CMSC 471:
Very Basic Intro to Neural Networks

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Outline

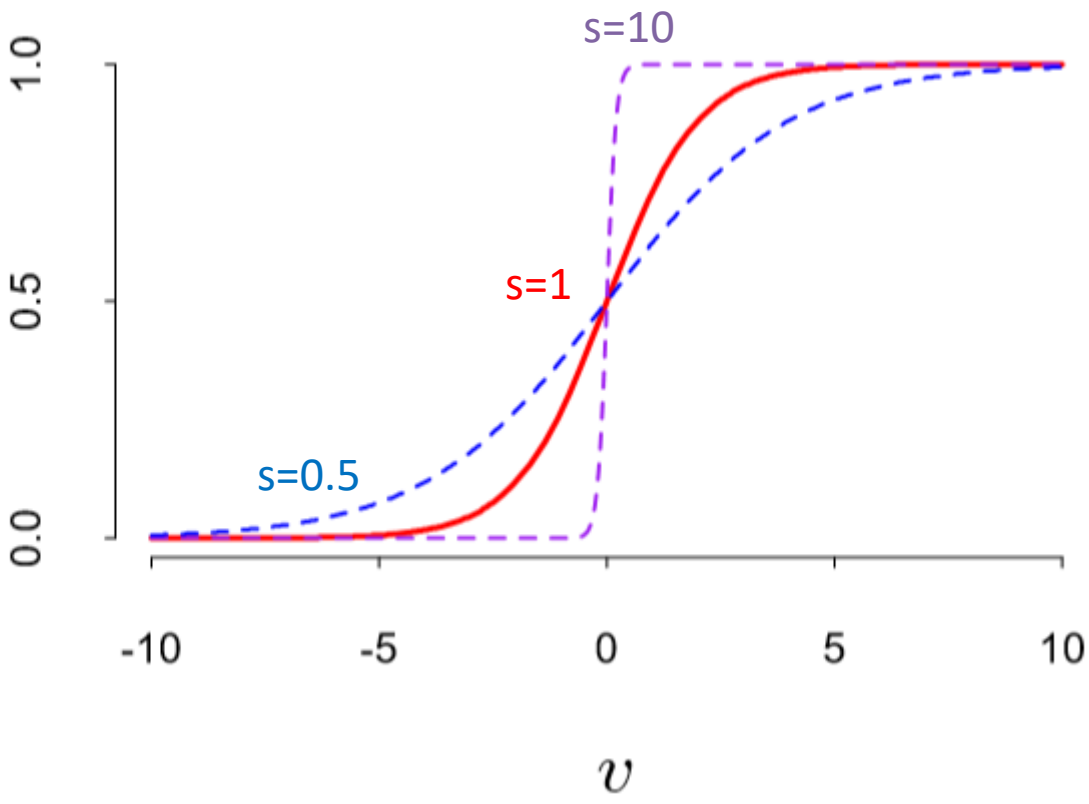
Neural networks: non-linear classifiers

Learning weights: backpropagation of error

Autodifferentiation (in reverse mode)

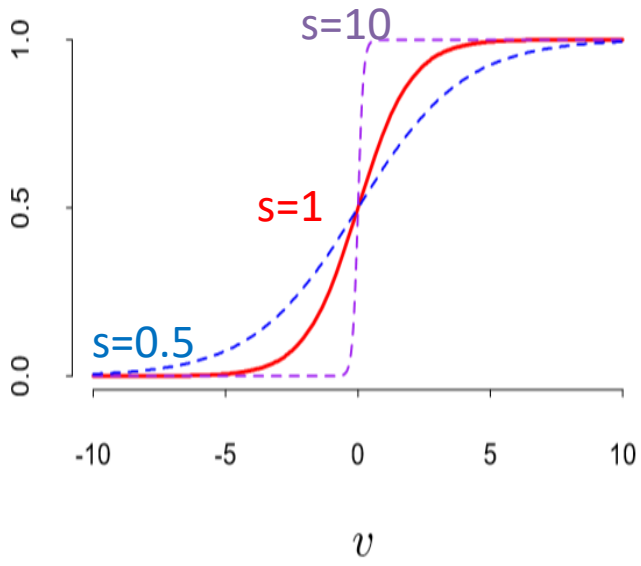
Sigmoid

$$\sigma(v) = \frac{1}{1 + \exp(-sv)}$$



Sigmoid

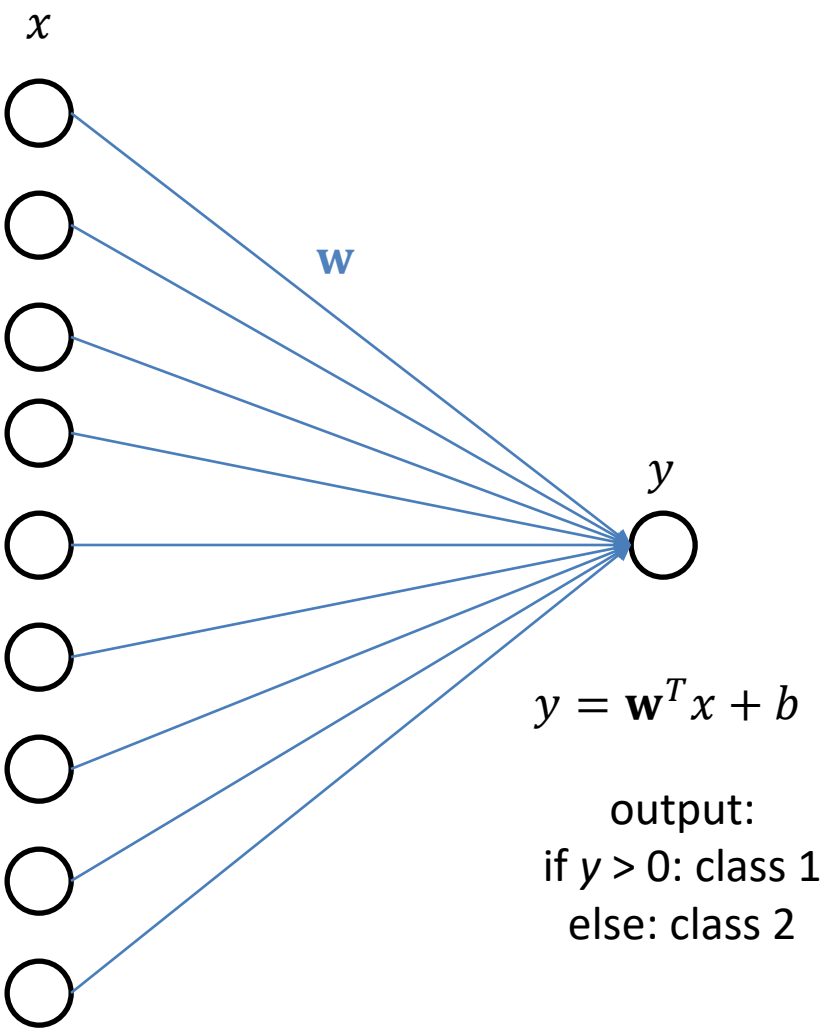
$$\sigma(v) = \frac{1}{1 + \exp(-sv)}$$



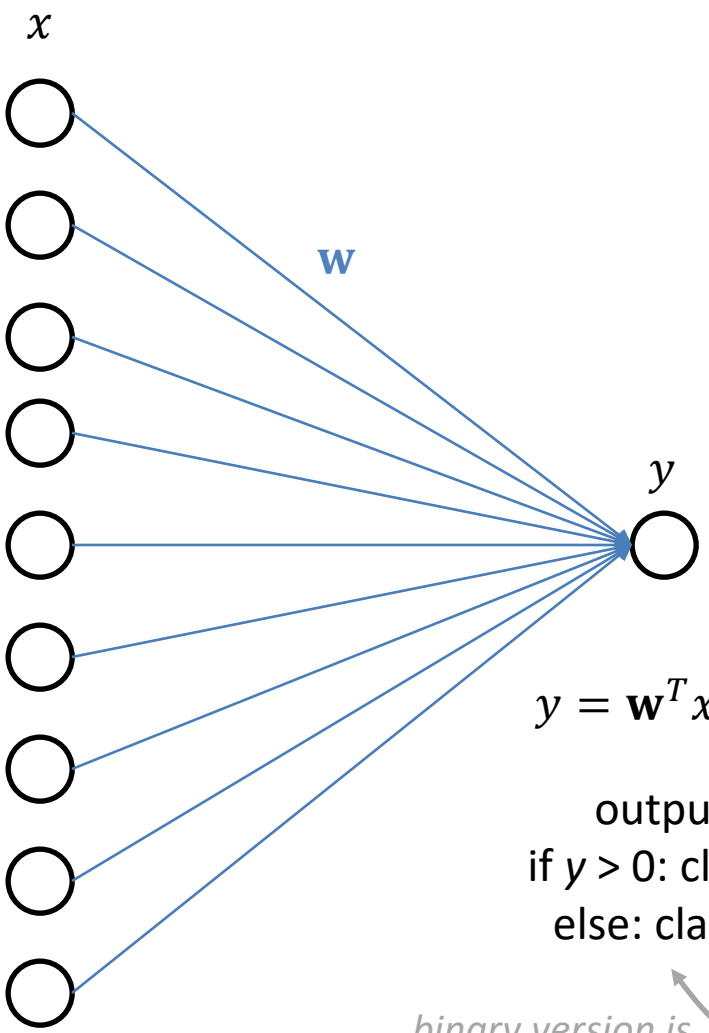
$$\frac{\partial \sigma(v)}{\partial v} = s * \sigma(v) * \big(1 - \sigma(v)\big)$$

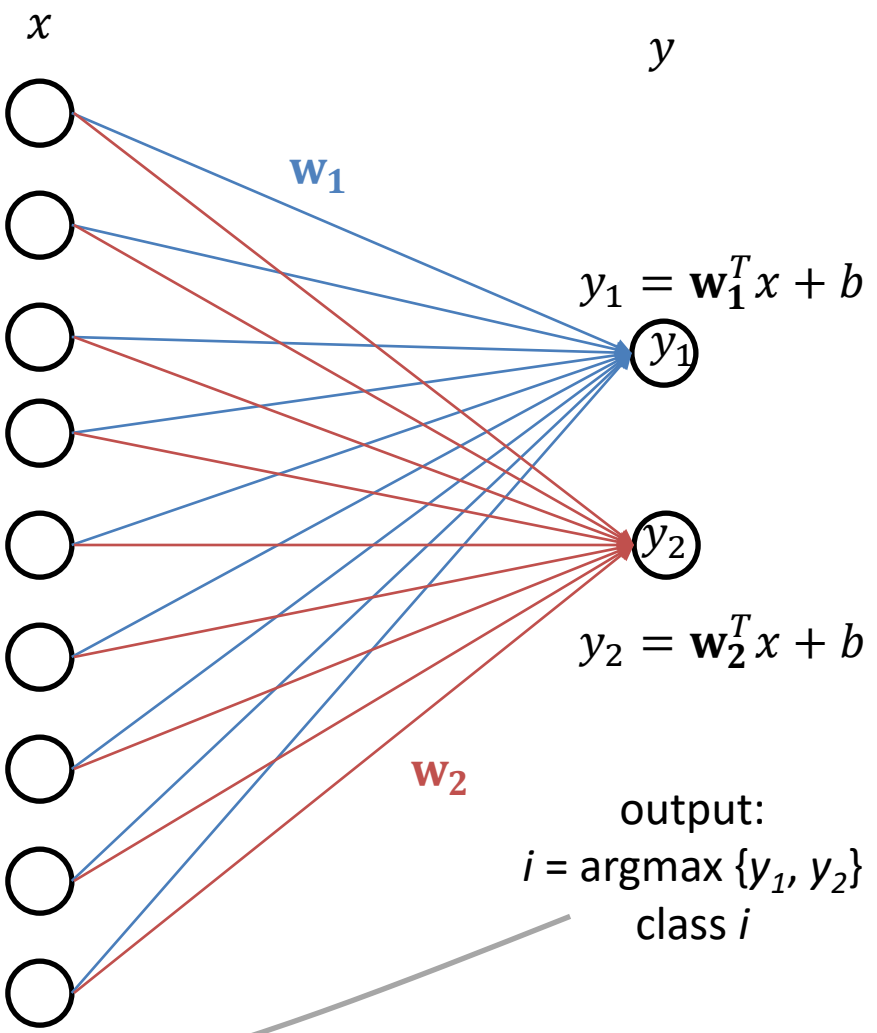
calc practice: verify for yourself

Remember Multi-class Linear Regression/Perceptron?



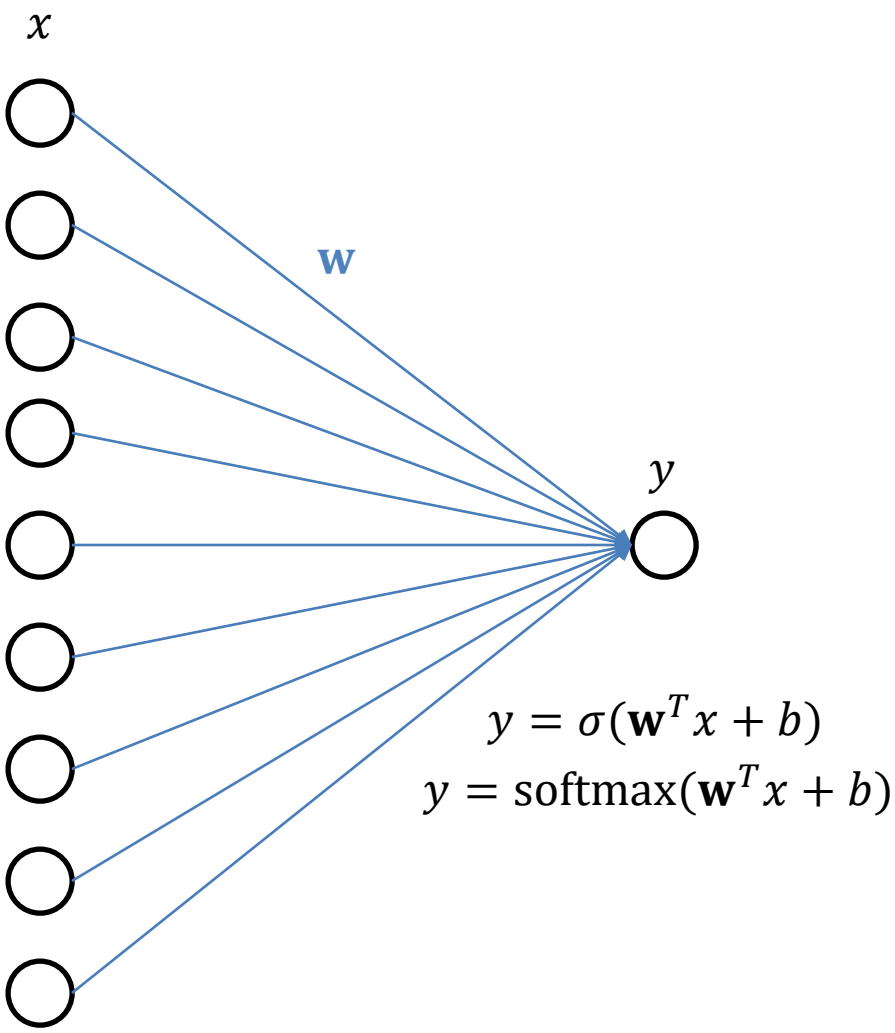
Linear Regression/Perceptron: A Per-Class View

