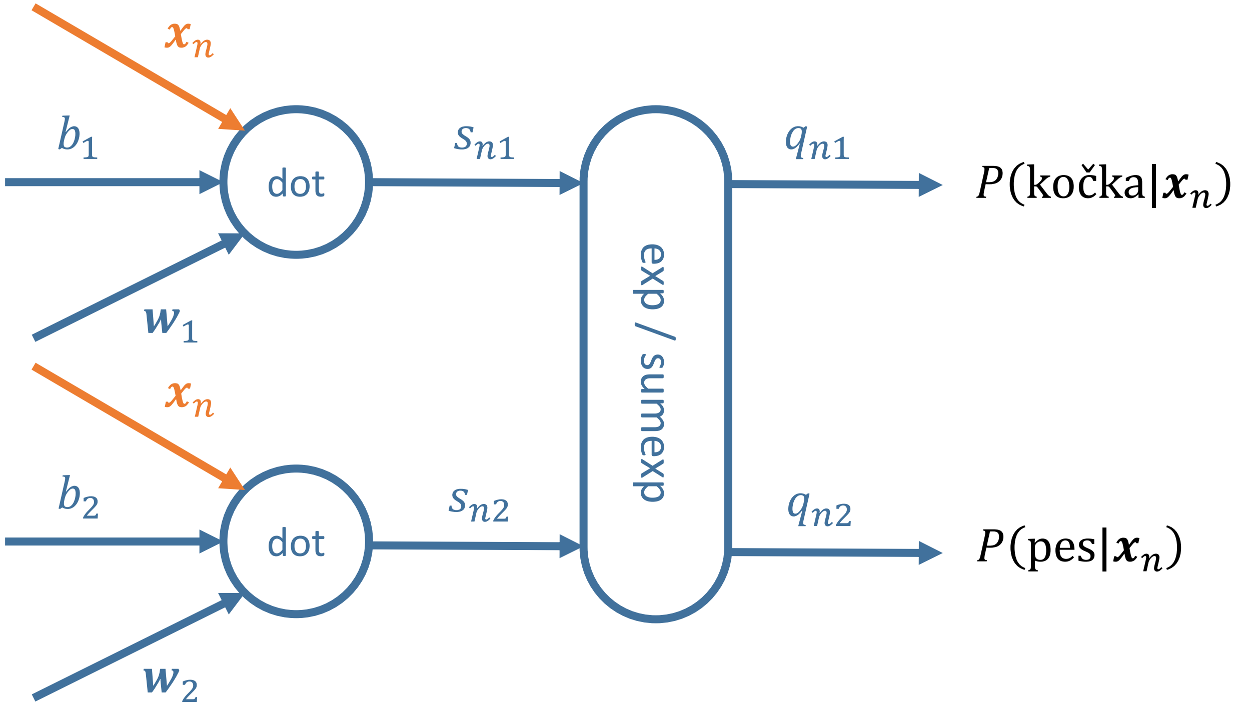
Aplikace neuronových sítí

Zpětná propagace

Multiclass logistická regrese (softmax klasifikátor)



$$q_{nc} = P(\text{třída } c|\boldsymbol{x}_n) = \frac{e^{s_{nc}}}{\sum_{i=1}^{C} e^{s_{ni}}}$$

Diferencovatelné výpočetní grafy

Řetízkové pravidlo (chain rule)

- Pro výpočet derivace složených funkcí formy $z = f(y) = f\big(g(x)\big)$ používáme

$$\boxed{\frac{\mathrm{d}z}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}y} \cdot \frac{\mathrm{d}y}{\mathrm{d}x}}$$

- “derivace vnější krát derivace vnitřní”

Příklad na řetízkové pravidlo

$$z = (\underbrace{x_1 + a x_2}_{g})^{2}$$

f

vnitřní funkce g:

$$y = x_1 + a x_2$$

$$\frac{\partial y}{\partial x_1} = 1 \qquad \frac{\partial y}{\partial x_2} = a$$

vnější funkce f:

$$z = y^2$$

$$\frac{\partial z}{\partial y} = 2y$$

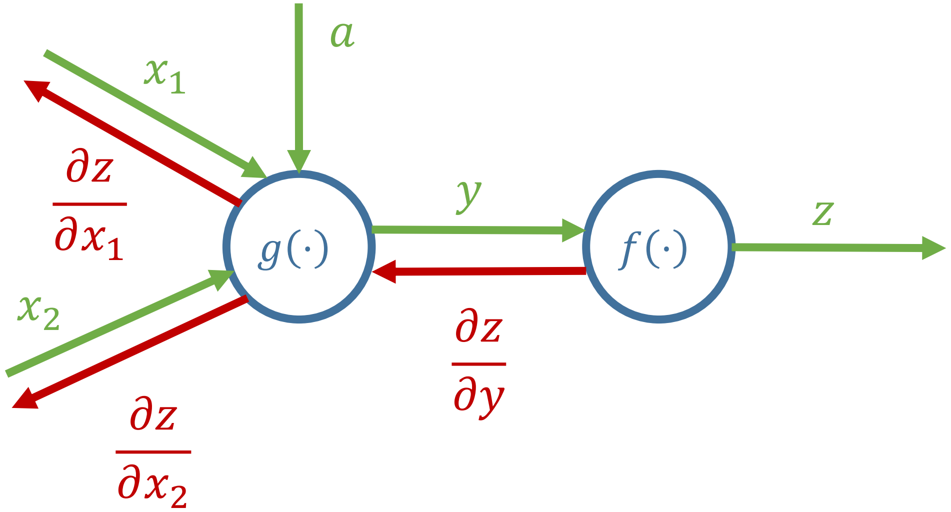
aplikace pravidla:

$$\frac{\partial z}{\partial x_1} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x_1} = 2y \cdot 1 = 2(x_1 + a x_2)$$

$$\frac{\partial z}{\partial x_2} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x_2} = 2y \cdot a = 2a(x_1 + a x_2)$$

Funkce $z = (x_1 + ax_2)^2$ jako graf

$$z = (x_1 + ax_2)^2$$



Funkce $z = (x_1 + ax_2)^2$ jako graf

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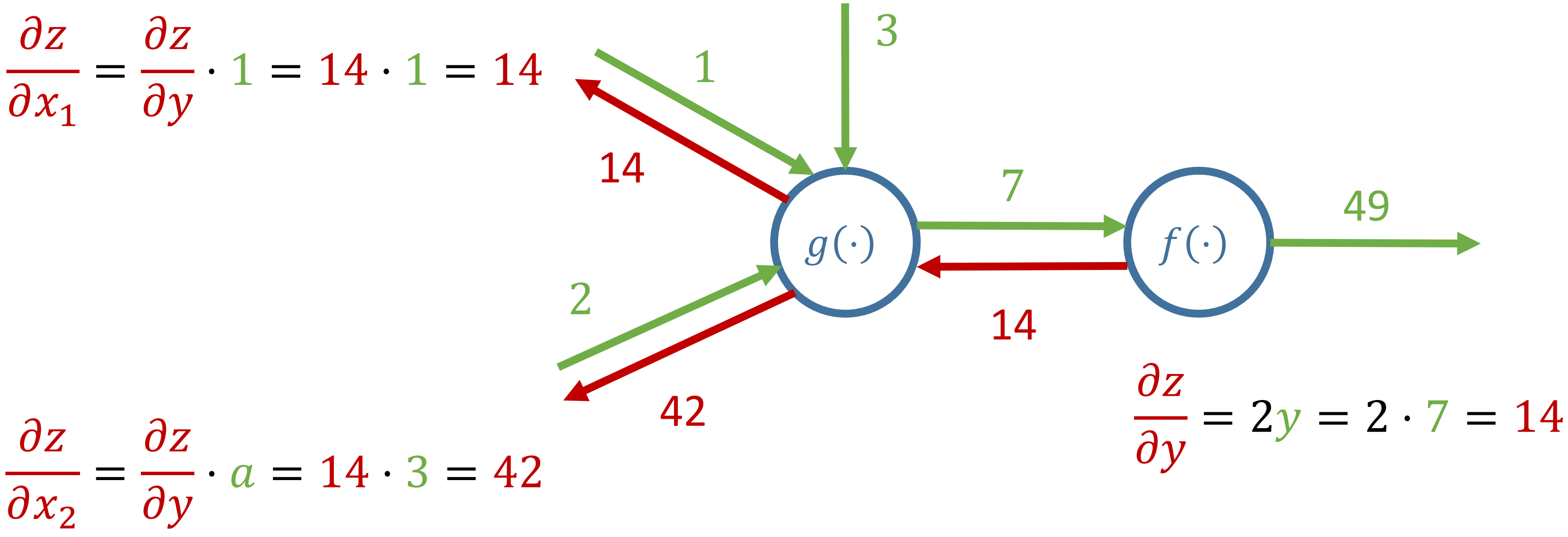


Funkce $z = (x_1 + ax_2)^2$ jako graf podrobně

dopředný průchod

(1) $x_2' \leftarrow ax_2$

(2) $y \leftarrow x_1 + x_2'$

(3) $z \leftarrow y^2$

zpětný průchod

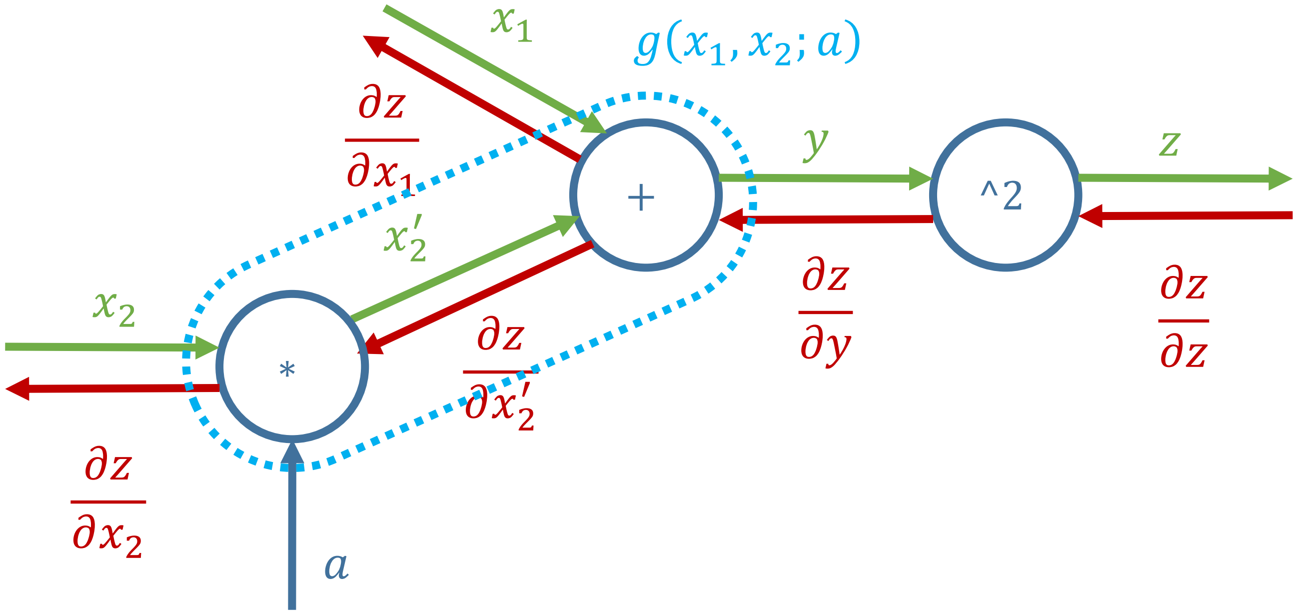
(0) $\frac{\partial z}{\partial z} = 1$

(1) $\frac{\partial z}{\partial y} \leftarrow \frac{\partial z}{\partial z} \cdot \frac{\partial z}{\partial y} = 2y$

(2) $\frac{\partial z}{\partial x_1} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x_1} = \frac{\partial z}{\partial y}$

$\frac{\partial z}{\partial x_2'} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x_2'} = \frac{\partial z}{\partial y}$

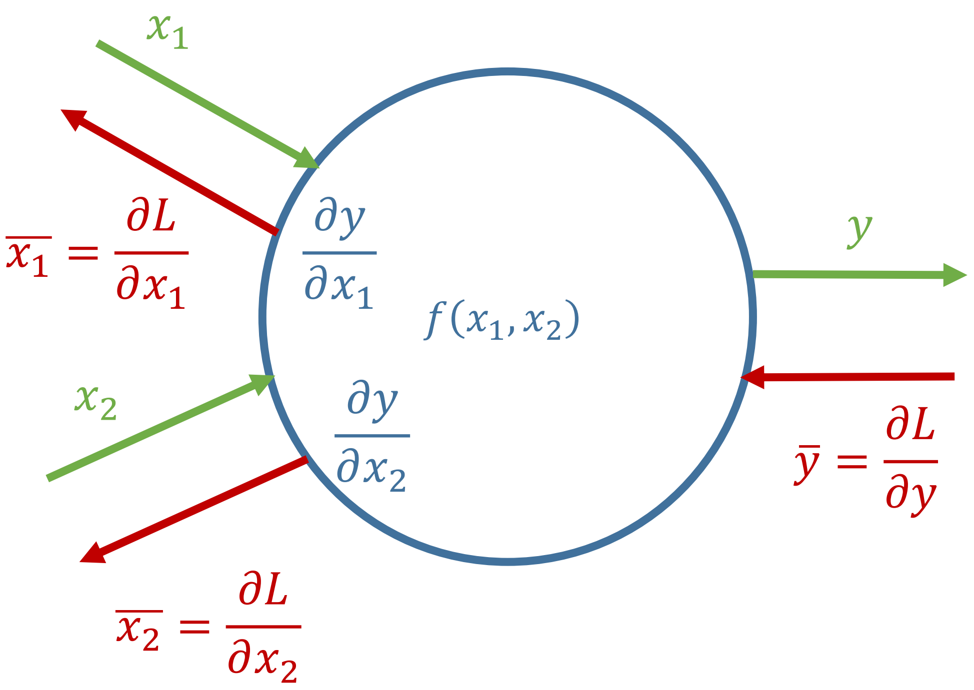
(3) $\frac{\partial z}{\partial x_2} = \frac{\partial z}{\partial x_2'} \cdot \frac{\partial x_2'}{\partial x_2} = \frac{\partial z}{\partial x_2'} \cdot a$



