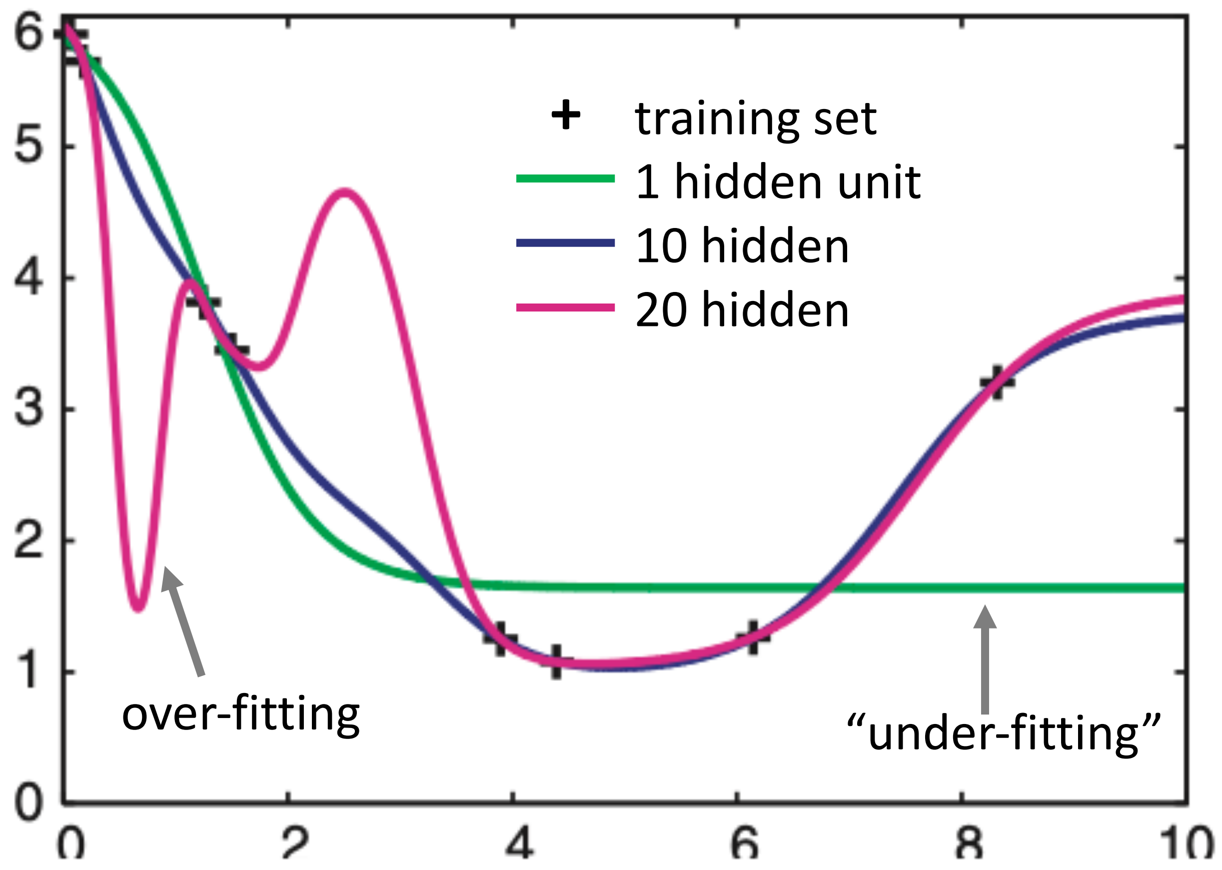
Neural Networks 2

Anders Krogh
Center for Health Data Science
University of Copenhagen

Over-fitting and generalization

- Many parameters and few training data leads to over-fitting
- If it over-fits, the network cannot generalize
- To generalize means to be able to predict on unseen (test) data



