
Computation Graphs

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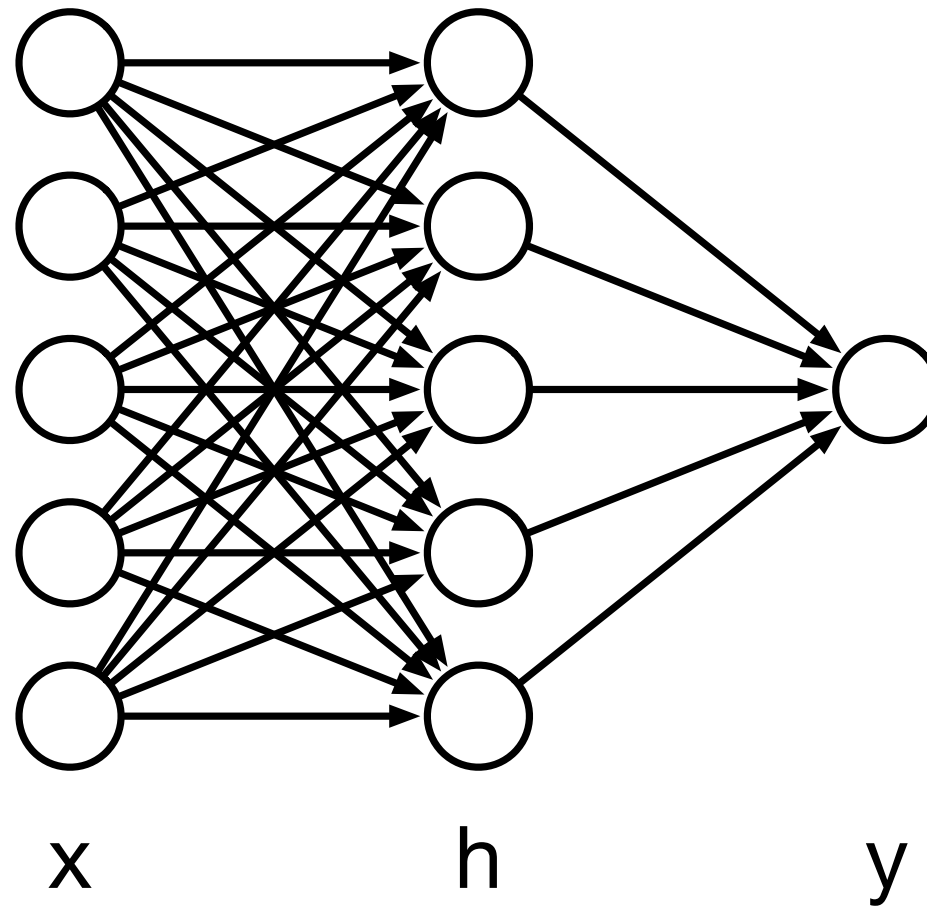
29 May 2024