Uzel grafu a lokální gradient

- Na funkci lze nahlížet jako na orientovaný výpočetní graf
- Jednotlivé operace jsou uzly
- Hrany repezentují návaznosti vstupů a výstupů
- **Jakobián:**

$$J = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_D} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_C}{\partial x_1} & \cdots & \frac{\partial y_C}{\partial x_D} \end{bmatrix}$$



pruhová notace: https://people.maths.ox.ac.uk/gilesm/files/NA-08-01.pdf

Python kód funkce $z = (x_1 + ax_2)^2$ se zpětnou propagací

dopředný průchod

(1) $x'_2 \leftarrow ax_2$

(2) $y \leftarrow x_1 + x'_2$

(3) $z \leftarrow y^2$

zpětný průchod

(0) $\frac{\partial z}{\partial z} = 1$

(1) $\frac{\partial z}{\partial y} \leftarrow \frac{\partial z}{\partial z} \cdot \frac{\partial z}{\partial y} = 2y$

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(3) $\frac{\partial z}{\partial x_2} = \frac{\partial z}{\partial x'_2} \cdot \frac{\partial x'_2}{\partial x_2} = \frac{\partial z}{\partial x'_2} \cdot a$

```
def forward(x1, x2, a):
    # (1) forward
    x2_ = a * x2

    # (2) forward
    y = x1 + x2_

    # (3) forward
    z = y * y

    cache = x2, a, y
    return z, cache
```

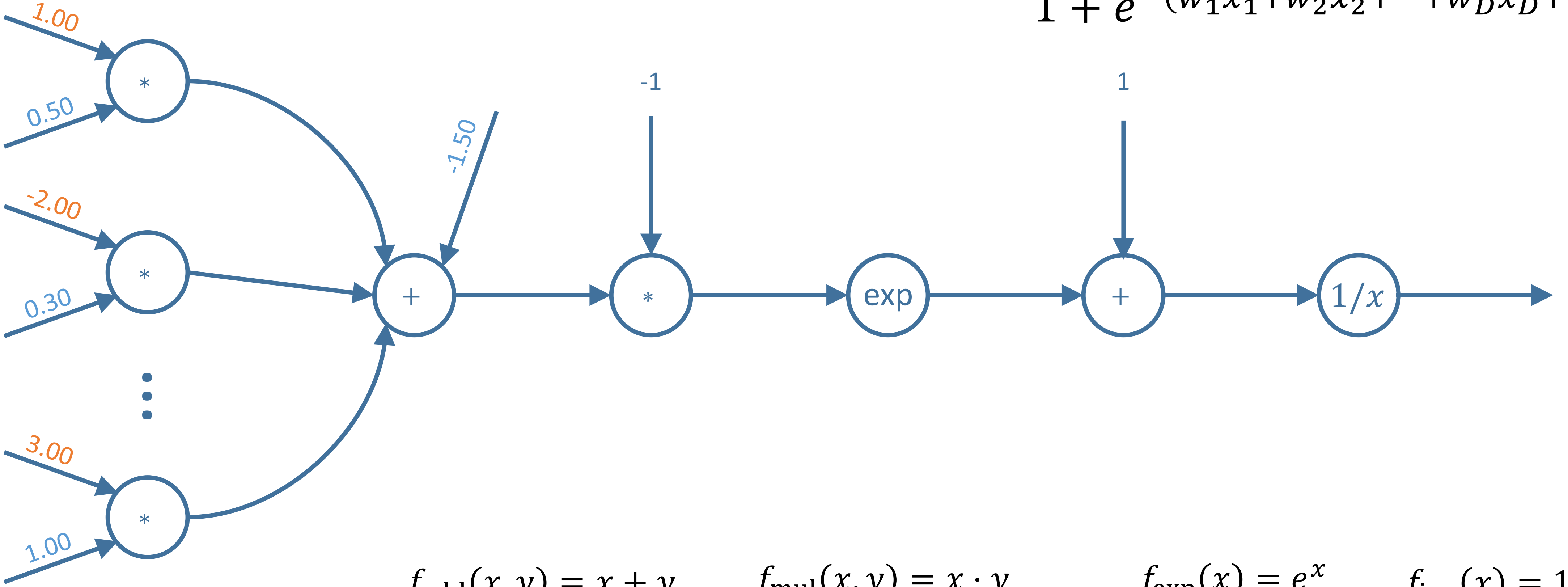
```
def backward(dz, cache):
    x2, a, y = cache

    # (3) backward
    dy = dz * 2 * y
    # (2) backward
    dx1 = dy
    dx2_ = dy
    # (1) backward
    dx2 = dx2_ * a
    da = dx2_ * x2
    return dx1, dx2, da
```

```
>>> x1, x2, a = 1, 2, 3
>>> z, cache = forward(x1, x2, a)
>>> dx1, dx2, da = backward(1.0, cache)
>>> dx1, dx2, da
(14.0, 42.0, 28.0)
```

Binární logistická regrese se sigmoidem jako graf

$\boldsymbol{x}_n = [1.00, -2.00, \dots, 3.00]^T$

$$q_n = \frac{1}{1 + e^{-(w_1 x_1 + w_2 x_2 + \cdots + w_D x_D + b)}}$$



$f_{\text{add}}(x, y) = x + y$ $\qquad$ $f_{\text{mul}}(x, y) = x \cdot y$ $\qquad$ $f_{\exp}(x) = e^x$ $\qquad$ $f_{\text{inv}}(x) = 1/x$

$\boldsymbol{w} = [0.50, 0.30, \dots, 1.00]^T$

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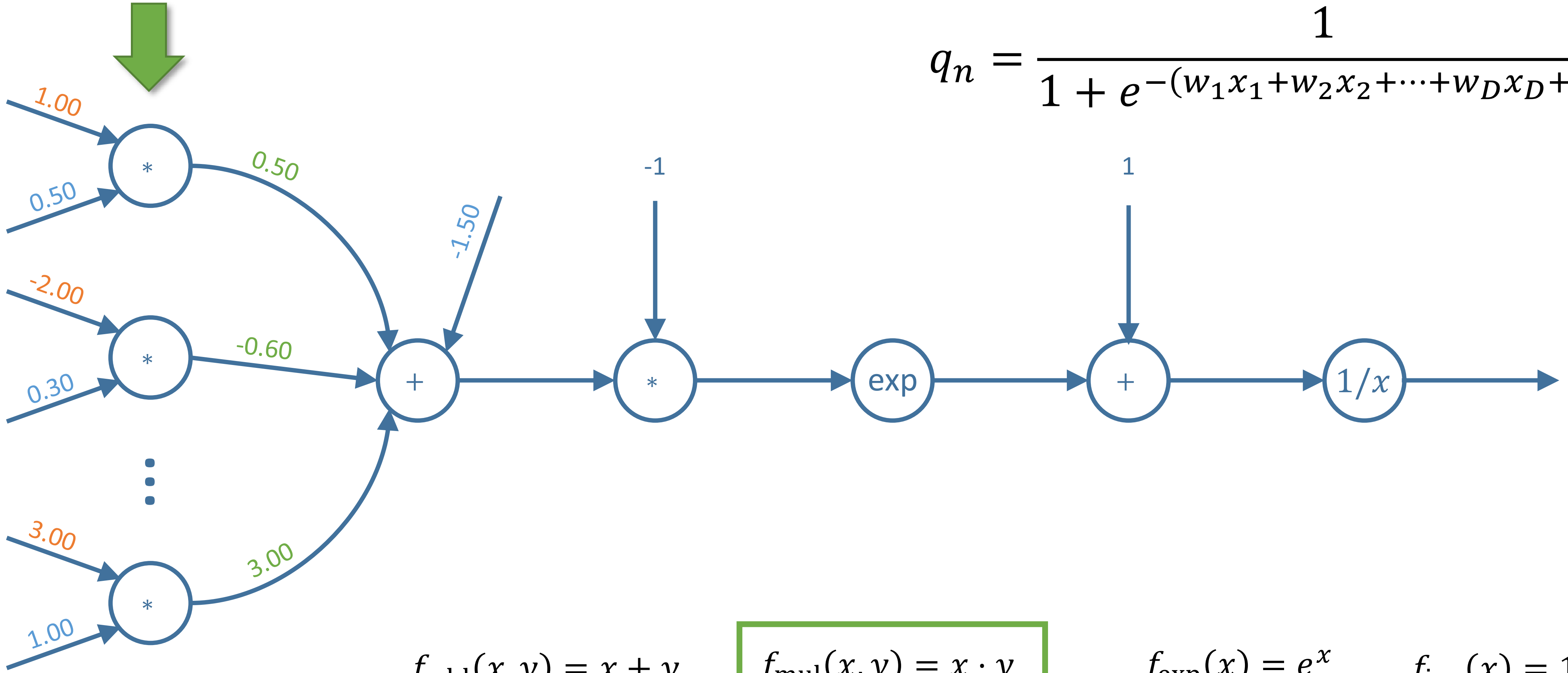

$f_{\text{add}}(x, y) = x + y$

$\frac{\partial f_{\text{add}}}{\partial x} = \frac{\partial f_{\text{add}}}{\partial y} = 1$

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$f_{\exp}(x) = e^x$

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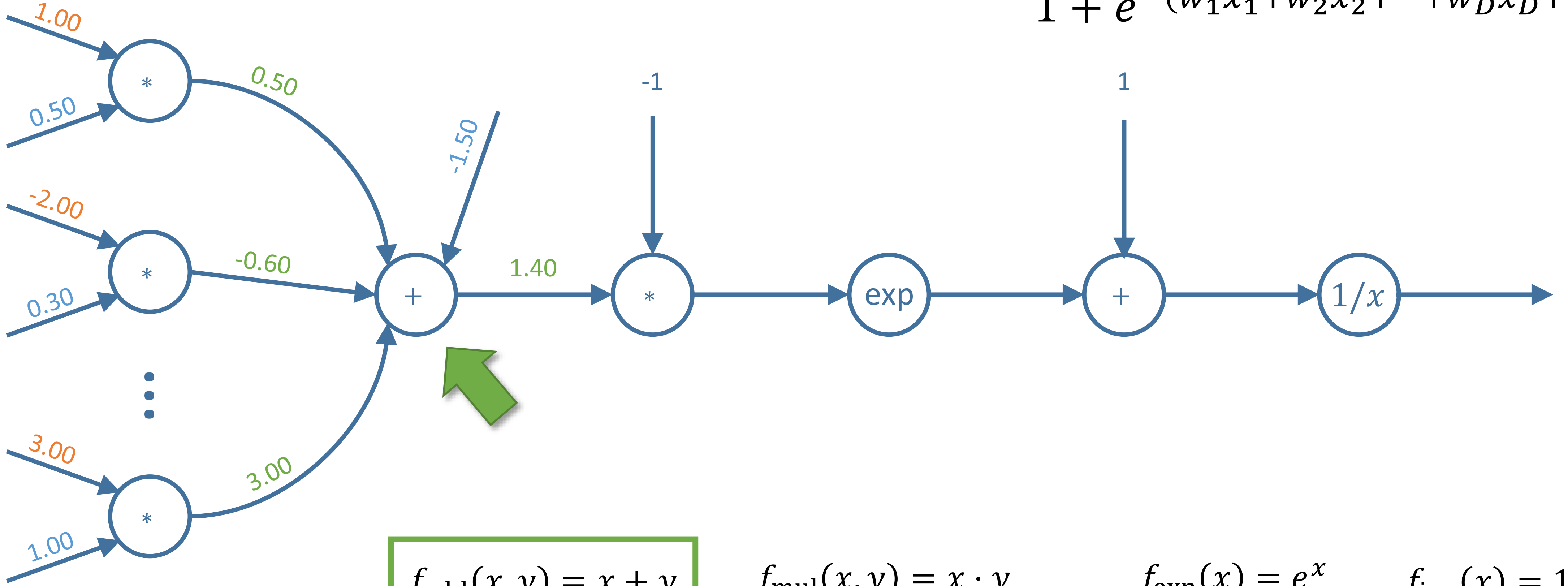

