

Deep Learning

A course about theory & practice



Flow Graphs & Automatic Differentiation

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Learning with Feed-Forward Neural Networks

Learning with FF Neural Networks

- Approximating a target function

$$y = f^*(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d$$

with **feed-forward neural network**

$$\tilde{y} = \mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + b, \quad \boldsymbol{\vartheta} = (\mathbf{W} \in \mathbb{R}^{h \times d}, \mathbf{w}, \mathbf{b} \in \mathbb{R}^h, b \in \mathbb{R})$$

parameters

ReLU has been chosen in this example

Objective: *minimizing* the loss function

$$L(D, \boldsymbol{\vartheta}) = \frac{1}{N} \sum_D (\mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x}^{(i)} + \mathbf{b}) + b - y^{(i)})^2$$

with respect to a dataset

$$D := \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$$

A set of data items

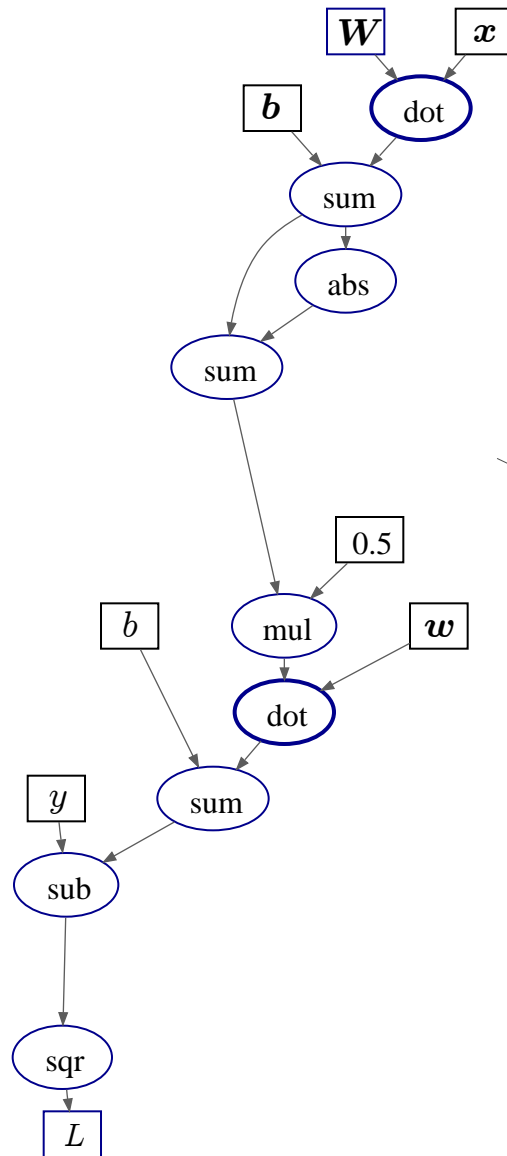
To apply *gradient descent* (any variant), we need to compute:

$$\frac{\partial}{\partial \boldsymbol{\vartheta}} L(\tilde{y}^{(i)}, y^{(i)}, \boldsymbol{\vartheta})$$

That is, the gradient of the loss function with respect to a data item

Flow Graphs *(a.k.a. Computation Graphs)*

Flow Graph

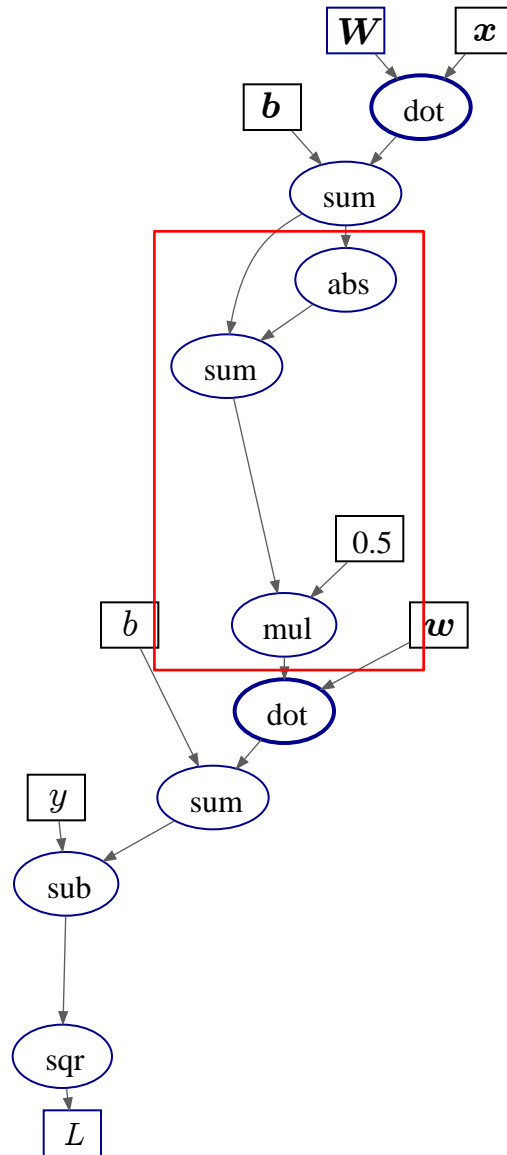


$$L(\tilde{y}, y) = (\mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + b - y)^2$$

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

The above expression translates into this flow graph

Flow Graph



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

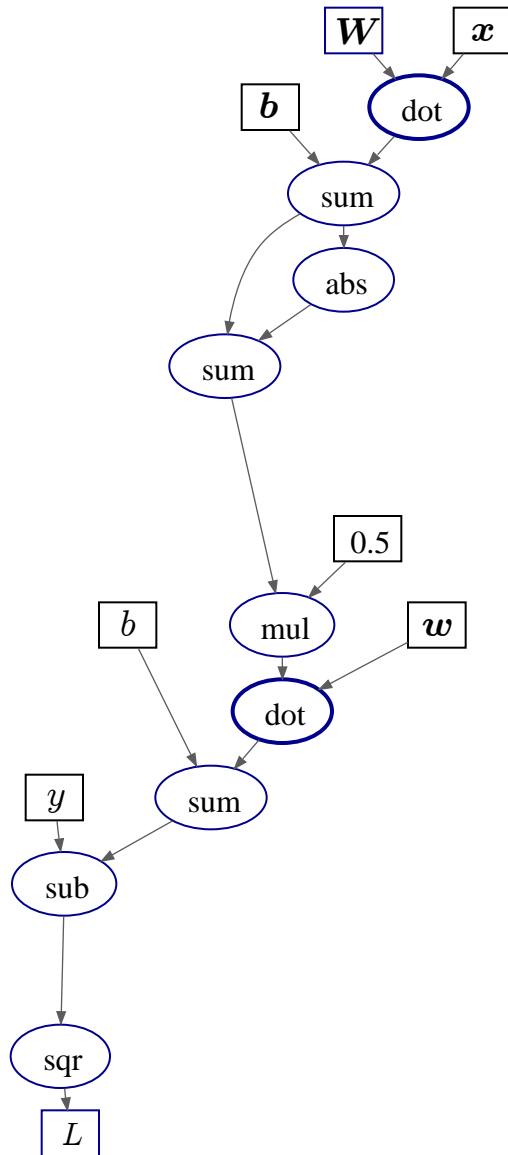
Item-wise loss function, FF neural network with ReLU as non-linearity

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

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

(equivalent expression)