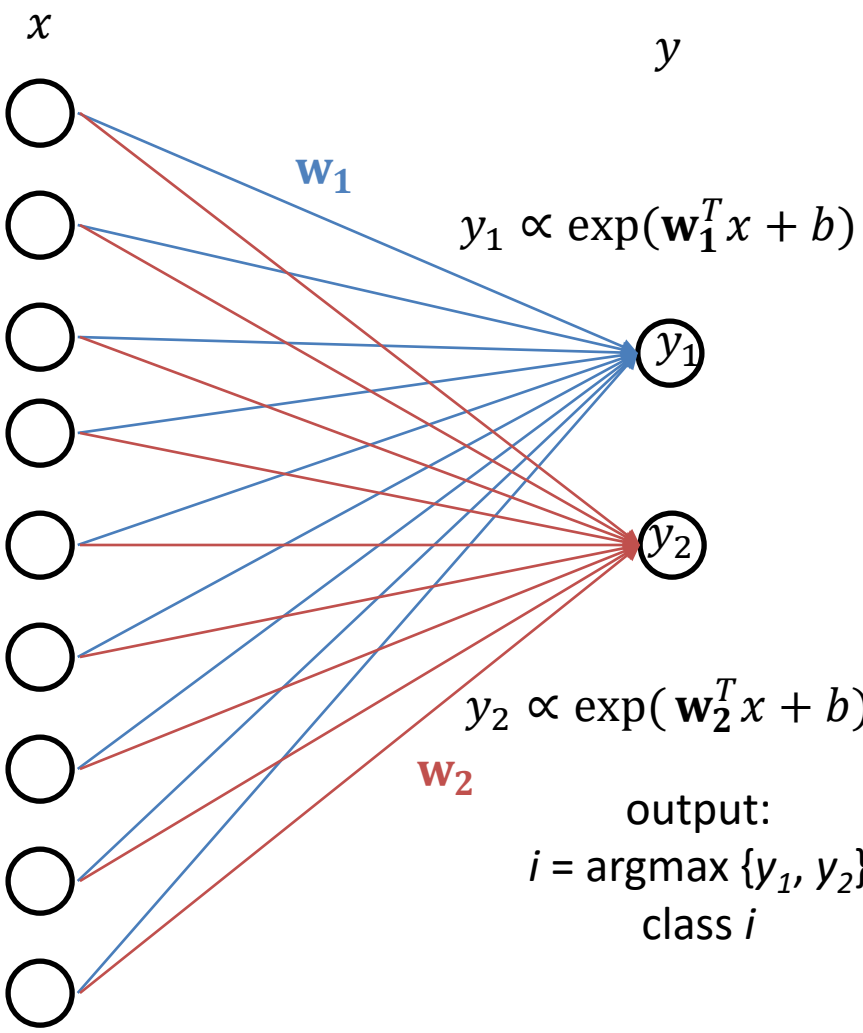




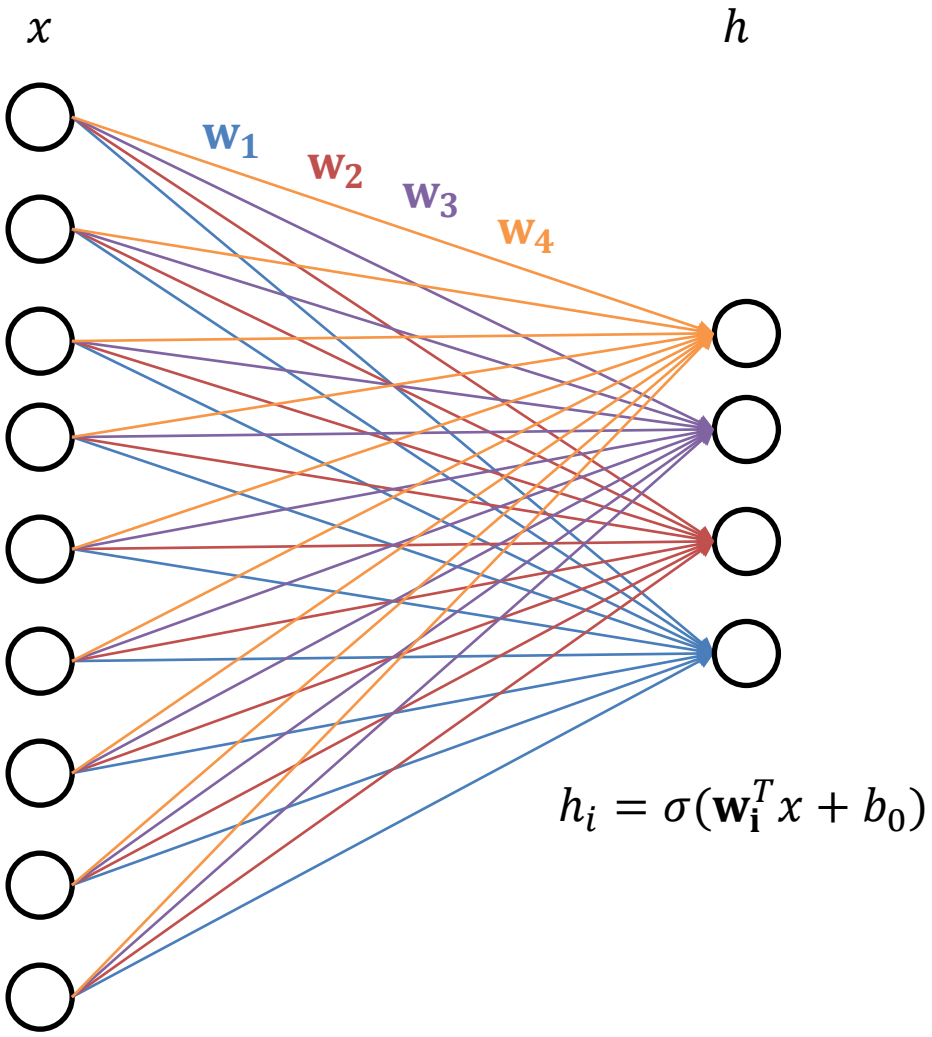
binary version is special case

Logistic Regression/Classification





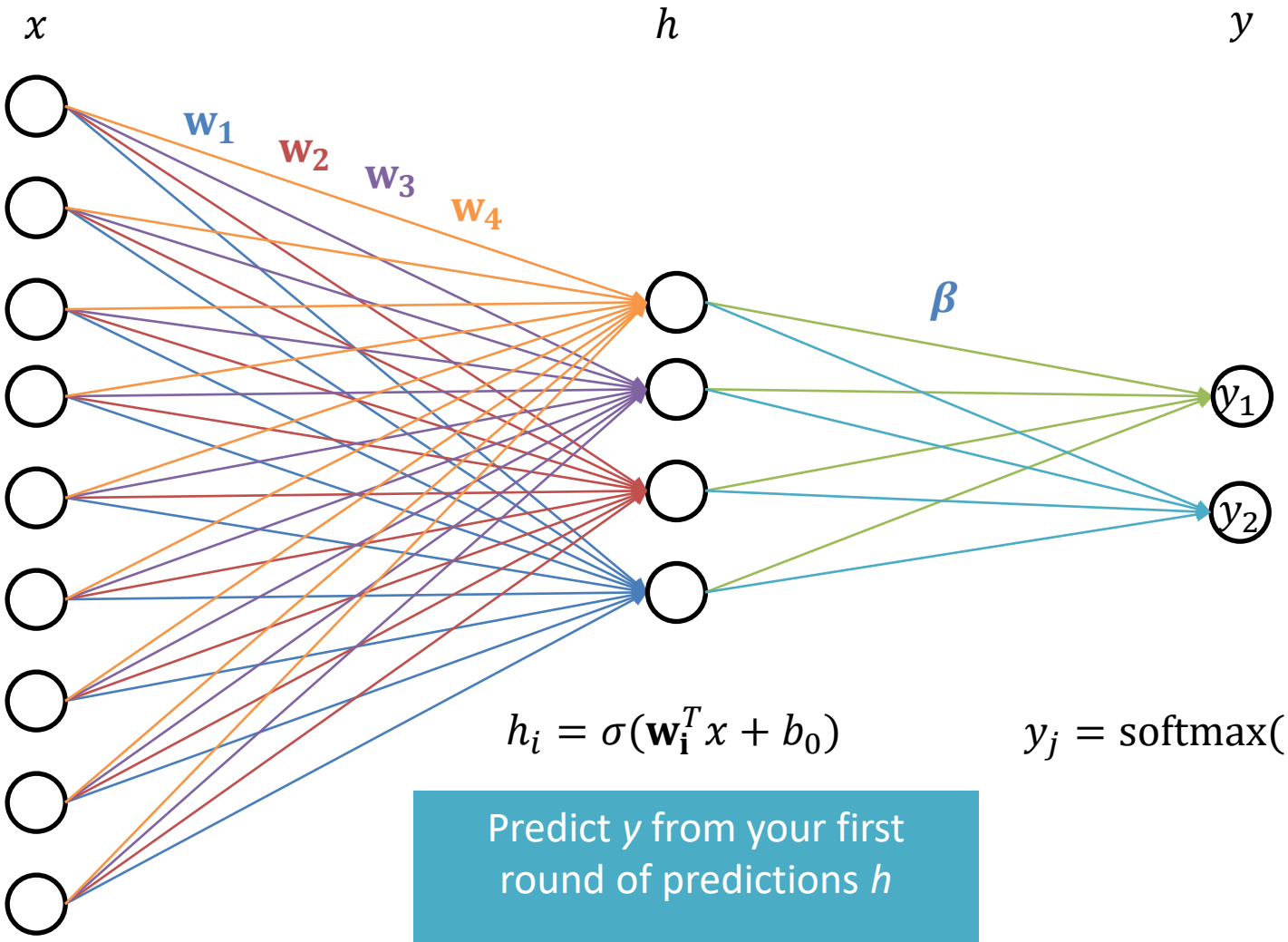
Stacking Logistic Regression



Goal: you still want to predict y

Idea: Can making an initial round of separate (independent) *binary* predictions *h* help?

Stacking Logistic Regression



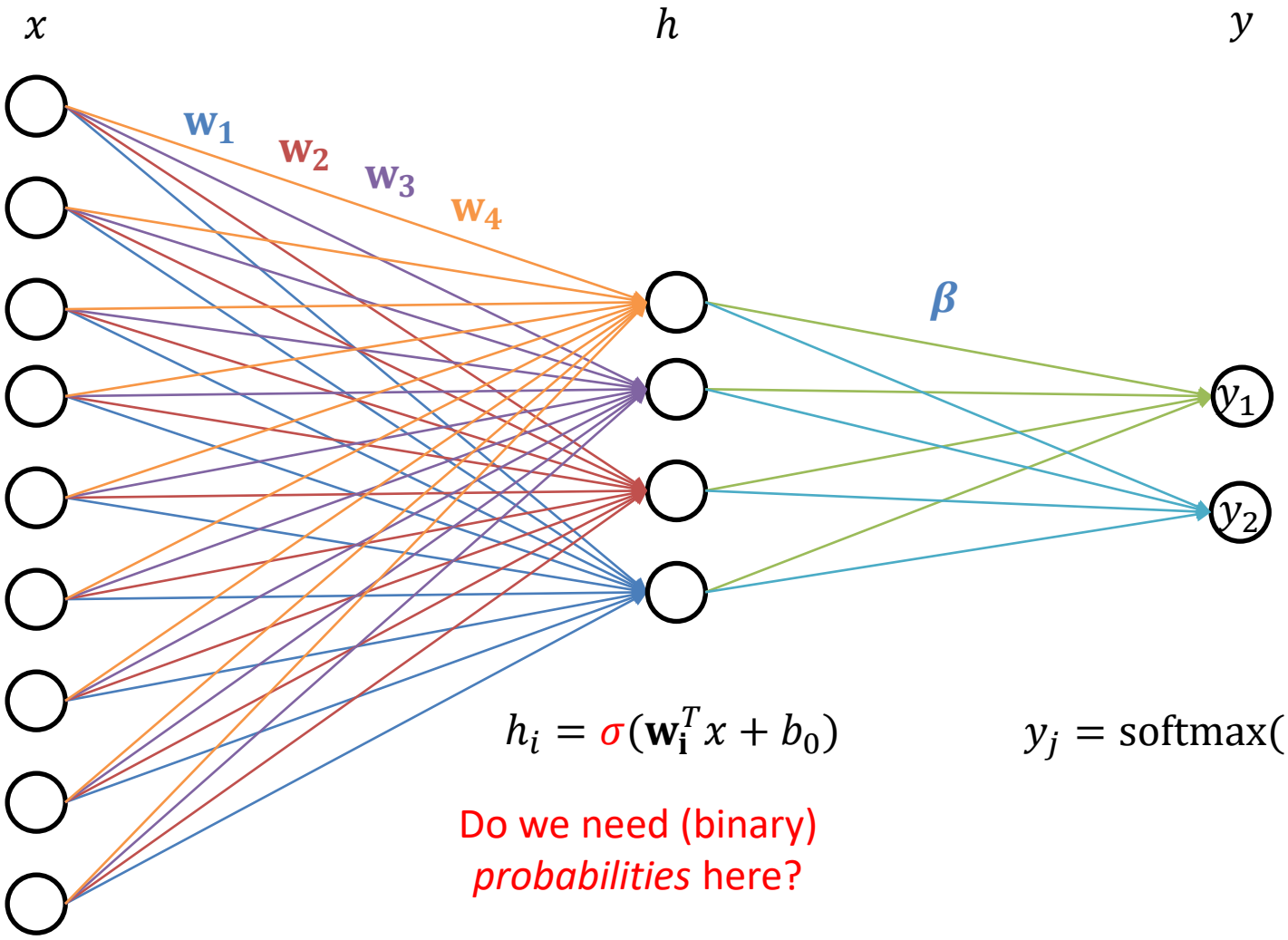
$$h_i = \sigma(\mathbf{w_i}^T x + b_0)$$

$$y_j = \text{softmax}(\boldsymbol{\beta_j}^T h + b_1)$$

Predict *y* from your first round of predictions *h*

Idea: data/signal compression

Stacking Logistic Regression

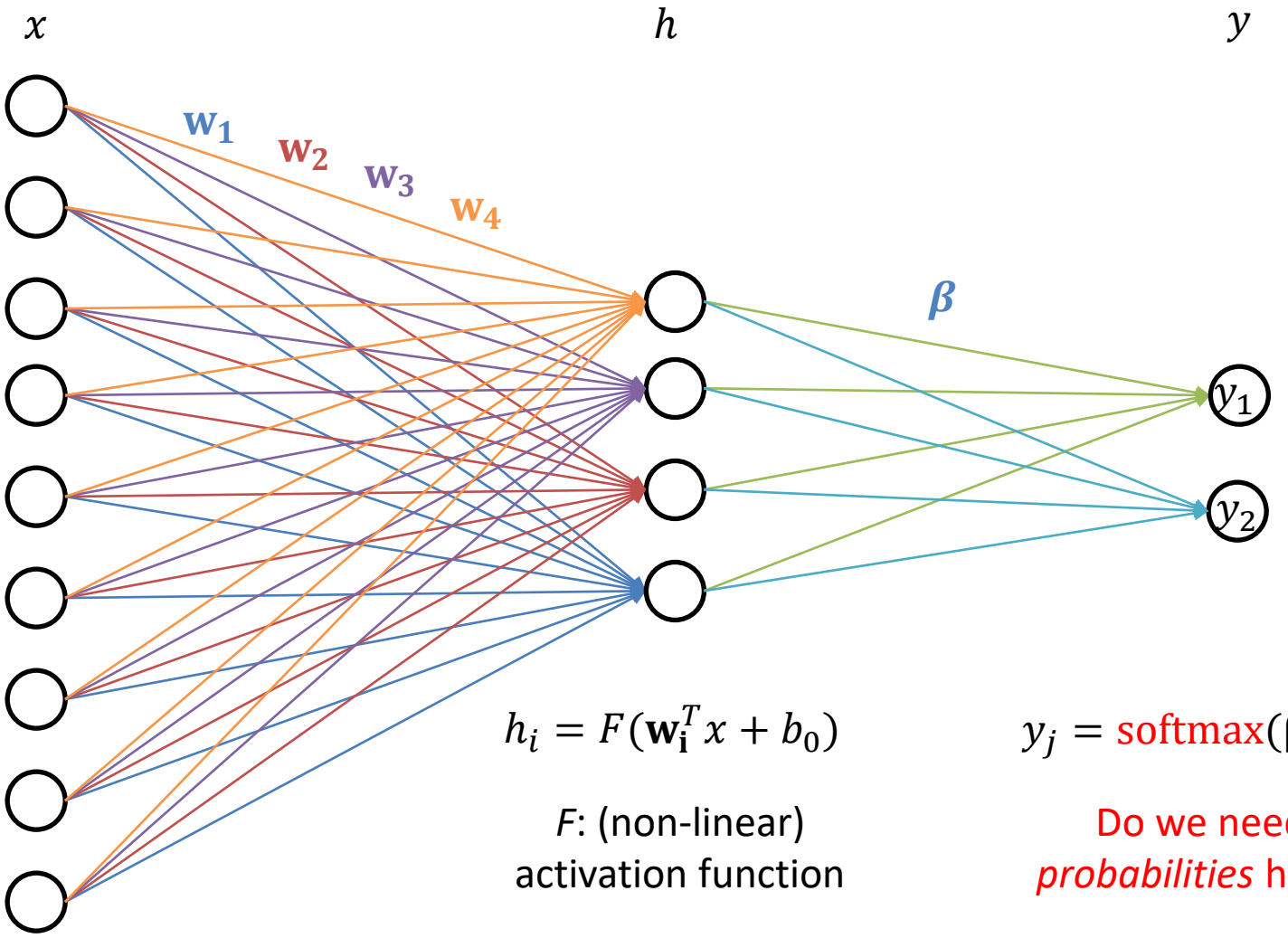


$$h_i = \sigma(\mathbf{w_i}^T x + b_0)$$

$$y_j = \text{softmax}(\boldsymbol{\beta_j}^T h + b_1)$$

Do we need (binary) *probabilities* here?

Stacking Logistic Regression



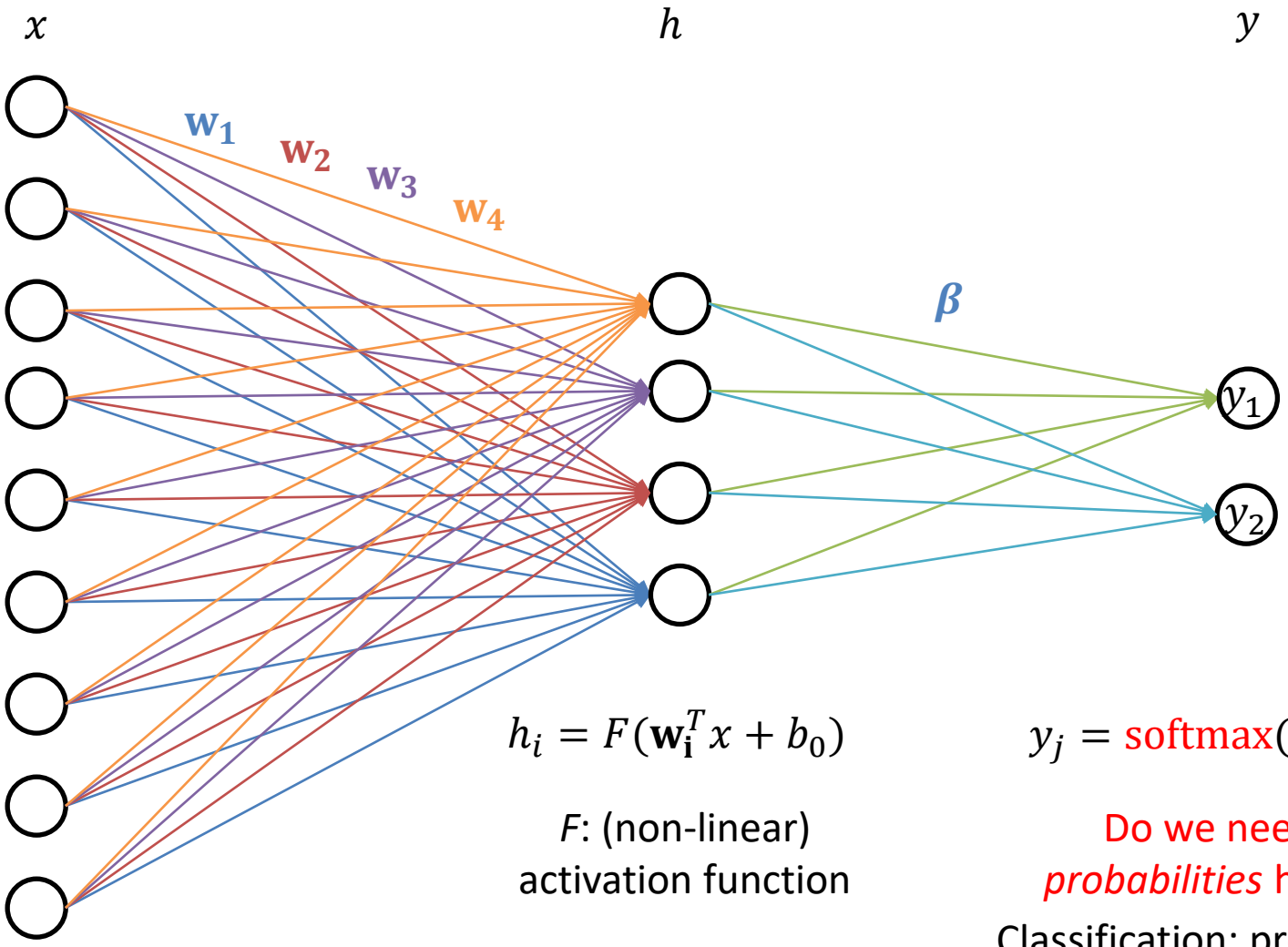
$$h_i = F(\mathbf{w_i}^T x + b_0)$$

F: (non-linear) activation function

$$y_j = \text{softmax}(\boldsymbol{\beta_j}^T h + b_1)$$

Do we need *probabilities* here?

