Computation Graphs

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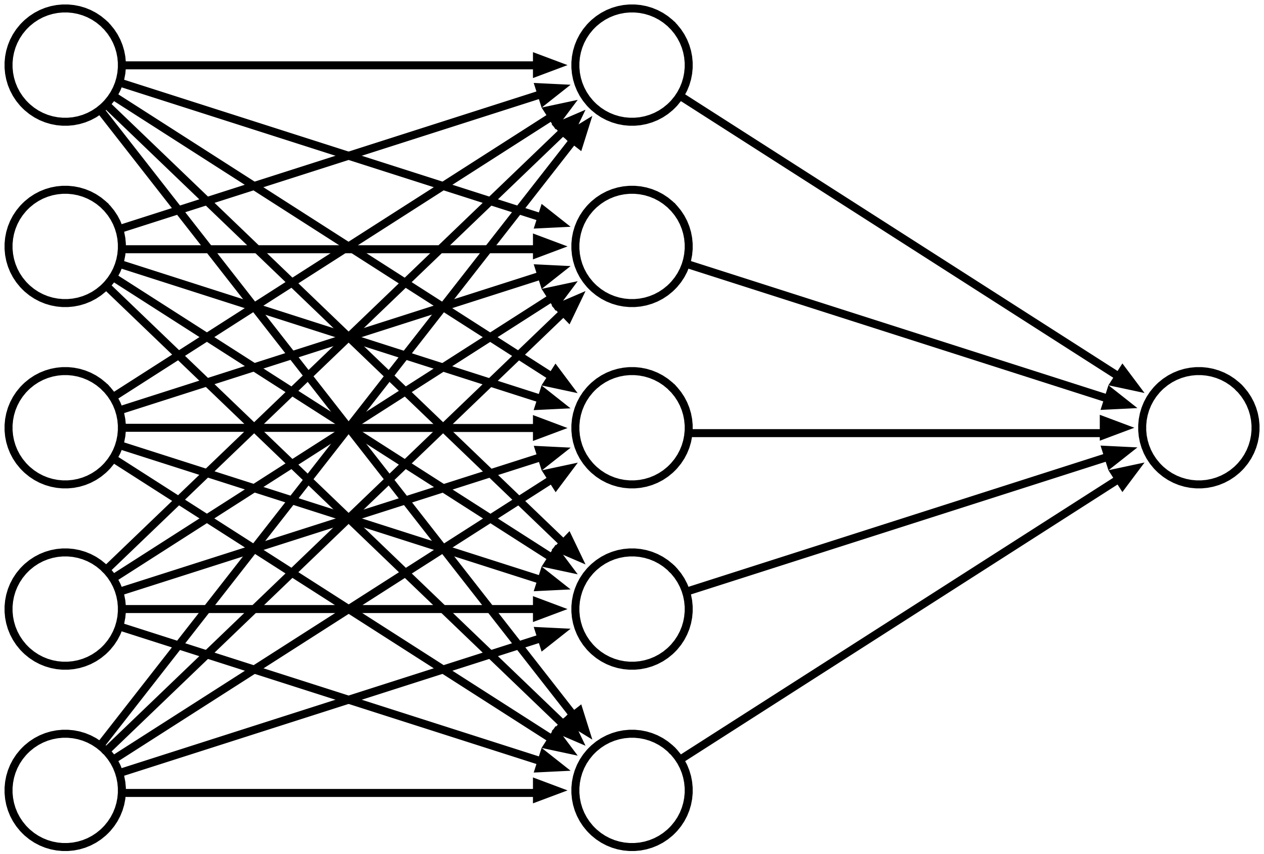
Neural Network Cartoon