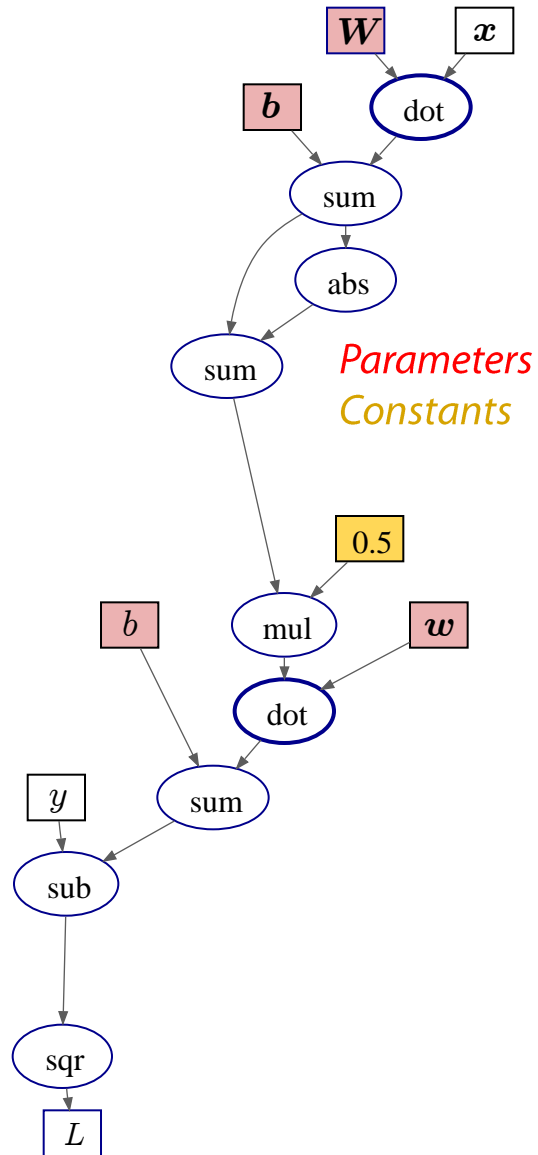
Flow Graph



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

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

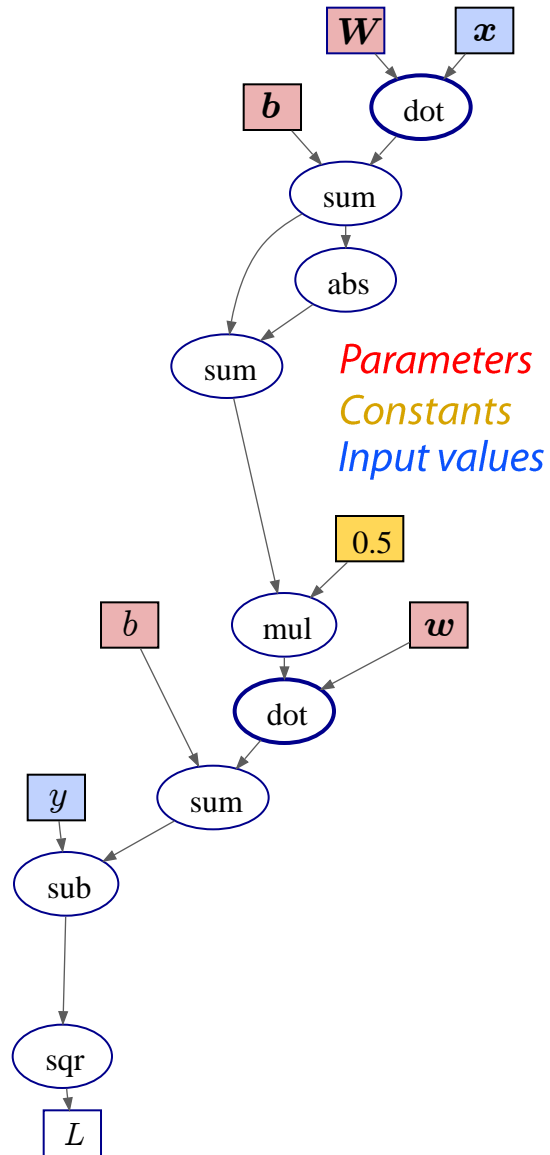
Flow Graph



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

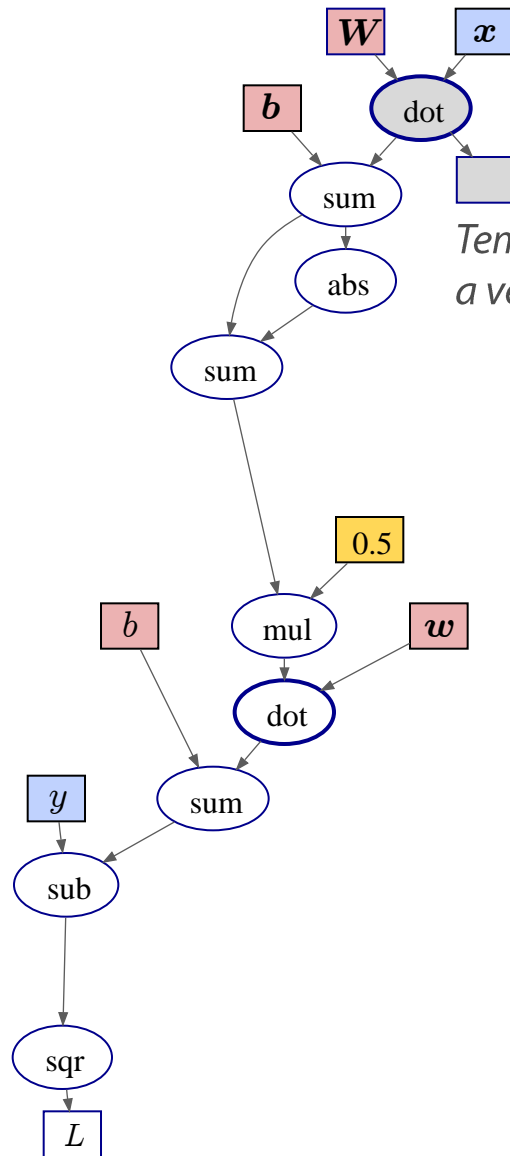
Flow Graph



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

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

Flow Graph

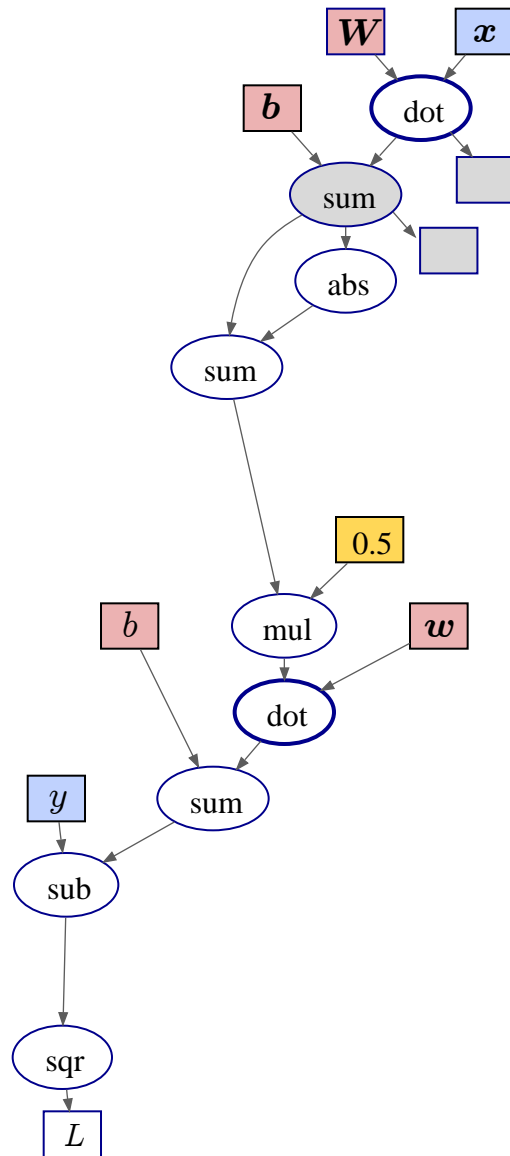


■ Computing the Flow Graph

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

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

Flow Graph



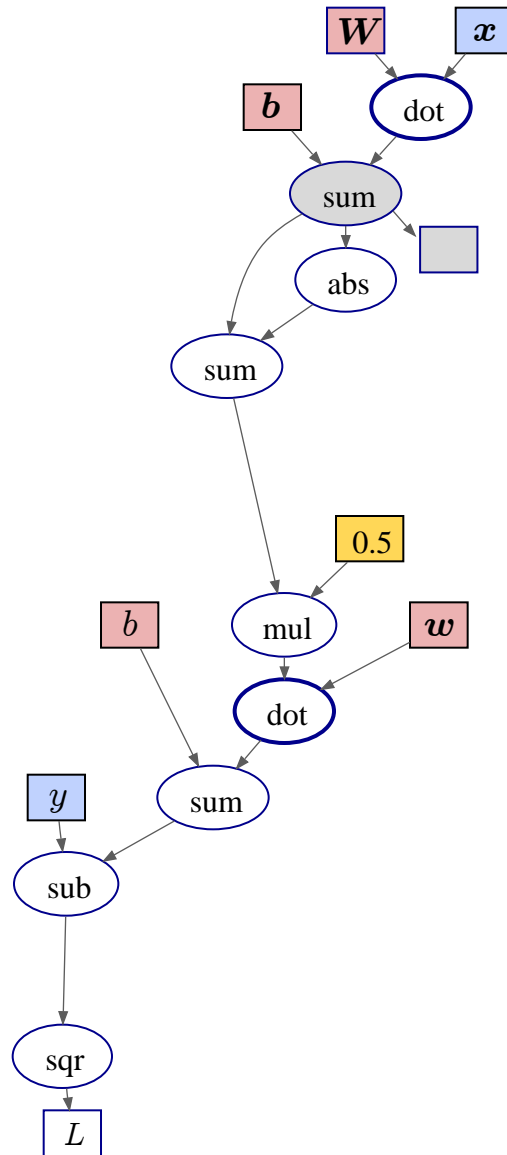
■ Computing the Flow Graph

This is no longer necessary

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

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

Flow Graph

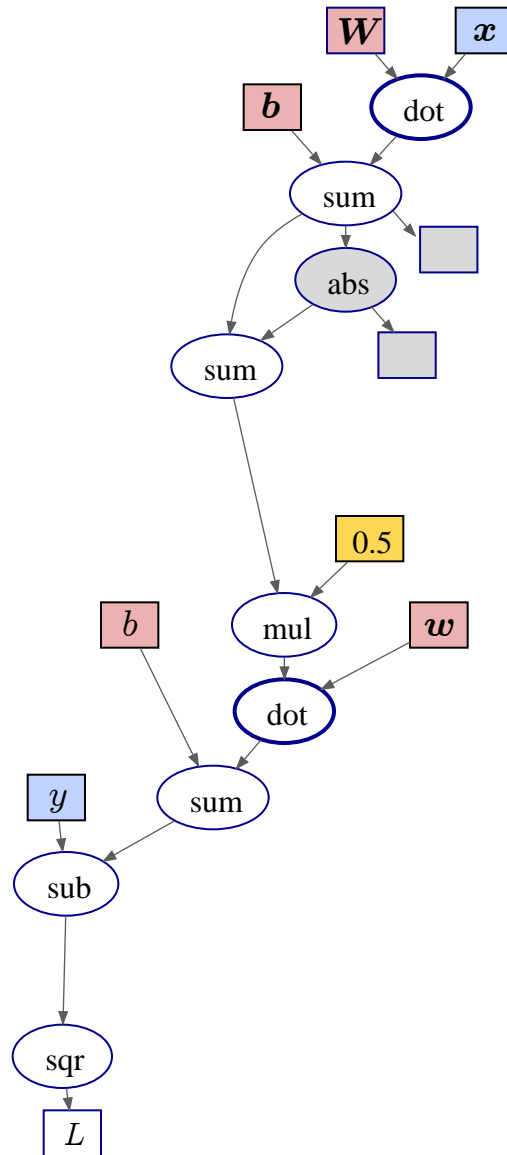


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Item-wise loss function, FF neural network with ReLU as non-linearity

Flow Graph

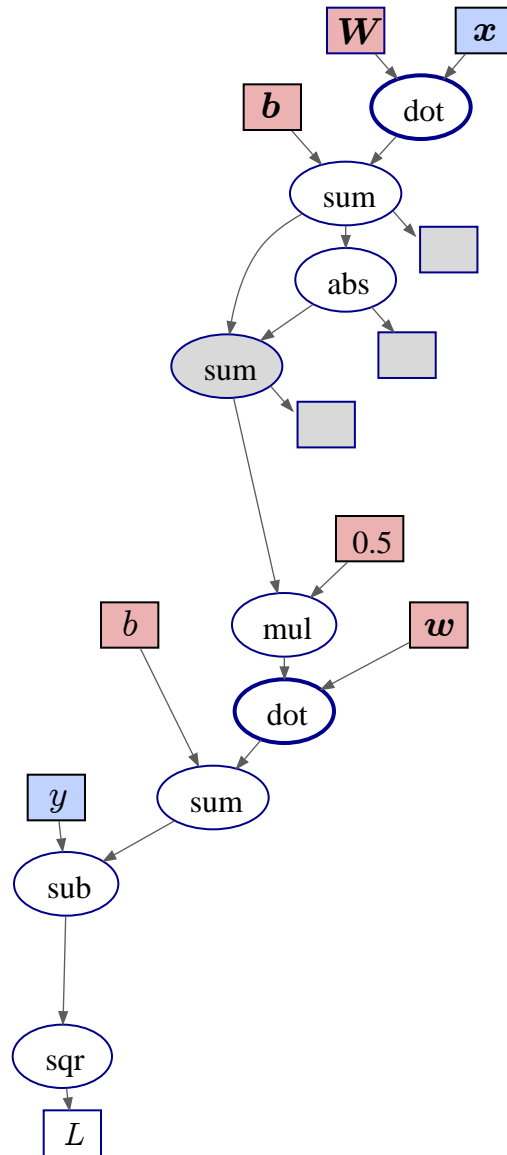


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Flow Graph

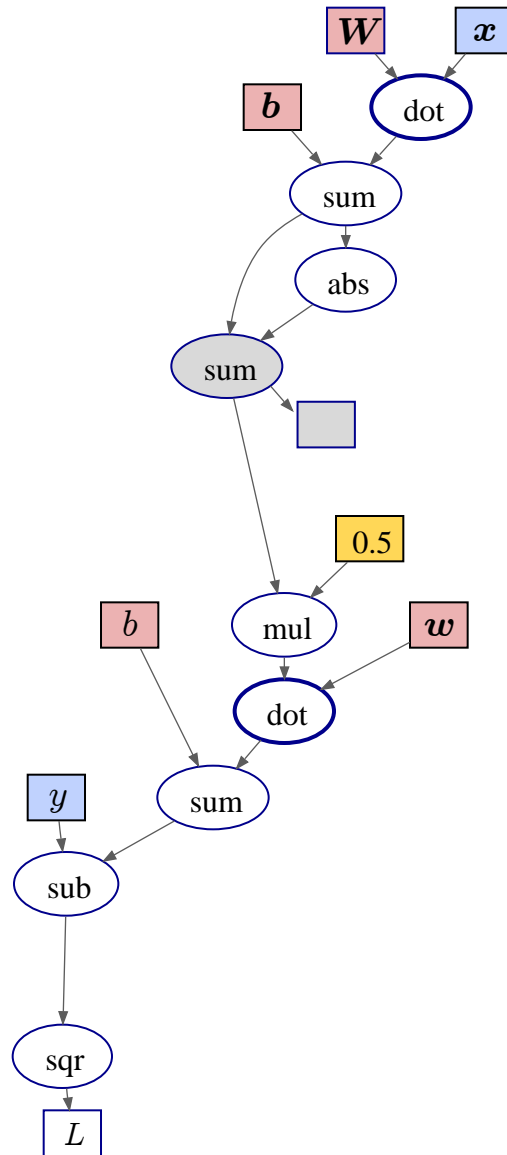


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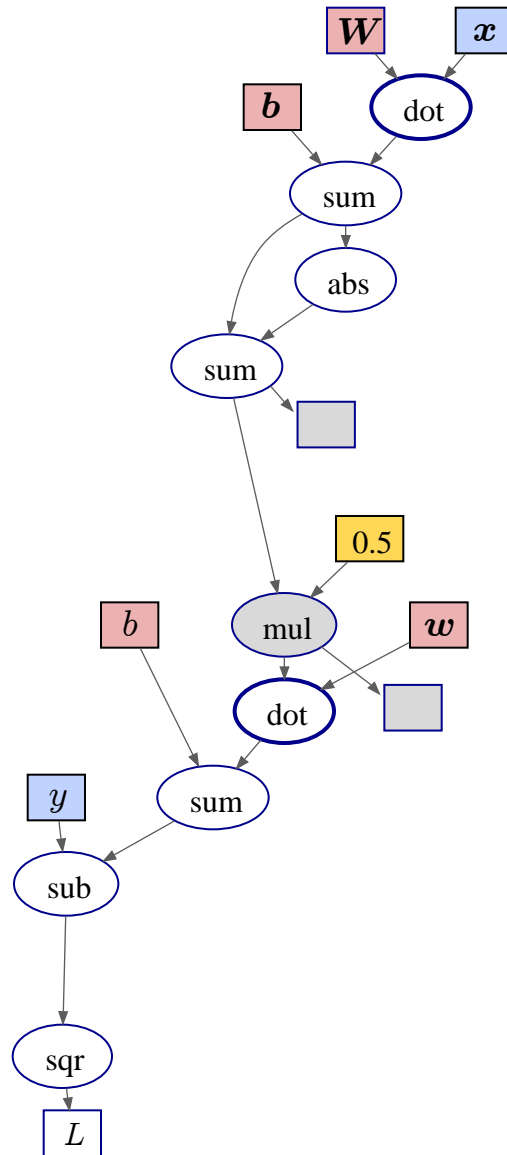


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Item-wise loss function, FF neural network with ReLU as non-linearity

