Lecture 11. Neural Network Fundamentals

COMP90051 Statistical Machine Learning

Lecturer: Dr Christine de Kock

Deep learning topic (lects 11-14)

- Fundamentals
  - Networks, layers, activation functions
  - Training by gradient backpropagation
  - Regularisation
- Network architectures:
  - Autoencoders
  - Convolutional networks (CNN)
  - Recurrent networks (RNNs)
  - Attention and the Transformer

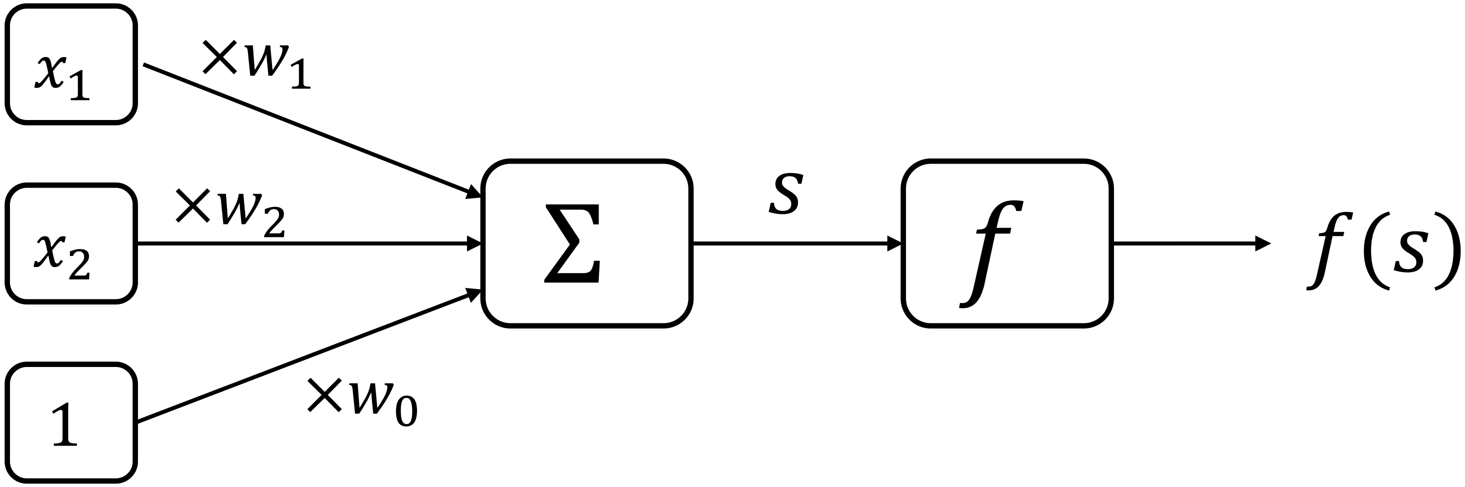
This lecture

- Deep learning
  - Multi-layer perceptron formulation
  - Deep models and representation learning
- Gradient backpropagation
  - Step-by-step derivation

Multilayer Perceptron

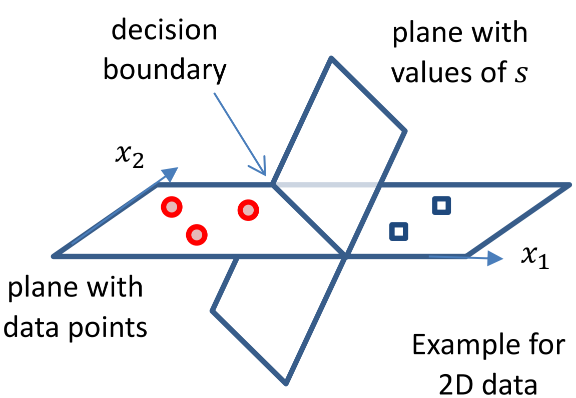
Modelling non-linearity via
function composition

Recap: Perceptron model



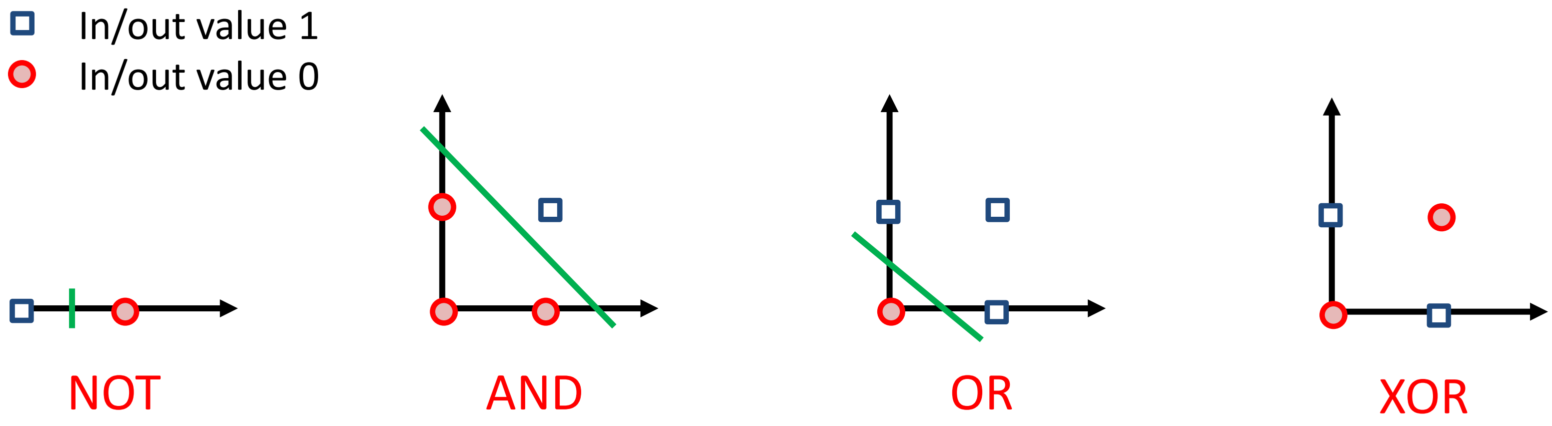
- x_1, x_2 – inputs
- w_1, w_2 – synaptic weights
- w_0 – bias weight
- f – activation function

A linear classifier



Limitations of linear models

Some problems are linearly separable, but many are not



Possible solution: composition

$x_1 \text{ XOR } x_2 = (x_1 \text{ OR } x_2) \text{ AND not}(x_1 \text{ AND } x_2)$

We are going to compose perceptrons …

Perceptron is *sort of* a building block for ANN

- ANNs are not restricted to binary classification
- Nodes in ANN can have various activation functions

Step function $f(s) = \begin{cases} 1, & if\ s \geq 0 \\ 0, & if\ s < 0 \end{cases}$

Sign function $f(s) = \begin{cases} 1, & if\ s \geq 0 \\ -1, & if\ s < 0 \end{cases}$