- A common way to illustrate a neural network



Neural Network Math

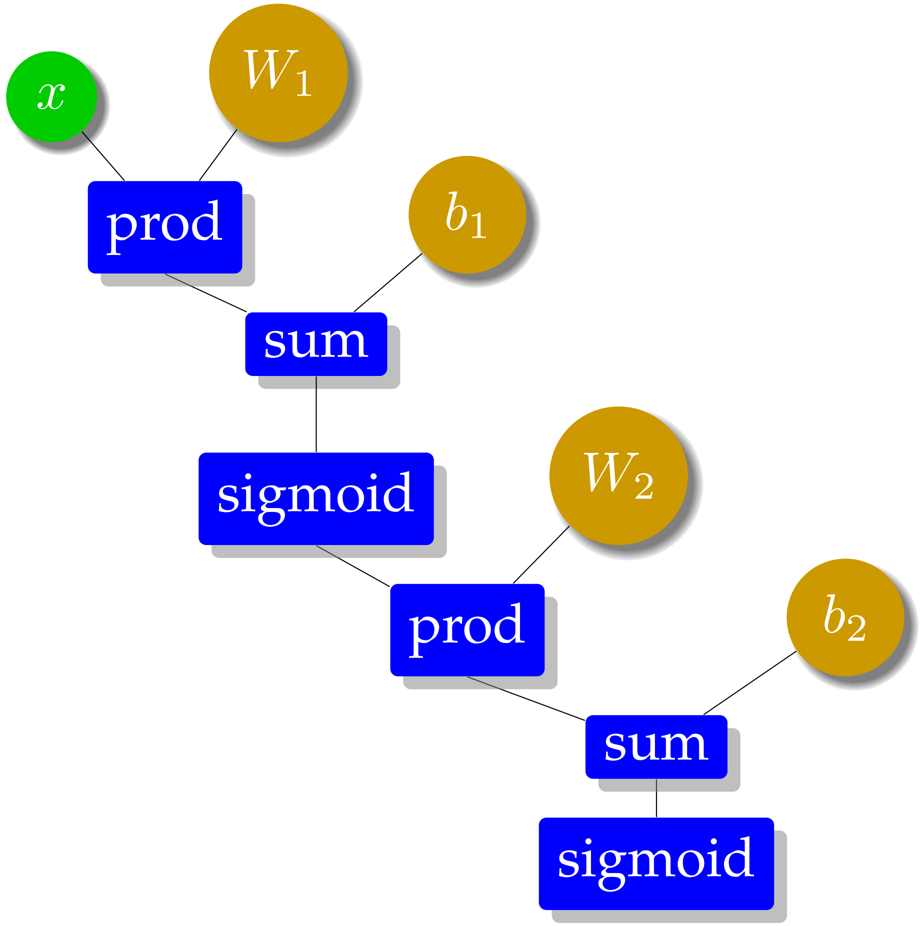
- Hidden layer

$$h = \text{sigmoid}(W_1 x + b_1)$$

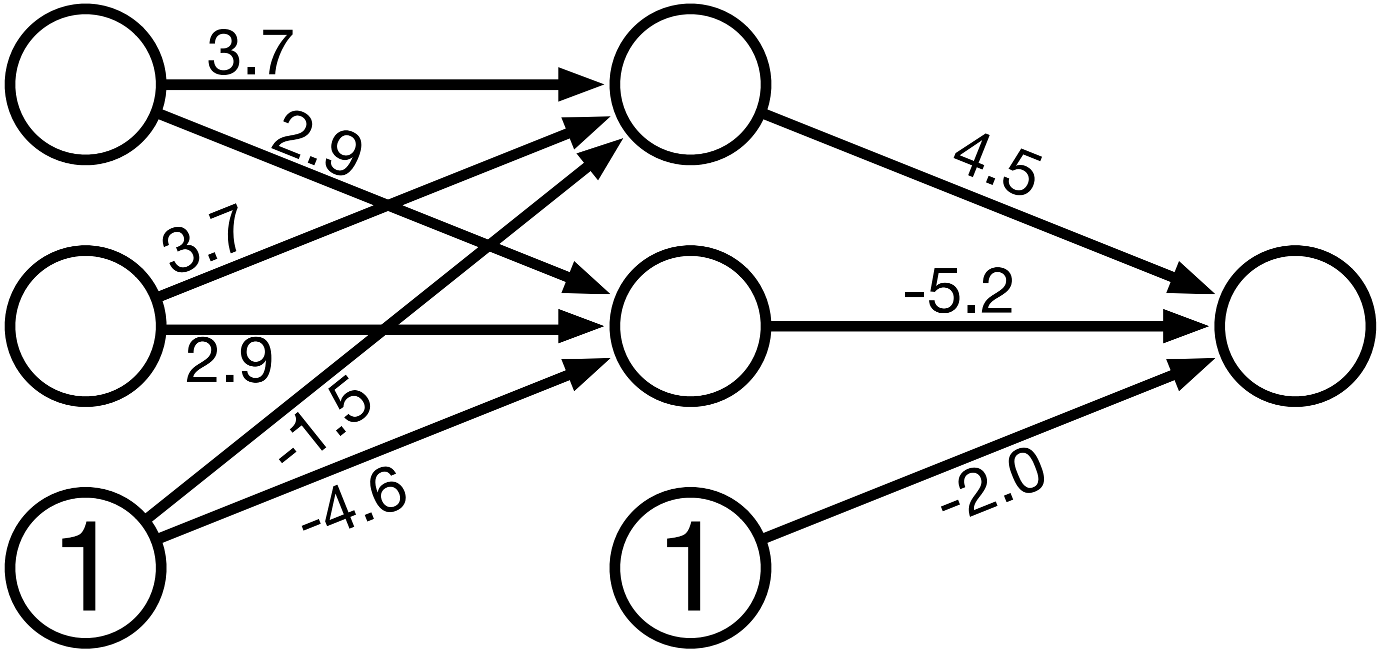
- Final layer

$$y = \text{sigmoid}(W_2 h + b_2)$$

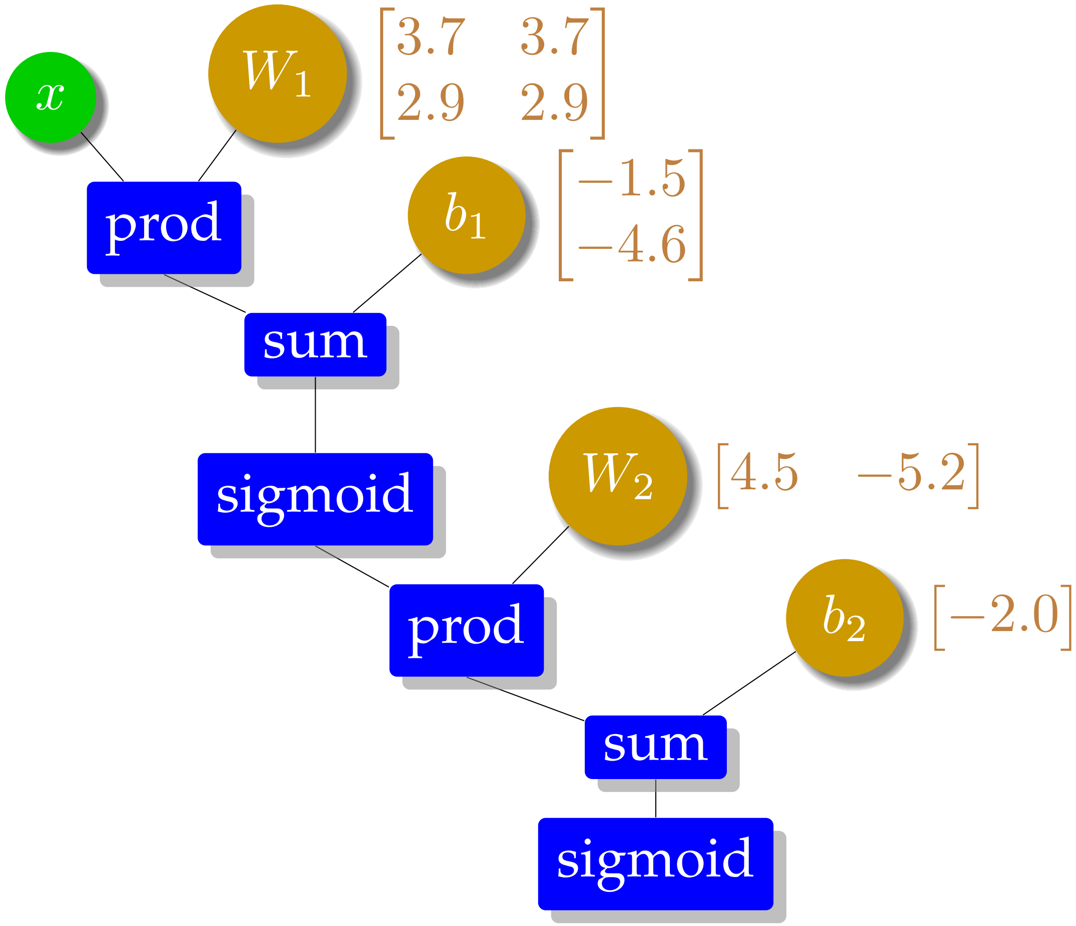
Computation Graph



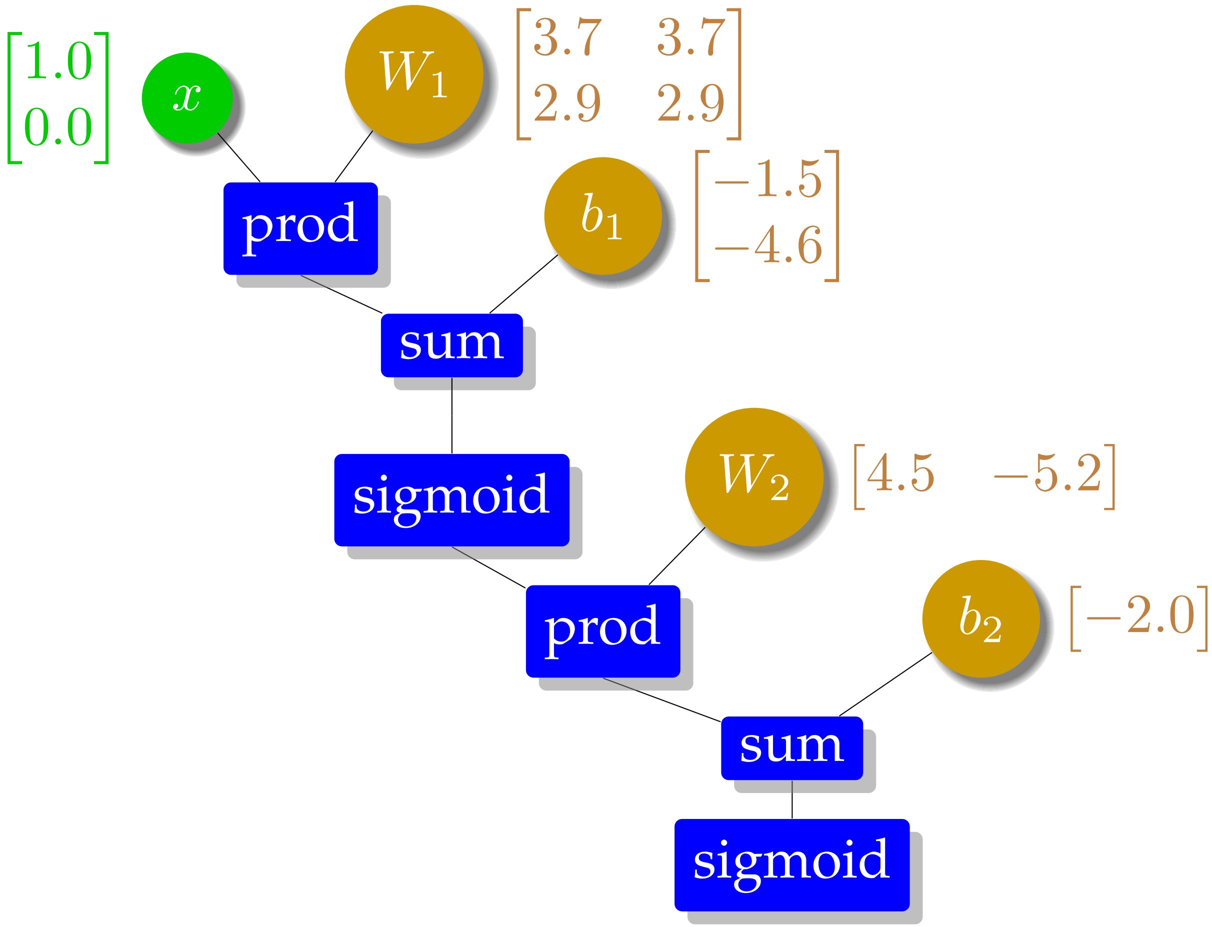
Simple Neural Network



Computation Graph



Processing Input



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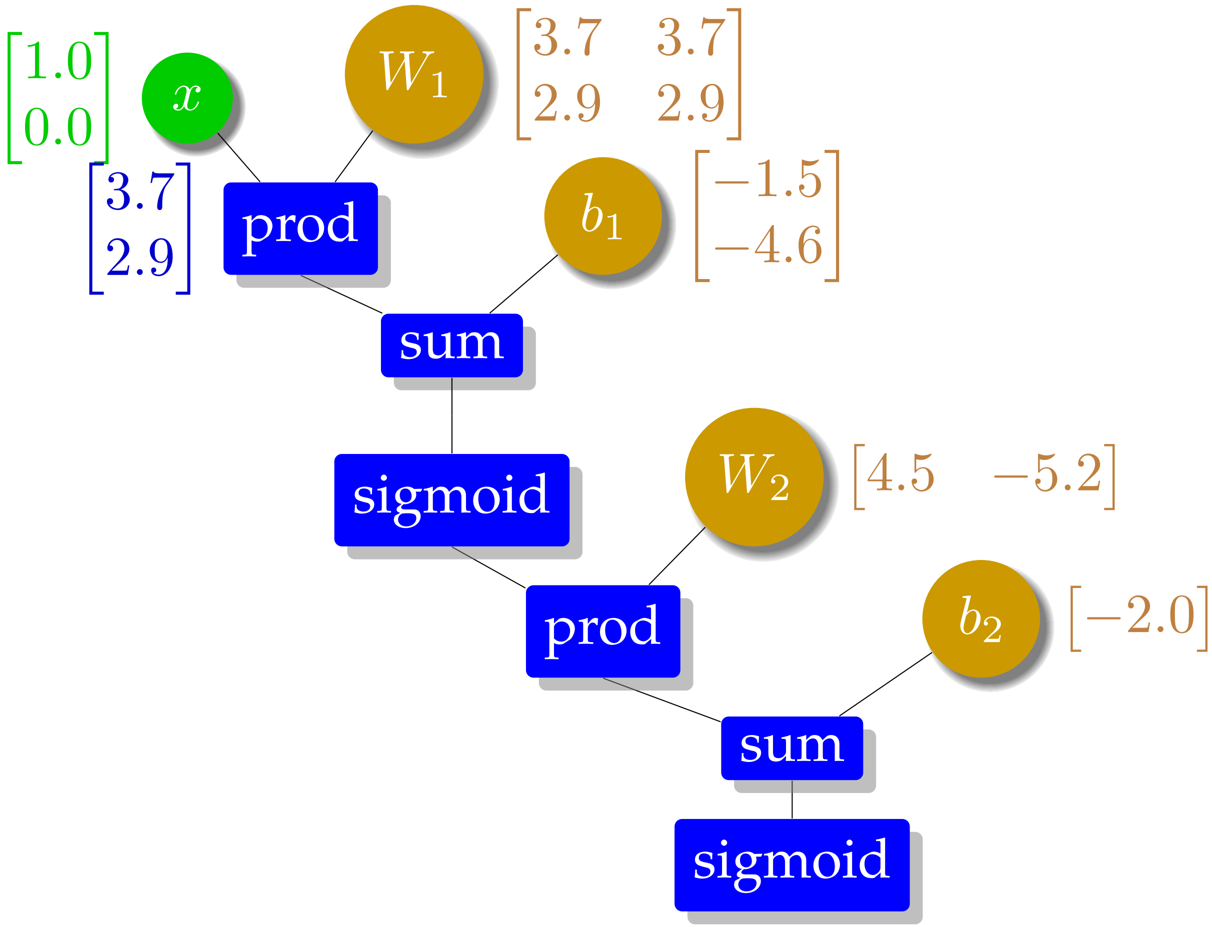