Flow Graph

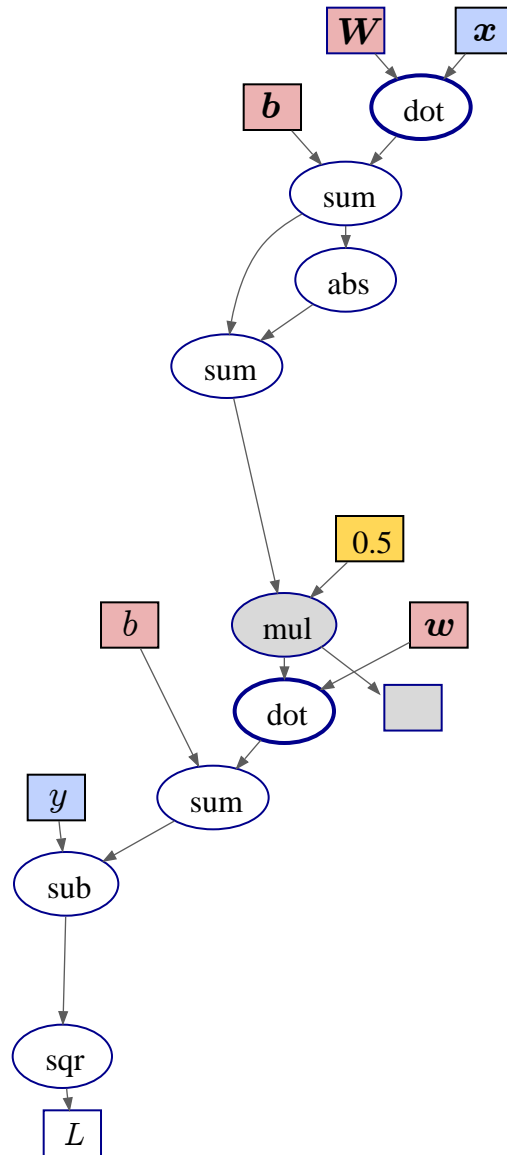


■ Computing the Flow Graph

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

Flow Graph

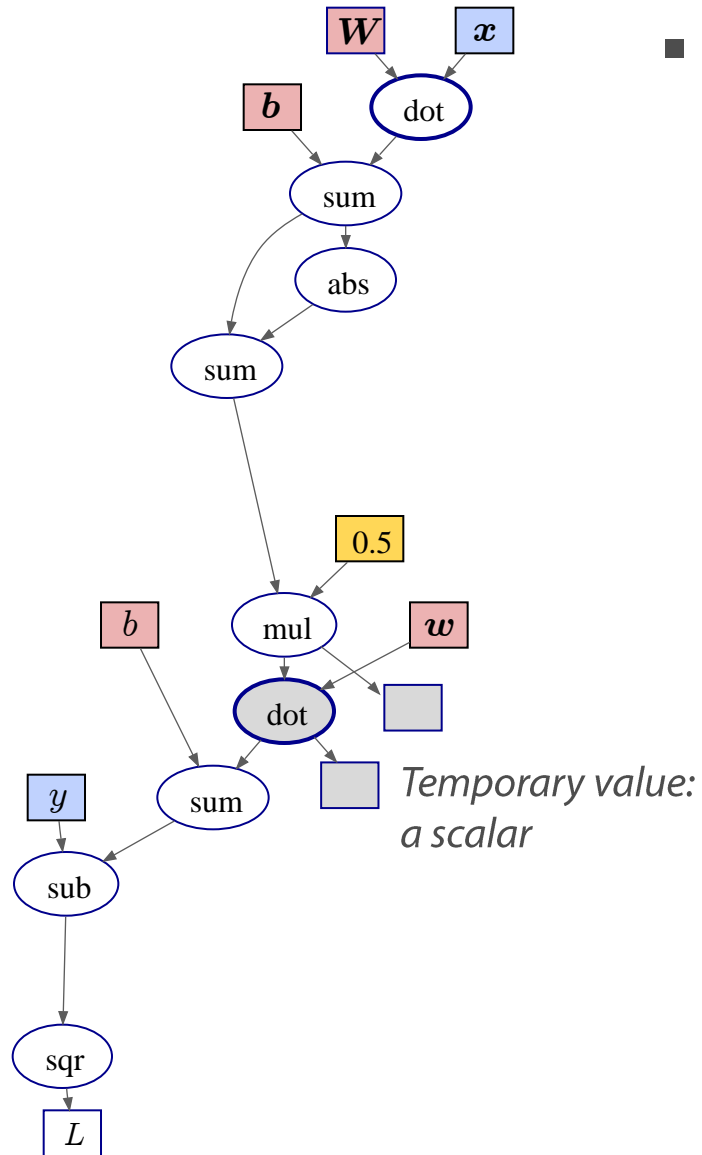


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Item-wise loss function, FF neural network with ReLU as non-linearity

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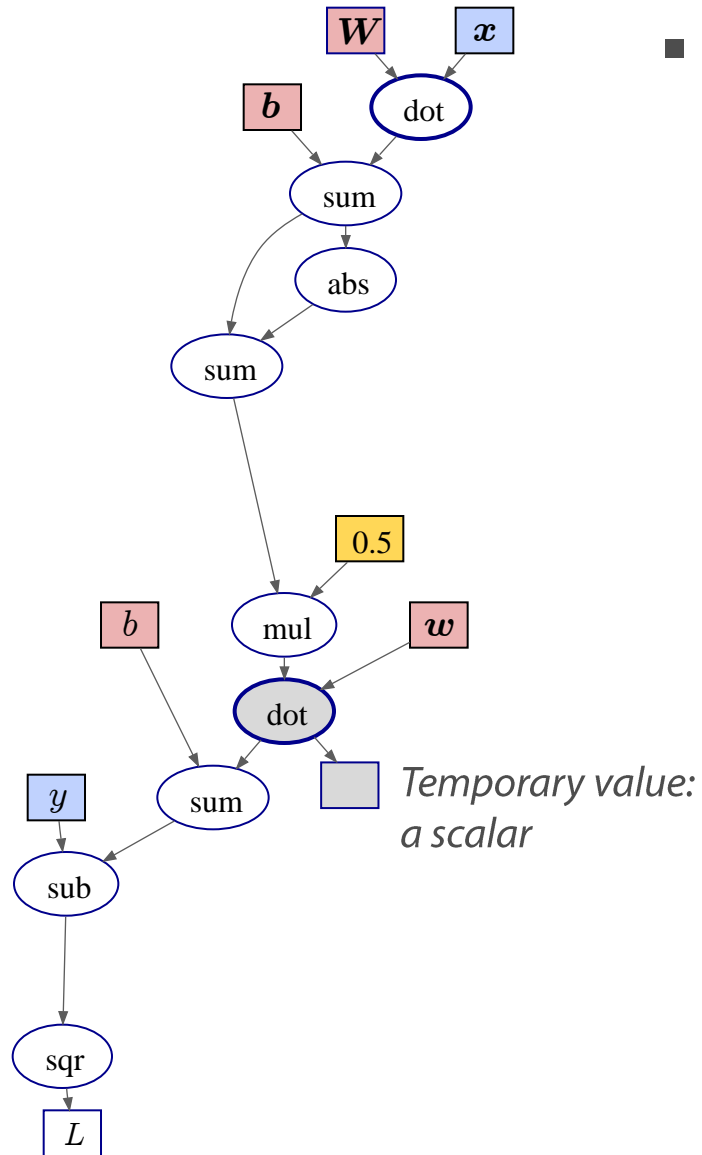


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Item-wise loss function, FF neural network with ReLU as non-linearity

Flow Graph

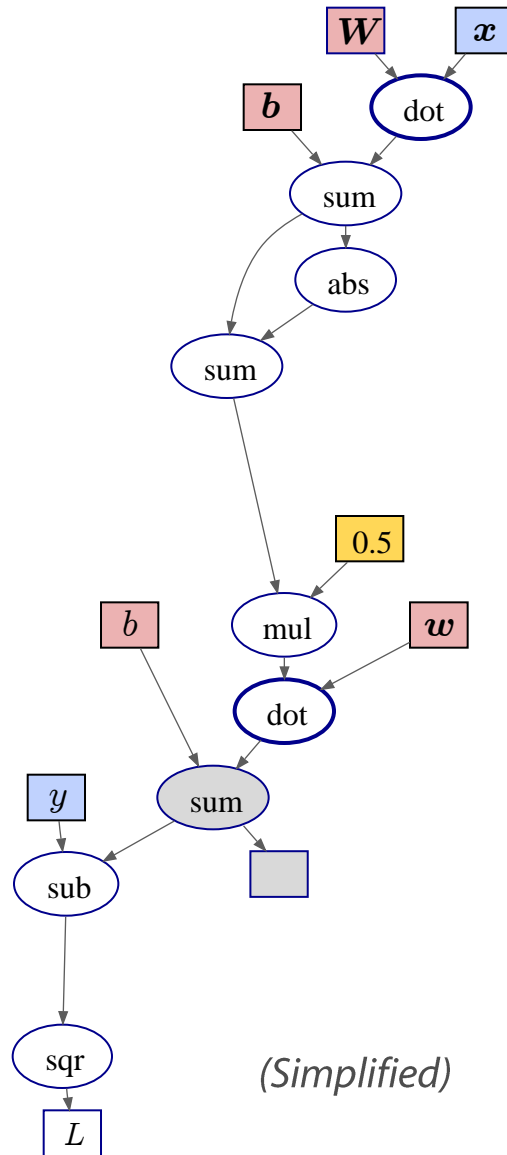


■ Computing the Flow Graph

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

Flow Graph

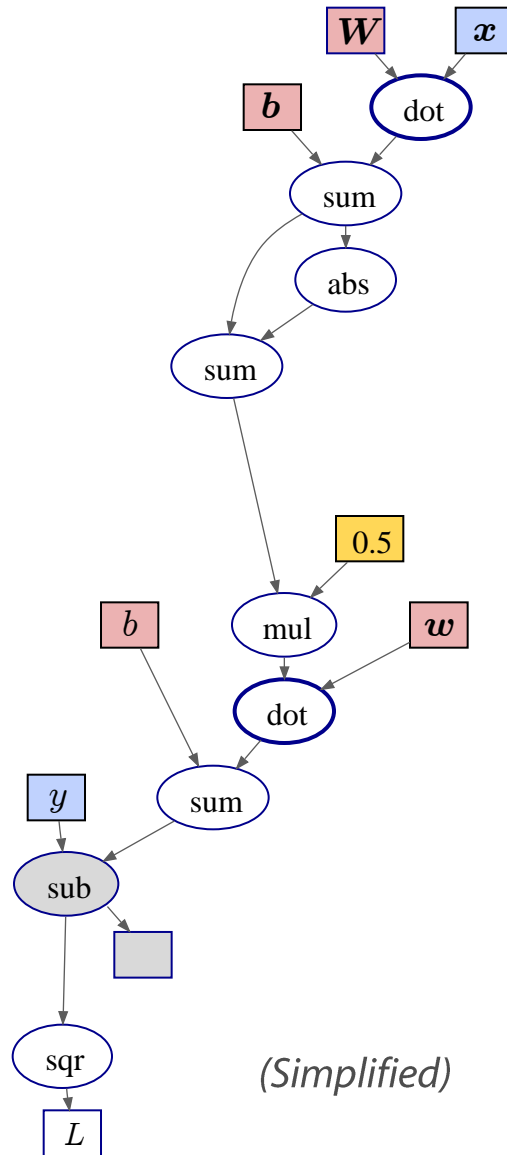


■ Computing the Flow Graph

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

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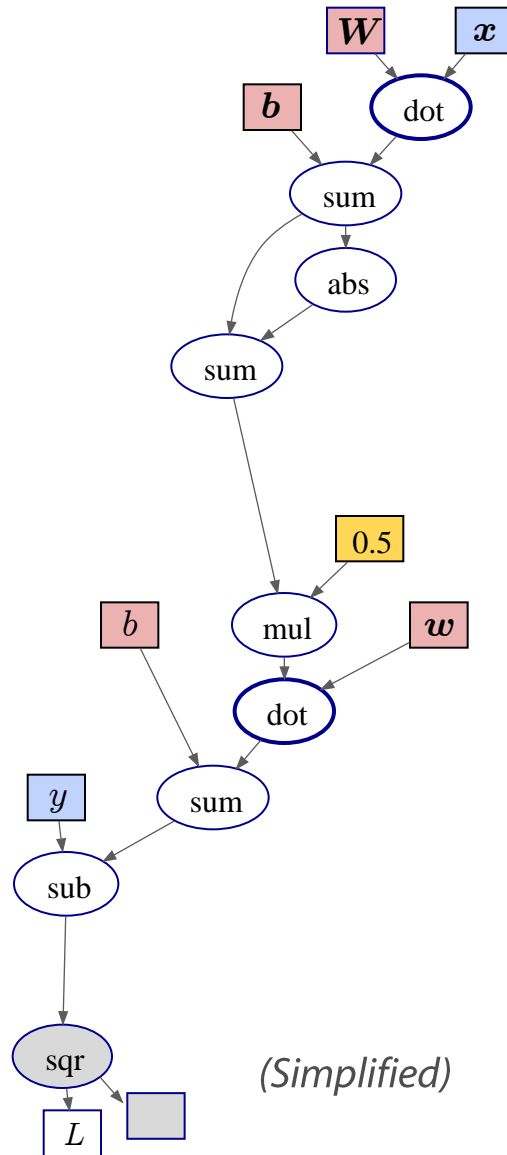


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Item-wise loss function, FF neural network with ReLU as non-linearity

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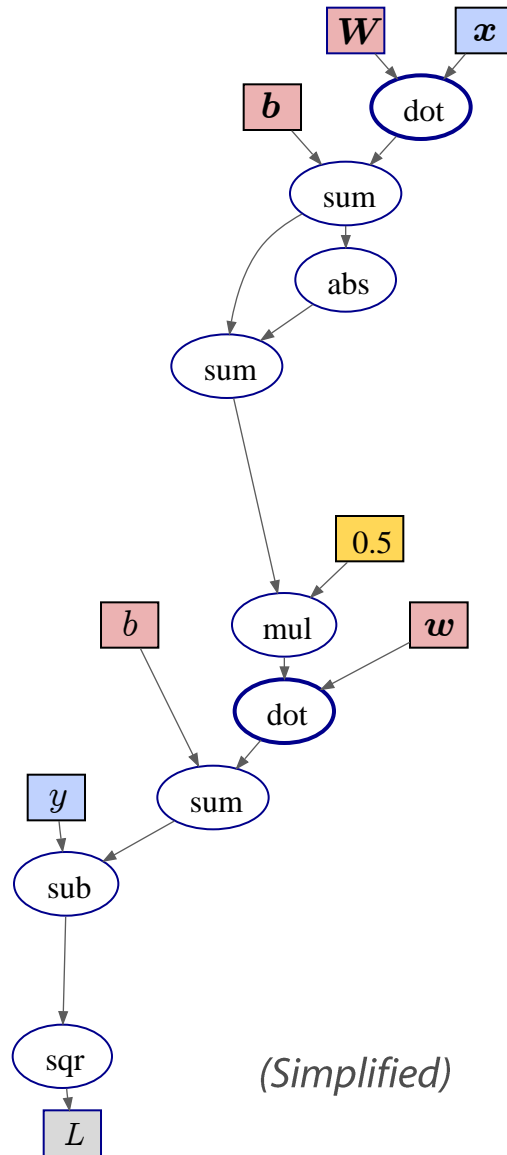


