165B
Machine Learning
Backpropagation

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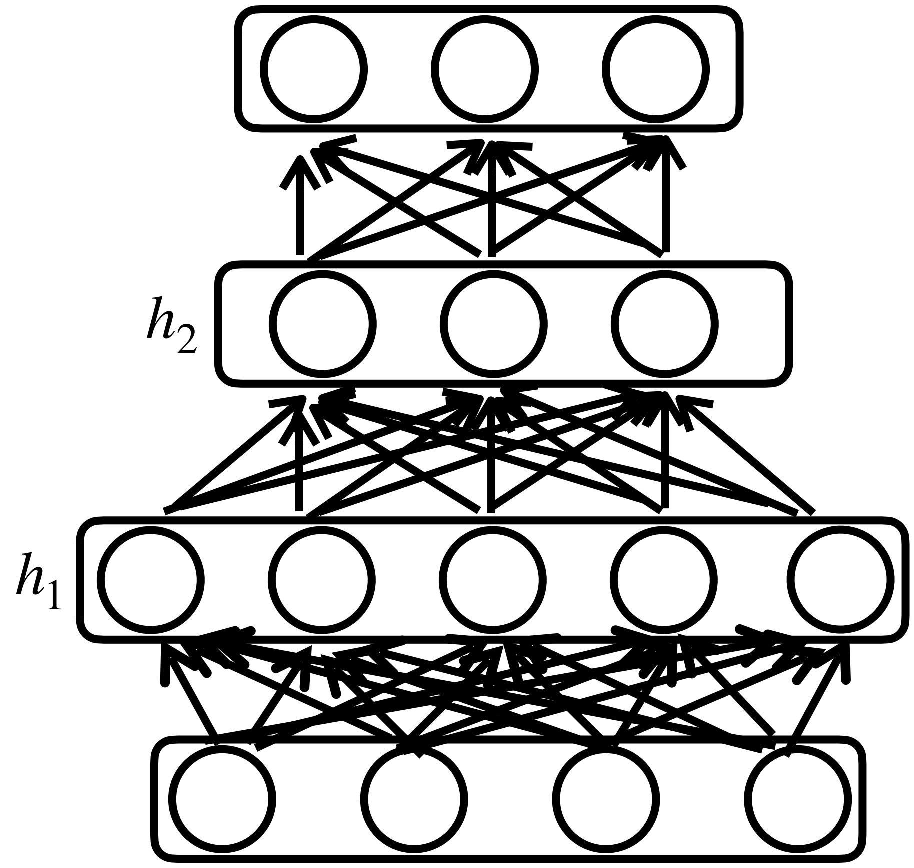
Acknowledgement: Slides borrowed from Bhiksha Raj's 11485 and Mu Li & Alex Smola's 157 courses on Deep Learning, with modification

Recap

- Feedforward network (also Multilayer Perceptron)
- Empirical Risk minimization framework for learning
- Loss function for classification and regression
- First-order optimality condition: gradient=0
- Gradient descent is an iterative algorithm to update the parameter towards the opposite direction of gradient

Feedforward Neural Net (FFN)

- also known as multilayer perceptron (MLP)
- Layers are connected sequentially
- Each layer has full-connection (each unit is connected to all units of next layer)
  - Linear project followed by
  - an element-wise nonlinear activation function
- There is no connection from output to input



Empirical Risk Minimization

- The expected risk is the average risk (loss) over the entire (x, y) data space

$$R(\theta) = E_{\langle x,y \rangle \in P}\left[\ell(y, f(x;\theta))\right] = \int \ell(y, f(x;\theta))dP(x,y)$$

- Instead, given a training set of empirical data $D = \{(x_n, y_n)\}_{n=1}^{N}$
- Minimize the empirical risk over training data

$$\hat{\theta} \leftarrow \arg\min_{\theta} L(\theta) = \frac{1}{N}\sum_{n} \ell(y_n, f(x_n;\theta))$$

Gradient Descent

- Update rule: $x_{t+1} = x_t - \eta \nabla f|_{x_t}$
- η is a hyper-parameter to control the learning rate

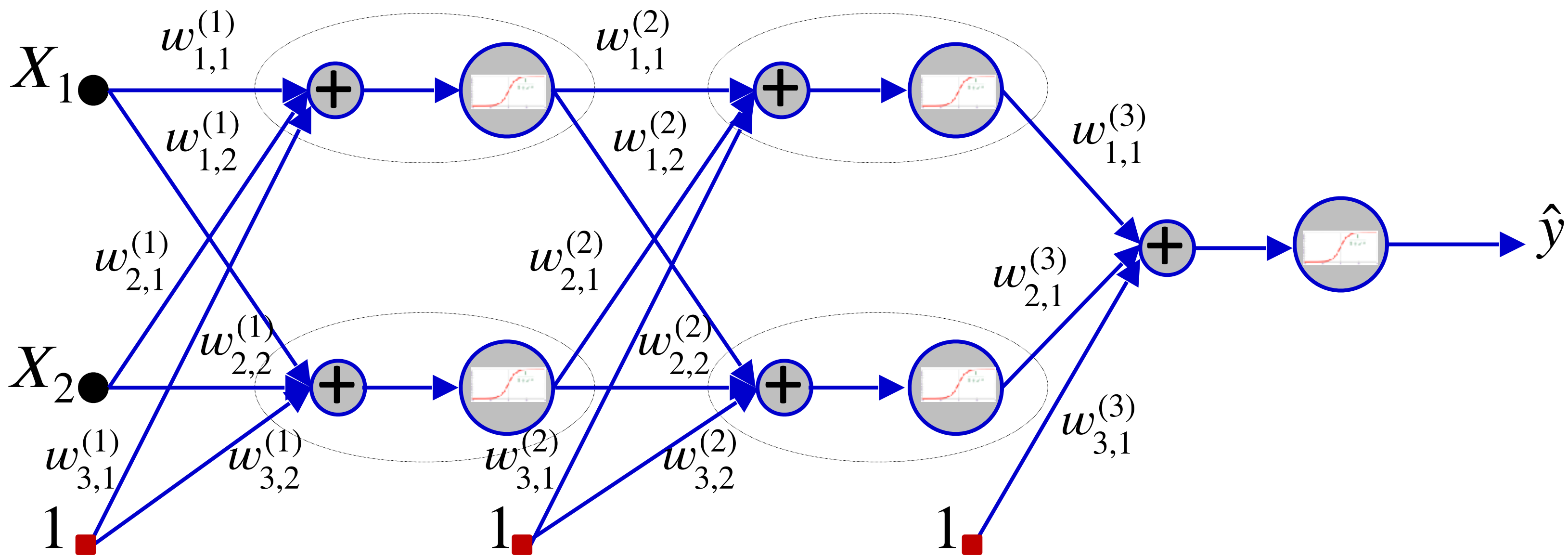
Computing Gradient for Neural Net

- Forward and back-propagation
- Suppose y=f(x), z=g(y), therefore z=g(f(x))
- Use the chain rule,

$$\nabla g(f(x))\,|_x = (\nabla f\,|_x)^T \cdot \nabla g\,|_y$$

- For a neural net and its loss $\ell(\theta)$
- First compute gradient with respect to last layer
- then using chain-rule to back propagate to second last, and so on

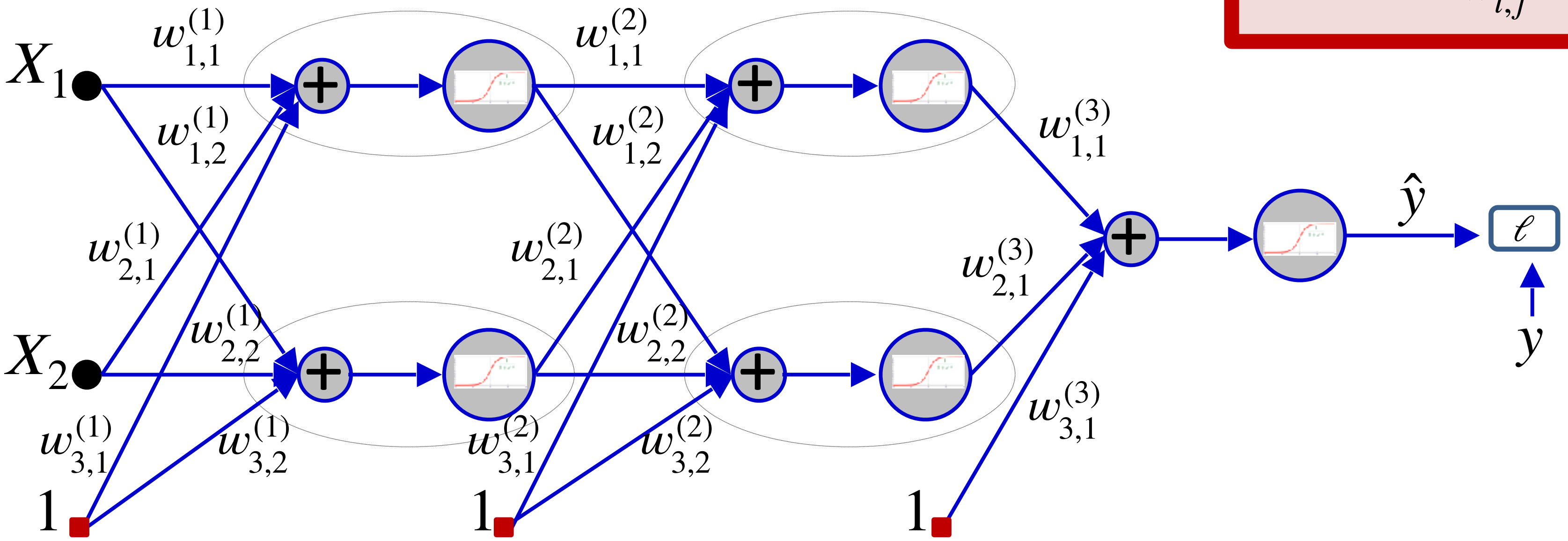
Example



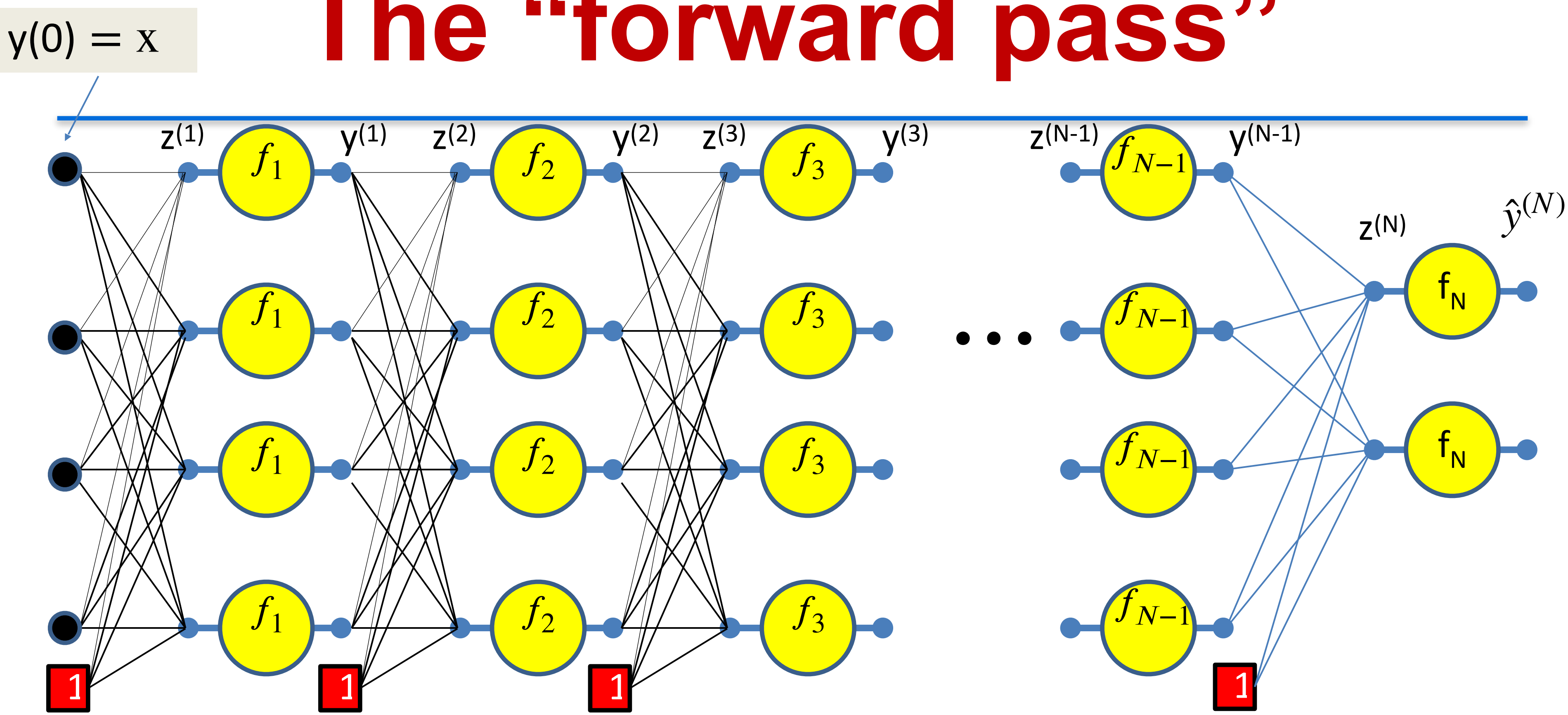
X_1
X_2
1
1
1
$w^{(1)}_{1,1}$
$w^{(1)}_{1,2}$
$w^{(1)}_{2,1}$
$w^{(1)}_{2,2}$
$w^{(1)}_{3,1}$
$w^{(1)}_{3,2}$
$w^{(2)}_{1,1}$
$w^{(2)}_{1,2}$
$w^{(2)}_{2,1}$
$w^{(2)}_{2,2}$
$w^{(2)}_{3,1}$
$w^{(2)}_{3,2}$
$w^{(3)}_{1,1}$
$w^{(3)}_{2,1}$
$w^{(3)}_{3,1}$
$\hat{y}$

Computing the Gradient

What is: $\dfrac{\partial \ell(y, \hat{y})}{\partial w_{i,j}^{(k)}}$



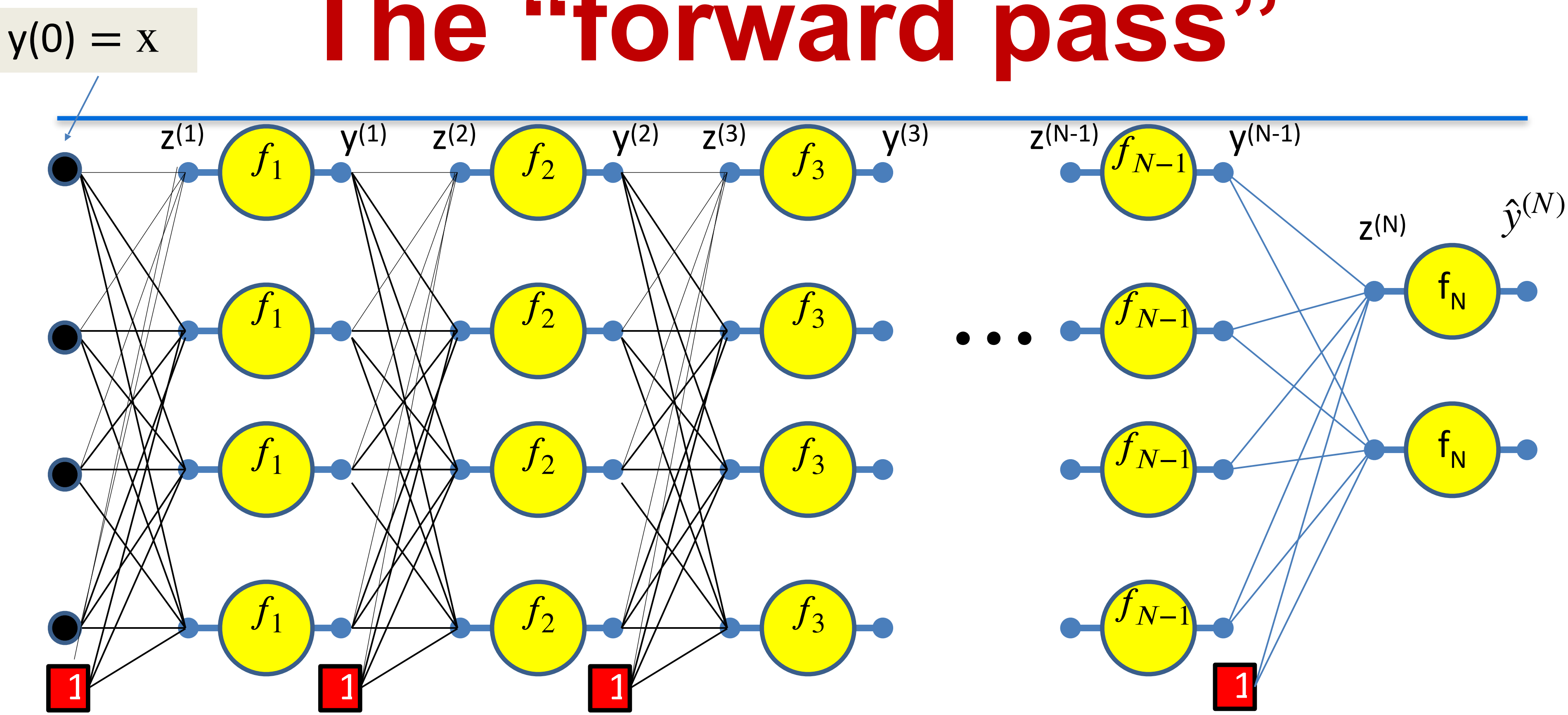
The "forward pass"



We will refer to the process of computing the output from an input as the forward pass