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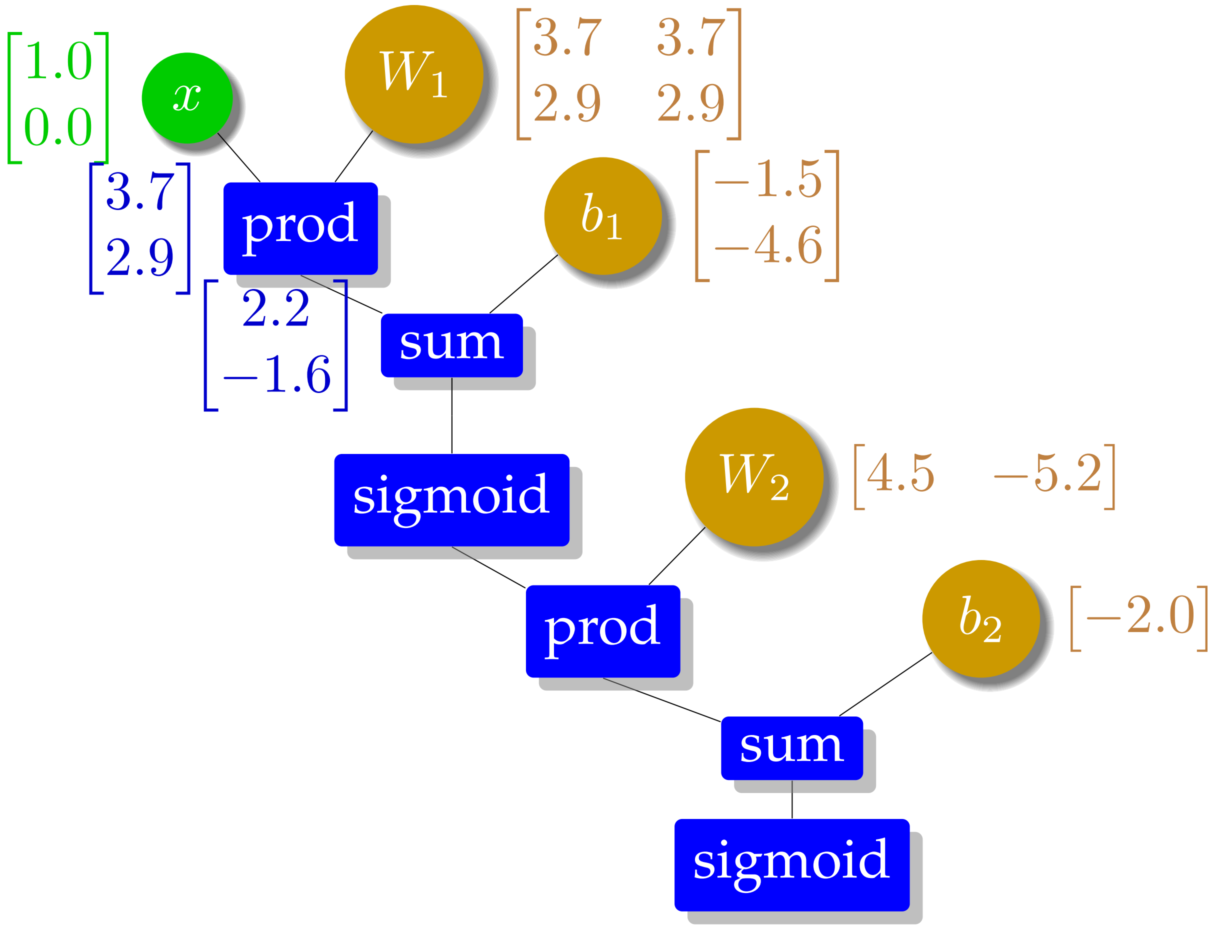

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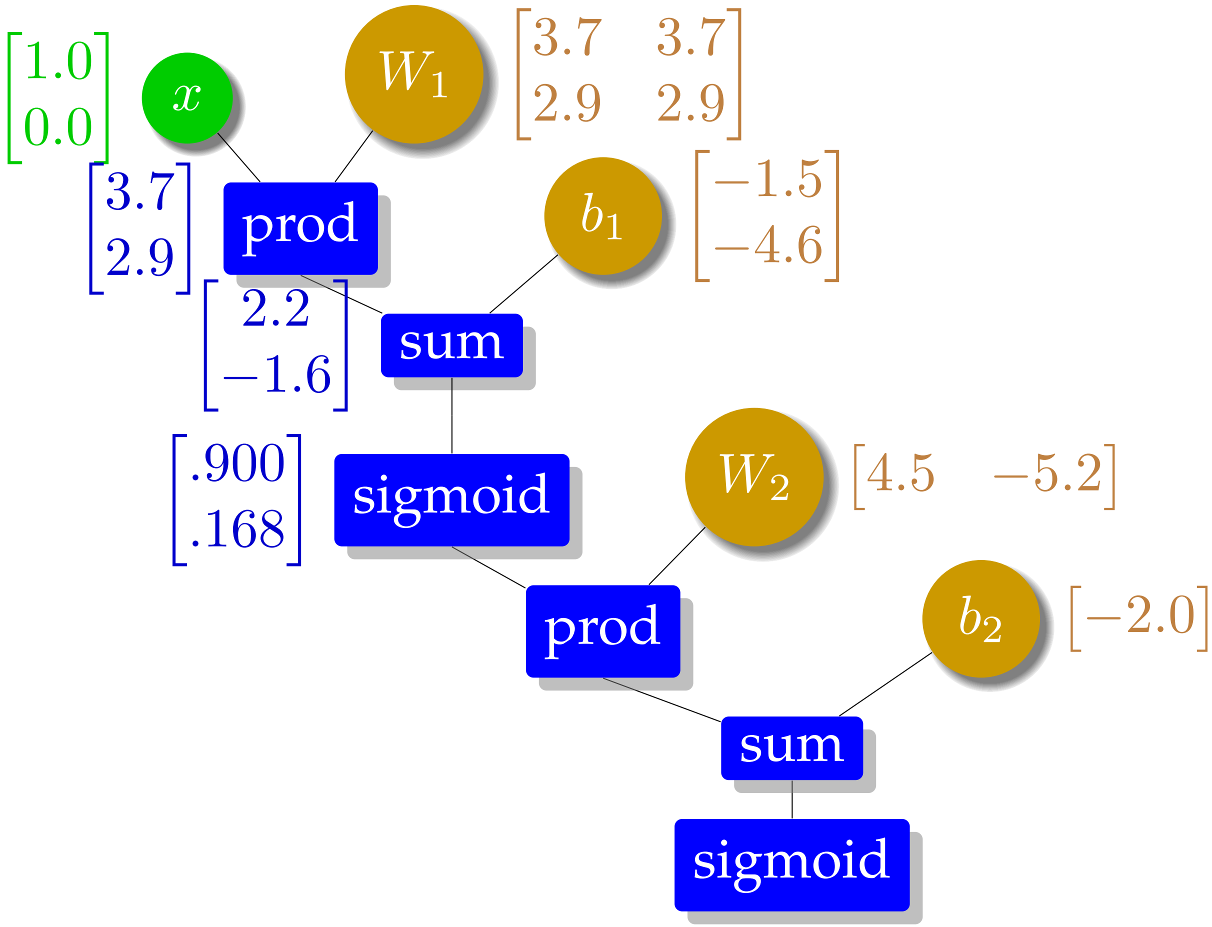

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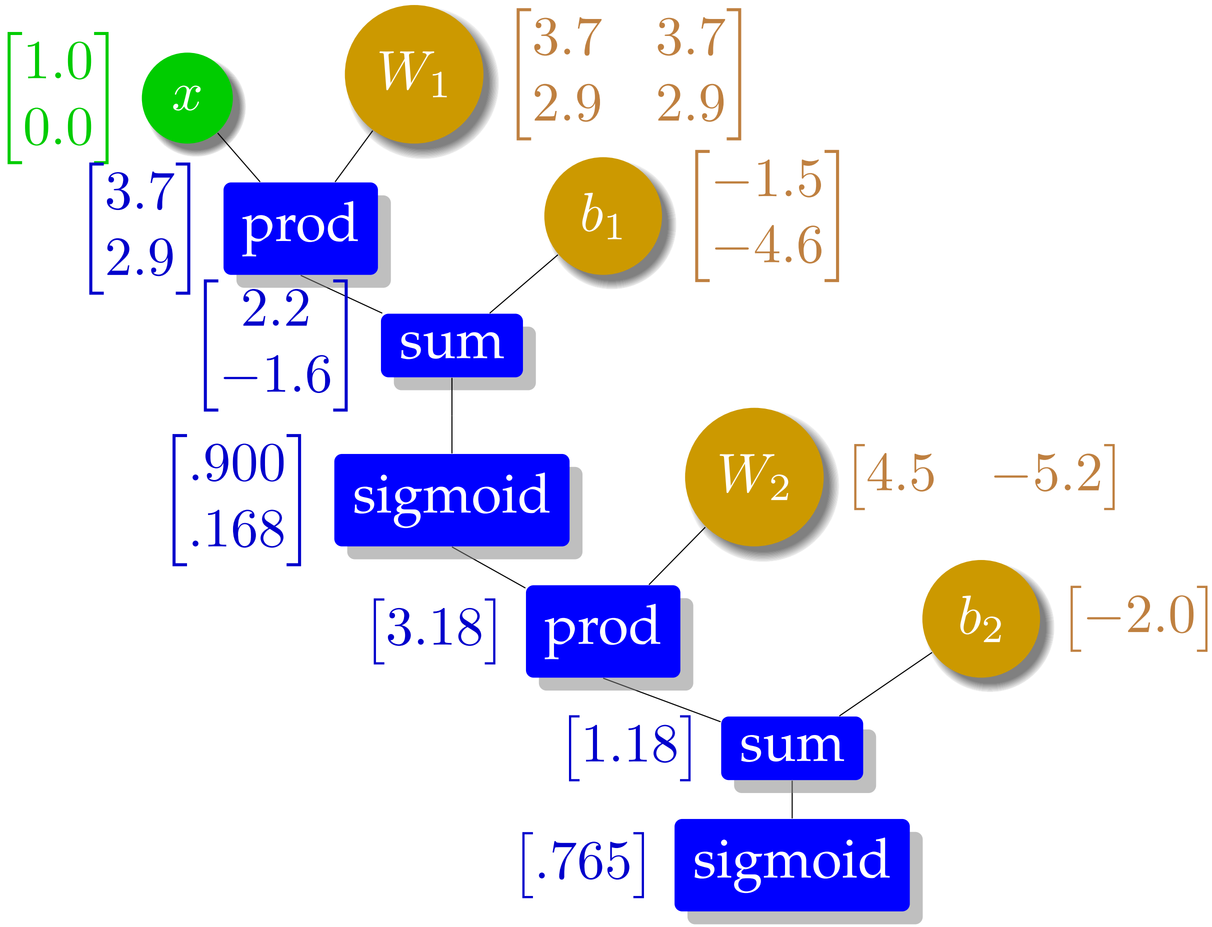