■ Computing the Flow Graph

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

Flow Graph



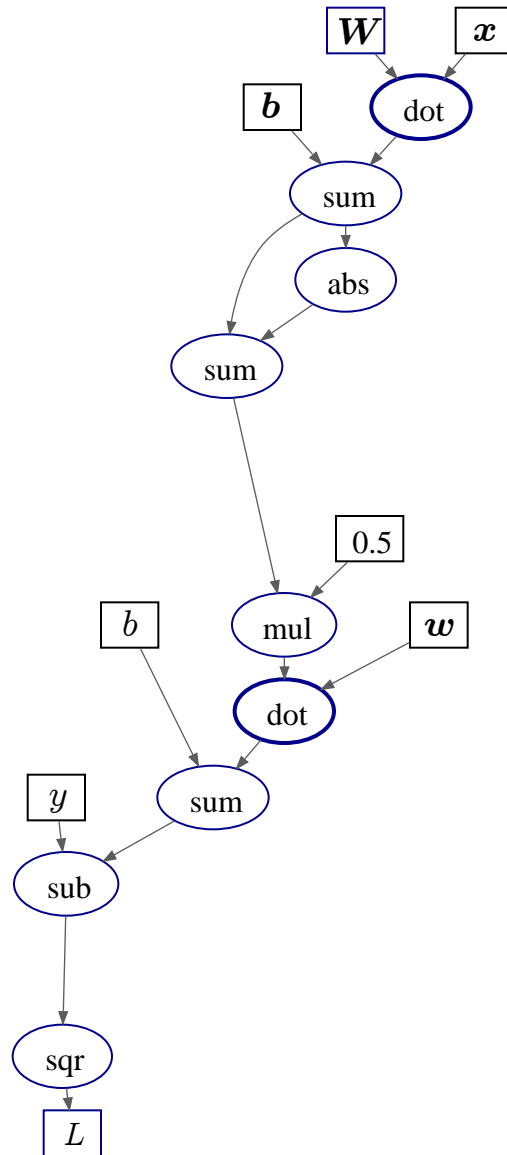
■ Computing the Flow Graph

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

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

Autograd: Automatic Differentiation of Flow Graphs

Computing Gradients

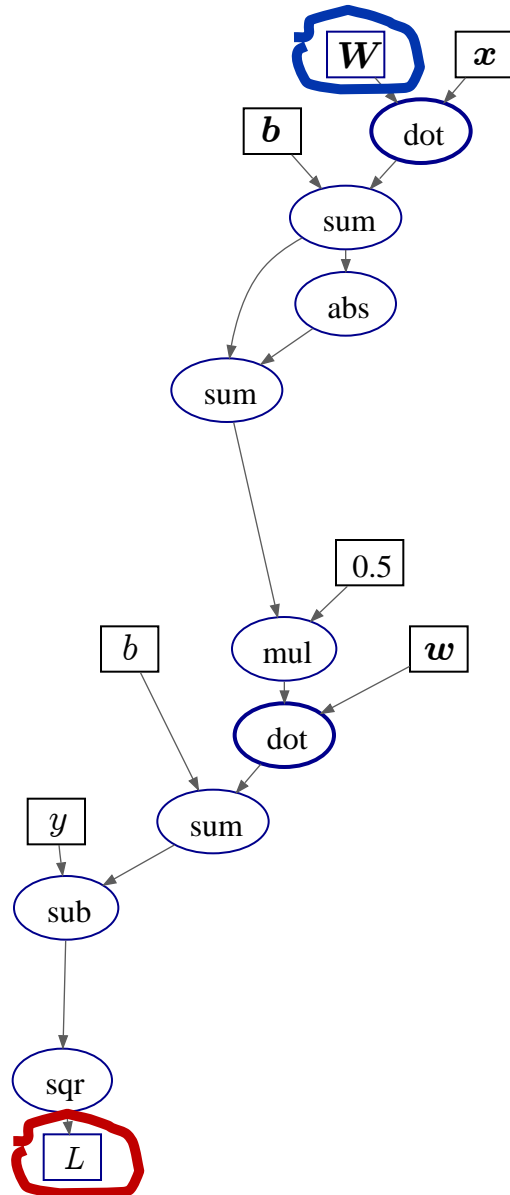


- **Computing one gradient of the flow graph**

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

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

Computing Gradients

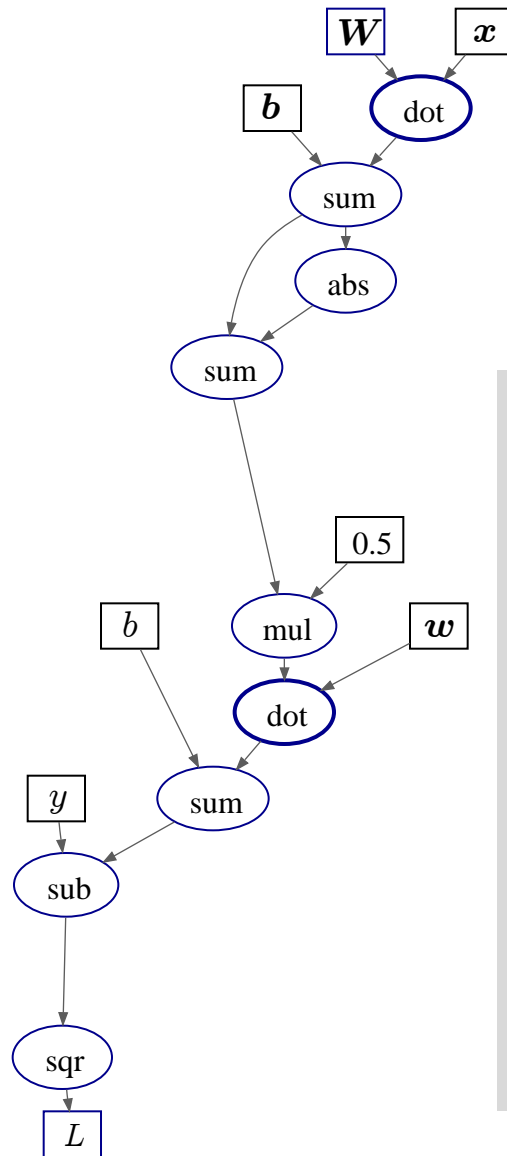


- **Computing one gradient of the flow graph**

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

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

Computing Gradients



■ Computing one gradient of the flow graph

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

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

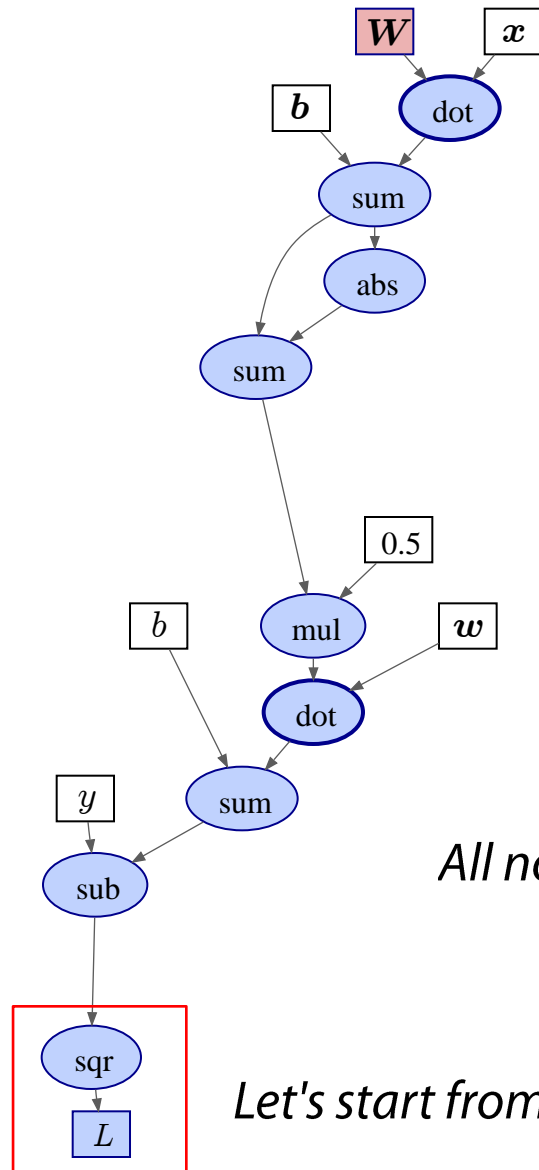
Chain rule for derivatives (*single argument*)

$$\frac{\partial}{\partial \mathbf{v}} f(g(\mathbf{v})) = \frac{\partial}{\partial g(\mathbf{v})} f(g(\mathbf{v})) \frac{\partial}{\partial \mathbf{v}} g(\mathbf{v})$$

Chain rule for derivatives (*multiple arguments*)

$$\frac{\partial}{\partial \mathbf{v}} f(g(\mathbf{v}), h(\mathbf{v})) = \frac{\partial}{\partial g(\mathbf{v})} f(g(\mathbf{v}), h(\mathbf{v})) \frac{\partial}{\partial \mathbf{v}} g(\mathbf{v}) + \frac{\partial}{\partial h(\mathbf{v})} f(g(\mathbf{v}), h(\mathbf{v})) \frac{\partial}{\partial \mathbf{v}} h(\mathbf{v})$$

Computing Gradients

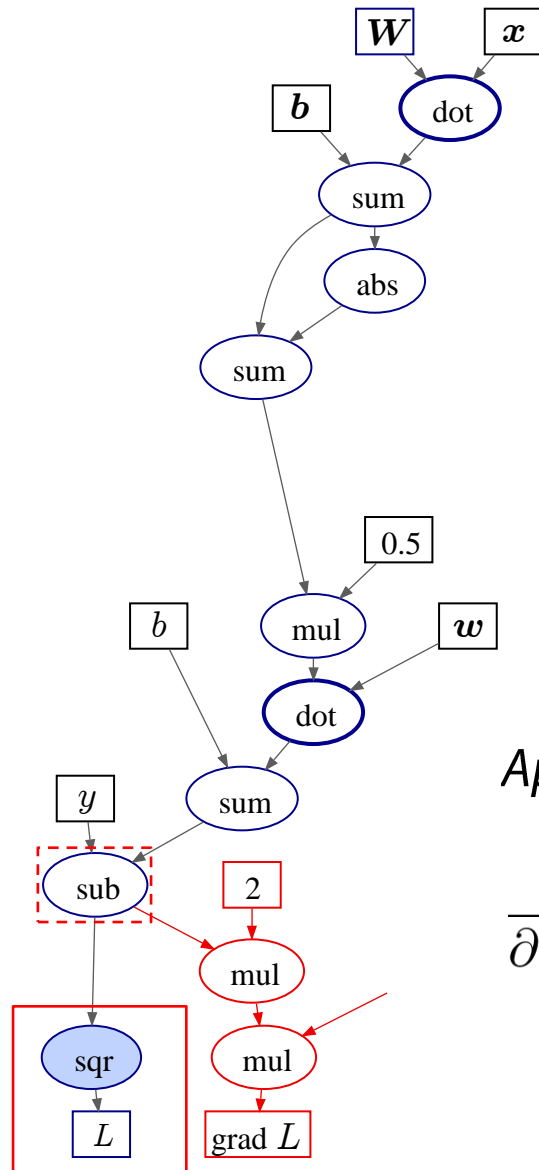


$$\frac{\partial}{\partial \mathbf{W}} (w \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + b - y)^2$$

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

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

Computing Gradients

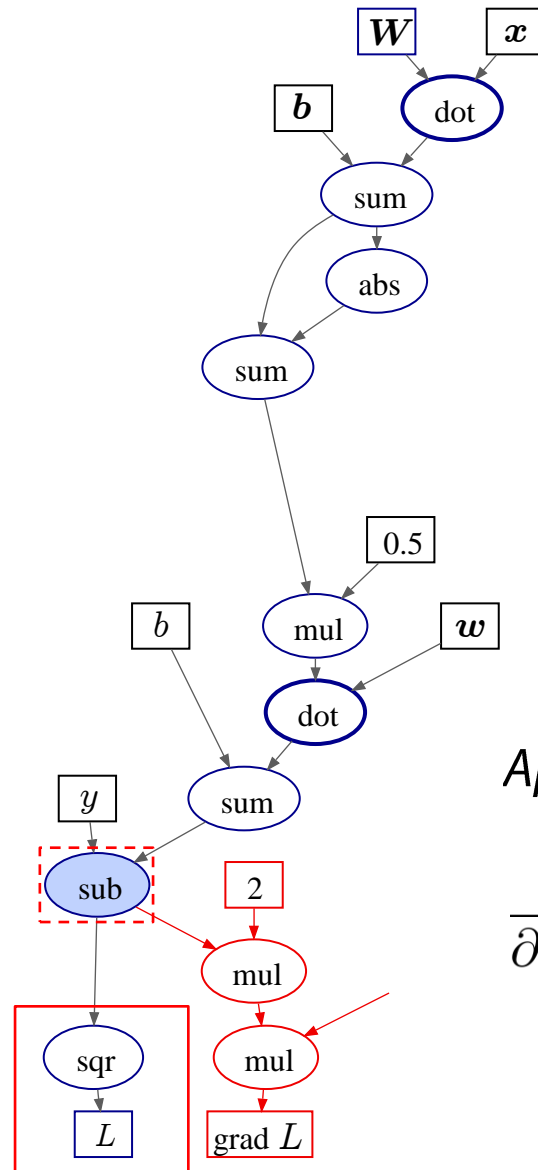


$$\frac{\partial}{\partial \mathbf{W}} (\mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + \mathbf{b} - y)^2$$