Logistic function $f(s) = \frac{1}{1 + e^{-s}}$

tanh function $f(s) = \frac{e^s - e^{-s}}{e^s + e^{-s}}$

Rectified linear unit $f(s) = \max\{0, s\}$

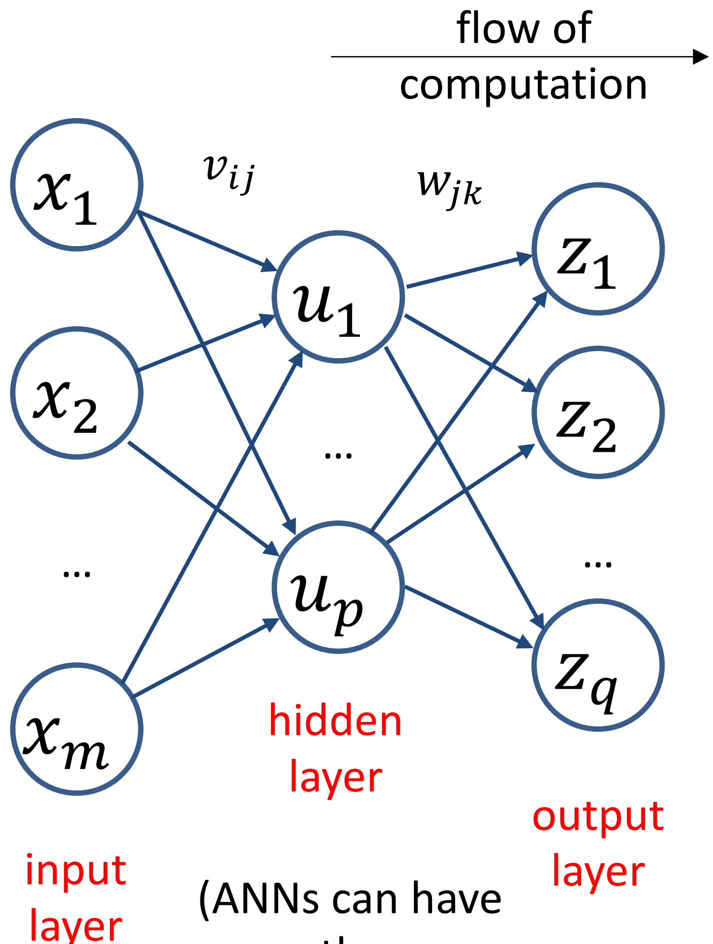
…many others, many variations…

Feed-forward Artificial Neural Network

x_i are inputs, i.e., attributes

note: here x_i are components of a single training instance $\boldsymbol{x}$

a training dataset is a set of instances



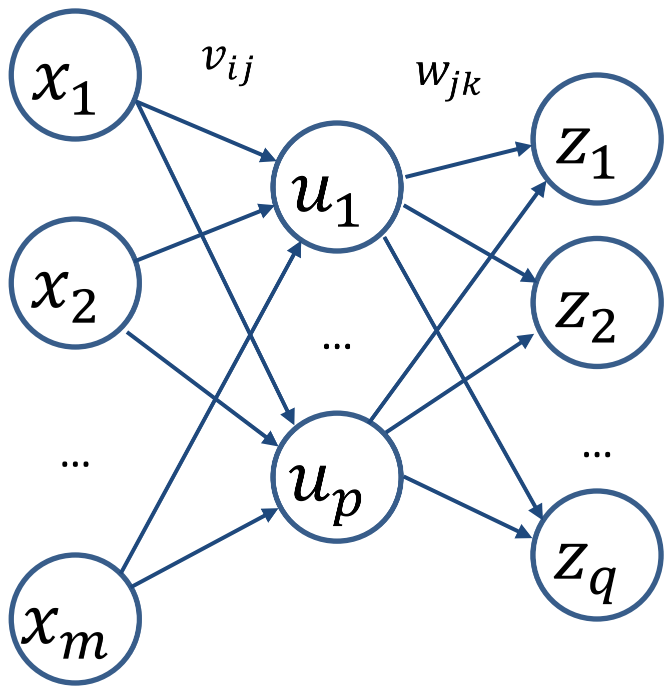
(ANNs can have more than one hidden layer)

z_i are outputs, i.e., predicted labels

note: ANNs naturally handle multidimensional output

e.g., for handwritten digits recognition, each output node can represent the probability of a digit

ANN as function composition



$u_j = g(r_j)$

$$r_j = v_{0j} + \sum_{i=1}^{m} x_i v_{ij}$$

$z_k = h(s_k)$

$$s_k = w_{0k} + \sum_{j=1}^{p} u_j w_{jk}$$

note that z_k is a function composition (a function applied to the result of another function, etc.)

here g, h are activation functions. These can be either same (e.g., both sigmoid) or different

you can add bias node $x_0 = 1$ to simplify equations: $r_j = \sum_{i=0}^{m} x_i v_{ij}$

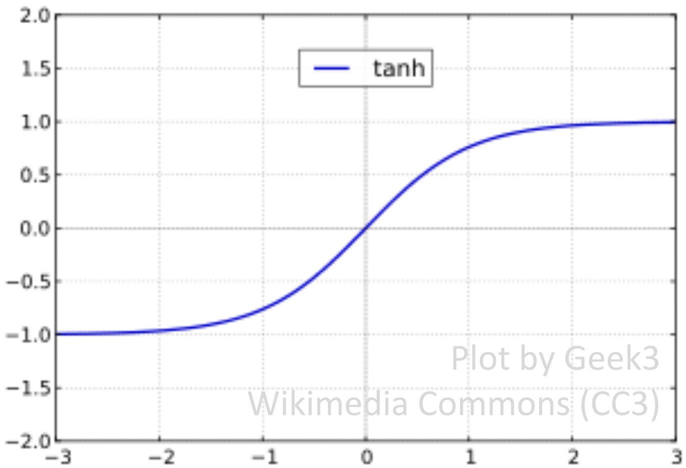
similarly you can add bias node $u_0 = 1$ to simplify equations: $s_k = \sum_{j=0}^{p} u_j w_{jk}$

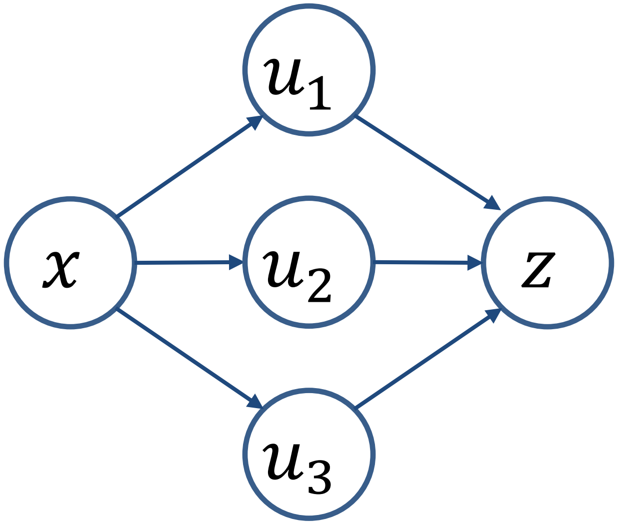
ANN in supervised learning

- ANNs can be naturally adapted to various supervised learning setups. Requires setting: output layer dimension, output layer activations, appropriate loss
- Univariate regression $y = f(\boldsymbol{x})$
  - e.g., linear regression earlier in the course
- Multivariate regression $\boldsymbol{y} = f(\boldsymbol{x})$
  - predicting values for multiple continuous outcomes
- Binary classification
  - e.g., predict whether a patient has type II diabetes
- Multiclass classification
  - e.g., handwritten digits recognition with labels “1”, “2”, etc.