We will illustrate the forward pass in the following slides

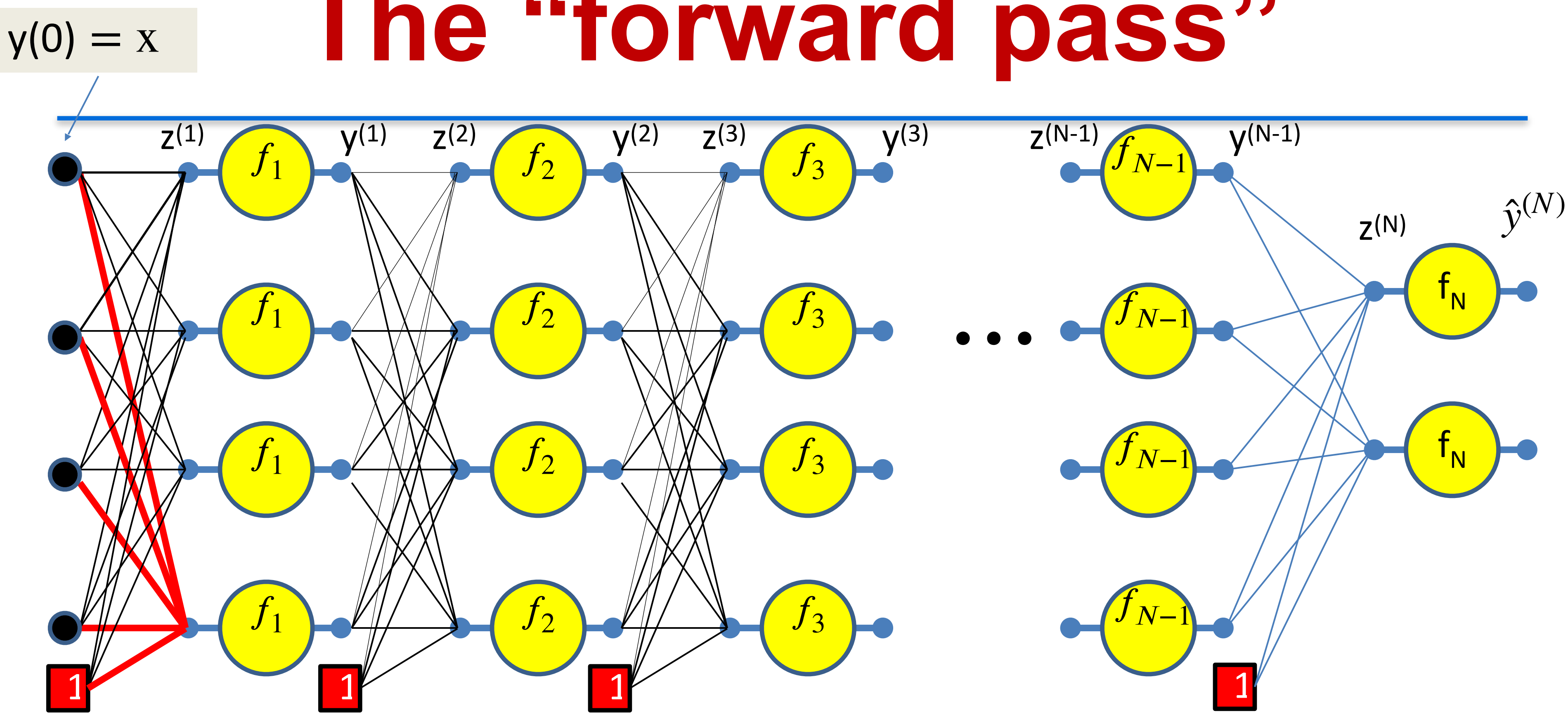
The “forward pass”



Setting $y_i^{(0)} = x_i$ for notational convenience

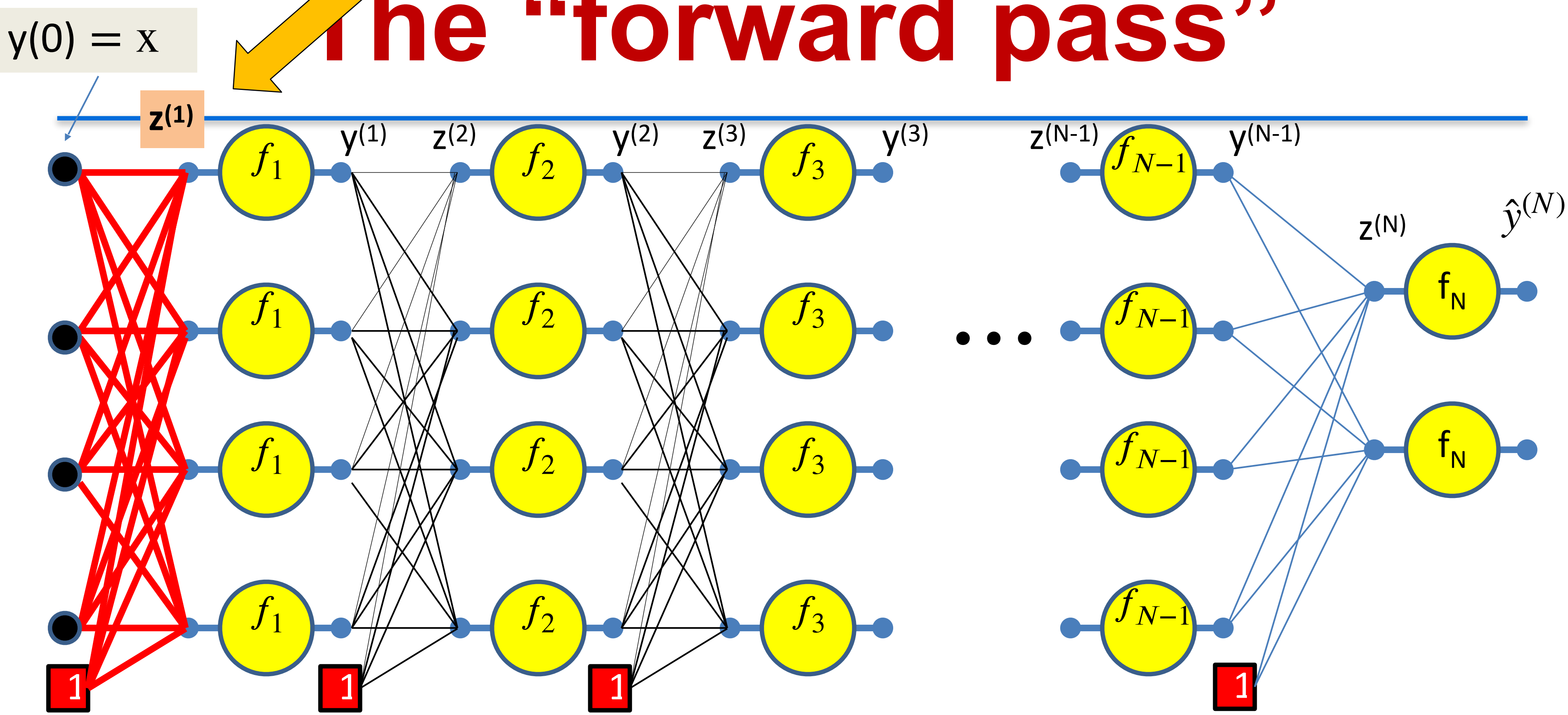
Assuming $w_{0j}^{(k)} = b_j^{(k)}$ and $y_0^{(k)} = 1$ -- assuming the bias is a weight and extending the output of every layer by a constant 1, to account for the biases

The “forward pass”

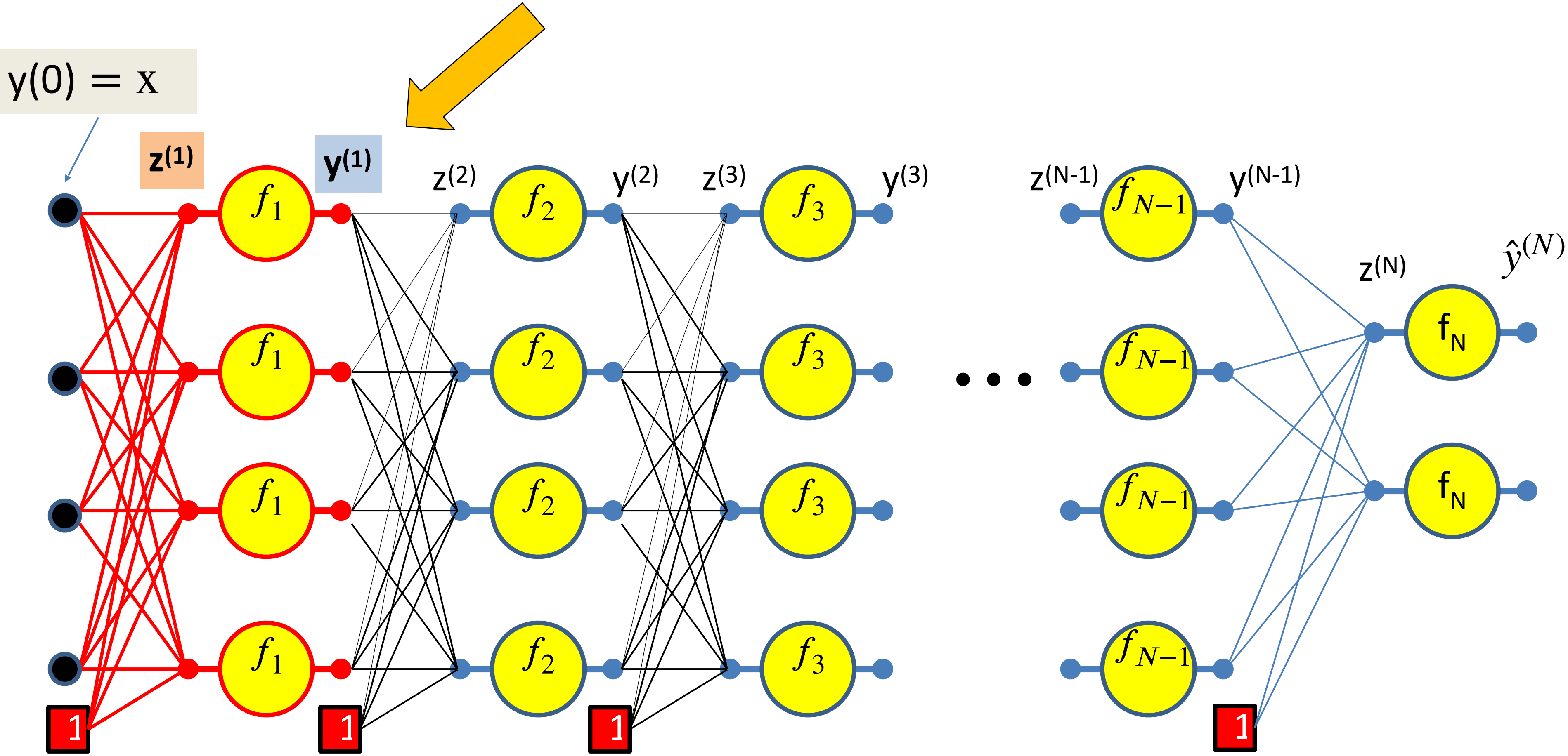


$$z_1^{(1)} = \sum_i w_{i1}^{(1)} y_i^{(0)}$$

The "forward pass"

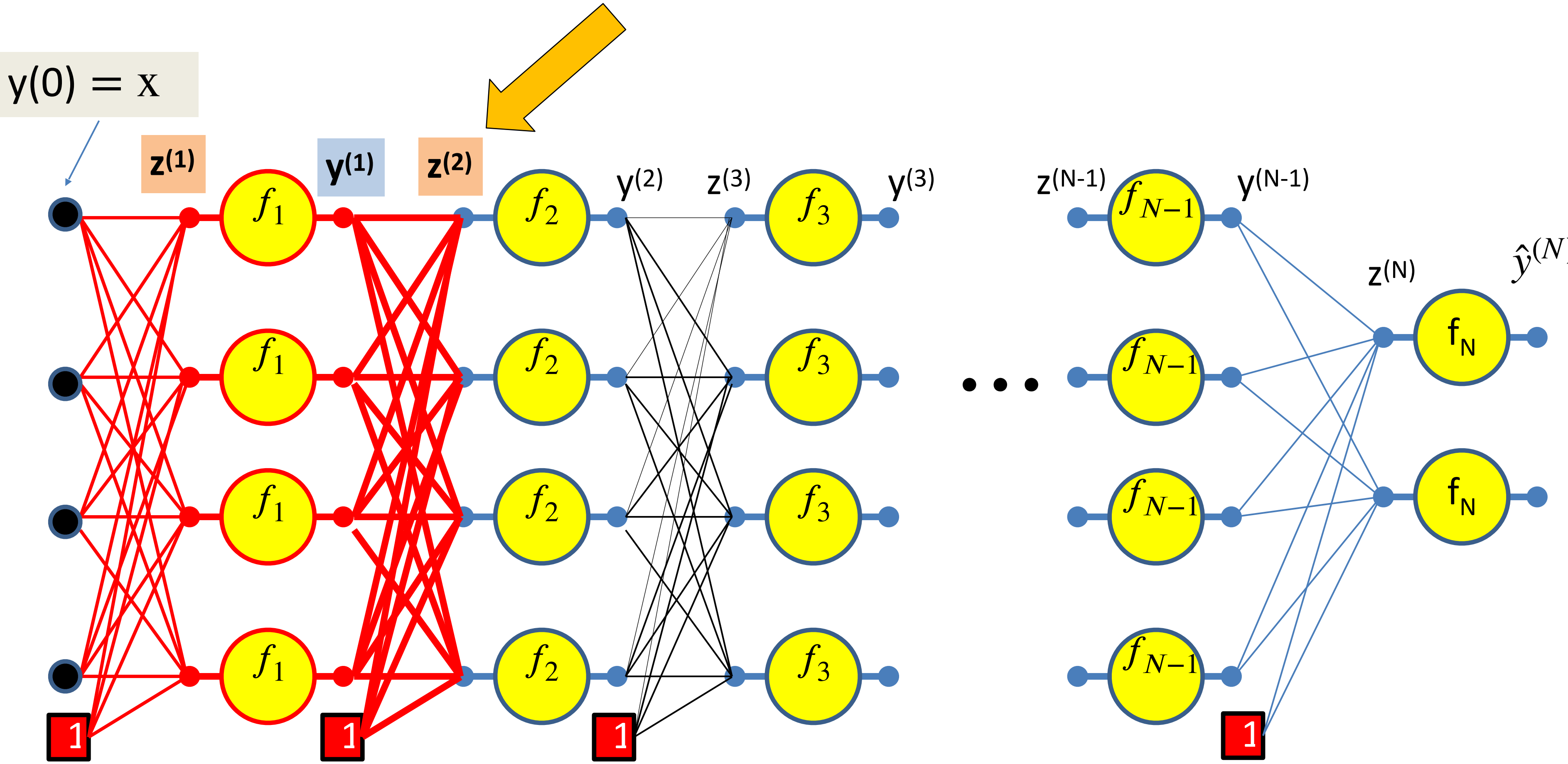


$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

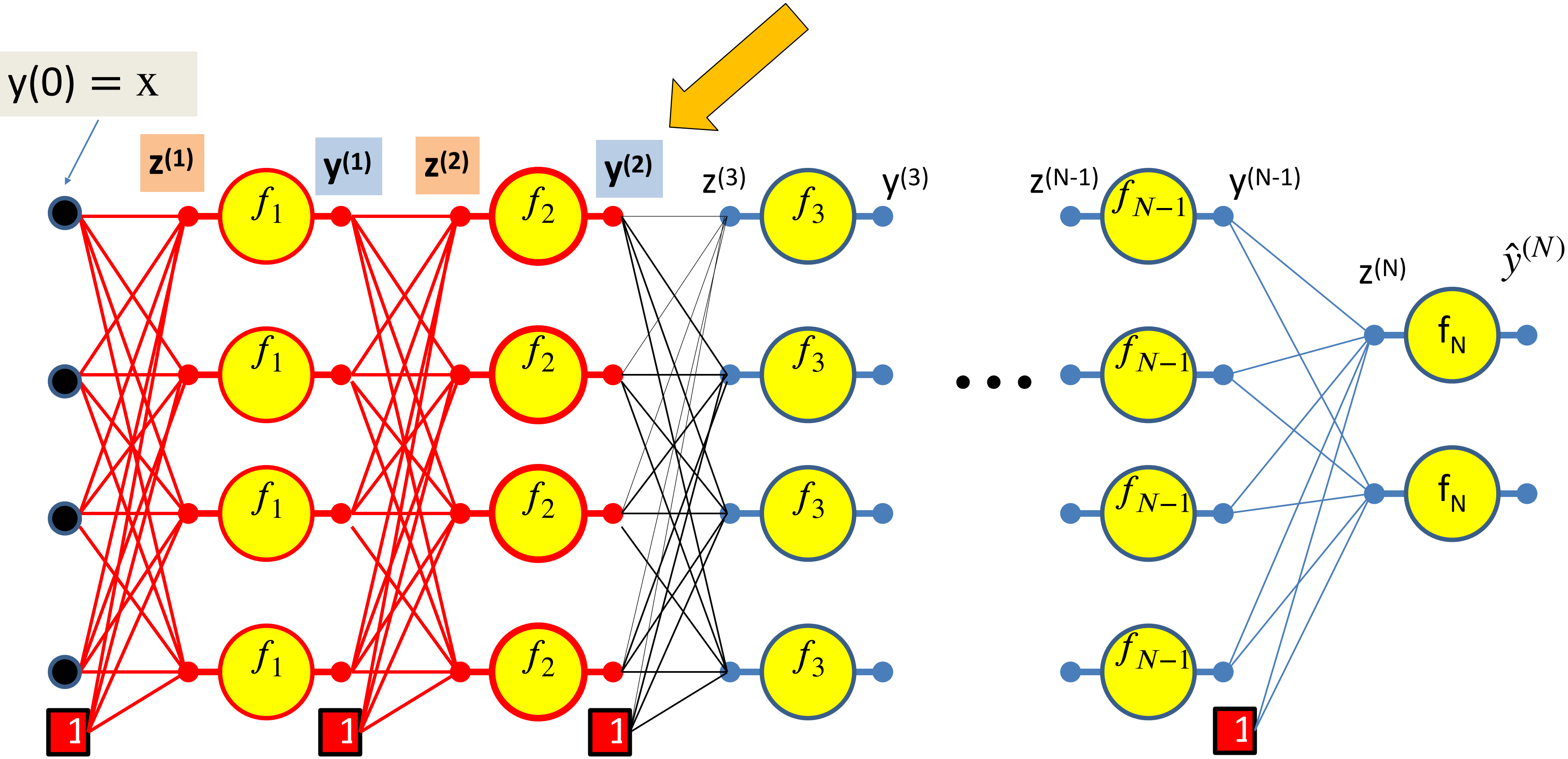
$$\boxed{y_j^{(1)} = f_1\left(z_j^{(1)}\right)}$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1\left(z_j^{(1)}\right)$$