Apply the chain rule to the sqr node

$$\begin{aligned} \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})^2 &= \frac{\partial}{\partial f(\mathbf{W})} f(\mathbf{W})^2 \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \\ &= 2 \cdot f(\mathbf{W}) \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \end{aligned}$$

Computing Gradients

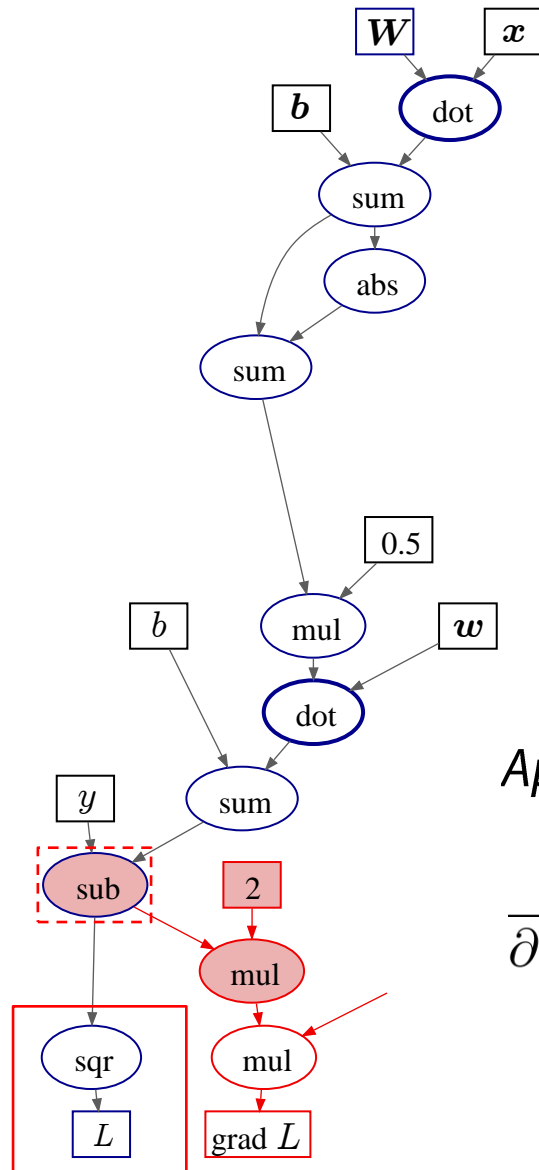


$$\frac{\partial}{\partial \mathbf{W}} (\mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + b - y)^2$$

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Computing Gradients

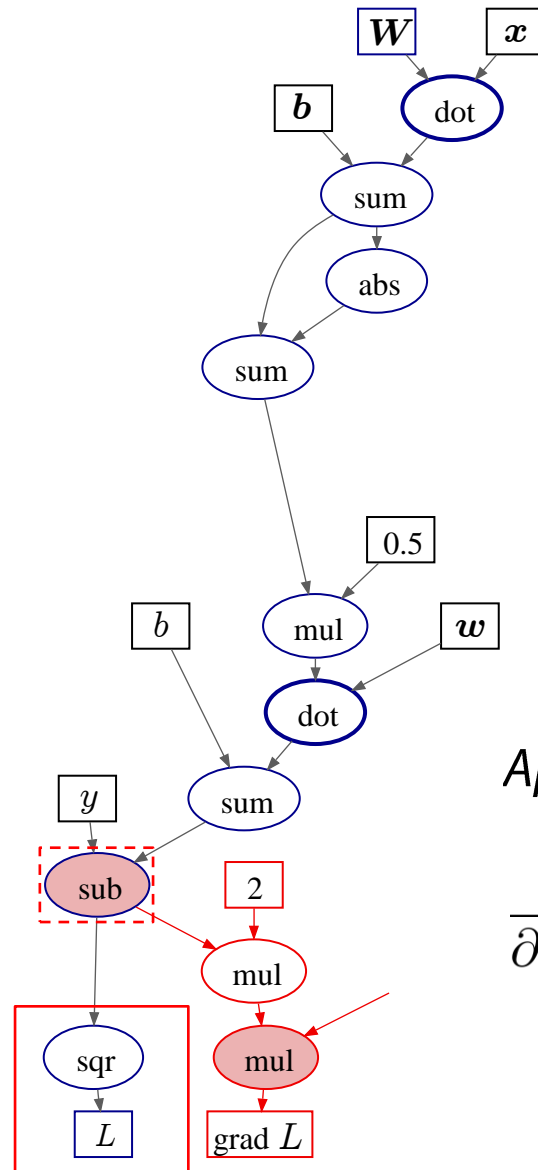


$$\frac{\partial}{\partial \mathbf{W}} (\mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + b - y)^2$$

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Computing Gradients

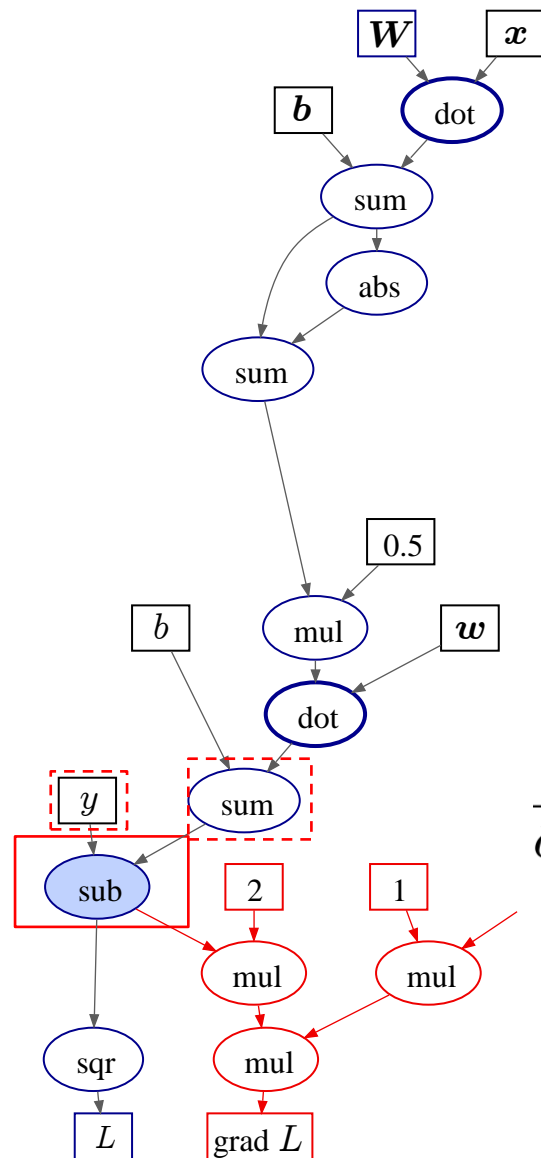


$$\frac{\partial}{\partial \mathbf{W}} (\mathbf{w} \cdot \text{ReLU}(\mathbf{W}\mathbf{x} + \mathbf{b}) + b - y)^2$$

Apply the chain rule to the sqr node

$$\begin{aligned} \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})^2 &= \frac{\partial}{\partial f(\mathbf{W})} f(\mathbf{W})^2 \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \\ &= 2 \cdot f(\mathbf{W}) \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \end{aligned}$$

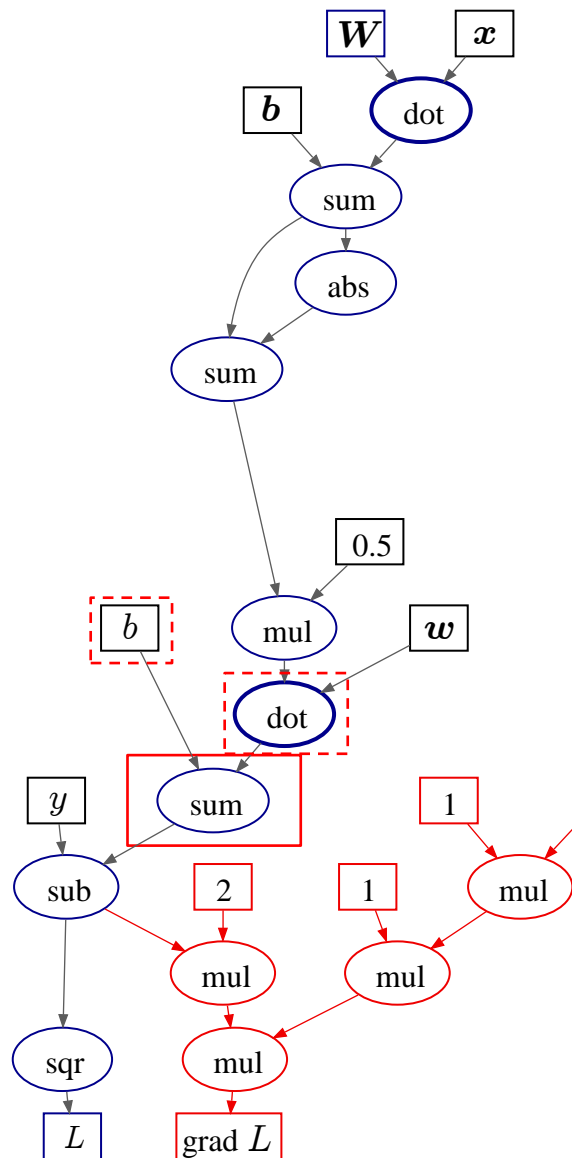
Computing Gradients



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

$$\begin{aligned}\frac{\partial}{\partial \mathbf{W}}(f(\mathbf{W}) - y) &= \frac{\partial}{\partial f(\mathbf{W})}(f(\mathbf{W}) - y) \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \\ &= 1 \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})\end{aligned}$$

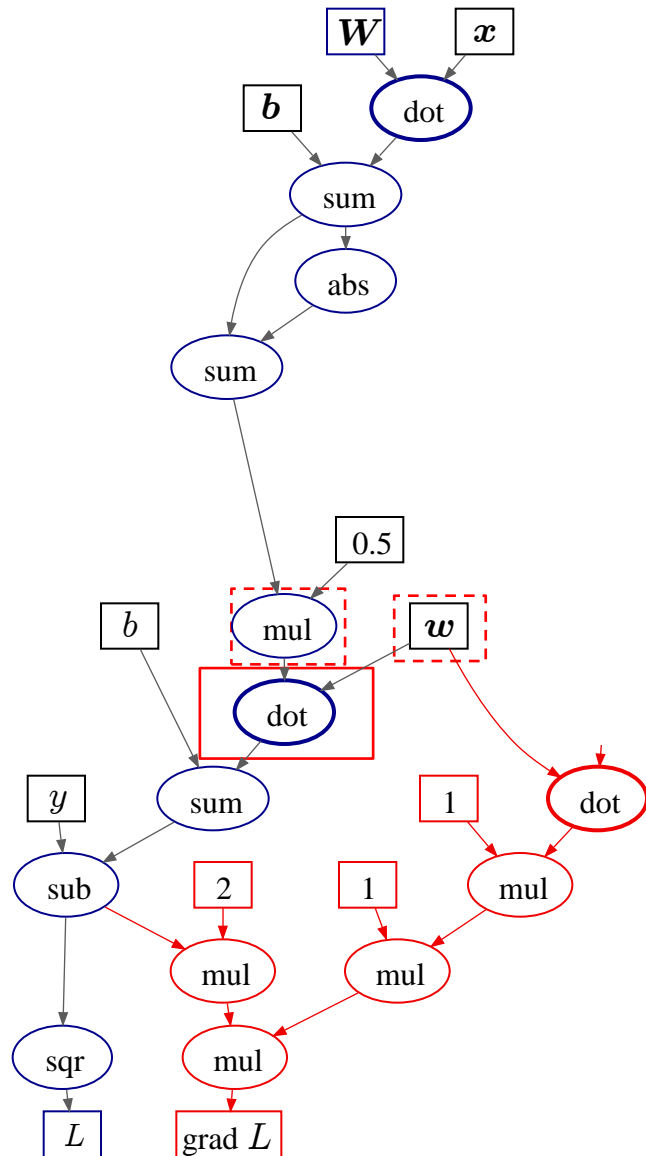
Computing Gradients



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

$$\begin{aligned}\frac{\partial}{\partial \mathbf{W}}(f(\mathbf{W}) + b) &= \frac{\partial}{\partial f(\mathbf{W})}(f(\mathbf{W}) + b) \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \\ &= 1 \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})\end{aligned}$$