The power of ANN as a non-linear model

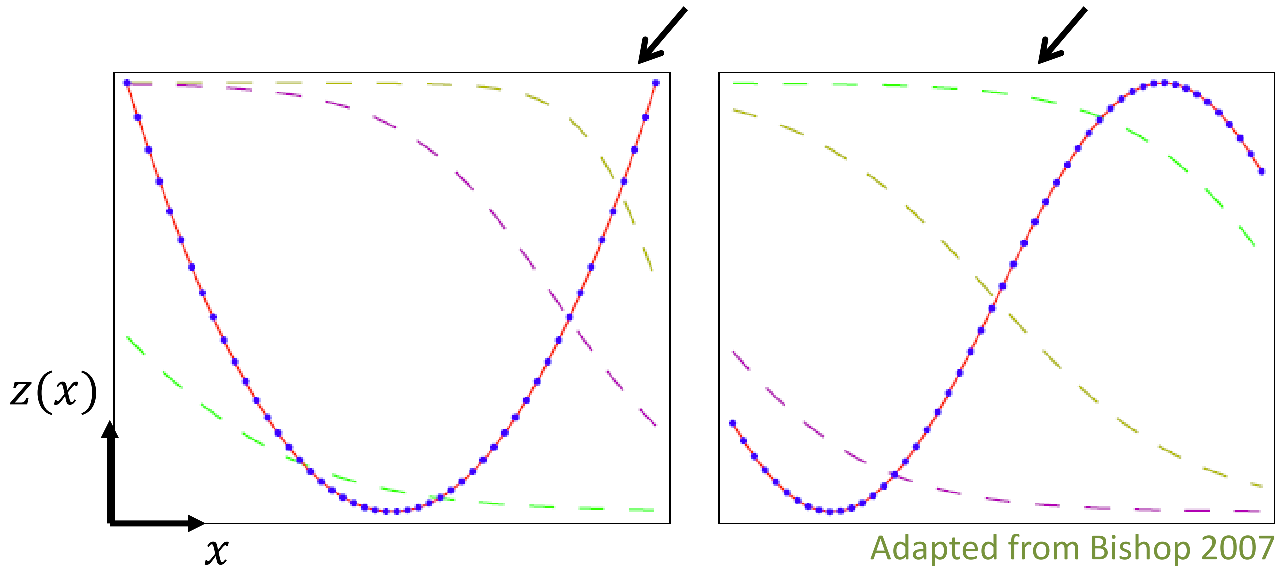
- ANNs are capable of approximating plethora non-linear functions, e.g., $z(x) = x^2$ and $z(x) = \sin x$
- For example, consider the following network. In this example, hidden unit activation functions are tanh





The power of ANN as a non-linear model

- ANNs are capable of approximating various non-linear functions, e.g., $z(x) = x^2$ and $z(x) = \sin x$



Adapted from Bishop 2007

Blue points are the function values evaluated at different x. Red lines are the predictions from the ANN. Dashed lines are outputs of the hidden units

- *Universal approximation theorem* *(Cybenko 1989)*: An ANN with a hidden layer with a finite number of units, and mild assumptions on the activation function, can approximate continuous functions on compact subsets of $\boldsymbol{R}^n$ arbitrarily well

Mini Summary

- Multiple layer networks
  - Model structure
  - Universal approximation

Next: Representation learning perspective

Deep Learning and Representation Learning

Hidden layers viewed as
feature space transformation

Representational capacity

- ANNs with a single hidden layer are universal approximators
- For example, such ANNs can represent any Boolean function

$$OR(x_1, x_2) \qquad u = g(x_1 + x_2 - 0.5)$$

$$AND(x_1, x_2) \qquad u = g(x_1 + x_2 - 1.5)$$

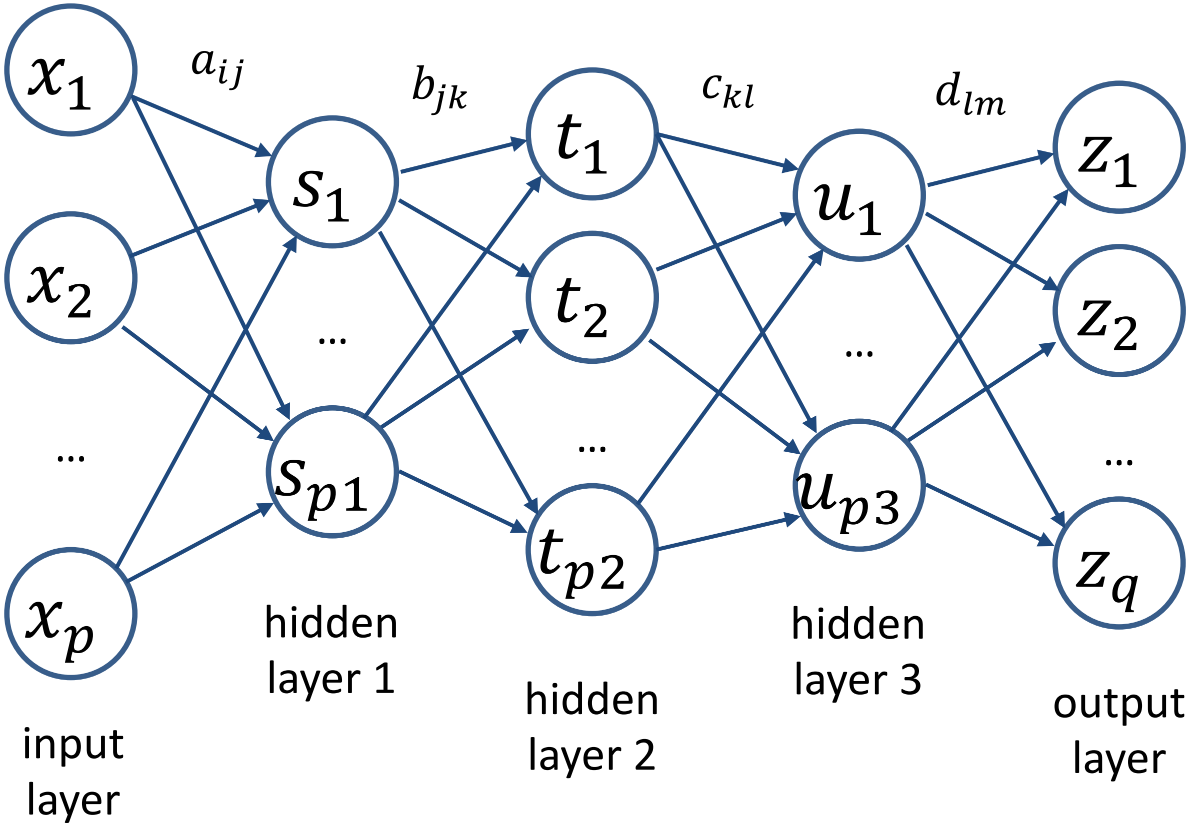
$$NOT(x_1) \qquad u = g(-x_1)$$

$g(r) = 1$ if $r \geq 0$ and $g(r) = 0$ otherwise

- Any Boolean function over m variables can be implemented using a hidden layer with up to 2^m elements
- More *efficient* to stack several hidden layers