Neural Network Cartoon



- A common way to illustrate a neural network



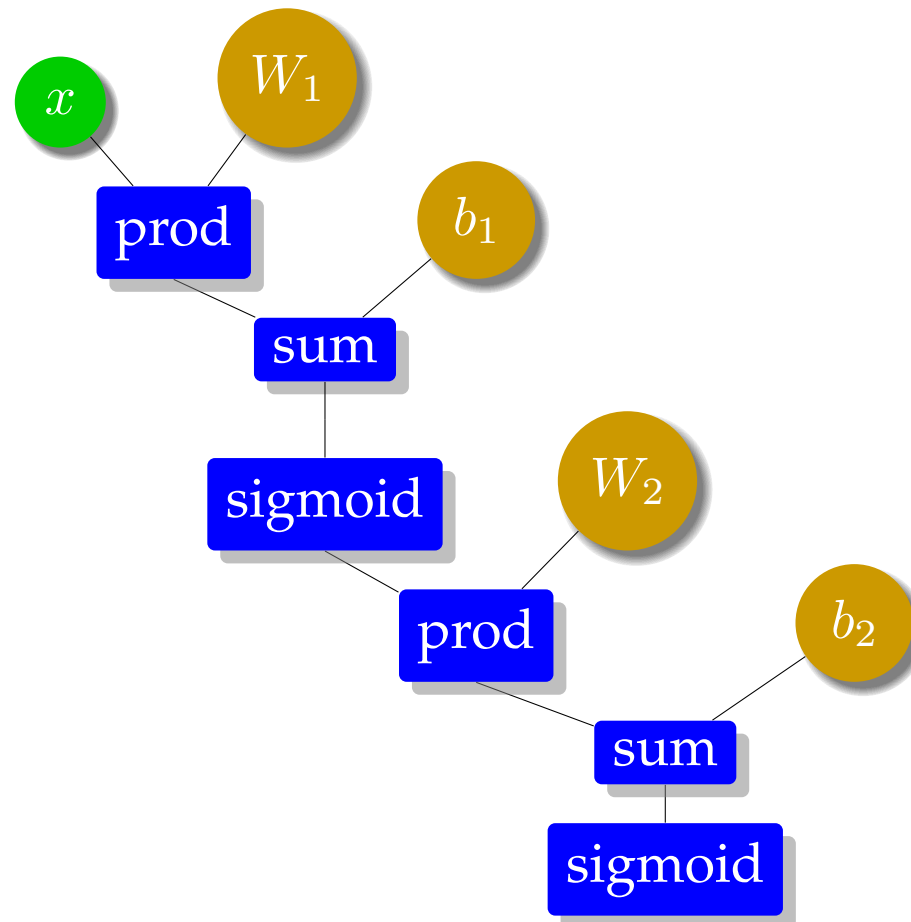
- Hidden layer

$$h = \text{sigmoid}(W_1x + b_1)$$

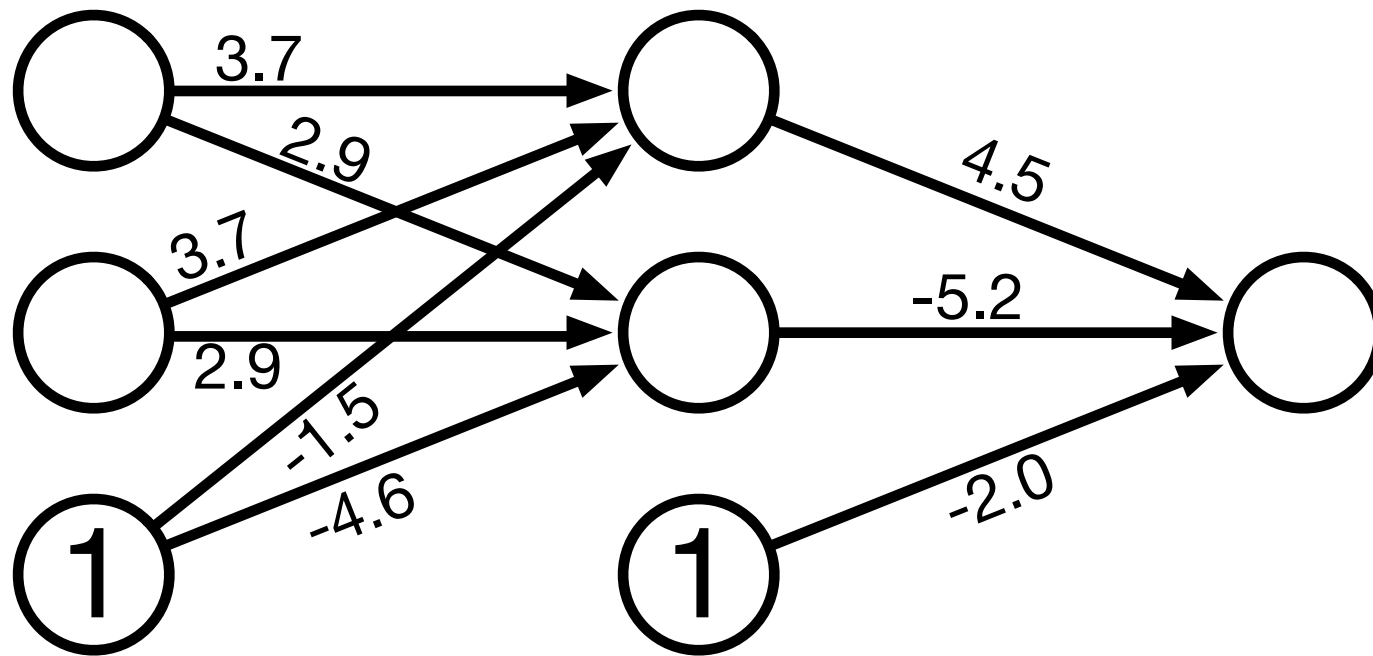
- Final layer

$$y = \text{sigmoid}(W_2h + b_2)$$

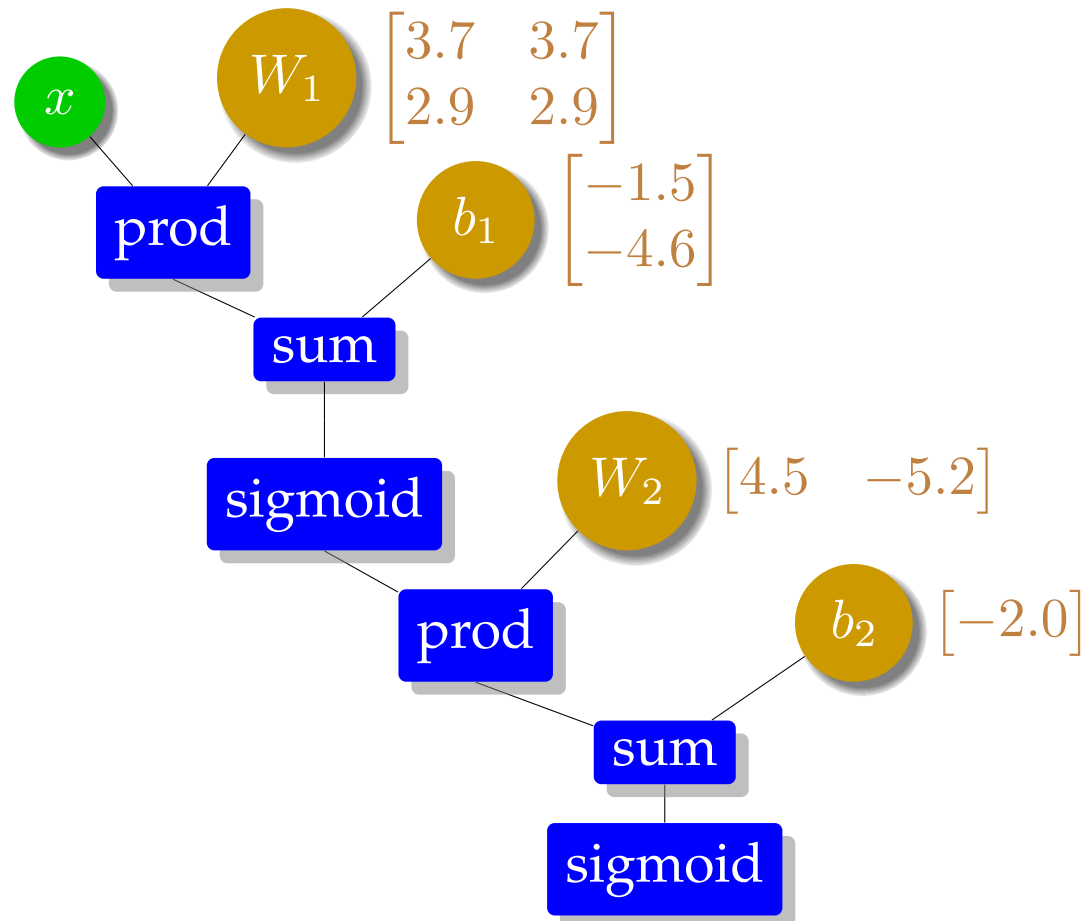
Computation Graph



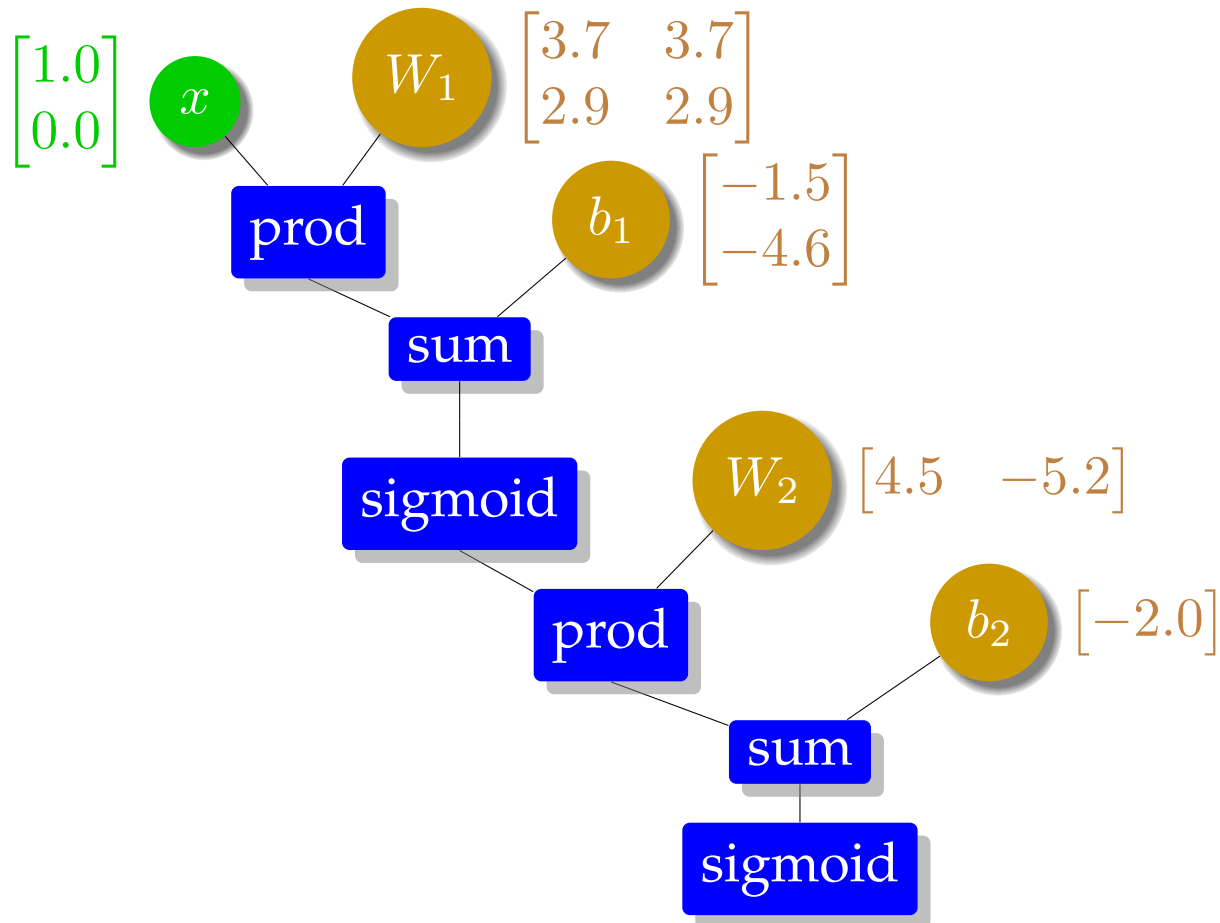
Simple Neural Network



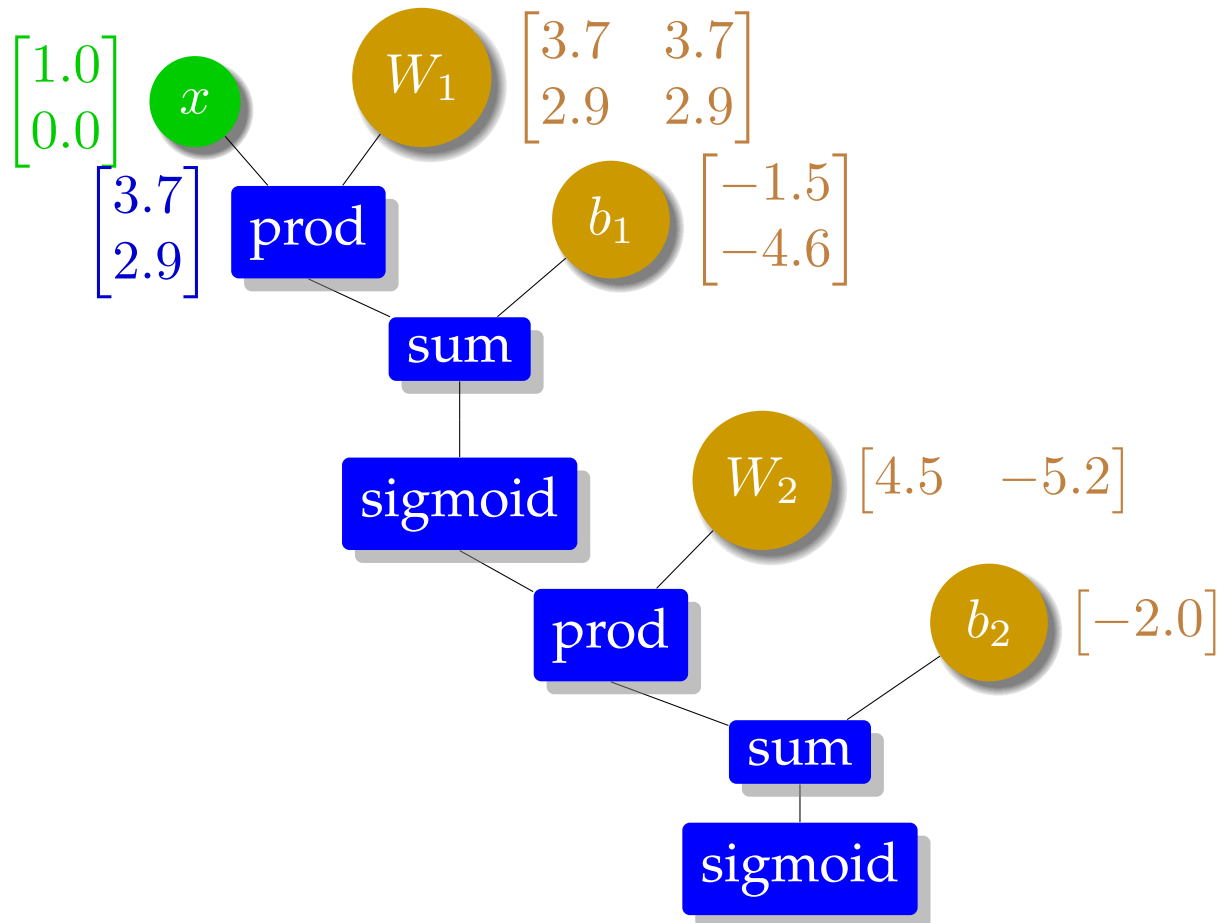
