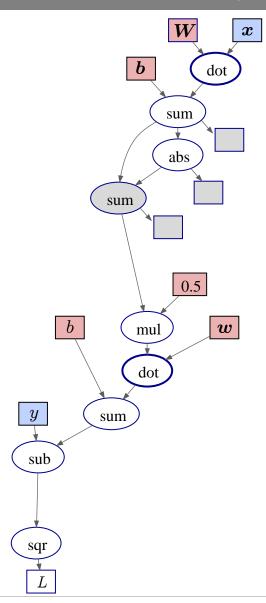
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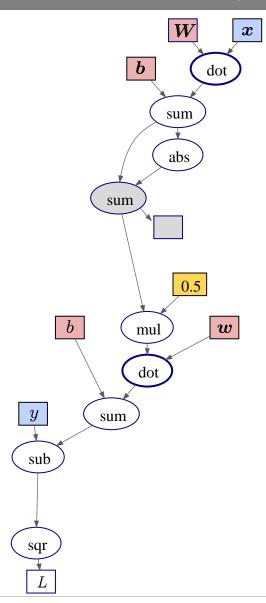
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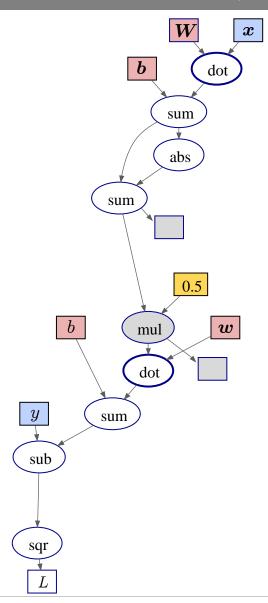
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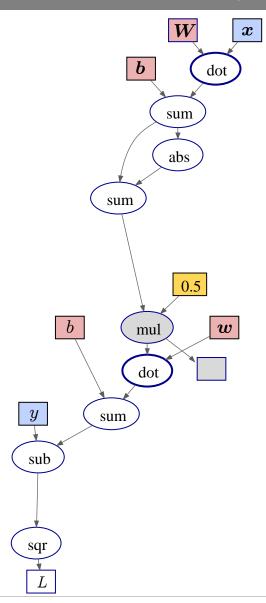
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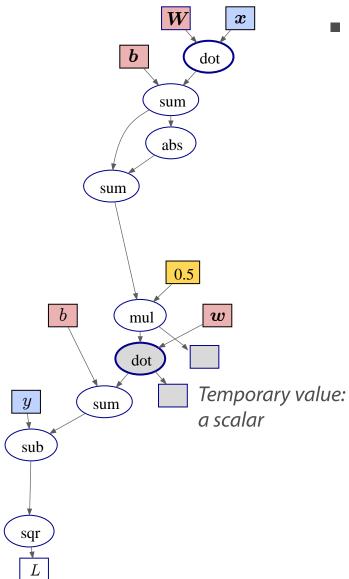
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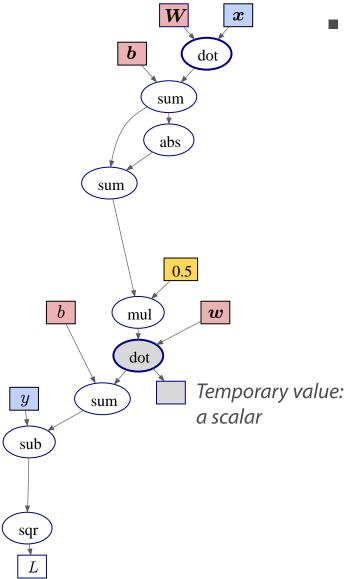
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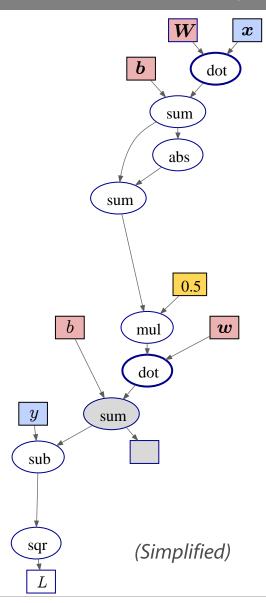
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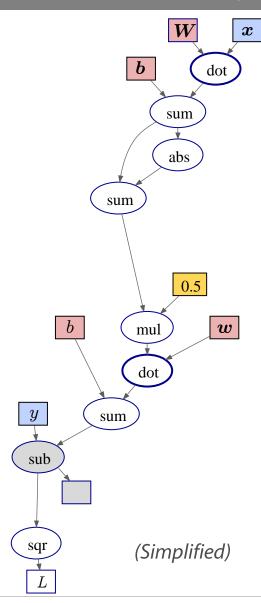
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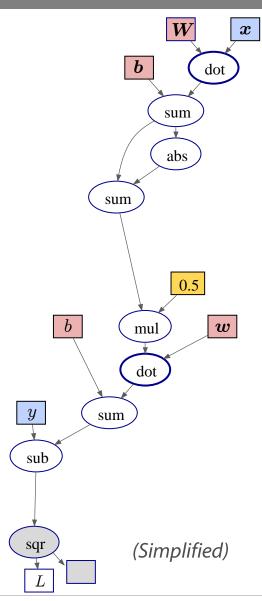
Computing the Flow Graph

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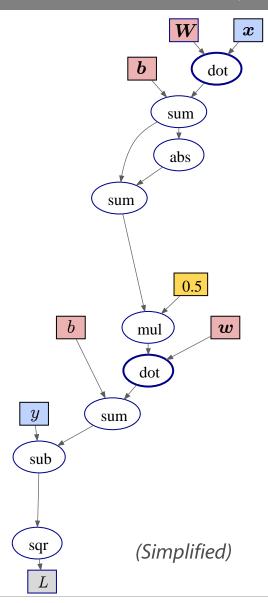
Computing the Flow Graph