Error Function

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

⇒ Cost function

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

- For instance L2 norm

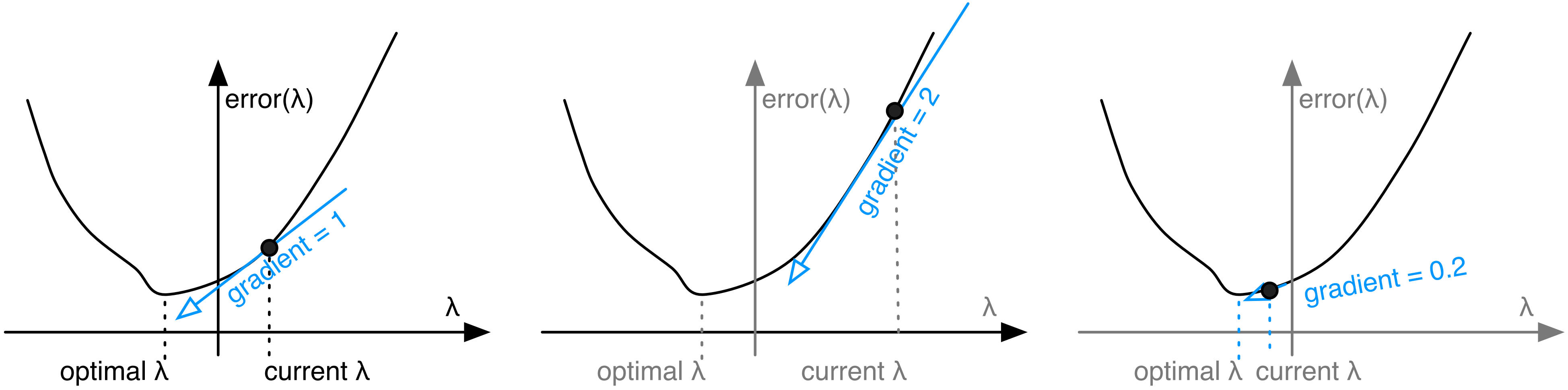
$$\text{error} = \frac{1}{2}(t - y)^2$$

Gradient Descent

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

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

- 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

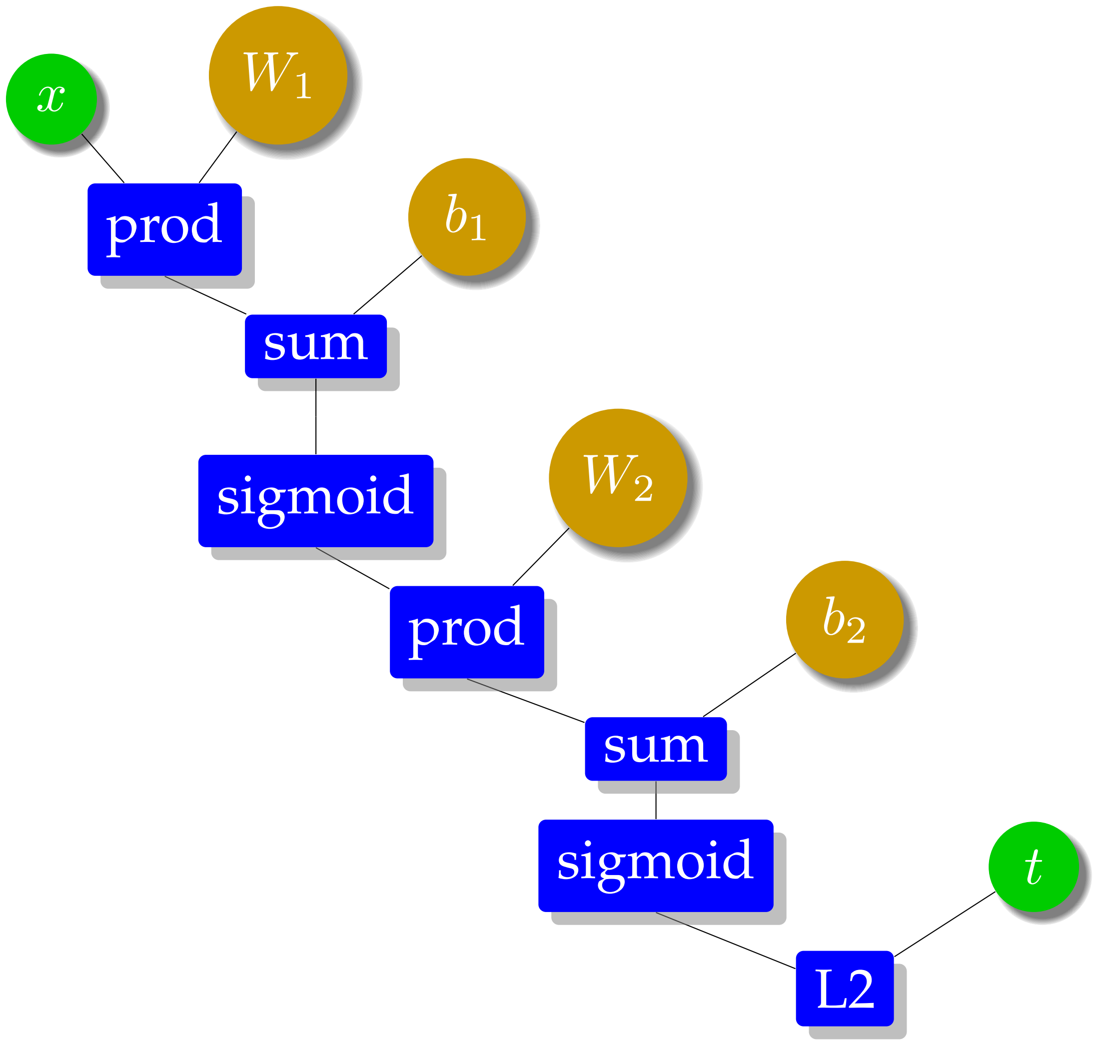
$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx} = f'(y)g'(x) = f'(g(x))g'(x)$$

Final Layer Update

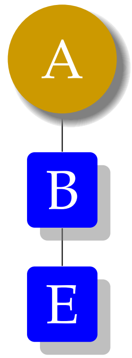
- Linear combination of weights $s = \sum_k w_k h_k$
- Activation function $y = \text{sigmoid}(s)$
- Error (L2 norm) $E = \frac{1}{2}(t - y)^2$
- Derivative of error with regard to one weight w_k