Computation Graph



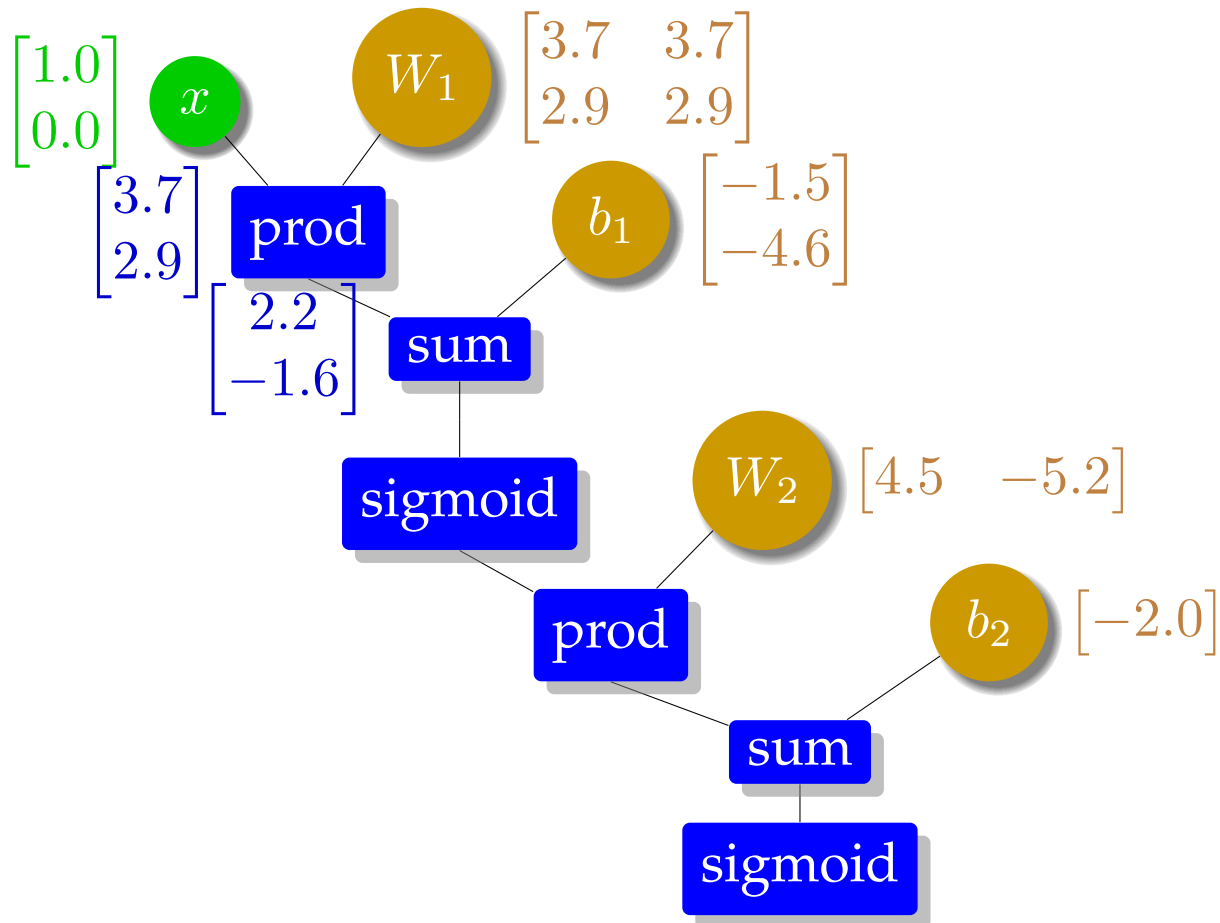
Processing Input



Processing Input



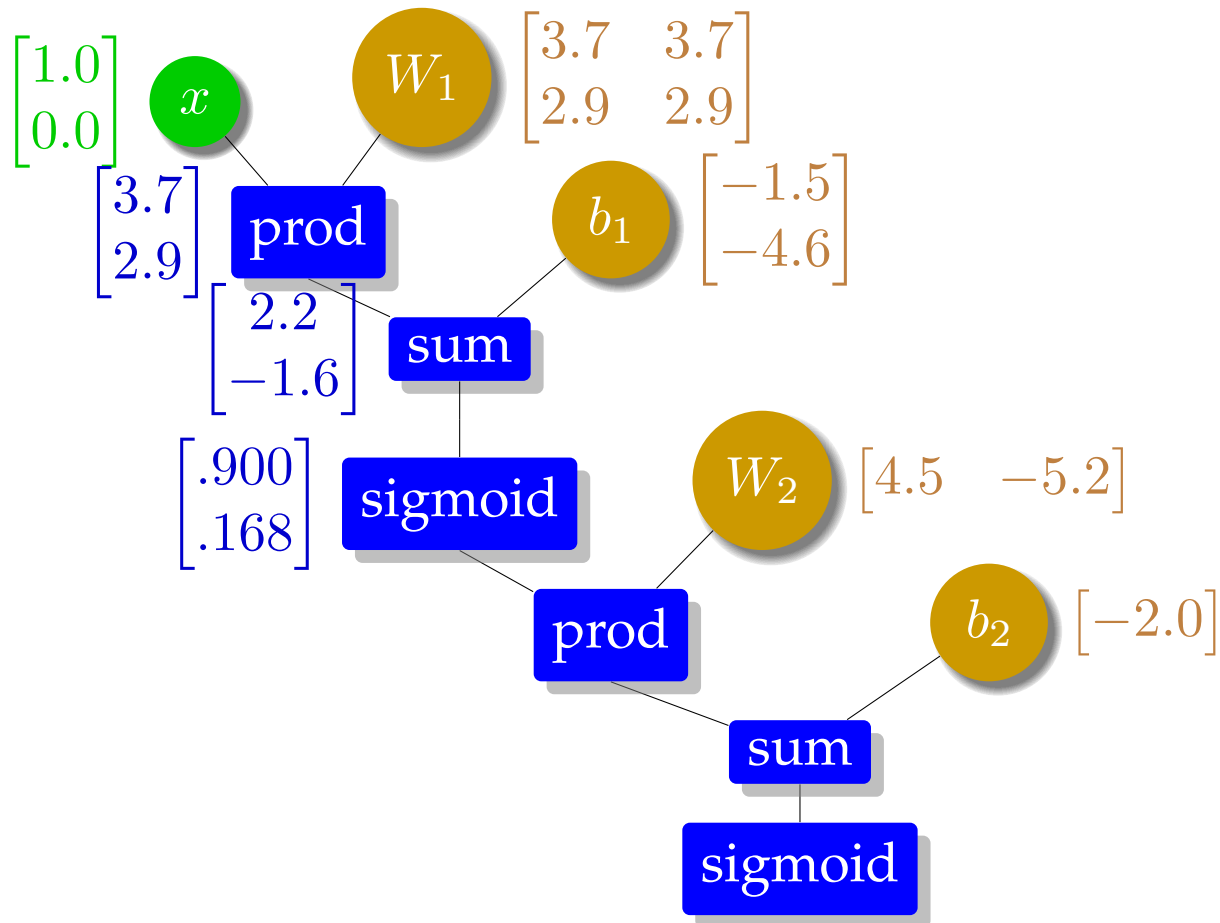
Processing Input



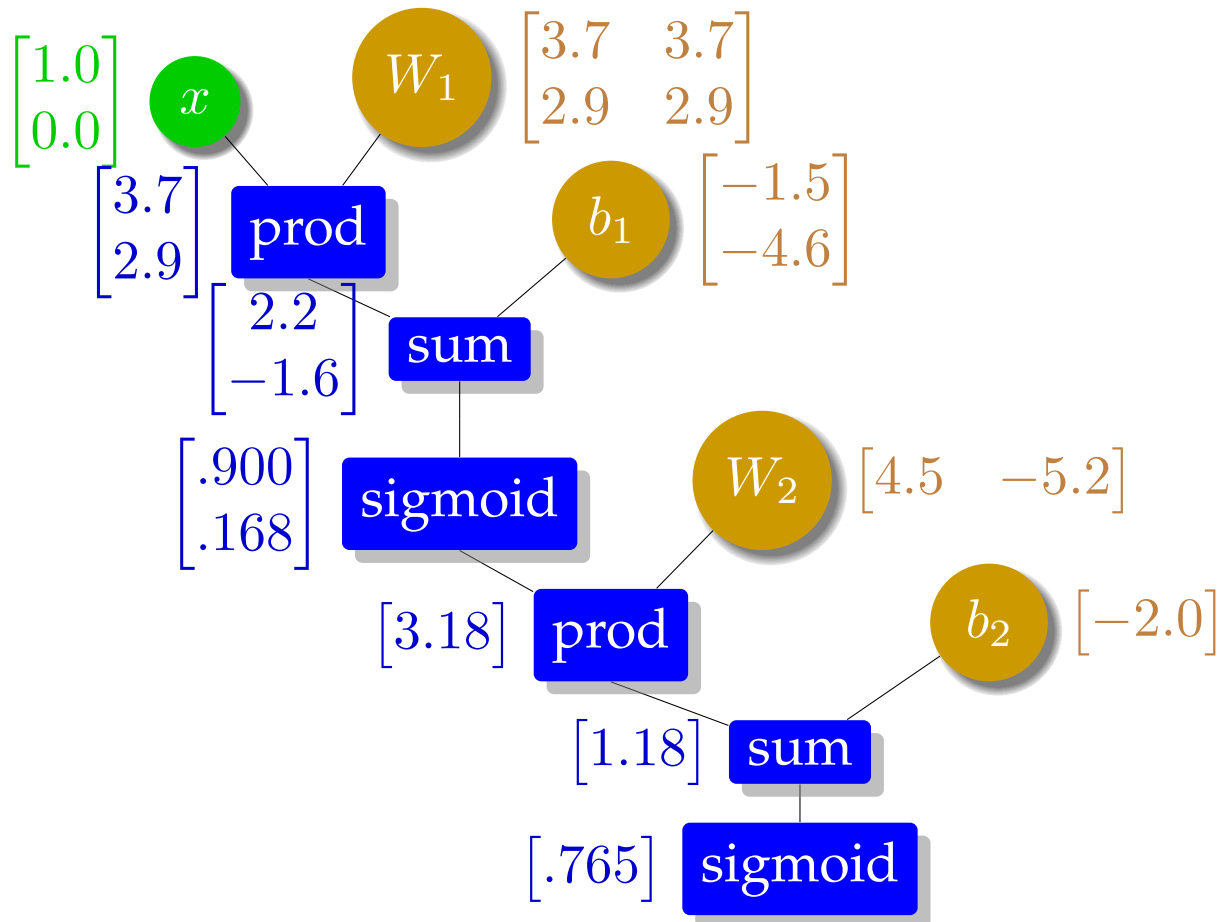
Processing Input



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Processing Input



Error Function

- For training, we need a measure how well we do

⇒ Cost function

also known as objective function, loss, gain, cost, ...