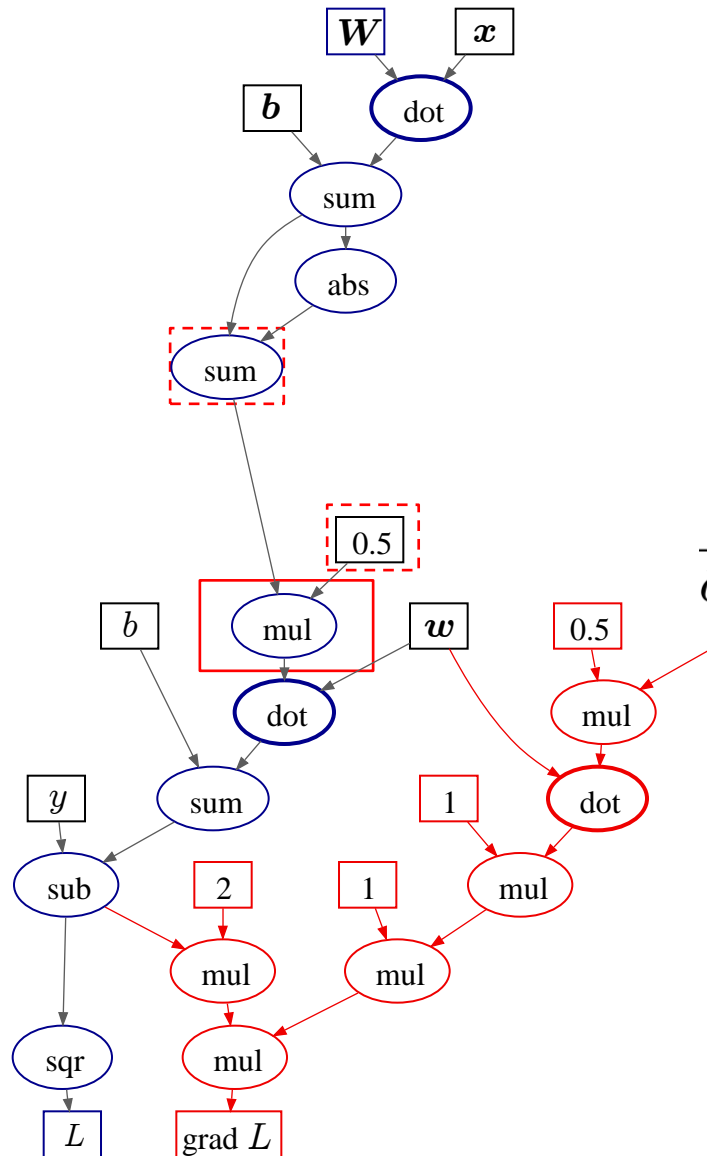
Computing Gradients



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

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

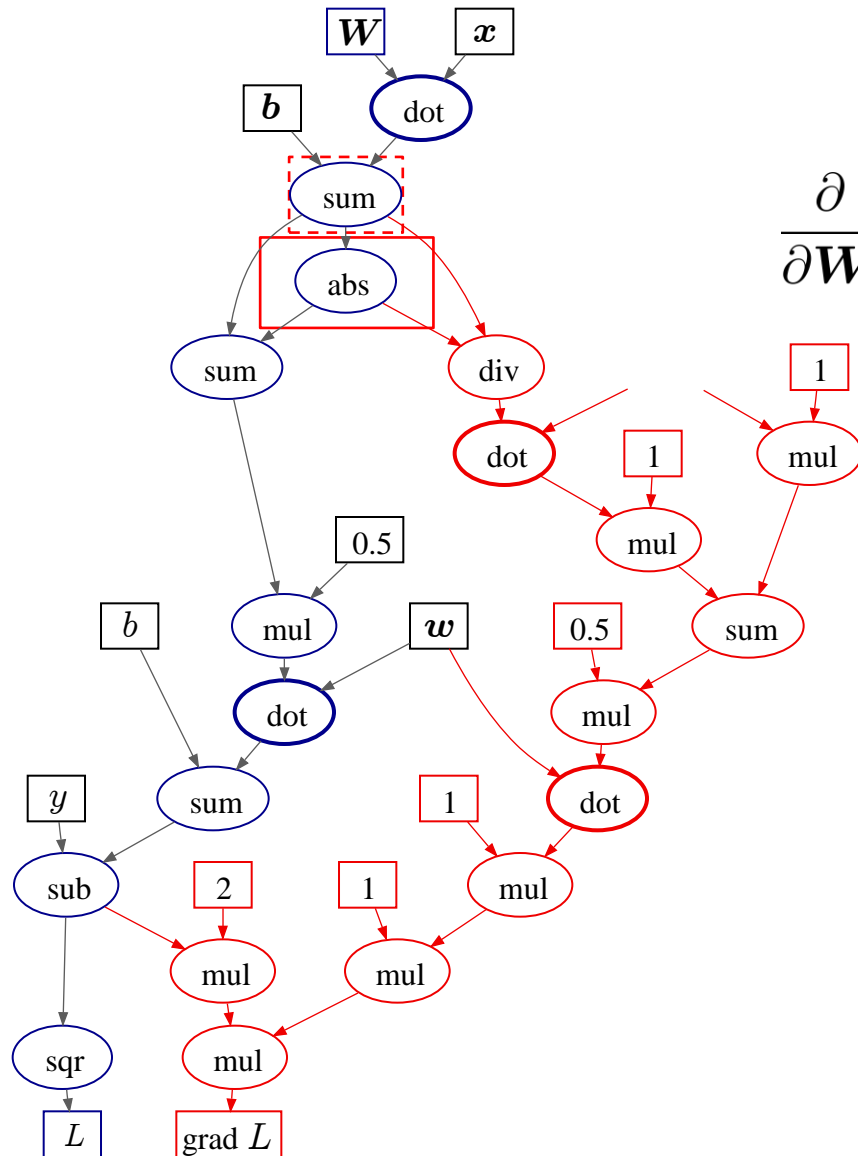
Computing Gradients




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

$$\begin{aligned} \frac{\partial}{\partial \mathbf{W}} (0.5 \cdot f(\mathbf{W})) &= \frac{\partial}{\partial f(\mathbf{W})} (0.5 \cdot f(\mathbf{W})) \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \\ &= 0.5 \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \end{aligned}$$

Computing Gradients

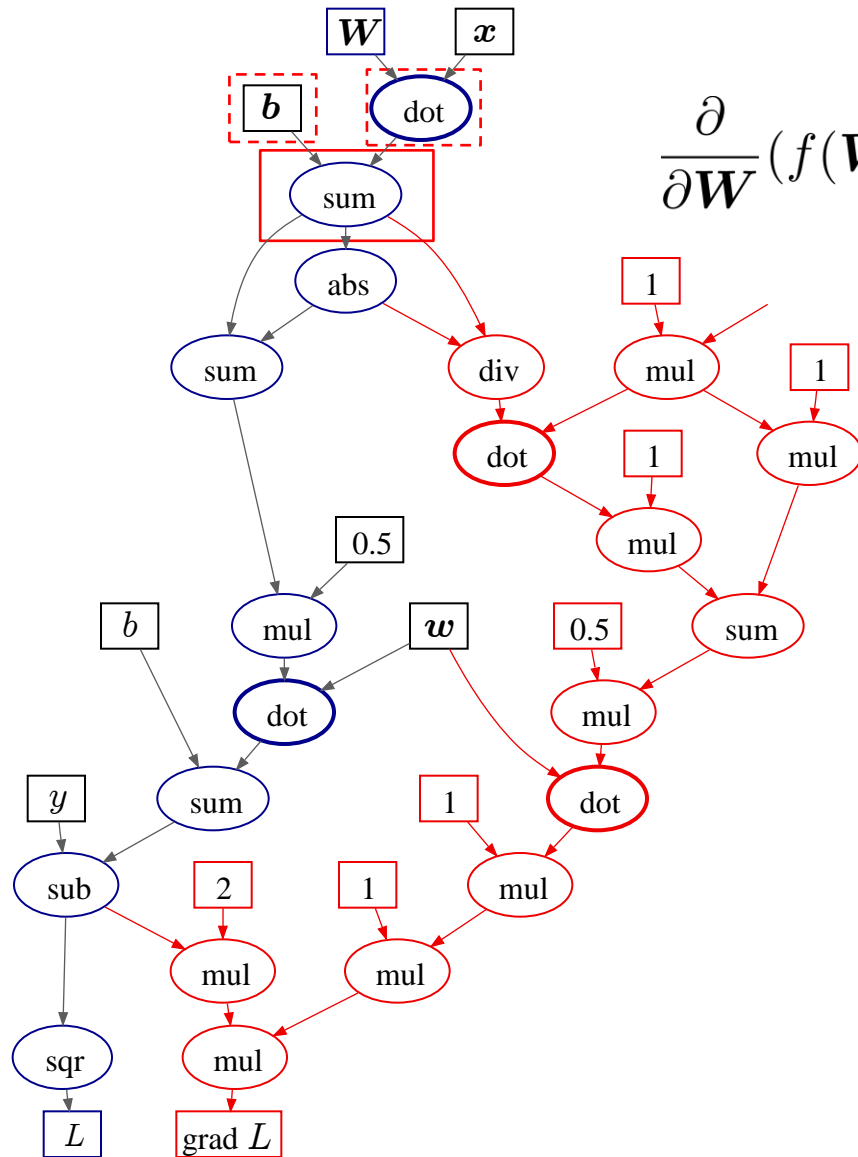


$$\frac{\partial}{\partial \mathbf{W}} |f(\mathbf{W})| = \frac{\partial}{\partial f(\mathbf{W})} |f(\mathbf{W})| \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W})$$

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


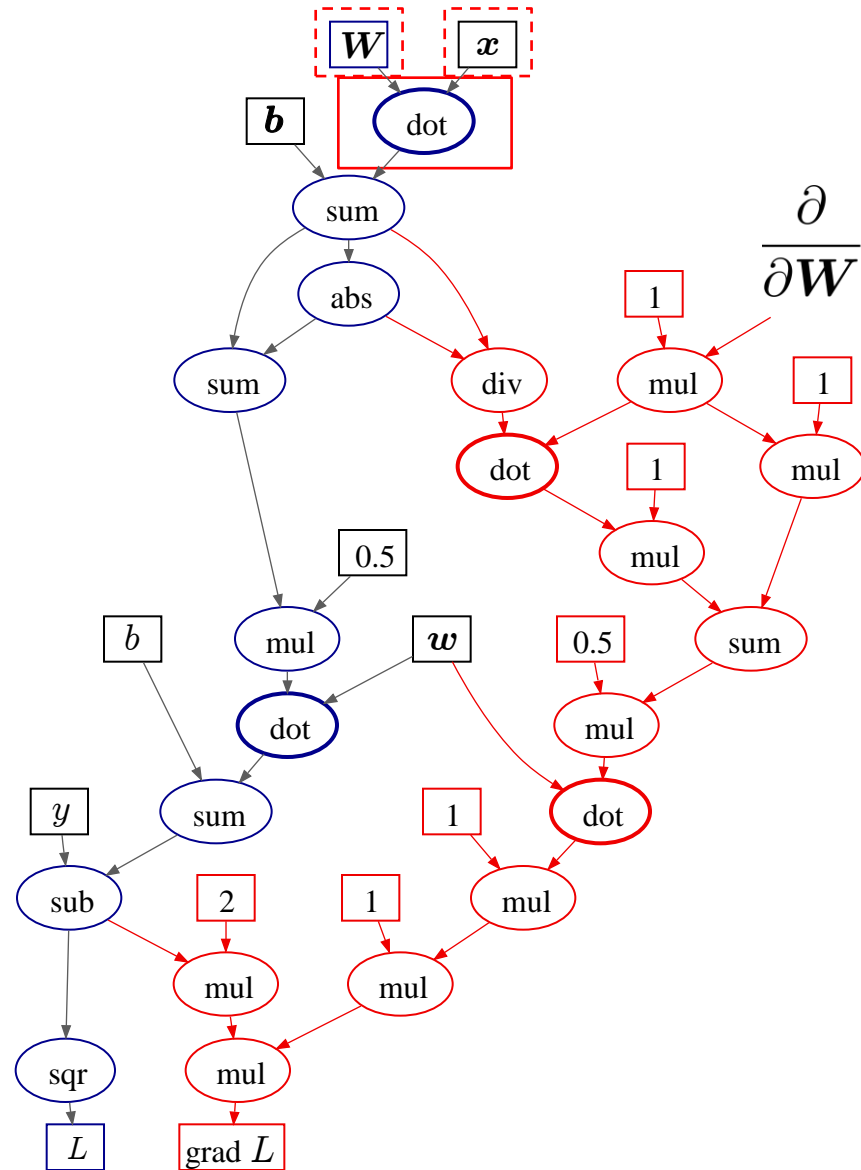
Clearly, this term is not defined for any $W_{ij} = 0$
 (Typically, this is a protected division $\frac{x}{0} := 1$)

Computing Gradients



$$\begin{aligned} \frac{\partial}{\partial \mathbf{W}} (f(\mathbf{W}) + b) &= \frac{\partial}{\partial f(\mathbf{W})} (f(\mathbf{W}) + b) \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \\ &= 1 \cdot \frac{\partial}{\partial \mathbf{W}} f(\mathbf{W}) \end{aligned}$$

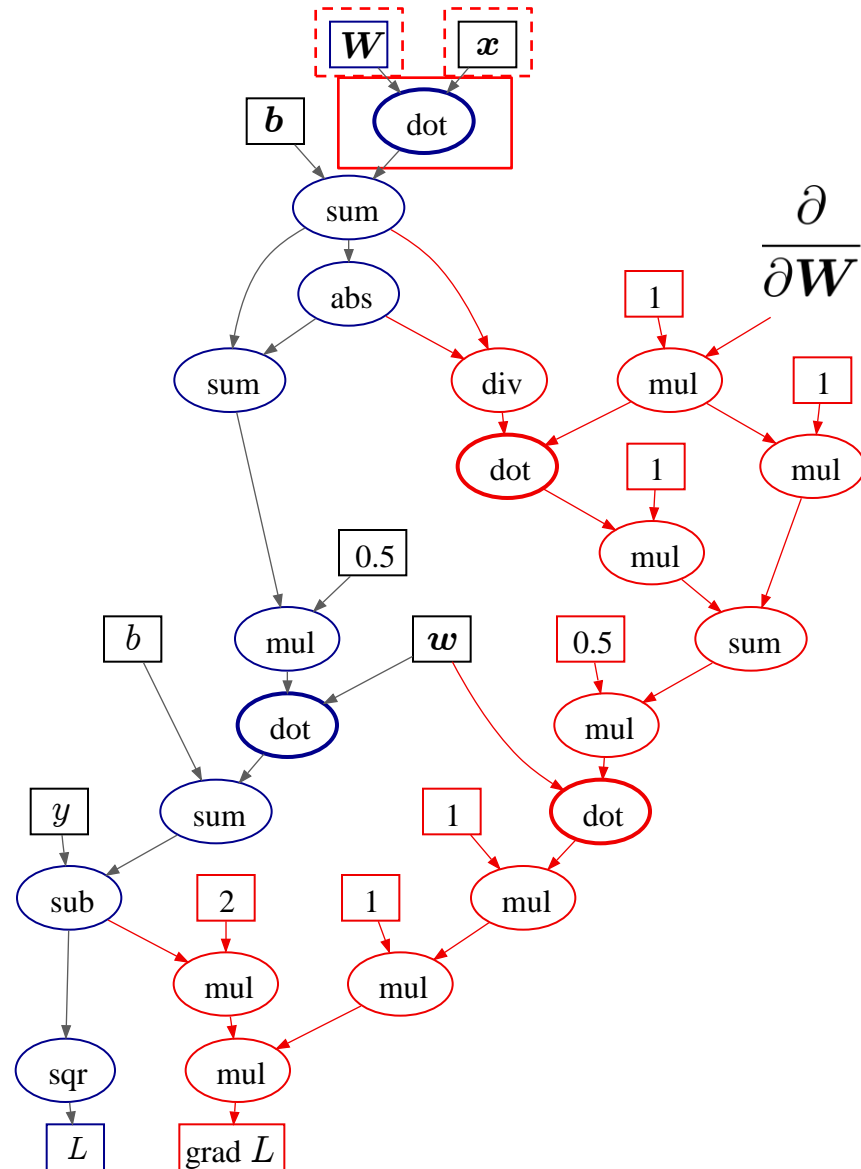
Computing Gradients



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

Well, this is tricky....