$$\frac{dE}{dw_k} = \frac{dE}{dy}\frac{dy}{ds}\frac{ds}{dw_k}$$

Error Computation in Computation Graph

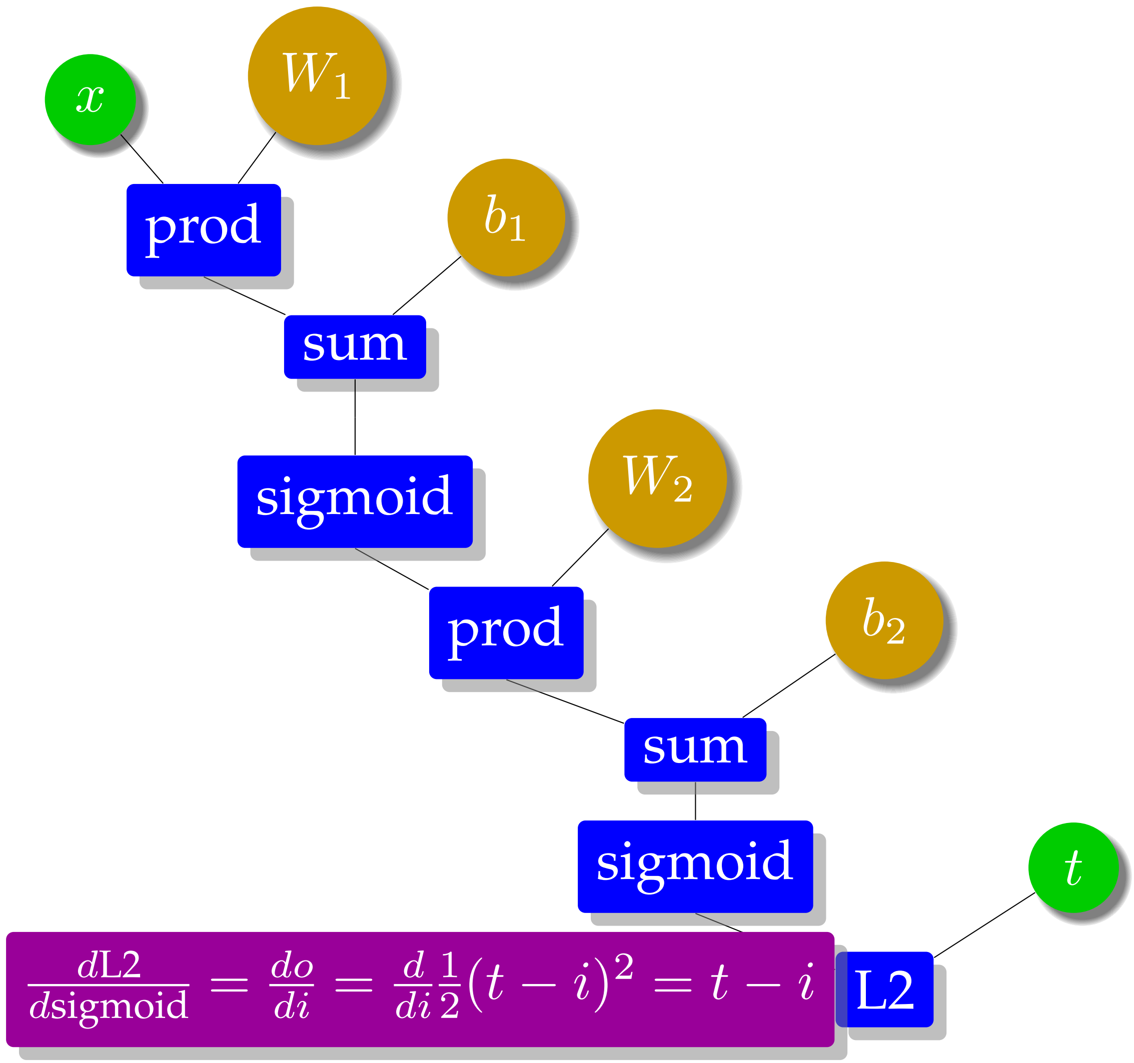


Error Propagation in Computation Graph

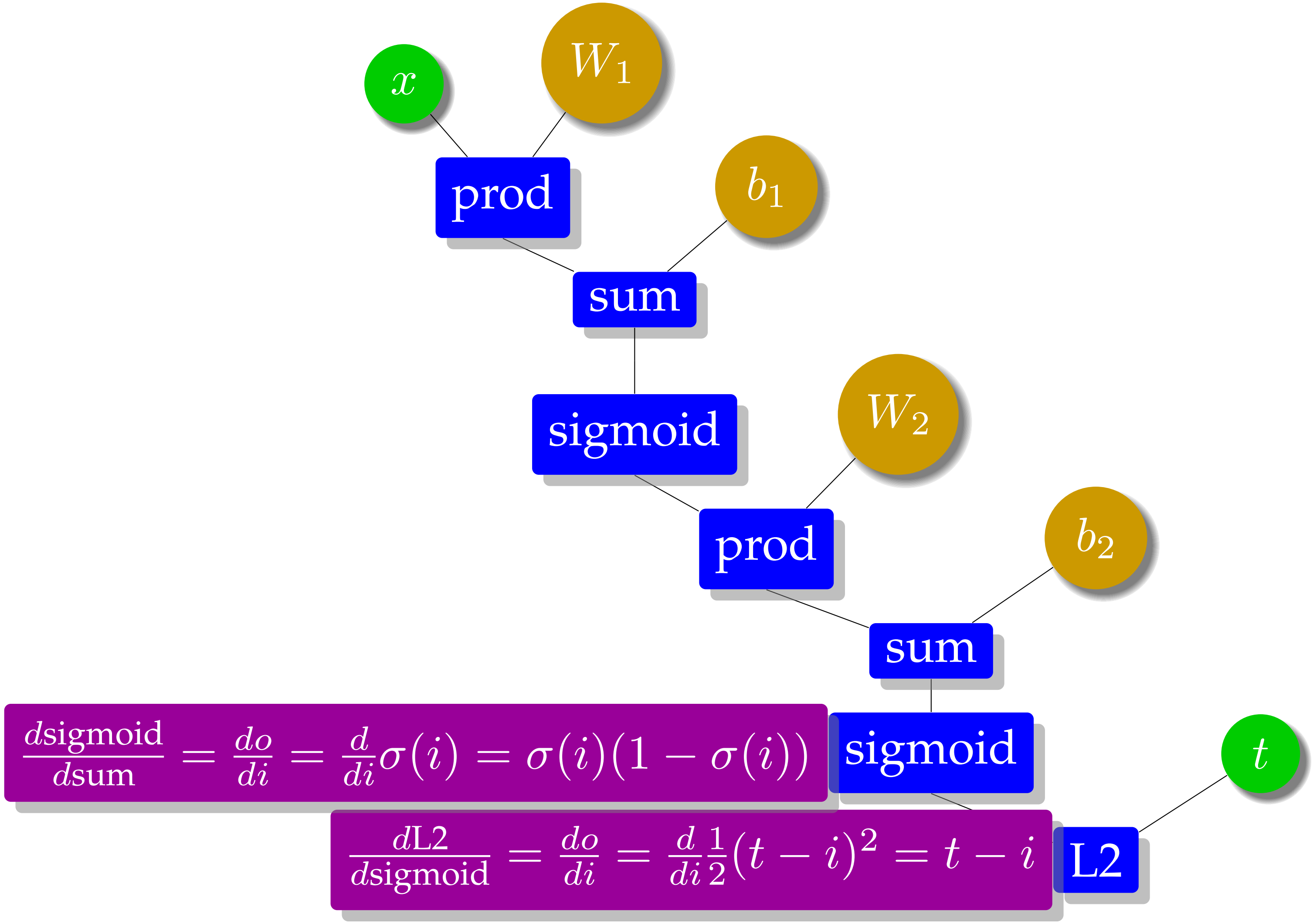


- Compute derivative at node A: $\frac{dE}{dA} = \frac{dE}{dB}\frac{dB}{dA}$
- Assume that we already computed $\frac{dE}{dB}$ (backward pass through graph)
- So now we only have to get the formula for $\frac{dB}{dA}$
- For instance B is a square node
  - forward computation: $B = A^2$
  - backward computation: $\frac{dB}{dA} = \frac{dA^2}{dA} = 2A$