- For instance L2 norm

$$\text{error} = \frac{1}{2}(t - y)^2$$

Gradient Descent

- We view the error as a function of the trainable parameters

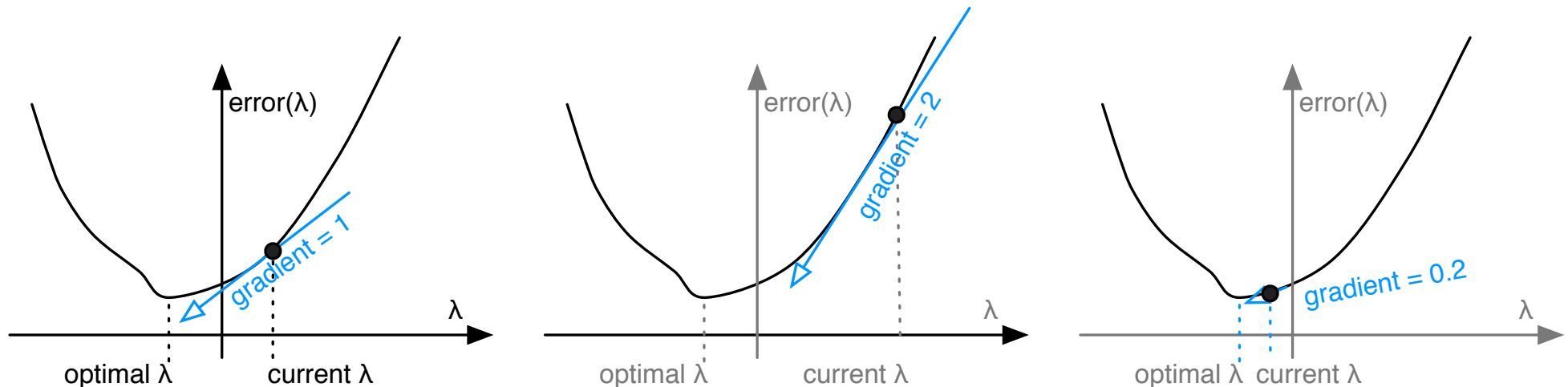
$$\text{error}(\lambda)$$

Gradient Descent

- We view the error as a function of the trainable parameters

$$\text{error}(\lambda)$$

- We want to optimize $\text{error}(\lambda)$ by moving it towards its optimum



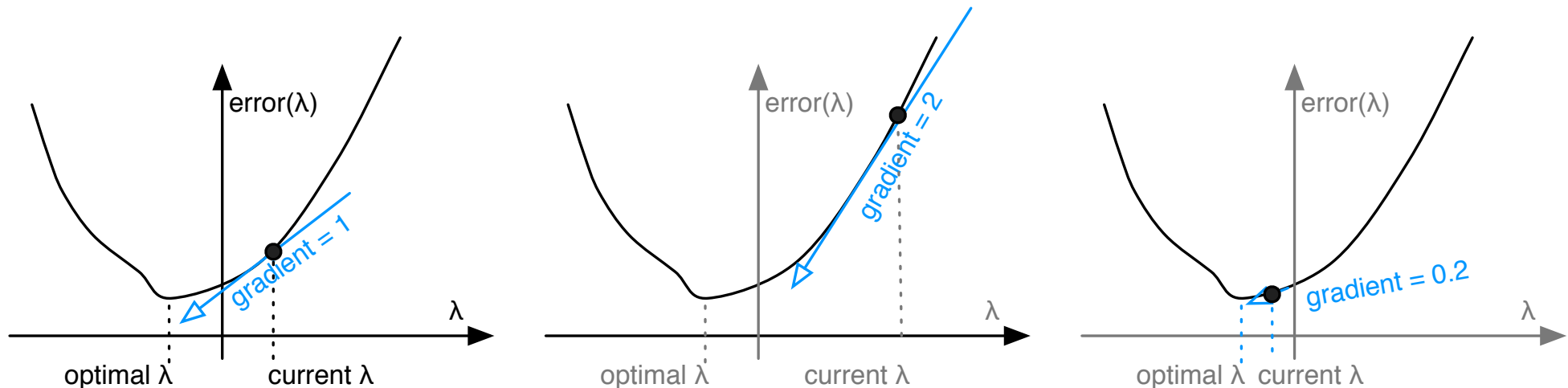
- Why not just set it to its optimum?

Gradient Descent

- We view the error as a function of the trainable parameters

$$\text{error}(\lambda)$$

- We want to optimize $\text{error}(\lambda)$ by moving it towards its optimum



- Why not just set it to its optimum?
 - we are updating based on one training example, do not want to overfit to it
 - we are also changing all the other parameters, the curve will look different

Calculus Refresher: Chain Rule

- Formula for computing derivative of composition of two or more functions
 - functions f and g
 - composition $f \circ g$ maps x to $f(g(x))$

- Chain rule

$$(f \circ g)' = (f' \circ g) \cdot g'$$

or

$$F'(x) = f'(g(x))g'(x)$$

- Leibniz's notation

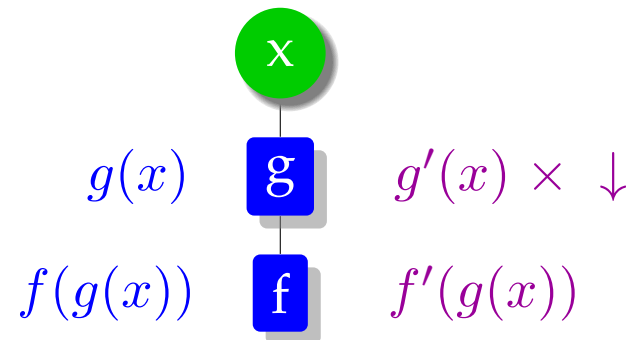
$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$$

if $z = f(y)$ and $y = g(x)$, then

$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx} = f'(y)g'(x) = f'(g(x))g'(x)$$

