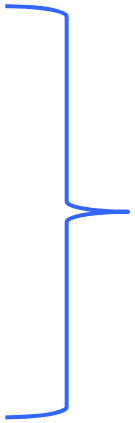
Today

- Neural networks and deep learning
  - Single layer neural networks
    - using keras package
    - architectures for different questions
      - regression, classification, multifunction
  - Multi-layer neural networks
  - Convolutional neural networks
  - U-net
  - Transformers



Neural network libraries

- PyTorch
  - torch (LUA, C): original Swiss nonprofit
  - Facebook/Meta, Linux foundation
  - Python (C++ backend)
  - most popular framework last 5 years
  - R torch library (PyTorch port)
    - developed over last few years
    - capability increasing
    - new book: Keydana 2023

Neural network libraries

- Tensorflow, keras
  - tensor: multidimensional array
  - Google
  - original: tensorflow C++ library
  - Python tensorflow library (2.0, 2019)
  - Python keras library (easier interface)
  - R tensorflow library > tensorflow R API
  - R keras library > Python keras

We will use keras since both R and Python; similar to PyTorch API

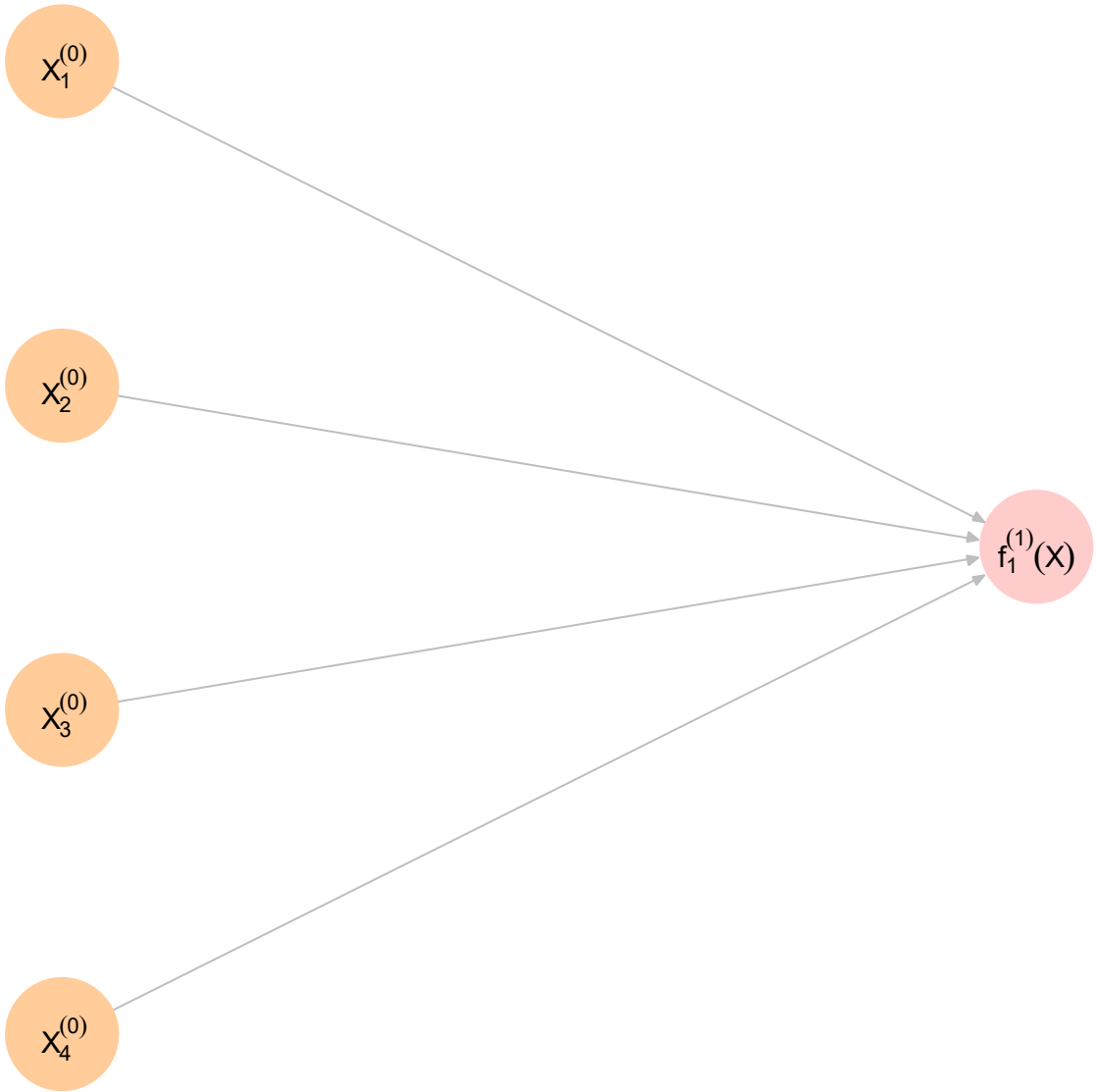
Reminder

- Data science framework
  - model algorithm
  - training algorithm
  - inference algorithm

Model algorithm: architecture

- How many units and how they are connected
- What activation functions are applied to each unit

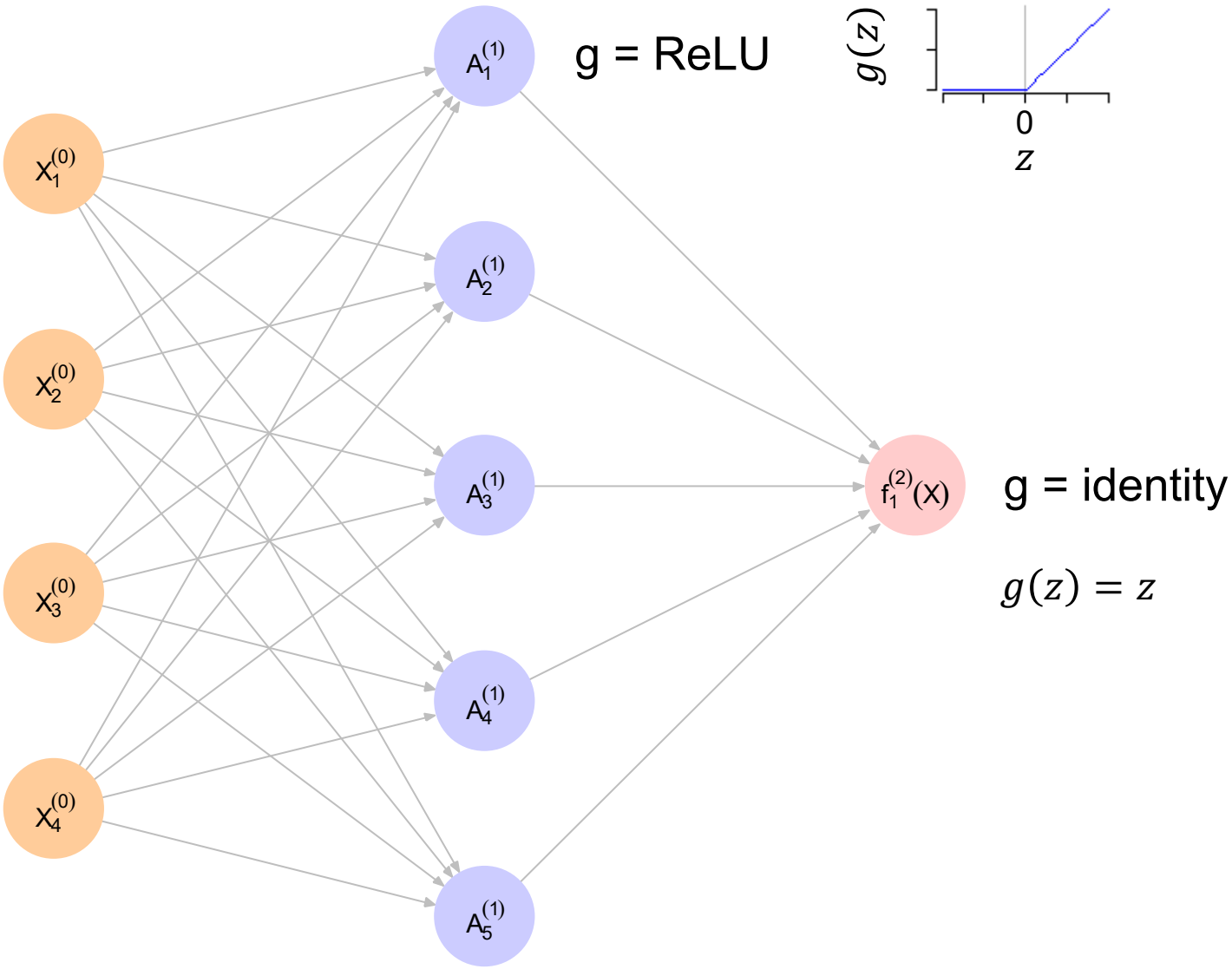
Architecture: multiple linear regression