$$\boxed{z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}}$$

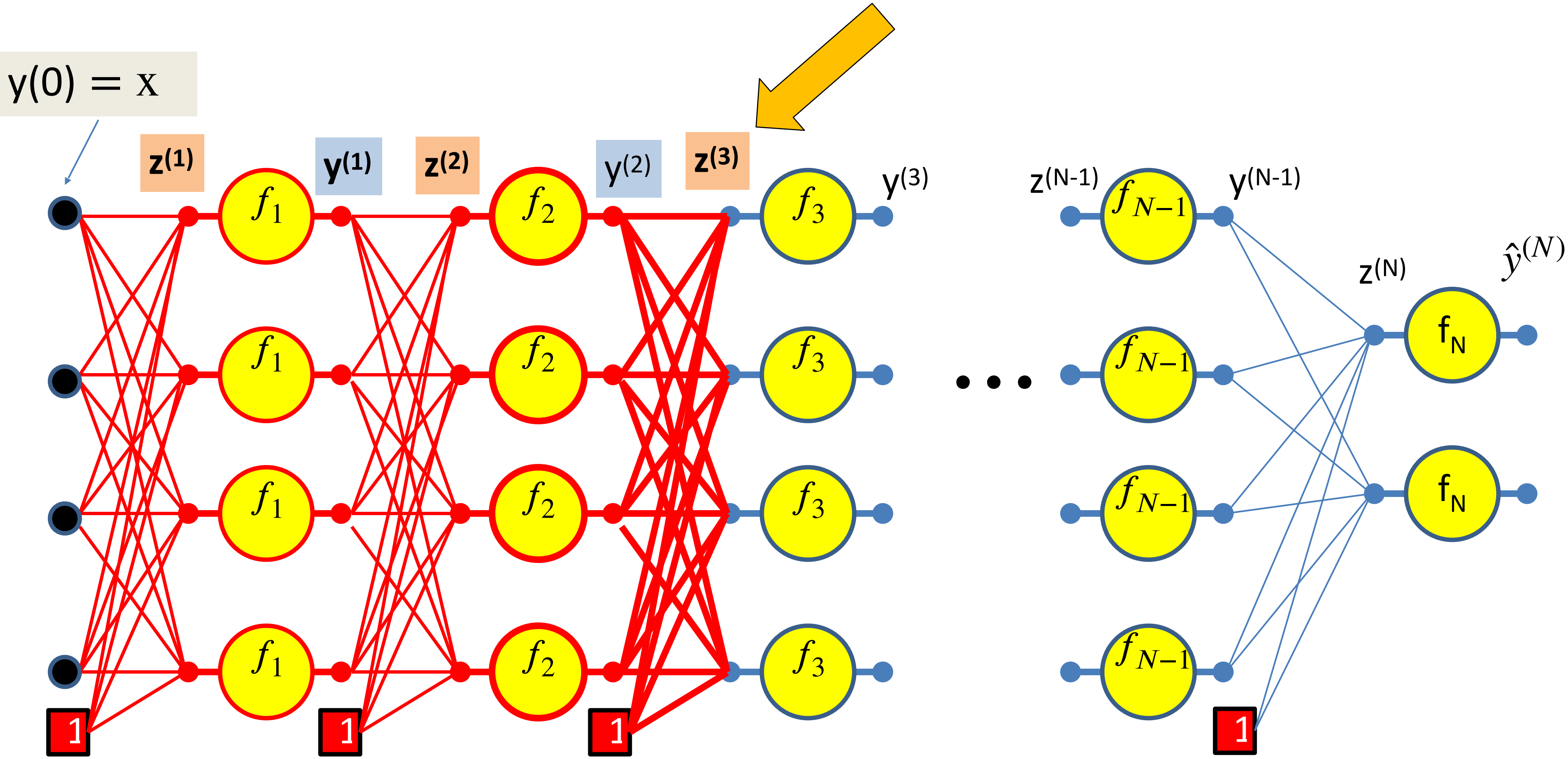


$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1\left(z_j^{(1)}\right)$$

$$z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}$$

$$\boxed{y_j^{(2)} = f_2\left(z_j^{(2)}\right)}$$



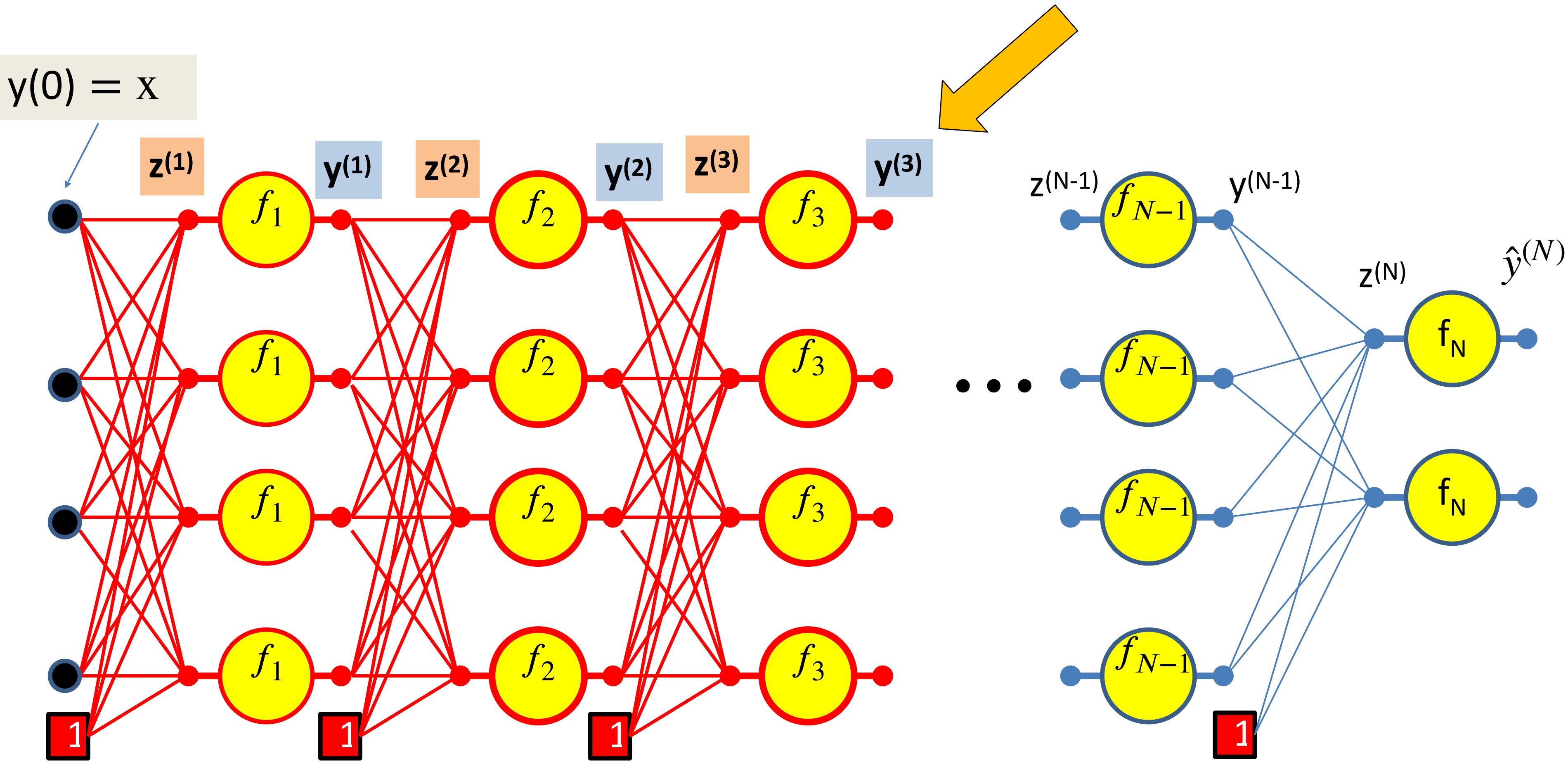
$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1\left(z_j^{(1)}\right)$$

$$z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}$$

$$y_j^{(2)} = f_2\left(z_j^{(2)}\right)$$

$$\boxed{z_j^{(3)} = \sum_i w_{ij}^{(3)} y_i^{(2)}}$$



$$z_j^{(1)} = \sum_i w_{ij}^{(1)} y_i^{(0)}$$

$$y_j^{(1)} = f_1\left(z_j^{(1)}\right)$$

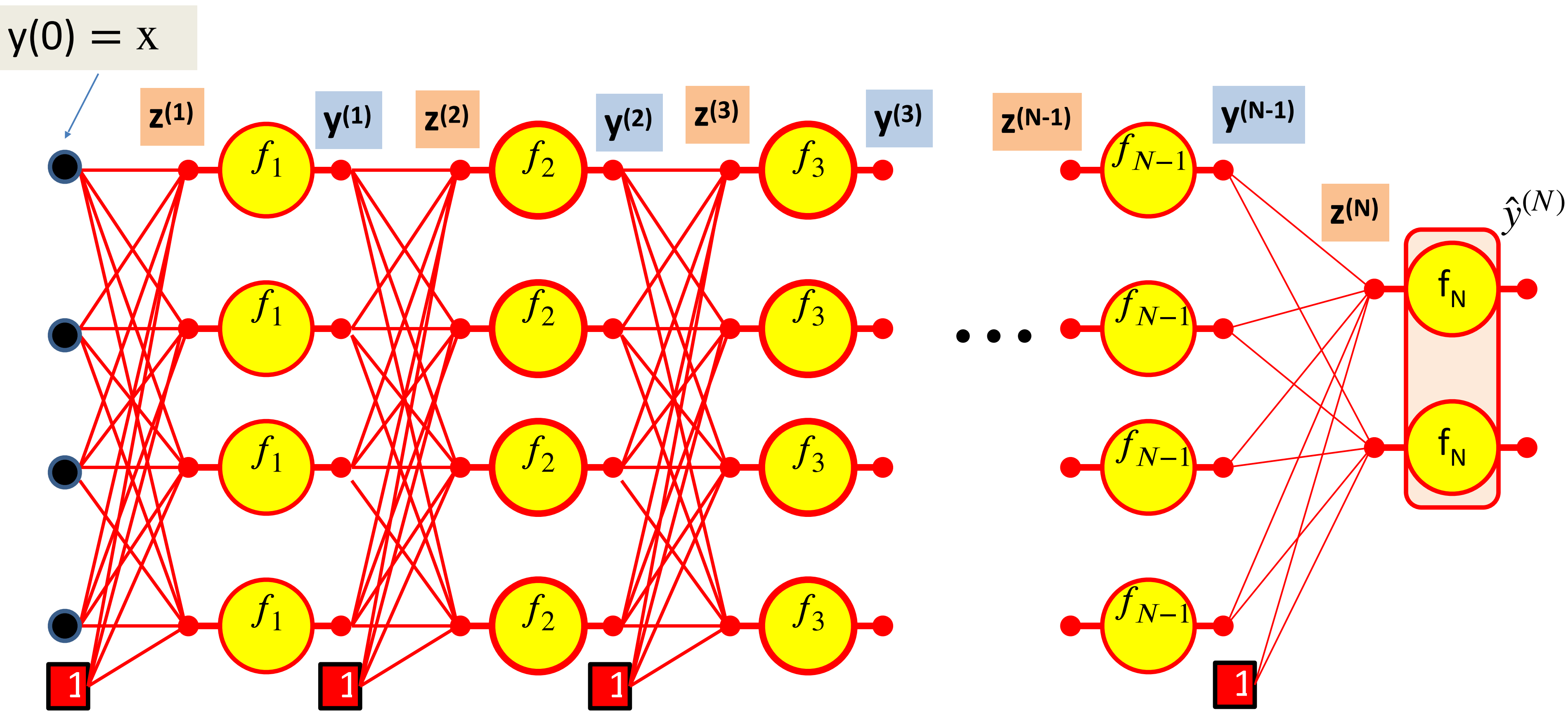
$$z_j^{(2)} = \sum_i w_{ij}^{(2)} y_i^{(1)}$$

$$y_j^{(2)} = f_2\left(z_j^{(2)}\right)$$

...

$$z_j^{(3)} = \sum_i w_{ij}^{(3)} y_i^{(2)}$$

$$\boxed{y_j^{(3)} = f_3\left(z_j^{(3)}\right)}$$



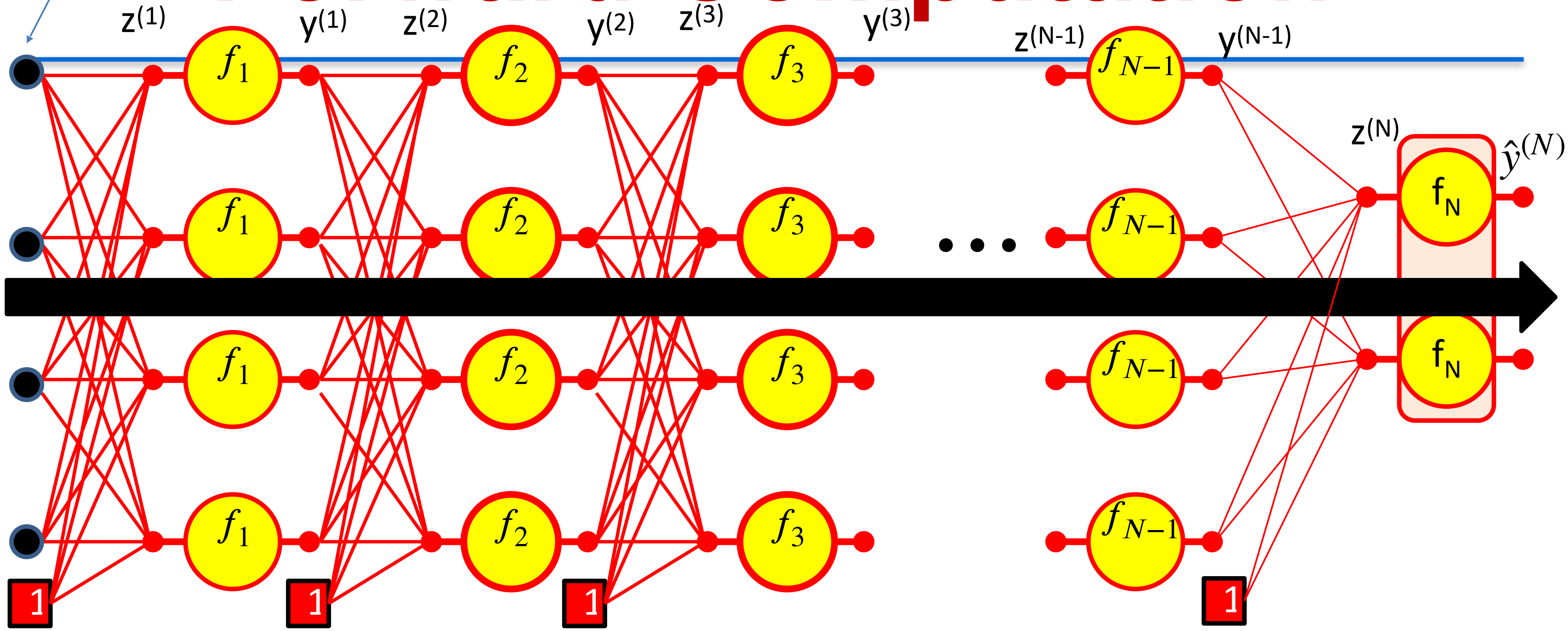
$$y_j^{(N-1)} = f_{N-1}\left(z_j^{(N-1)}\right)$$

$$z_j^{(N)} = \sum_i w_{ij}^{(N)} y_i^{(N-1)}$$

$$\boldsymbol{y}^{(N)} = f_N\left(\boldsymbol{z}^{(N)}\right)$$

Forward Computation

$y(0) = x$



ITERATE FOR k = 1:N

for j = 1:layer-width

$$y_i^{(0)} = x_i$$

$$z_j^{(k)} = \sum_i w_{ij}^{(k)} y_i^{(k-1)}$$

$$y_j^{(k)} = f_k\left(z_j^{(k)}\right)$$

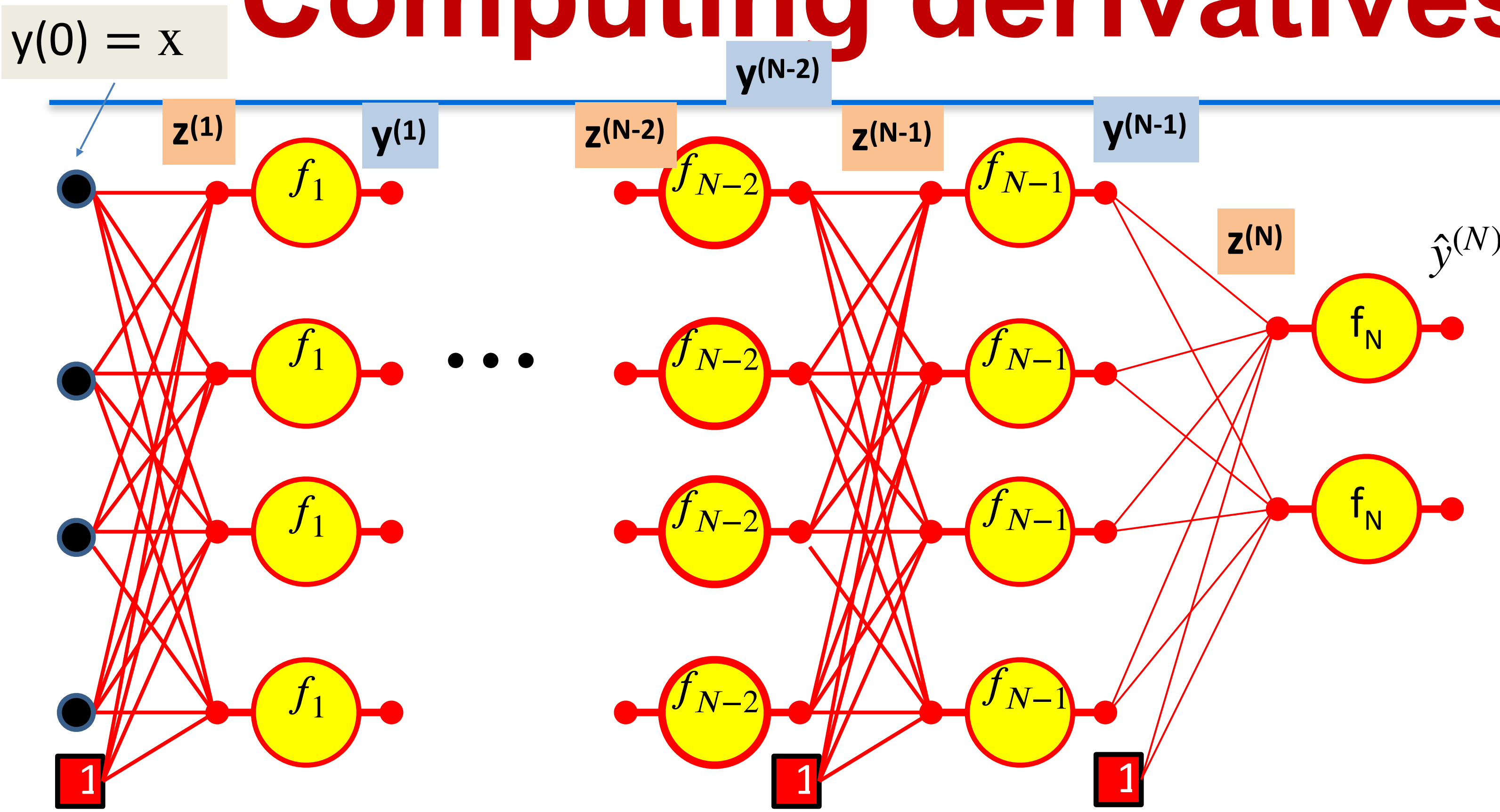
Forward "Pass"