Stacking Logistic Regression



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F: (non-linear) activation function

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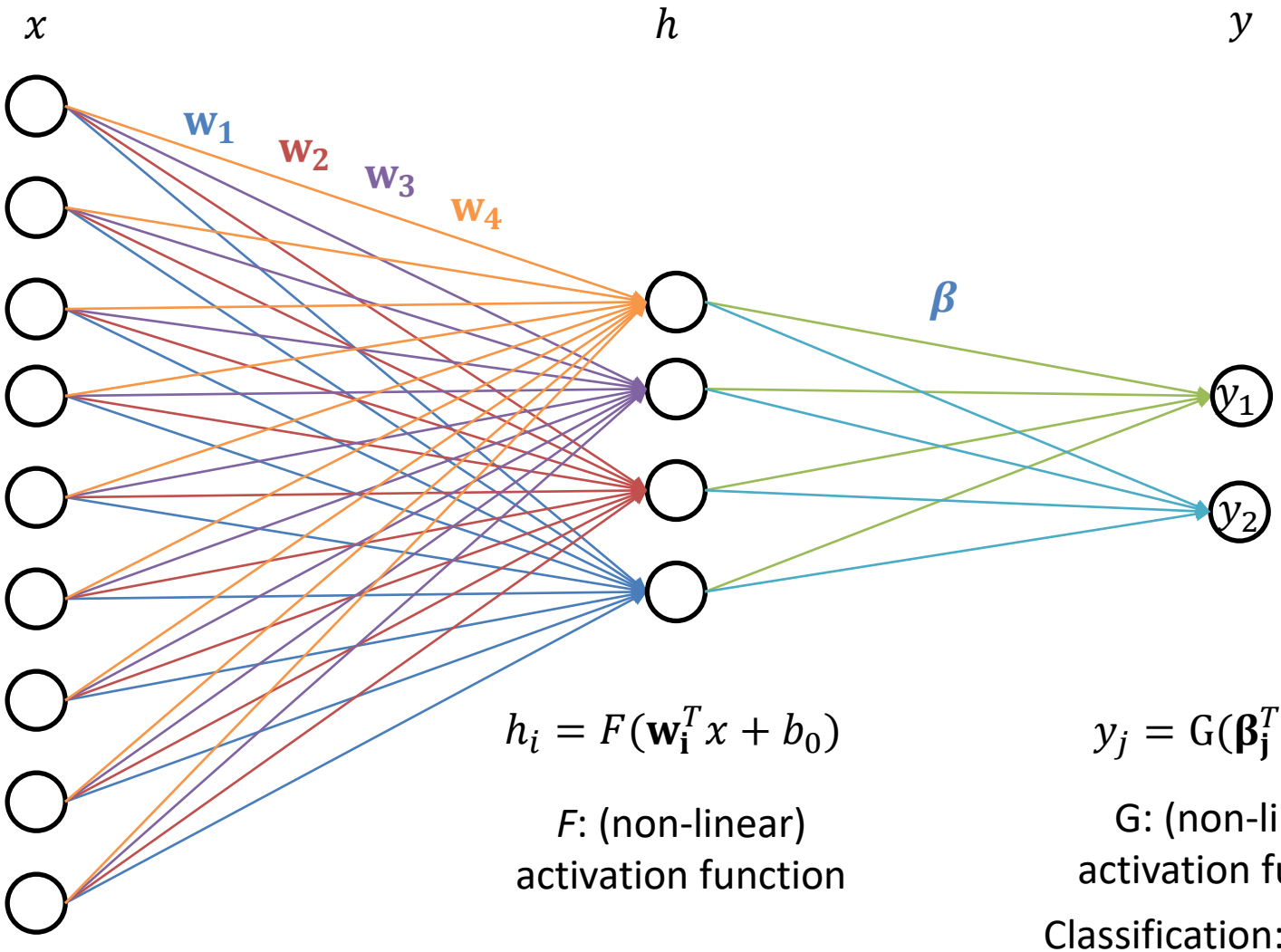
Do we need *probabilities* here?

Classification: probably

Regression: not really

Stacking Logistic Regression



$$h_i = F(\mathbf{w_i}^T x + b_0)$$

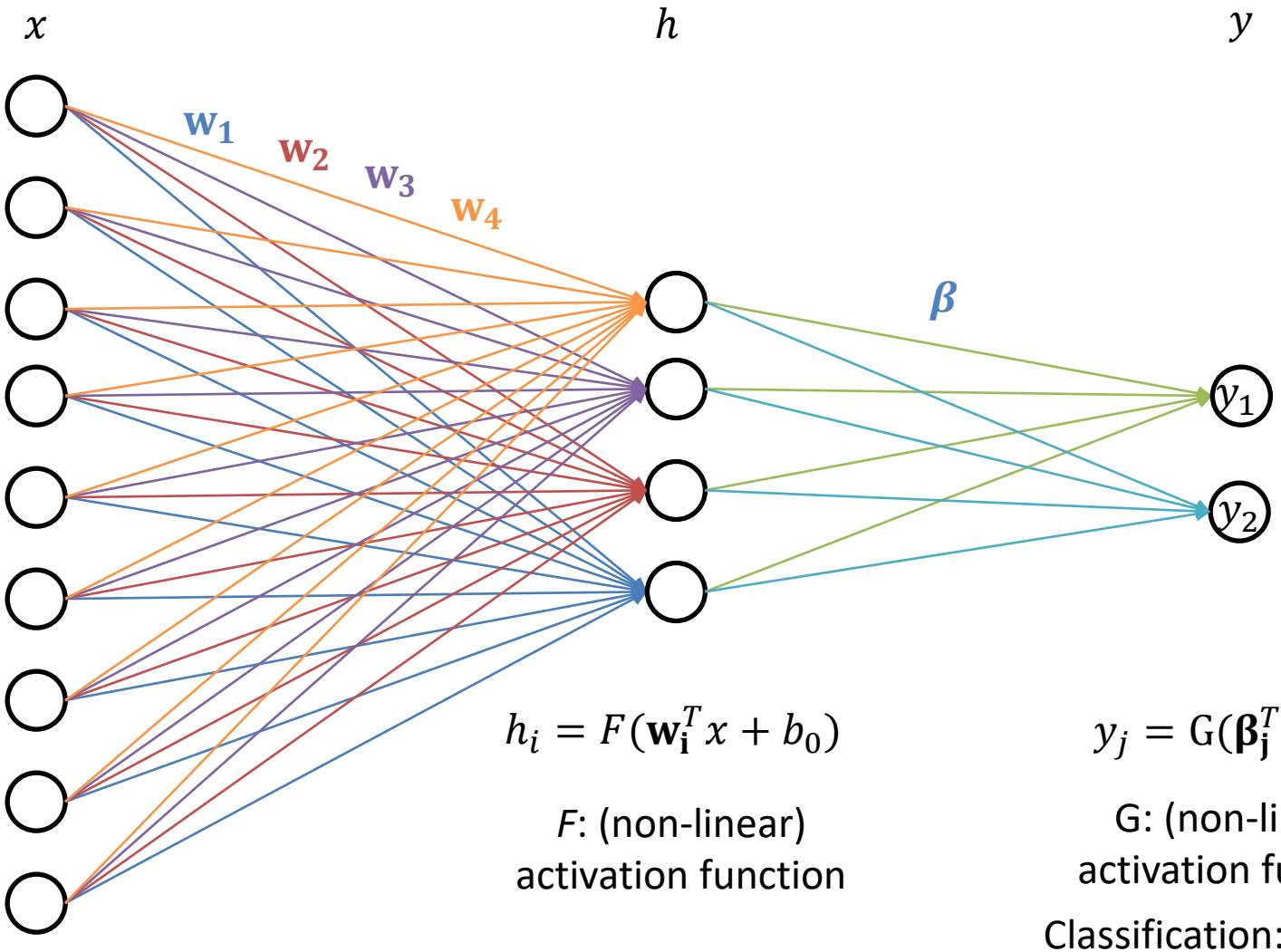
F: (non-linear) activation function

$$y_j = \mathrm{G}(\boldsymbol{\beta_j}^T h + b_1)$$

G: (non-linear) activation function

Classification: softmax
Regression: identity

Multilayer Perceptron, a.k.a. Feed-Forward Neural Network



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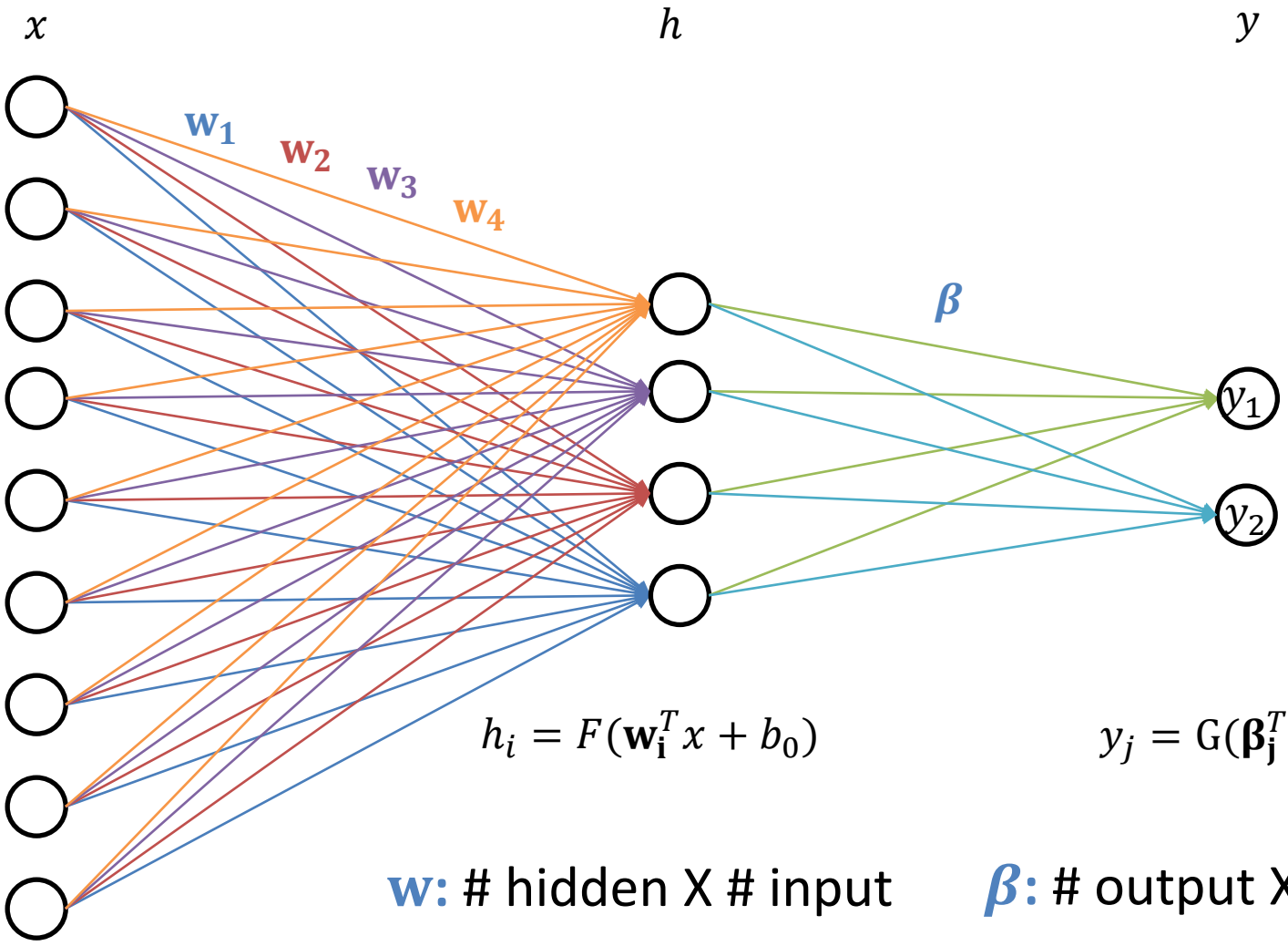
Classification: softmax

Regression: identity

Feed-Forward Neural Network



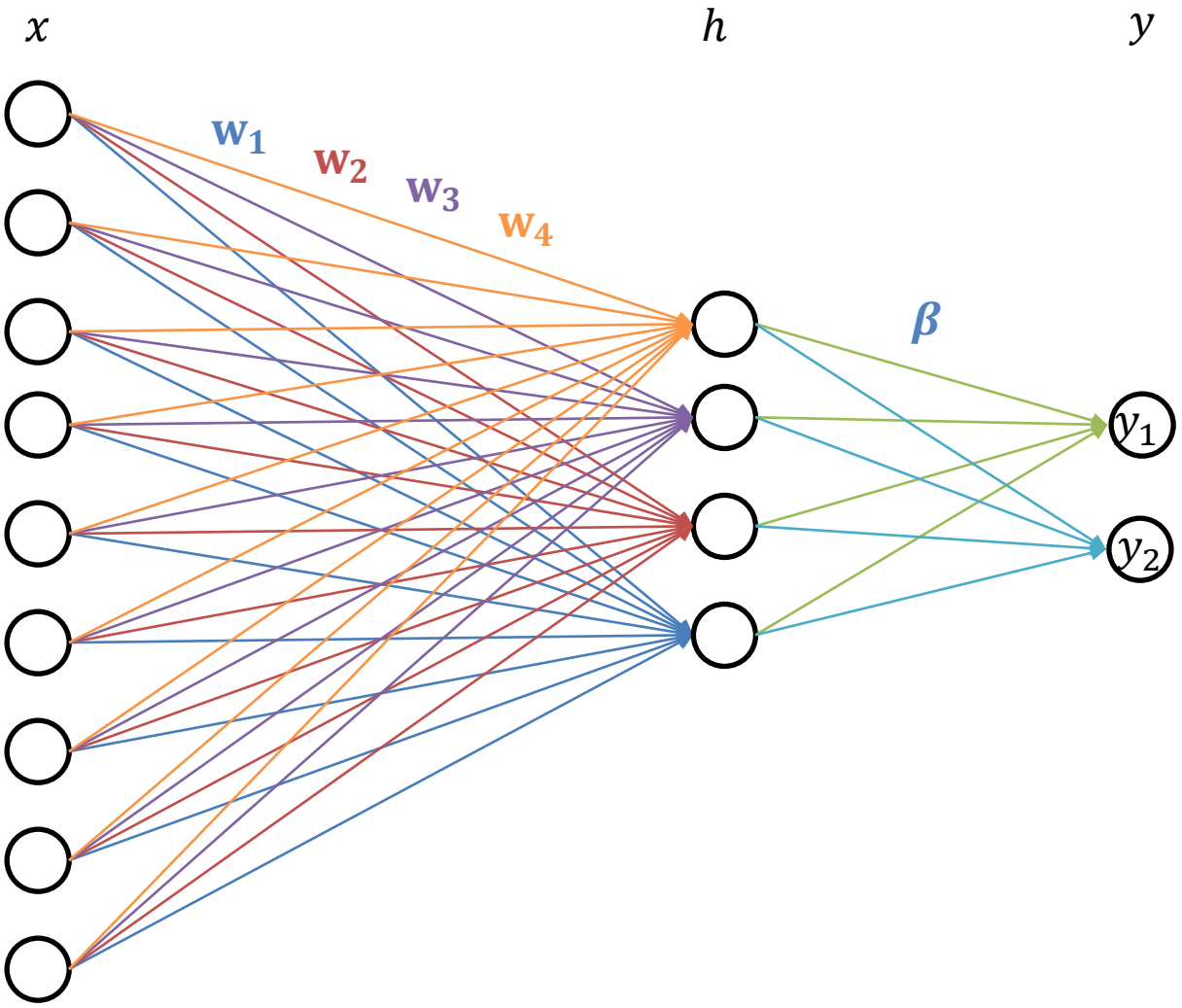
$$h_i = F(\mathbf{w_i}^T x + b_0)$$

$$y_j = \mathrm{G}(\boldsymbol{\beta_j}^T h + b_1)$$

w: # hidden X # input

$\boldsymbol{\beta}$: # output X # hidden

Why Non-Linear?