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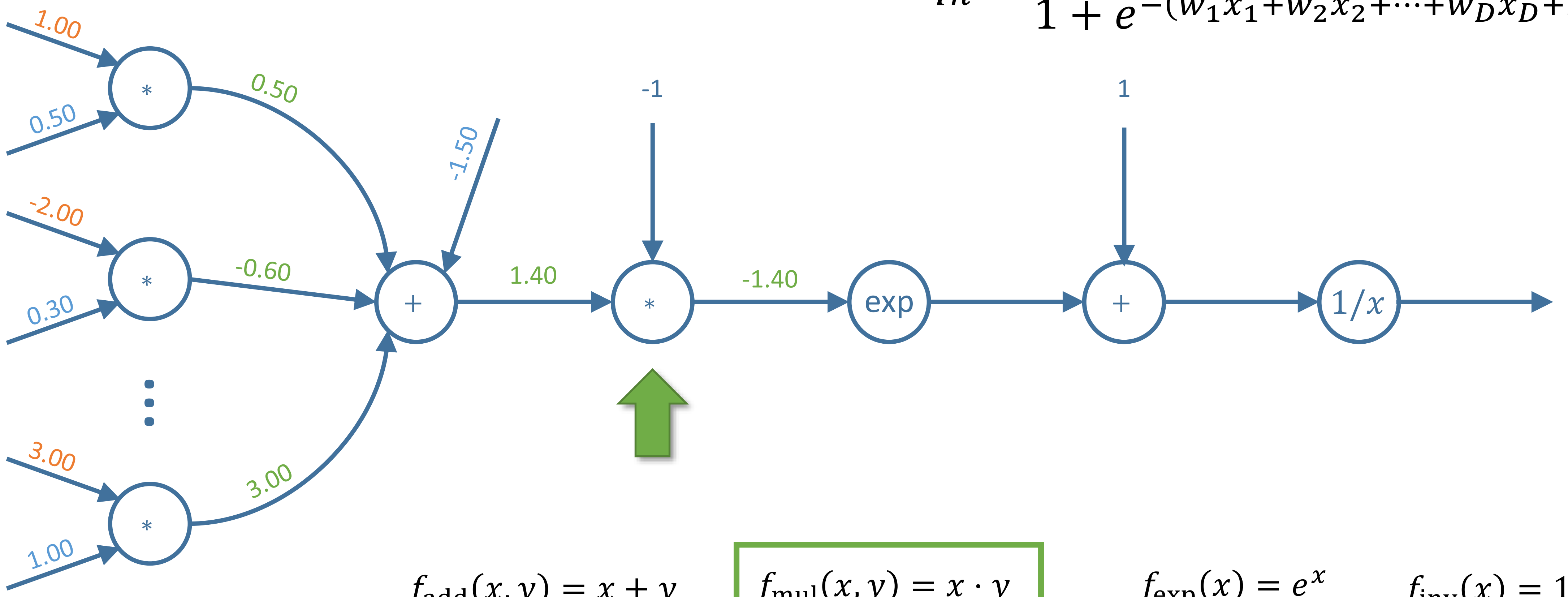

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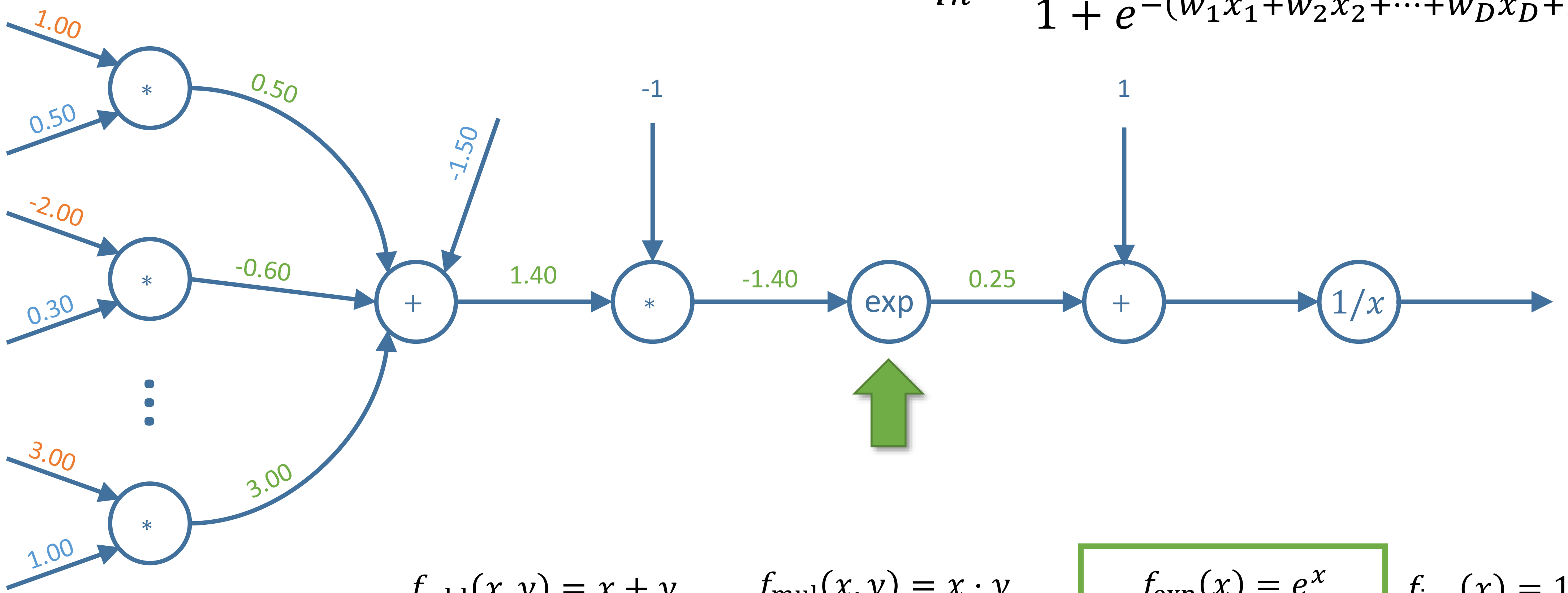

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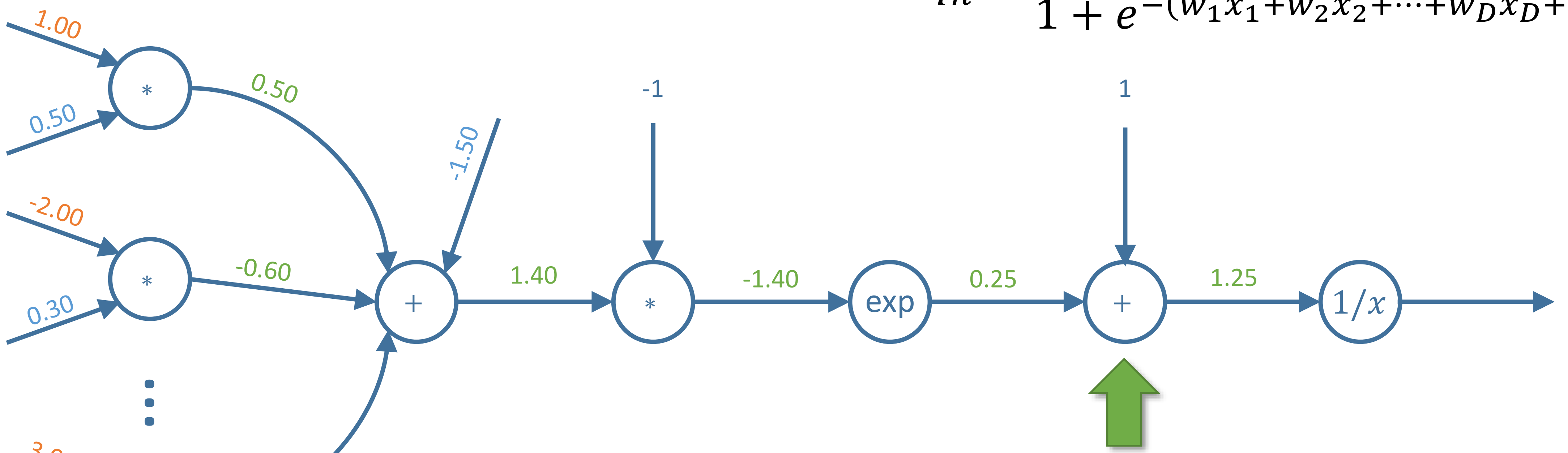

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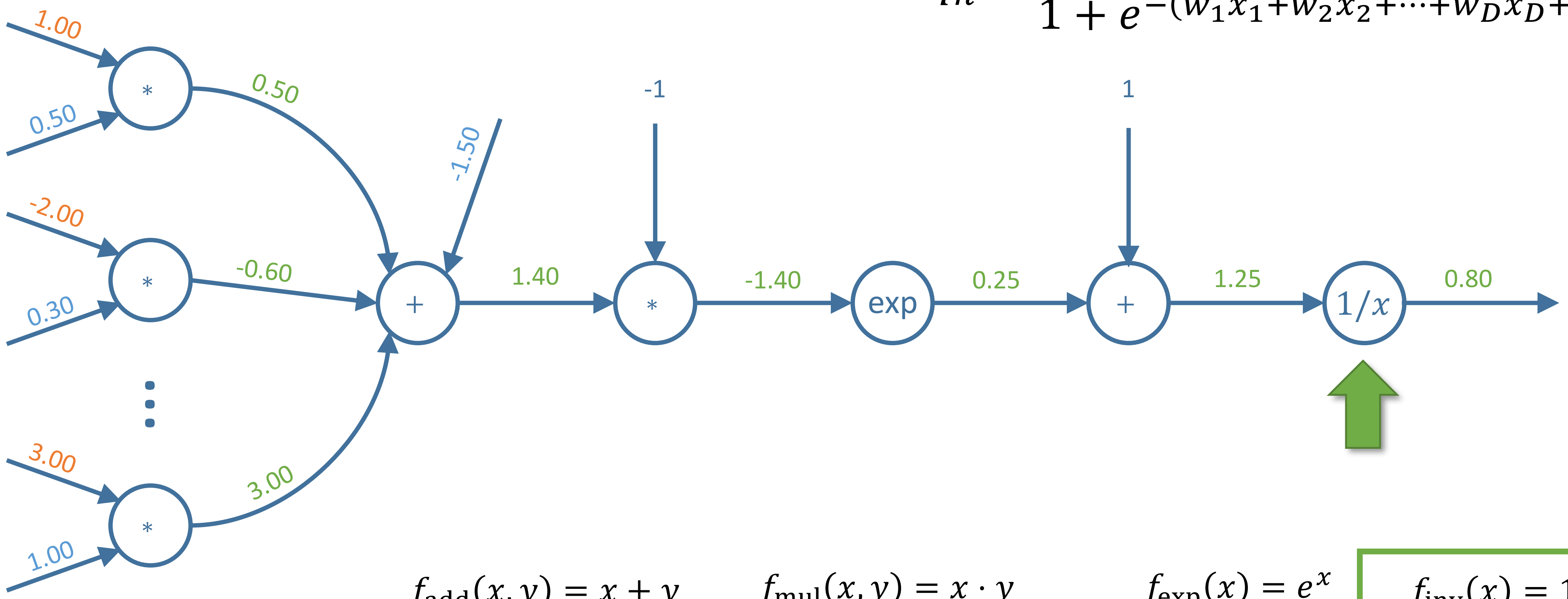

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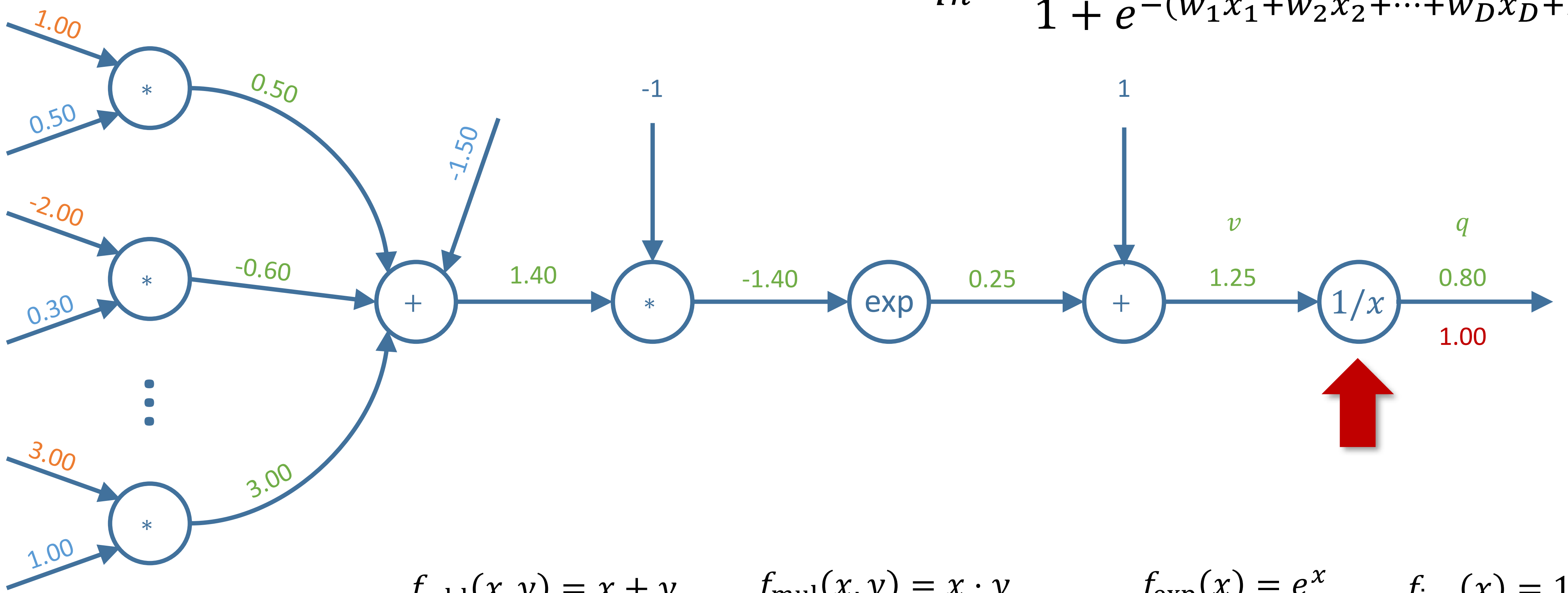