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



Computing the Flow Graph

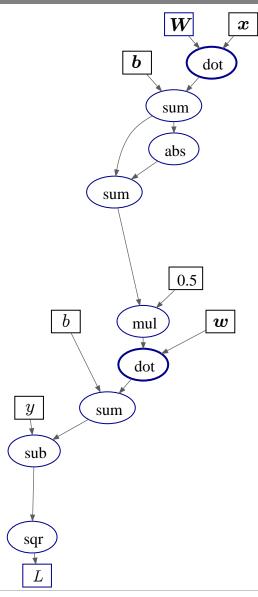
$$L(\tilde{y}, y) = (\boldsymbol{w} \cdot \text{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$



Computing the Flow Graph

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

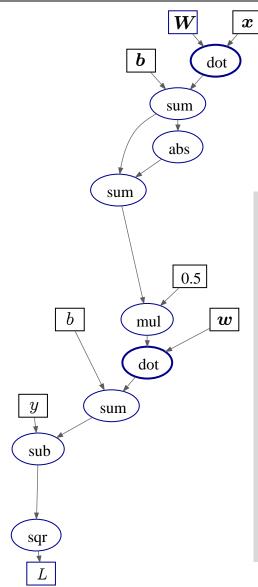
Autodiff: Automatic Differentiation of Flow Graphs



Computing one gradient of the flow graph

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

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



Computing one gradient of the flow graph

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

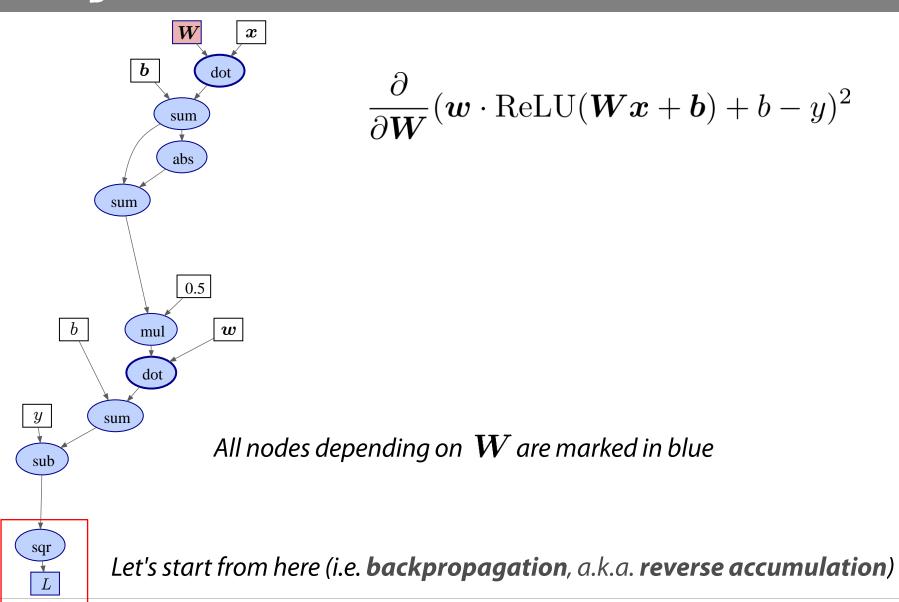
This is the gradient we want to compute (remember this is just one of the four)

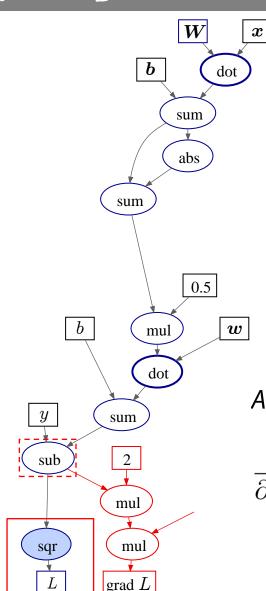
Chain rule for derivatives (single argument)

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

Chain rule for derivatives (multiple arguments)

$$\begin{split} \frac{\partial}{\partial \boldsymbol{\vartheta}} f(g(\boldsymbol{\vartheta}), h(\boldsymbol{\vartheta})) &= \\ \frac{\partial}{\partial g(\boldsymbol{\vartheta})} f(g(\boldsymbol{\vartheta}), h(\boldsymbol{\vartheta})) \frac{\partial}{\partial \boldsymbol{\vartheta}} g(\boldsymbol{\vartheta}) \ + \ \frac{\partial}{\partial h(\boldsymbol{\vartheta})} f(g(\boldsymbol{\vartheta}), h(\boldsymbol{\vartheta})) \frac{\partial}{\partial \boldsymbol{\vartheta}} h(\boldsymbol{\vartheta}) \end{split}$$

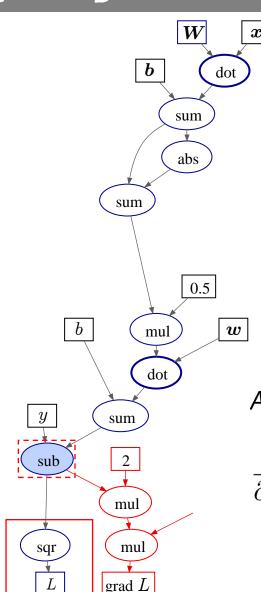




$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \text{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