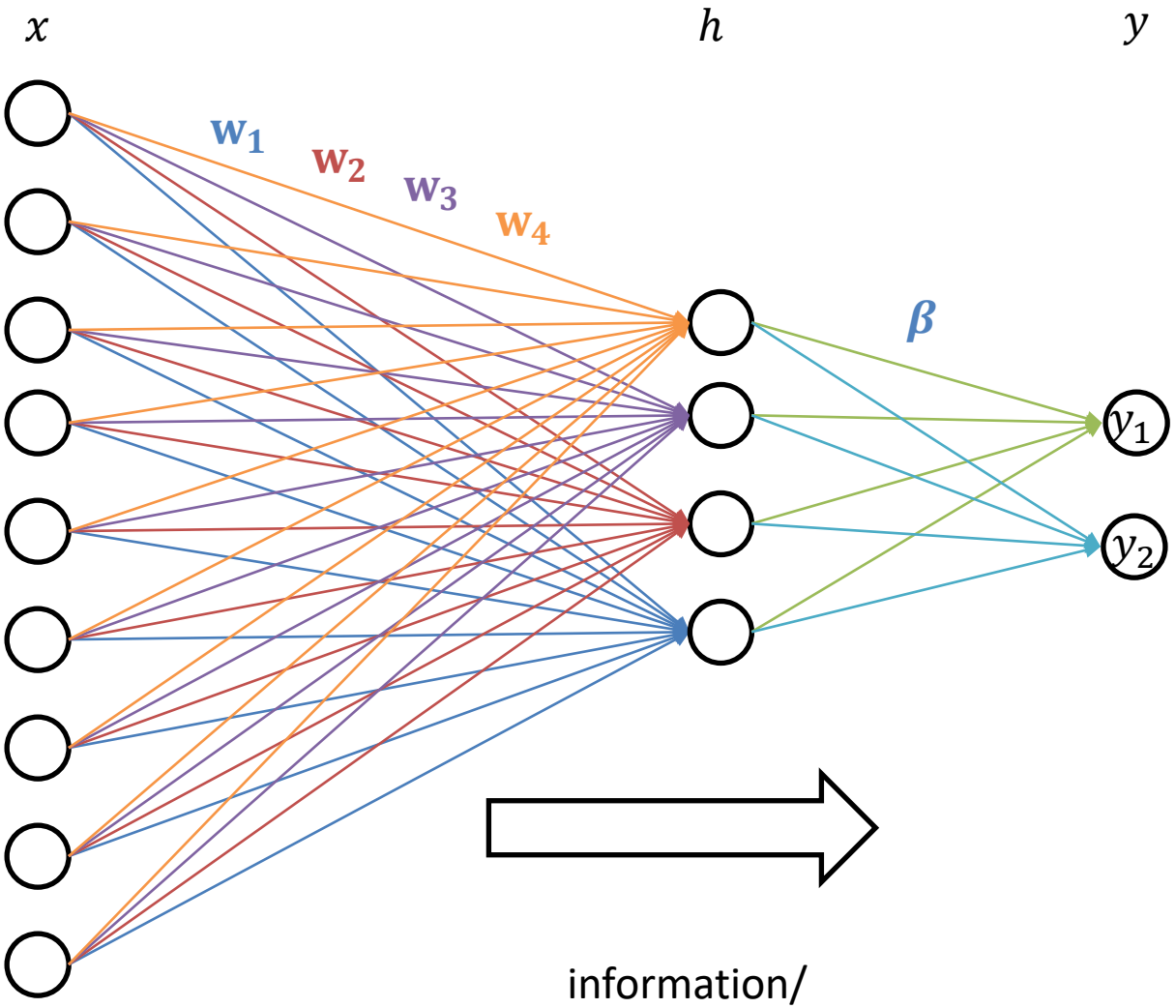


$$y_j = \mathrm{G}\left(\boldsymbol{\beta}_j^T h + b_1\right)$$

$$\Downarrow$$

$$y_j = G\left(\beta_j^T\left(F\left(w_i^T x + b_0\right)\right)_i\right)$$

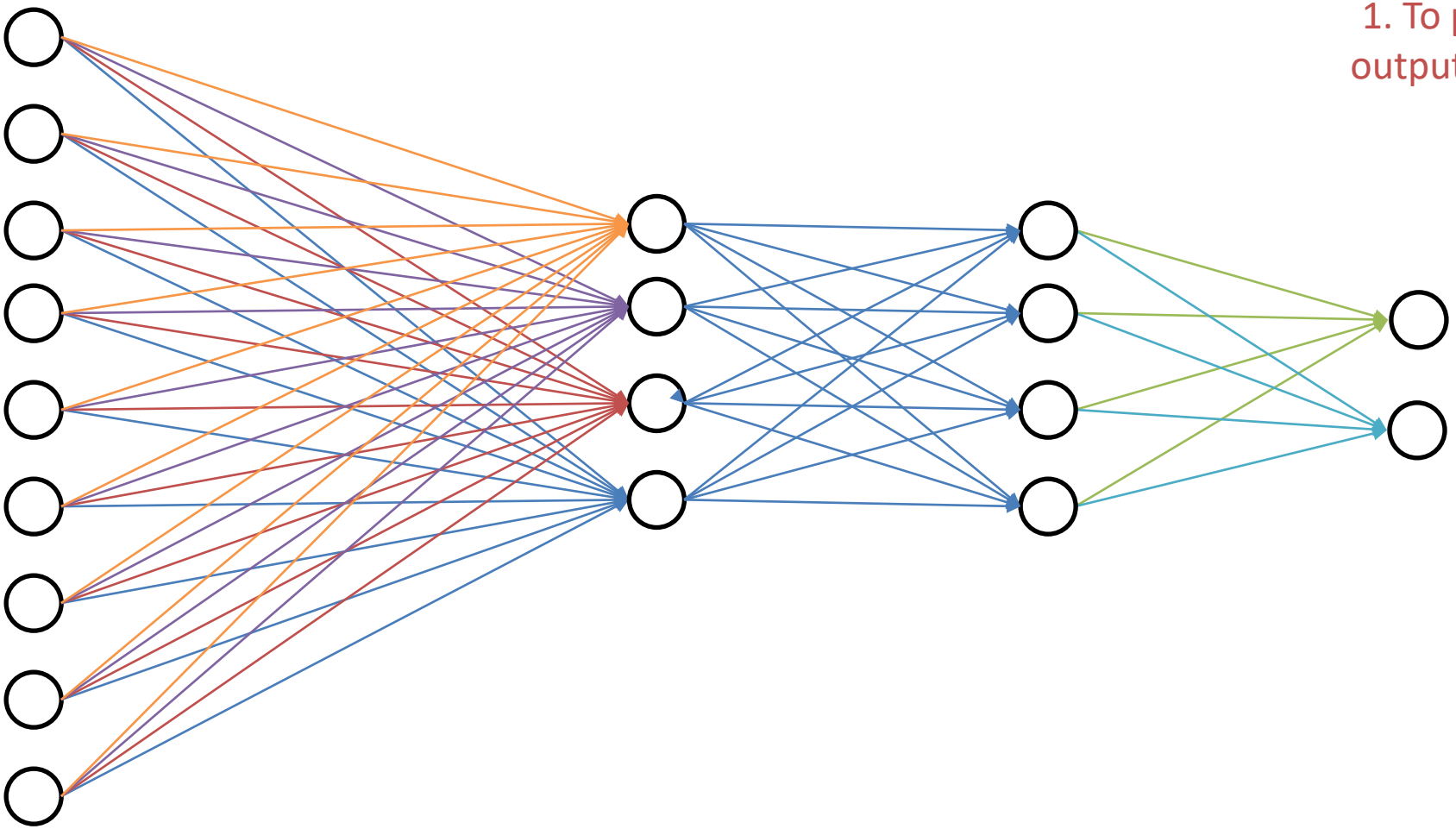
Feed-Forward



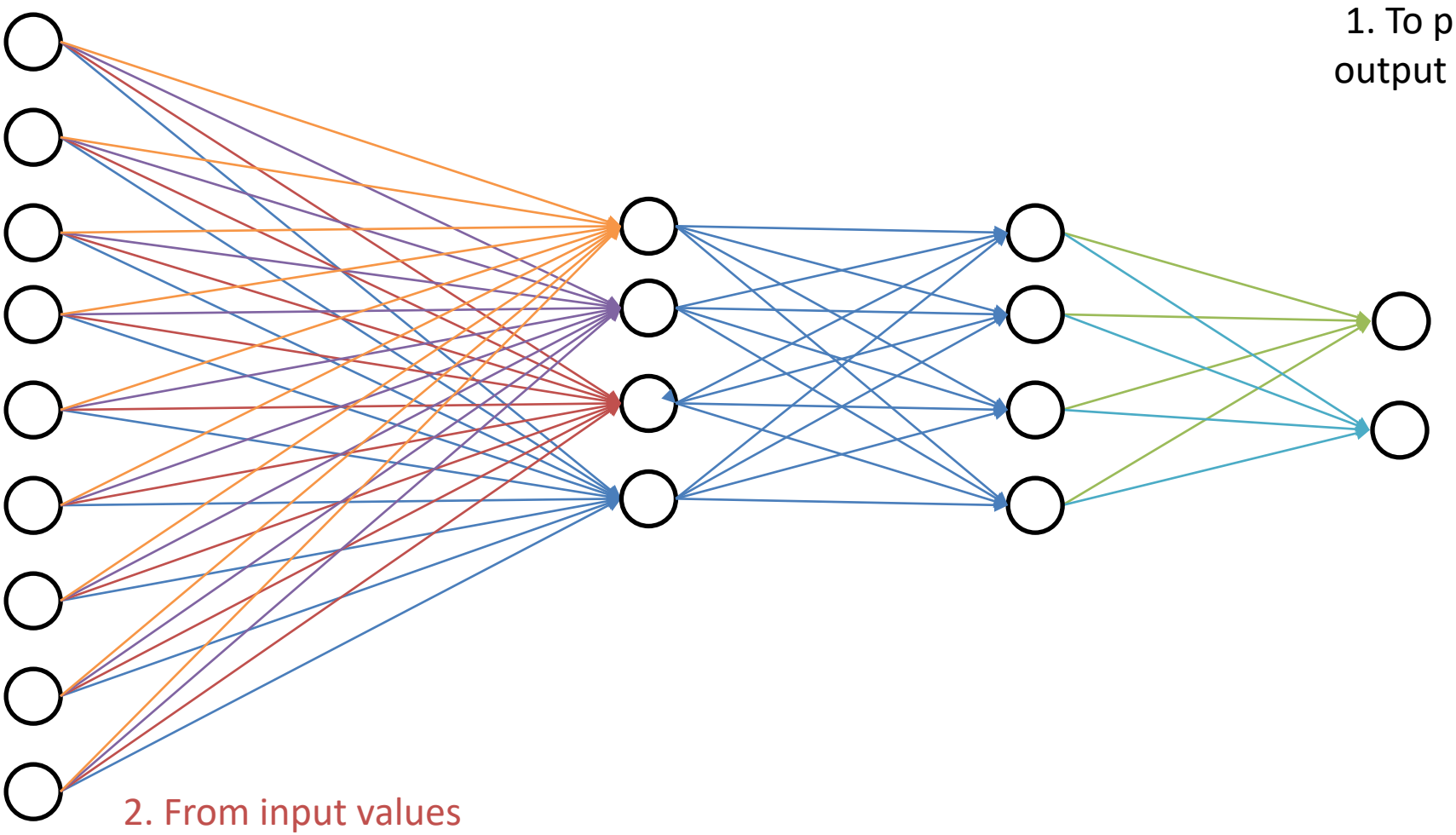
information/
computation flow

no self-loops
(recurrence/reuse of weights)

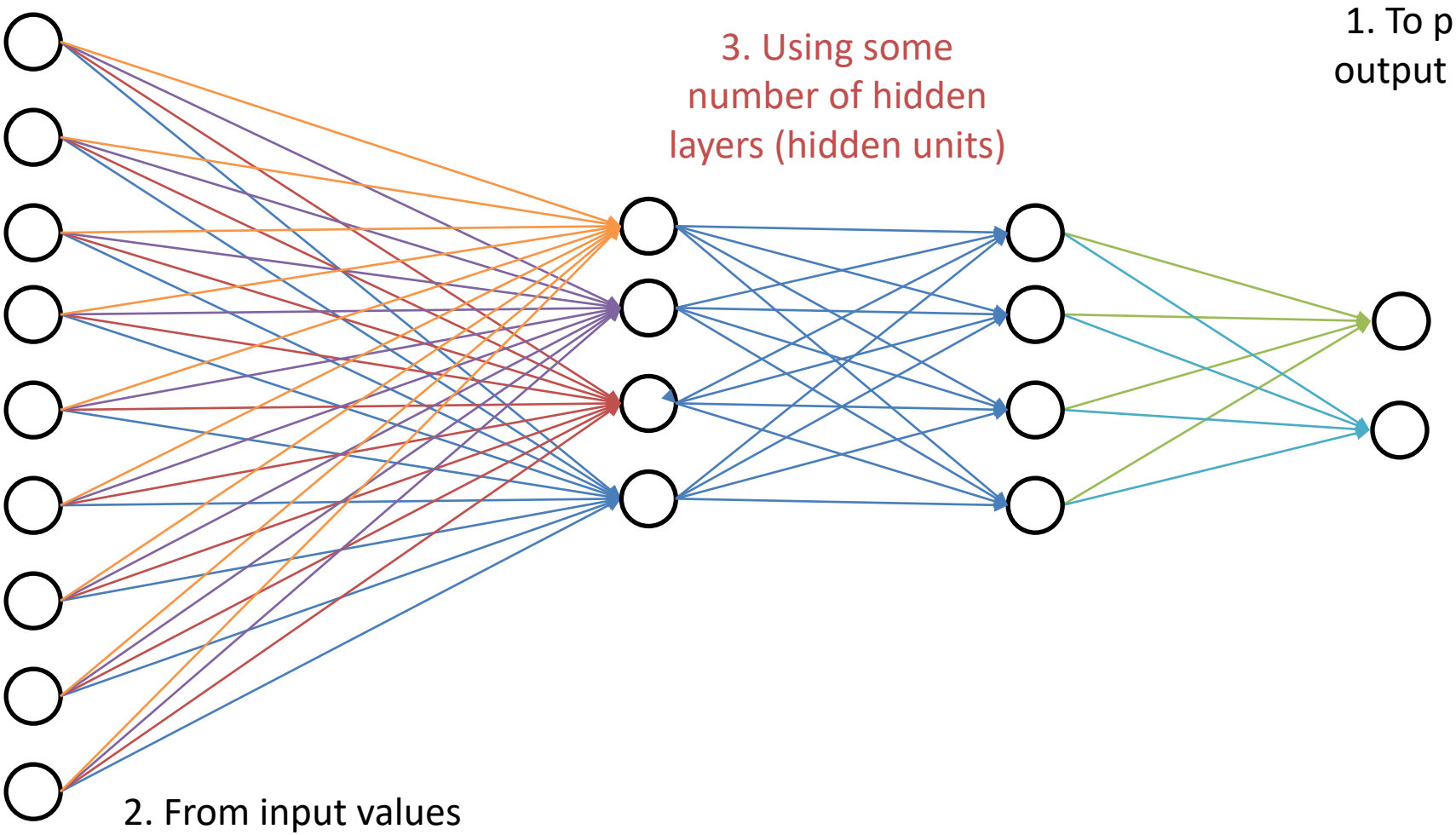
A Neural Network is a Machine Learning System…



A Neural Network is a Machine Learning System…



A Neural Network is a Machine Learning System…



Universal Function Approximator

Theorem [Kurt Hornik et al., 1989]: Let F be a continuous function on a bounded subset of D-dimensional space. Then there exists a two-layer network G with finite number of hidden units that approximates F arbitrarily well. For all x in the domain of F, $|F(x) - G(x)| < \varepsilon$

"a two-layer network can approximate any function"

Going from one to two layers dramatically improves the representation power of the network

How Deep Can They Be?

So many choices:

Architecture

# of hidden layers

# of units per hidden layer

Computational Issues:

Vanishing gradients

Gradients shrink as one moves away from the output layer

Convergence is slow

Opportunities:

Training deep networks is an active area of research

Layer-wise initialization (perhaps using unsupervised data)

Engineering: GPUs to train on massive labelled datasets

Slide courtesy Hamed Pirsiavash

Some Results: Digit Classification

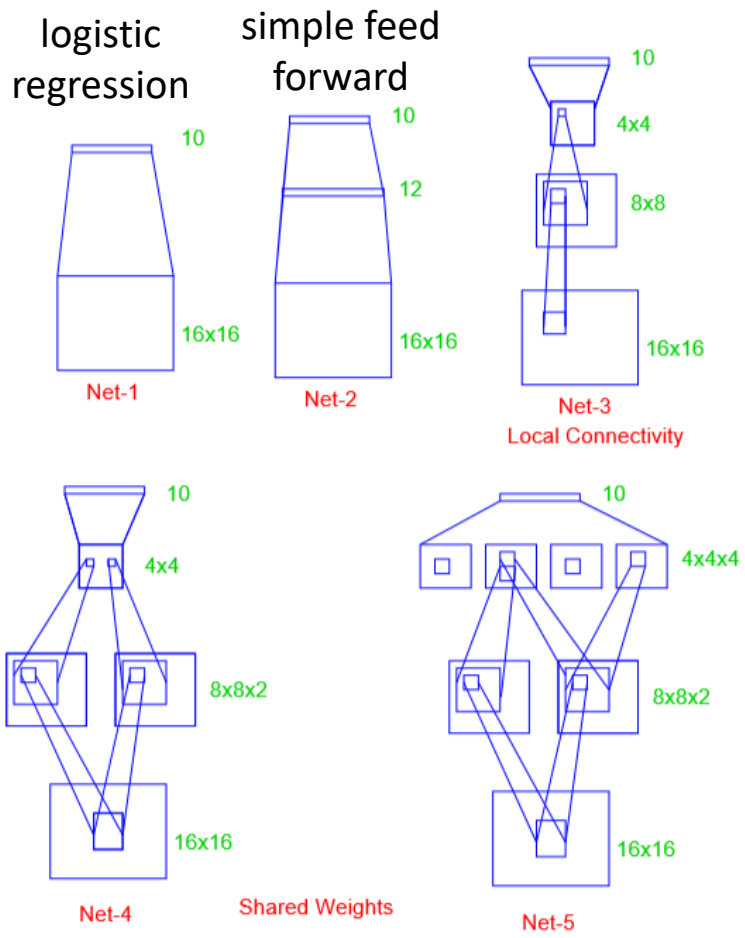


FIGURE 11.10. *Architecture of the five networks used in the ZIP code example.*

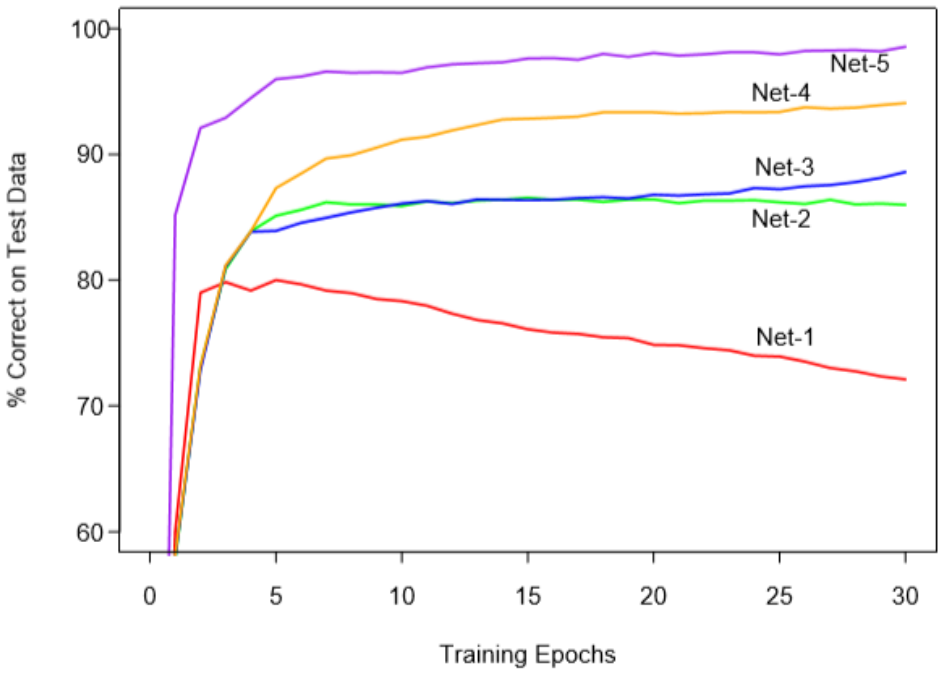


FIGURE 11.11. *Test performance curves, as a function of the number of training epochs, for the five networks of Table 11.1 applied to the ZIP code data.*