From A Krogh (2008) Nat. Biotech. 26, p. 195

Over-fitting and generalization

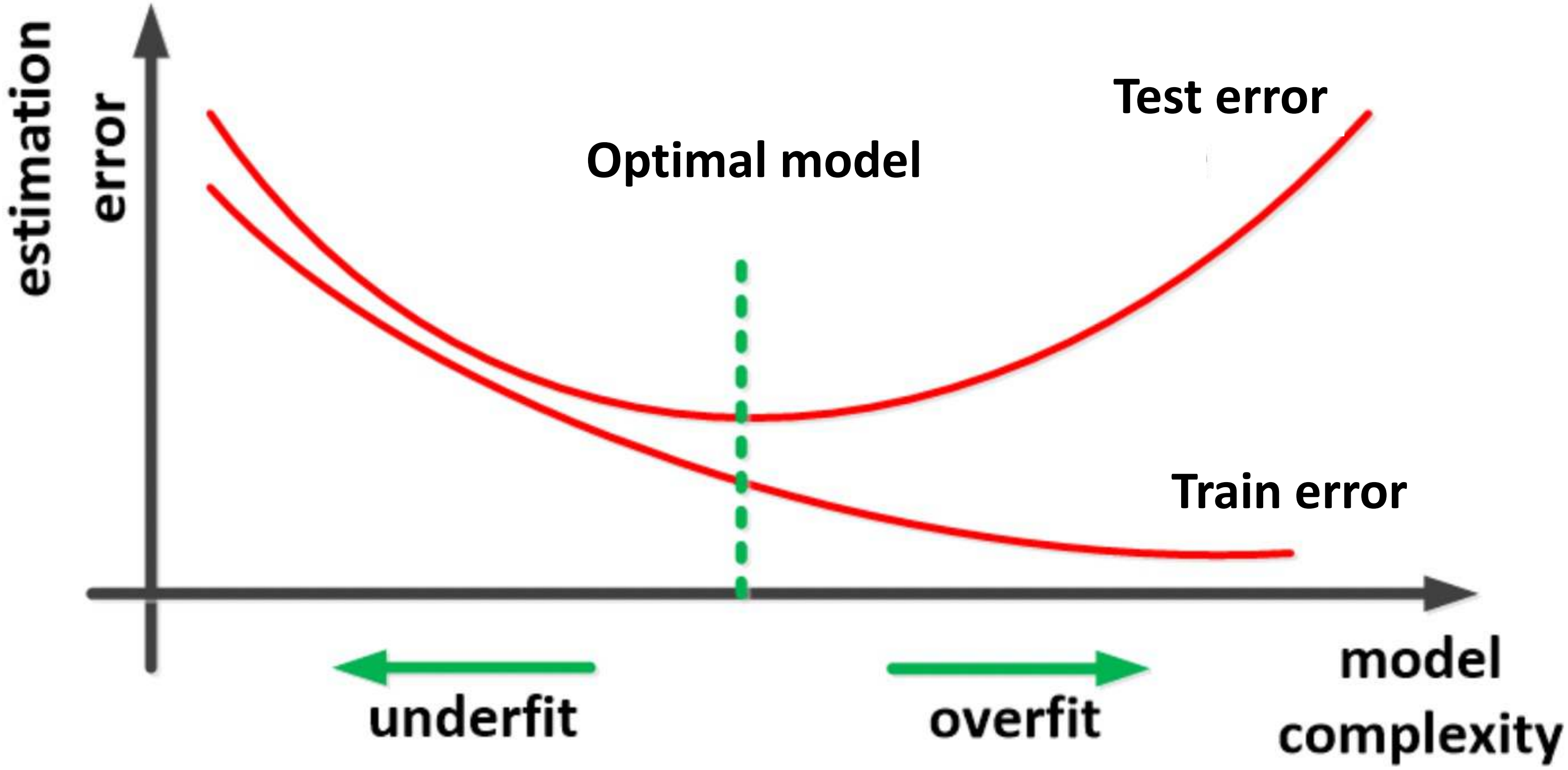