Apply the chain rule to the sqr node

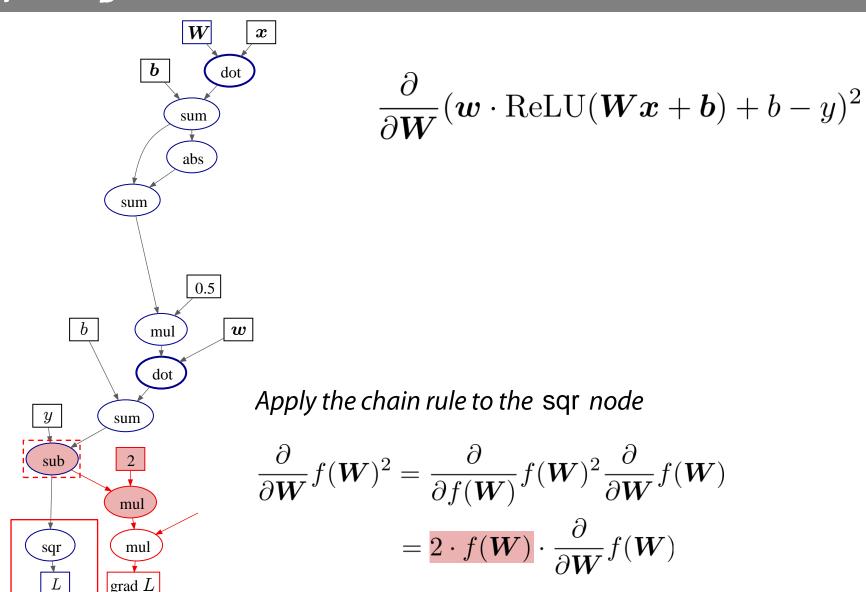
$$\frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})^{2} = \frac{\partial}{\partial f(\mathbf{W})} f(\mathbf{W})^{2} \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})$$
$$= 2 \cdot f(\mathbf{W}) \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})$$

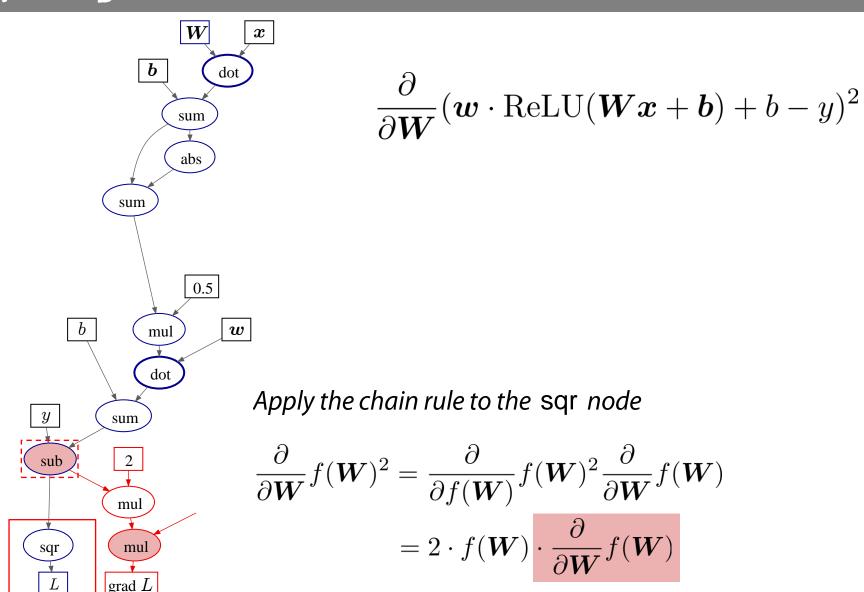


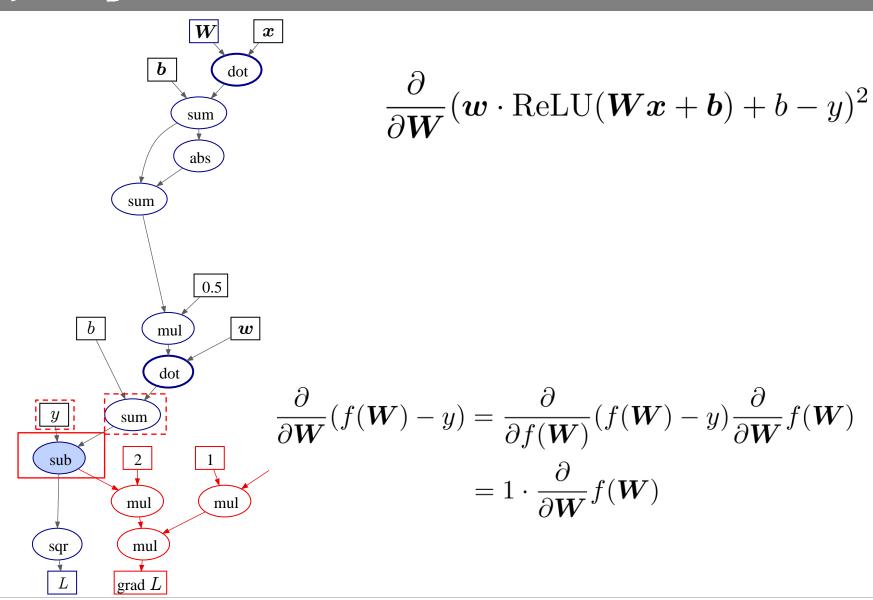
$$\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{w} \cdot \text{ReLU}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) + b - y)^2$$