- Input: D dimensional vector $\mathbf{x} = [x_j, \quad j = 1 \ldots D]$
- Set:
  - $D_0 = D,$ is the width of the 0th (input) layer
  - $y_j^{(0)} = x_j, \quad j = 1 \ldots D;$ $\quad y_0^{(k=1 \ldots N)} = x_0 = 1$
- For layer $k = 1 \ldots N$
  - For $j = 1 \ldots D_k$

    D_k is the size of the kth layer

    - $z_j^{(k)} = \sum_{i=0}^{D_{k-1}} w_{i,j}^{(k)} y_i^{(k-1)}$
    - $y_j^{(k)} = f_k\left(z_j^{(k)}\right)$
- Output:
  - $Y = y_j^{(N)}, \; j = 1..D_N$

Computing derivatives



We have computed all these intermediate values in the forward computation

We must remember them – we will need them to compute the derivatives

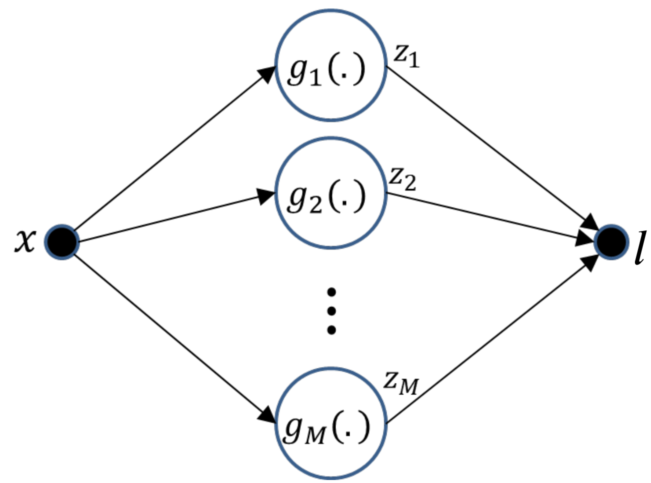
Calculus Refresher: Chain rule

For any nested function $l = f(y)$ where $y = g(z)$

$$\boxed{\frac{dl}{dz} = \frac{dl}{dy}\frac{dy}{dz}}$$

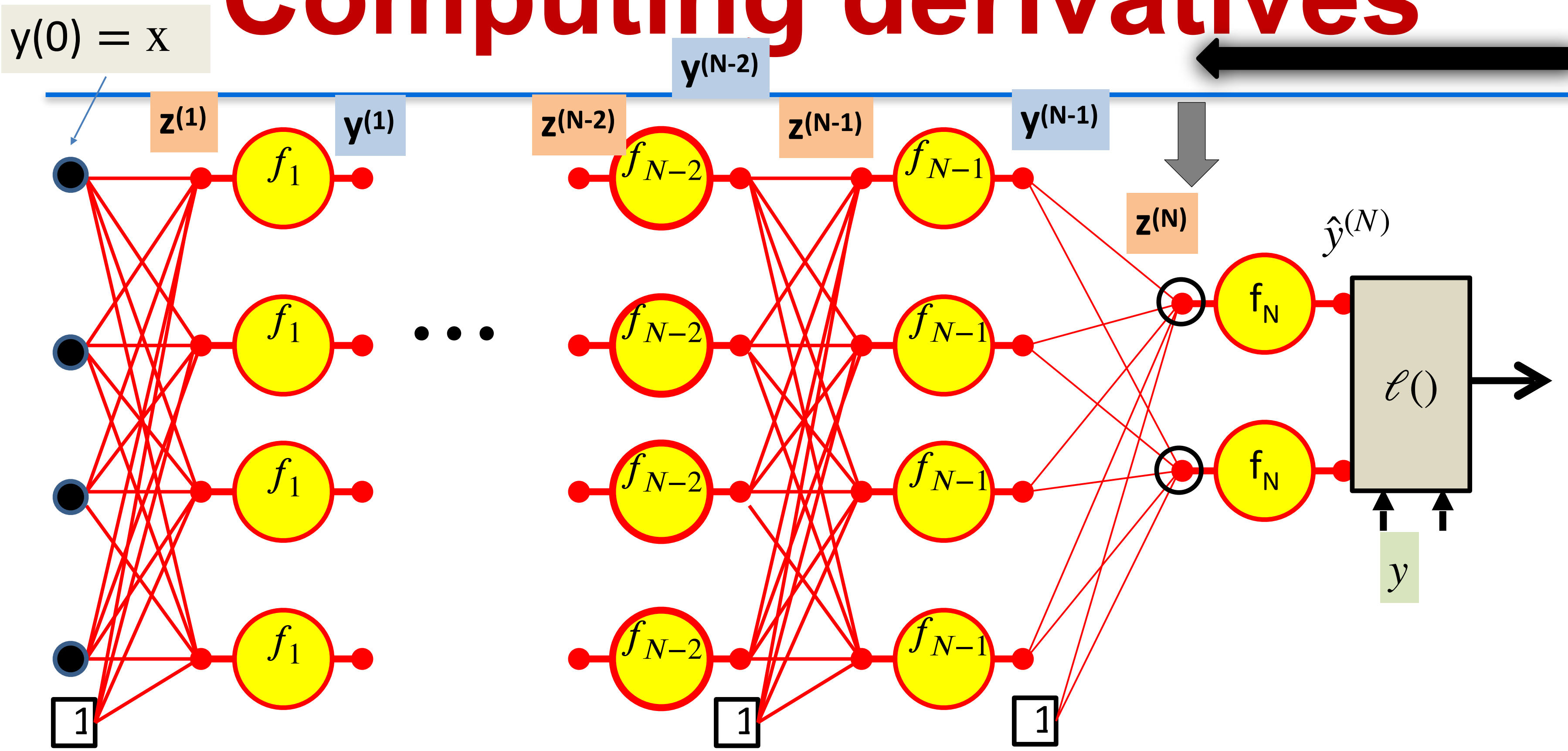
For $l = f(z_1, z_2, \ldots, z_M)$

where $z_i = g_i(x)$

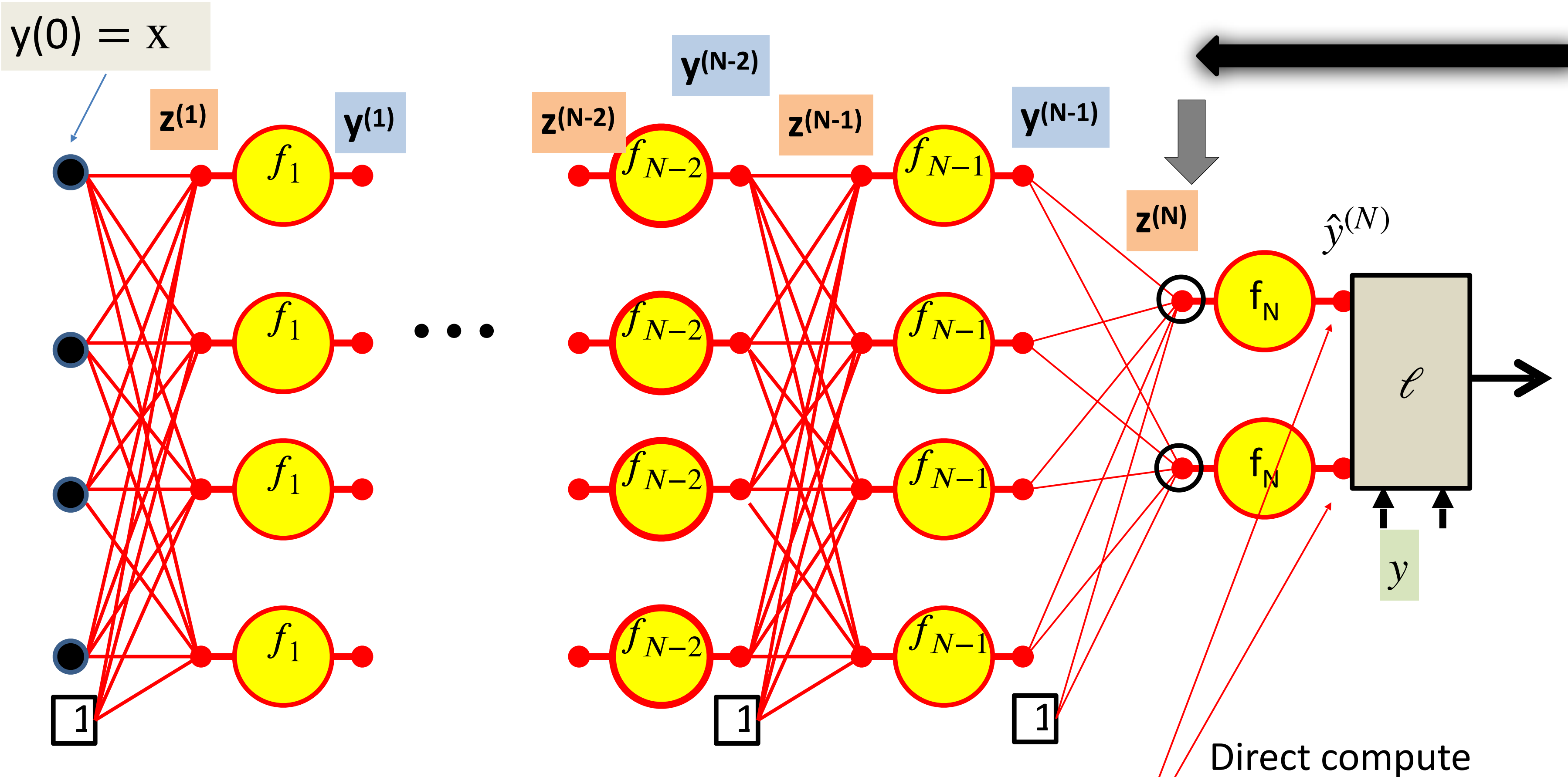


$$\boxed{\frac{dl}{dx} = \frac{\partial l}{\partial z_1}\frac{dz_1}{dx} + \frac{\partial l}{\partial z_2}\frac{dz_2}{dx} + \ldots + \frac{\partial l}{\partial z_M}\frac{dz_M}{dx}}$$

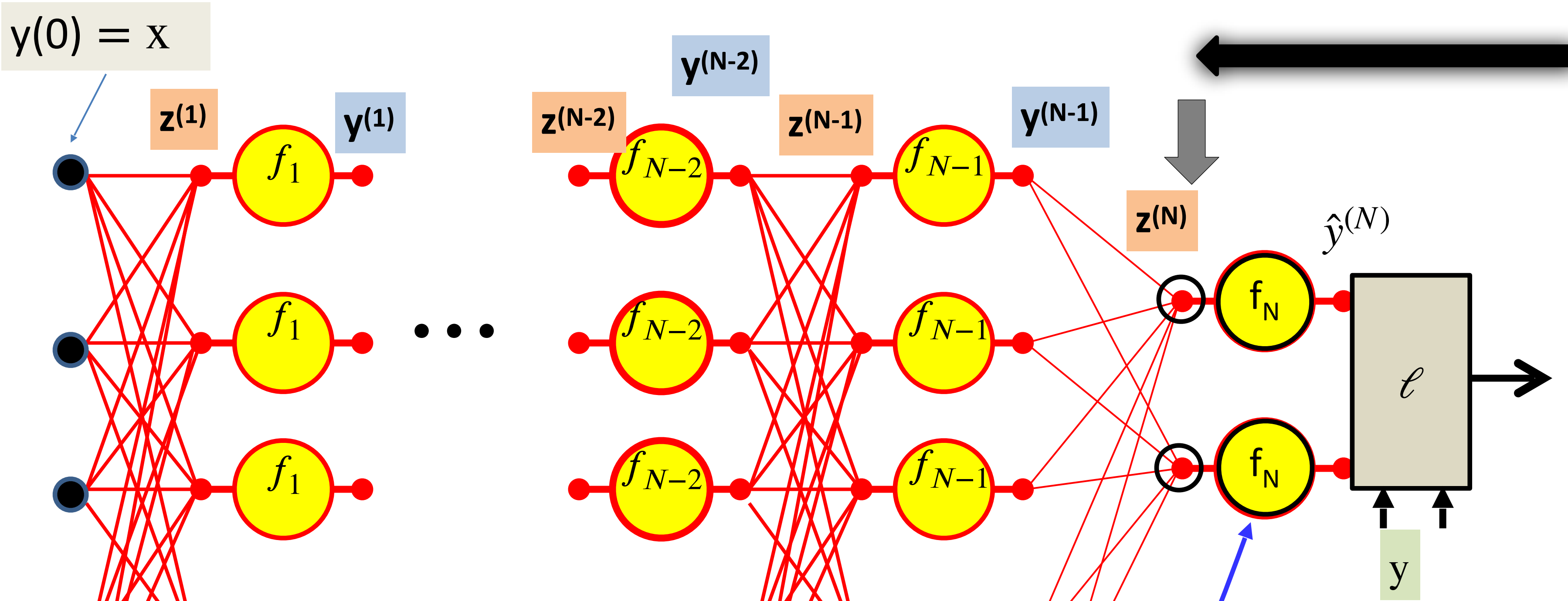
Computing derivatives



$$\frac{\partial \ell}{\partial z_i^{(N)}} = \frac{\partial \hat{y}}{\partial z_i^{(N)}} \frac{\partial \ell}{\partial \hat{y}_i^{(N)}}$$



$$\frac{\partial \ell}{\partial z_i^{(N)}} = \frac{\partial \hat{y}}{\partial z_i^{(N)}} \frac{\partial \ell}{\partial \hat{y}_i^{(N)}}$$