Figure adapted from Ghojogh & Crowley (2019). https://arxiv.org/abs/1905.12787

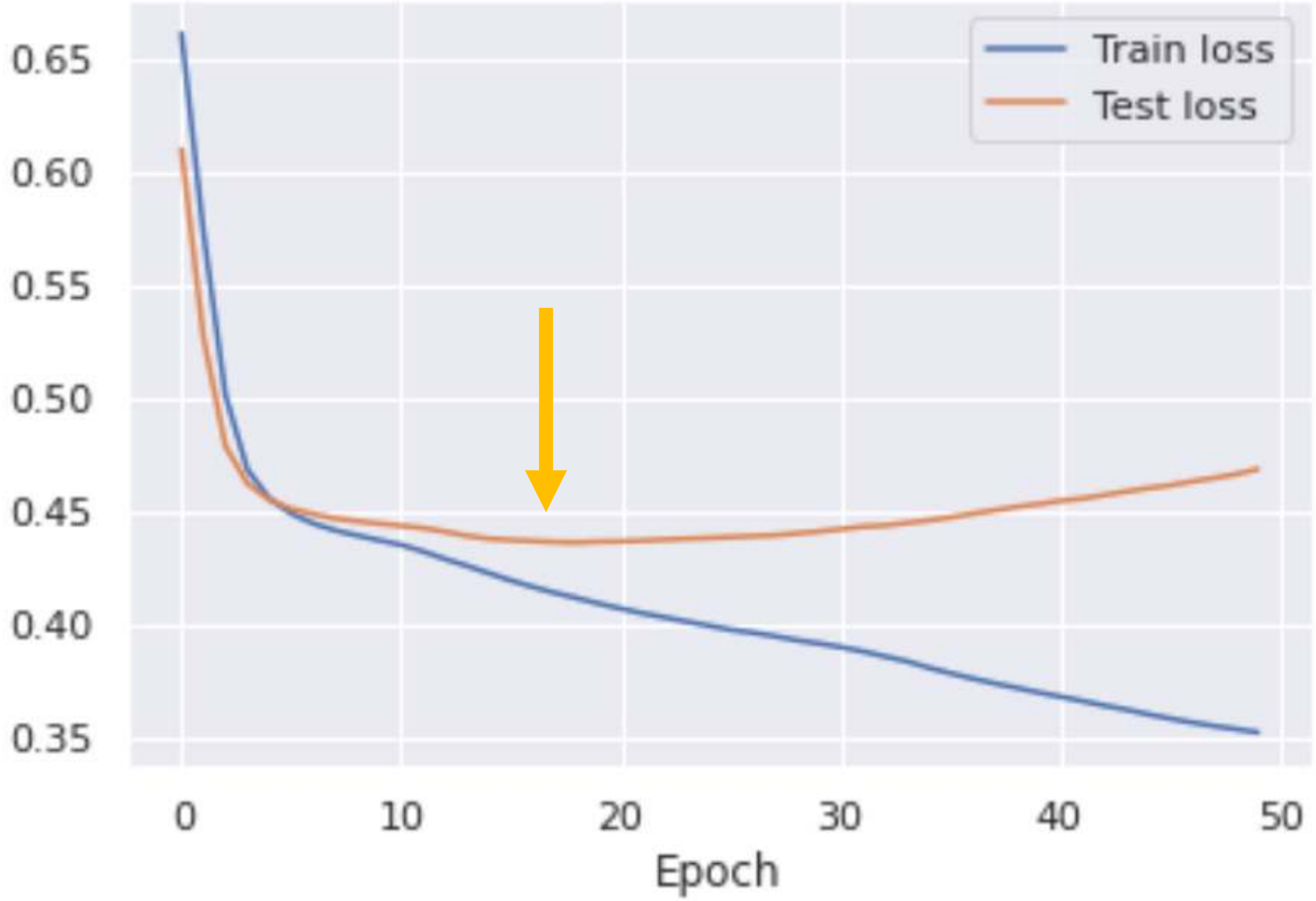
Over-fitting

Sign of over-fitting:

Test error starts to grow while training error decreases

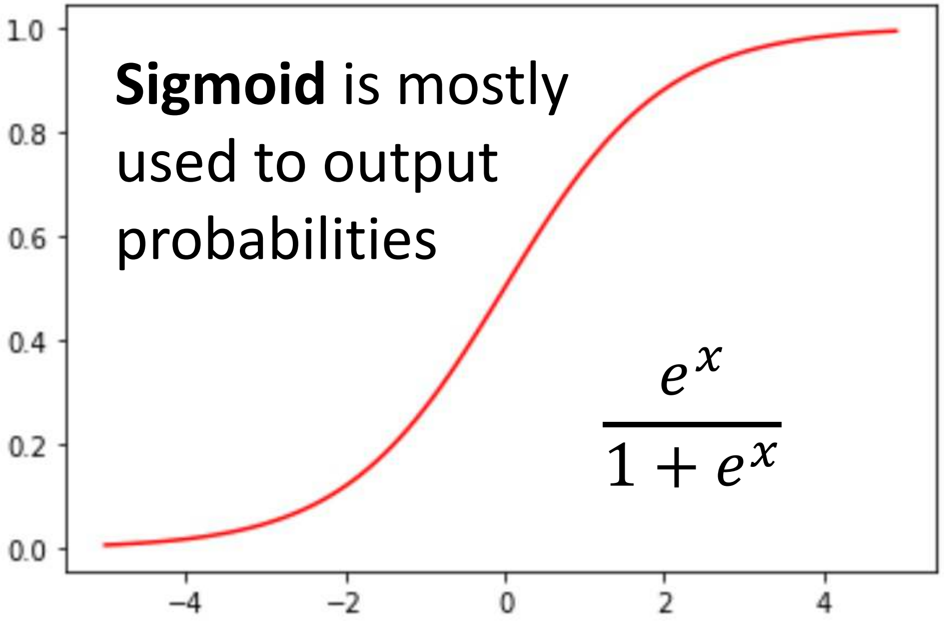
The network size can be decreased if it over-fits (e.g. fewer hidden units)

Alternatively, a weight decay can mitigate over-fitting



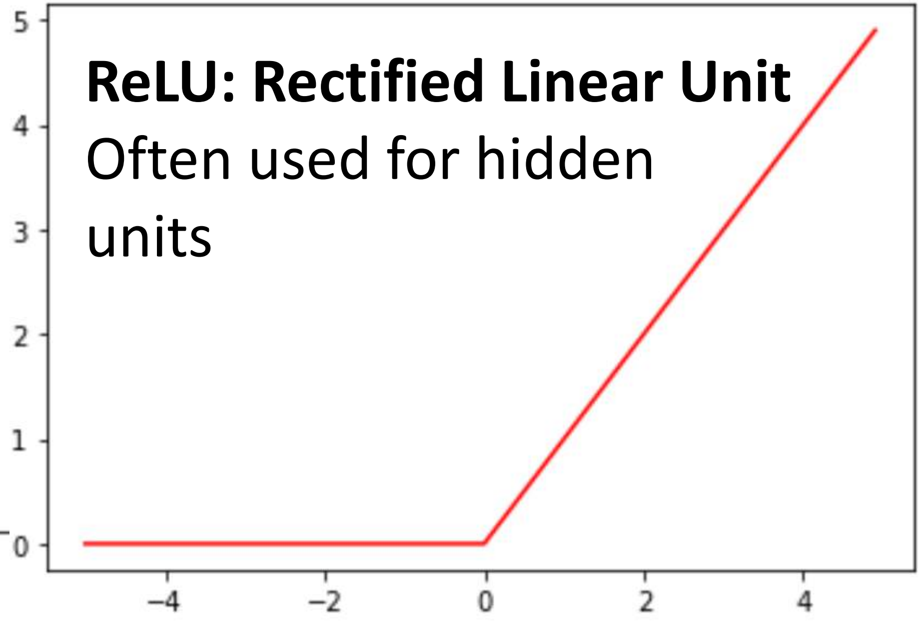
Weight decay: a term λw is subtracted from a weight w in each iteration. λ is normally small, 10^{-2} to 10^{-6}