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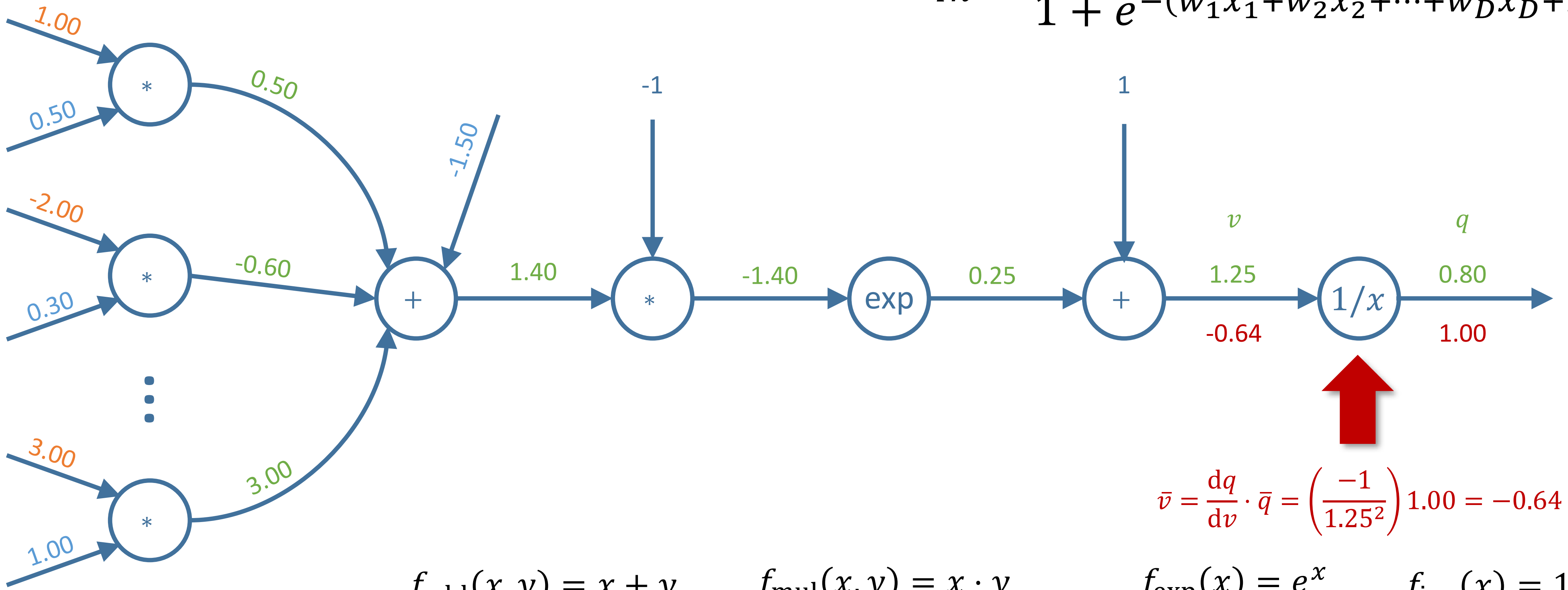

$$\bar{v} = \frac{\mathrm{d}q}{\mathrm{d}v} \cdot \bar{q} = \left(\frac{-1}{1.25^2}\right) 1.00 = -0.64$$

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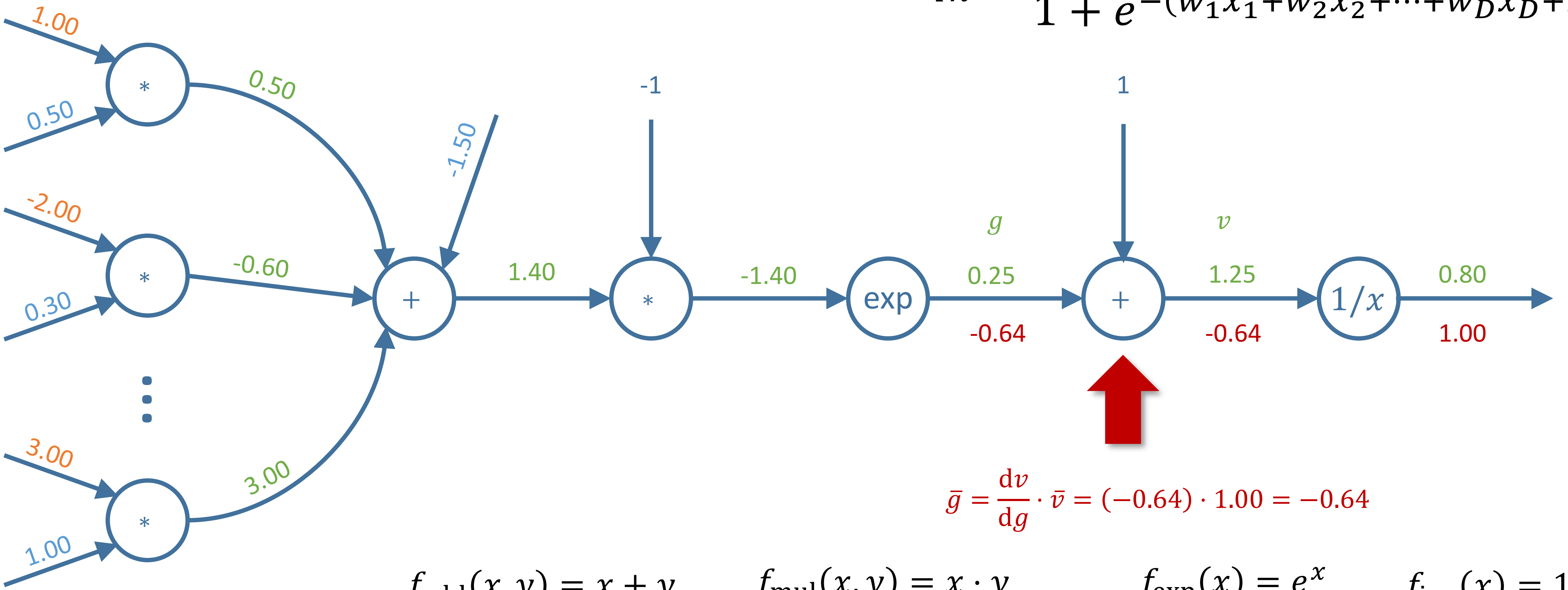

$$\bar{g} = \frac{\mathrm{d}v}{\mathrm{d}g} \cdot \bar{v} = (-0.64) \cdot 1.00 = -0.64$$

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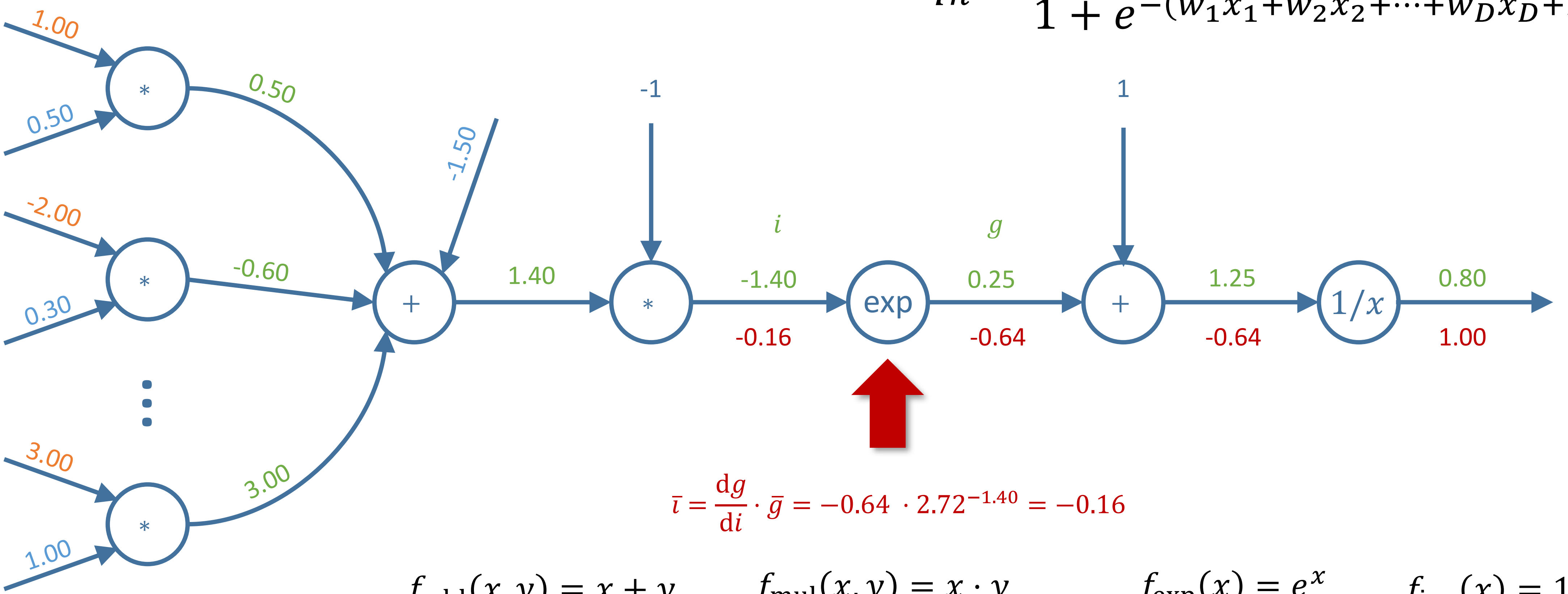

$$\bar{i} = \frac{\mathrm{d}g}{\mathrm{d}i} \cdot \bar{g} = -0.64 \cdot 2.72^{-1.40} = -0.16$$

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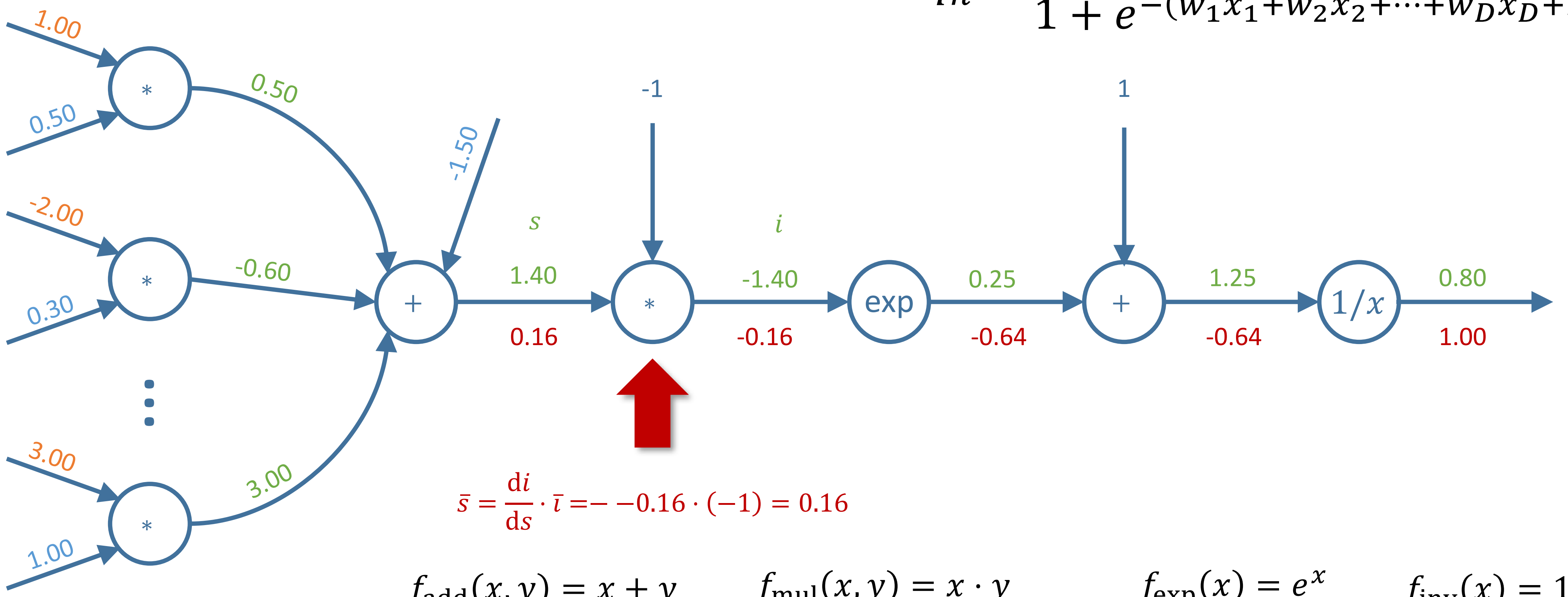

$$\bar{s} = \frac{\mathrm{d}i}{\mathrm{d}s} \cdot \bar{\imath} =- -0.16 \cdot (-1) = 0.16$$