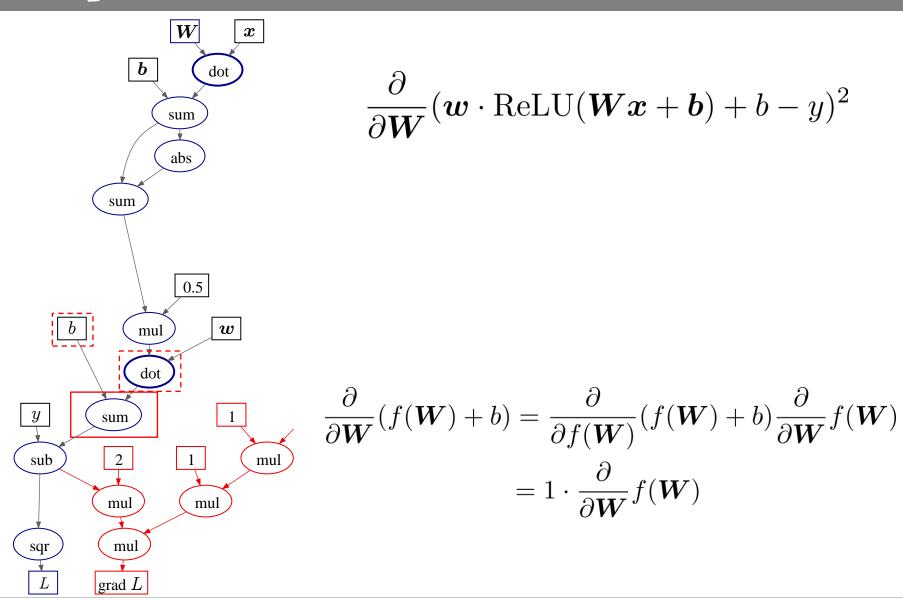
Apply the chain rule to the sqr node

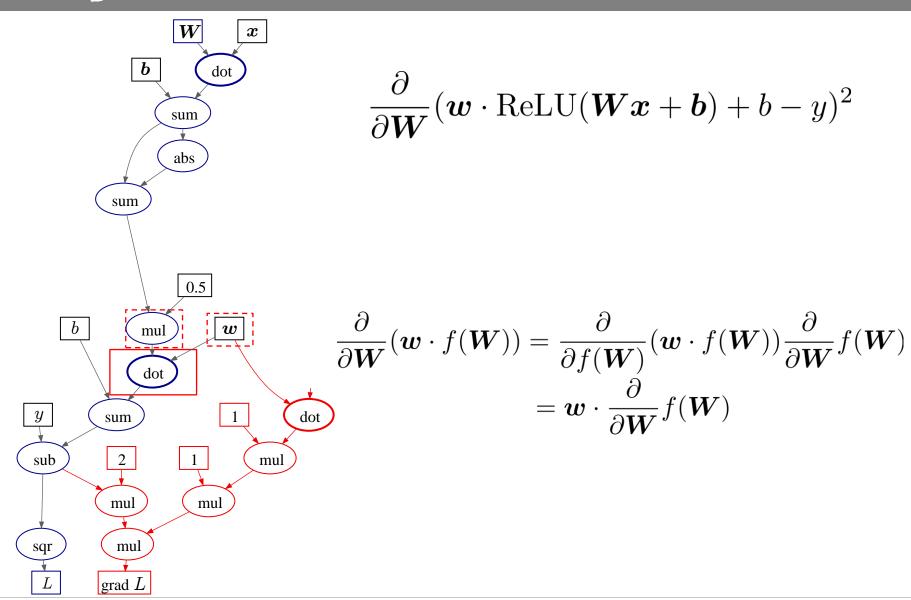
$$\frac{\partial}{\partial \mathbf{W}} \mathbf{f(W)}^2 = \frac{\partial}{\partial f(\mathbf{W})} f(\mathbf{W})^2 \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})$$
$$= 2 \cdot f(\mathbf{W}) \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})$$