"Depth" refers to number of hidden layers

Deep networks



$$\boldsymbol{s} = \tanh(\boldsymbol{A}'\boldsymbol{x}) \quad \boldsymbol{t} = \tanh(\boldsymbol{B}'\boldsymbol{s}) \quad \boldsymbol{u} = \tanh(\boldsymbol{C}'\boldsymbol{t}) \quad \boldsymbol{z} = \tanh(\boldsymbol{D}'\boldsymbol{u})$$

Deep ANNs as representation learning

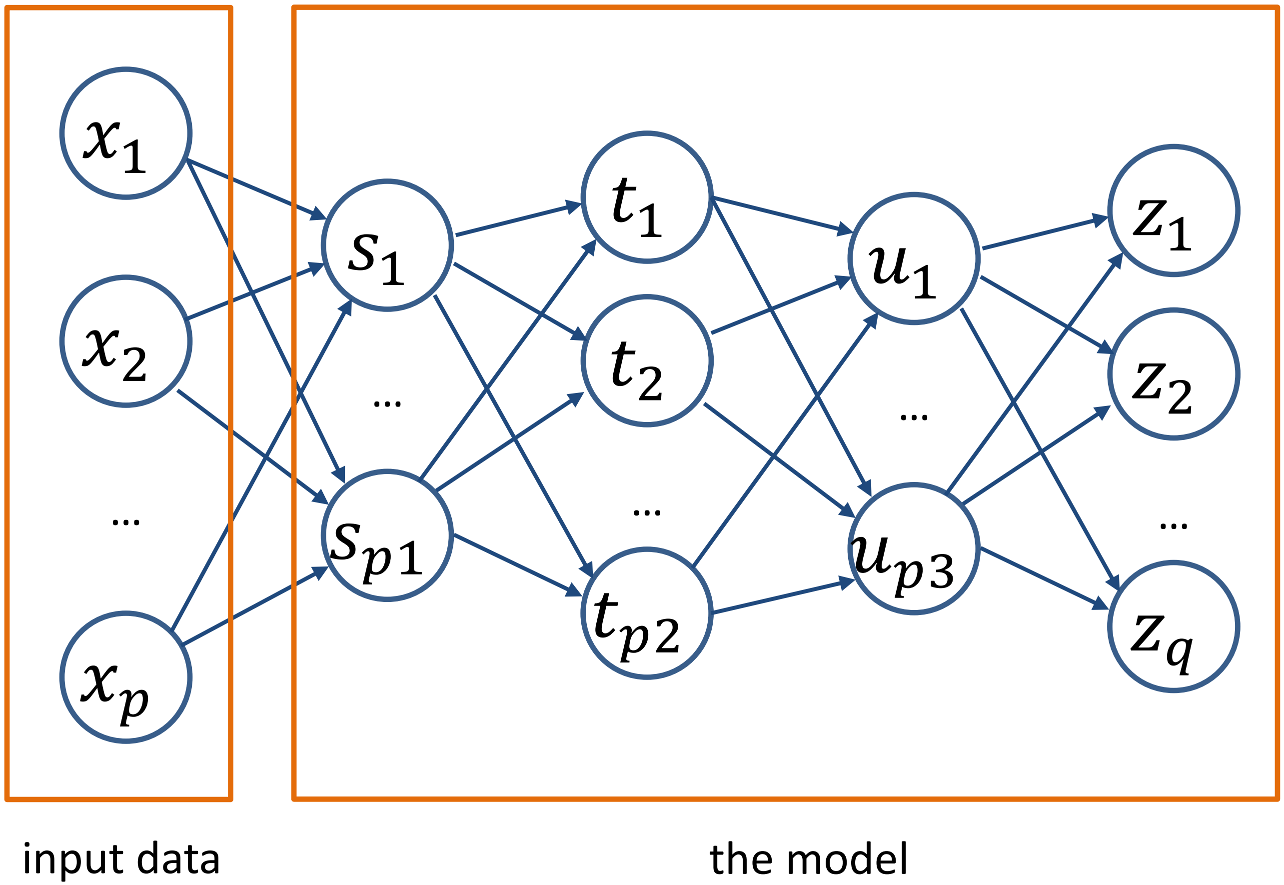
- Consecutive layers form representations of the input of increasing complexity
- An ANN can have a simple *linear* output layer, but using complex *non-linear* representation

$$\boldsymbol{z} = \tanh\left(\boldsymbol{D}'\left(\tanh\left(\boldsymbol{C}'\left(\tanh\left(\boldsymbol{B}'\left(\tanh(\boldsymbol{A}'\boldsymbol{x})\right)\right)\right)\right)\right)\right)$$