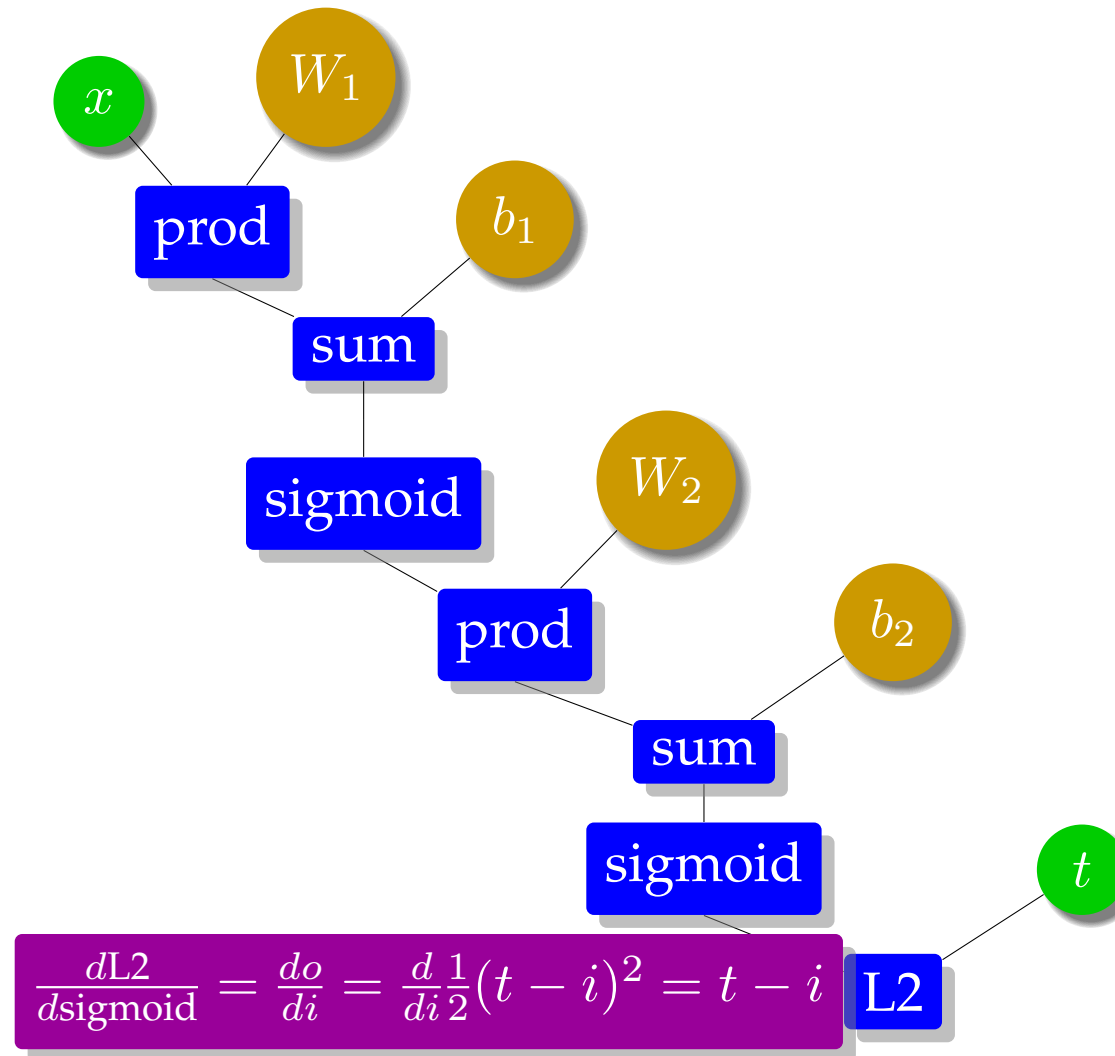
Chain Rule in the Computation Graph

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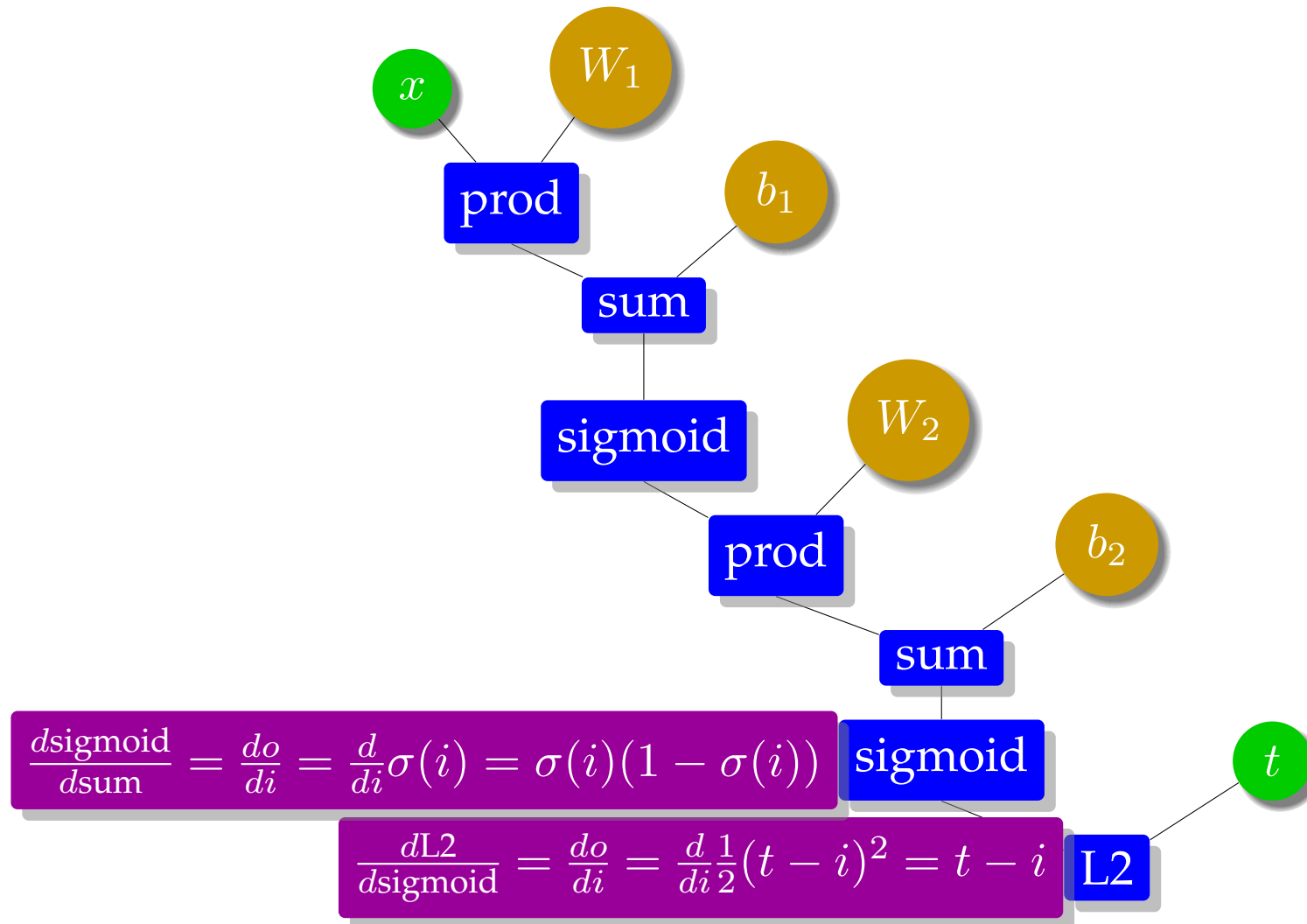


$\underbrace{f'(g(x))}_{\text{recurse down the graph}}$
 $\underbrace{\times}_{\text{multiply values}}$
 $\underbrace{g'(x)}_{\text{apply derivative of function to forward value}}$