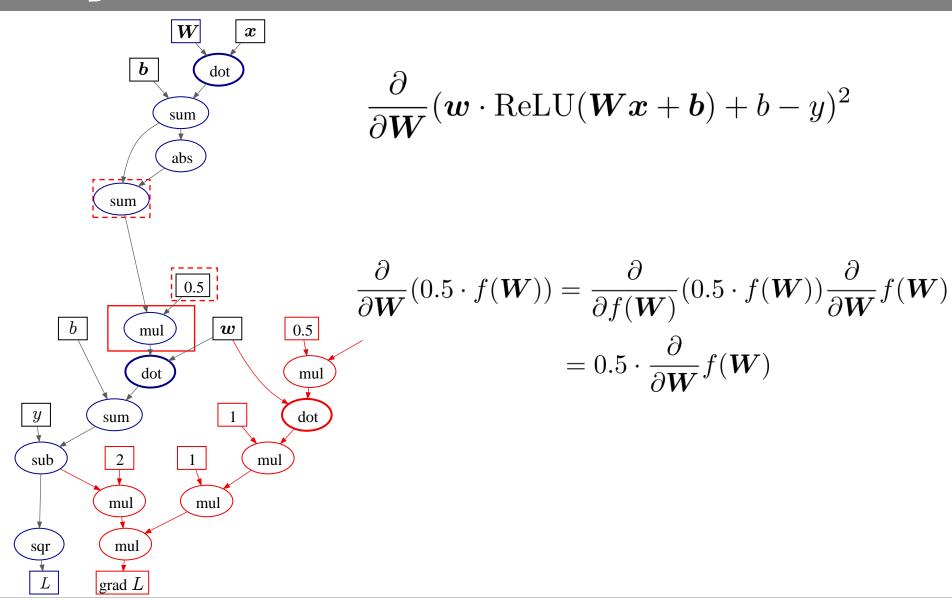


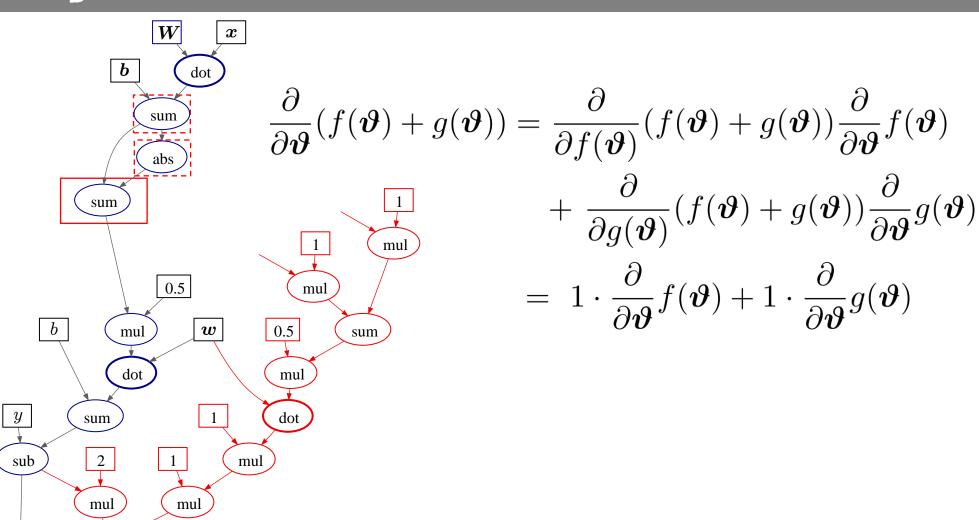






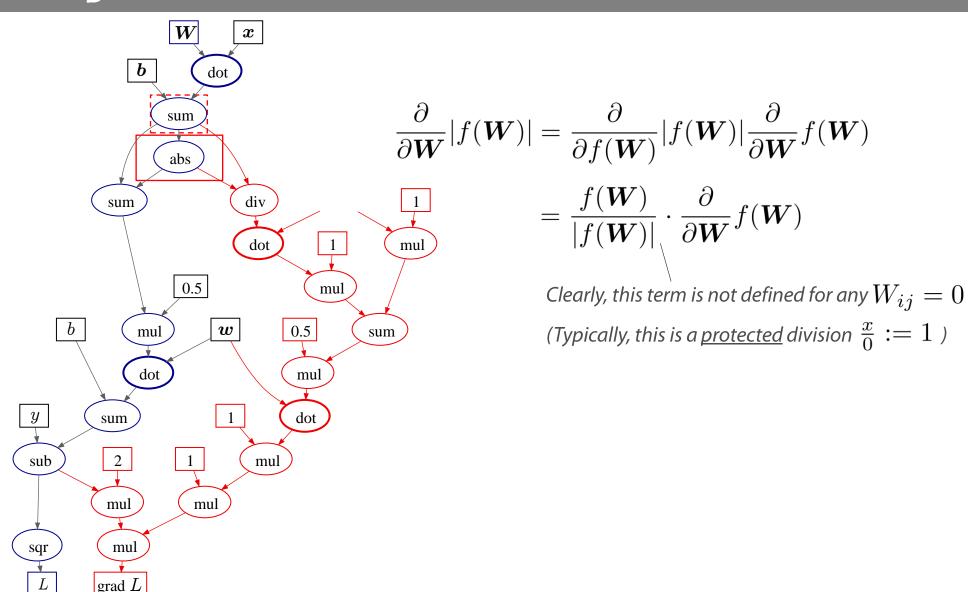


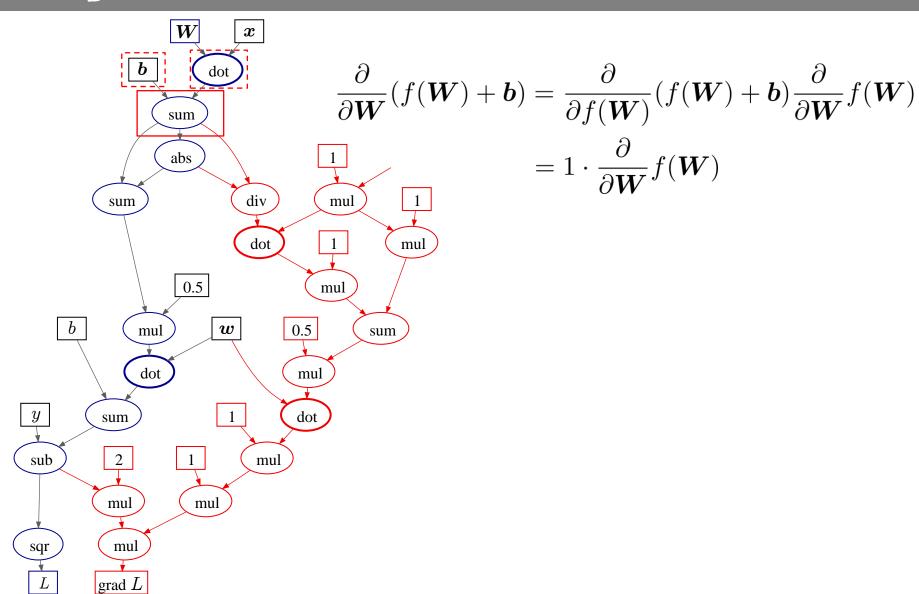


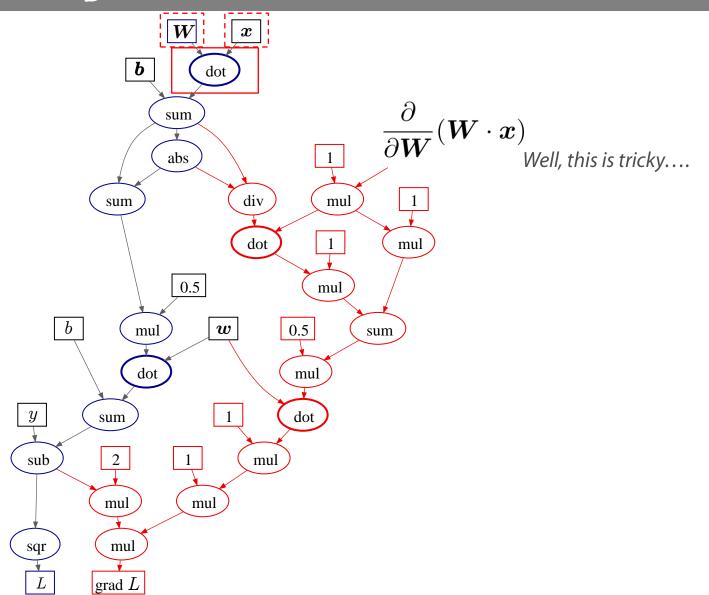