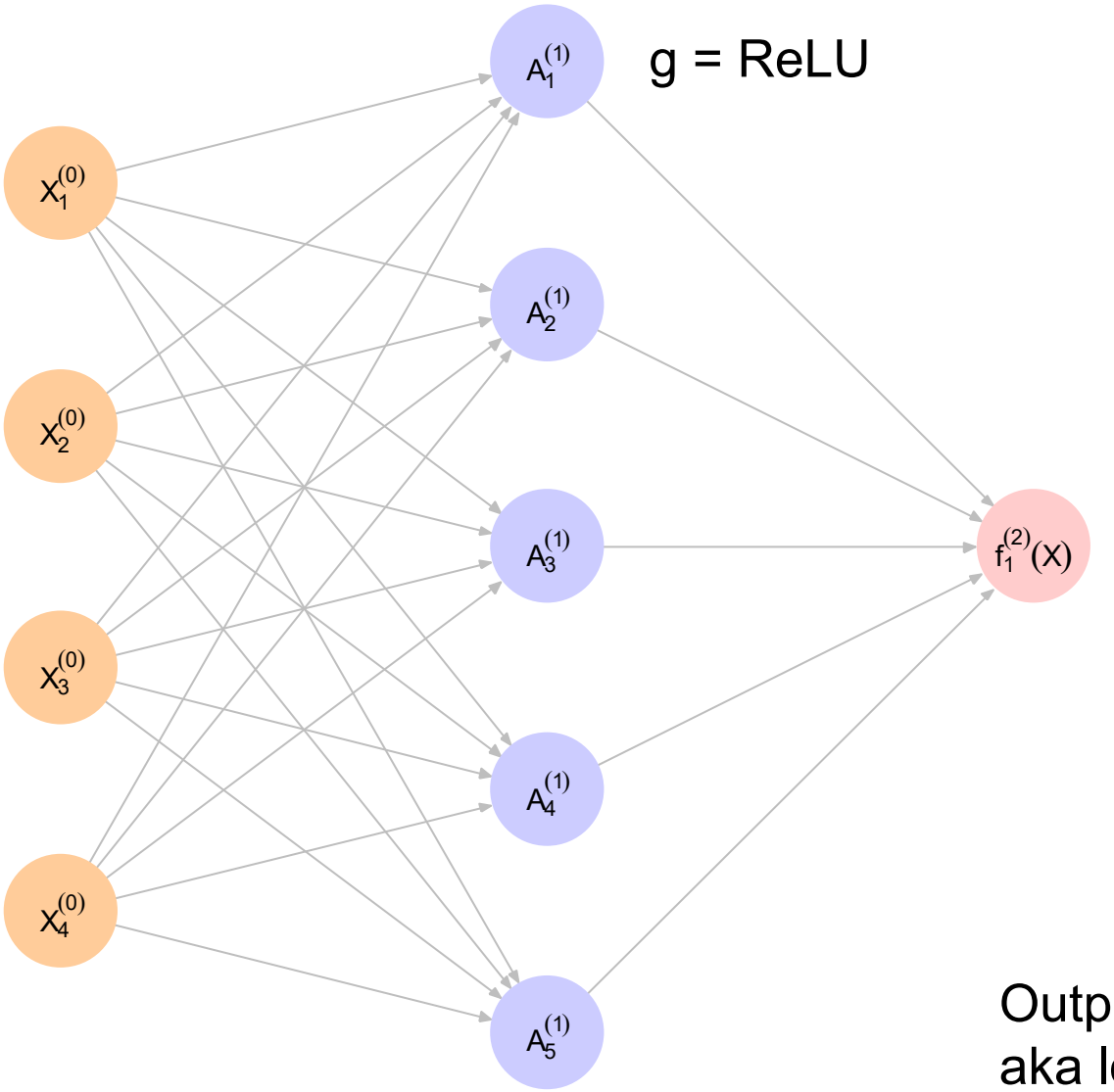
g = identity

$g(z) = z$

Architecture: regression

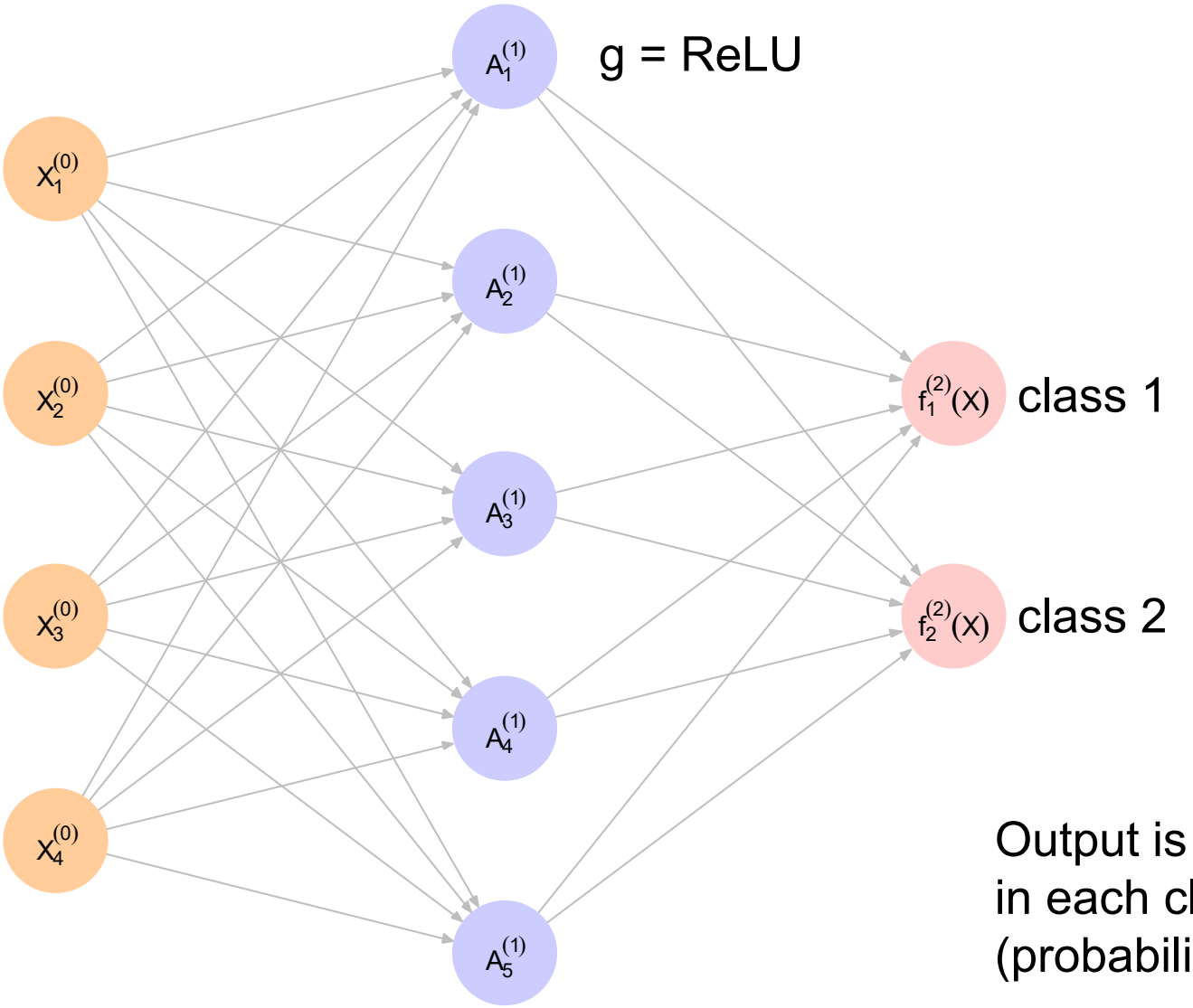


Architecture: binary classification (opt 1)



Output is probability
aka logistic regression