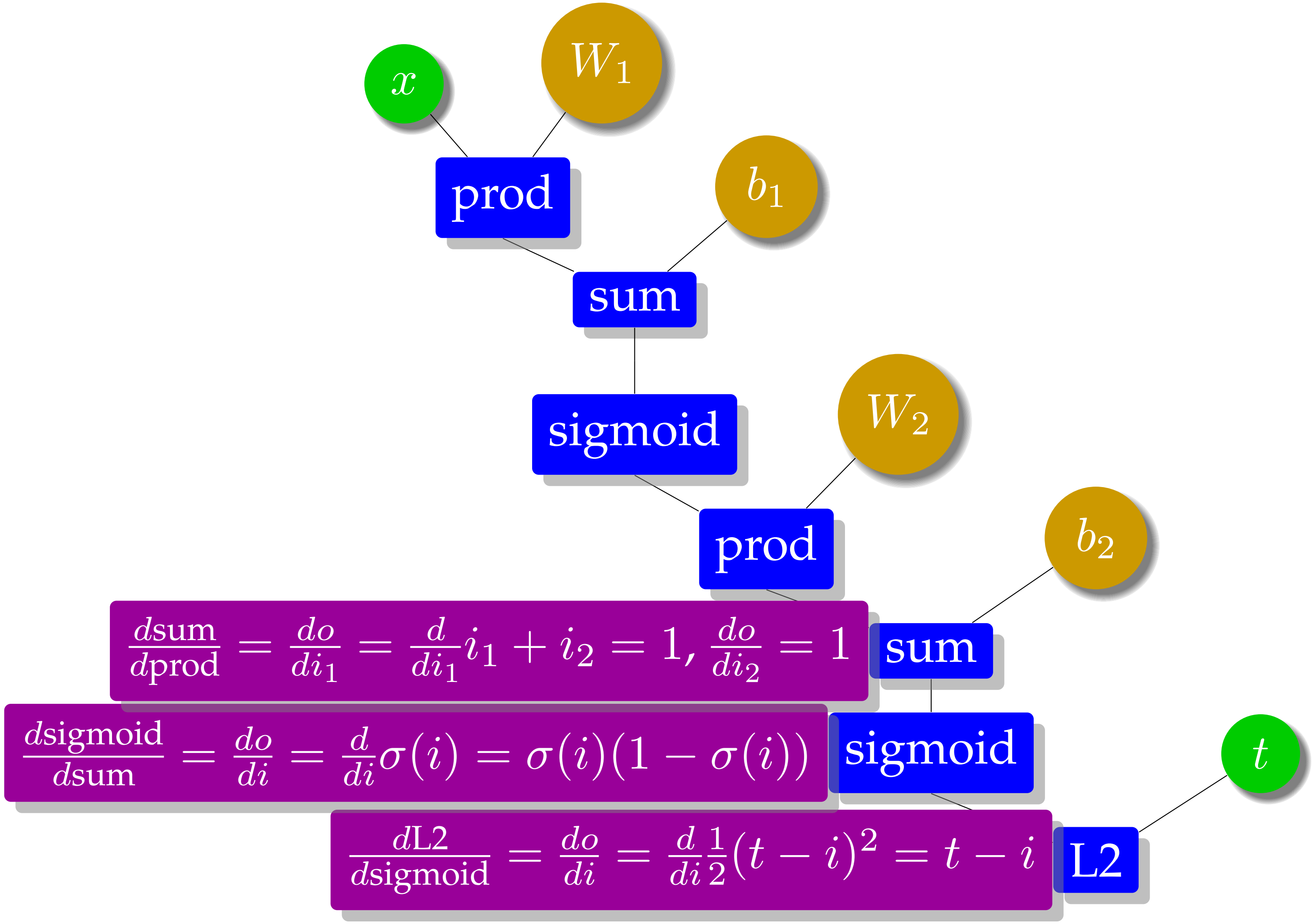
Derivatives for Each Node



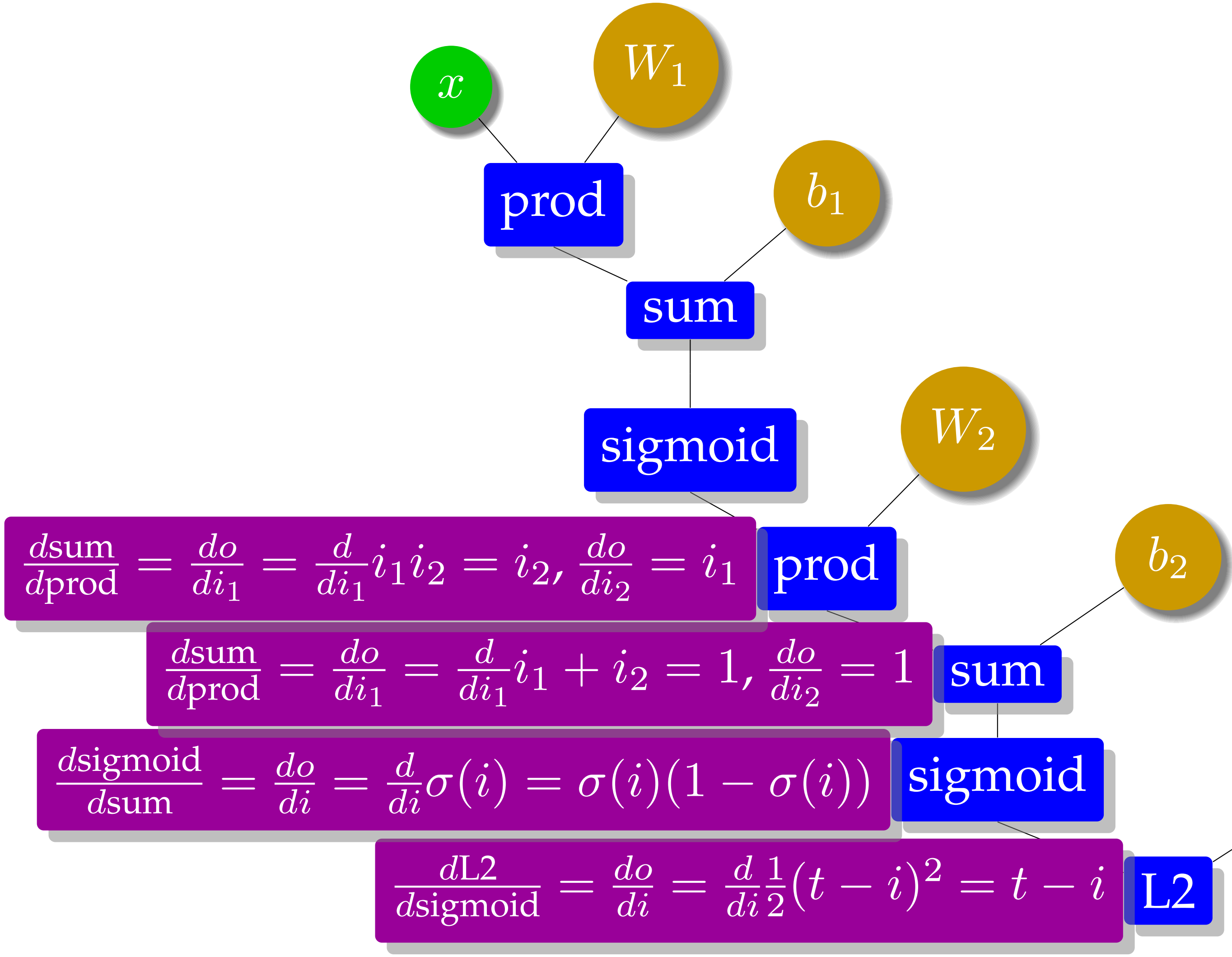
Derivatives for Each Node



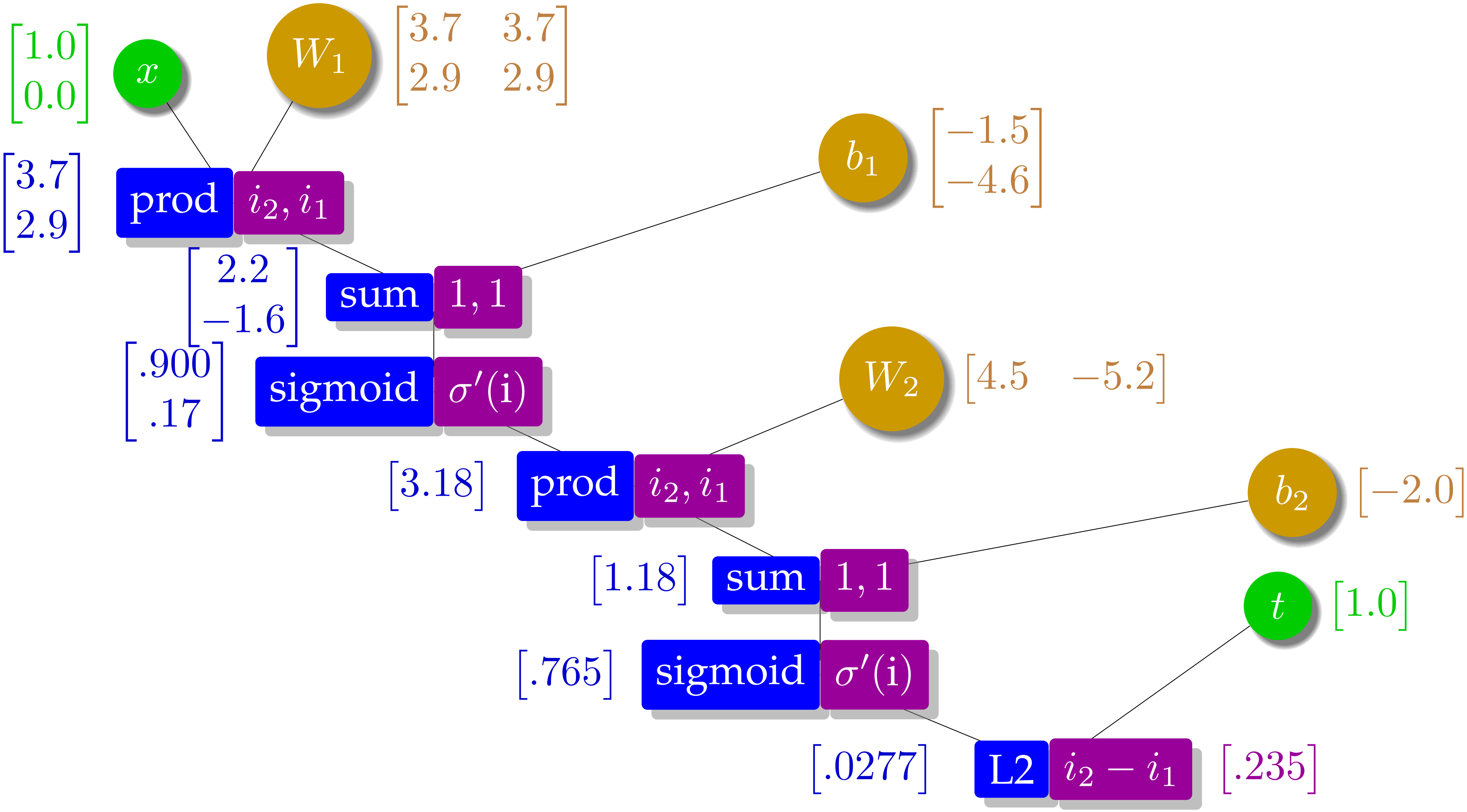
Derivatives for Each Node



Derivatives for Each Node



Backward Pass: Derivative Computation



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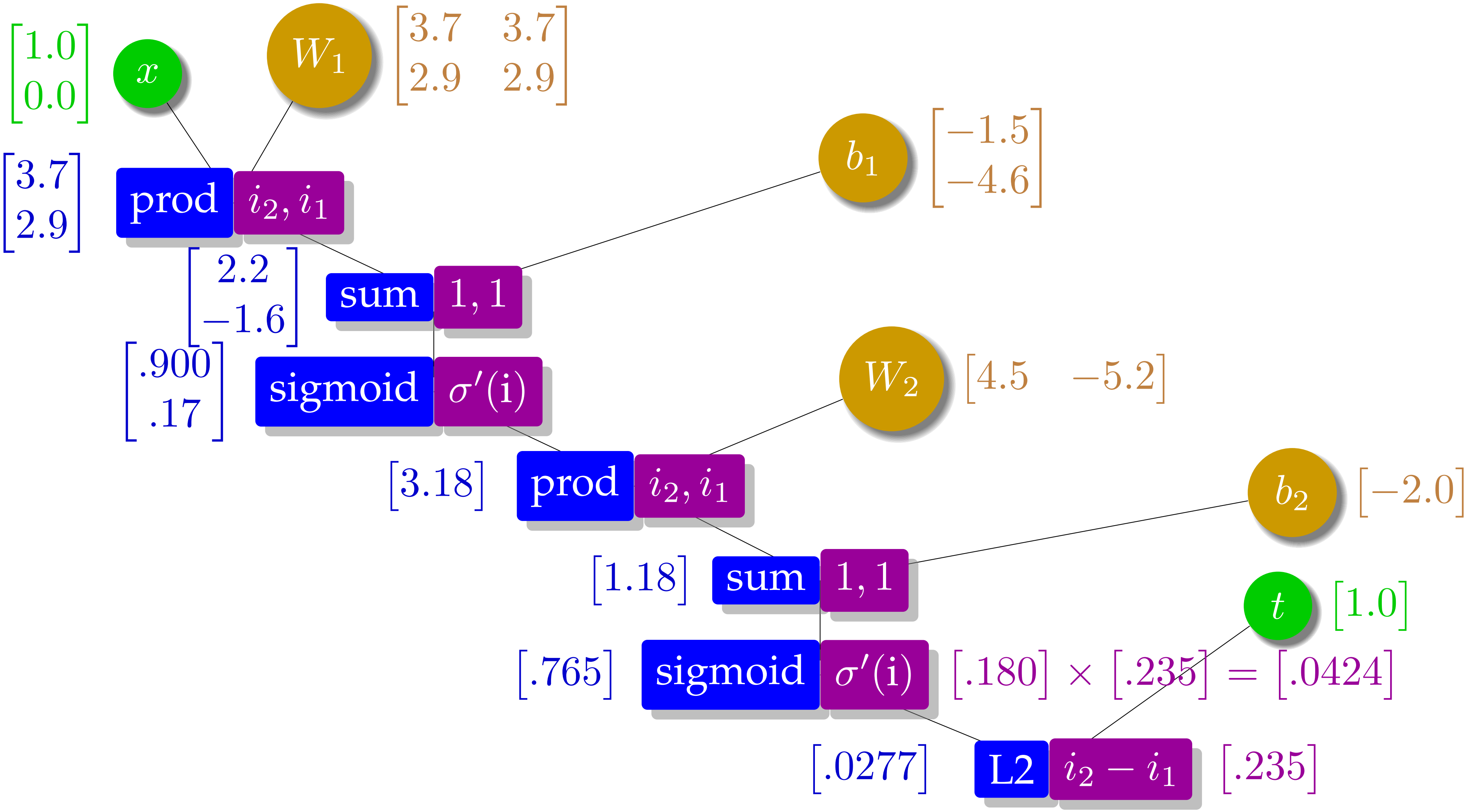