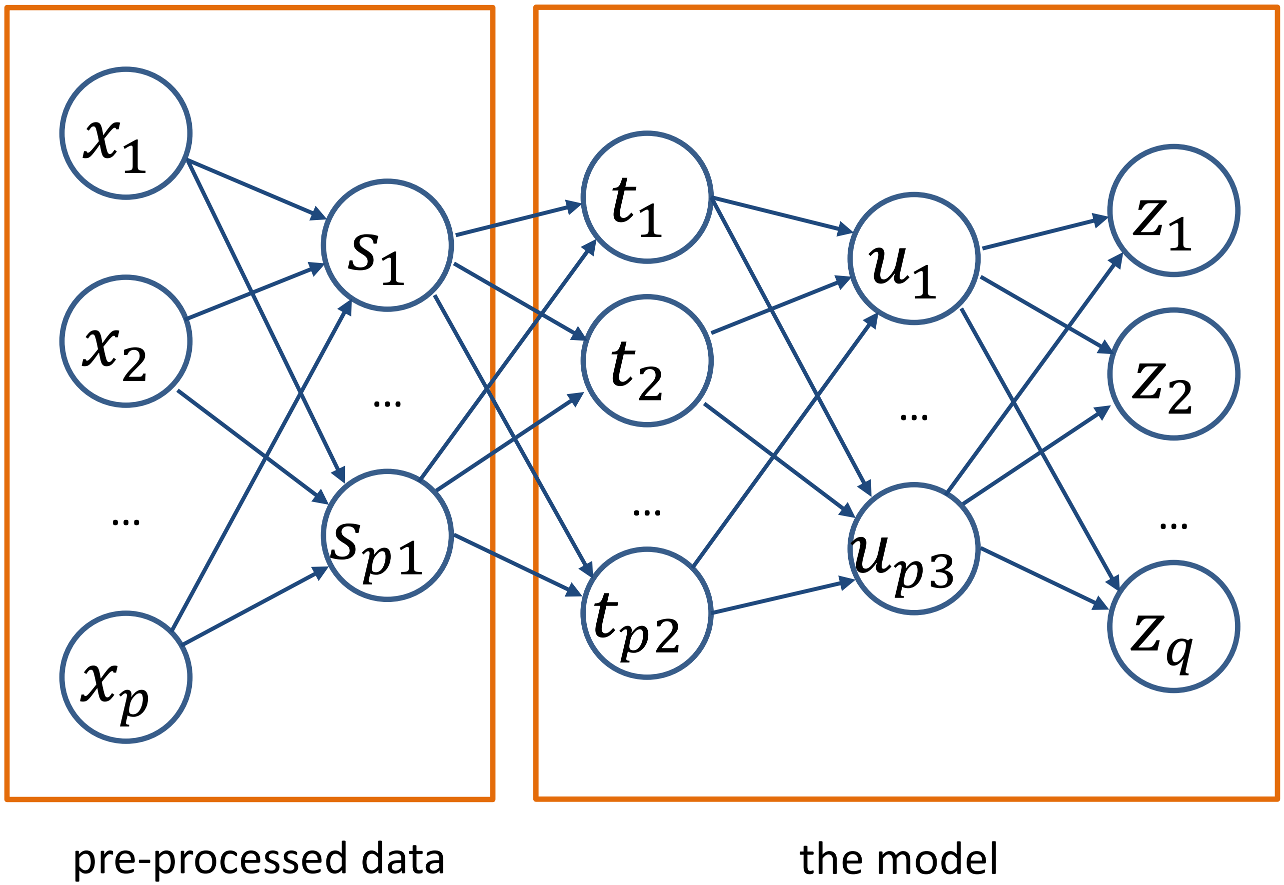
- Equivalently, a hidden layer can be thought of as the transformed feature space, e.g., $\boldsymbol{u} = \varphi(\boldsymbol{x})$
  compare to basis expansion / kernel learning
- Parameters of such a transformation are learned from data