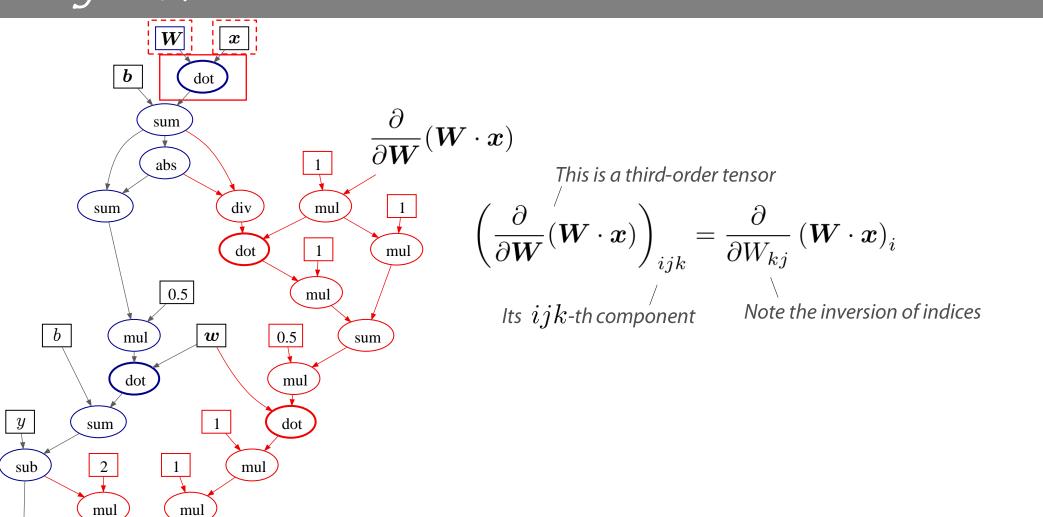
mul

grad L



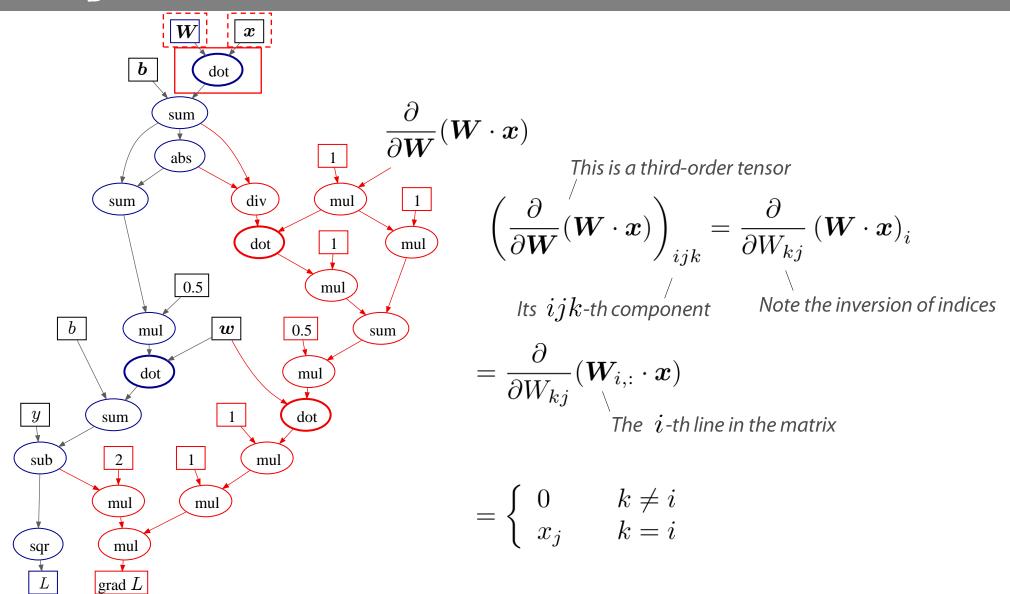




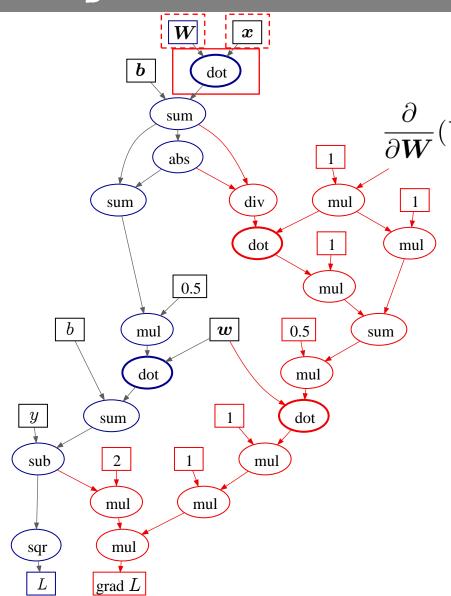


mul

 $\operatorname{grad} L$



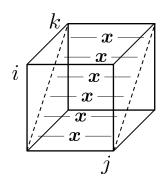
[39]