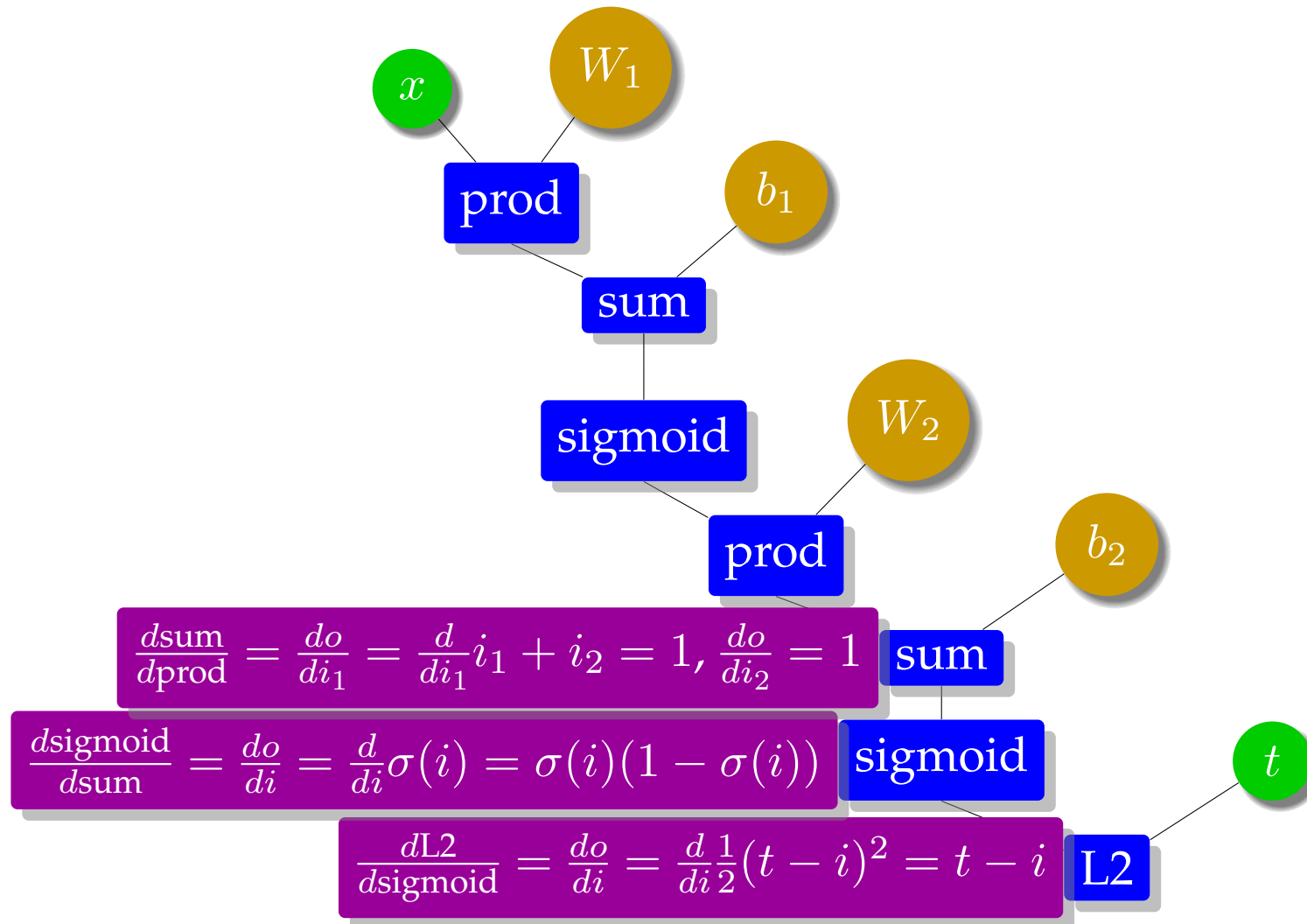
Derivatives for Each Node



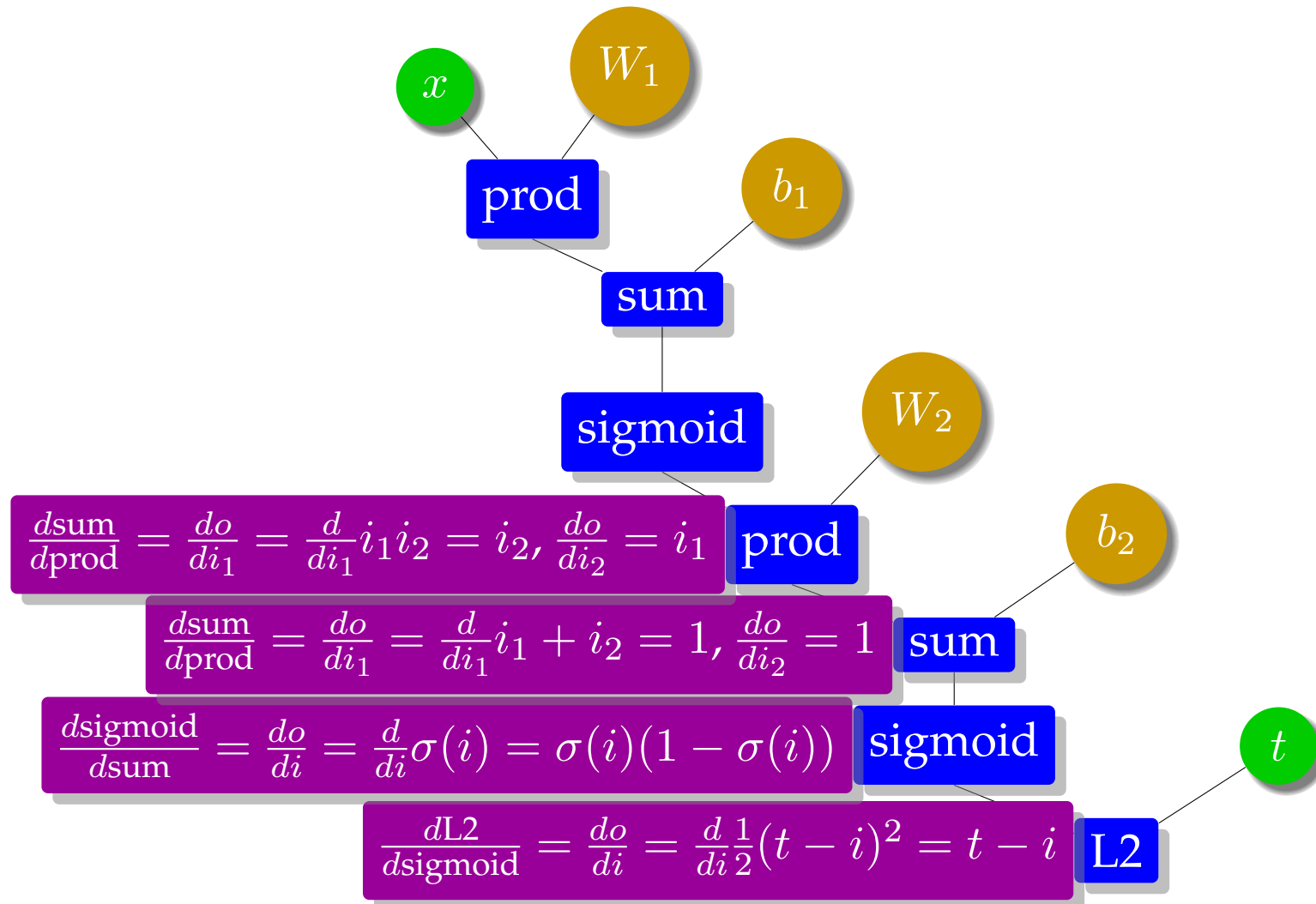
Derivatives for Each Node



Derivatives for Each Node

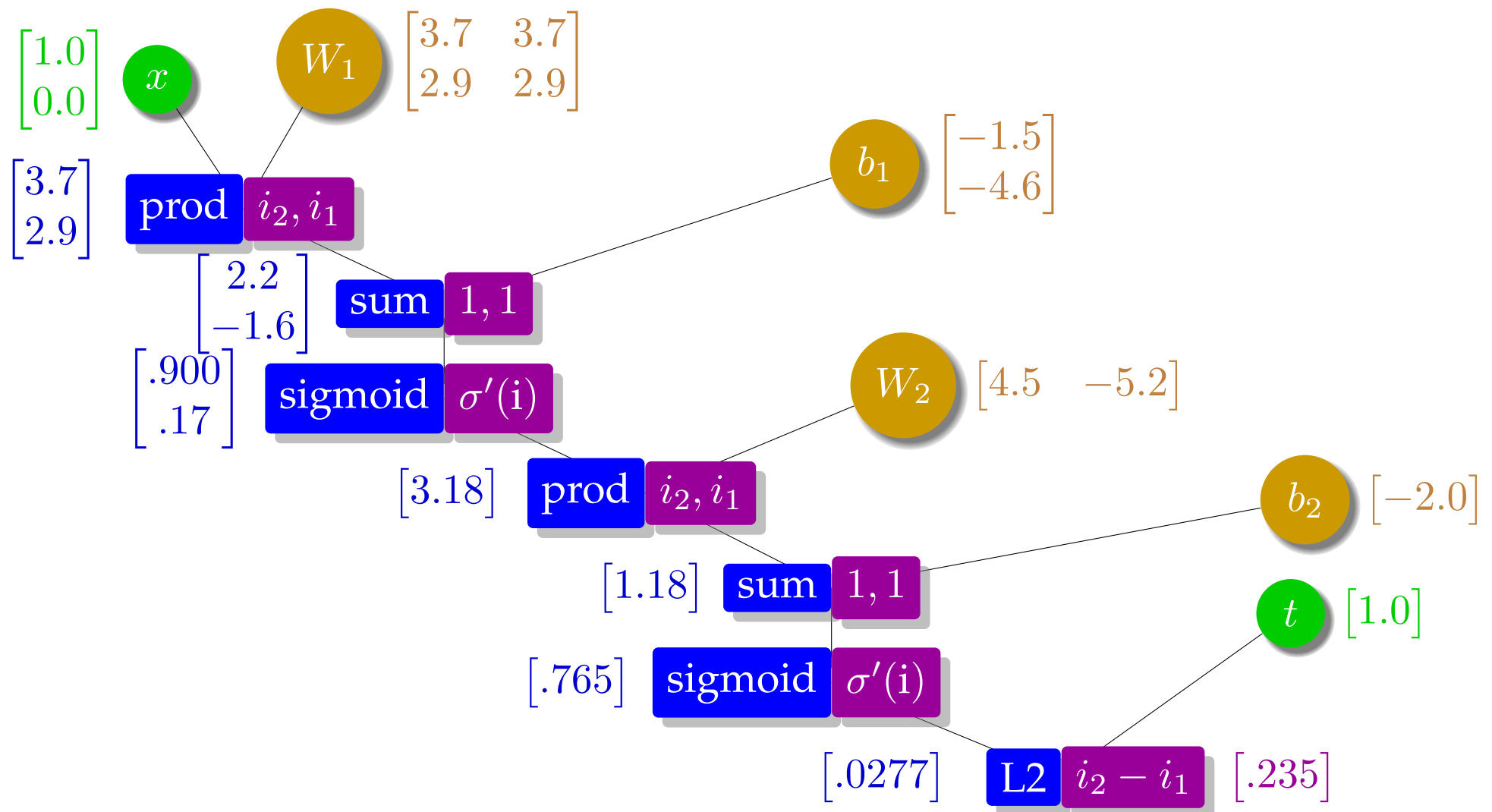