Bias terms are omitted for simplicity

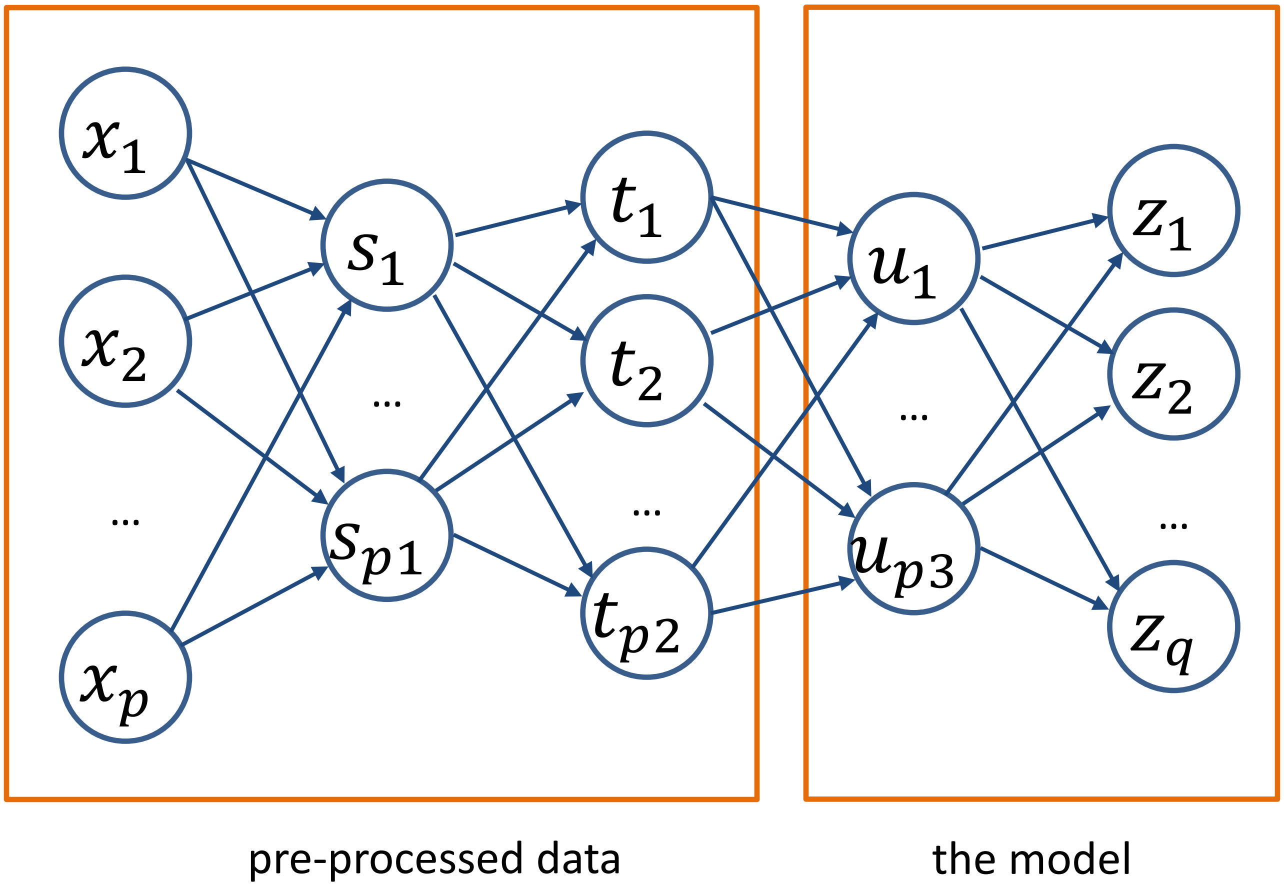
ANN layers as data transformation



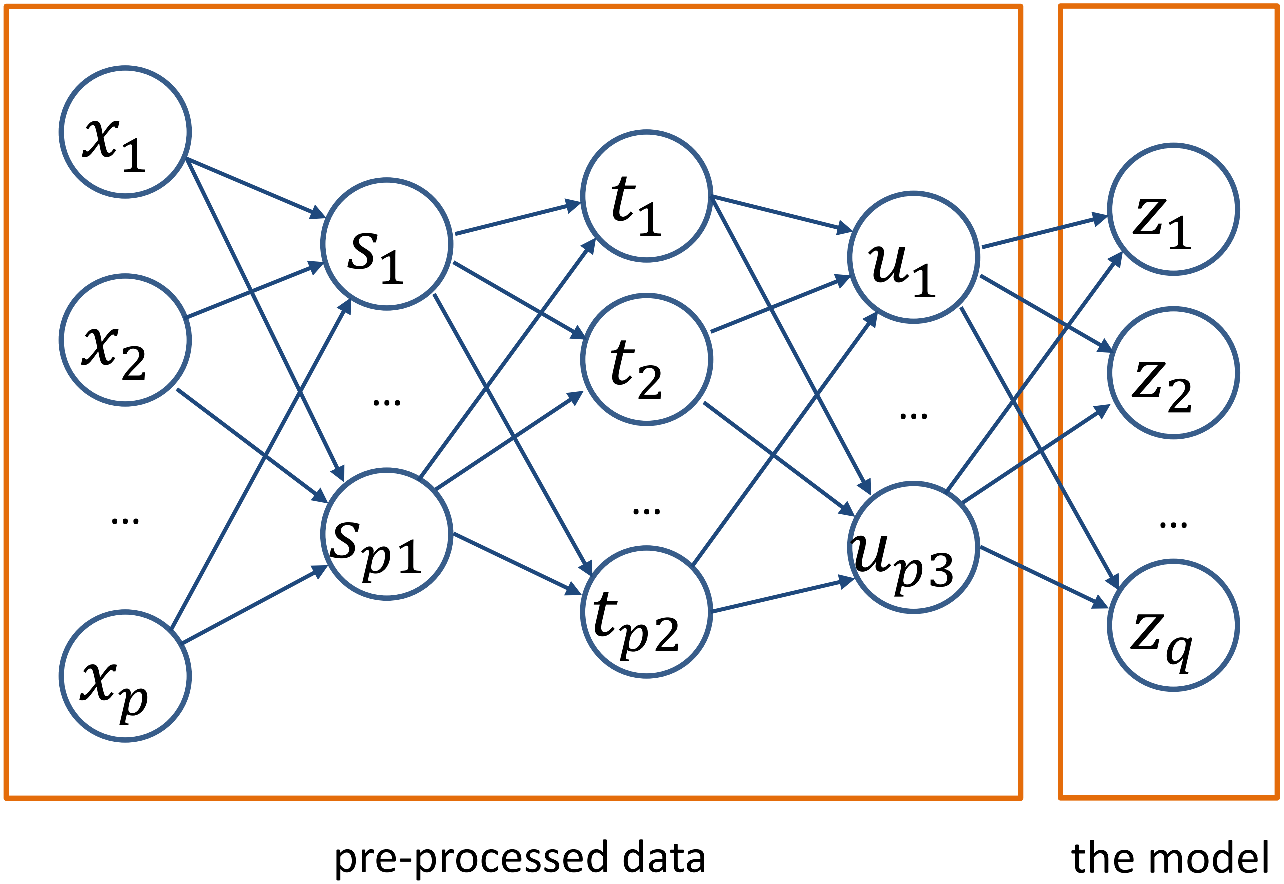
ANN layers as data transformation



ANN layers as data transformation



ANN layers as data transformation



Depth vs width

- A single arbitrarily wide layer in theory gives a universal approximator
- However (empirically) depth yields more accurate models

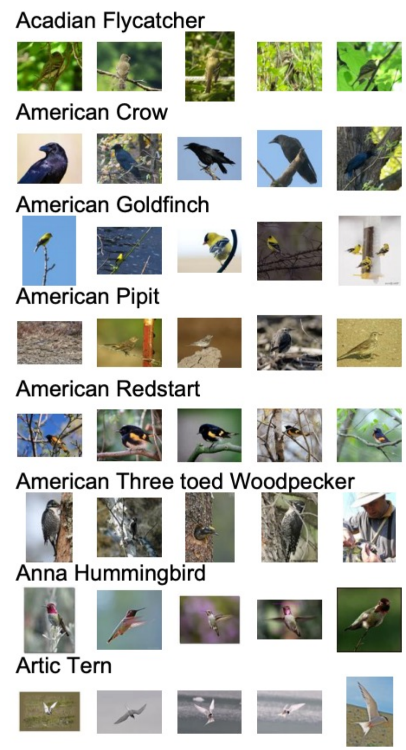
  Biological inspiration from the eye:
  - first detect small edges and color patches;
  - compose these into smaller shapes;
  - building to more complex detectors, of e.g. textures, faces, etc.
- Seek to mimic layered complexity in a network
- However vanishing gradient problem affects learning with very deep models

Vs manual feature representation

- Standard pipeline
  - input → feature engineering → classification algorithm
- Deep learning automates feature engineering
  - no need for expert analysis

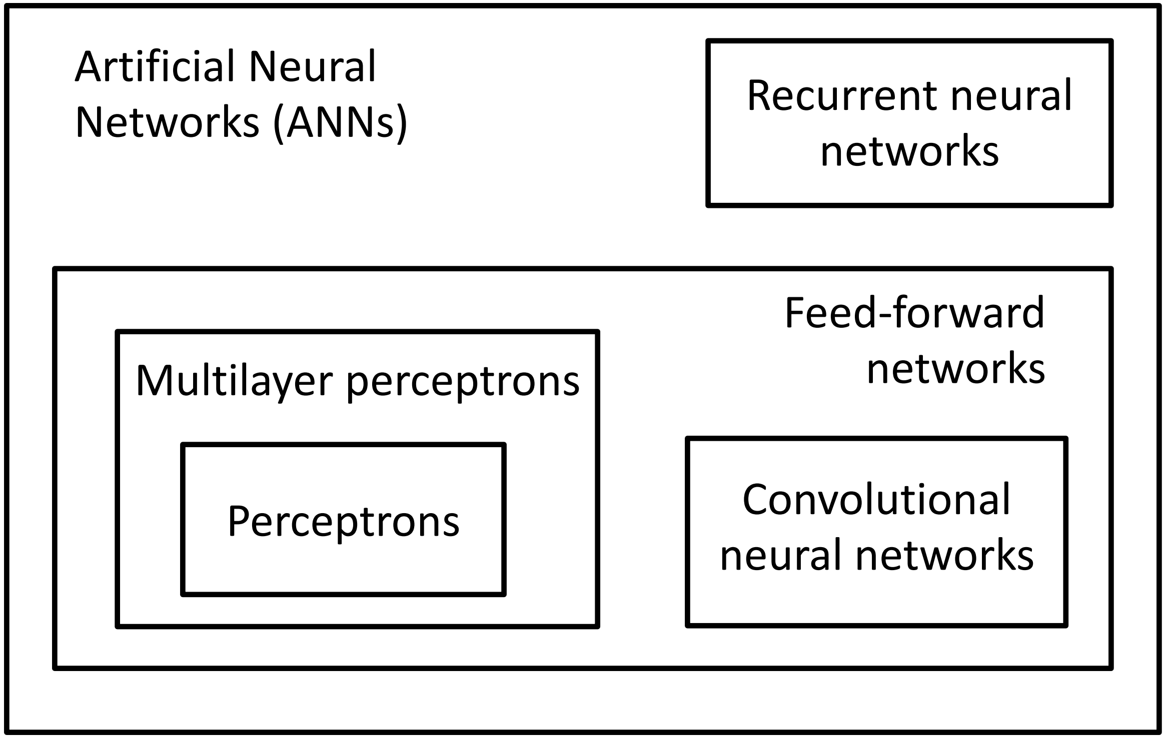
forehead_color	**black**	**black**	**black**
breast_pattern	**solid**	**solid**	**solid**
breast_color	**white**	**white**	**white**
head_pattern	**plain**	**capped**	plain
back_color	**white**	white	**black**
wing_color	grey/white	**grey**	**white**
leg_color	**orange**	orange	**orange**
size	**medium**	large	**medium**
bill_shape	needle	dagger	**dagger**
wing_shape	**pointed**	**tapered**	**long**
...	...	...	...
primary_color	white	white	white