Architecture: binary classification (opt 2)

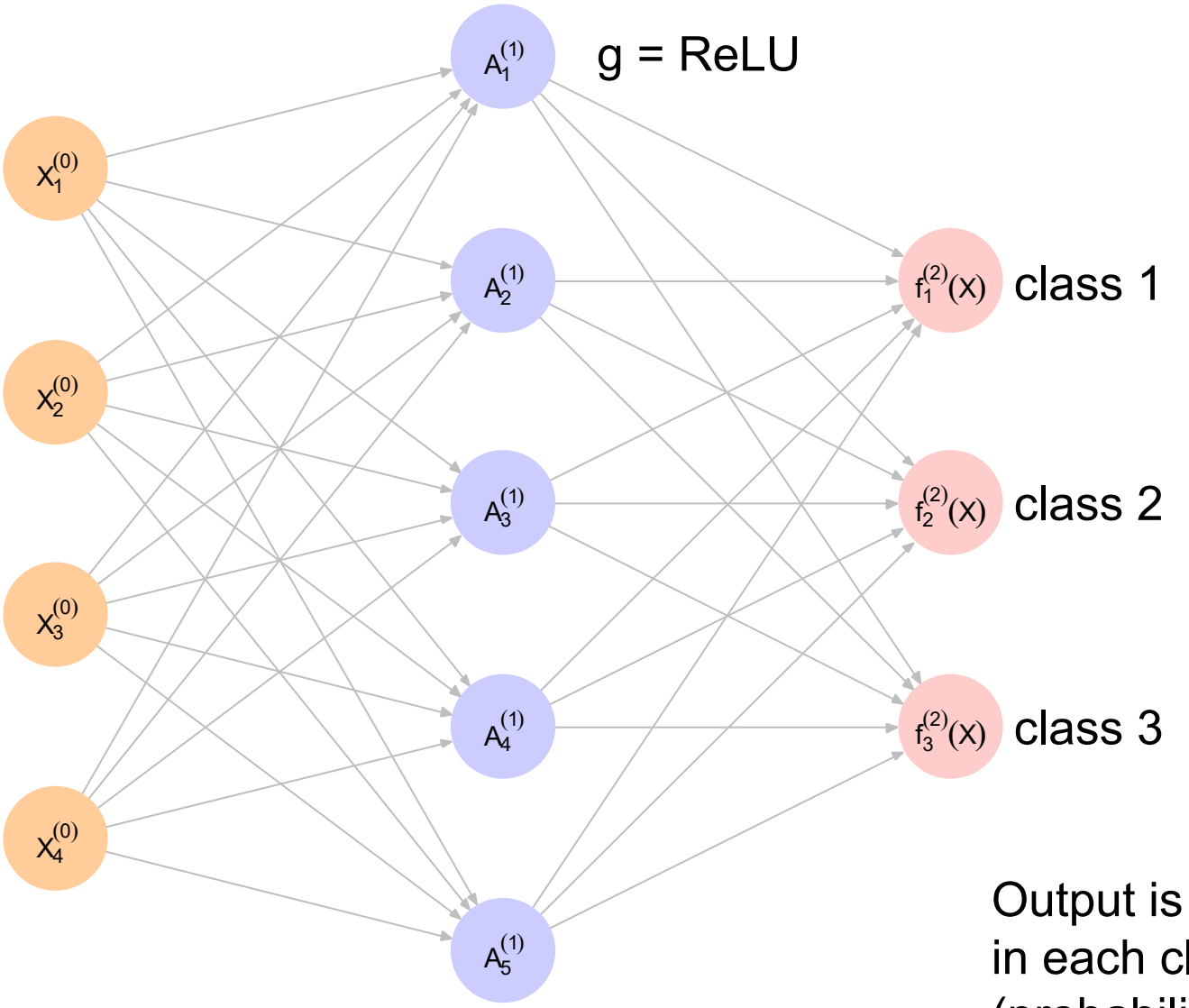


g = softmax

$$g_m(z) = \frac{e^{z_m}}{\sum_{l=1}^{K} e^{z_l}}$$

Output is probability
in each class
(probability sums to 1)