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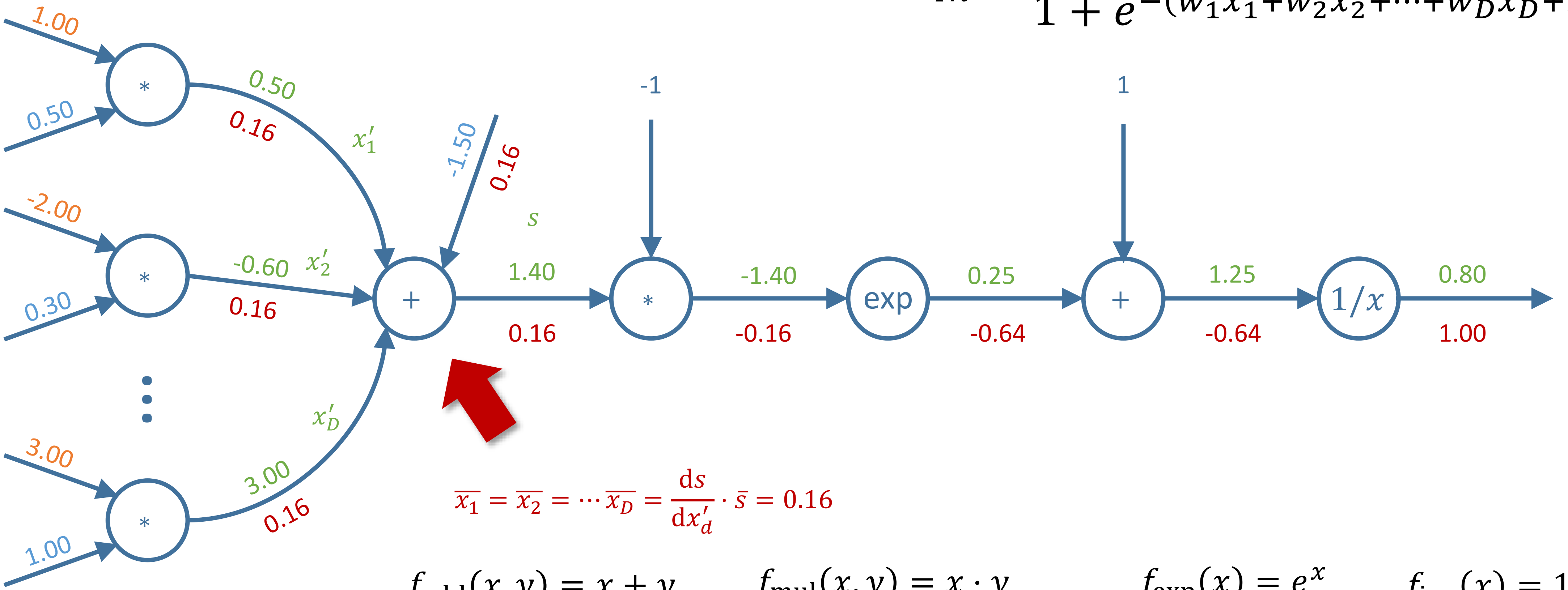

$$\overline{x_1} = \overline{x_2} = \cdots \overline{x_D} = \frac{\mathrm{d}s}{\mathrm{d}x_d'} \cdot \bar{s} = 0.16$$

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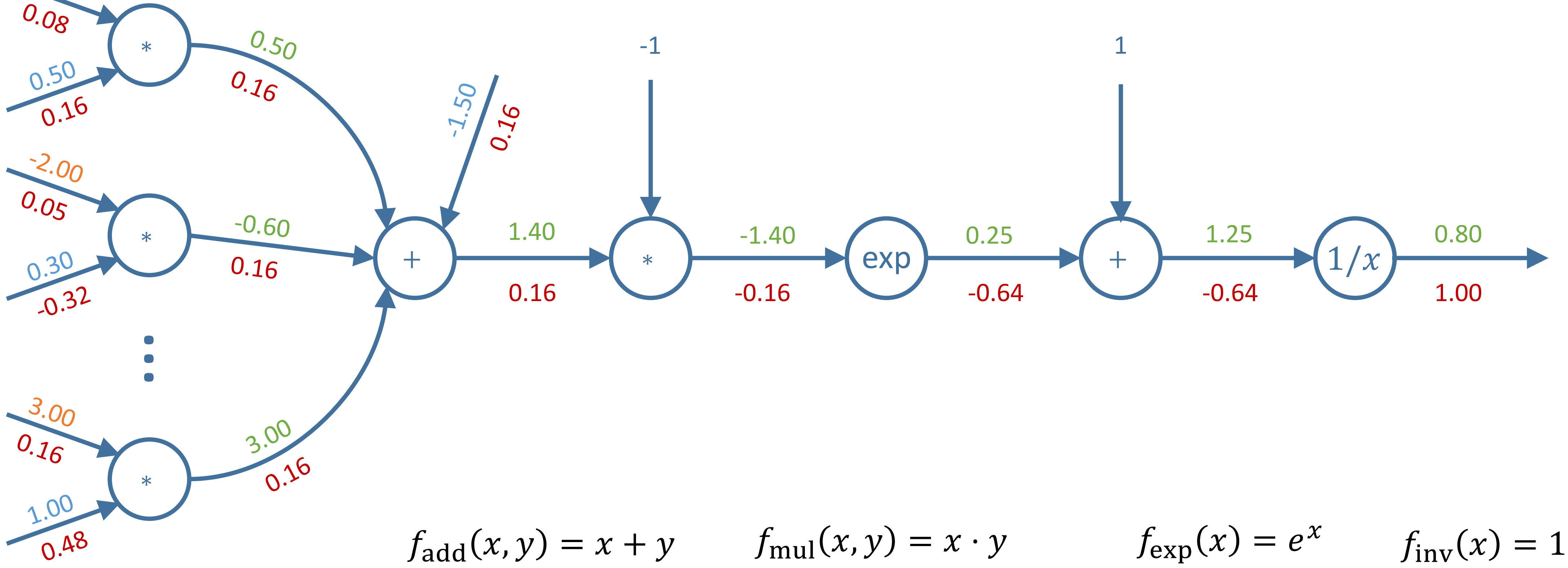

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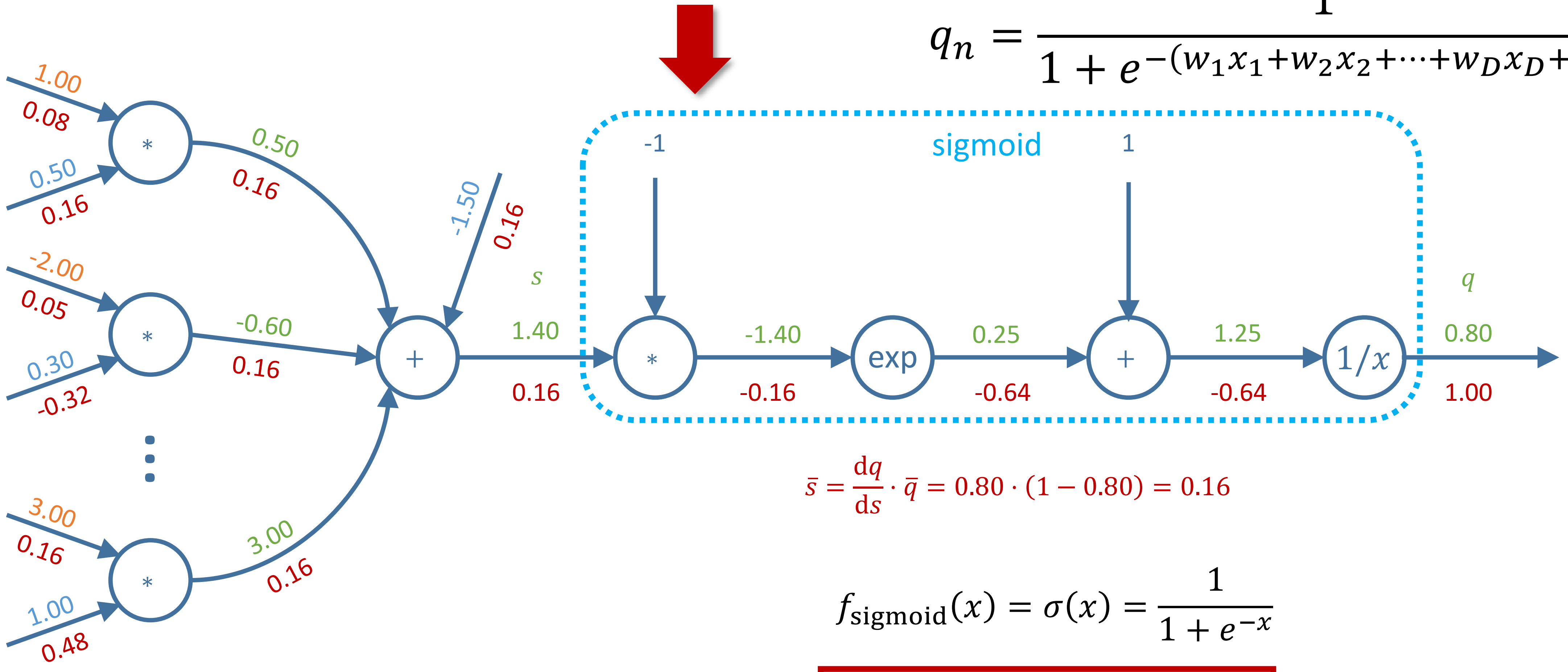


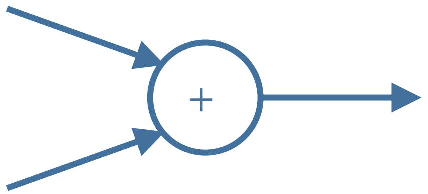
$$\bar{s} = \frac{\mathrm{d}q}{\mathrm{d}s} \cdot \bar{q} = 0.80 \cdot (1 - 0.80) = 0.16$$

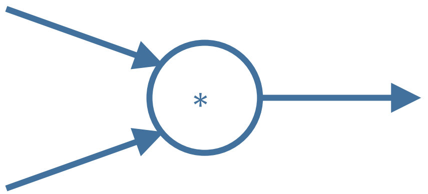
$$f_{\text{sigmoid}}(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$

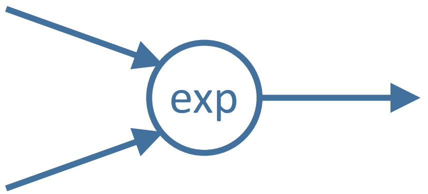
$$\boxed{\frac{\partial f_{\text{sigmoid}}}{\partial x} = \sigma(x)\big(1 - \sigma(x)\big)}$$

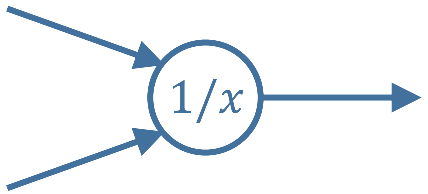
Druhy operací

- Operace v grafu se opakují → platí i pro výpočet gradientu
- V grafu se opakují pouze 4 typy **vrstev**:
    1. součet
    2. násobení
    3. exponenciální funkce
    4. inverze









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$$\frac{\partial f_{\text{add}}}{\partial x} = \frac{\partial f_{\text{add}}}{\partial y} = 1$$

$$f_{\text{mul}}(x, y) = x \cdot y$$

$$\frac{\partial f_{\text{mul}}}{\partial x} = y, \frac{\partial f_{\text{mul}}}{\partial y} = x$$

$$f_{\text{exp}}(x) = e^x$$

$$\frac{\partial f_{\text{exp}}}{\partial x} = e^x$$

$$f_{\text{inv}}(x) = 1/x$$

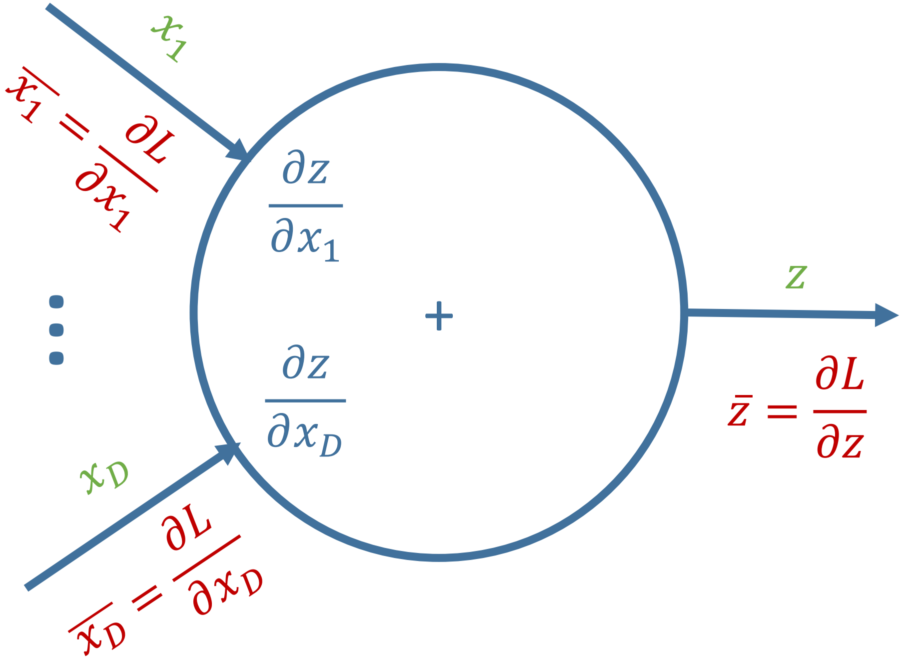
$$\frac{\partial f_{\text{inv}}}{\partial x} = -1/x^2$$