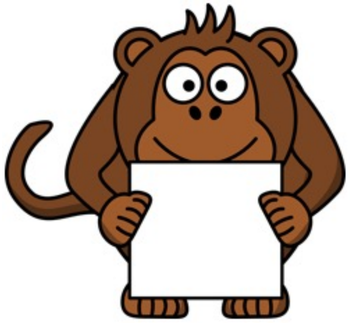
→ class = *Artic Tern*



https://vision.cornell.edu/se3/wp-content/uploads/2014/09/WelinderEtal10_CUB-200.pdf

Mini Summary





art: OpenClipartVectors
at pixabay.com (CC0)

- Deep models and representation learning

Next: Backpropagation learning algorithm

Backpropagation

= “backward propagation of errors”

Calculating the gradient of loss of a composition

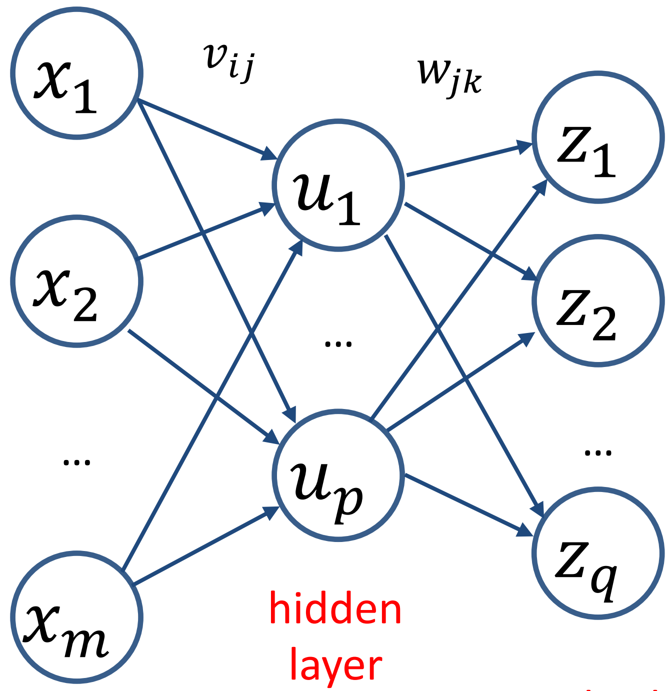
Recap: Feed-forward Artificial Neural Network

flow of computation →

x_i are inputs, i.e., attributes

note: here x_i are components of a single training instance $\boldsymbol{x}$

a training dataset is a set of instances



input layer

hidden layer

output layer

(ANNs can have more than one hidden layer)

z_i are outputs, i.e., predicted labels

Loss function L used to compare outputs with gold, gradient used for training **v**, **w**

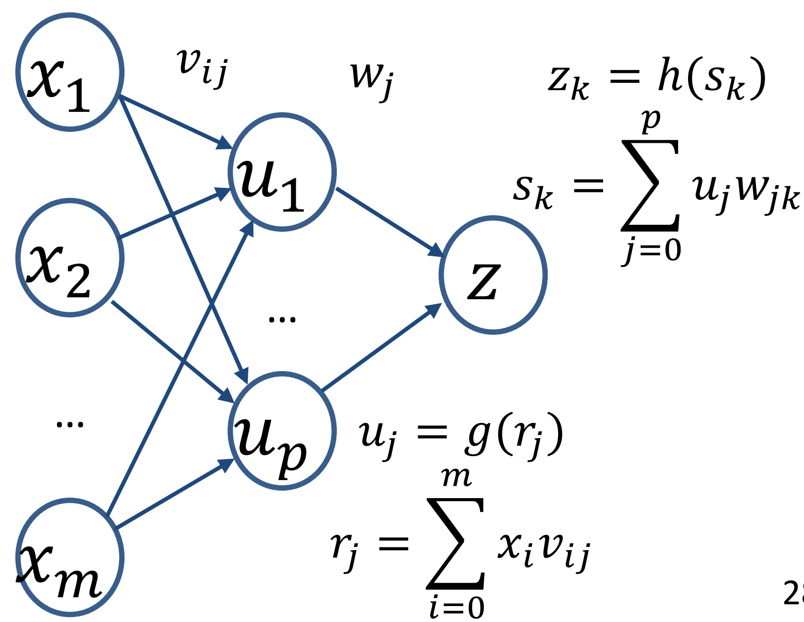
Backpropagation: start with the chain rule

- Recall that the output z of an ANN is a function composition, and hence $L(z)$ is also a composition
  - $L = 0.5(z-y)^2 = 0.5(h(s)-y)^2 = 0.5(s-y)^2$
  - $= 0.5\left(\sum_{j=0}^{p} u_j w_j - y\right)^2 = 0.5\left(\sum_{j=0}^{p} g(r_j) w_j - y\right)^2 = \cdots$

- Backpropagation makes use of this fact by applying the chain rule for derivatives

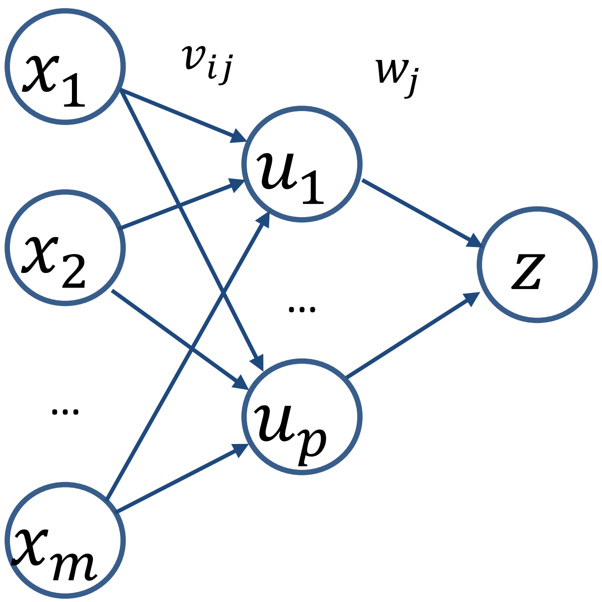
- $\frac{\partial L}{\partial w_j} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial s}\frac{\partial s}{\partial w_j}$

- $\frac{\partial L}{\partial v_{ij}} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial s}\frac{\partial s}{\partial u_j}\frac{\partial u_j}{\partial r_j}\frac{\partial r_j}{\partial v_{ij}}$