Architecture: multicategory classification



g = softmax

$$g_m(z) = \frac{e^{z_m}}{\sum_{l=1}^{K} e^{z_l}}$$

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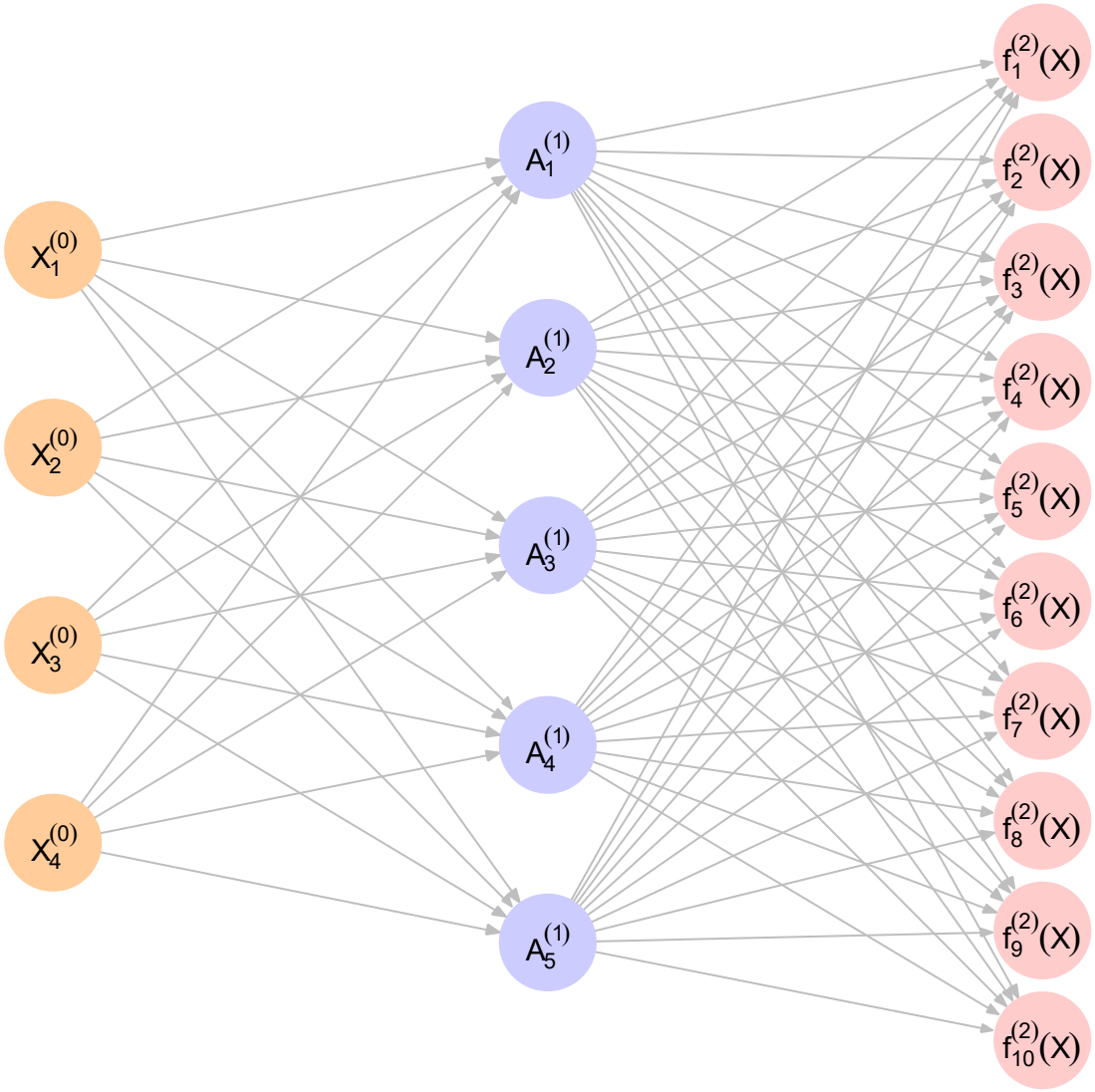
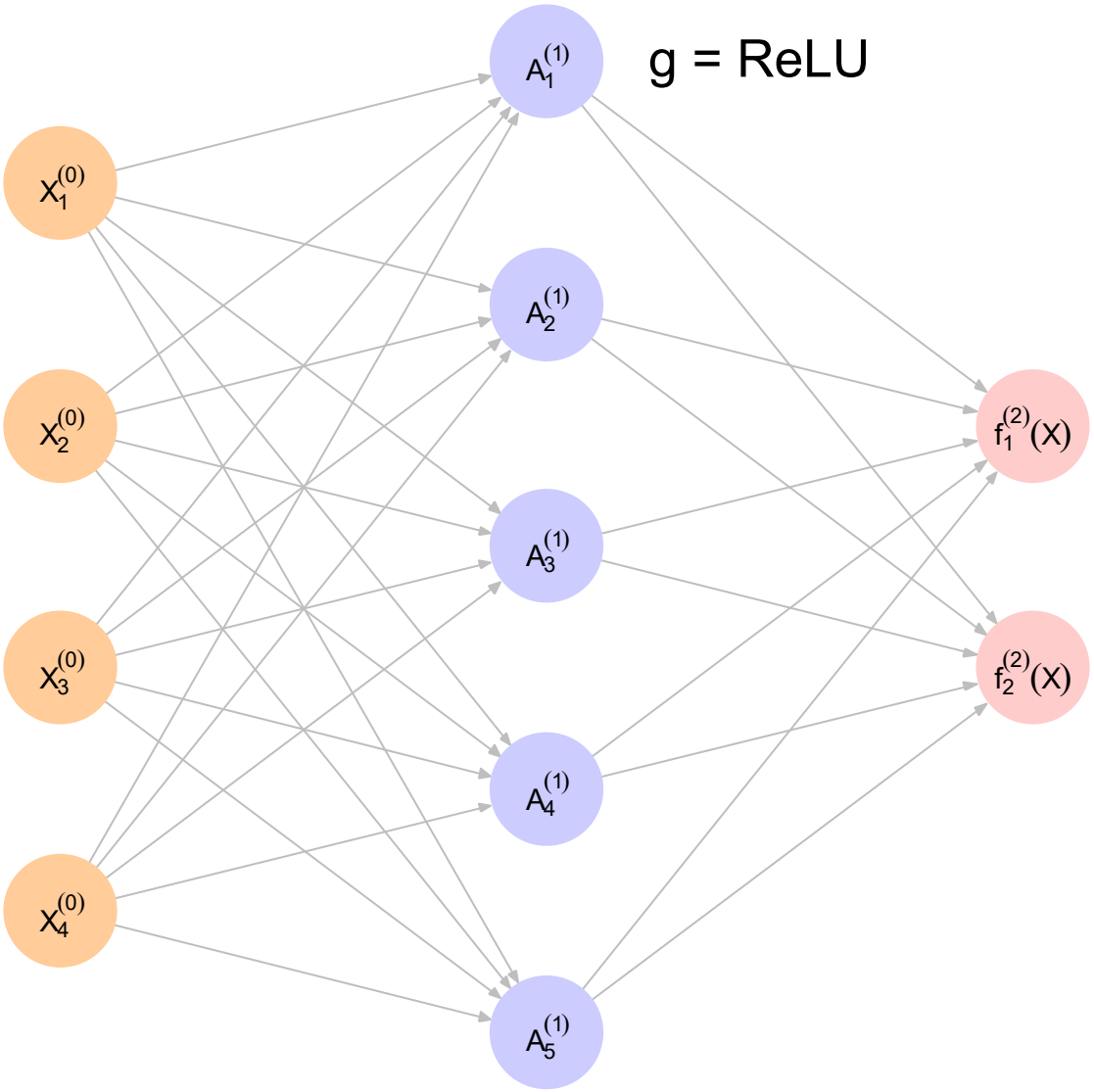
Architecture: multicategory classification



Could have any number of categories

Architecture: multifunction (examples)