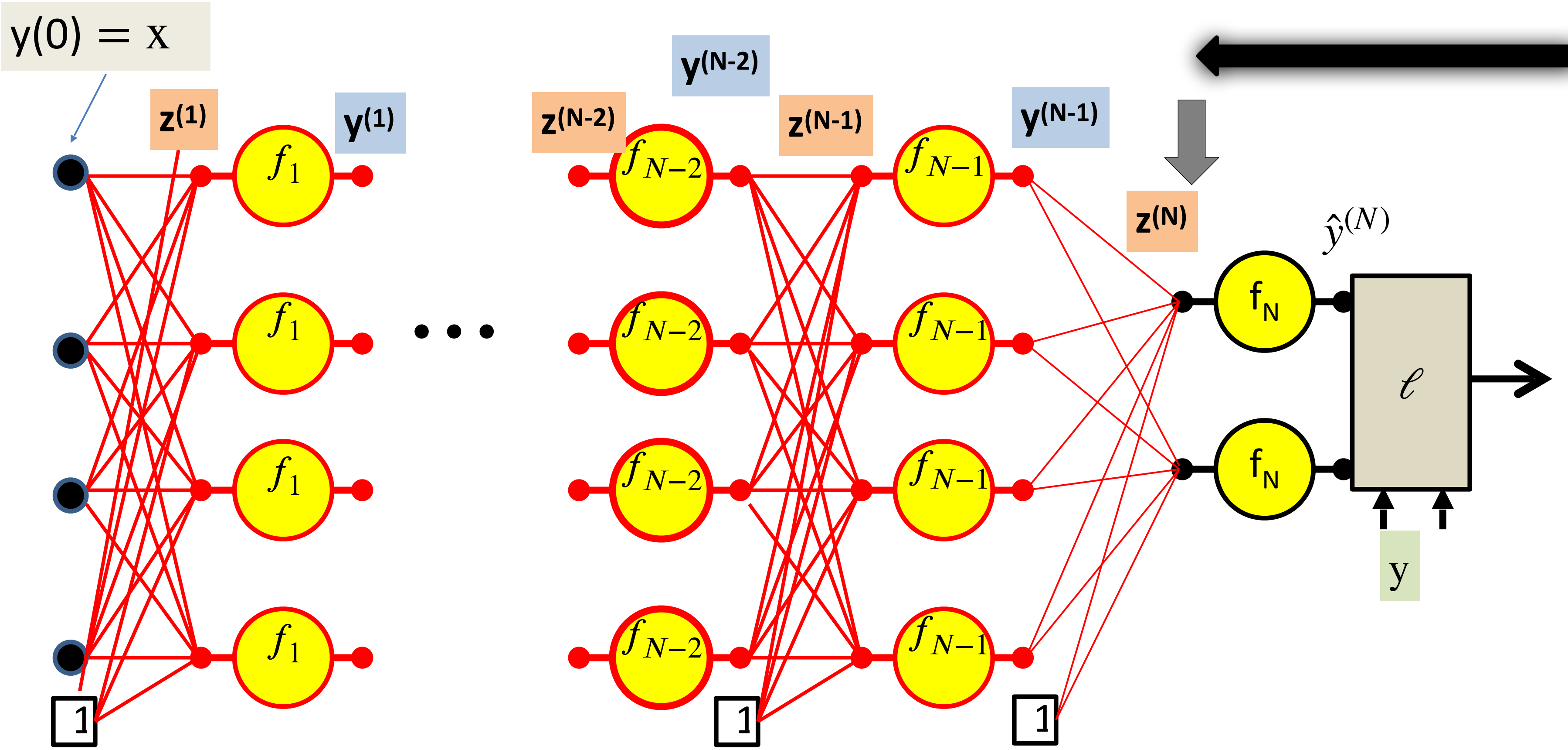


$f'_N\left(z_i^{(N)}\right)$

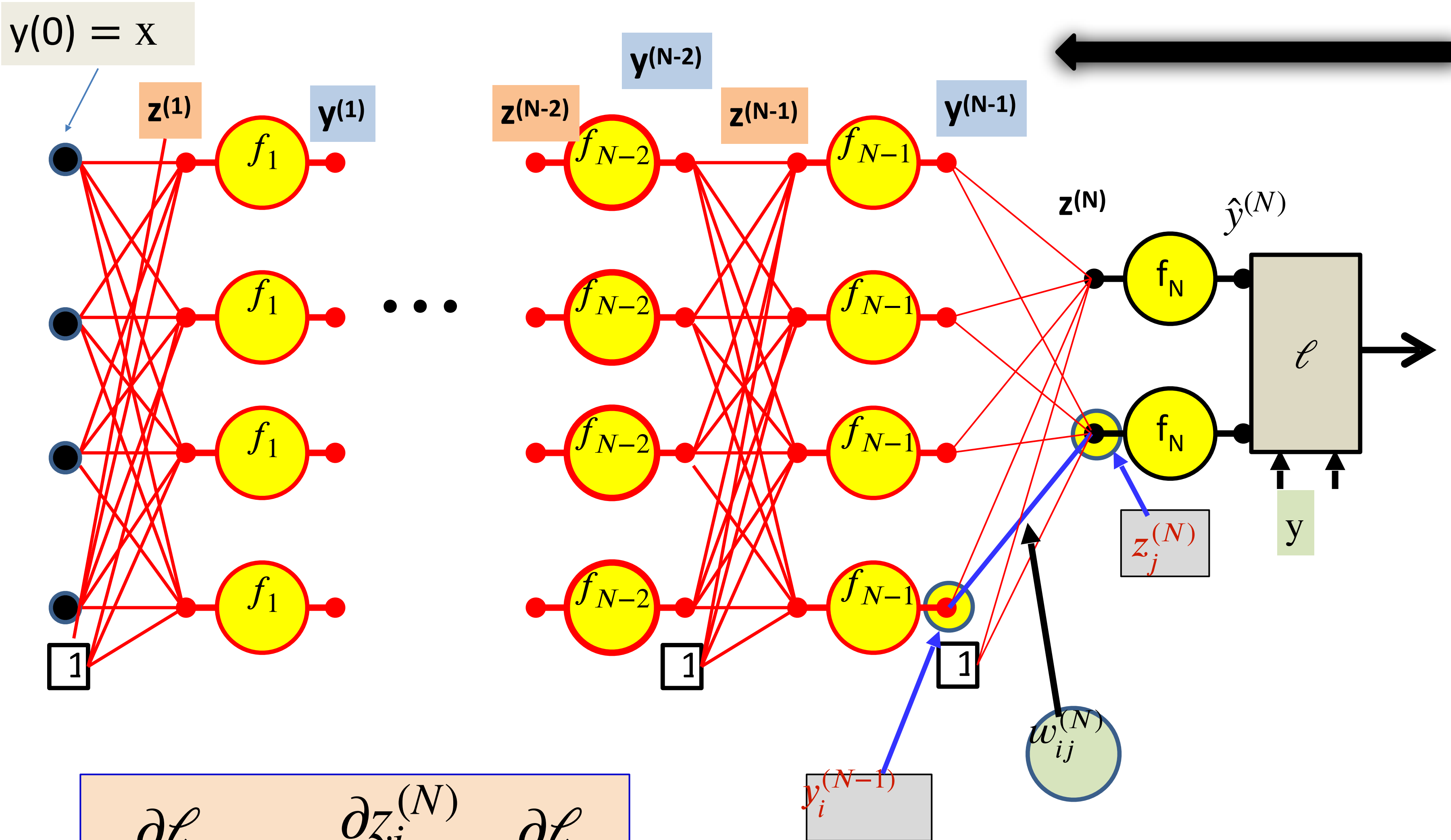
Derivative of activation function

$$\frac{\partial \ell}{\partial z_i^{(N)}} = \frac{\partial \hat{y}}{\partial z_i^{(N)}} \frac{\partial \ell}{\partial \hat{y}_i^{(N)}}$$

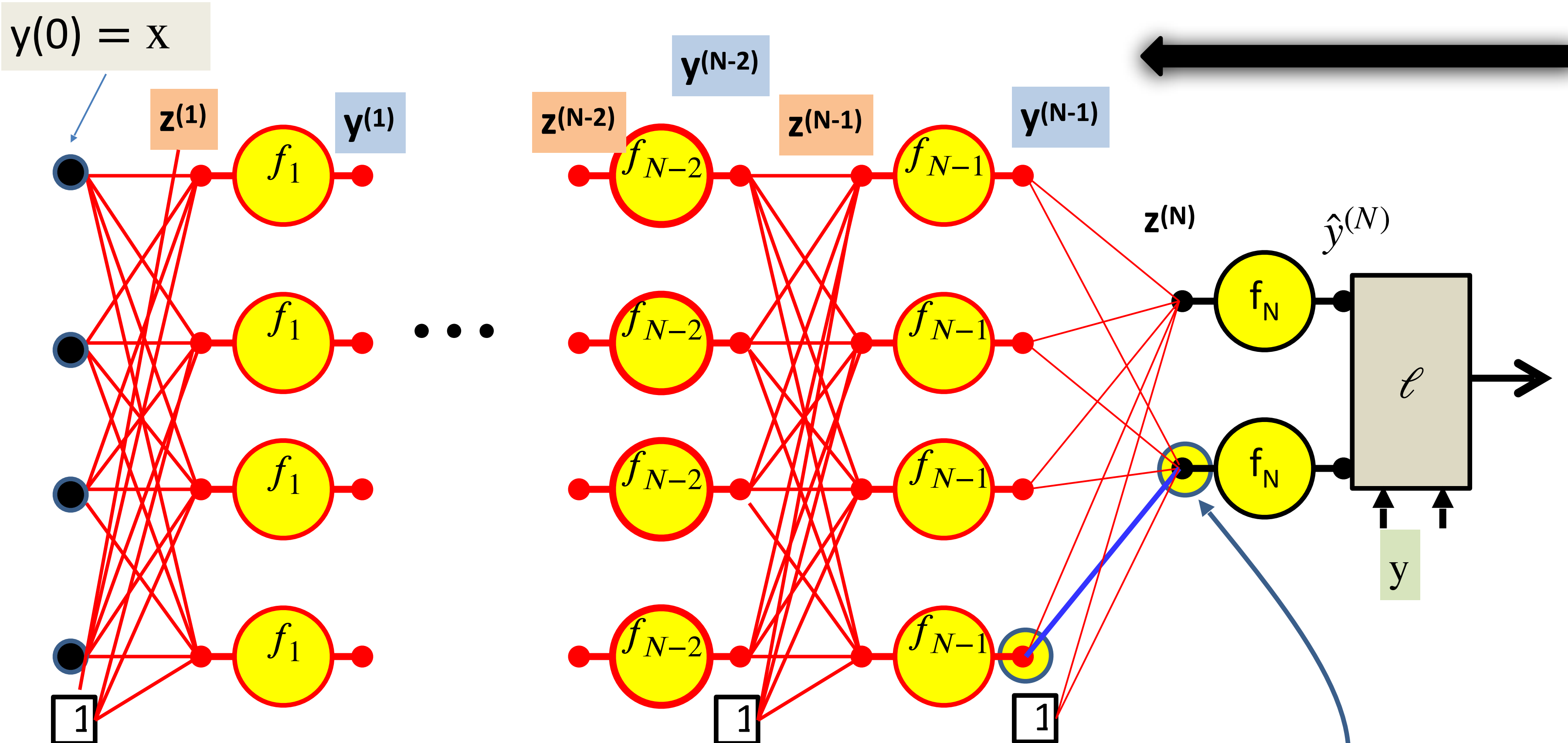
Computed in forward pass



$$\frac{\partial \ell}{\partial z_i^{(N)}} = f_N'(z_i^{(N)}) \frac{\partial \ell}{\partial \hat{y}_i^{(N)}}$$

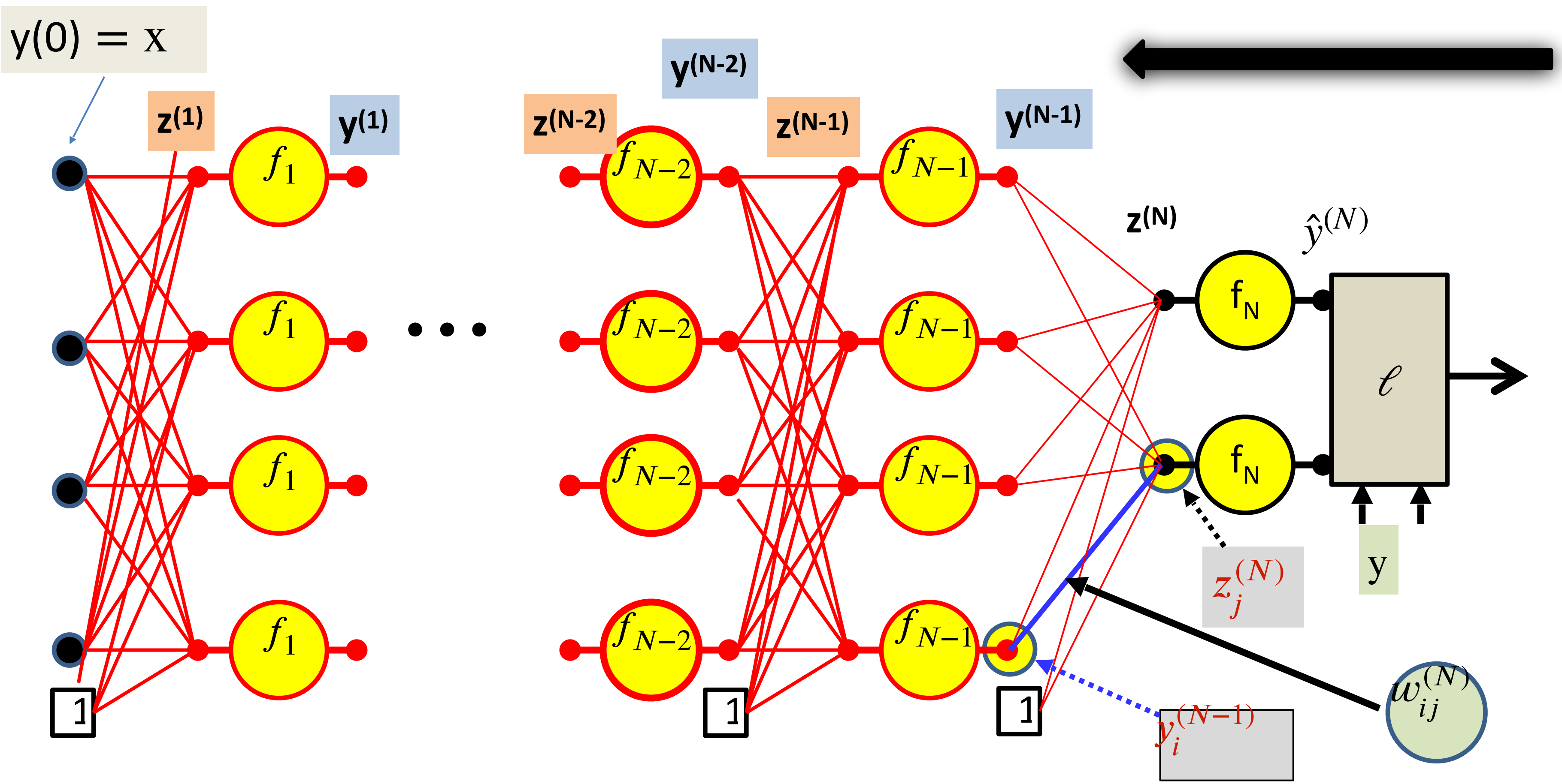


$$\frac{\partial \ell}{\partial w_{ij}^{(N)}} = \frac{\partial z_j^{(N)}}{\partial w_{ij}^{(N)}} \frac{\partial \ell}{\partial z_j^{(N)}}$$



$$\frac{\partial \ell}{\partial w_{ij}^{(N)}} = \frac{\partial z_j^{(N)}}{\partial w_{ij}^{(N)}} \frac{\partial \ell}{\partial z_j^{(N)}}$$

Just computed



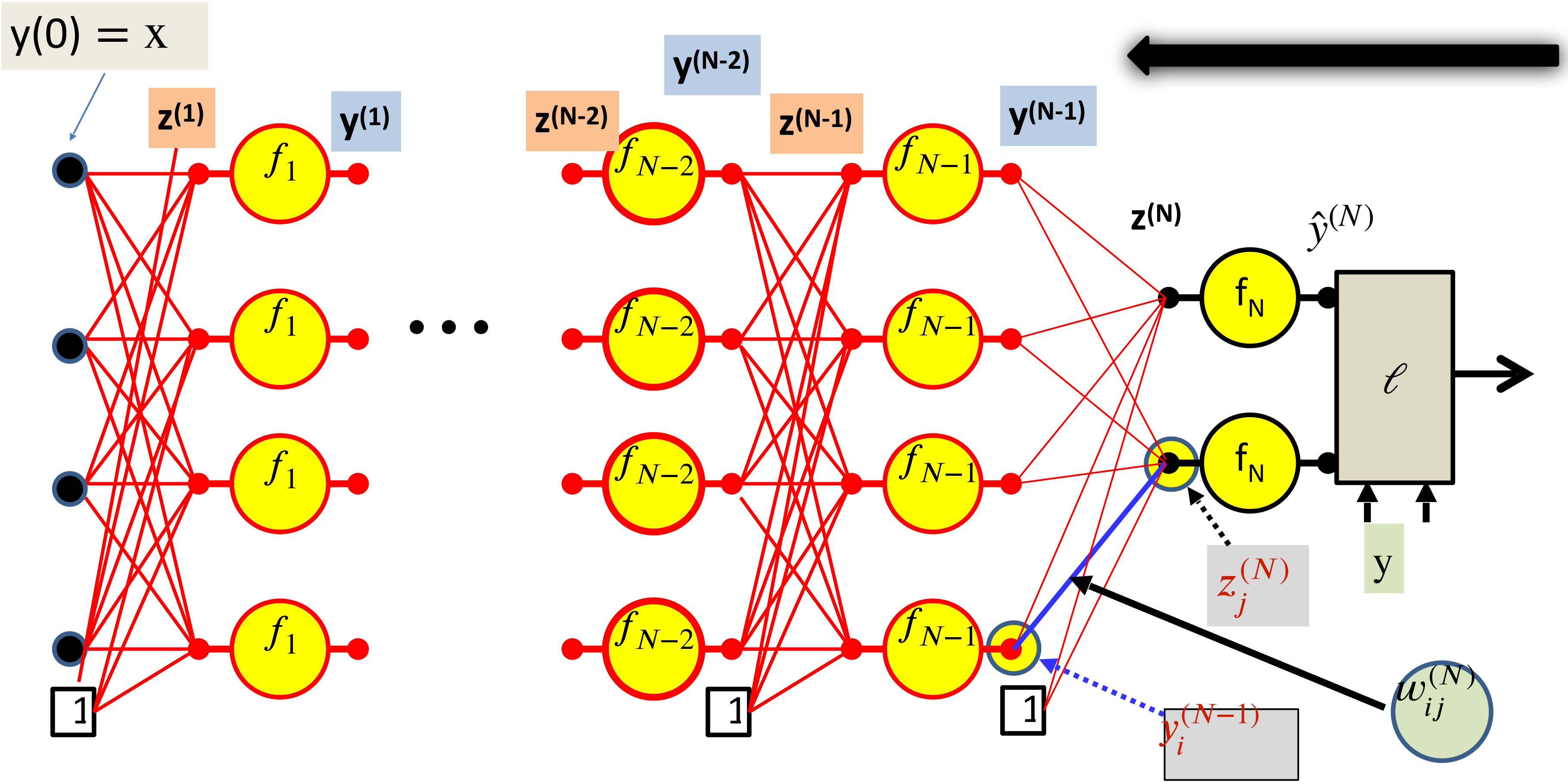
$$\frac{\partial \ell}{\partial w_{ij}^{(N)}} = \frac{\partial z_j^{(N)}}{\partial w_{ij}^{(N)}} \frac{\partial \ell}{\partial z_j^{(N)}}$$