Activation functions



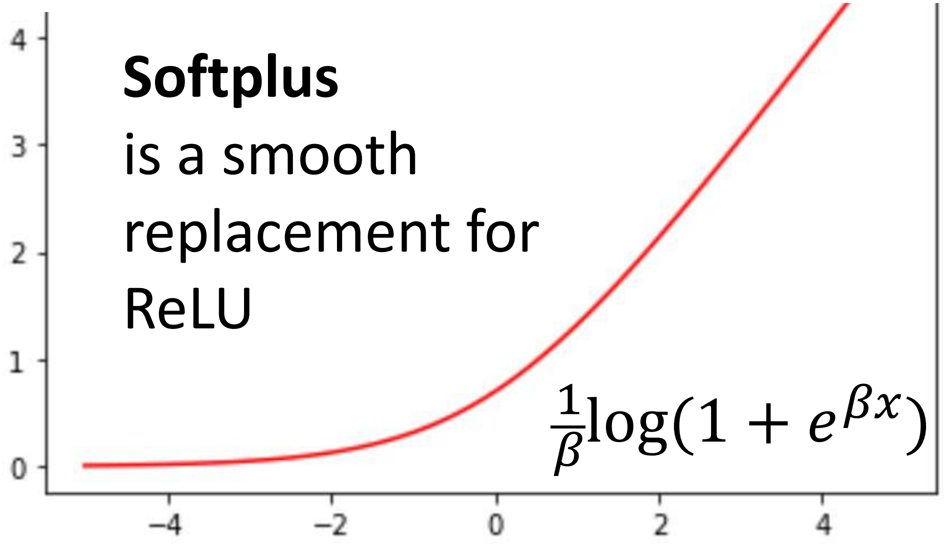
Sigmoid is mostly used to output probabilities