Sčítání

```
class AddNode(object):

    def forward(x_vec):
        # cache
        self.dim = x_vec.shape[0]
        z = np.sum(x_vec)
        return z

    def backward(dz):
        dx_vec = dz * np.ones(self.dim)
        return dx_vec
```



ve zpětném režimu “rozdistribuje” příchozí gradient do všech vstupů:

$$\overline{x_d} = \bar{z}, \qquad d = 1, \dots, D$$

forward: $z = \sum_{d=1}^{D} x_d$

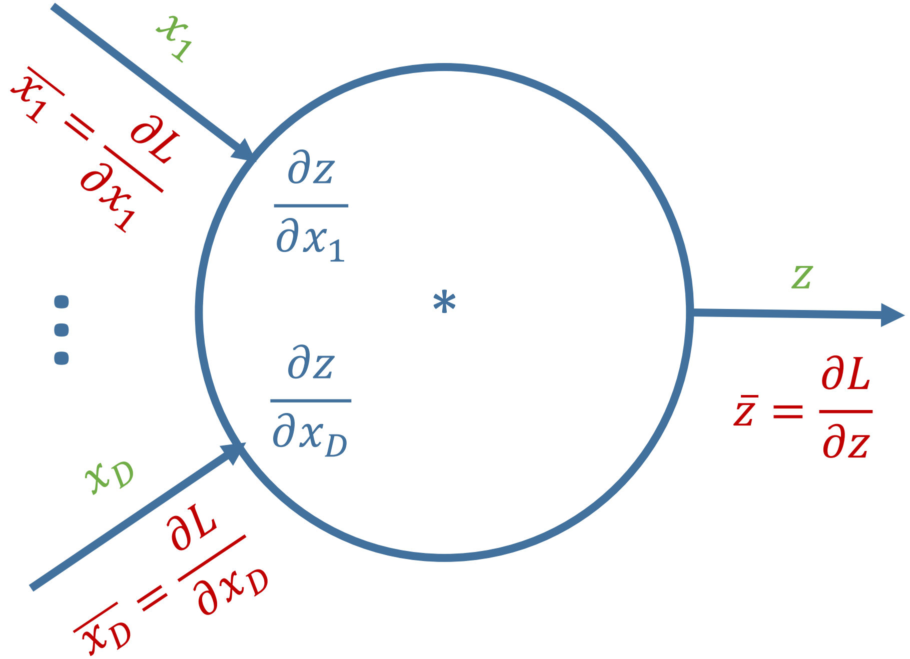
backward: $\frac{\partial z}{\partial x_d} = 1$

Násobení

```python
class MultiplyNode(object):

    def forward(x_vec):
        # cache
        self.x = x_vec
        self.z = np.prod(self.x)
        return self.z

    def backward(dz):
        # dx1 = (x1 * x2 * ... xD) / x1
        dx_vec = dz * self.z / self.x
        return dx_vec
```



forward: $z = \prod_{d=1}^{D} x_d$

backward: $\frac{\partial z}{\partial x_d} = \prod_{i \neq d} x_i$

Výpočetní graf pro zabalení funkcí do jednoho bloku

graf nesmí obsahovat cykly!

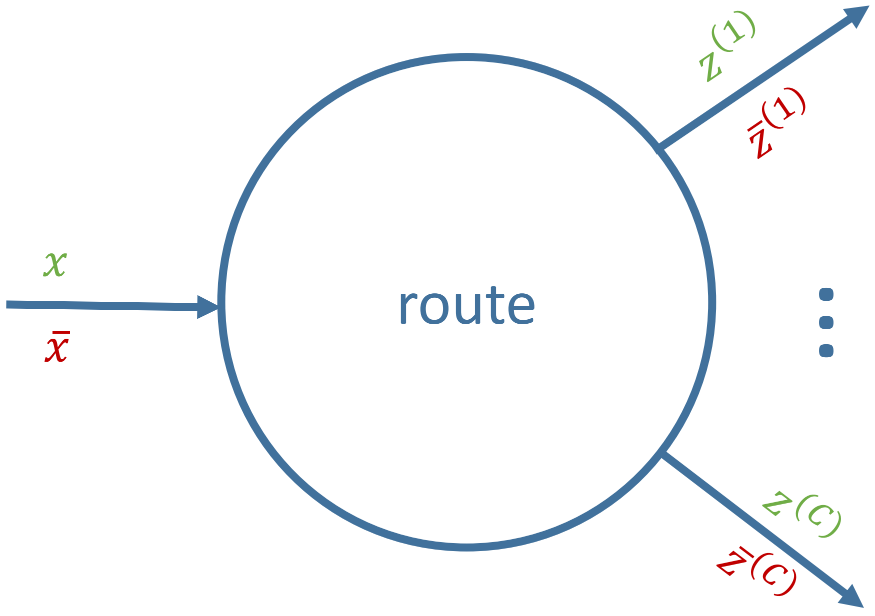
```
class ComputationalGraph(object):
    def add_node(node, *parents):
        self.nodes.append(node)
        self.parents[node] = parents

    def forward(*inputs):
        for node in topologically_sorted(self.nodes):
            inputs = [self.outputs[p] for p in self.parents[node]]
            self.outputs[node] = node.forward(*inputs)
        return top_nodes_outputs  # napr. loss (treba cross entropy)

    def backward(dout):
        for node in reversed(topologically_sorted(self.nodes)):
            node_grads = node.backward(self.grads[node])  # retizkove pravidlo
            for p, g in zip(self.parents[node], node_grads):
                self.grads[p] = g
        return bottom_nodes_grads
```

Opakované použití jednoho výstupu

- Výstup vstupuje do více než jednoho bloku v další vrstvě
- Konečný výsledek (např. loss) je závislý na obou mezivýsledcích
- Všimněme si duality vůči bloku sčítání



forward: $z^{(c)} = x$

backward: $\bar{x} = \sum_{c=1}^{C} \bar{z}^{(c)}$

https://math.stackexchange.com/questions/1566376/derivation-of-the-multivariate-chain-rule

Příklad: “lineární” vrstva, gradient na vstup

- Lineární (afinní) vrstva

$$\boldsymbol{s} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

- Rozvinutý zápis

$$\begin{bmatrix} s_1 \\ \vdots \\ s_C \end{bmatrix} = \begin{bmatrix} w_{11} & \cdots & w_{1D} \\ \vdots & \ddots & \vdots \\ w_{C1} & \cdots & w_{CD} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ \vdots \\ x_D \end{bmatrix} + \begin{bmatrix} b_1 \\ \vdots \\ b_C \end{bmatrix}$$

- c-tý výstup

$$s_c = \sum_{d=1}^{D} w_{cd} x_d + b_c$$

- Gradient pro jeden vstup a výstup

$$\frac{\partial s_c}{\partial x_d} = w_{cd}$$

- Každé x_d je ale použito C-krát: vyskytuje se ve výpočtech všech $s_1, \ldots, s_C$, a proto

$$\overline{x_d} = \sum_{c=1}^{C} w_{cd} \overline{s_c} = \boldsymbol{w}_{:,d} \overline{\boldsymbol{s}}$$

kde $\boldsymbol{w}_{:,d}$ je d-tý sloupec $\boldsymbol{W}$

- Celý gradient vektorově:

$$\overline{\boldsymbol{x}} = \boldsymbol{W}^\top \overline{\boldsymbol{s}}$$

Příklad: “lineární” vrstva, gradient na váhy

- Pro c-tý výstup pouze c-tý řádek – např. s_1 nezávisí na $w_{21}, \dots, w_{2D}$

$$s_c = \sum_{d=1}^{D} w_{cd} x_d + b_c \quad \Longrightarrow \quad \frac{\partial s_c}{\partial w_{id}} = \begin{cases} x_d & \text{když} \quad i = c \\ 0 & \text{když} \quad \mathrm{i} \neq c \end{cases}$$

- Celkový gradient tedy je

$$\overline{w_{cd}} = \sum_{i=1}^{C} \overline{s_i} \cdot \frac{\partial s_i}{\partial w_{cd}} = \overline{s_c} \cdot x_d$$

$\boldsymbol{x}$ co bylo na vstupu při dopředném průchodu → **cache!**

- Vektorově

$$\overline{\boldsymbol{W}} = \frac{\partial L}{\partial \boldsymbol{W}} = \begin{bmatrix} \overline{s_1} \\ \vdots \\ \overline{s_C} \end{bmatrix} \cdot [x_1, \dots, x_D] = \begin{bmatrix} \overline{s_1} \cdot x_1 & \dots & \overline{s_1} \cdot x_D \\ \vdots & \ddots & \vdots \\ \overline{s_C} \cdot x_1 & \dots & \overline{s_C} \cdot x_D \end{bmatrix} = \overline{\boldsymbol{s}} \cdot \boldsymbol{x}^{\top}$$

Sigmoid jako vrstva

- Dopředný průchod

$$q = \sigma(x) = \frac{1}{1 + e^{-x}}$$

- Derivace funkce sigmoid

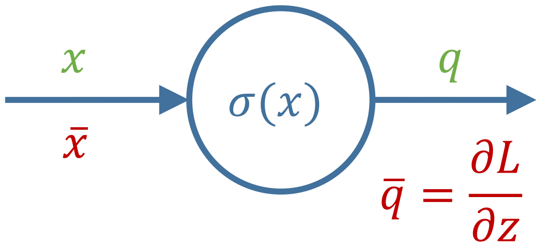
$$\frac{\mathrm{d}\sigma(x)}{\mathrm{d}x} = \sigma(x)\big(1 - \sigma(x)\big)$$

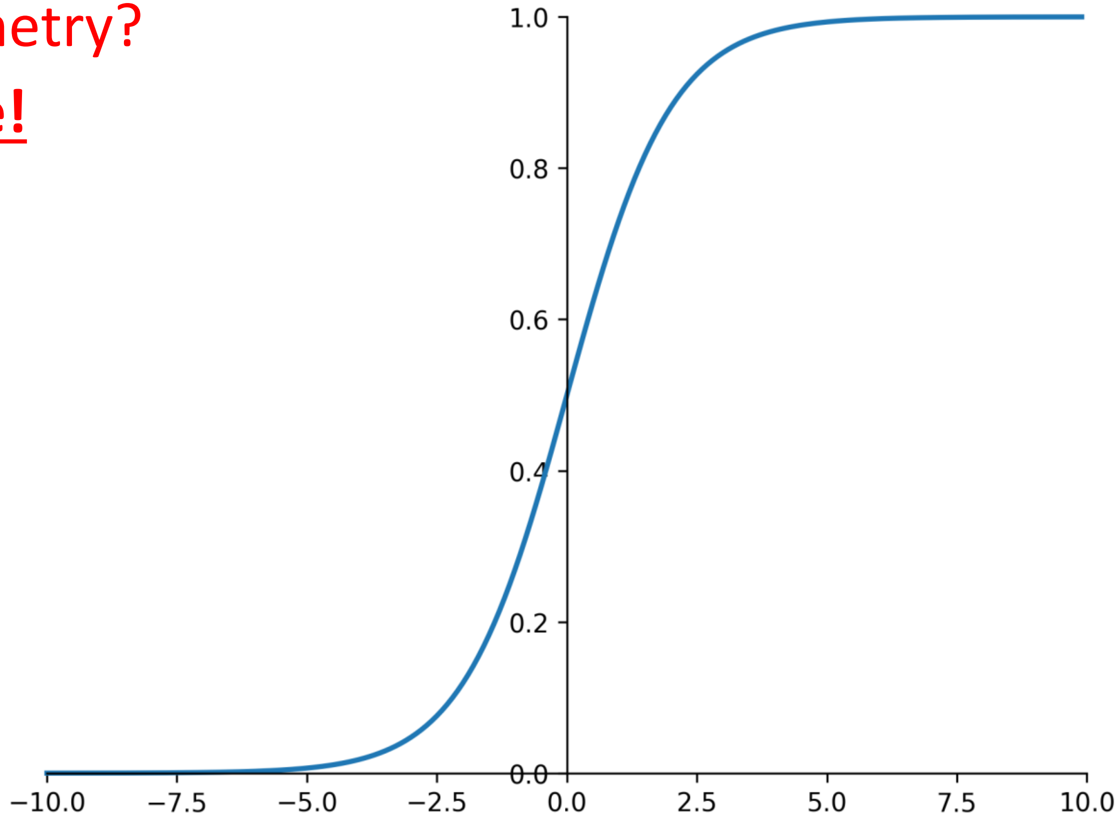
- Zpětný průchod

$$\bar{x} = \bar{q} \cdot \frac{\mathrm{d}q}{\mathrm{d}x} = \bar{q} \cdot q \cdot (1 - q)$$