$y_i^{(N-1)}$

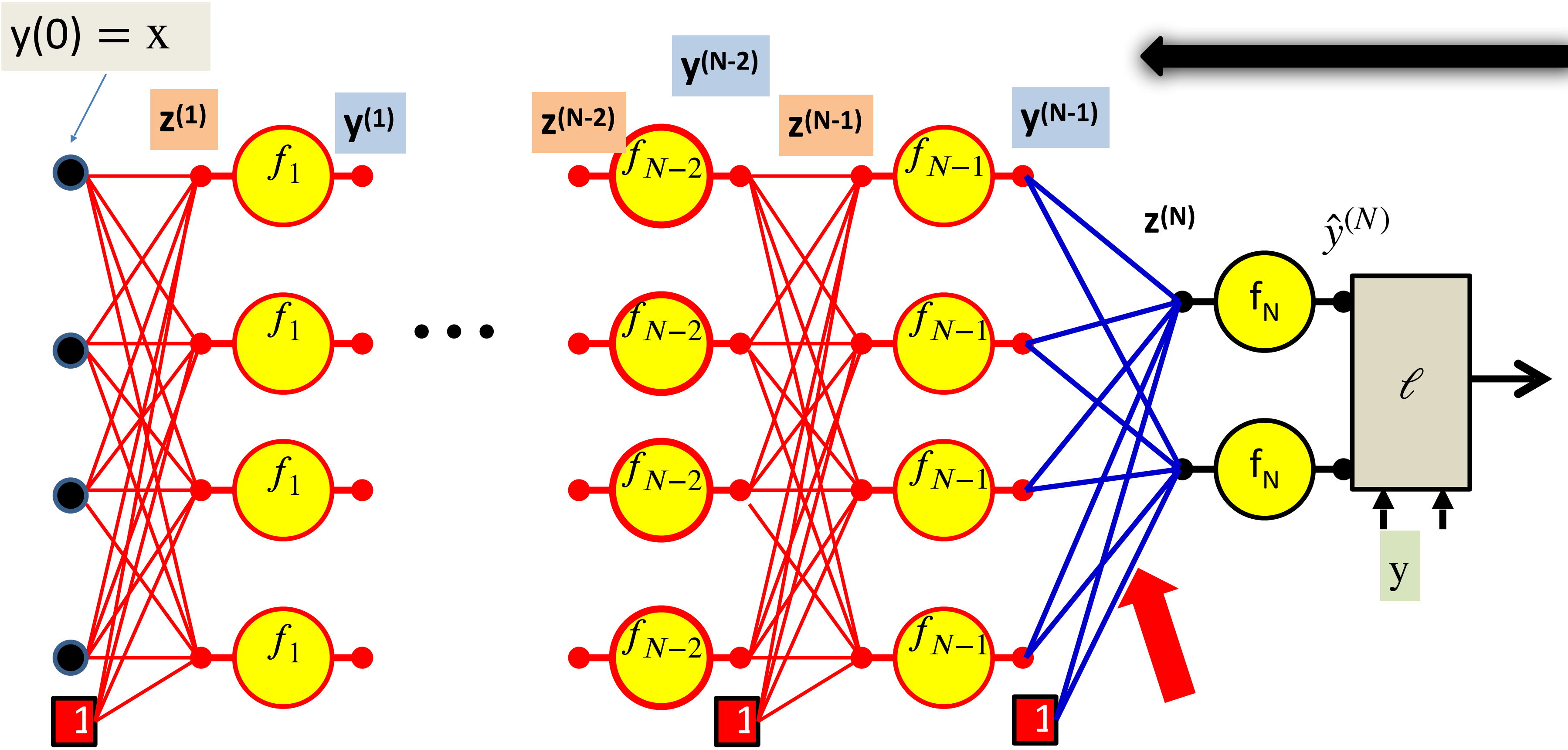
Computed in forward pass

Because

$$z_j^{(N)} = w_{ij}^{(N)} y_i^{(N-1)} + \text{other terms}$$

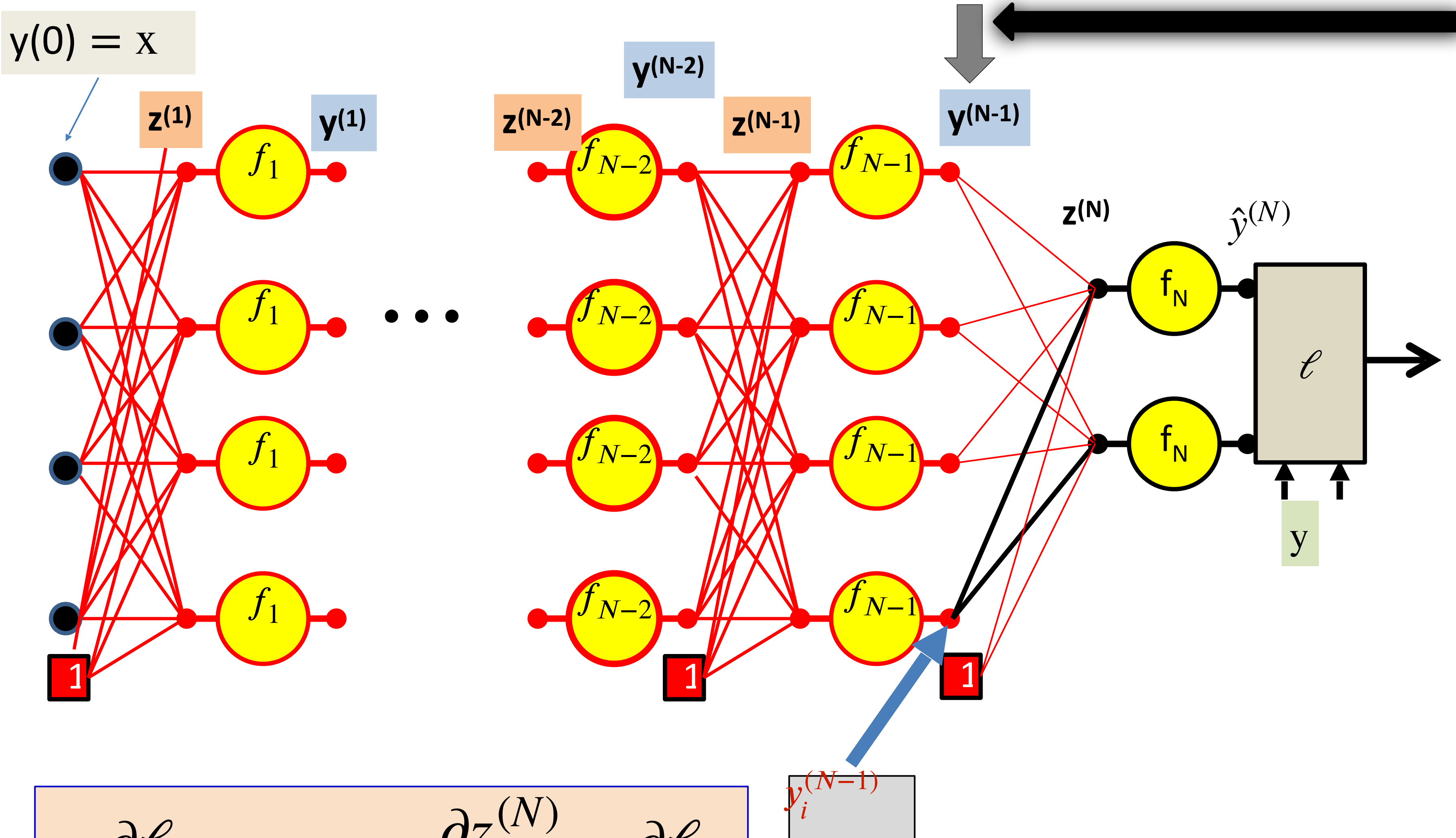


$$\frac{\partial \ell}{\partial w_{ij}^{(N)}} = y_i^{(N-1)} \frac{\partial \ell}{\partial z_j^{(N)}}$$

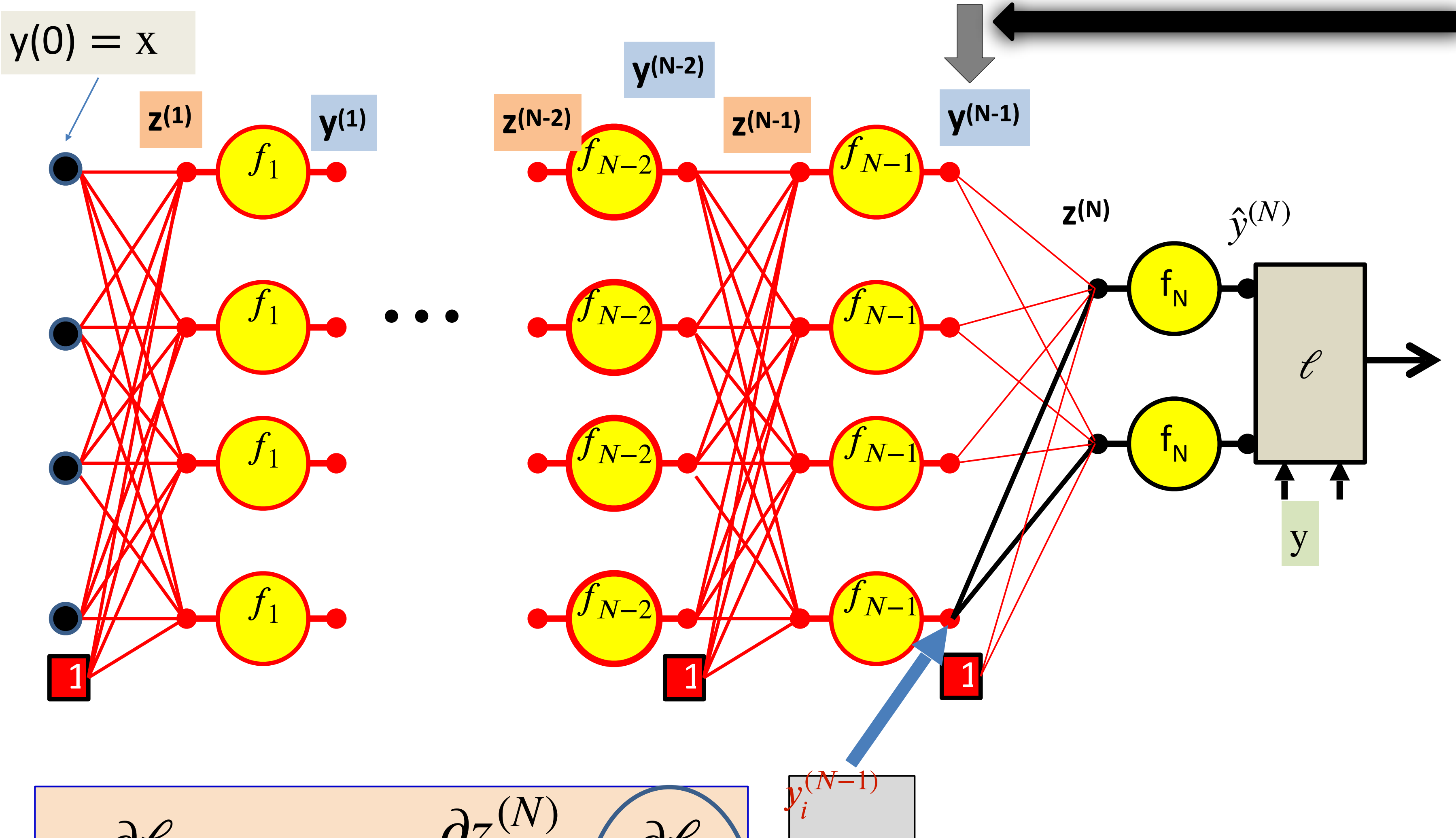


$$\frac{\partial \ell}{\partial w_{ij}^{(N)}} = y_i^{(N-1)} \frac{\partial \ell}{\partial z_j^{(N)}}$$

For the bias term $y_0^{(N-1)} = 1$

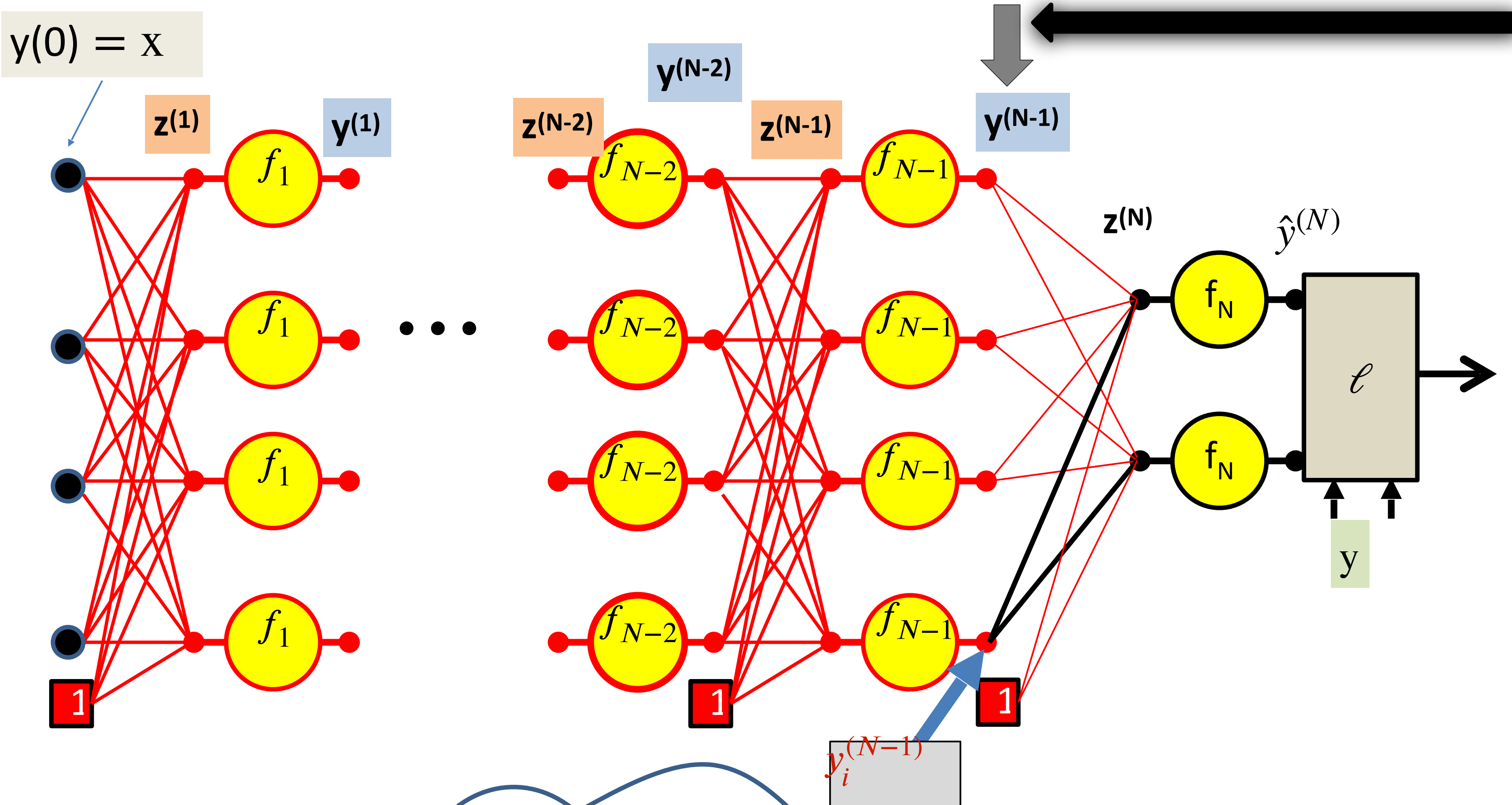


$$\frac{\partial \ell}{\partial y_i^{(N-1)}} = \sum_j \frac{\partial z_j^{(N)}}{\partial y_i^{(N-1)}} \frac{\partial \ell}{\partial z_j^{(N)}}$$



$$\frac{\partial \ell}{\partial y_i^{(N-1)}} = \sum_j \frac{\partial z_j^{(N)}}{\partial y_i^{(N-1)}} \frac{\partial \ell}{\partial z_j^{(N)}}$$