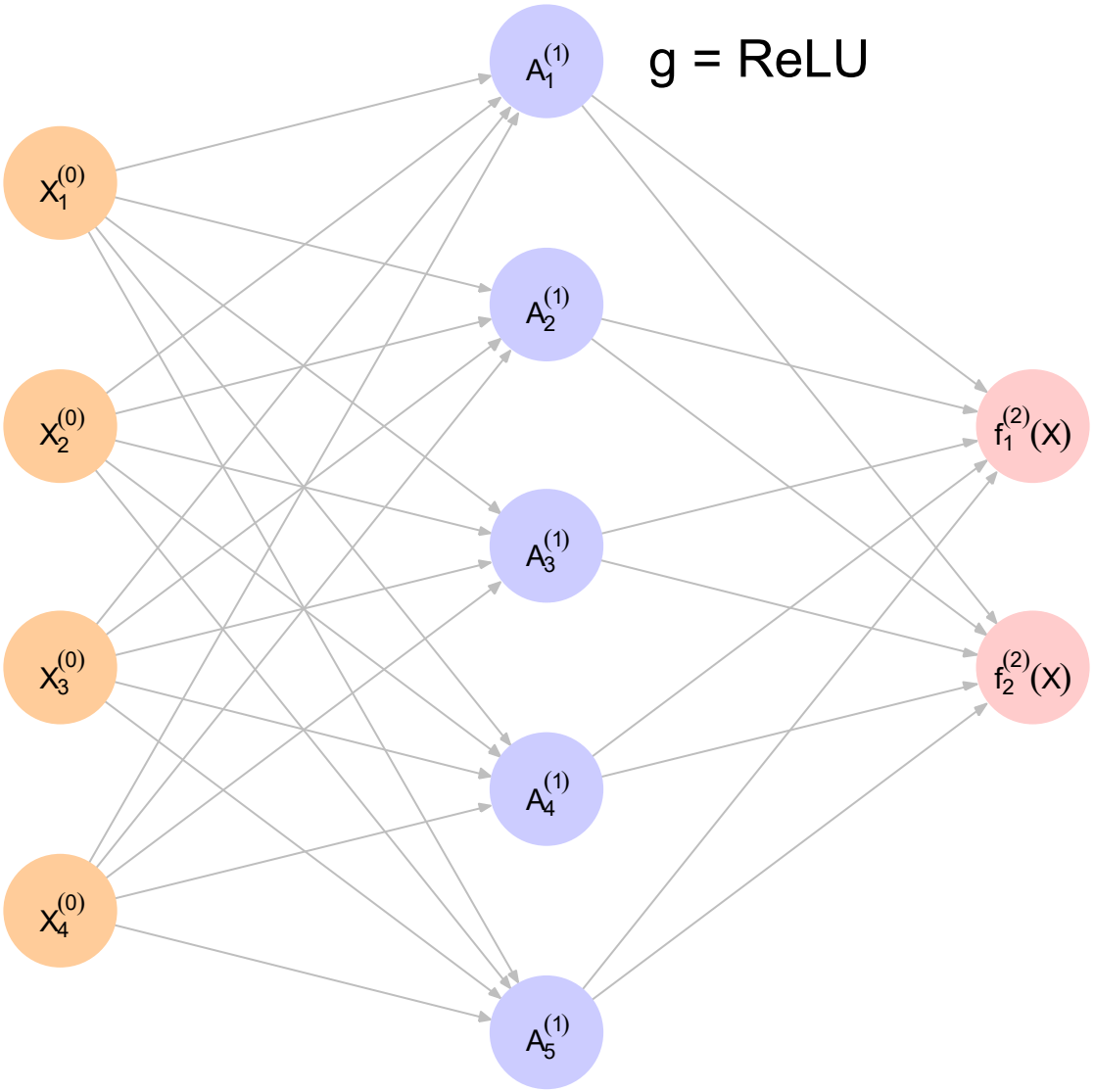
Joint species abundance model for 2 species

g = identity
Y1 = abun species 1

g = identity
Y2 = abun species 2

Output is a prediction for two different outcome variables Y1, Y2

Architecture: multifunction (examples)



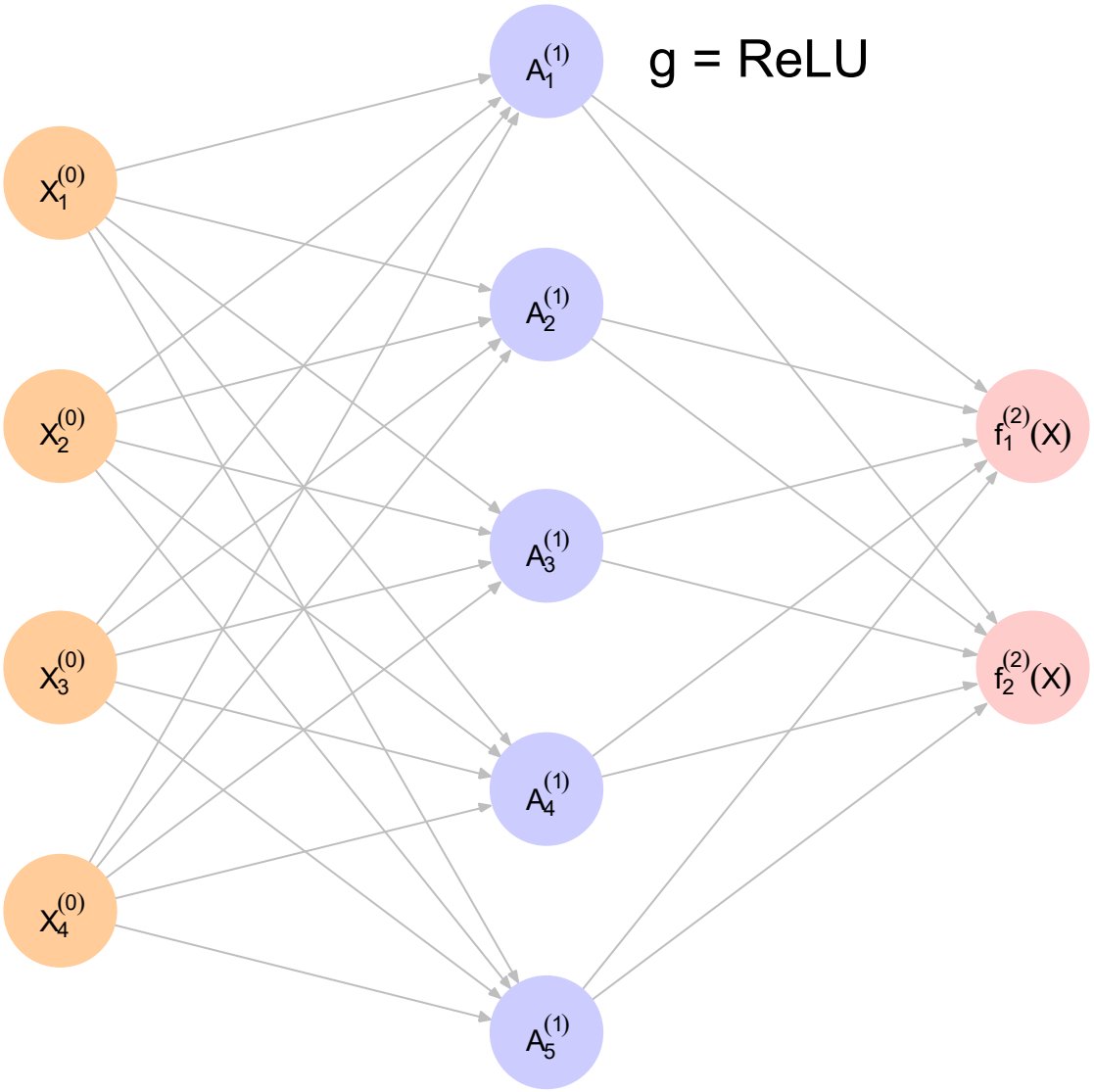
Joint species distribution model for 2 species

g = sigmoid
Y1 = prob species 1

g = sigmoid
Y2 = prob species 2

Output is a prediction for two different outcome variables Y1, Y2

Architecture: multifunction (examples)