Derivatives for Each Node

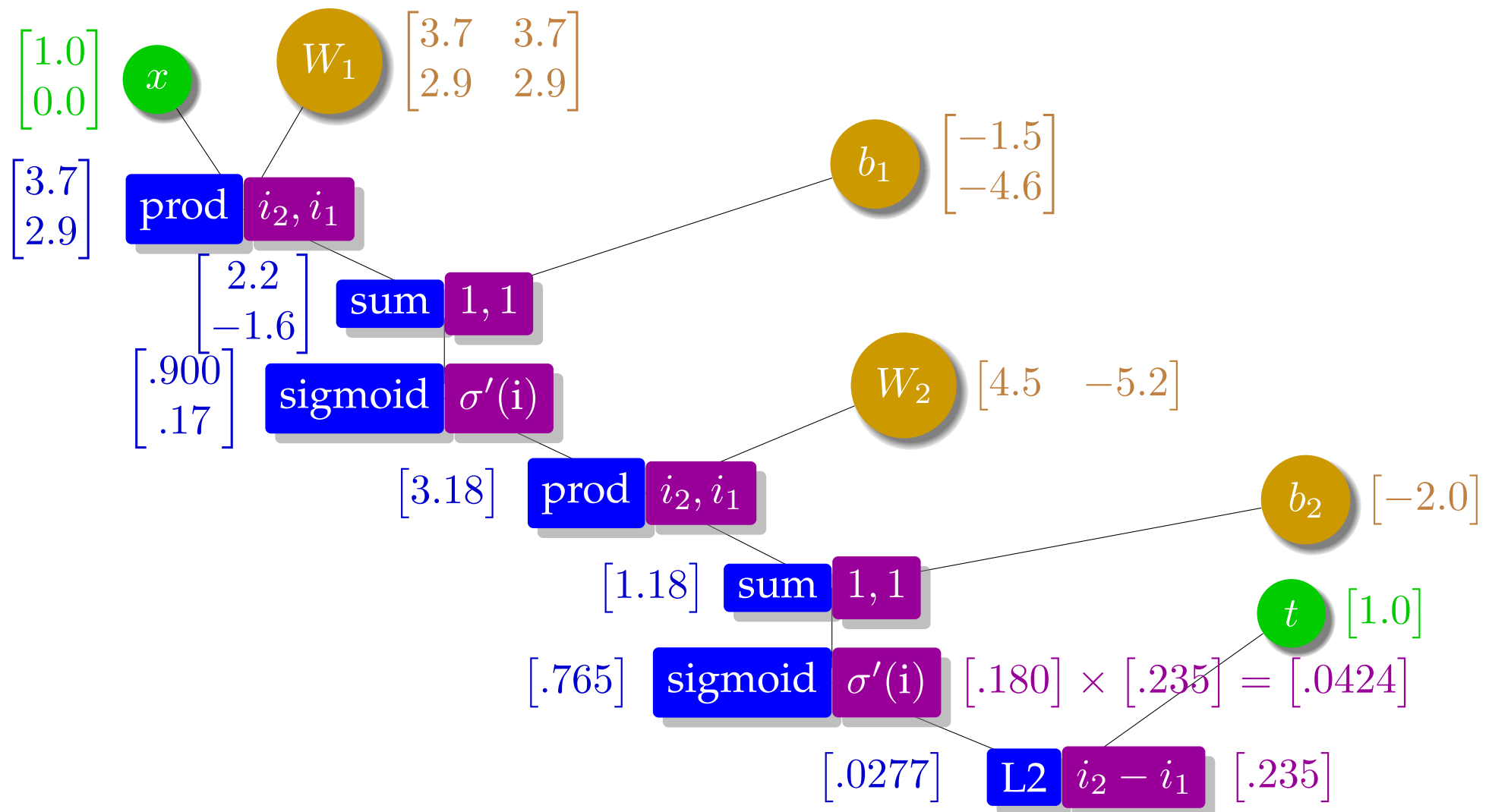


Backward Pass: Derivative Computation

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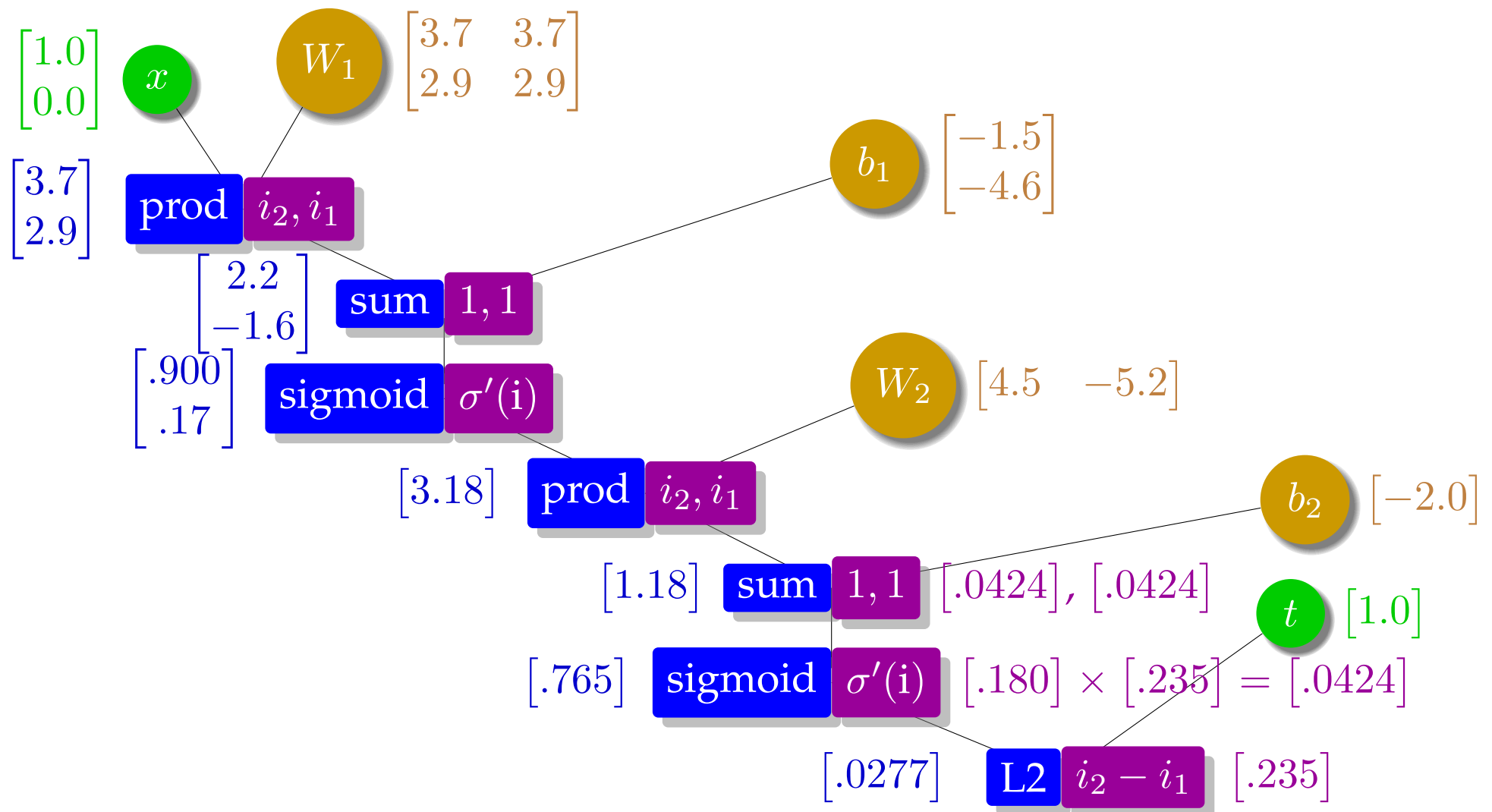