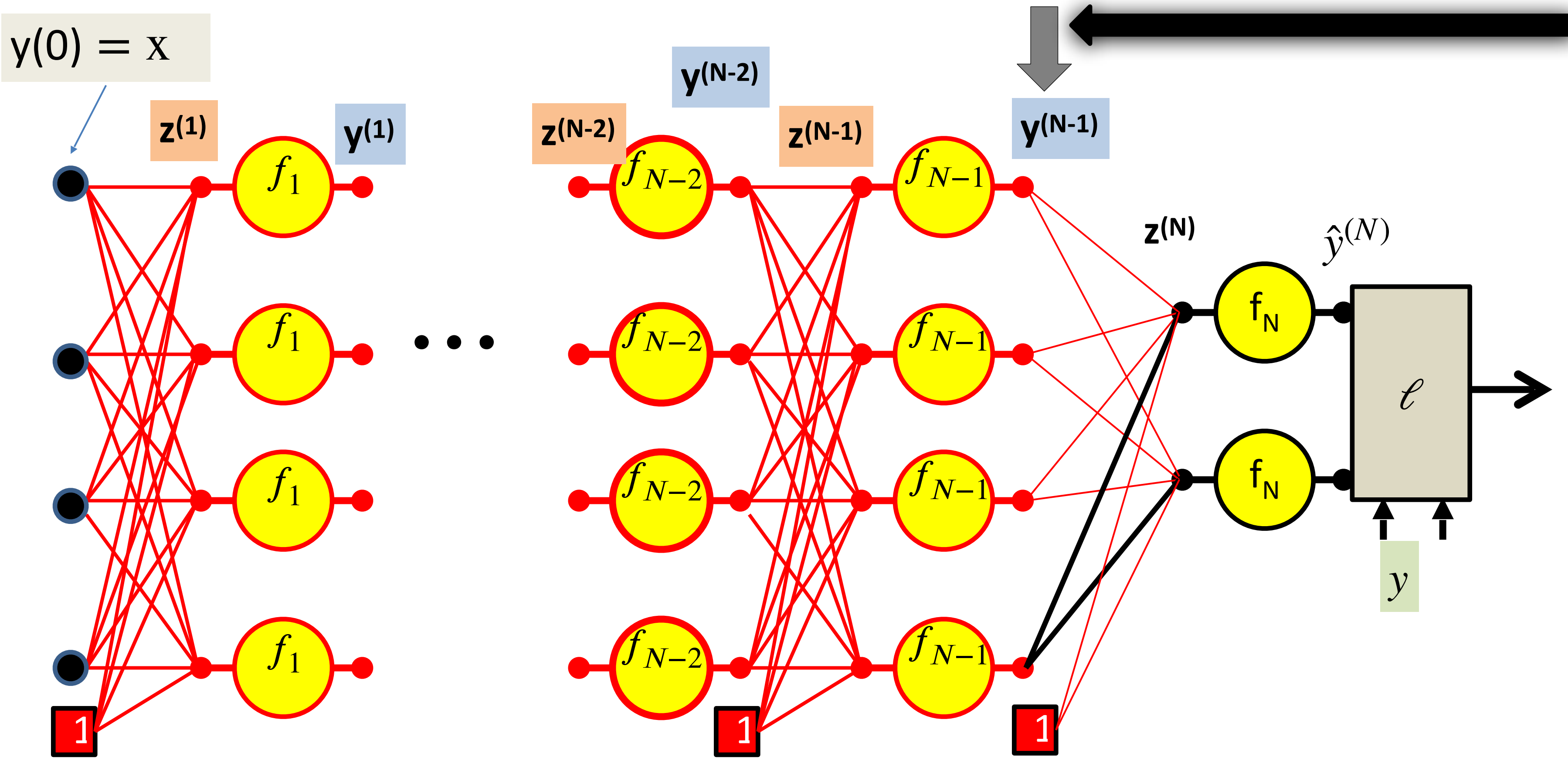
Already computed



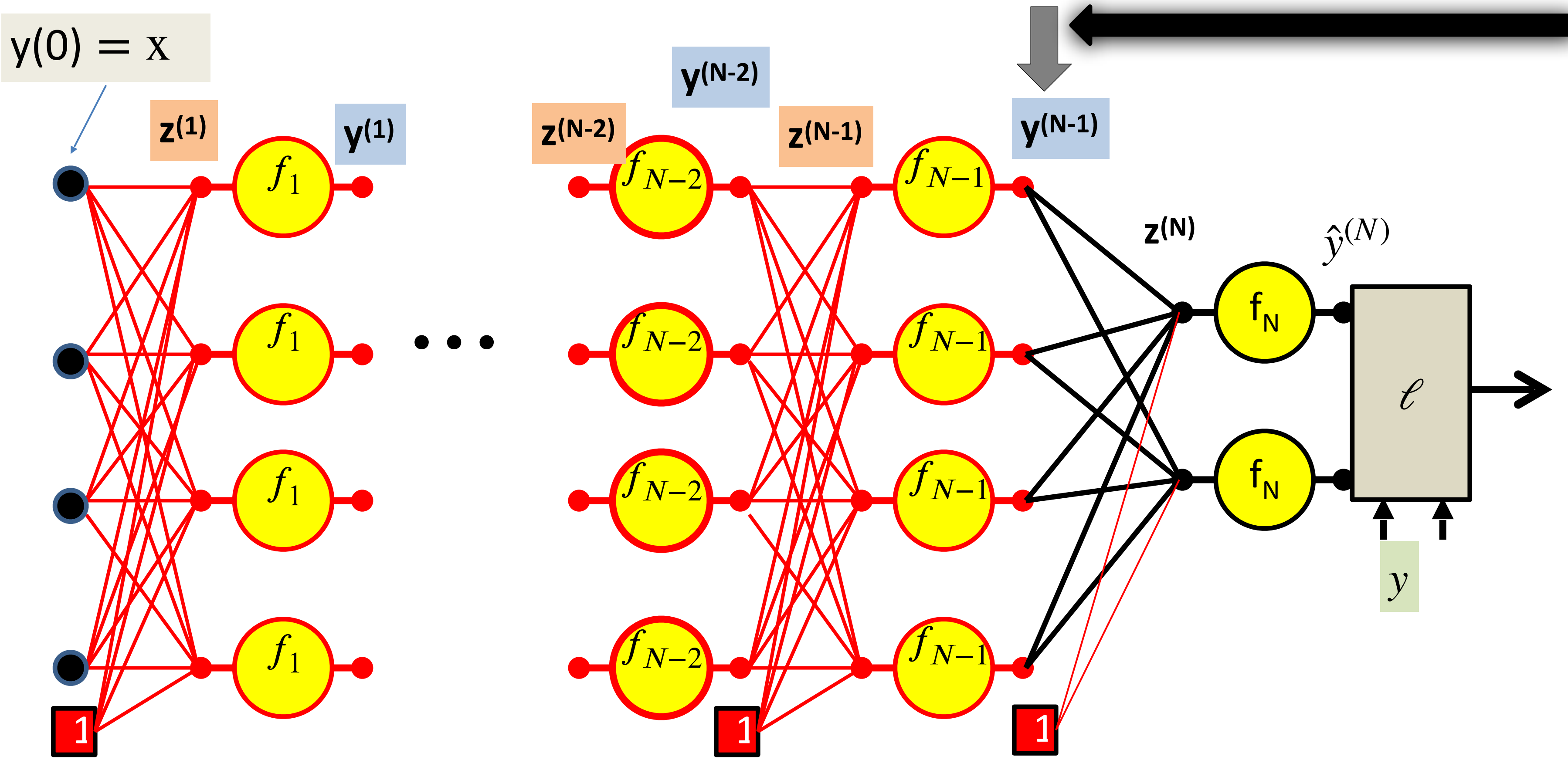
$$\frac{\partial \ell}{\partial y_i^{(N-1)}} = \sum_j \frac{\partial z_j^{(N)}}{\partial y_i^{(N-1)}} \frac{\partial \ell}{\partial z_j^{(N)}}$$

Because

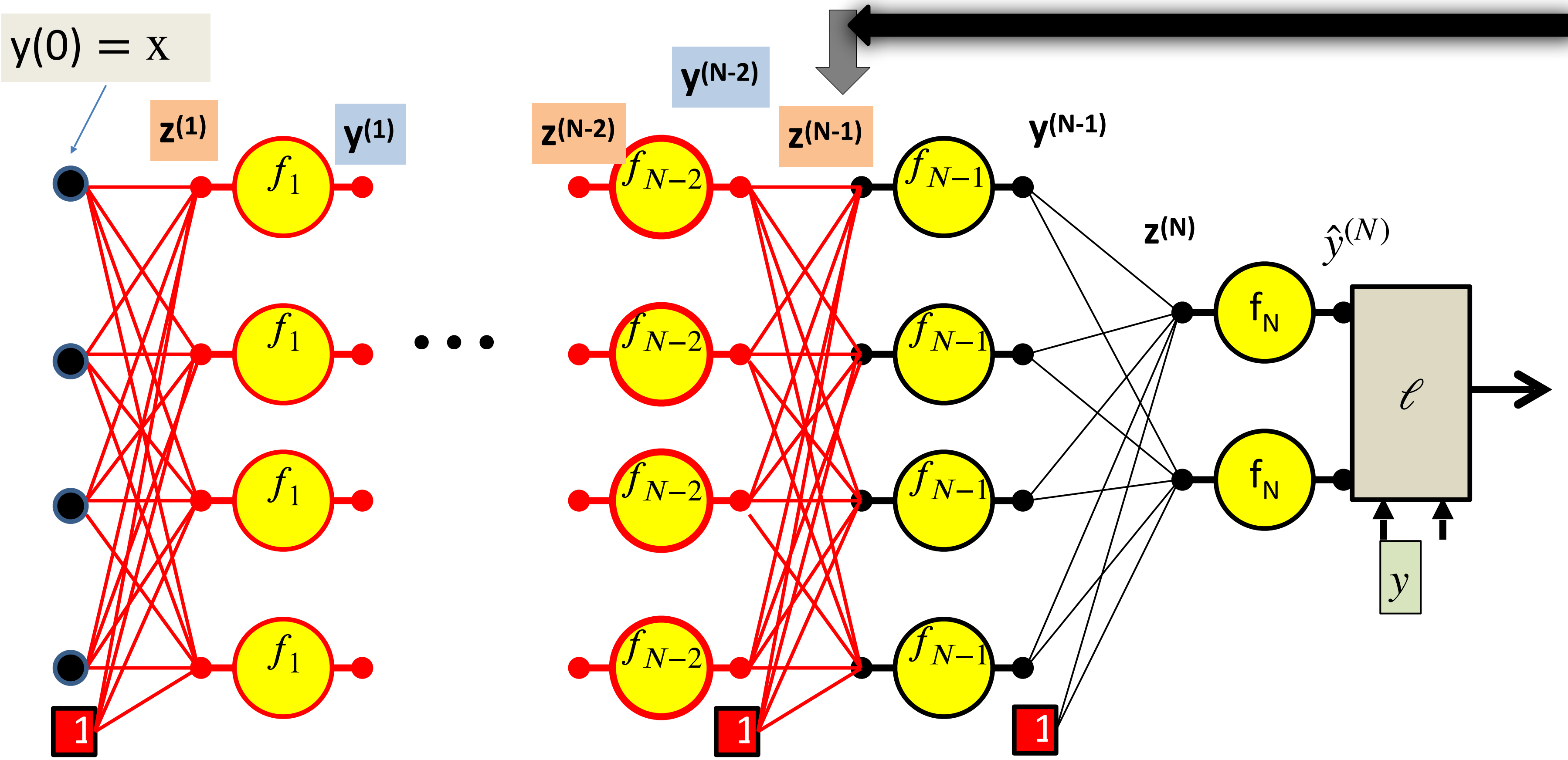
$$z_j^{(N)} = w_{ij}^{(N)} y_i^{(N-1)} + \text{other terms}$$



$$\frac{\partial \ell}{\partial y_i^{(N-1)}} = \sum_j w_{ij}^{(N)} \frac{\partial \ell}{\partial z_j^{(N)}}$$

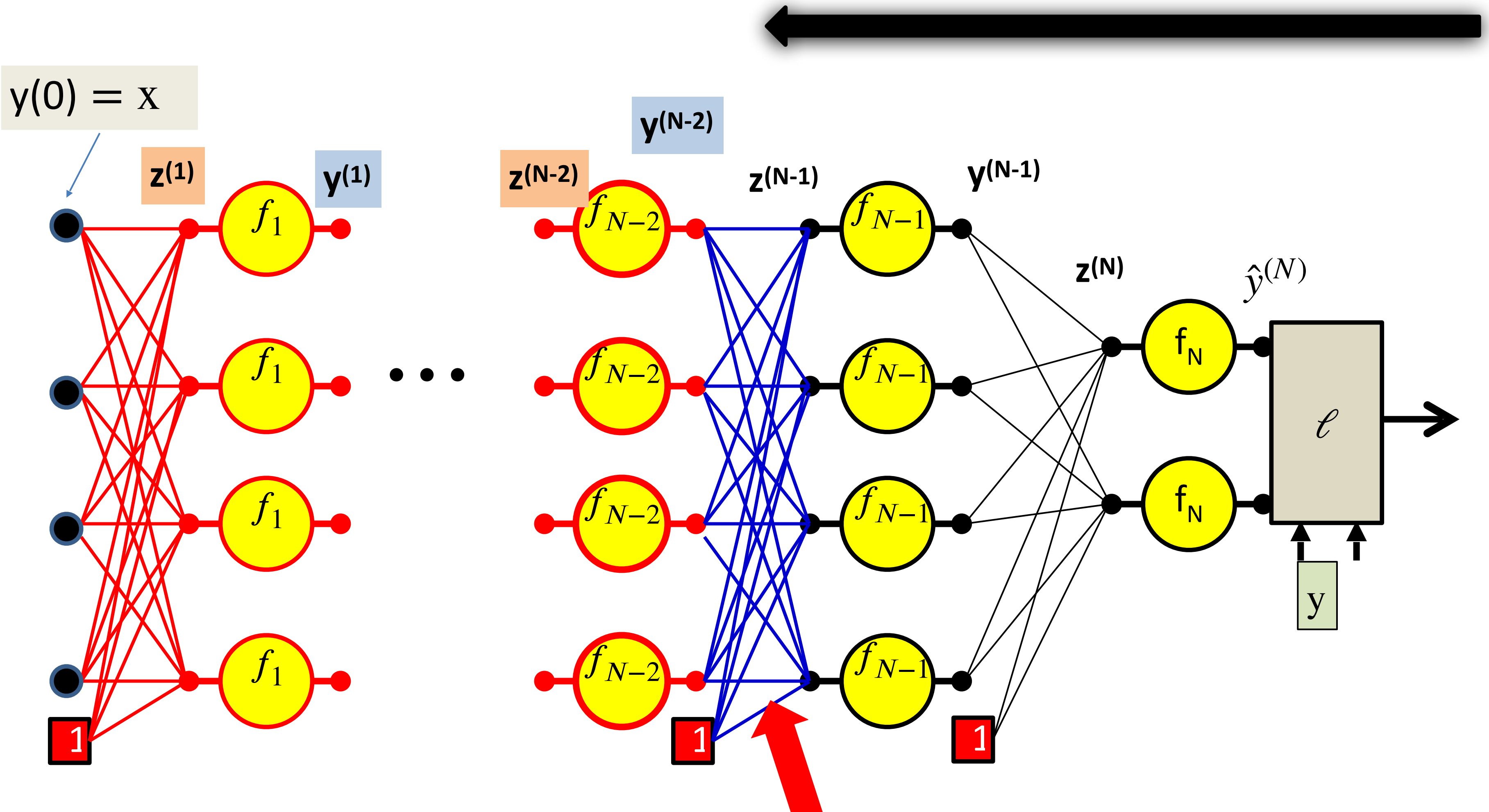


$$\frac{\partial \ell}{\partial y_i^{(N-1)}} = \sum_j w_{ij}^{(N)} \frac{\partial \ell}{\partial z_j^{(N)}}$$



We continue our way backwards in the order shown

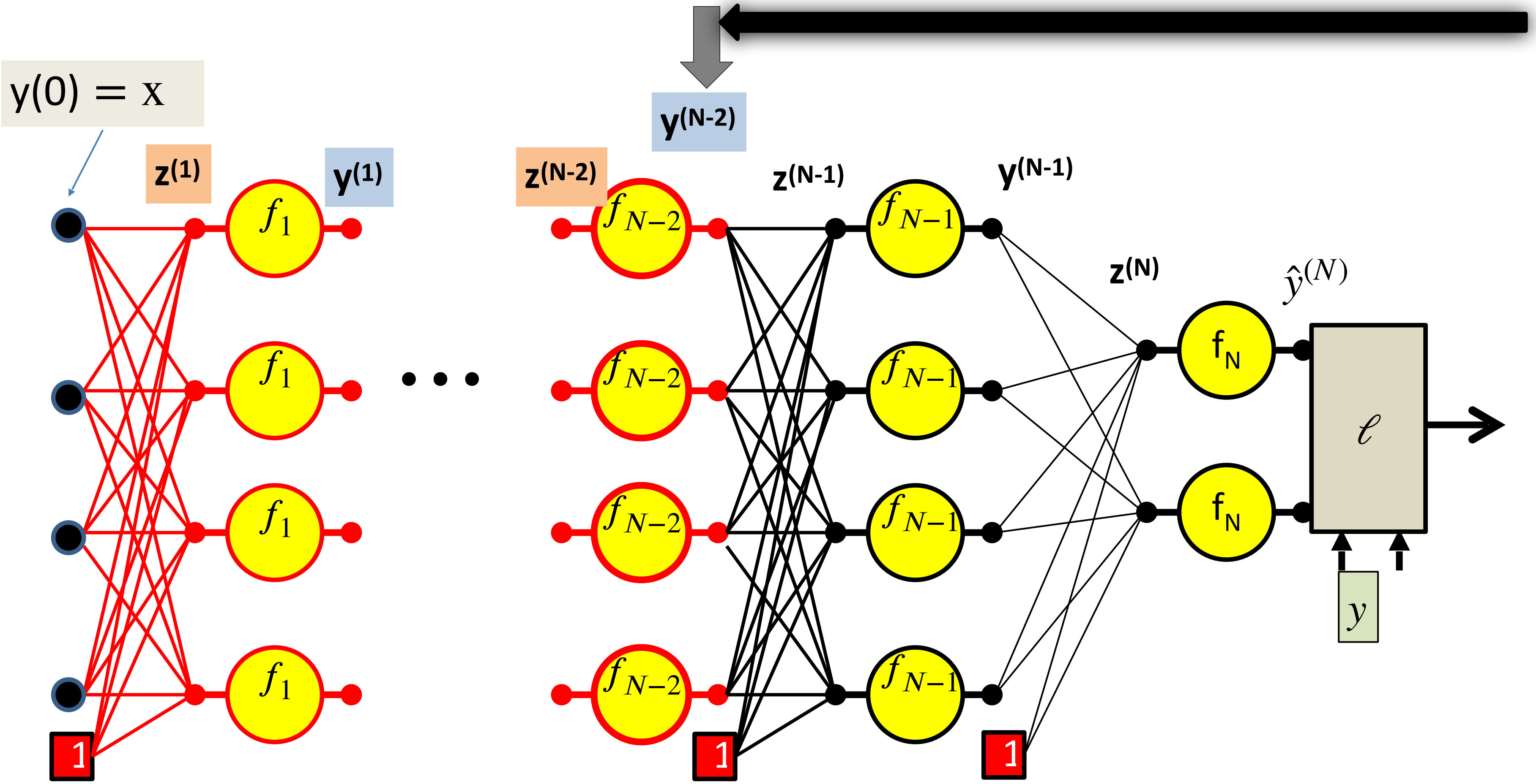
$$\frac{\partial \ell}{\partial z_i^{(N-1)}} = f'_{N-1}(z_i^{(N-1)}) \frac{\partial \ell}{\partial \hat{y}_i^{(N-1)}}$$