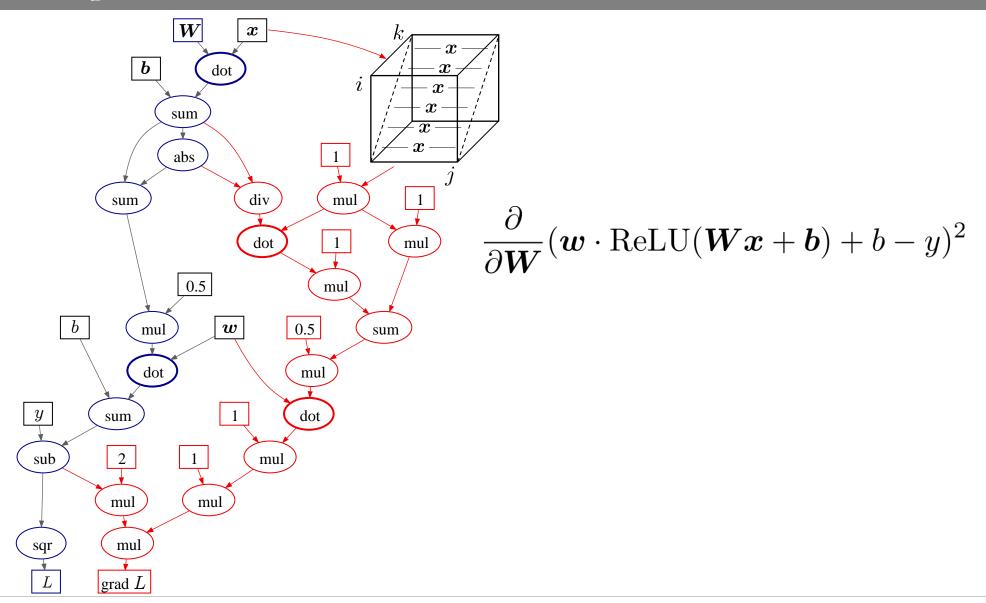


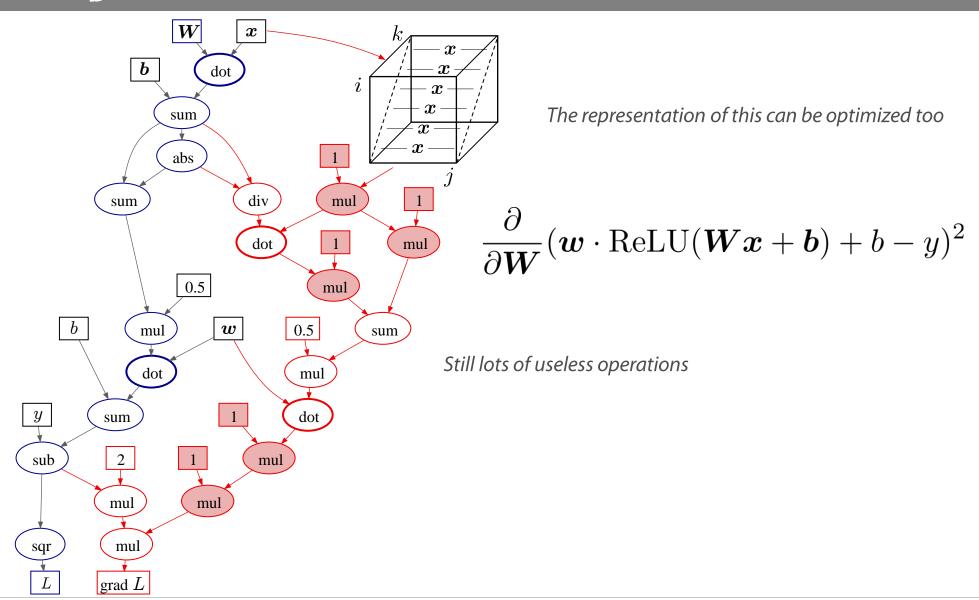
Putting it all together...

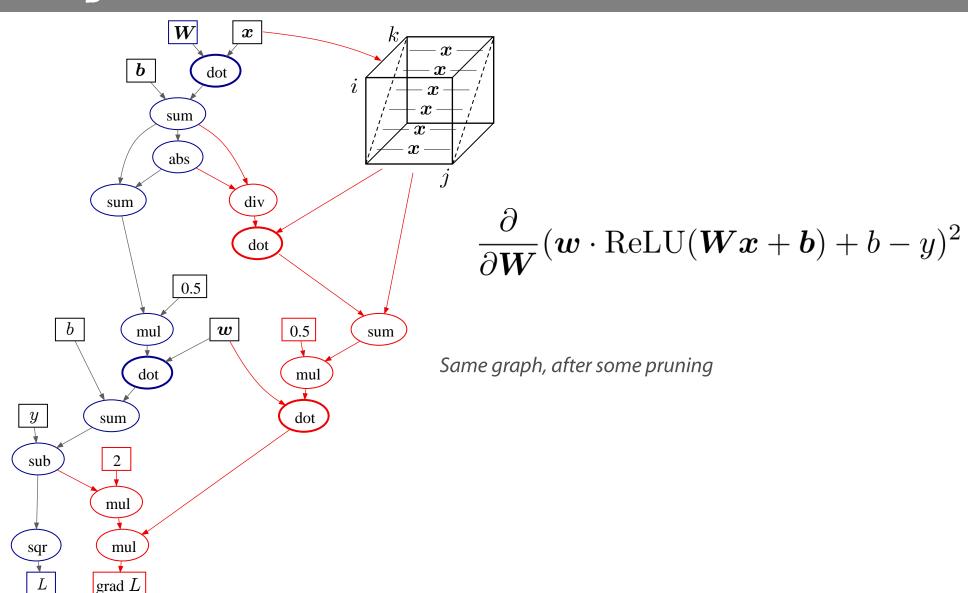
$$\left(\frac{\partial}{\partial \mathbf{W}}(\mathbf{W} \cdot \mathbf{x})\right)_{ijk} = \begin{cases} 0 & k \neq i \\ x_j & k = i \end{cases}$$