q … **cache!**

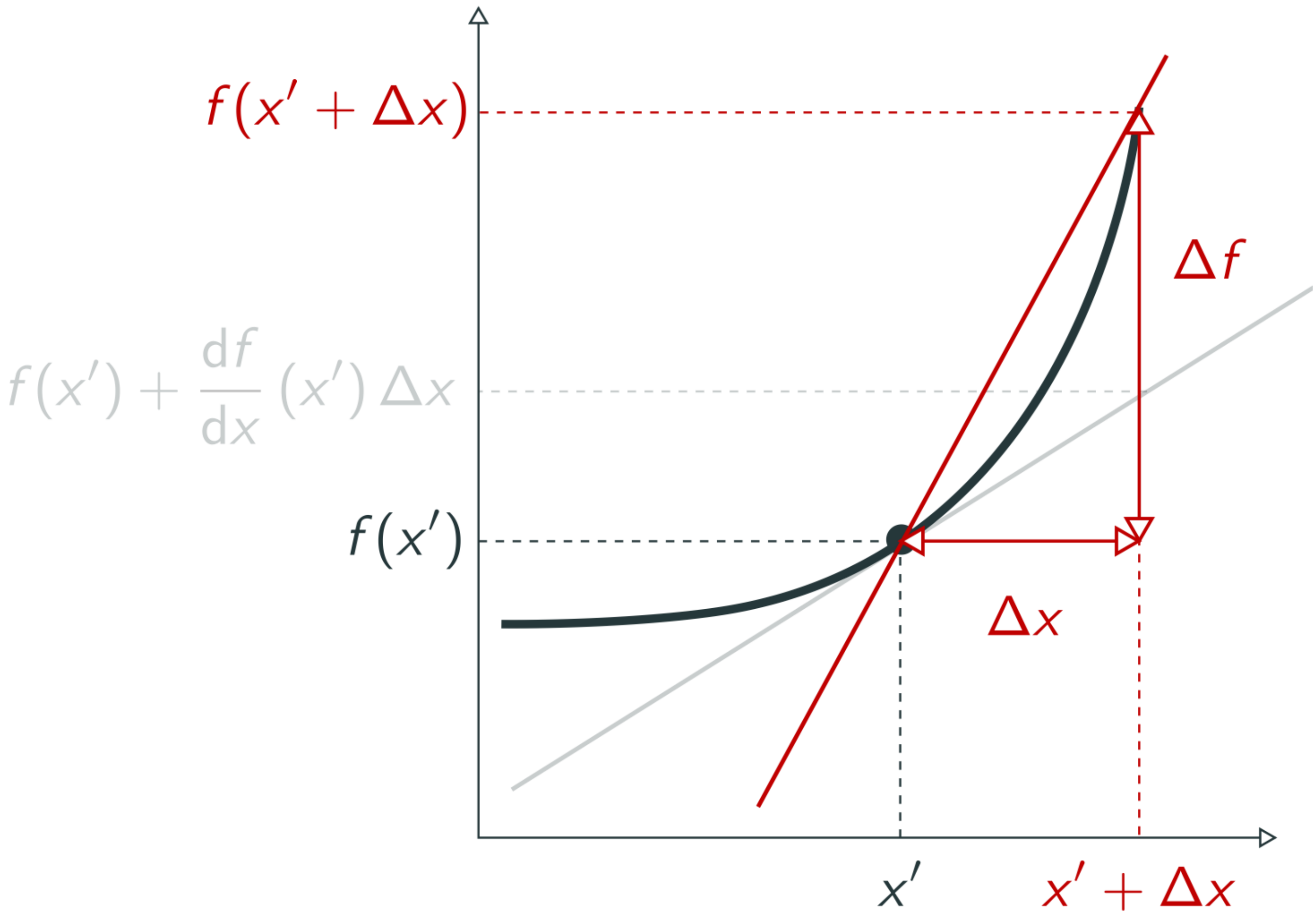
Parametry?
Žádné!





Numerický gradient

Aproximace derivace dopřednou diferencí



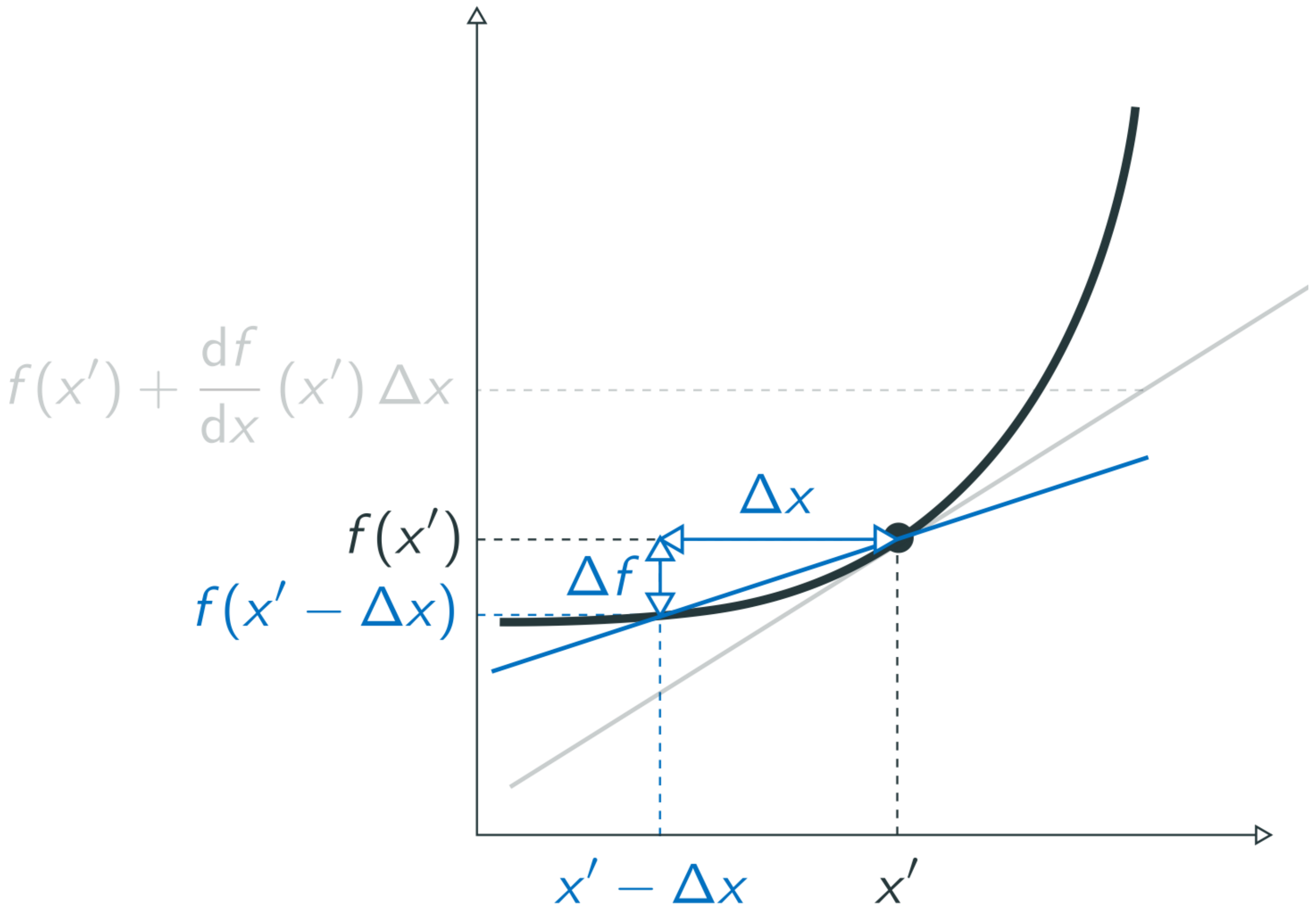
Derivace:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x}$$

Aproximace dopředně:

$$\frac{df}{dx} \approx \frac{f(x' + \Delta x) - f(x')}{\Delta x}$$

Aproximace derivace zpětnou diferencí



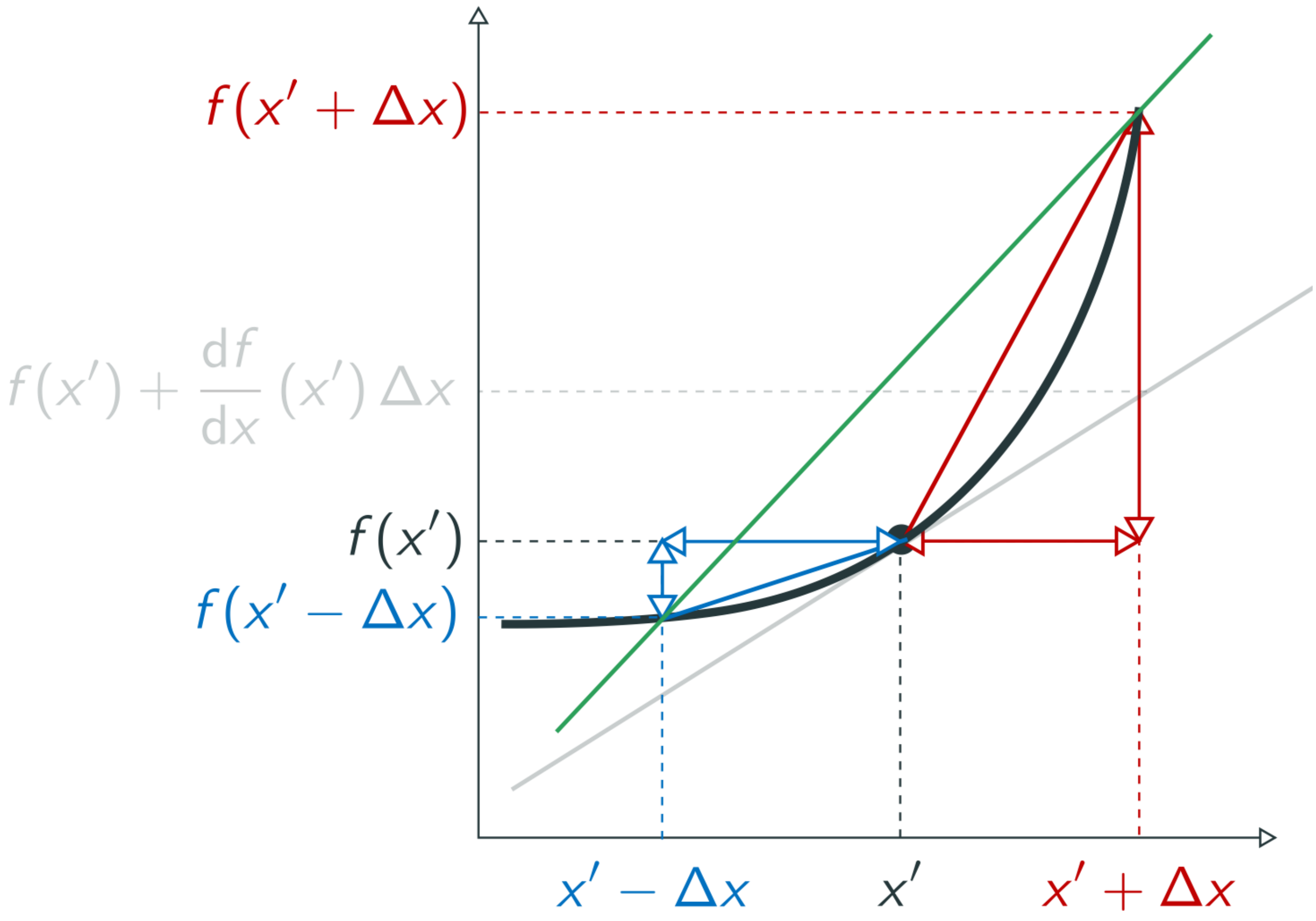
Derivace:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x}$$

Aproximace zpětně:

$$\frac{df}{dx} \approx \frac{f(x') - f(x' + \Delta x)}{\Delta x}$$

Aproximace derivace centrální diferencí



Derivace:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x}$$

Aproximace centrálně:

$$\frac{df}{dx} \approx \frac{f(x' + \Delta x) - f(x' - \Delta x)}{\Delta x}$$

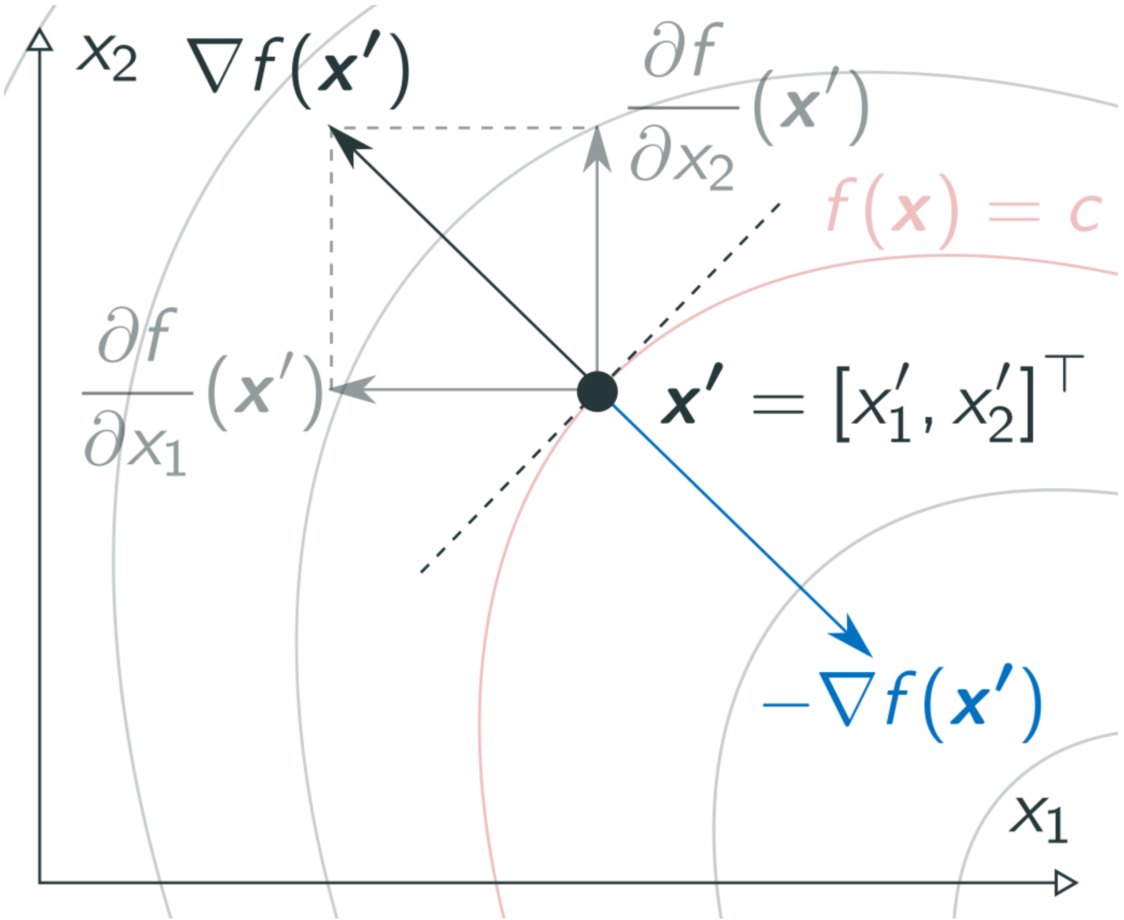
výhodou menší chyba aproximace $O(\Delta x^2)$ → častější použití než jednostranné