$$\frac{e^x}{1+e^x}$$



ReLU: Rectified Linear Unit

Often used for hidden units



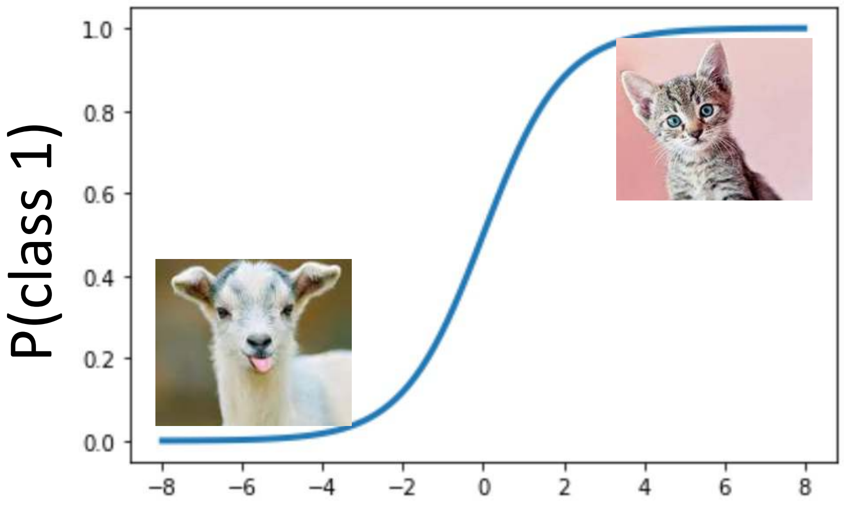
Softplus

is a smooth replacement for ReLU

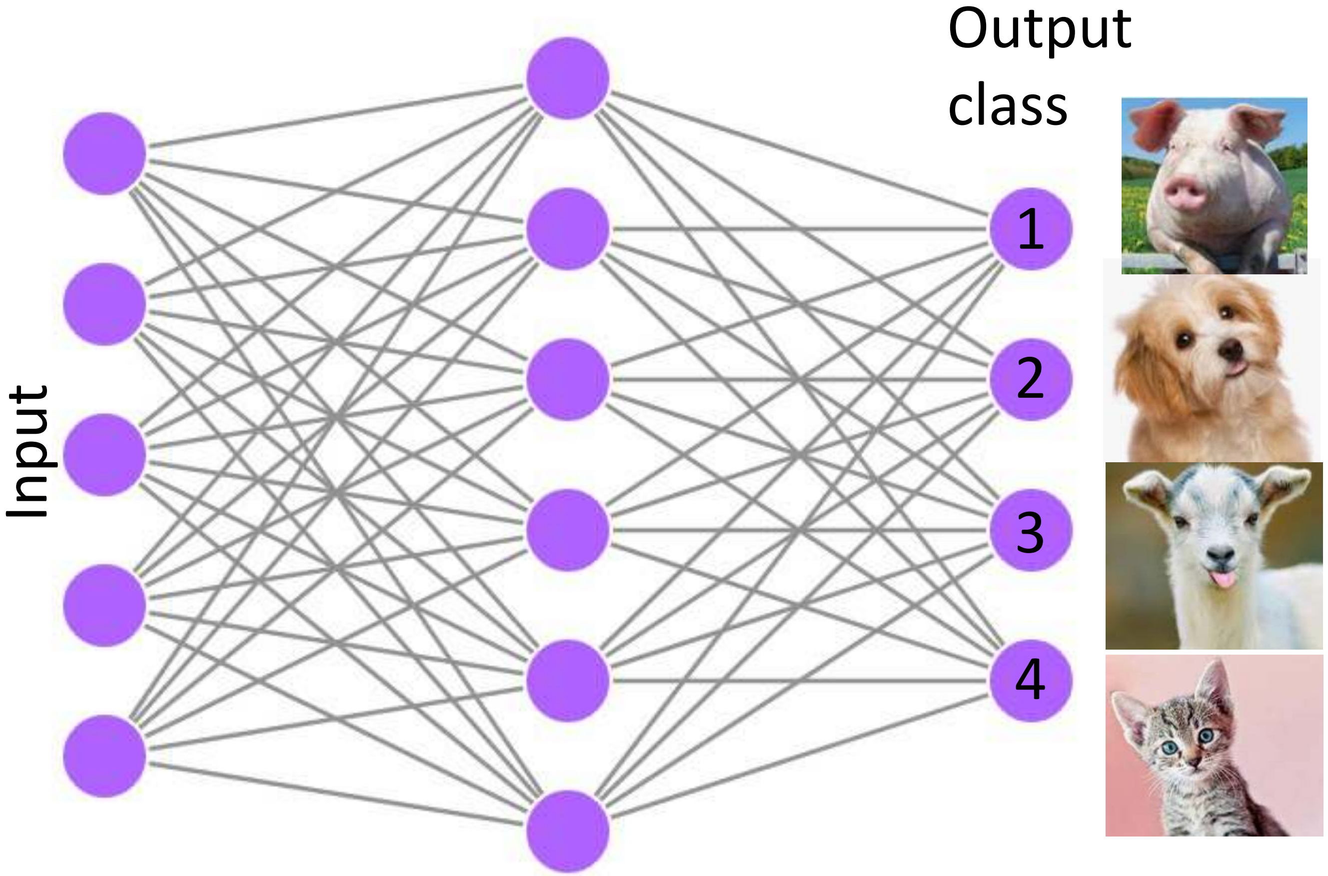
$$\frac{1}{\beta}\log(1+e^{\beta x})$$

What if we have multiple classes?

Sigmoid for two classes



P(class 0) = 1–P(class 1)