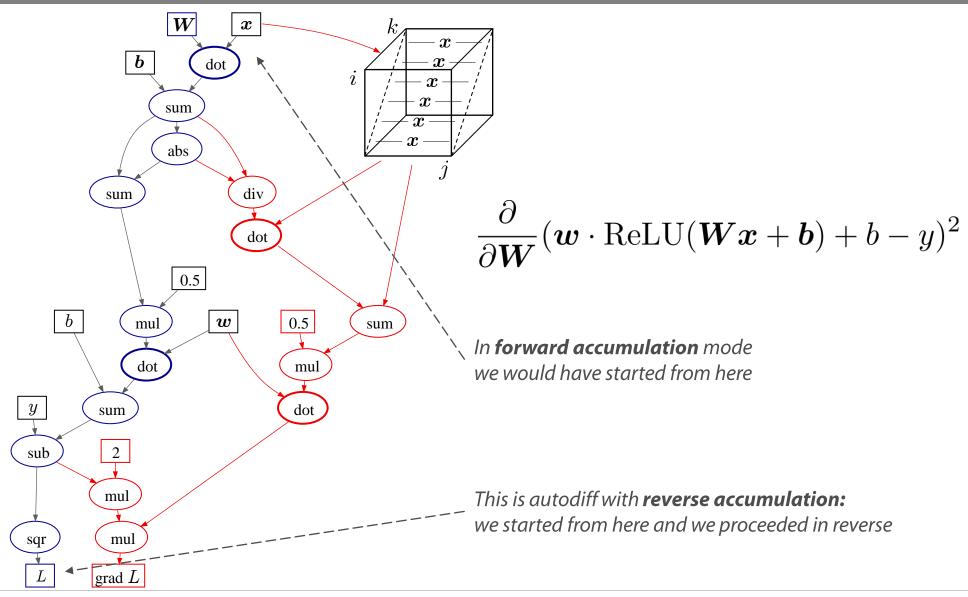
This 'thing' is a cube having copies of $oldsymbol{x}$ on one diagonal 'plane' and zeros elsewhere











(Mini) Batches in Matrix Form

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

Wx

by defining

$$m{X} := egin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$$
 input data in matrix form (item index first)

Then we can write

$$oldsymbol{W}oldsymbol{X}^T = egin{bmatrix} | & & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & & | & | & & | & & | & | & & | & | & & | & | & & | & & | & | & | & & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | & | &$$

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

$$\hat{m{X}} := egin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} & 1 \ drawtriangledows & \ddots & drawtriangledows & drawtriangledows & arphi & arphi & drawtriangledows & arphi & a$$

$$\hat{m{W}} := \left[egin{array}{ccc} m{W} & m{b} \ dots & dots \end{array}
ight]$$

Then we could write

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

Consider then
$$(\boldsymbol{W}\boldsymbol{x}+\boldsymbol{b})$$
 and let's 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

Say it with matrices...

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

Consider then
$$({m W}{m x}+{m b})$$
 and let's keep the definition ${m X}:=egin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \ \vdots & \ddots & \vdots \ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$

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

This is called **broadcasting**

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

$$m{X} := egin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ draingle & \ddots & draingle \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix} \qquad m{y} := egin{bmatrix} y^{(1)} \\ draingle \\ y^{(N)} \end{bmatrix}$$

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

$$L(D) = rac{1}{N}((m{w}\cdotm{g}(m{W}m{X}^T+m{b})+b)-m{y})^2$$
 This is a matrix $g(m{W}m{X}^T+m{b})\in\mathbb{R}^{h imes N}$

(Note the **broadcast** with +)

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** <u>vectors</u> automatically, as required)

NOTE: automatic transposition applies **to vectors only**! For any tensor beyond dimension 1, you need to do that on your own

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

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

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

Say it with matrices...

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

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

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

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

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

$$L(D) = \frac{1}{N}((m{w} \cdot g(m{W}m{X}^T + m{b}) + b) - m{y})^2$$
 ... 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 (Also, the — operator **transposes** vectors automatically, as required)

A similar behavior of operators is standard in









Say it with matrices...

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

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

$$L(D) = rac{1}{N}((m{w}\cdot g(m{W}m{X}^T + m{b}) + b) - m{y})^2$$
 This is a matrix $\mbox{m{W}}m{X}^T \in \mathbb{R}^{h imes N}$ Ouch! No item index first \dots

Say it with matrices...

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

$$L(D) = rac{1}{N}((g(m{X}m{W}^T + m{b}) \cdot m{w} + b) - m{y})^2$$
 This is a matrix $m{X}m{W}^T \in \mathbb{R}^{N imes h}$ [tem index first!

Say it with matrices...

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

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

$$\text{This is a } \boldsymbol{column} \text{ vector } \in \mathbb{R}^h$$

$$\text{This is a matrix } \boldsymbol{X}\boldsymbol{W}^T \in \mathbb{R}^{N \times h} \text{ (it will be transposed automatically)}$$

$$\text{Item index first!}$$