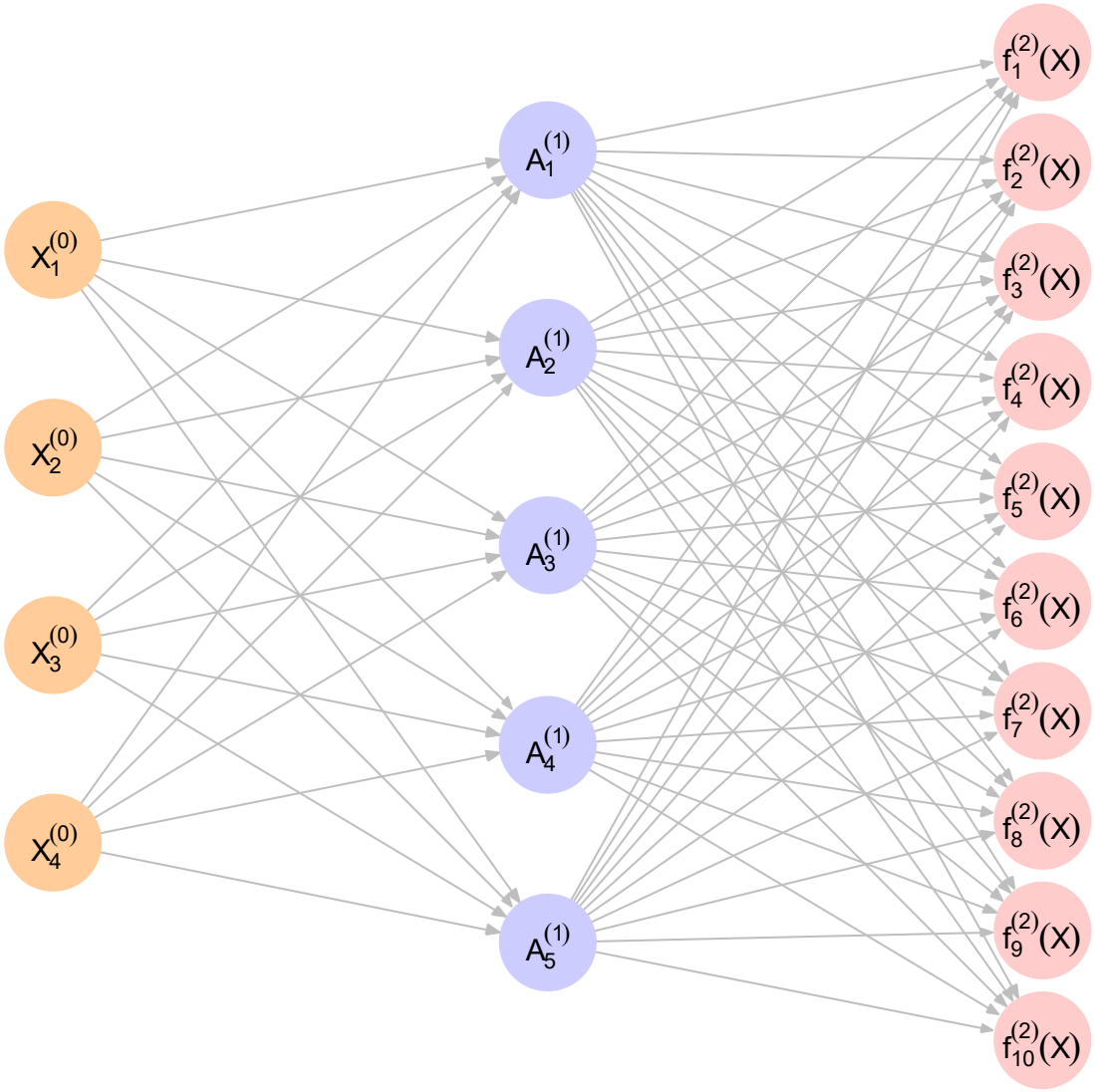
Joint presence-abundance model for a single species

g = sigmoid
Y1 = prob presence

g = identity
Y2 = abundance

Output is a prediction for two different outcome variables Y1, Y2

Architecture: multifunction (examples)



Could be quite complex with different g(z) for many different output variables

Deep learning

- Multilayer neural networks
  - aka deep feedforward networks
  - aka multilayer perceptrons (MLP)
- Model algorithm
  - expressiveness
    - ability to approximate complex nonlinearity
  - architecture: width versus depth
  - depth = number of layers
  - width = number of nodes in a layer

Expressiveness

Universal approximation theorem (1989)

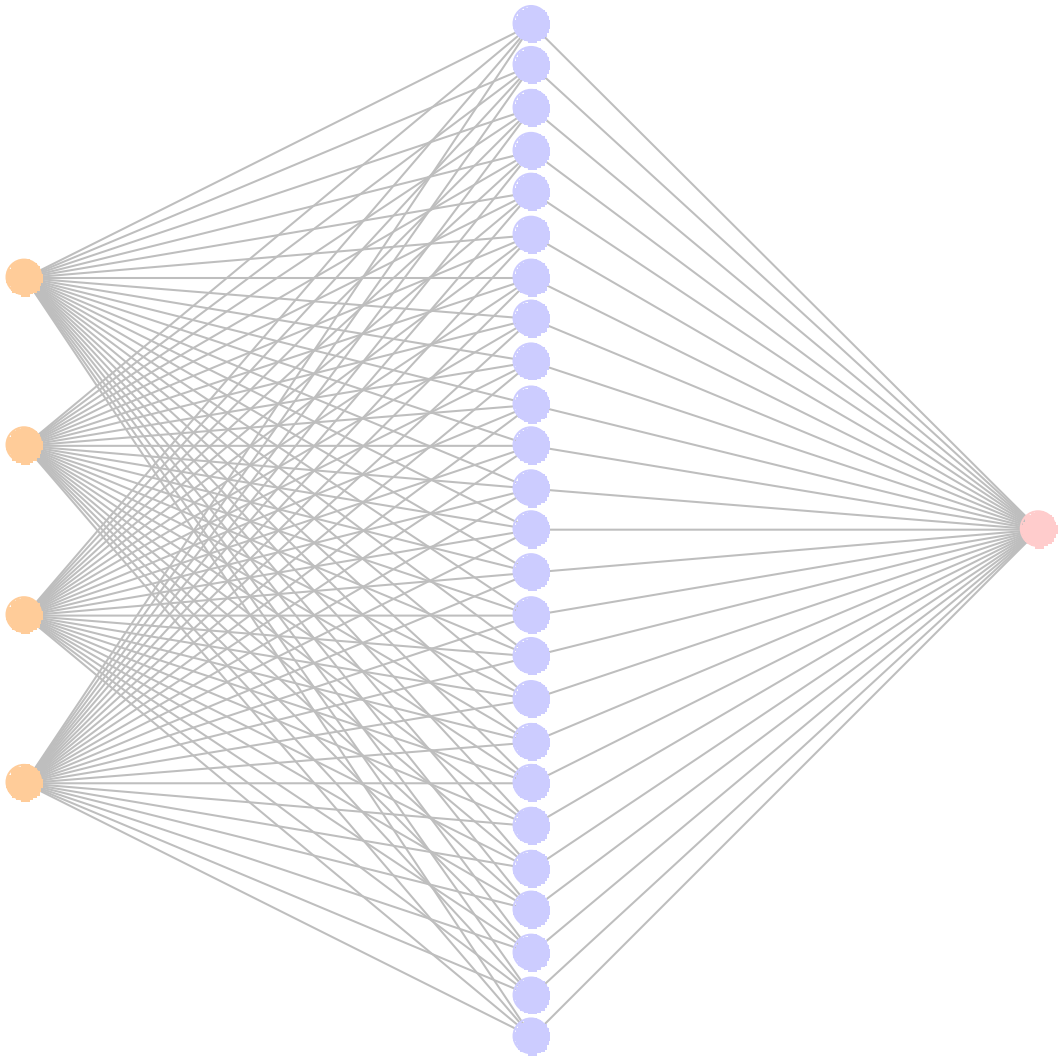
A feedforward neural network with at least one hidden layer can approximate any mapping