Backpropagation: intermediate step

- Apply the chain rule
- $\frac{\partial L}{\partial w_j} = \boxed{\frac{\partial L}{\partial z}\frac{\partial z}{\partial s}}\frac{\partial s}{\partial w_j}$
- $\frac{\partial L}{\partial v_{ij}} = \boxed{\frac{\partial L}{\partial z}\frac{\partial z}{\partial s}\frac{\partial s}{\partial u_j}\frac{\partial u_j}{\partial r_j}}\frac{\partial r_j}{\partial v_{ij}}$



- Now define

$$\delta \equiv \frac{\partial L}{\partial s} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial s}$$

$$\varepsilon_j \equiv \frac{\partial L}{\partial r_j} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial s}\frac{\partial s}{\partial u_j}\frac{\partial u_j}{\partial r_j}$$

- Here $L = 0.5(z-y)^2$ and $z = s$

  Thus $\boxed{\delta = (z-y)}$

- Here $s = \sum_{j=0}^{p} u_j w_j$ and $u_j = g(r_j)$

  Thus $\boxed{\varepsilon_j = \delta w_j g'(r_j)}$

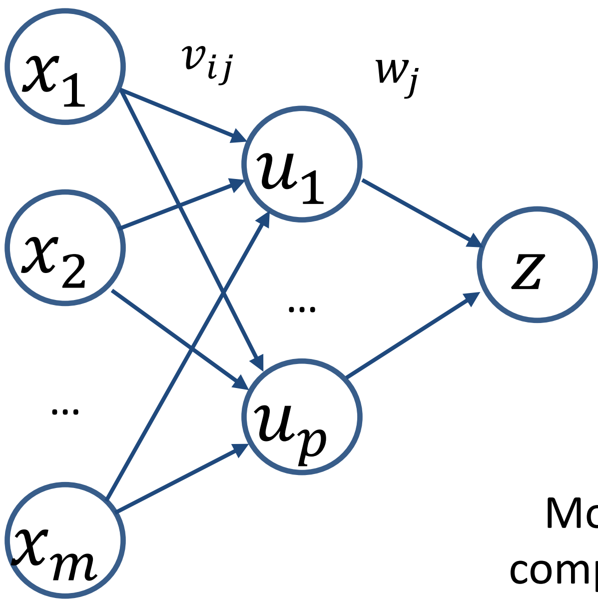
Backpropagation equations

- We have
  * $\frac{\partial L}{\partial w_j} = \delta \boxed{\frac{\partial s}{\partial w_j}}$
  * $\frac{\partial L}{\partial v_{ij}} = \varepsilon_j \boxed{\frac{\partial r_j}{\partial v_{ij}}}$

... where

* $\delta = \frac{\partial L}{\partial s} = (z - y)$
* $\varepsilon_j = \frac{\partial L}{\partial r_j} = \delta w_j g'(r_j)$

- Recall that
  * $s = \sum_{j=0}^{p} u_j w_j$
  * $r_j = \sum_{i=0}^{m} x_i v_{ij}$



- So $\frac{\partial s}{\partial w_j} = u_j$ and $\frac{\partial r_j}{\partial v_{ij}} = x_i$

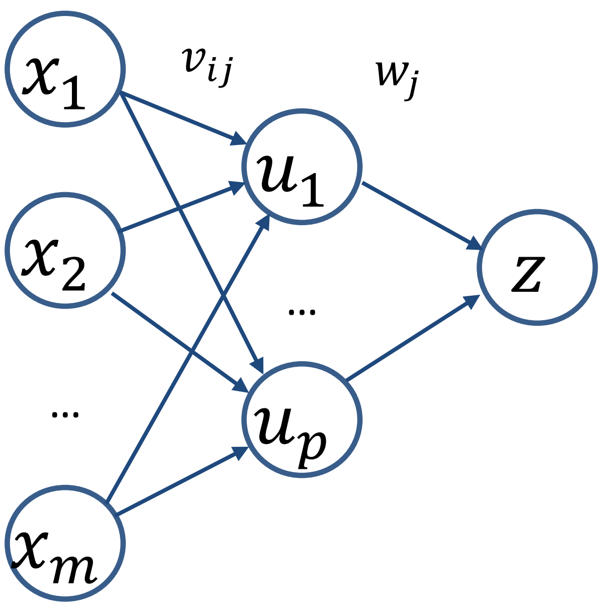
- We have
  * $\frac{\partial L}{\partial w_j} = \delta u_j = (z - y) u_j$
  * $\frac{\partial L}{\partial v_{ij}} = \varepsilon_j x_i = \delta w_j g'(r_j) x_i$

Modern DNN libraries have active derivatives pre-computed; autodiff computes derivatives efficiently

Forward propagation

- Use current estimates of v_{ij} and w_j

- Calculate r_j, u_j, s and z

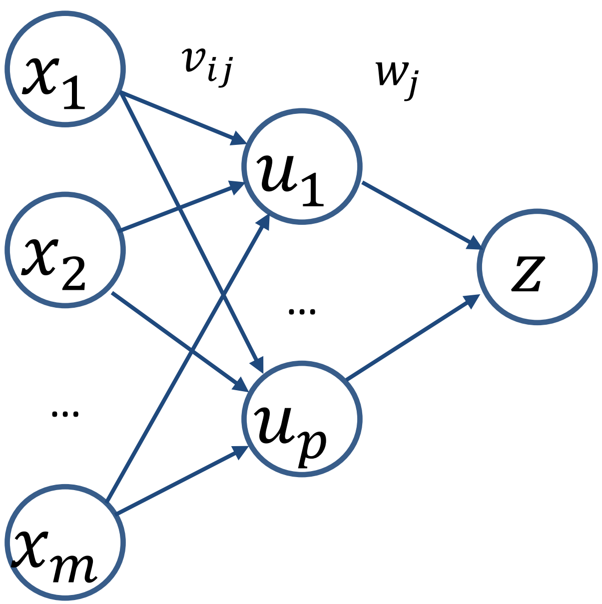


- Backpropagation equations
  * $\frac{\partial L}{\partial w_j} = \delta u_j = (z - y)u_j$
  * $\frac{\partial L}{\partial v_{ij}} = \varepsilon_j x_i = \delta w_j g'(r_j) x_i$

Backward propagation of errors

$$\frac{\partial L}{\partial v_{ij}} = \varepsilon_j x_i \quad \Leftarrow \quad \varepsilon_j = \delta w_j g'(r_j) \quad \Leftarrow \quad \frac{\partial L}{\partial w_j} = \delta u_j \quad \Leftarrow \quad \delta = (z - y)$$

Notice how intermediate values get reused.



- Backpropagation equations
  - $\frac{\partial L}{\partial w_j} = \delta u_j = (z - y)u_j$
  - $\frac{\partial L}{\partial v_{ij}} = \varepsilon_j x_i = \delta w_j g'(r_j) x_i$

This lecture

- Multi-layer perceptron
- Representation learning: learned bases
- Backpropagation
  - derivative chain rule
  - algorithm to compute gradients in backwards pass over network graph

Next lecture: Deep net training, autoencoders