Backward Pass: Derivative Computation

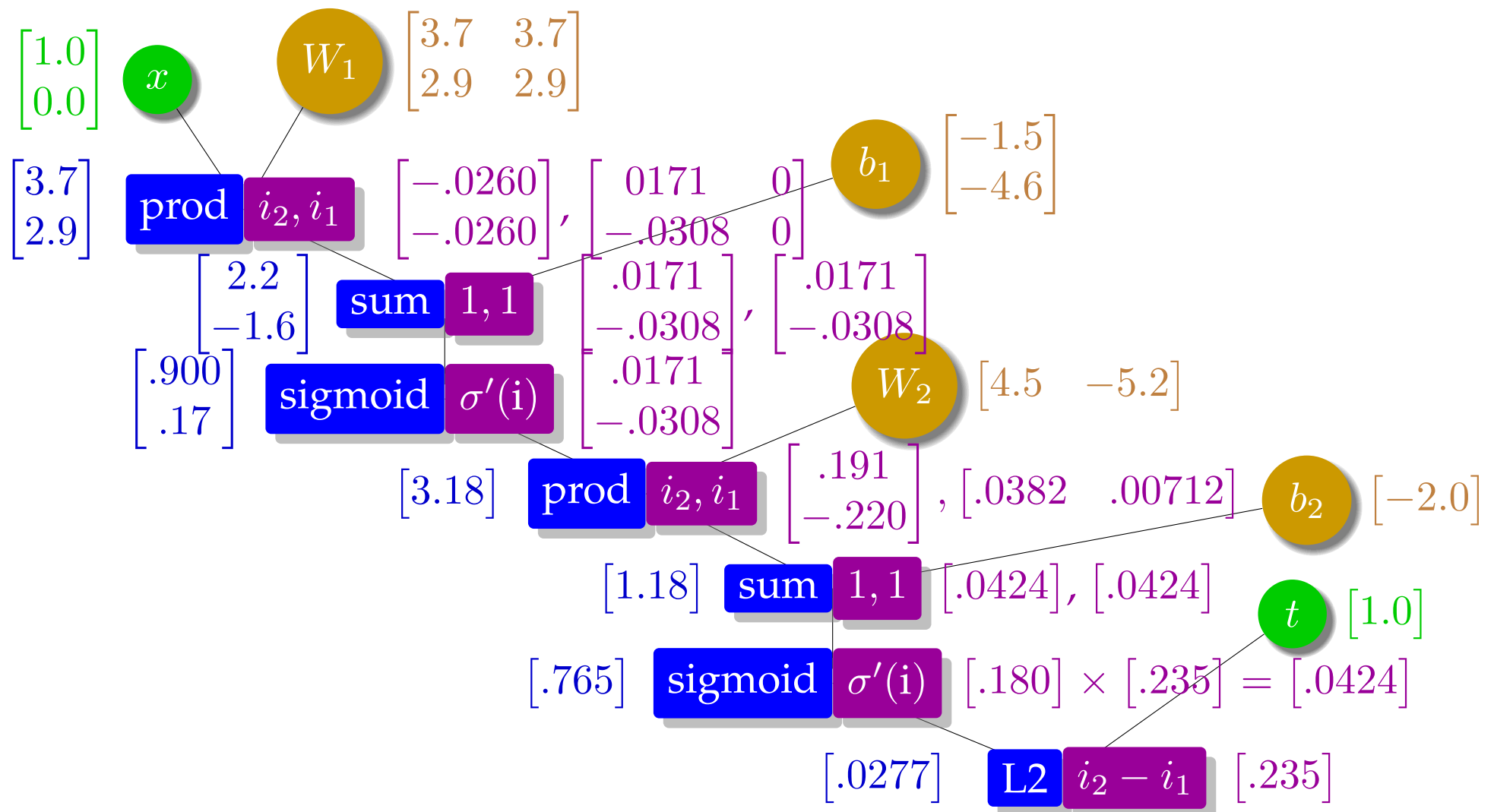


Backward Pass: Derivative Computation

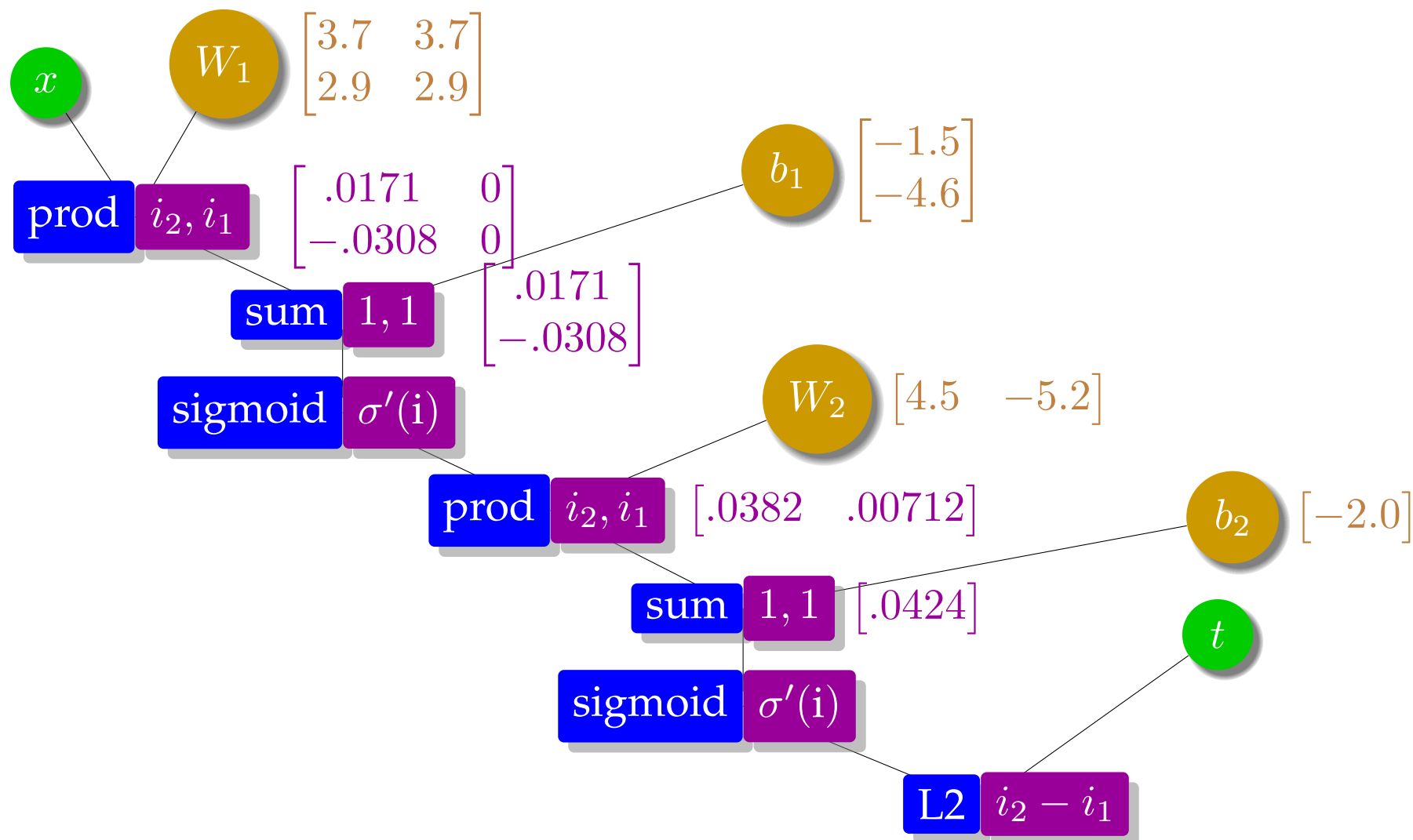
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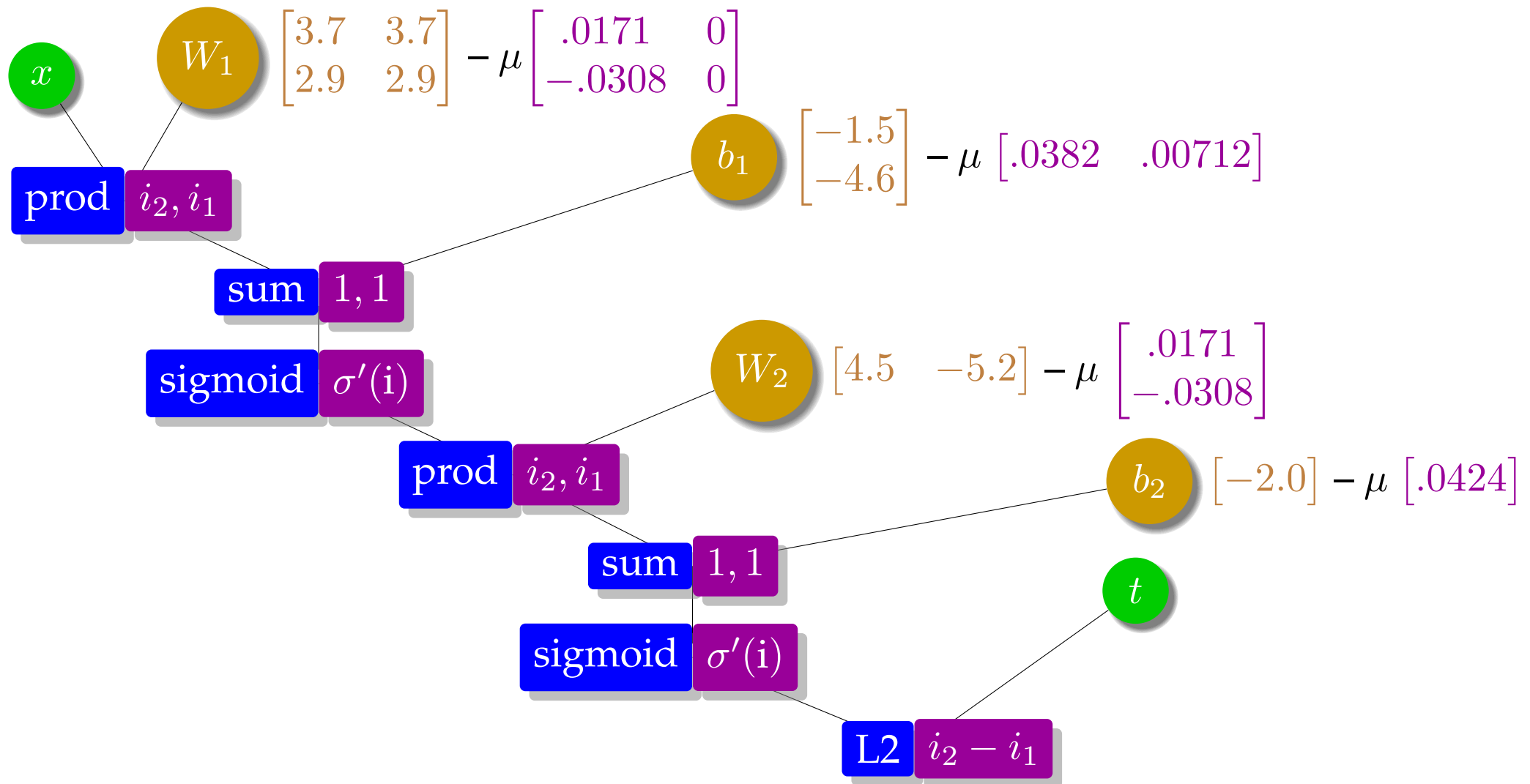
Backward Pass: Derivative Computation



Gradients for Parameter Update



Parameter Update



toolkits

Explosion of Deep Learning Toolkits

- University of Montreal: Theano (early, now defunct)
- Google: Tensorflow
- Facebook: Torch, pyTorch
- Microsoft: CNTK
- Amazon: MX-Net
- CMU: Dynet
- AMU/Edinburgh/Microsoft: Marian
- ... and many more

- Machine learning architectures around computations graphs very powerful
 - define a computation graph
 - provide data and a training strategy (e.g., batching)
 - toolkit does the rest
 - seamless support of GPUs

Example: PyTorch

- Installation

```
pip install torch
```

- Usage

```
import torch
```

Some Data Types

- PyTorch data type for parameter vectors, matrices etc., called `torch.tensor`

```
W = torch.tensor([[3,4],[2,3]], requires_grad=True, dtype=torch.float)
b = torch.tensor([-2,-4], requires_grad=True, dtype=torch.float)
W2 = torch.tensor([5,-5], requires_grad=True, dtype=torch.float)
b2 = torch.tensor([-2], requires_grad=True, dtype=torch.float)
```

- Definition of variables includes
 - specification of their basic data type (`float`)
 - indication to compute gradients (`requires_grad=True`)
- Input and output

```
x = torch.tensor([1,0], dtype=torch.float)
t = torch.tensor([1], dtype=torch.float)
```


- Computation graph

```
s = W.mv(x) + b
h = torch.nn.Sigmoid()(s)

z = torch.dot(W2, h) + b2
y = torch.nn.Sigmoid()(z)

error = 1/2 * (t - z) ** 2
```

- Note

- PyTorch sigmoid function `torch.nn.Sigmoid()`
- multiplication between matrix `W` and vector `x` is `mv`
- multiplication between two vectors `W2` and `h` is `torch.dot`.

Backward Computation

- Here it is:

```
error.backward()
```

- No need to derive gradients — all is done automatically

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- We can look up computed gradients

```
>>> W2.grad  
tensor([-0.0360, -0.0059])
```

Backward Computation

- Here it is:

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error.backward()
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- No need to derive gradients — all is done automatically
- We can look up computed gradients

```
>>> W2.grad  
tensor([-0.0360, -0.0059])
```

- Note
 - when you run this code multiple times, then gradients accumulate
 - reset them with, e.g., `W2.grad.data.zero_()`

Training Data

- Our training set consists of the four examples of binary XOR operations.

x	y	$x \oplus y$
0	0	0
0	1	1
1	0	1
1	1	0

- Placed into array

```
training_data =  
    [ [ torch.tensor([0.,0.]), torch.tensor([0.]) ],  
      [ torch.tensor([1.,0.]), torch.tensor([1.]) ],  
      [ torch.tensor([0.,1.]), torch.tensor([1.]) ],  
      [ torch.tensor([1.,1.]), torch.tensor([0.]) ] ]
```

Training Loop: Forward

```
mu = 0.1

for epoch in range(1000):
    total_error = 0

    for item in training_data:
        x = item[0]
        t = item[1]

        # forward computation
        s = W.mv(x) + b
        h = torch.nn.Sigmoid()(s)
        z = torch.dot(W2, h) + b2
        y = torch.nn.Sigmoid()(z)
        error = 1/2 * (t - y) ** 2
        total_error = total_error + error
```

Training Loop: Backward and Updates

```
# backward computation
error.backward()

# weight updates
W.data = W - mu * W.grad.data
b.data = b - mu * b.grad.data
W2.data = W2 - mu * W2.grad.data
b2.data = b2 - mu * b2.grad.data

W.grad.data.zero_()
b.grad.data.zero_()
W2.grad.data.zero_()
b2.grad.data.zero_()

print("error: ", total_error/4)
```

Batch Training

- We computed gradients for each training example, update model immediately
- More common: process examples in batches, update after batch processed
- Instead

```
error.backward()
```

- Run back-propagation on accumulated error

```
total_error.backward()
```


Training Data Batch

```
x = torch.tensor([ [0.,0.], [1.,0.], [0.,1.], [1.,1.]  ])
t = torch.tensor([ 0., 1., 1., 0.  ])
```

- Change to computation graph (input now a matrix, output a vector)

```
s = x.mm(W) + b
h = torch.nn.Sigmoid()(s)
z = h.mv(W2) + b2
y = torch.nn.Sigmoid()(z)
```

- Convert error vector into single number

```
error = 1/2 * (t - y) ** 2
mean_error = error.mean()
mean_error.backward()
```

Parameter Updates (Optimizer)

- Our code has explicit parameter update computations

```
# weight updates
W.data = W - mu * W.grad.data
b.data = b - mu * b.grad.data
W2.data = W2 - mu * W2.grad.data
b2.data = b2 - mu * b2.grad.data
```

- But fancier optimizers are typically used (Adam, etc.)
- This requires more complex implementation

- Neural network model is defined as class derived from torch.nn.Module

```
class ExampleNet(torch.nn.Module):  
    def __init__(self):  
        super(ExampleNet, self).__init__()  
        self.layer1 = torch.nn.Linear(2,2)  
        self.layer2 = torch.nn.Linear(2,1)  
        self.layer1.weight = torch.nn.Parameter(torch.tensor([[3.,2.],[4.,3.])))  
        self.layer1.bias = torch.nn.Parameter(torch.tensor([-2.,-4.])))  
        self.layer2.weight = torch.nn.Parameter(torch.tensor([[5.,-5.])))  
        self.layer2.bias = torch.nn.Parameter(torch.tensor([-2.])))  
  
    def forward(self, x):  
        s = self.layer1(x)  
        h = torch.nn.Sigmoid()(s)  
        z = self.layer2(h)  
        y = torch.nn.Sigmoid()(z)  
        return y
```

Optimizer Definition

- Instantiation of neural network object

```
net = ExampleNet()
```

- Optimizer definition

```
optimizer = torch.optim.SGD(net.parameters(), lr=0.1)
```

Training Loop

```
for iteration in range(1000):  
    optimizer.zero_grad()  
    out = net.forward( x )  
    error = 1/2 * (t - out) ** 2  
    mean_error = error.mean()  
    print("error:  ",mean_error.data)  
    mean_error.backward()  
    optimizer.step()
```

code available on web page for textbook

<http://www.statmt.org/nmt-book/>