$$X \rightarrow f(X)$$

with arbitrarily low error provided it has enough units

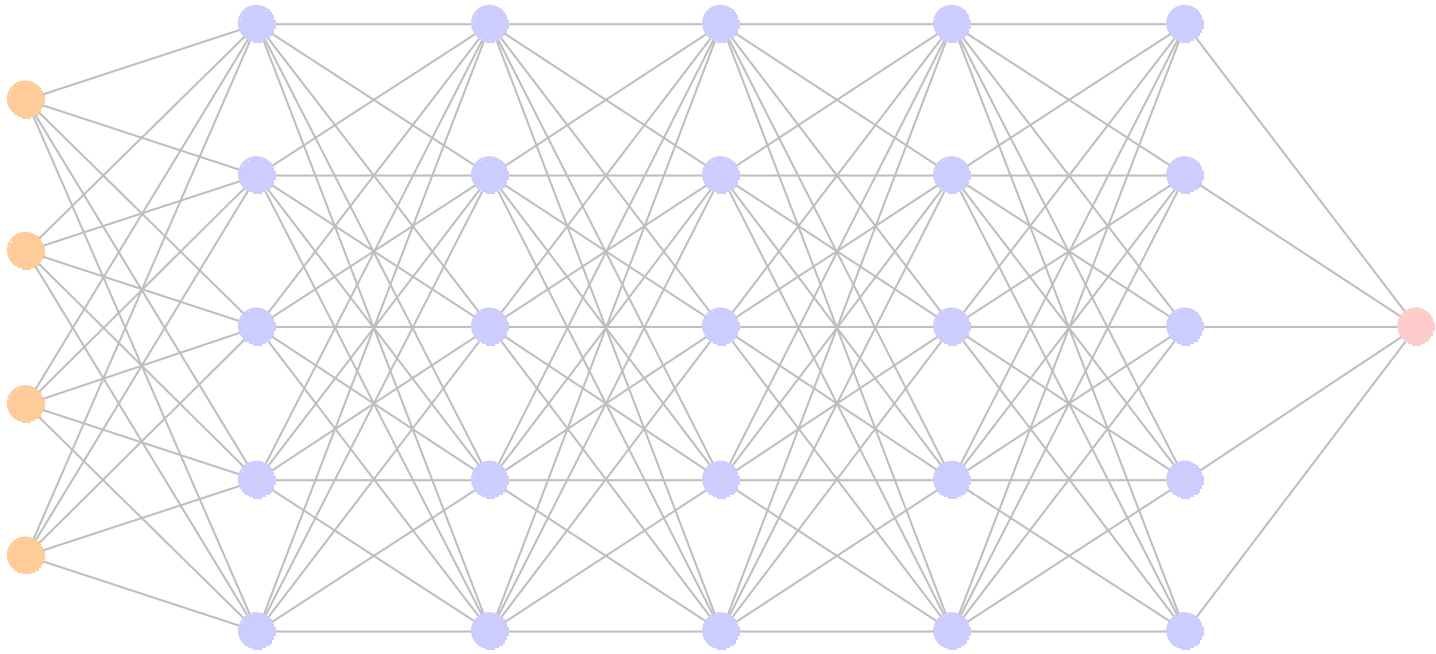
Can be wide or deep

Wide: 25 hidden units

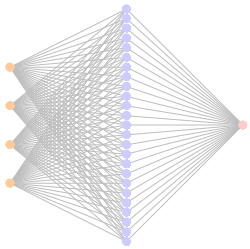


125 connections

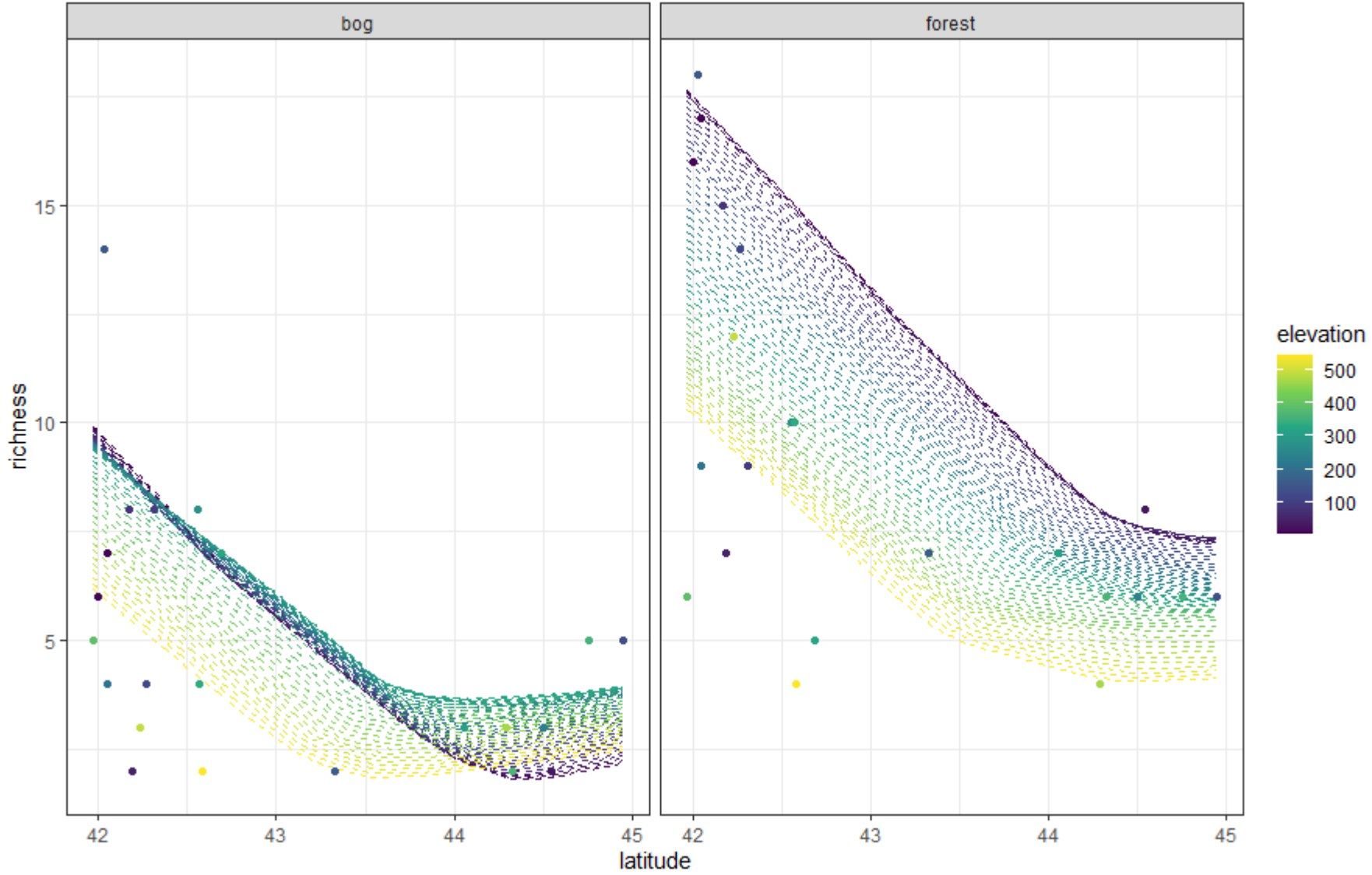
Deep: 25 hidden units

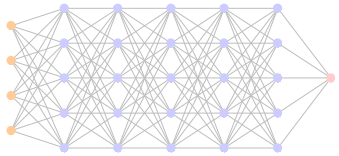


125 connections