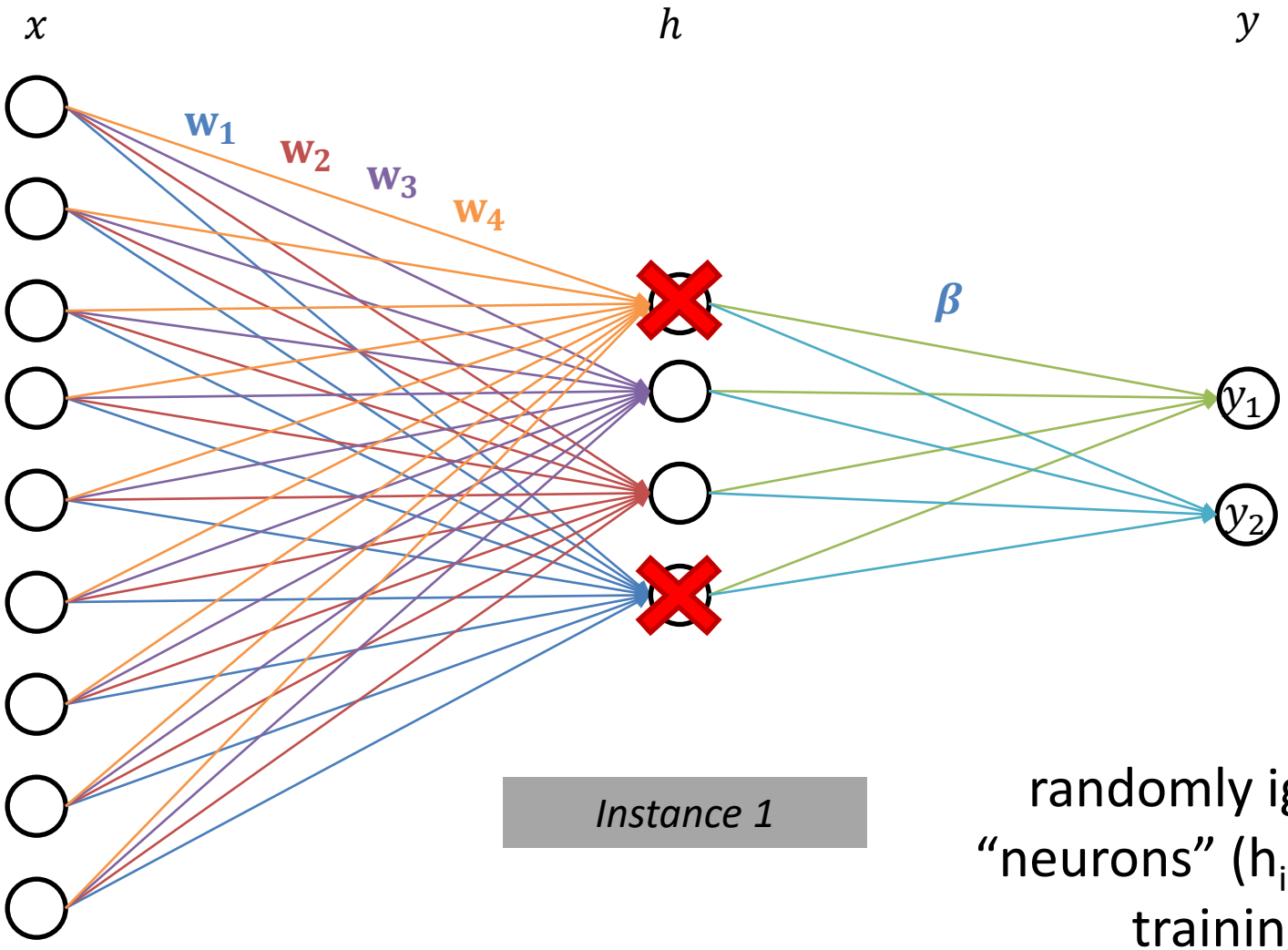
Tensorflow Playground

http://playground.tensorflow.org

Experiment with small (toy) data neural networks in your browser

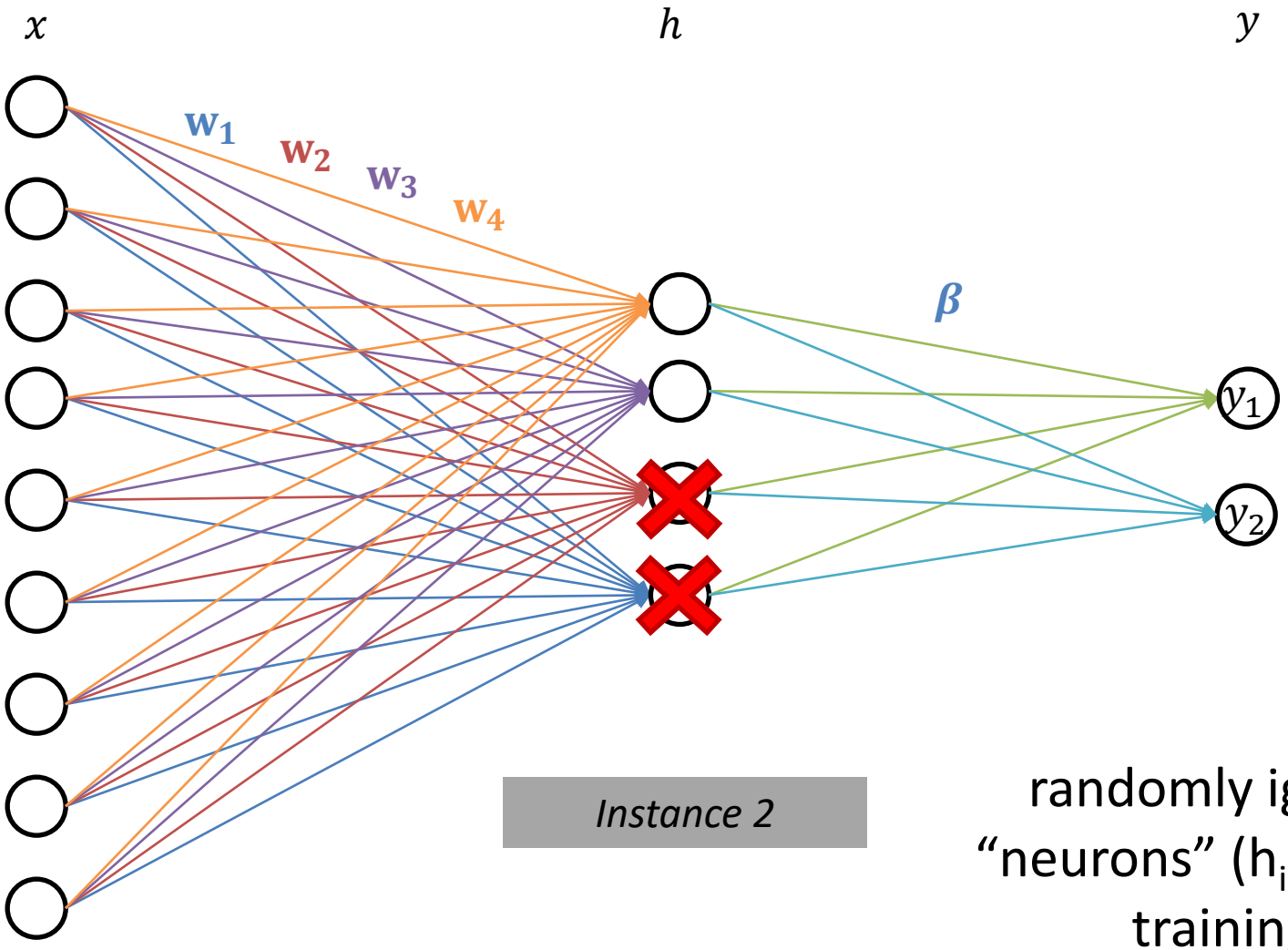
Feel free to use this to gain an intuition

Dropout: Regularization in Neural Networks



randomly ignore "neurons" (h_i) during training

Dropout: Regularization in Neural Networks



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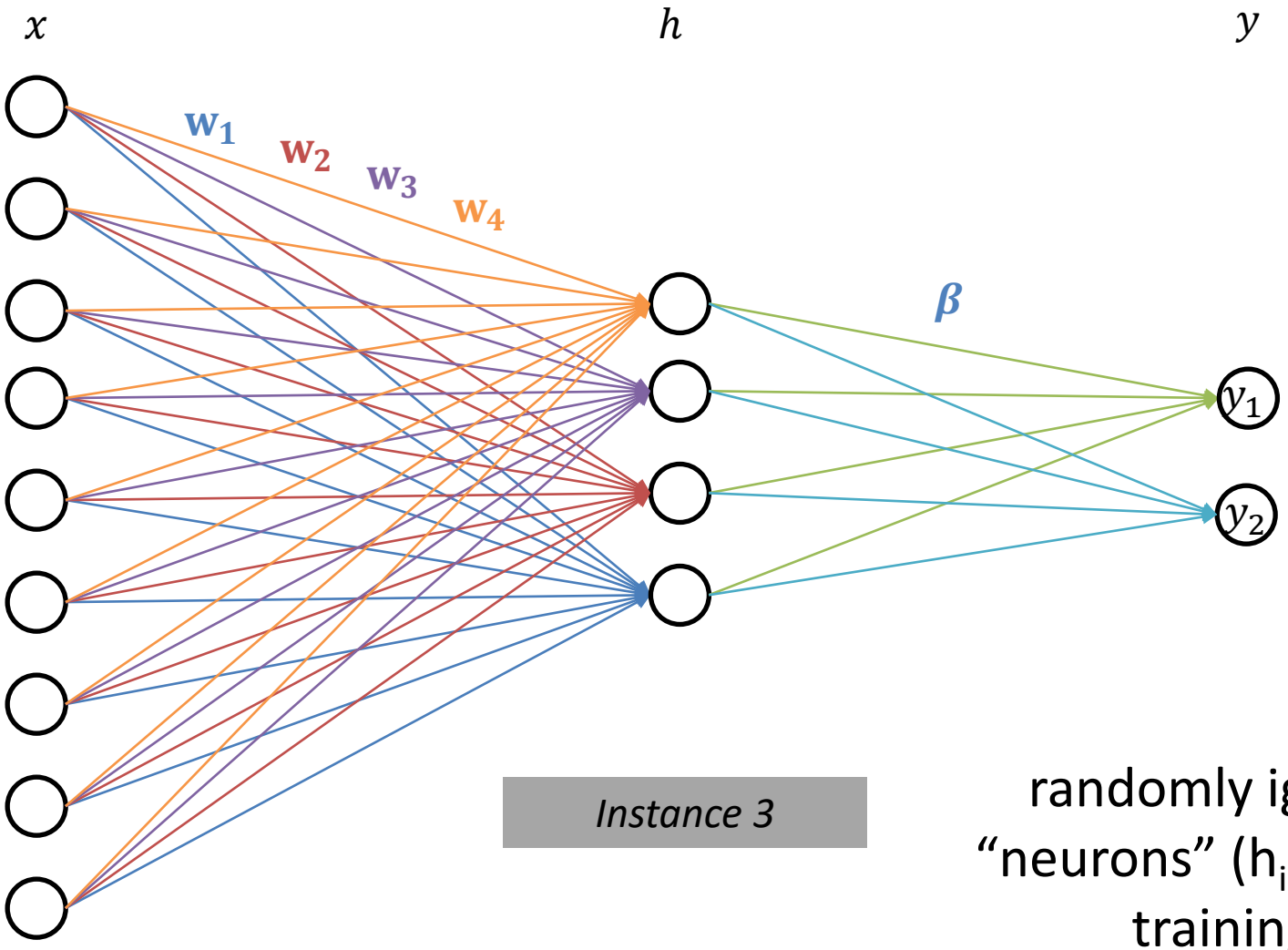
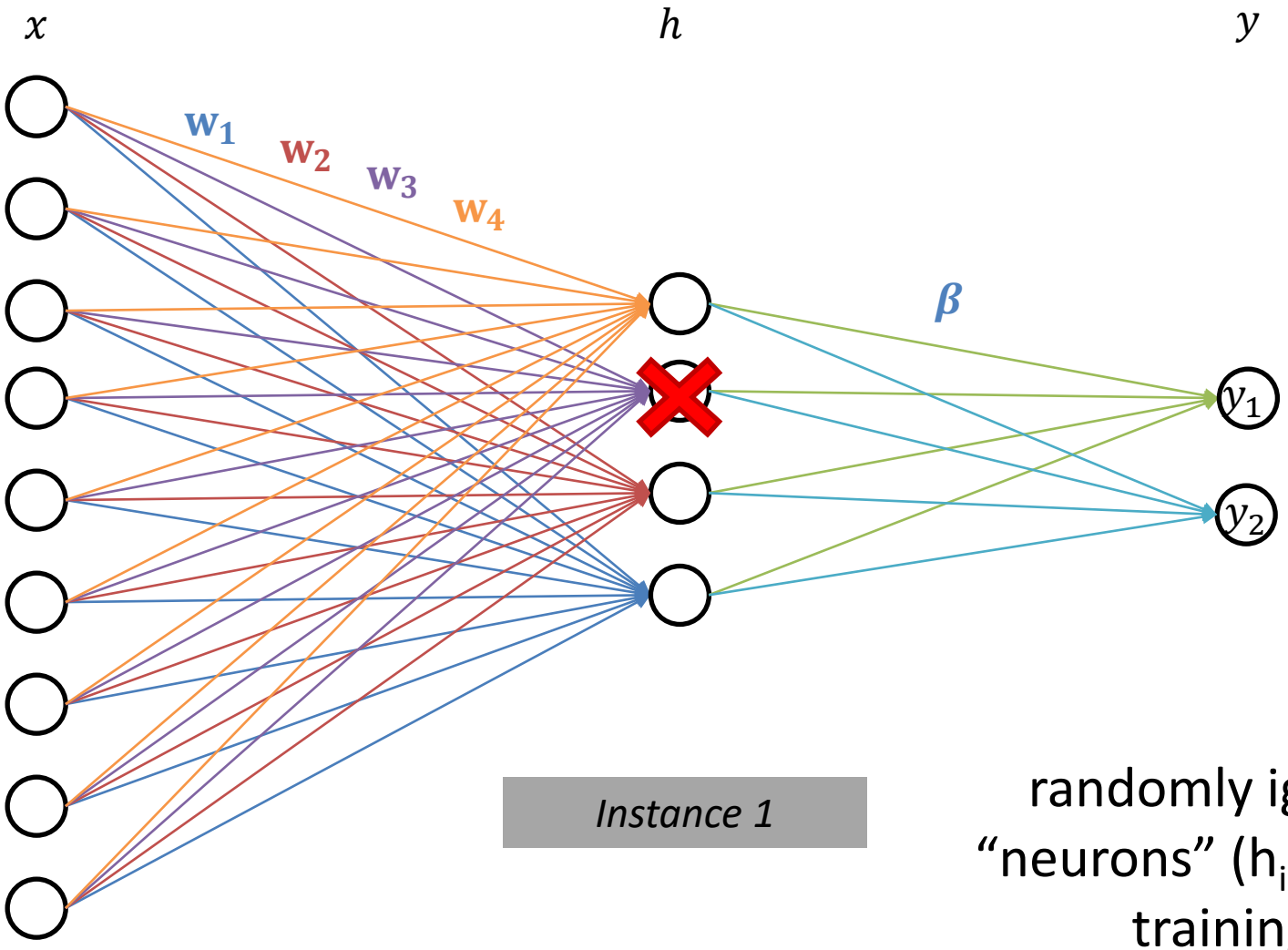


randomly ignore "neurons" (h_i) during training

Dropout: Regularization in Neural Networks

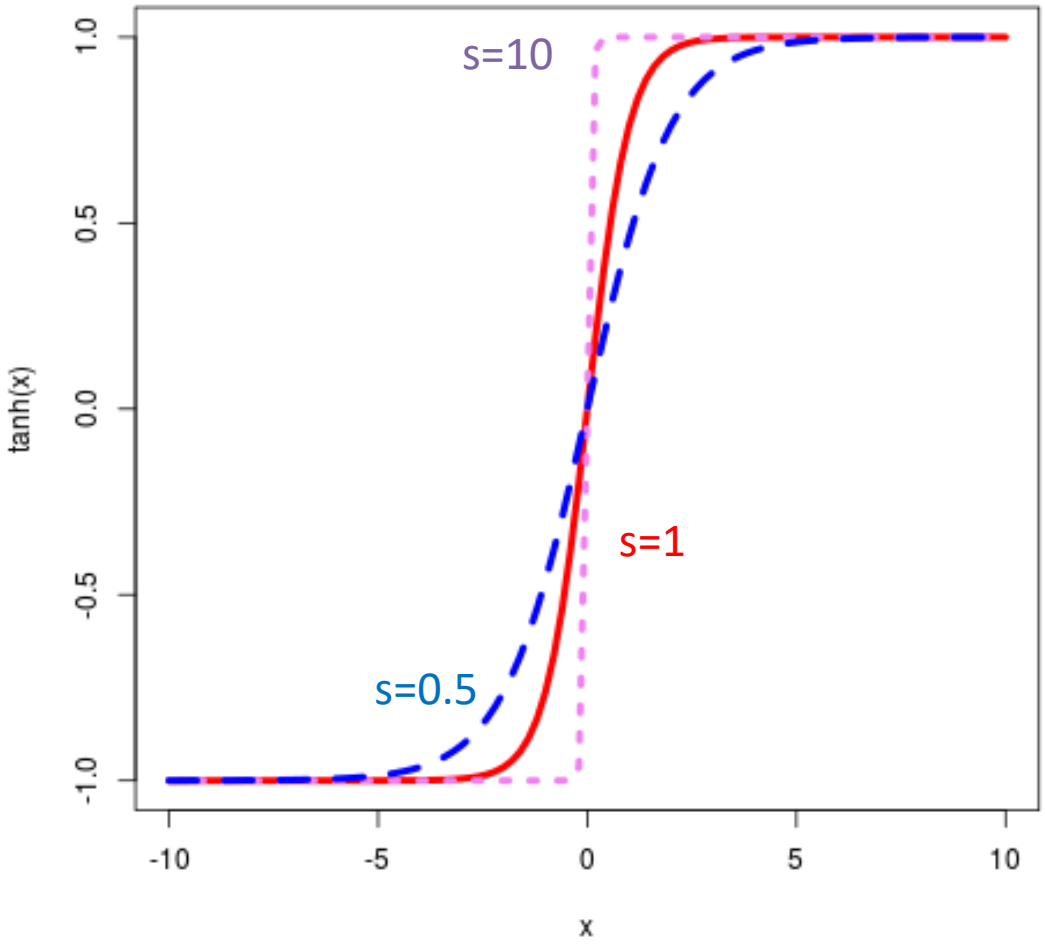


randomly ignore "neurons" (h_i) during training

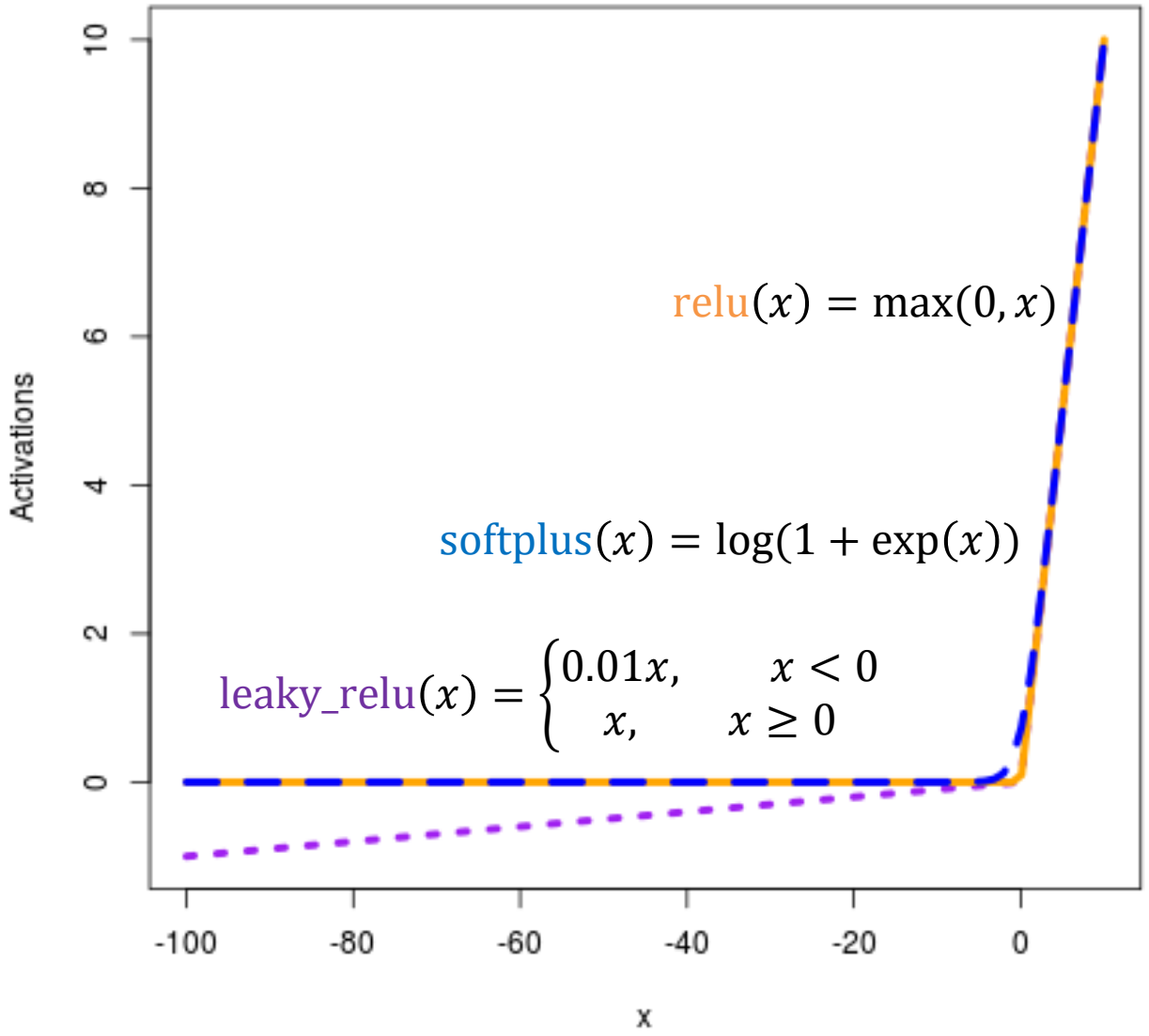
tanh Activation

$$\tanh_s(x) = \frac{2}{1 + \exp(-2 * s * x)} - 1$$

$$= 2\sigma_s(x) - 1$$

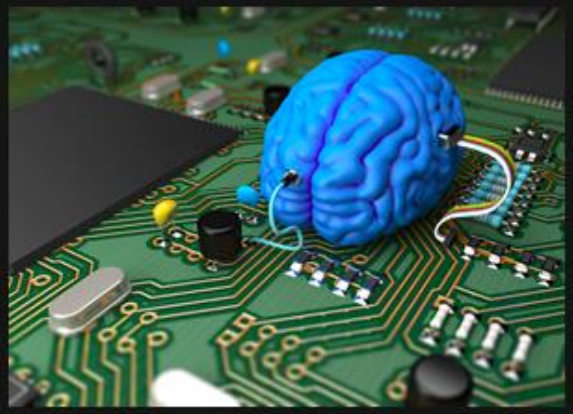


Rectifiers Activations



Deep Learning

What society thinks I do



What my friends think I do

What other computer scientists think I do

What mathematicians think I do

What I think I do

```
from [redacted] import *
```

keras
torch

What I actually do

Typical Python Libraries

numpy, scipy

- Basic mathematical libraries for dealing with matrices and scientific/mathematical functions

pandas, matplotlib

- Libraries for data science & plotting

sklearn (scikit-learn)

- A whole bunch of implemented classifiers

torch (pytorch) and tensorflow

- Frameworks for building neural networks

Lots of documentation available for all of these online!