Computing Gradients



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

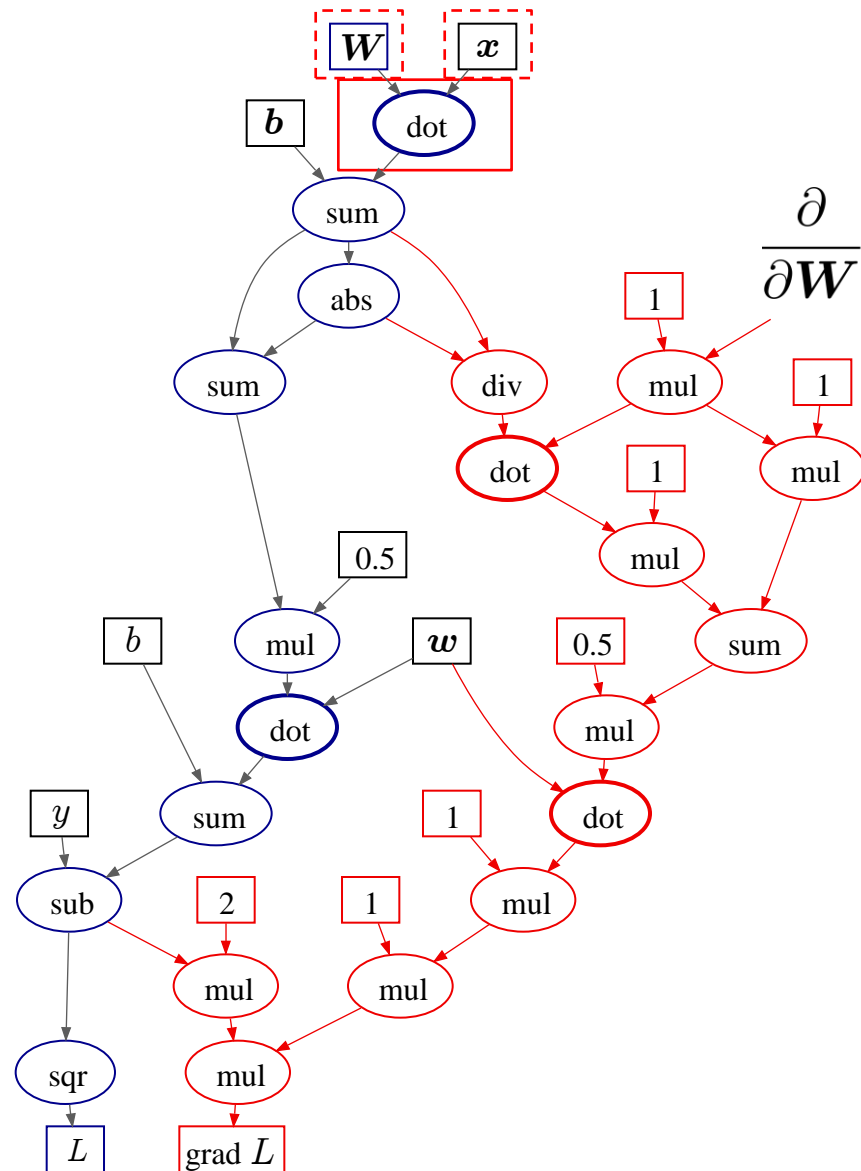
This is a third-order tensor

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

Its ijk -th component

Note the inversion of indices

Computing Gradients



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

This is a third-order tensor

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

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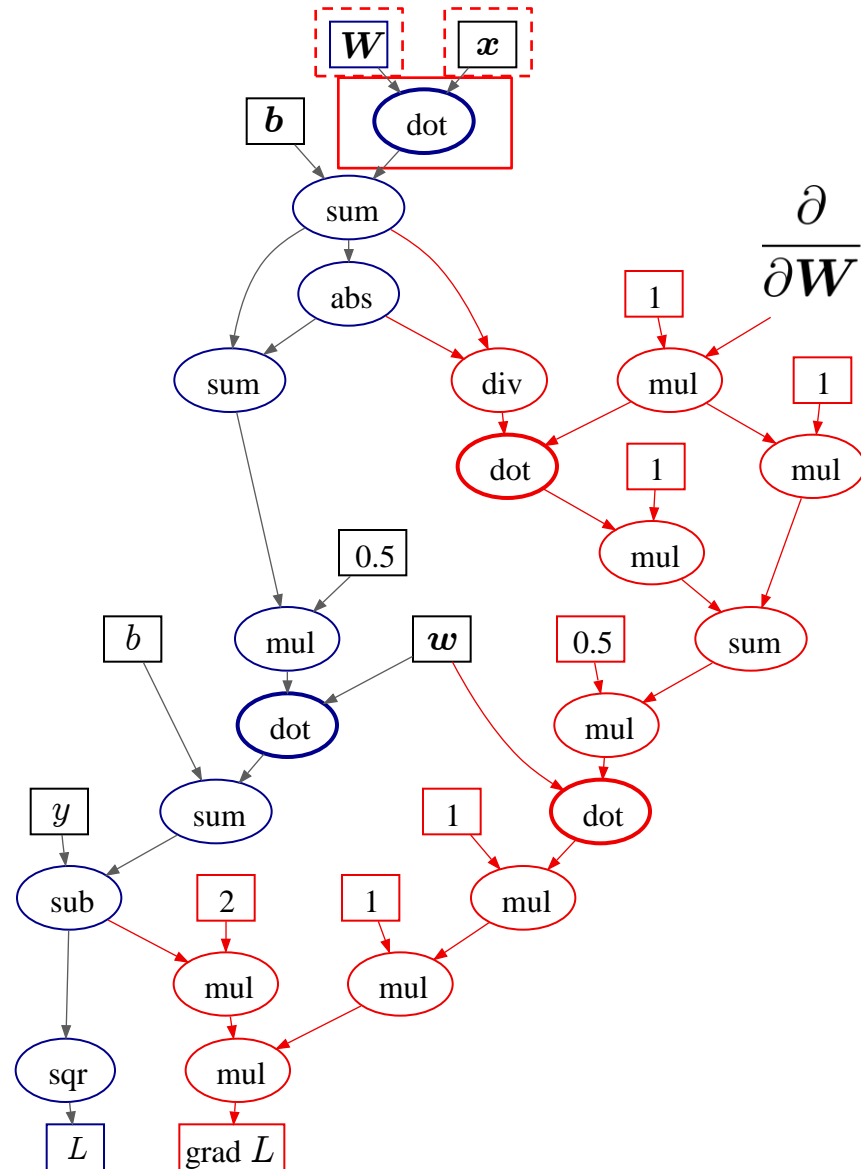
Note the inversion of indices

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

The i -th line in the matrix

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

Computing Gradients

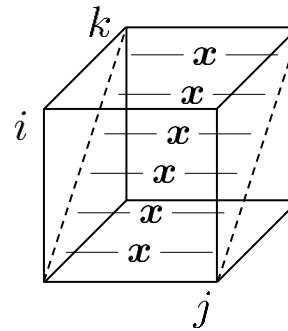


$$\frac{\partial}{\partial \mathbf{W}} (\mathbf{W} \cdot \mathbf{x})$$

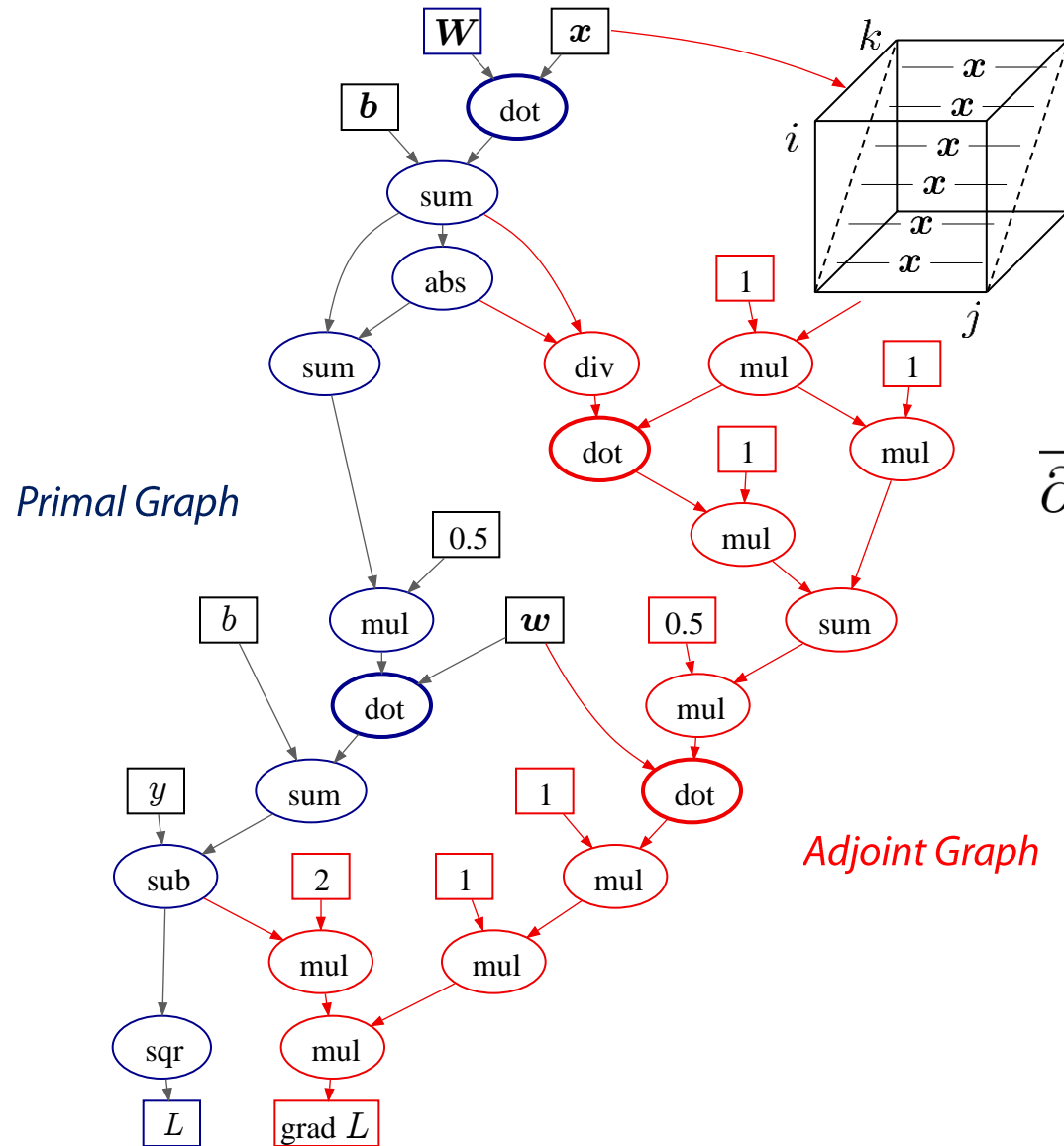
Putting it all together...