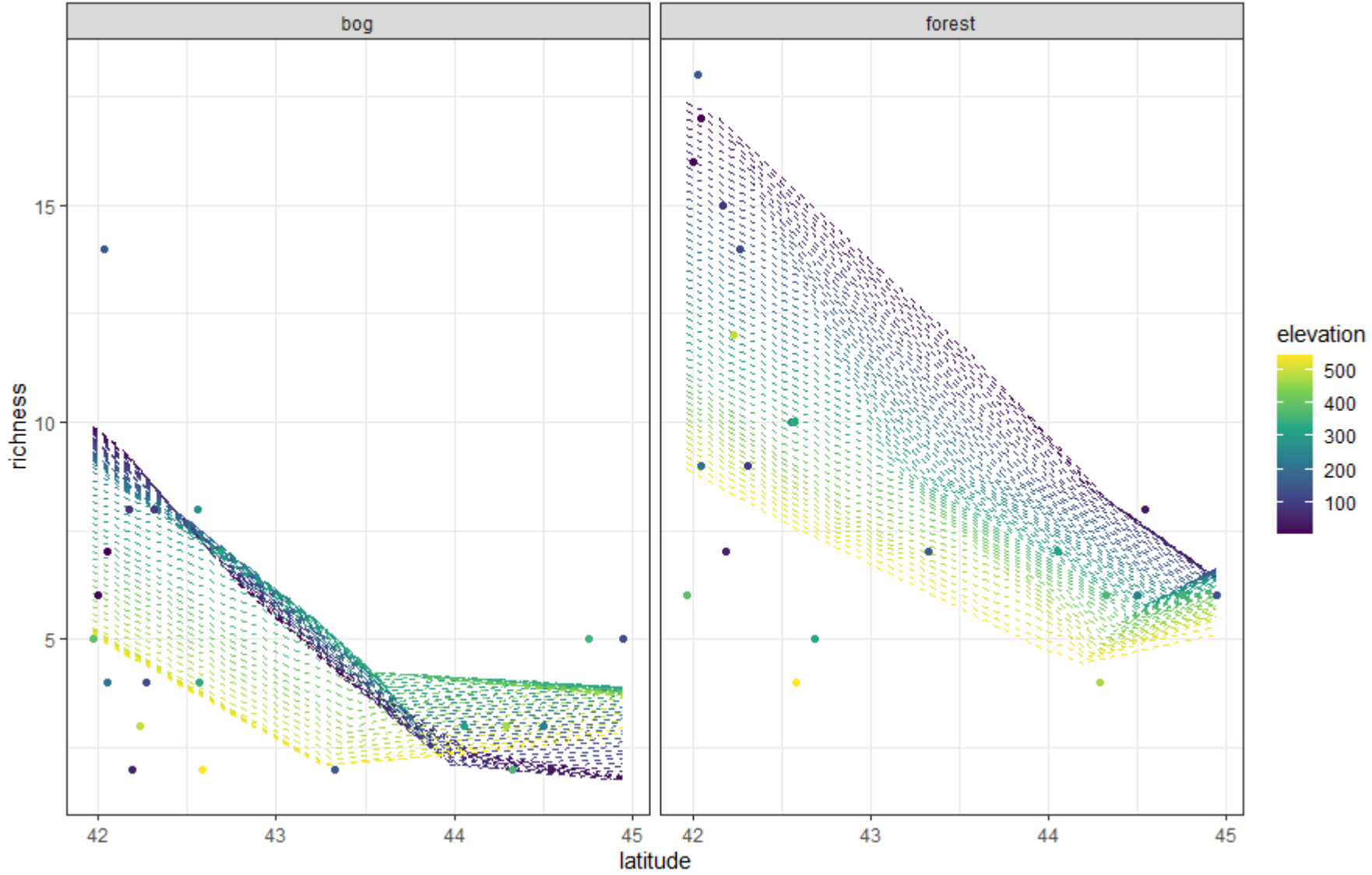


Ants data: wide



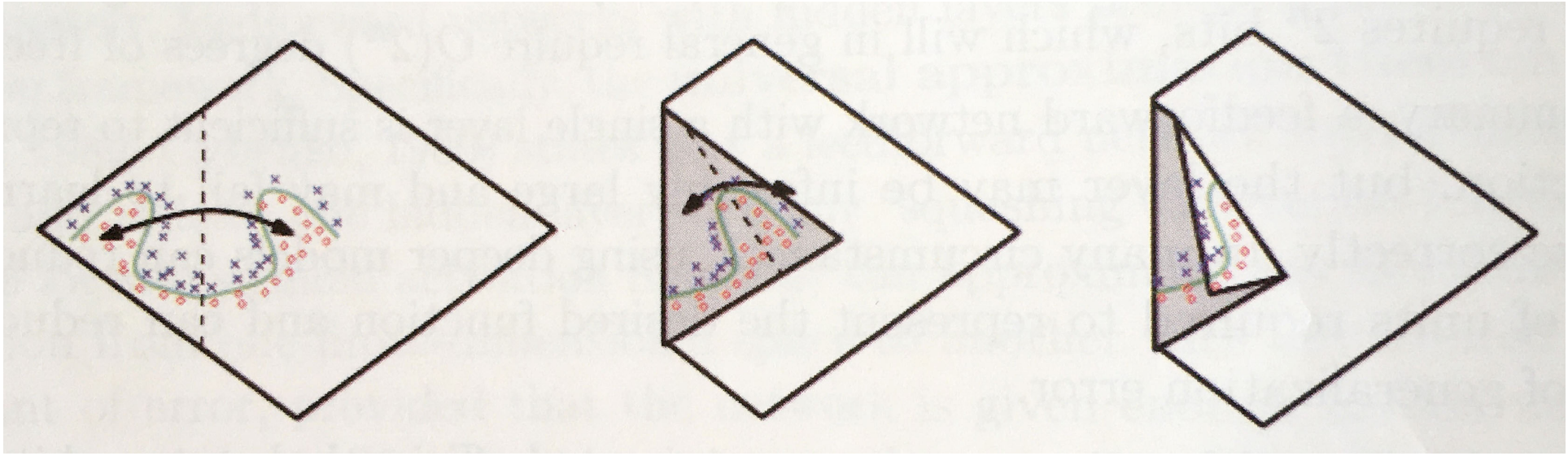


Ants data: deep



Deep: expressiveness

1 layer **2 layers** **3 layers**



Deeper networks (more layers) allow more folds, which can represent the same complex function more efficiently by finding symmetries

Goodfellow et al 2016 Deep Learning