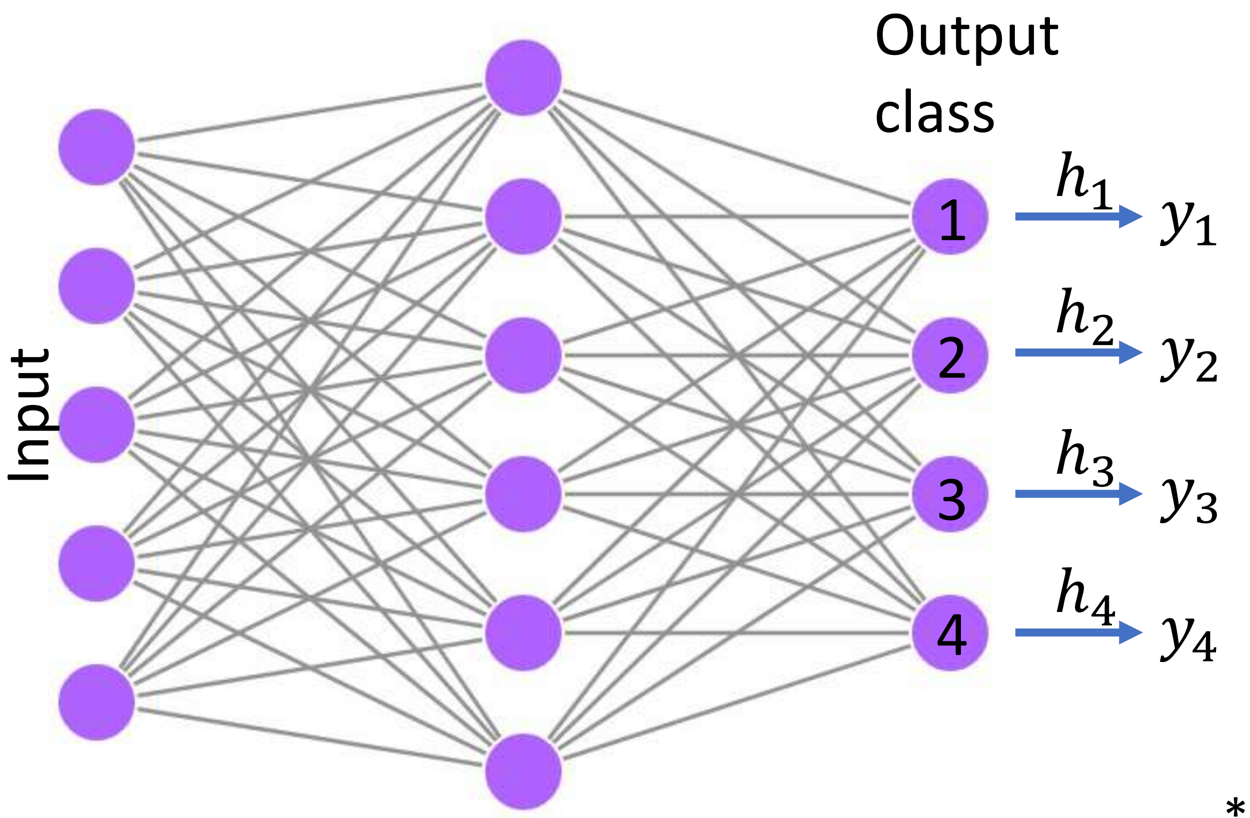


We would like the network to output the probability of each class

Neural net drawing made at http://alexlenail.me/NN-SVG/index.html

Multiple classes: Softmax

Use the softmax function to ensure probabilities sum to one



Weighted sum for the last layer is called h_i for class i

Output for class i:

$$y_i = \text{softmax}(h_i) = \frac{e^{h_i}}{\sum_{j=1}^{n} e^{h_j}}$$

- **Loss function**: cross entropy *
- In pytorch, the softmax is built into the loss function: it takes h_i instead of y_i.

*) Cross entropy loss is similar to binary case.

$E(w) = -\sum_i t_i \log y_i$ where target t_i is 1 or 0

The optimizer

- In plain stochastic gradient descent (torch.optim.SGD) you need to set parameters (learning rate and momentum)
- The Adam optimizer is usually a better choice
  - It automatically adapts the learning rate and momentum in clever ways
  - It is based on SGD and uses mini-batches
  - you can set a weight decay

Example of code using the Adam optimizer:

```
optimizer = torch.optim.Adam(nn.parameters())
for epoch in range(nepochs):
  for x,t in train_loader:
    optimizer.zero_grad()
    y = nn(x)
    loss = lossfunc(y,t)
    loss.backward()
    optimizer.step()
```

You can set parameters in Adam, such as

- learning rate (e.g. “lr=1.e-4”)
- “weight_decay=1.e-5”

All the choices you have to make …

- There are many parameters you can vary in a Neural Network.
- It is a good idea to make an initial “grid search” where you systematically test performance by varying
  - the number of hidden layers and their size
  - other parameters one by one
- This is sometimes done on a reduced data set and or with quite few iterations

Exercise with gene expression data

- Explain the data a bit