For Spring 2021 CMSC 471: Everything after this slide is beyond the normal course scope. You are not responsible for knowing it.

Outline

Neural networks: non-linear classifiers

Learning weights: backpropagation of error

Autodifferentiation (in reverse mode)

Empirical Risk Minimization

Cross entropy loss

$$\ell^{\text{xent}}\left(\overrightarrow{y^*}, y\right) = -\sum_k \overrightarrow{y^*}[k] \log p(y = k)$$

mean squared error/L2 loss

$$\ell^{\text{L2}}(y^*, y) = (y^* - y)\text{^}2$$

squared expectation loss

$$\ell^{\text{sq-expt}}\left(\overrightarrow{y^*}, y\right) = \left|\overrightarrow{y^*} - p(y)\right|_2^2$$

hinge loss

$$\ell^{\text{hinge}}\left(\overrightarrow{y^*}, y\right) = \max\left\{0, 1 + \max_{j \neq y^*}\left(y[j] - \overrightarrow{y^*}[j]\right)\right\}$$

Gradient Descent: Backpropagate the Error

Set t = 0

Pick a starting value θ_t

Until converged:

for example(s) i:

1. Compute loss l on x_i
2. Get gradient $g_t = l'(x_i)$
3. Get scaling factor ρ_t
4. Set $\theta_{t+1} = \theta_t - \rho_t * g_t$
5. Set t += 1

(mini)batch

epoch

epoch: a single run over all training data

(mini-)batch: a run over a subset of the data

Flavors of Gradient Descent

"Online"

Set t = 0
Pick a starting value θ_t
Until converged:

for example i in full data:

1. Compute loss l on x_i
2. Get gradient $g_t = l'(x_i)$
3. Get scaling factor ρ_t
4. Set $\theta_{t+1} = \theta_t - \rho_t * g_t$
5. Set t += 1

done

"Minibatch"

Set t = 0
Pick a starting value θ_t
Until converged:
get batch B ⊂ full data
set $g_t = 0$
for example(s) i in B:

1. Compute loss l on x_i
2. Accumulate gradient g_t += $l'(x_i)$

done
Get scaling factor ρ_t
Set $\theta_{t+1} = \theta_t - \rho_t * g_t$
Set t += 1

"Batch"

Set t = 0
Pick a starting value θ_t
Until converged:

set $g_t = 0$
for example(s) i in full data:

1. Compute loss l on x_i
2. Accumulate gradient g_t += $l'(x_i)$

done
Get scaling factor ρ_t
Set $\theta_{t+1} = \theta_t - \rho_t * g_t$
Set t += 1

Gradients for Feed Forward Neural Network

$$y_k = \sigma\left(\beta_k^T \underbrace{\left(\sigma\left(w_j^T x + b_0\right)\right)_j}_{h}\right)$$

h: a vector

$$\mathcal{L} = -\sum_k \overrightarrow{y^*}[k] \log y_k$$

$$\frac{\partial \mathcal{L}}{\partial \beta_{kj}} = \frac{-1}{y_{y^*}} \frac{\partial y_{y^*}}{\partial \beta_{kj}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{jl}}$$

Gradients for Feed Forward Neural Network

$$y_k = \sigma\left(\beta_k^T \underbrace{\left(\sigma\left(w_j^T x + b_0\right)\right)_j}_{h\text{: a vector}}\right) \qquad \mathcal{L} = -\sum_k \overrightarrow{y^*}[k] \log y_k$$

$$\frac{\partial \mathcal{L}}{\partial \beta_{kj}} = \frac{-1}{y_{y^*}} \frac{\partial y_{y^*}}{\partial \beta_{kj}} = \frac{-\sigma'\left(\beta_{y^*}^T h\right)}{\sigma\left(\beta_{y^*}^T h\right)} \frac{\partial \beta_k^T h}{\partial \beta_{kj}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{jl}}$$

Gradients for Feed Forward Neural Network

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$$\frac{\partial \mathcal{L}}{\partial w_{jl}}$$

Gradients for Feed Forward Neural Network

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h: a vector

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$$= \left(1 - \sigma\left(\beta_{y^*}^T h\right)\right) h_j$$

$$\frac{\partial \mathcal{L}}{\partial w_{jl}} = \left(1 - \sigma\left(\beta_{y^*}^T h\right)\right) \left(\beta_{y^* j} \sigma'\left(w_j^T x\right) x_l\right)$$

Gradients for Feed Forward Neural Network

$$y_k = \sigma\left(\beta_k^T \underbrace{\left(\sigma\left(w_j^T x + b_0\right)\right)_j}_{h\text{: a vector}}\right) \qquad \mathcal{L} = -\sum_k \overrightarrow{y^*}[k] \log y_k$$

$$\frac{\partial \mathcal{L}}{\partial \beta_{kj}} = \left(1 - \sigma\left(\beta_{y^*}^T h\right)\right) h_j$$

$$\frac{\partial \mathcal{L}}{\partial w_{jl}} = \left(1 - \sigma\left(\beta_{y^*}^T h\right)\right)\left(\beta_{y^* j}\sigma'\left(w_j^T x\right)x_l\right)$$

Debugging can be hard to do!

Gradients for Feed Forward Neural Network

$$y_k = \sigma\left(\beta_k^T \underbrace{\left(\sigma\left(w_j^T x + b_0\right)\right)_j}_{h\text{: a vector}}\right)$$

$$\mathcal{L} = -\sum_k \overrightarrow{y^*}[k] \log y_k$$

$$\frac{\partial \mathcal{L}}{\partial \beta_{kj}} = \left(1 - \sigma\left(\beta_{y^*}^T h\right)\right) h_j$$

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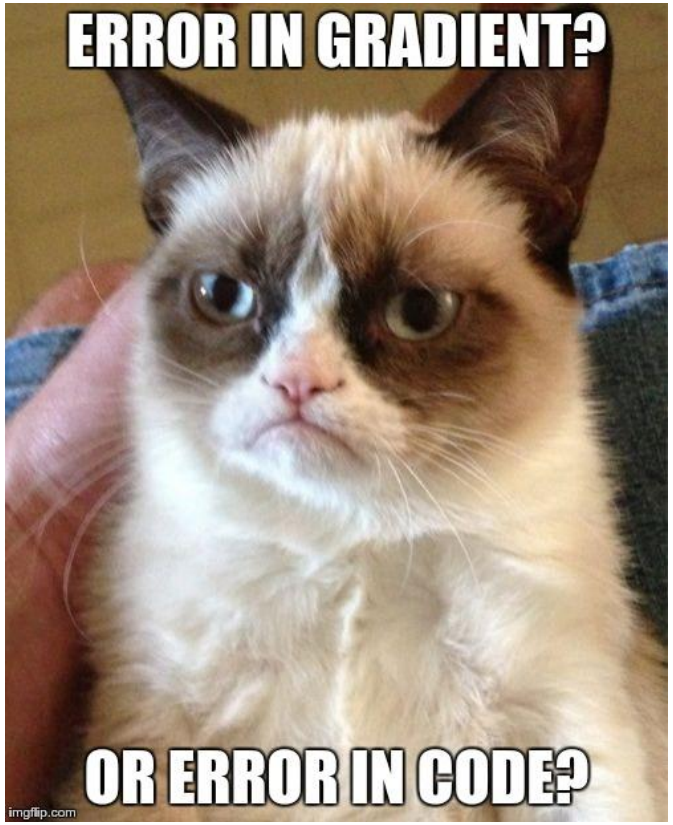


Outline

Neural networks: non-linear classifiers

Learning weights: backpropagation of error

Autodifferentiation (in reverse mode)

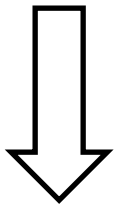
Finding Gradients

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

what are the partial derivatives?

Finding Gradients

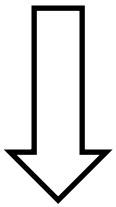
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$



$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 + a(x_1 - x_2)^{a-1} - \frac{2x_1}{x_1^2 + x_2^2}$$

Finding Gradients

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$



chain rule (multiple times)

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 + a(x_1 - x_2)^{a-1} - \frac{2x_1}{x_1^2 + x_2^2}$$

$$\frac{\partial f(x_1, x_2)}{\partial x_2} = -a(x_1 - x_2)^{a-1} - \frac{2x_2}{x_1^2 + x_2^2}$$

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

"straight line" program

autodiff: a way of finding gradients

mechanistic/procedural

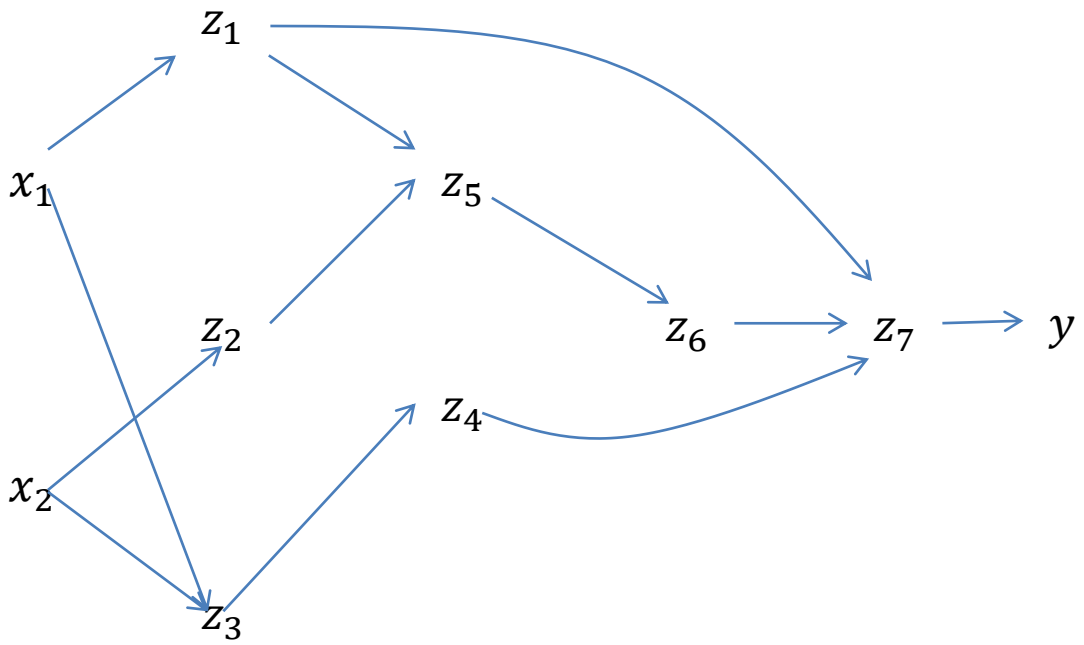
two (standard) modes: forward and reverse

ML often uses reverse mode

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$



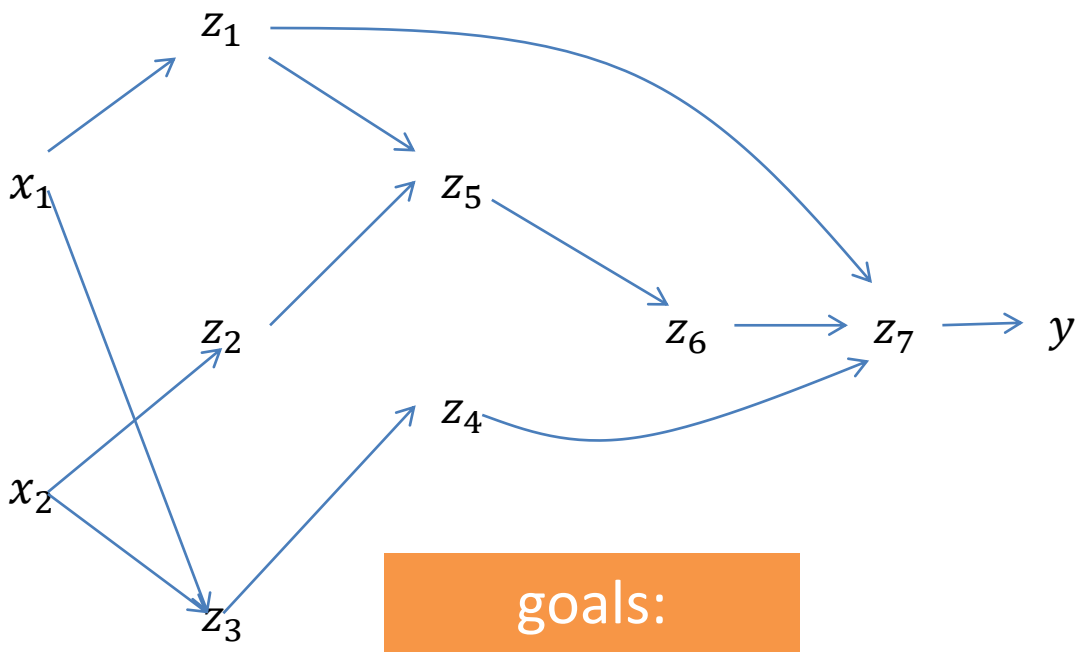
"straight line" program

computation graph

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$



"straight line" program

goals:

$$\frac{\partial y}{\partial x_1} \quad \frac{\partial y}{\partial x_2}$$

Autodifferentiation

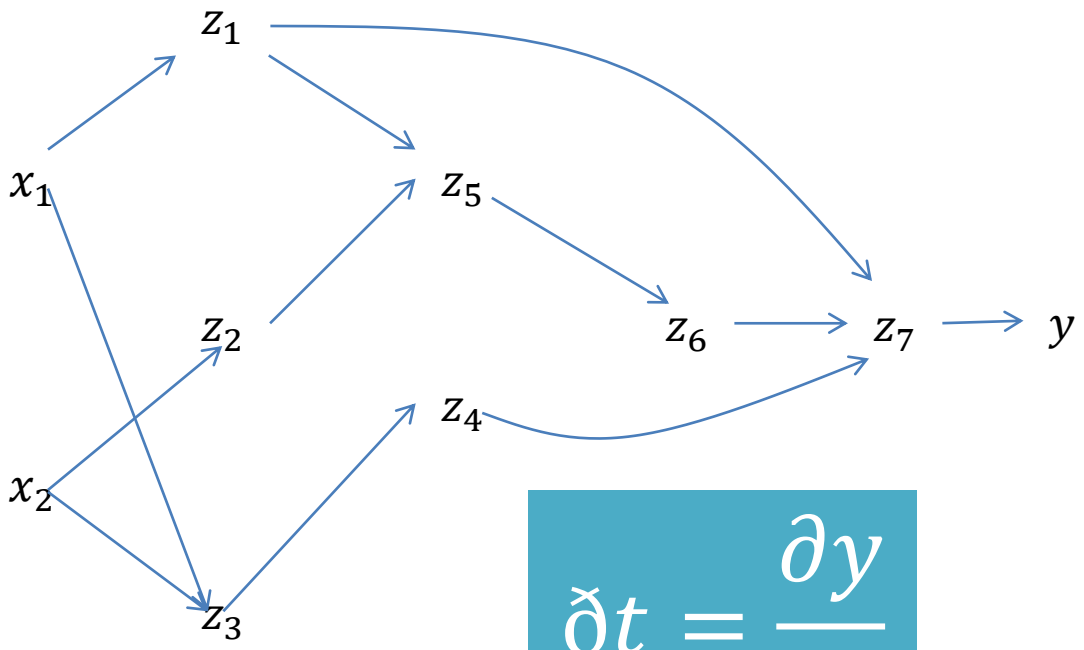
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$ðt = \frac{\partial y}{\partial t}$$

adjoint

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

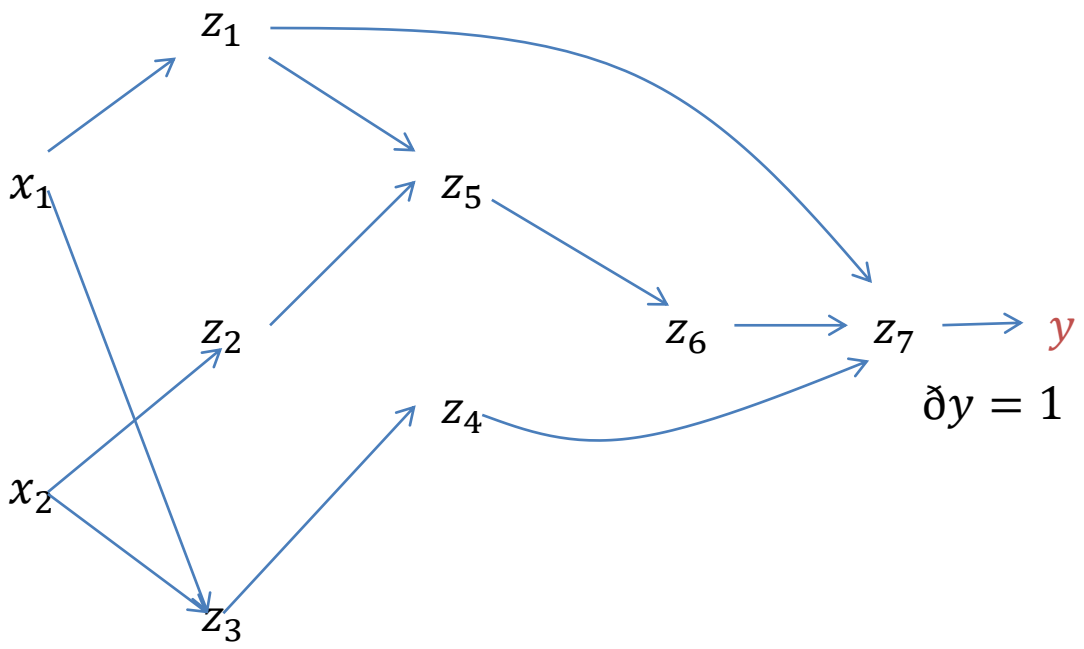
goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint



Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

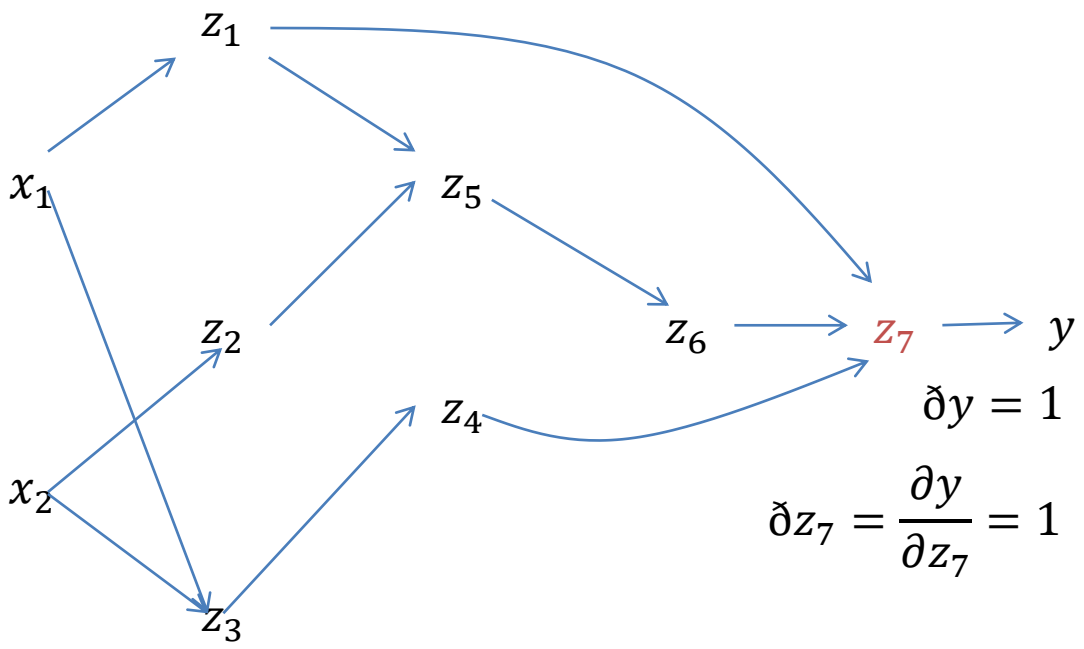
goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint



Autodifferentiation

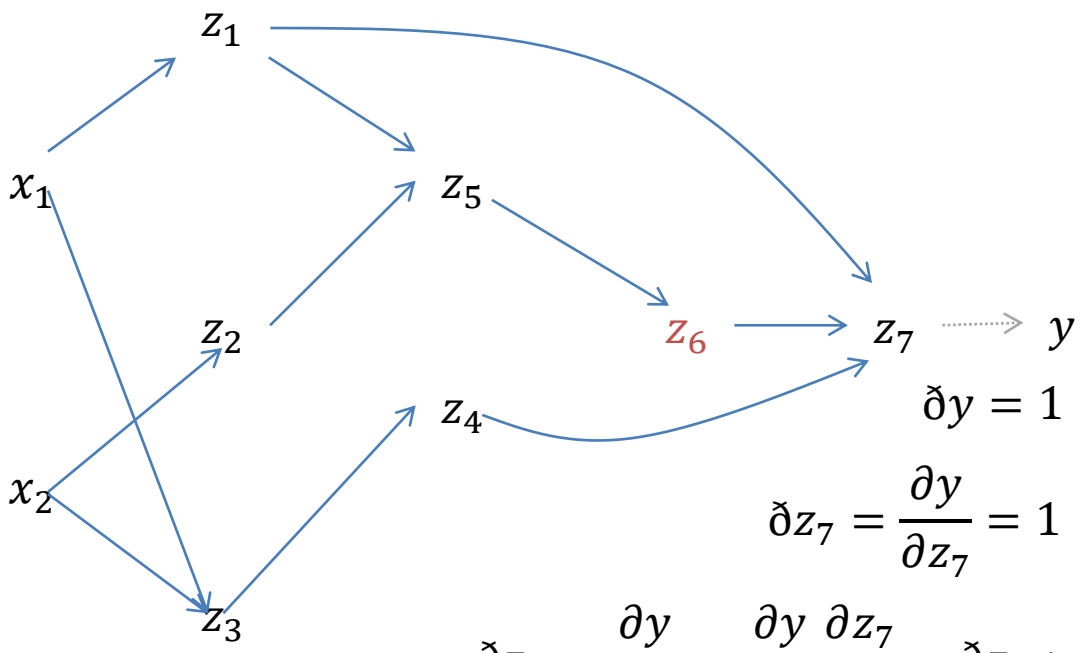
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \frac{\partial y}{\partial z_6} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_6} = \eth z_7 * -1$$

Autodifferentiation

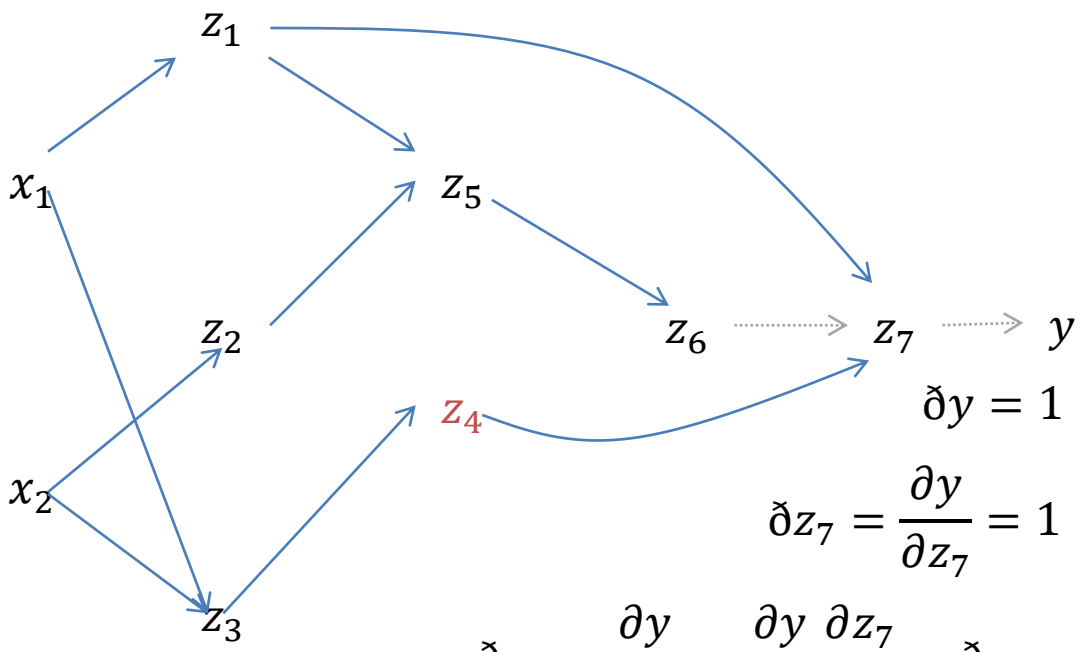
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \frac{\partial y}{\partial z_6} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_6} = \eth z_7 * -1$$

$$\eth z_4 = \frac{\partial y}{\partial z_4} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_4} = \eth z_7 * 1$$

Autodifferentiation

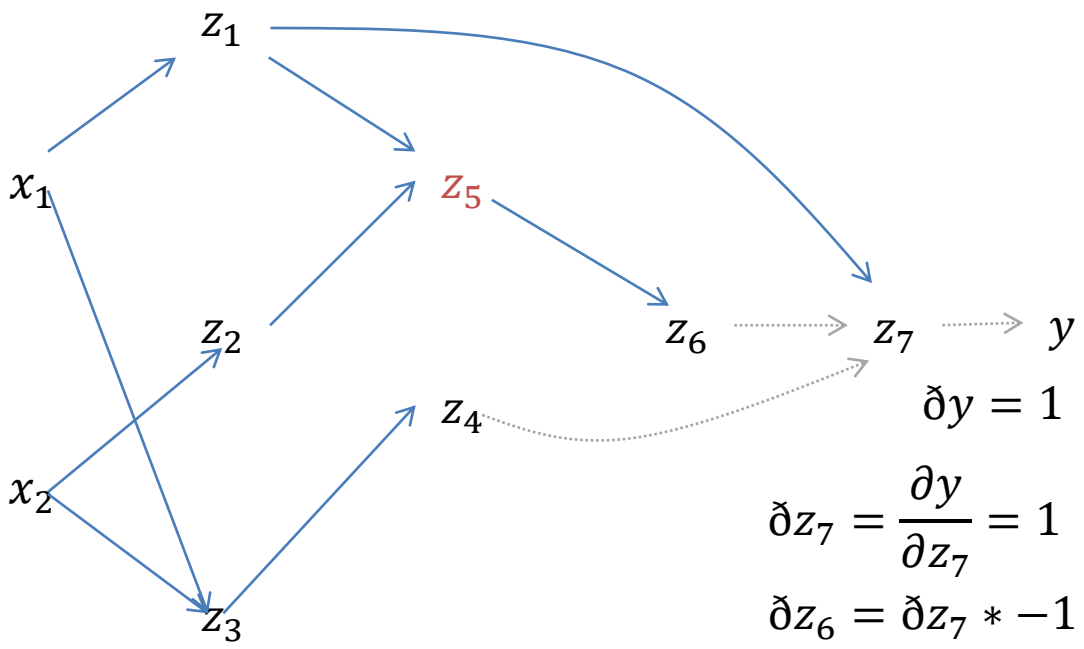
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \frac{\partial y}{\partial z_5} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_5} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_6}\frac{\partial z_6}{\partial z_5}$$

Autodifferentiation

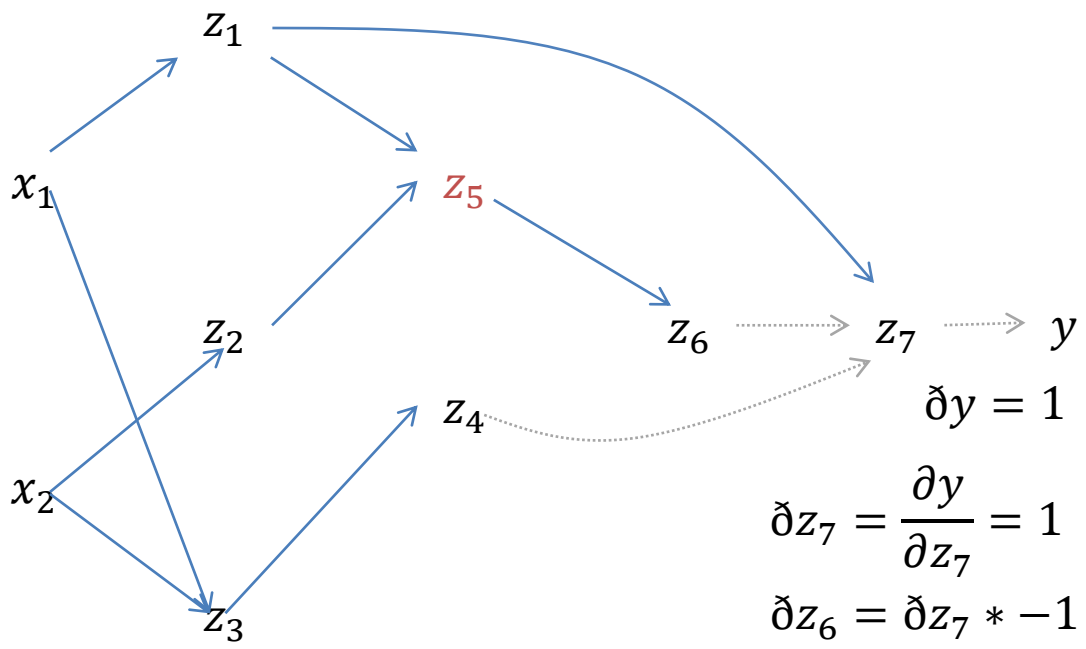
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \frac{\partial y}{\partial z_5} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_5} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_6}\frac{\partial z_6}{\partial z_5} = \eth z_6 * \frac{1}{z_5}$$

Autodifferentiation

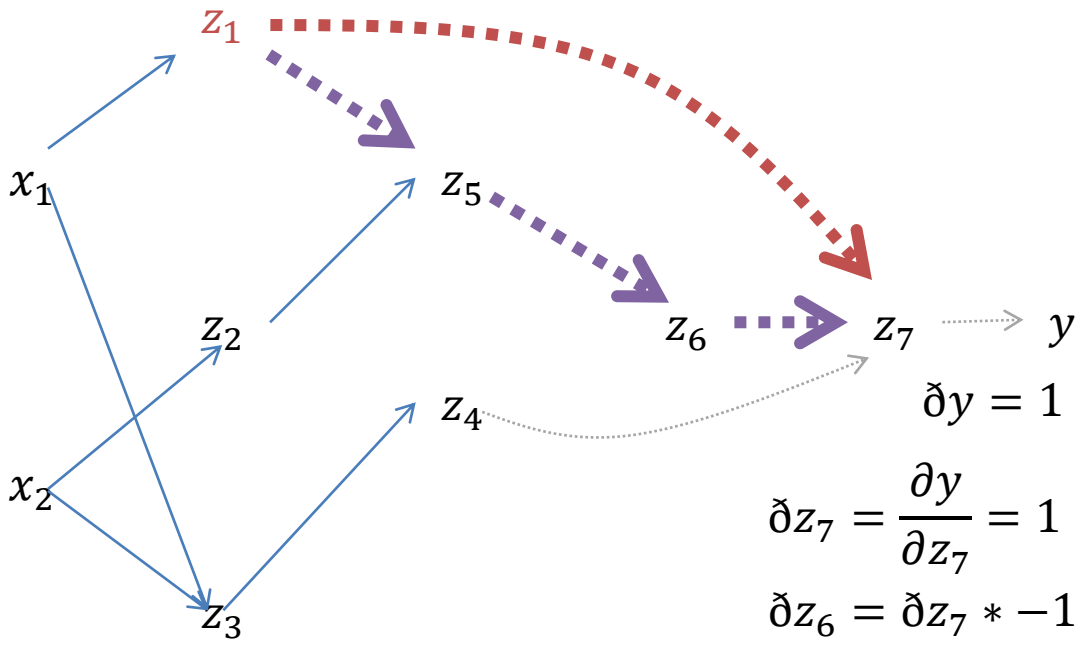
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \eth z_6 * \frac{1}{z_5}$$

$$\eth z_1 = \frac{\partial y}{\partial z_1} = \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_1} + \frac{\partial y}{\partial z_7}\frac{\partial z_7}{\partial z_6}\frac{\partial z_6}{\partial z_5}\frac{\partial z_5}{\partial z_1}$$

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

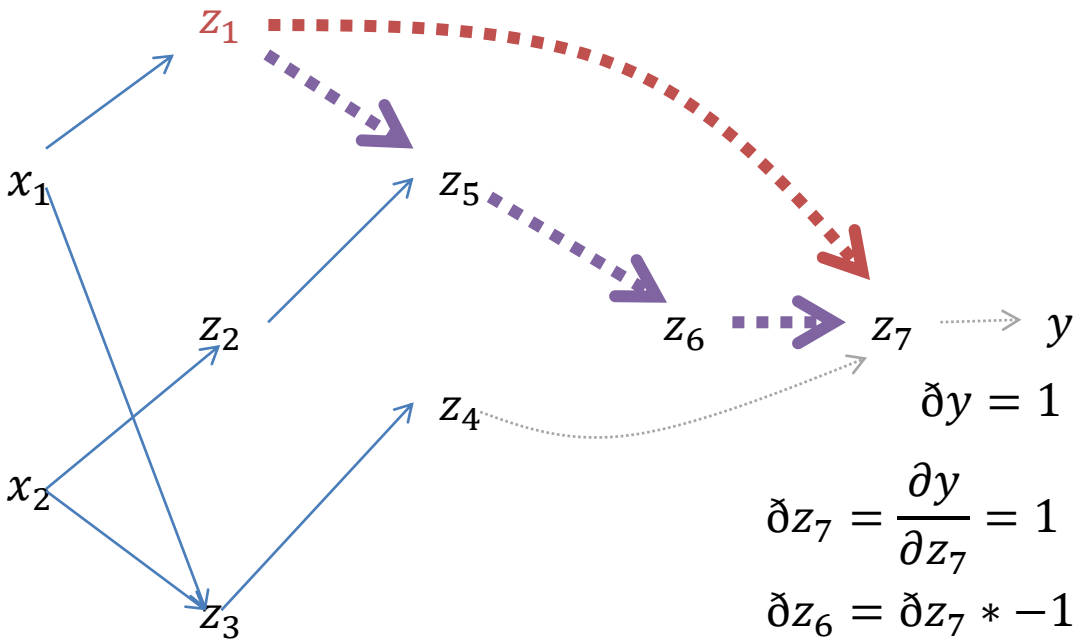
goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint



$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \eth z_6 * \frac{1}{z_5}$$

$$\eth z_1 = \frac{\partial y}{\partial z_1} = \eth z_7 * 1 + \eth z_5 * 1$$

Autodifferentiation

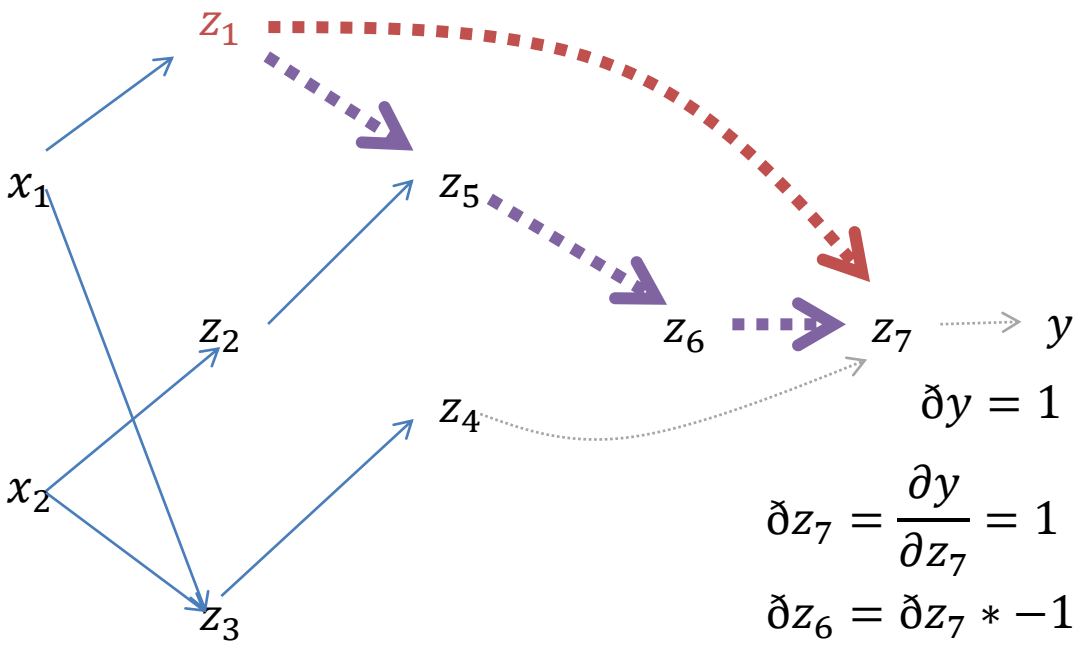
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \eth z_6 * \frac{1}{z_5}$$

$$\eth z_1 \mathrel{+}= \eth z_7 * 1$$

$$\eth z_1 \mathrel{+}= \eth z_5 * 1$$

Autodifferentiation

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

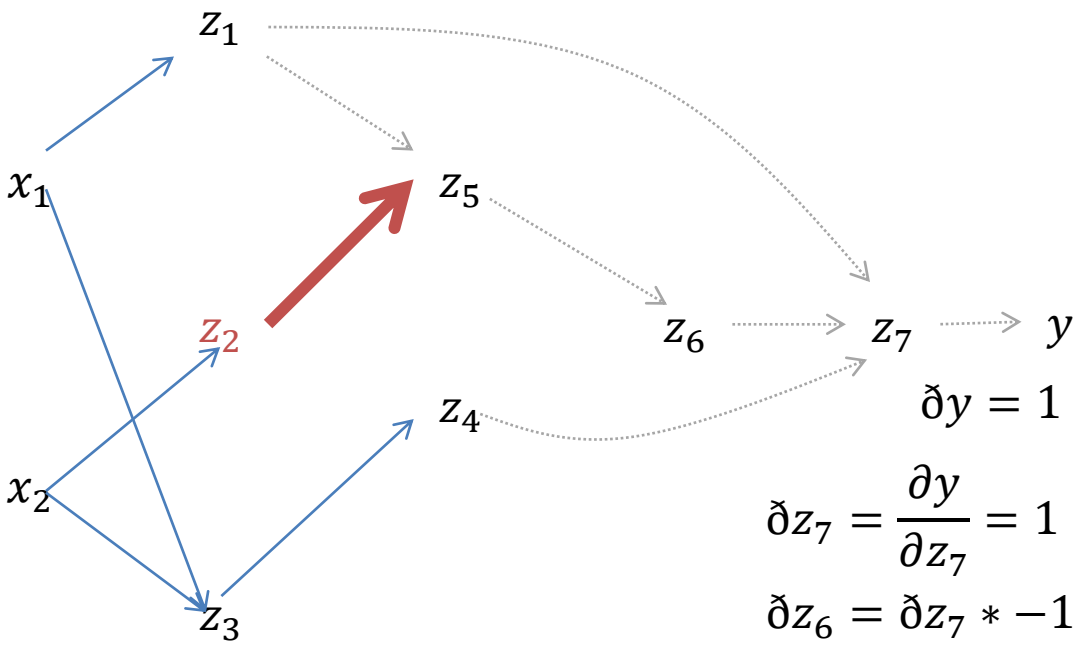
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$
$$\eth z_6 = \eth z_7 * -1$$
$$\eth z_4 = \eth z_7 * 1$$
$$\eth z_5 = \eth z_6 * \frac{1}{z_5}$$
$$\eth z_1 \mathrel{+}= \eth z_7 * 1$$
$$\eth z_1 \mathrel{+}= \eth z_5 * 1$$