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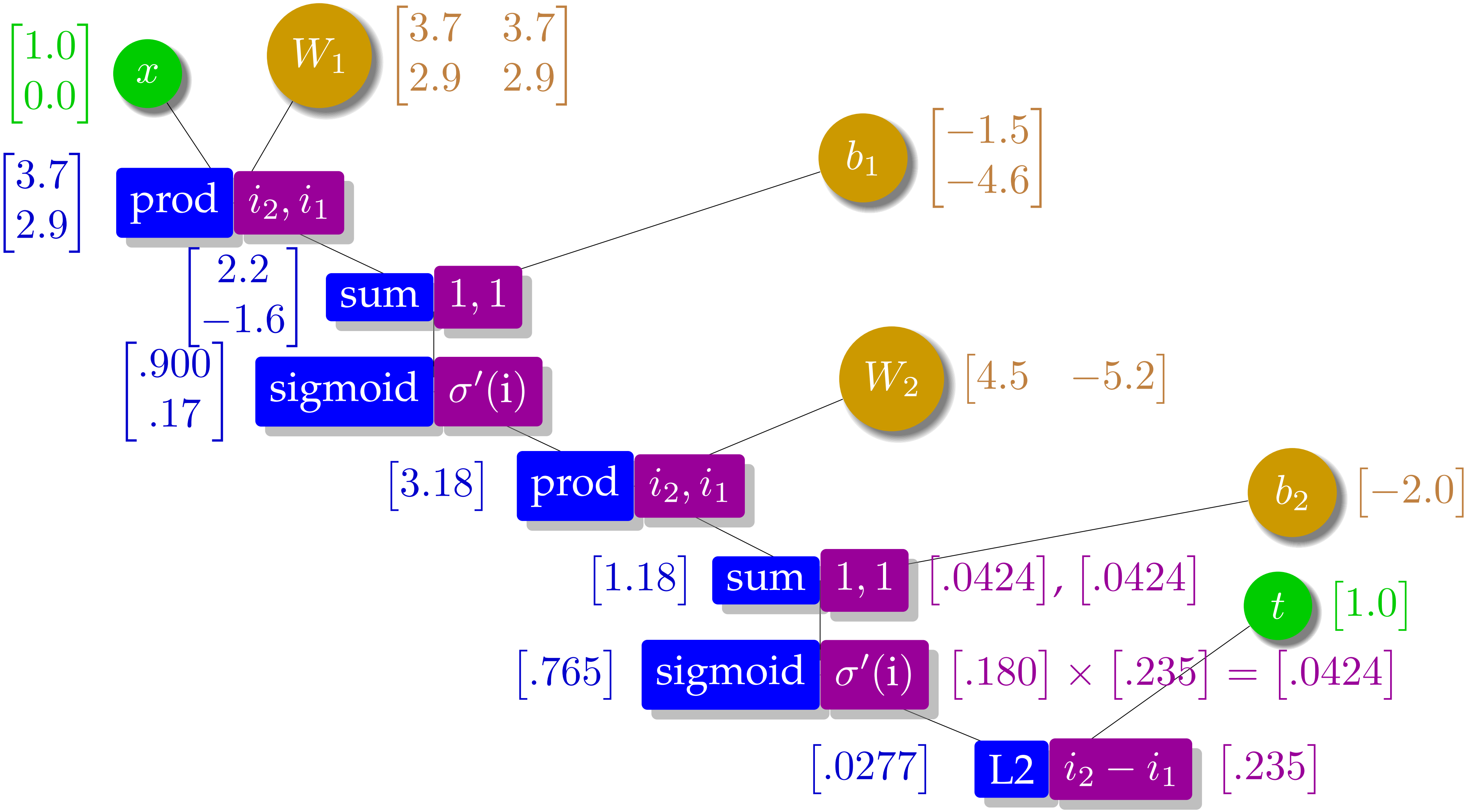
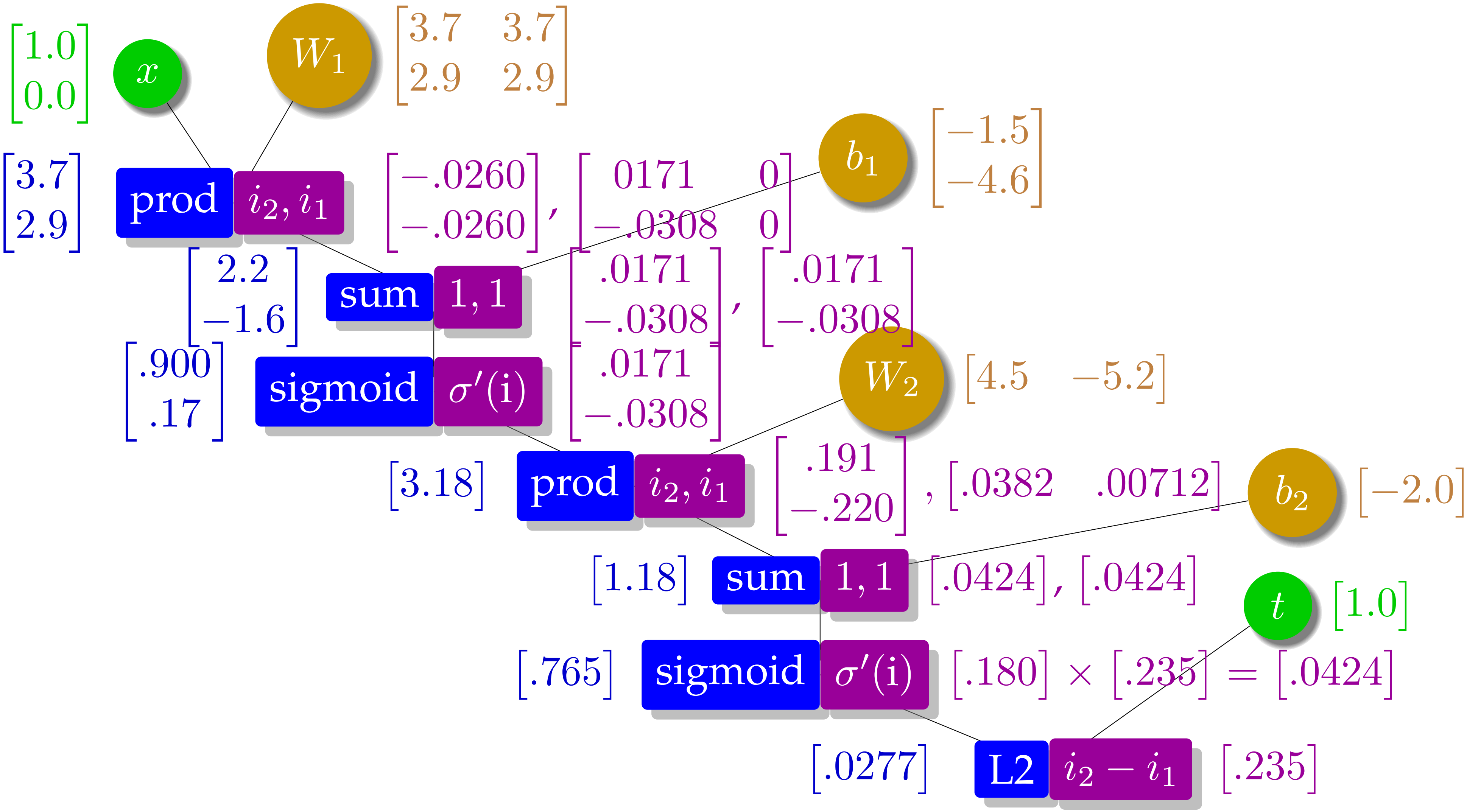
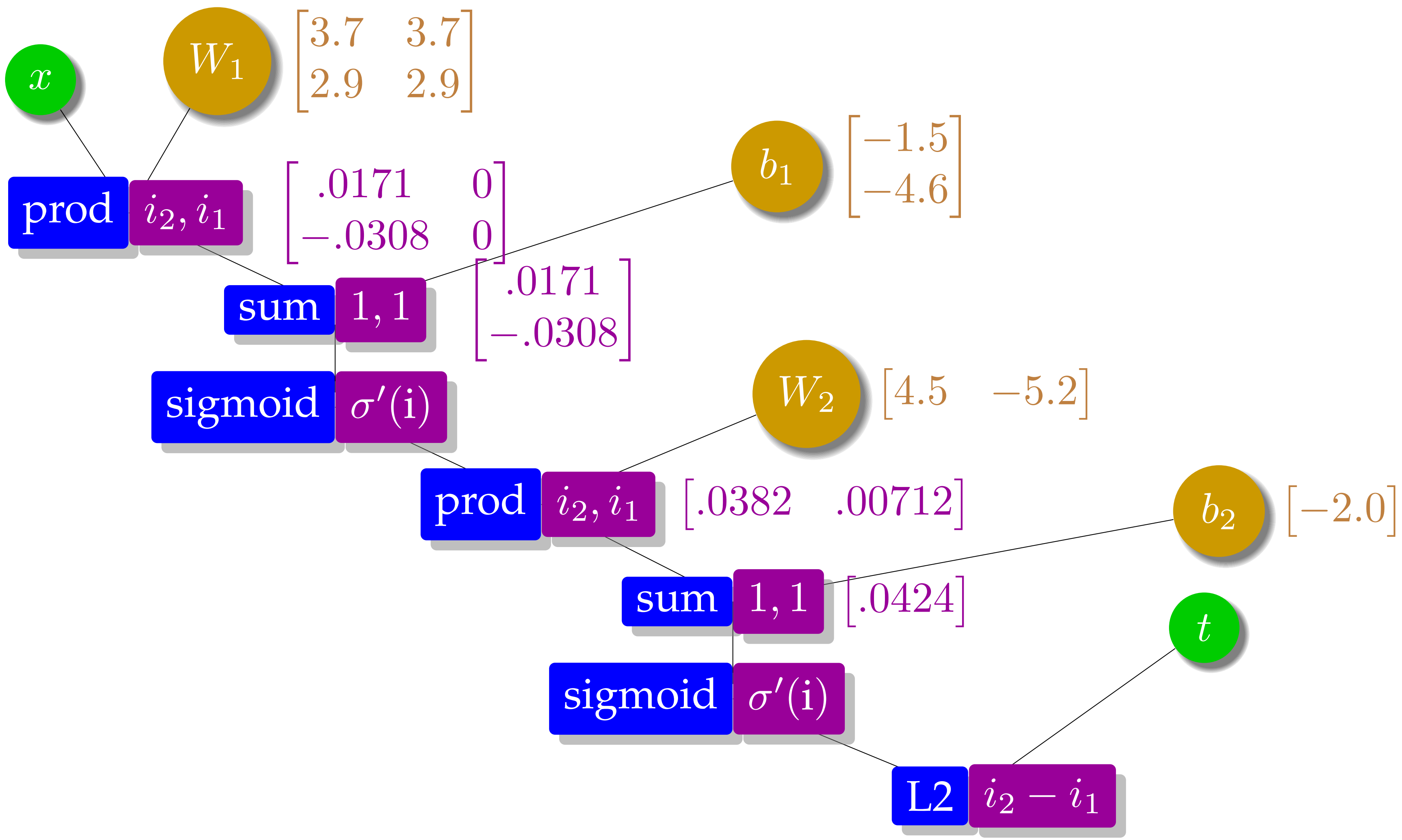