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

This 'thing' (tensor) is a cube having copies of \mathbf{x} on one diagonal 'plane' and zeros elsewhere

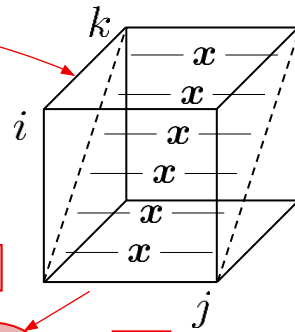
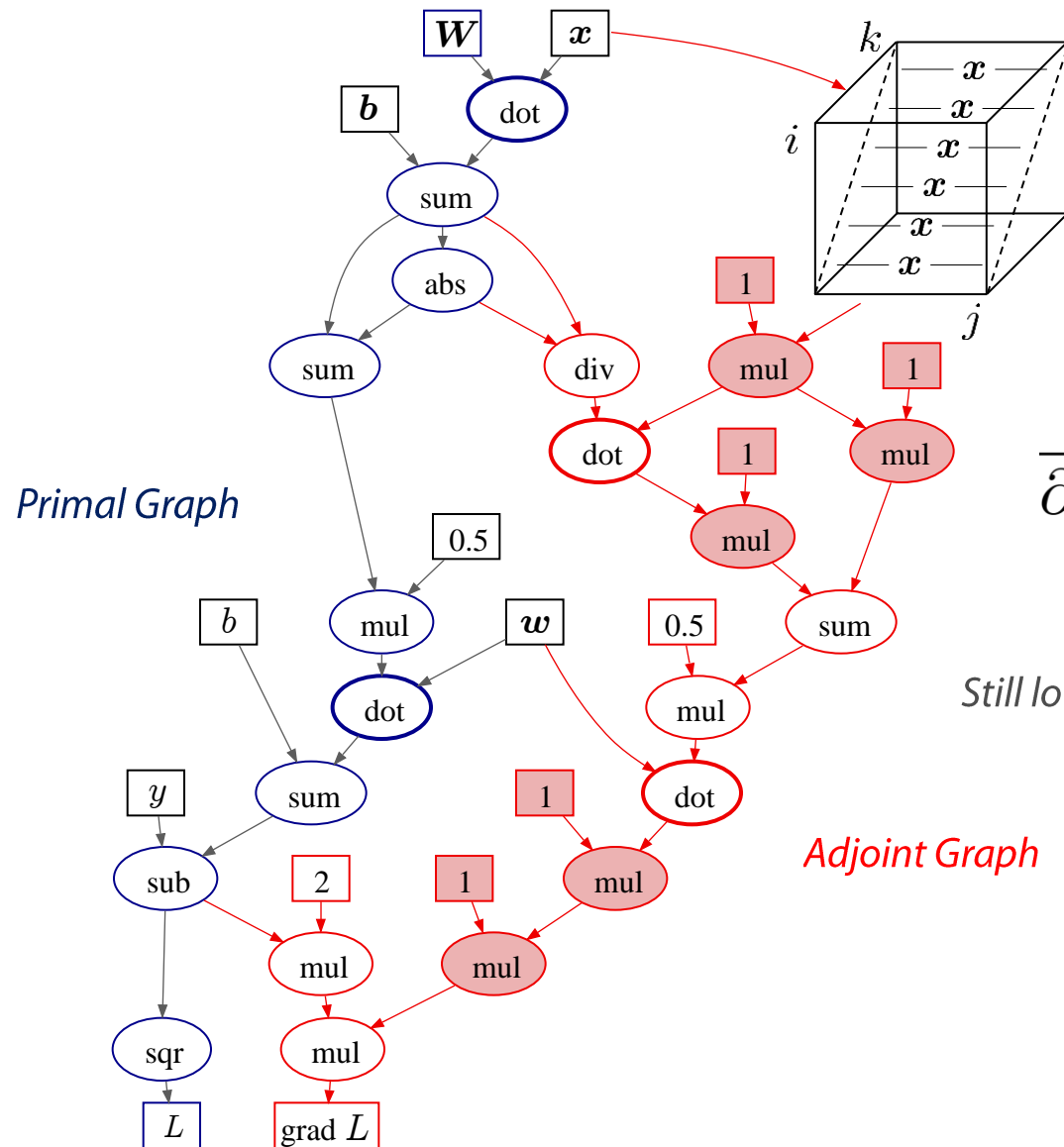


Computing Gradients



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

Computing Gradients

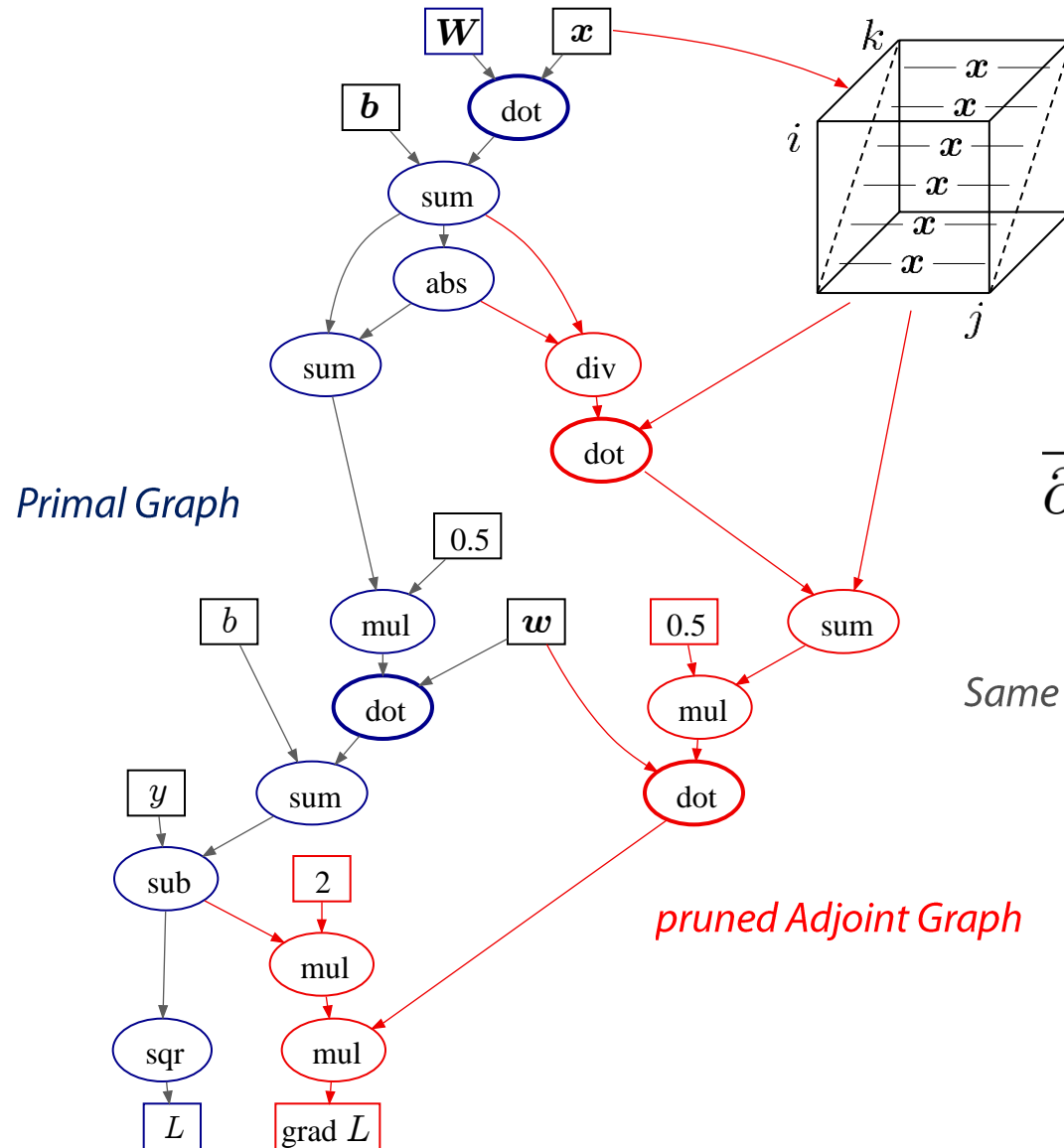


The representation of this can be optimized too

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

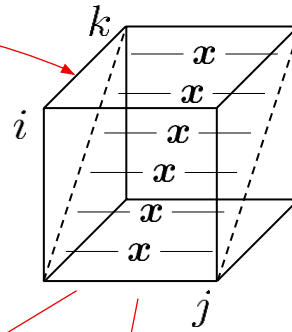
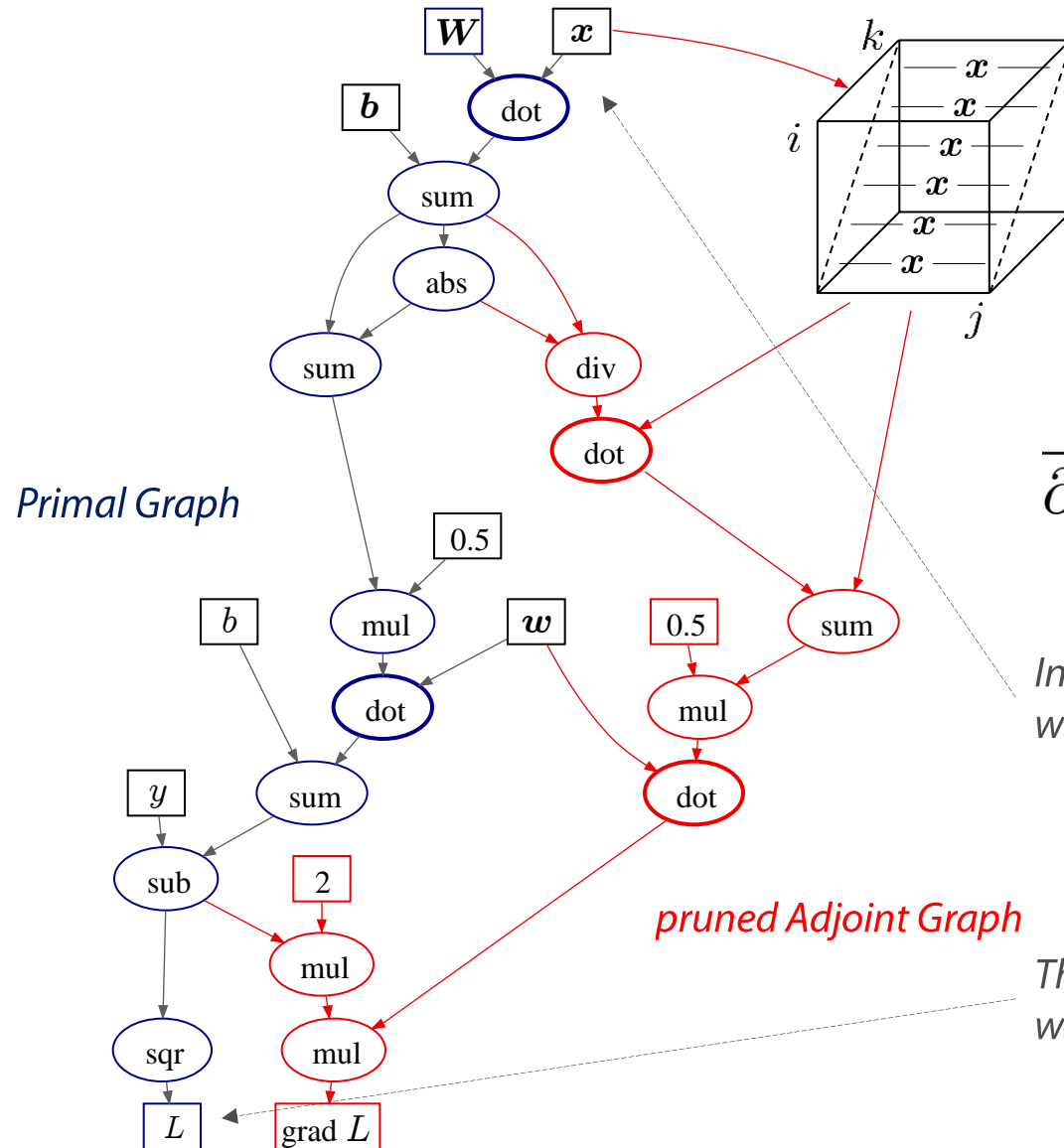
Still lots of useless operations

Computing Gradients



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

Computing Gradients



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

In **forward accumulation** mode
we would have started from here

This is autograd with **reverse (backward) accumulation**:
we started from here and we proceeded in reverse

(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

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

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

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

Then we can write

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

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

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

by defining

$$\hat{\mathbf{X}} := \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} & 1 \end{bmatrix} \quad \hat{\mathbf{W}} := \left[\begin{array}{c|c} \mathbf{W} & \mathbf{b} \end{array} \right]$$

Then we could write

$$\hat{\mathbf{W}} \hat{\mathbf{X}}^T = \left[\begin{array}{c|c} \mathbf{W} \mathbf{x}^{(1)} + \mathbf{b} & \dots & \mathbf{W} \mathbf{x}^{(N)} + \mathbf{b} \end{array} \right]$$

Matrix $\hat{\mathbf{W}}$
includes two parameters: \mathbf{W} and \mathbf{b}

*this may be inconvenient for Autograd,
due to the lack of modularity
(more to follow)*

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

Consider then $(\mathbf{W}\mathbf{x} + \mathbf{b})$
and let's keep the definition

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

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

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

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Say it with matrices...

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

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

Consider then $(\mathbf{W}\mathbf{x} + \mathbf{b})$
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It could be convenient to redefine the operator $+$ such that is interpreted as

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

\ This is called **broadcasting**

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Say it with matrices...

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

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

Using broadcasting, we would express the above as

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

But it does NOT work

Matrix $\mathbf{W} \mathbf{X}^T \in \mathbb{R}^{h \times N}$ and vector $\mathbf{b} \in \mathbb{R}^h$ are not aligned
(for **broadcasting**, the operands' **shapes** must be right-aligned)

More on Matrix Forms

Say it with matrices...

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

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

Using broadcasting, we would express the above as

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

But it does NOT work yet

Now matrix $\mathbf{W} \mathbf{X}^T \in \mathbb{R}^{N \times h}$ and vector $\mathbf{b} \in \mathbb{R}^h$ are right-aligned in shape
Moreover, the resulting matrix is **data item index first**

Vector $\mathbf{w} \in \mathbb{R}^h$ cannot be left-multiplied with a matrix in $\mathbb{R}^{N \times h}$

More on Matrix Forms

Say it with matrices...

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

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

Using broadcasting, we can express the above as

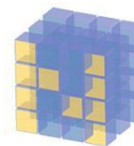
$$L(D) = \frac{1}{N} ((g(\mathbf{X}\mathbf{W}^T + \mathbf{b})\mathbf{w} + b) - \mathbf{y})^2$$

The result is a vector in \mathbb{R}^N

Broadcasting applies

This is a vector in \mathbb{R}^N

A similar behavior of operators is standard in



NumPy