$$\eth z_2 = \frac{\partial y}{\partial z_2} = \eth z_5 * 1$$

Autodifferentiation

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

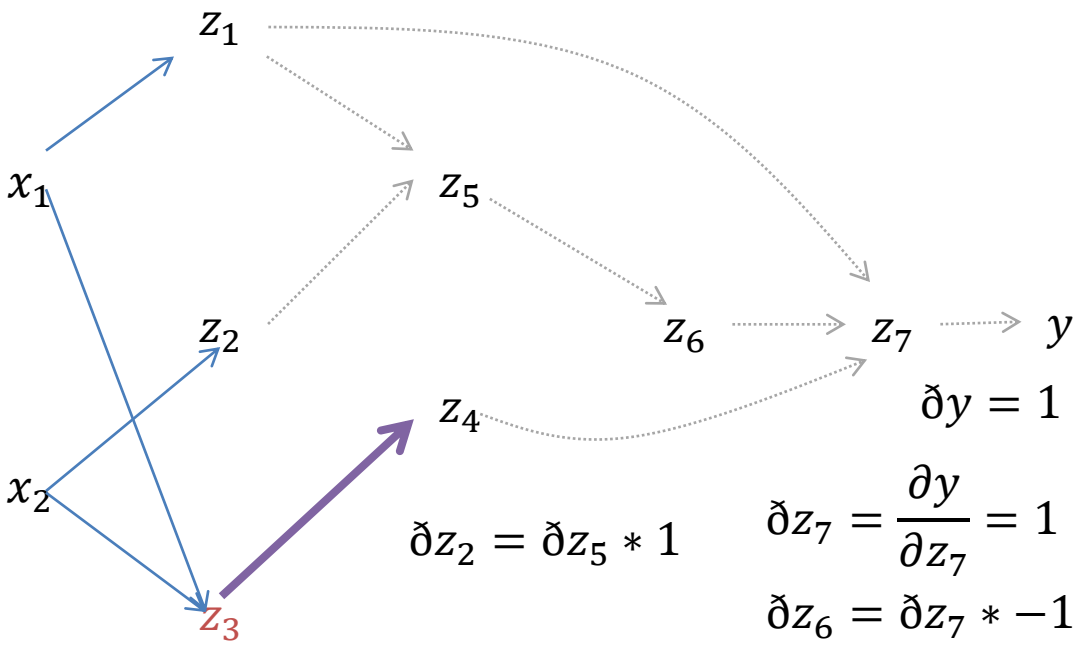
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_2 = \eth z_5 * 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \eth z_6 * \frac{1}{z_5}$$

$$\eth z_1 \mathrel{+}= \eth z_7 * 1$$

$$\eth z_1 \mathrel{+}= \eth z_5 * 1$$

$$\eth z_3 = \frac{\partial y}{\partial 3} = \eth z_4 * a * z_3^{a-1}$$

Autodifferentiation

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$\eth t = \frac{\partial y}{\partial t}$$

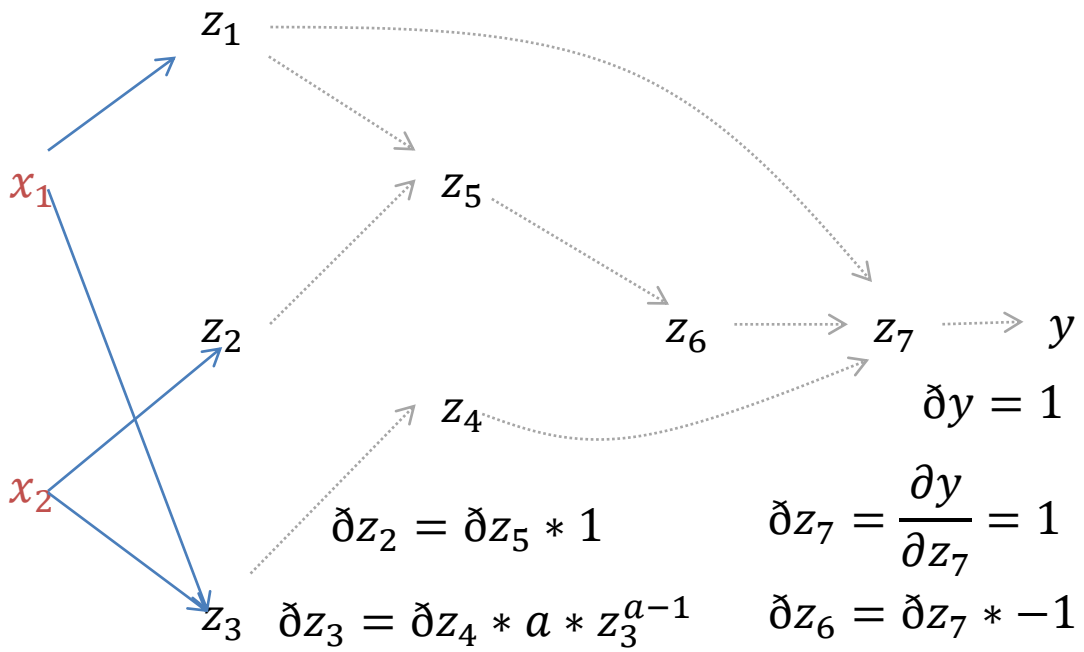
adjoint

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$$\eth y = 1$$

$$\eth z_7 = \frac{\partial y}{\partial z_7} = 1$$

$$\eth z_6 = \eth z_7 * -1$$

$$\eth z_4 = \eth z_7 * 1$$

$$\eth z_5 = \eth z_6 * \frac{1}{z_5}$$

$$\eth z_1 \mathrel{+}= \eth z_7 * 1$$

$$\eth z_1 \mathrel{+}= \eth z_5 * 1$$

$$\eth z_2 = \eth z_5 * 1$$

$$\eth z_3 = \eth z_4 * a * z_3^{a-1}$$

$$\eth x_1 \mathrel{+}= \eth z_1 * 2x_1$$

$$\eth x_1 \mathrel{+}= \eth z_3 * 1$$

$$\eth x_2 \mathrel{+}= \eth z_2 * 2x_2$$

$$\eth x_2 \mathrel{+}= \eth z_3 * -1$$

Autodifferentiation

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

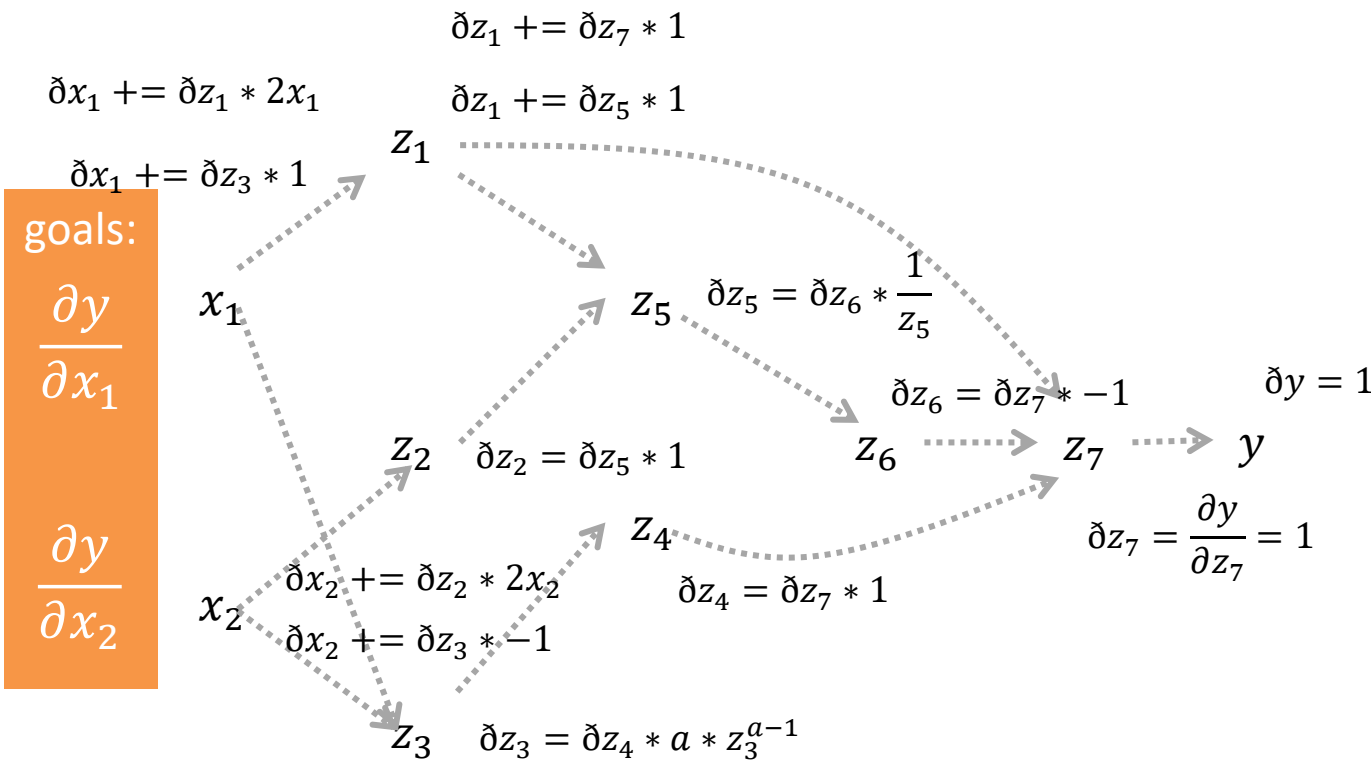
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



Autodifferentiation

$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

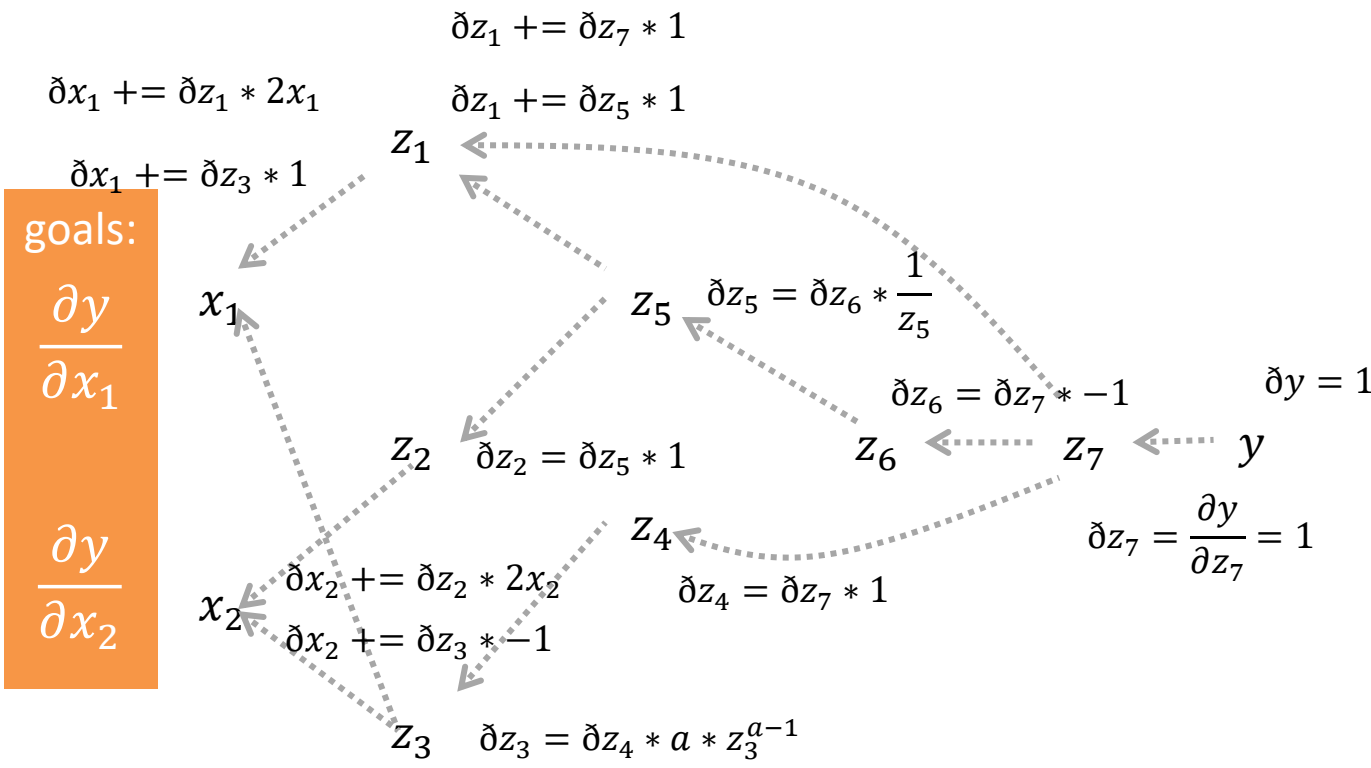
$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



autodifferentiation in reverse mode

Autodifferentiation in Reverse Mode

$$f(x_1, x_2) = x_1^2 + (x_1 - x_2)^a - \log(x_1^2 + x_2^2)$$

$$z_1 = x_1^2$$
$$z_2 = x_2^2$$
$$z_3 = (x_1 - x_2)$$
$$z_4 = z_3^a$$
$$z_5 = z_1 + z_2$$
$$z_6 = \log z_5$$
$$z_7 = z_1 + z_4 - z_6$$
$$y = z_7$$

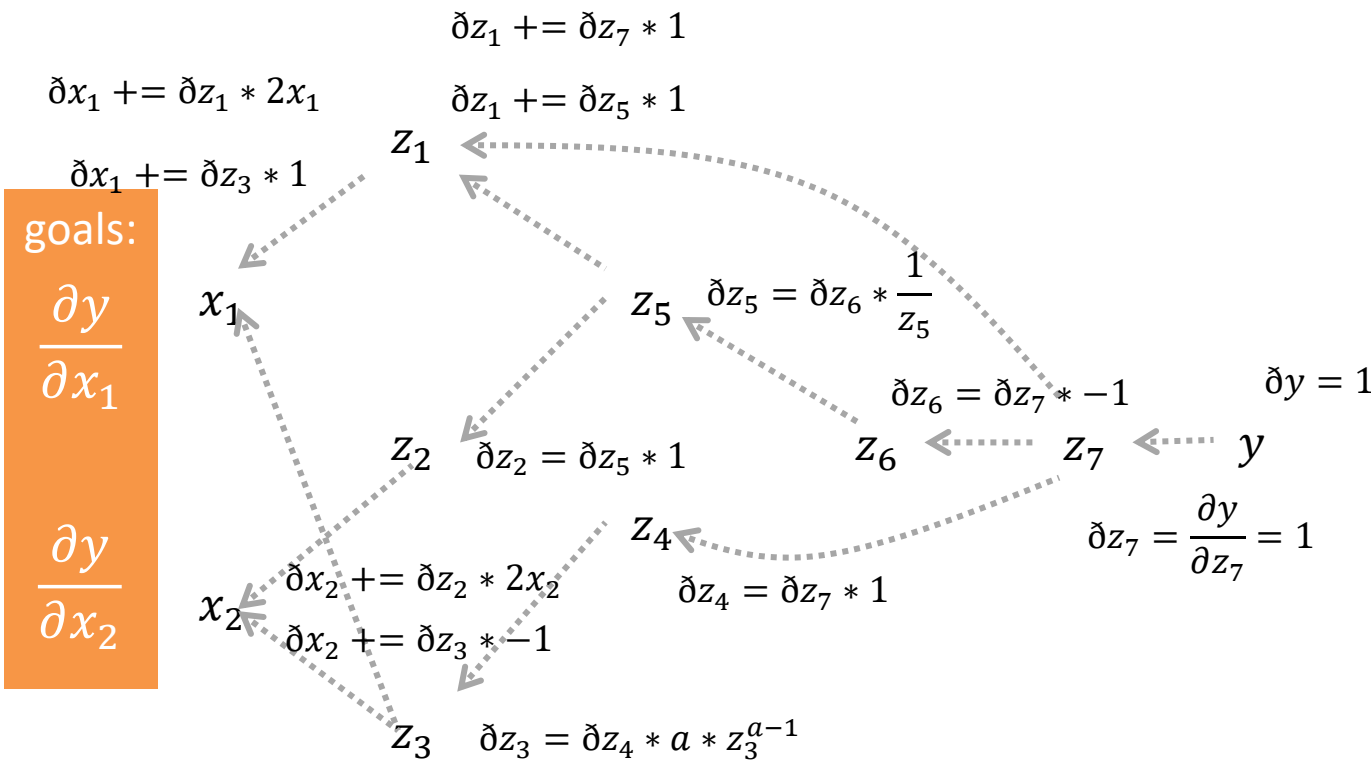
$$\eth t = \frac{\partial y}{\partial t}$$

adjoint

goals:

$$\frac{\partial y}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2}$$



$x_1 = 2$
$x_2 = 1$
$a = 1$

$$f(x_1 = 2, x_2 = 1) \approx 3.390562$$

$\nabla_x = (4.2, -1.4)$

by exact gradients

$\nabla_x = (4.2, -1.4)$

by autodiff

Code Proof of Autodiff

```
>> def f(x1, x2):
        return x1**2 + (x1-x2)**1 - numpy.log(x1**2+x2**2)
```

```
>> def autodiff(x1,x2,a=1.0):
        z1=x1**2
        z2=x2**2
        z3=(x1-x2)
        z4=z3**a
        z5=z1+z2
        z6=numpy.log(z5)
        z7=z1+z4-z6
        y=z7
        dy=1
        dz7=dy
        dz6=dz7*-1.0
        dz5=dz6*1.0/z5
        dz4=dz7*1.0
        dz3=dz4*a*z3**(a-1)
        dz2=dz5*1.0
        dz1=dz7*1.0 +dz5*1.0
        dx1=dz1*2*x1+dz3*1.0
        dx2=dz2*2*x2+dz3*-1.0
        return dx1, dx2
```

```
>> autodiff(2,1)
(4.2, -1.4)
```

Code Proof of Autodiff

```
>> def f(x1, x2):
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        z5=z1+z2
        z6=numpy.log(z5)
        z7=z1+z4-z6
        y=z7
        dy=1
        dz7=dy
        dz6=dz7*-1.0
        dz5=dz6*1.0/z5
        dz4=dz7*1.0
        dz3=dz4*a*z3**(a-1)
        dz2=dz5*1.0
        dz1=dz7*1.0 +dz5*1.0
        dx1=dz1*2*x1+dz3*1.0
        dx2=dz2*2*x2+dz3*-1.0
        return dx1, dx2
```

forward pass

backward pass

```
>> autodiff(2,1)
(4.2, -1.4)
```

Outline

Neural networks: non-linear classifiers

Learning weights: backpropagation of error

Autodifferentiation (in reverse mode)

Gradient Descent: Backpropagate the Error

Set t = 0

Pick a starting value θ_t

Until converged:

for example(s) i:

1. Compute loss l on x_i
2. Get gradient $g_t = l'(x_i)$
3. Get scaling factor ρ_t
4. Set $\theta_{t+1} = \theta_t - \rho_t * g_t$
5. Set t += 1