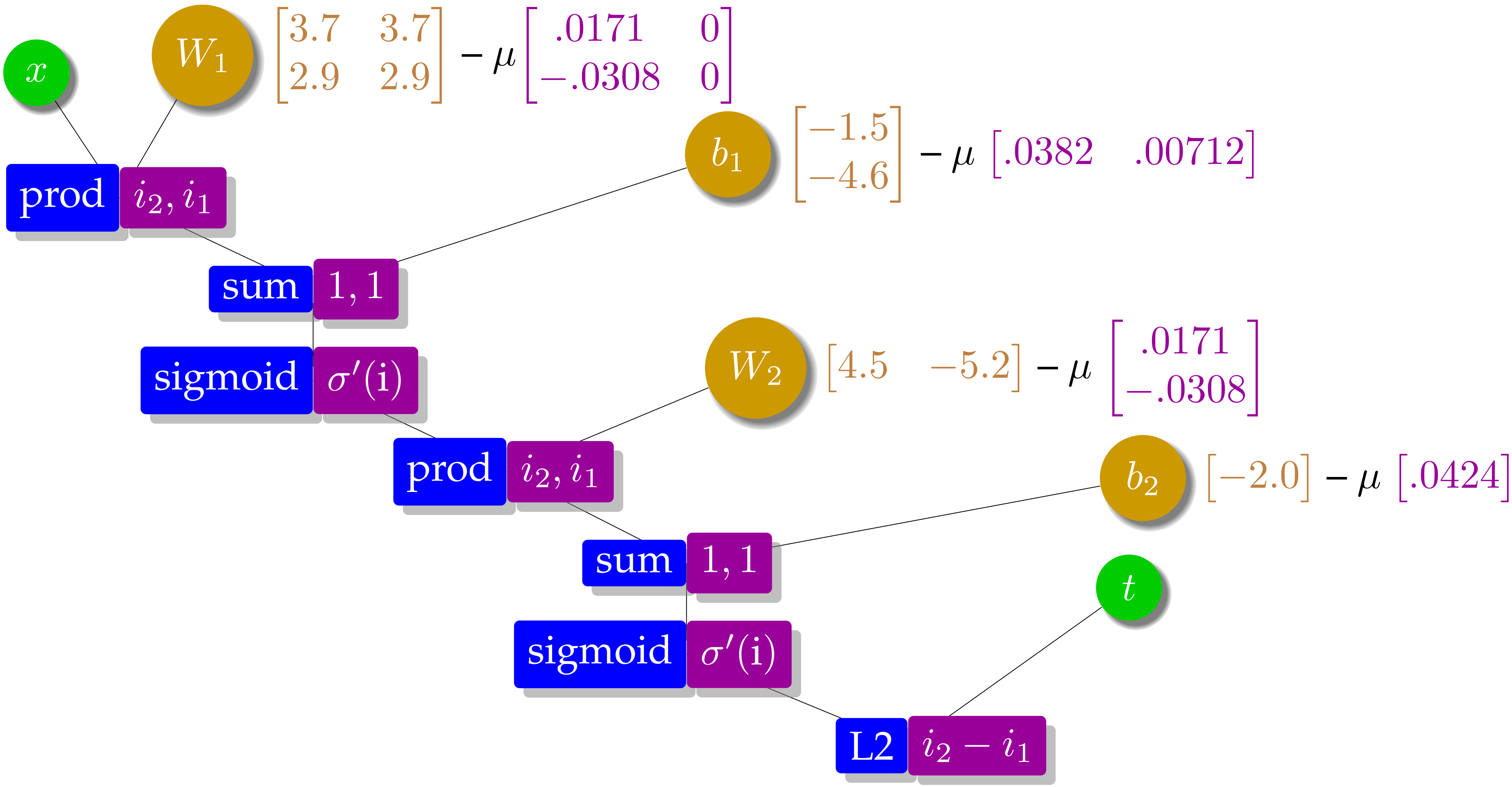
Backward Pass: Derivative Computation



Gradients for Parameter Update



Parameter Update



toolkits

Explosion of Deep Learning Toolkits

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

Toolkits

- 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

Example: Theano

- Deep learning toolkit for Python

- Included as library

```
> import numpy
> import theano
> import theano.tensor as T
```

Example: Theano

- Definition of parameters

```
> x = T.dmatrix()
> W = theano.shared(value=numpy.array([[3.0,2.0],[4.0,3.0]]))
> b = theano.shared(value=numpy.array([-2.0,-4.0]))
```

- Definition of feed-forward layer

```
> h = T.nnet.sigmoid(T.dot(x,W)+b)
```

note: `x` is matrix → process several training examples (sequence of vectors).

- Define as callable function

```
> h_function = theano.function([x], h)
```

- Apply to data

```
> h_function([[1,0]])
array([[ 0.73105858, 0.11920292]])
```

Example: Theano

- Same setup for hidden→output layer

```
W2 = theano.shared(value=numpy.array([5.0,-5.0] ))
b2 = theano.shared(-2.0)
y_pred = T.nnet.sigmoid(T.dot(h,W2)+b2)
```

- Define as callable function `> predict = theano.function([x], y_pred)`

- Apply to data

```
> predict([[1,0]])
array([[ 0.7425526]])
```

Model Training

- First, define the variable for the correct output

```
> y = T.dvector()
```

- Definition of a cost function (we use the L2 norm).

```
> l2 = (y-y_pred)**2
> cost = l2.mean()
```

- Gradient descent training: computation of the derivative

```
> gW, gb, gW2, gb2 = T.grad(cost, [W,b,W2,b2])
```

- Update rule (with learning rate 0.1)

```
> train = theano.function(inputs=[x,y],outputs=[y_pred,cost],
     updates=((W, W-0.1*gW), (b, b-0.1*gb),
             (W2, W2-0.1*gW2), (b2, b2-0.1*gb2)))
```

Model Training

- Training data

```
> DATA_X = numpy.array([[0,0],[0,1],[1,0],[1,1]])
> DATA_Y = numpy.array([0,1,1,0])
```

- Predict output for training data

```
> predict(DATA_X)
array([ 0.18333462, 0.7425526 , 0.7425526 , 0.33430961])
```

Model Training

- Train with training data

```
> train(DATA_X,DATA_Y)
[array([ 0.18333462, 0.7425526 , 0.7425526 , 0.33430961]),
array(0.06948320612438118)]
```

- Prediction after training

```
> train(DATA_X,DATA_Y)
[array([ 0.18353091, 0.74260499, 0.74321824, 0.33324929]),
array(0.06923193686092949)]
```

example: dynet

Dynet

- Our example: static computation graph, fixed set of data
- But: language requires different computation data for different data items (sentences have different length)

$\Rightarrow$ Dynamically create a computation graph for each data item

Example: Dynet

```
model = dy.model()
W_p = model.add_parameters((20, 100))
b_p = model.add_parameters(20)
E = model.add_lookup_parameters((20000, 50))
trainer = dy.SimpleSGDTrainer(model)
for epoch in range(num_epochs):
    for in_words, out_label in training_data:
        dy.renew_cg()
        W = dy.parameter(W_p)
        b = dy.parameter(b_p)
        score_sym = dy.softmax(
            W*dy.concatenate([E[in_words[0]],E[in_words[1]]])+b)
        loss_sym = dy.pickneglogsoftmax(score_sym, out_label)
        loss_sym.forward()
        loss_sym.backward()
        trainer.update()
```

Model Parameters

```
model = dy.model()
W_p = model.add_parameters((20, 100))
b_p = model.add_parameters(20)
E = model.add_lookup_parameters((20000, 50))
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        loss_sym = dy.pickneglogsoftmax(score_sym, out_label)
        loss_sym.forward()
        loss_sym.backward()
        trainer.update()
```

Model holds the values for the weight matrices and weight vectors

Training Setup


```
model = dy.model()
W_p = model.add_parameters((20, 100))
b_p = model.add_parameters(20)
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        loss_sym.forward()
        loss_sym.backward()
        trainer.update()
```

Defines the model update function (could be also Adagrad, Adam, ...)

Setting up Computation Graph

```
model = dy.model()
W_p = model.add_parameters((20, 100))
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trainer = dy.SimpleSGDTrainer(model)
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        loss_sym.backward()
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```

Create a new computation graph. Inform it about parameters.

Operations


```
model = dy.model()
W_p = model.add_parameters((20, 100))
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E = model.add_lookup_parameters((20000, 50))
trainer = dy.SimpleSGDTrainer(model)
for epoch in range(num_epochs):
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        W = dy.parameter(W_p)
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        score_sym = dy.softmax(
              W*dy.concatenate([E[in_words[0]],E[in_words[1]]])+b)
        loss_sym = dy.pickneglogsoftmax(score_sym, out_label)
        loss_sym.forward()
        loss_sym.backward()
        trainer.update()
```

Builds the computation graph by defining operations.

Training Loop


```
model = dy.model()
W_p = model.add_parameters((20, 100))
b_p = model.add_parameters(20)
E = model.add_lookup_parameters((20000, 50))
trainer = dy.SimpleSGDTrainer(model)
for epoch in range(num_epochs):
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        b = dy.parameter(b_p)
        score_sym = dy.softmax(
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        loss_sym = dy.pickneglogsoftmax(score_sym, out_label)
        loss_sym.forward()
        loss_sym.backward()
        trainer.update()
```

Process training data. Computations are done in `forward` and `backward`.