We continue our way backwards in the order shown

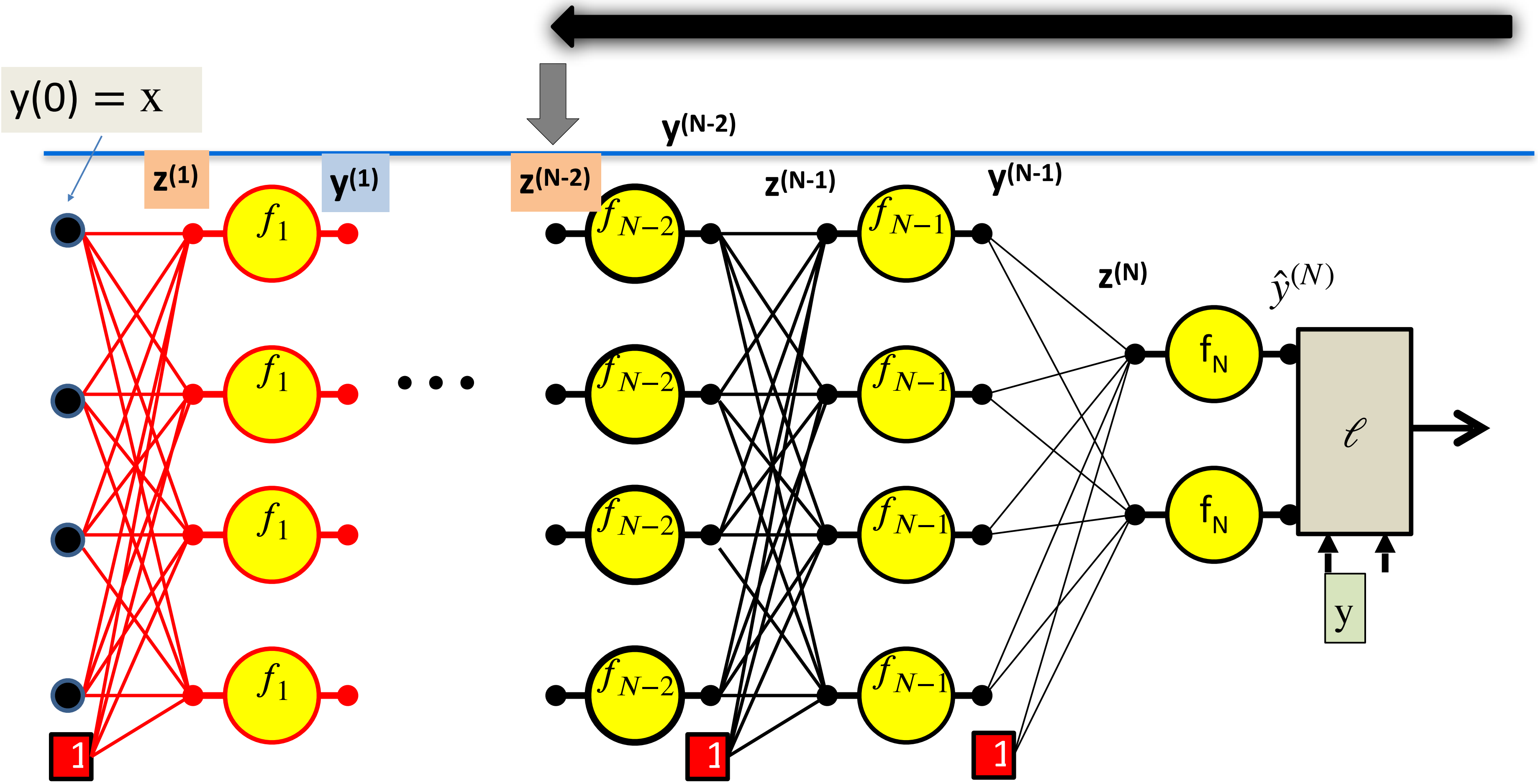
$$\boxed{\frac{\partial \ell}{\partial w_{ij}^{(N-1)}} = y_i^{(N-2)} \frac{\partial \ell}{\partial z_j^{(N-1)}}}$$

the bias term $y_0^{(N-2)} = 1$



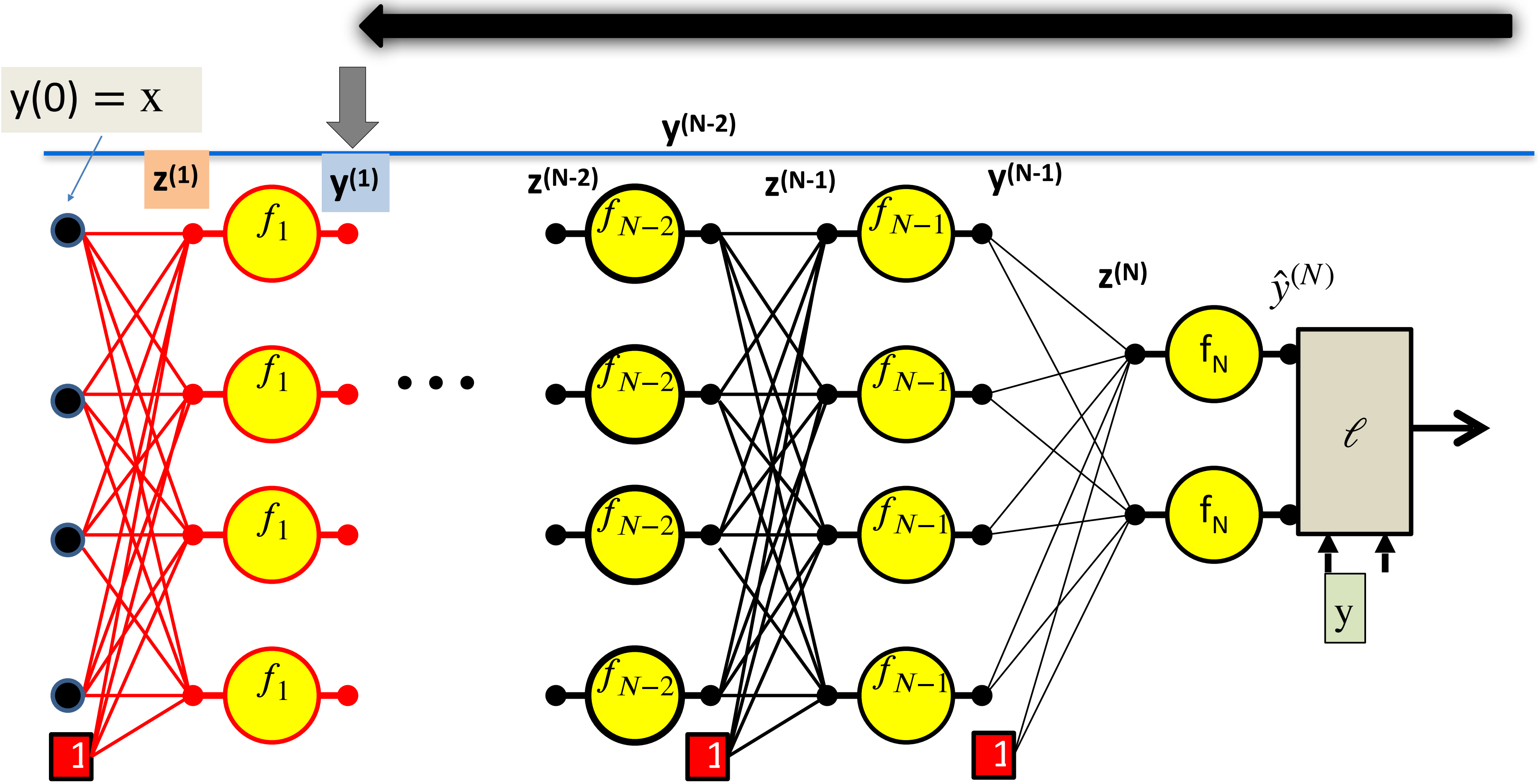
We continue our way backwards in the order shown

$$\boxed{\frac{\partial \ell}{\partial y_i^{(N-2)}} = \sum_j w_{ij}^{(N-1)} \frac{\partial \ell}{\partial z_j^{(N-1)}}}$$



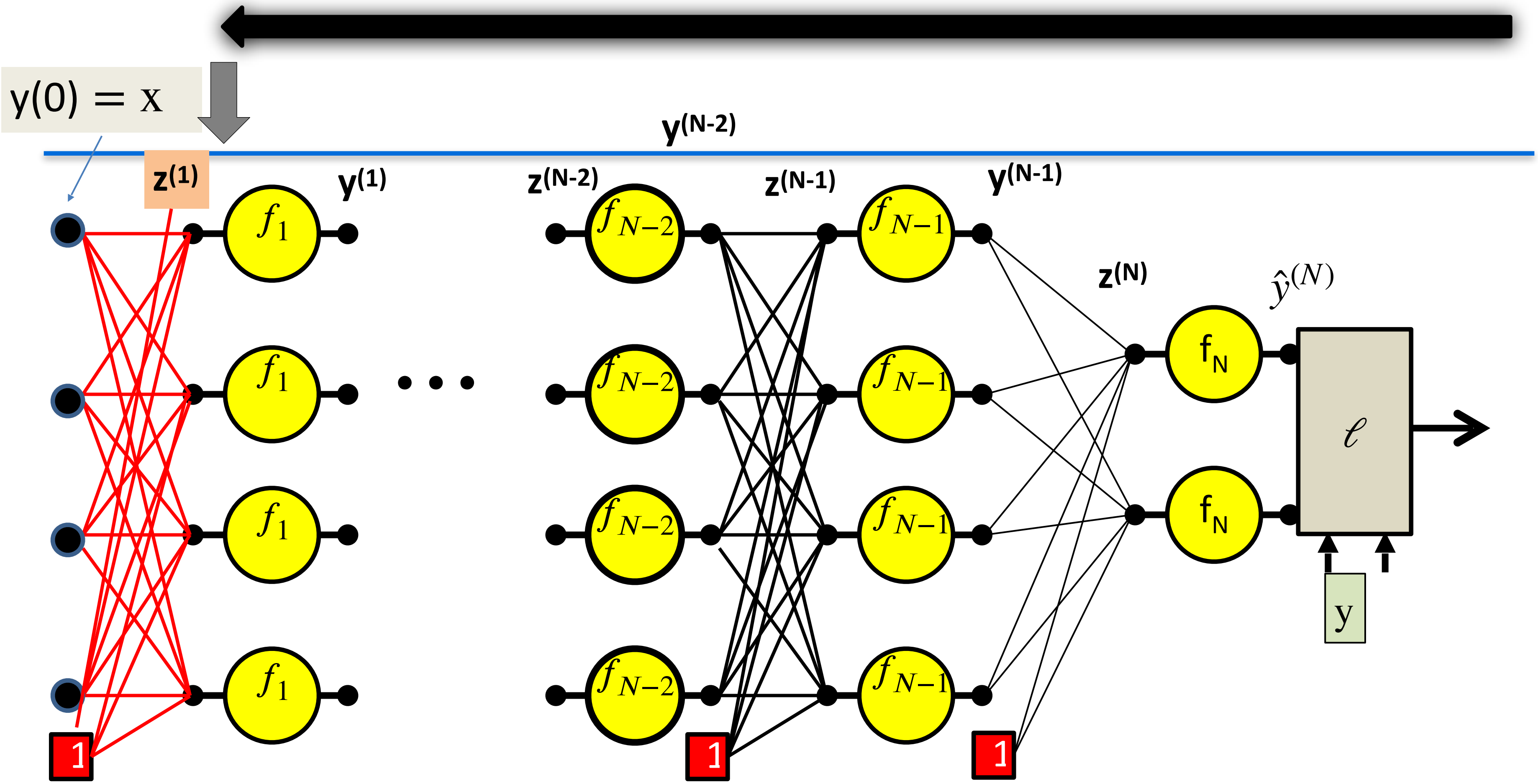
We continue our way backwards in the order shown

$$\frac{\partial \ell}{\partial z_i^{(N-2)}} = f'_{N-2}(z_i^{(N-2)}) \frac{\partial \ell}{\partial \hat{y}_i^{(N-2)}}$$



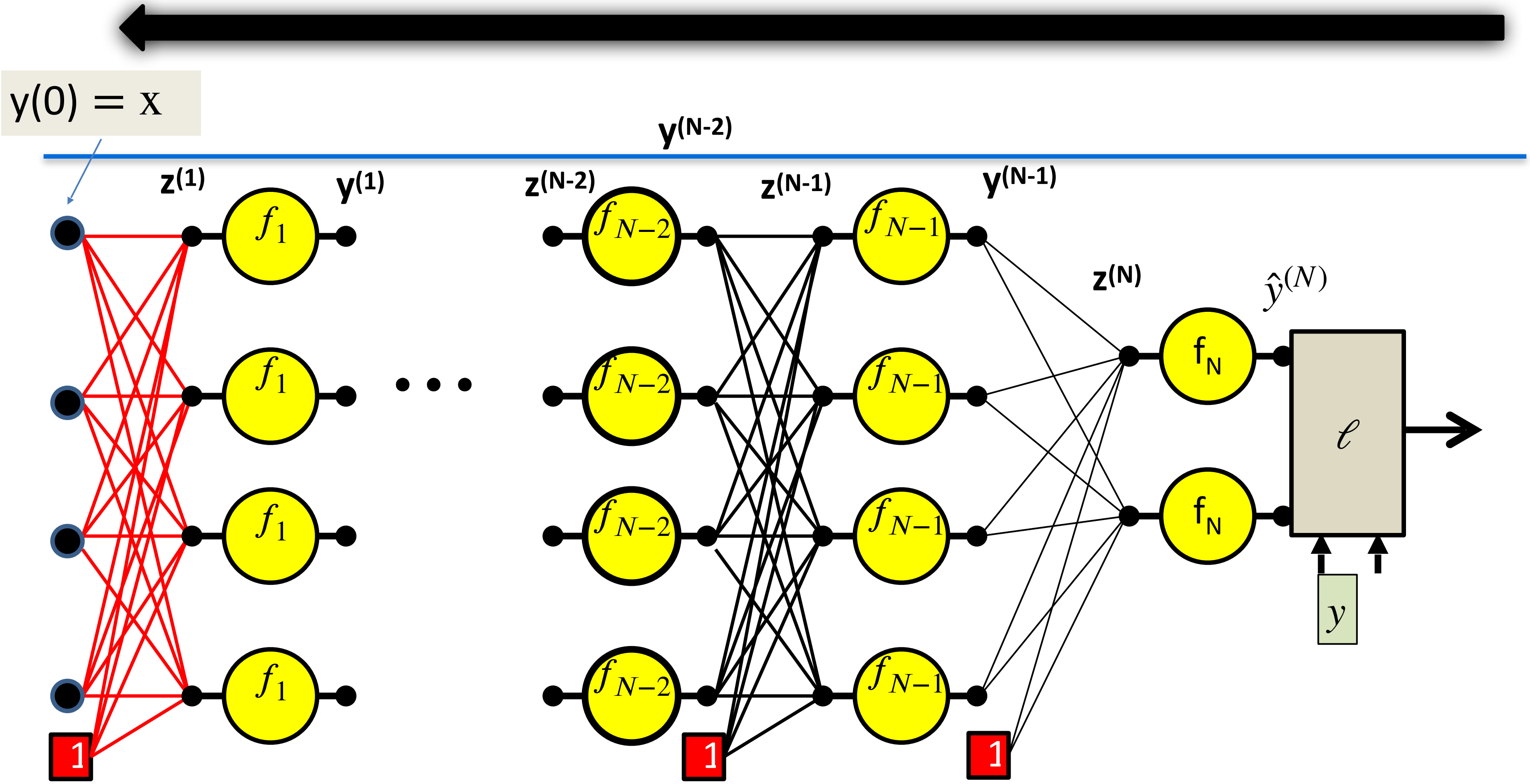
We continue our way backwards in the order shown

$$\frac{\partial \ell}{\partial y_i^{(1)}} = \sum_j w_{ij}^{(2)} \frac{\partial \ell}{\partial z_j^{(2)}}$$



We continue our way backwards in the order shown

$$\boxed{\frac{\partial \ell}{\partial z_i^{(1)}} = f_1'(z_i^{(1)}) \frac{\partial \ell}{\partial \hat{y}_i^{(1)}}}$$



We continue our way backwards in the order shown

$$\frac{\partial \ell}{\partial w_{ij}^{(1)}} = x_i \frac{\partial \ell}{\partial z_j^{(1)}}$$

Backward Pass

- Output layer (N) :
  - For $i = 1 \ldots D_N$
    - $$\frac{\partial \ell}{\partial z_i^{(N)}} = f_N'(z_i^{(N)}) \frac{\partial \ell}{\partial \hat{y}_i^{(N)}}$$
    - $$\frac{\partial \ell}{\partial w_{ij}^{(N)}} = y_i^{(N-1)} \frac{\partial \ell}{\partial z_j^{(N)}} \text{ for each j}$$
- For layer $k = N - 1 \; downto \; 1$
  - For $i = 1 \ldots D_k$
    - $$\frac{\partial \ell}{\partial y_i^{(k-1)}} = \sum_j w_{ij}^{(k)} \frac{\partial \ell}{\partial z_j^{(k)}}$$
    - $$\frac{\partial \ell}{\partial z_i^{(k)}} = f_k'(z_i^{(k)}) \frac{\partial \ell}{\partial y_i^{(k)}}$$
    - $$\frac{\partial \ell}{\partial w_{ij}^{(k)}} = y_i^{(k-1)} \frac{\partial \ell}{\partial z_j^{(k)}} \text{ for each j}$$

Called "Backpropagation" because the derivative of the loss is propagated "backwards" through the network

Very analogous to the forward pass:

Backward weighted combination of next layer

Backward equivalent of activation

Recap

- Compute the gradient through Back-propagation algorithm
  – with forward pass and backward pass
  – backward pass is application of chain rule

Example

- simple_model.html

Autograd

- No need to write forward and backward explicitly
- Only need to specify the network
- Supported in pytorch and tensorflow

FFN in Pytorch

```
import torch
import math

x = …
y = …

model = torch.nn.Sequential(
    torch.nn.Linear(2, 3),
    torch.nn.ReLU(),
    torch.nn.Linear(3, 1),
    torch.nn.Flatten(0, 1)
)

loss_fn =
torch.nn.MSELoss(reduction='sum')

learning_rate = 1e-3
optimizer =
torch.optim.SGD(model.parameters()
, lr=learning_rate)
for t in range(2000):

    # Forward pass
    y_pred = model(xx)
```

```
    loss = loss_fn(y_pred, y)
    if t % 100 == 99:
        print(t, loss.item())
    model.zero_grad()

    # Backward pass
    loss.backward()

    # Update the weights using
stochastic gradient descent.
    optimizer.step()

# You can access the first layer
linear_layer = model[0]

# For linear layer, its parameters
are stored as `weight` and `bias`.
print(f'Result: y =
{linear_layer.bias.item()} +
{linear_layer.weight[:, 0].item()}
x + {linear_layer.weight[:,
1].item()} x^2 +
{linear_layer.weight[:, 2].item()}
x^3')
```

Next Up

- More on optimization
- Training/testing procedure
- Generalization problem
- Regularization tricks