Aproximace ve více rozměrech

- Gradient je vektor parciálních derivací

$$\nabla f(x') = \left[\frac{\partial f}{\partial x_1}(x_1'), \dots, \frac{\partial f}{\partial x_D}(x_D')\right]^\top$$

- Aproximace tedy nutné provést **pro každou** proměnnou funkce f



Příklad aproximace derivace numerickou diferencí

$$f(\boldsymbol{x}) = \sum_{d=1}^{D} x_d^2 \qquad \boldsymbol{x} = [1.0, 0.8, 1.3]^\top$$

numerický odhad:

$$\widehat{\nabla f(x)} = \begin{bmatrix} \frac{f(x_1 + \Delta x, x_2, x_3) - f(x_1, x_2, x_3)}{\Delta x} \\ \frac{f(x_1, x_2 + \Delta x, x_3) - f(x_1, x_2, x_3)}{\Delta x} \\ \frac{f(x_1, x_2, x_3 + \Delta x) - f(x_1, x_2, x_3)}{\Delta x} \end{bmatrix} = \begin{bmatrix} \frac{f(1.0 + 0.001, 0.8, 1.3) - f(1.0, 0.8, 1.3)}{0.001} \\ \frac{f(1.0, 0.8 + 0.001, 1.3) - f(1.0, 0.8, 1.3)}{0.001} \\ \frac{f(1.0, 0.8, 1.3 + 0.001) - f(1.0, 0.8, 1.3)}{0.001} \end{bmatrix} = \begin{bmatrix} 2.001 \\ 1.601 \\ 2.601 \end{bmatrix}$$

skutečný gradient:

$$\nabla f(\boldsymbol{x}) = [2x_1, 2x_2, 2x_3]^\top = [2.0, 1.6, 2.6]^\top$$

hluboké neurosítě bežně miliony parametrů → pro vyčíslení gradientu nutné vyhodnotit jejich výstup min. jednou pro každý parametr a to v každém kroku gradient descentu!

Centrální diference v numpy

```
def eval_numerical_gradient_array(f, x, df, h=1e-5):
    grad = np.zeros_like(x)
    it = np.nditer(x, flags=['multi_index'], op_flags=['readwrite'])
    while not it.finished:
        ix = it.multi_index

        oldval = x[ix]
        x[ix] = oldval + h
        pos = f(x).copy()
        x[ix] = oldval - h
        neg = f(x).copy()
        x[ix] = oldval

        grad[ix] = np.sum((pos - neg) * df) / (2 * h)
        it.iternext()
        return grad
```

http://cs231n.github.io/

Kontrola gradient (gradient check)

- Numerická aproximace je sice **pomalá**, ale vždy až na toleranci **správná** → vhodná **pouze pro kontrolu** implementace backward metody
- V příkladu vyšlo

$$\widehat{\nabla f(\boldsymbol{x})} = [2.001, 1.601, 2.601]^T$$
$$\nabla f(\boldsymbol{x}) = [2.0, 1.6, 2.6]^T$$

- Relativní chyba

$$\delta = \max \frac{\left|\widehat{\nabla f(\boldsymbol{x})} - \nabla f(\boldsymbol{x})\right|}{\left|\widehat{\nabla f(\boldsymbol{x})}\right| + |\nabla f(\boldsymbol{x}))|} = \max\left(\frac{0.001}{4.001}, \frac{0.001}{3.201}, \frac{0.001}{5.201}\right) = 3.124 \cdot 10^{-4}$$

- Kód v numpy z předmetu cs231n Stanfordovy univerzity:

```
>>> def rel_error(x, y):
>>>     return np.max(np.abs(x - y) / (np.maximum(1e-8, np.abs(x) + np.abs(y))))
>>> rel_error(np.array([2.001, 1.601, 2.601]), np.array([2.0, 1.6, 2.6]))
0.00031240237425800993
```

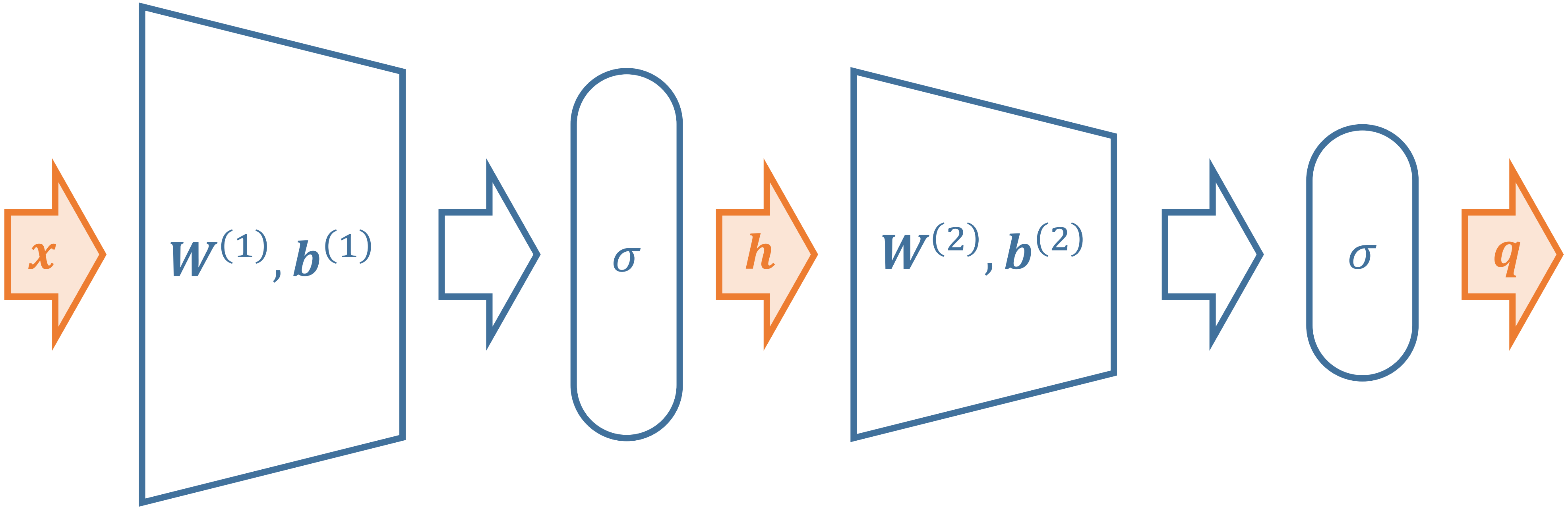
Vícevrstvé sítě

Vícevrstvý perceptron

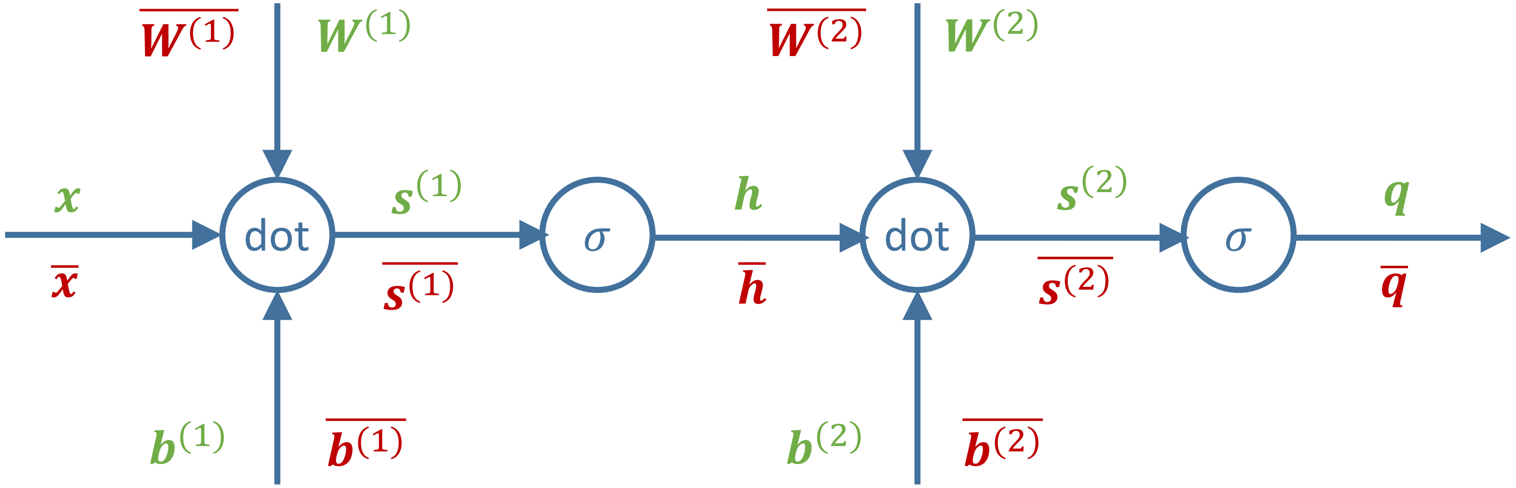
- Bloky s definovaným forward a backward chováním lze libovolně skládat za sebe
- Např. dvouvrstvý perceptron

$$\boldsymbol{q} = \sigma\{\boldsymbol{W}^{(2)}\boxed{\sigma(\boldsymbol{W}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)})} + \boldsymbol{b}^{(2)}\}$$

$\boldsymbol{h}$ … skrytá reprezentace



Vícevrstvý perceptron



forward:

$\boldsymbol{x}$

$$\boldsymbol{s}^{(1)} \leftarrow \boldsymbol{W}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)}$$

$$\boldsymbol{h} \leftarrow \sigma\left(\boldsymbol{s}^{(1)}\right)$$

$$\boldsymbol{s}^{(2)} \leftarrow \boldsymbol{W}^{(2)}\boldsymbol{h} + \boldsymbol{b}^{(2)}$$

$$\boldsymbol{q} \leftarrow \sigma\left(\boldsymbol{s}^{(2)}\right)$$

backward:

$$\overline{\boldsymbol{x}} \leftarrow \boldsymbol{W}^{(1)\top}\overline{\boldsymbol{s}^{(1)}}$$

$$\overline{\boldsymbol{W}^{(1)}} \leftarrow \overline{\boldsymbol{s}^{(1)}}\boldsymbol{h}^{\top}$$

$$\overline{\boldsymbol{b}^{(1)}} \leftarrow \overline{\boldsymbol{s}^{(1)}}$$

$$\overline{\boldsymbol{s}^{(1)}} \leftarrow \boldsymbol{h}(1-\boldsymbol{h})\overline{\boldsymbol{h}}$$

$$\overline{\boldsymbol{h}} \leftarrow \boldsymbol{W}^{(2)\top}\overline{\boldsymbol{s}^{(2)}}$$

$$\overline{\boldsymbol{W}^{(2)}} \leftarrow \overline{\boldsymbol{s}^{(2)}}\boldsymbol{h}^{\top}$$

$$\overline{\boldsymbol{b}^{(2)}} \leftarrow \overline{\boldsymbol{s}^{(2)}}$$

$$\overline{\boldsymbol{s}^{(2)}} \leftarrow \boldsymbol{q}(1-\boldsymbol{q})\overline{\boldsymbol{q}}$$

$\overline{\boldsymbol{q}}$

Dvouvrstvý perceptron v numpy na 11 řádků

```
X = np.array([[0, 0, 1], [0, 1, 1], [1, 0, 1], [1, 1, 1]])
y = np.array([[0, 1, 1, 0]]).T
syn0 = 2*np.random.random((3, 4)) - 1
syn1 = 2*np.random.random((4, 1)) - 1
for j in xrange(60000):
    l1 = 1 / (1 + np.exp(-(np.dot(X, syn0))))
    l2 = 1 / (1 + np.exp(-(np.dot(l1, syn1))))
    l2_delta = (y - l2) * (l2 * (1 - l2))
    l1_delta = l2_delta.dot(syn1.T) * (l1 * (1 - l1))
    syn1 += l1.T.dot(l2_delta)
    syn0 += X.T.dot(l1_delta)
```

http://iamtrask.github.io/2015/07/12/basic-python-network/