Advanced Machine Learning

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Deep Neural Networks

Deep neural networks

- Networks with more than one hidden layer
- Intuition becomes more difficult

Deep neural networks

- Composing two networks
- Combining the two networks into one
- Hyperparameters
- Notation change and general case
- Shallow vs. deep networks

Composing two networks.

$$h_1 = \mathbf{a}[\theta_{10} + \theta_{11}x]$$

Network 1:

$$h_3 = \mathbf{a}[\theta_{30} + \theta_{31}x]$$

$$h_2 = a[\theta_{20} + \theta_{21}x]$$
 $y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$

$$h_1' = a[\theta_{10}' + \theta_{11}'y]$$

Network 2:

$$h_3' = a[\theta_{30}' + \theta_{31}'y]$$

$$h'_2 = a[\theta'_{20} + \theta'_{21}y]$$
 $y' = \phi'_0 + \phi'_1h'_1 + \phi'_2h'_2 + \phi'_3h'_3$

Composing two networks.

$$h_1 = \mathbf{a}[\theta_{10} + \theta_{11}x]$$

Network 1:

Network 2:

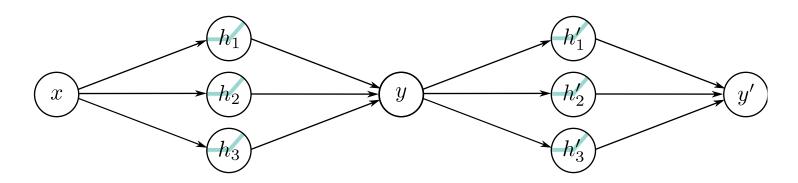
$$h_3 = \mathbf{a}[\theta_{30} + \theta_{31}x]$$

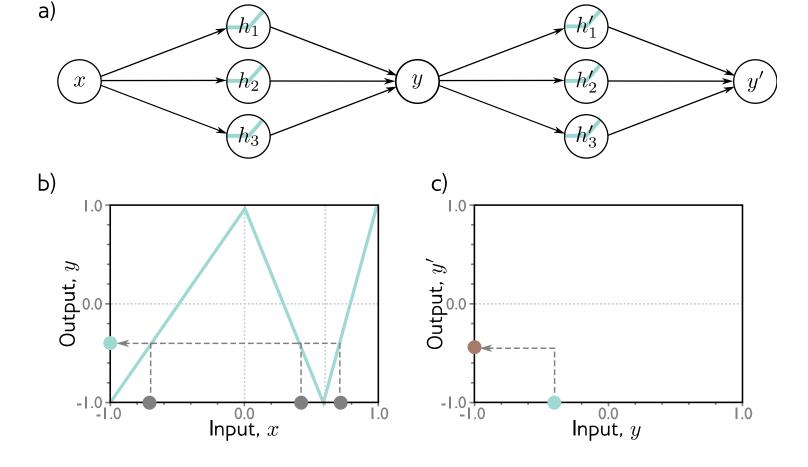
$$h_2 = a[\theta_{20} + \theta_{21}x]$$
 $y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$

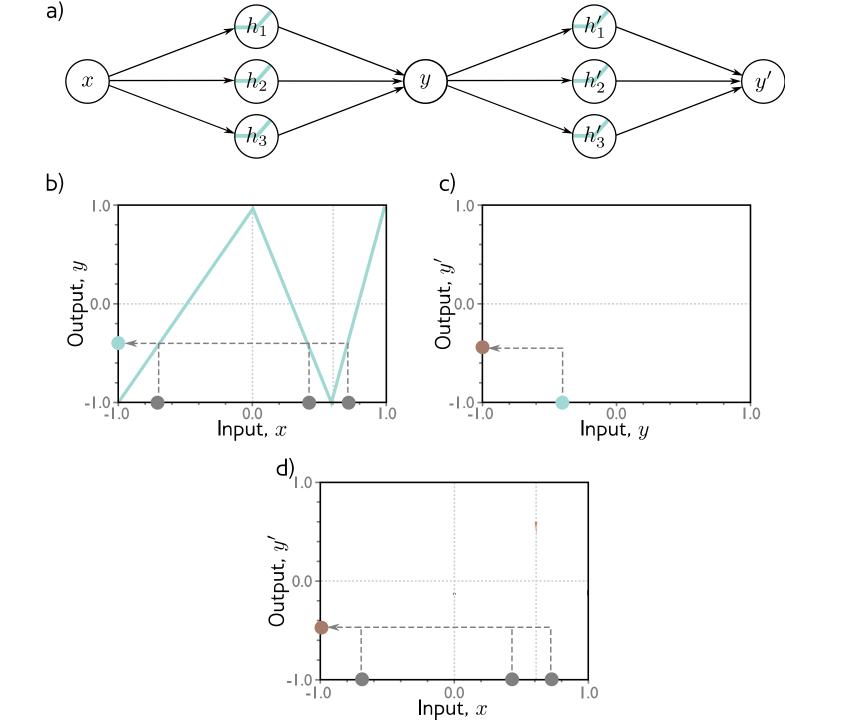
$$h_1' = a[\theta_{10}' + \theta_{11}'y]$$

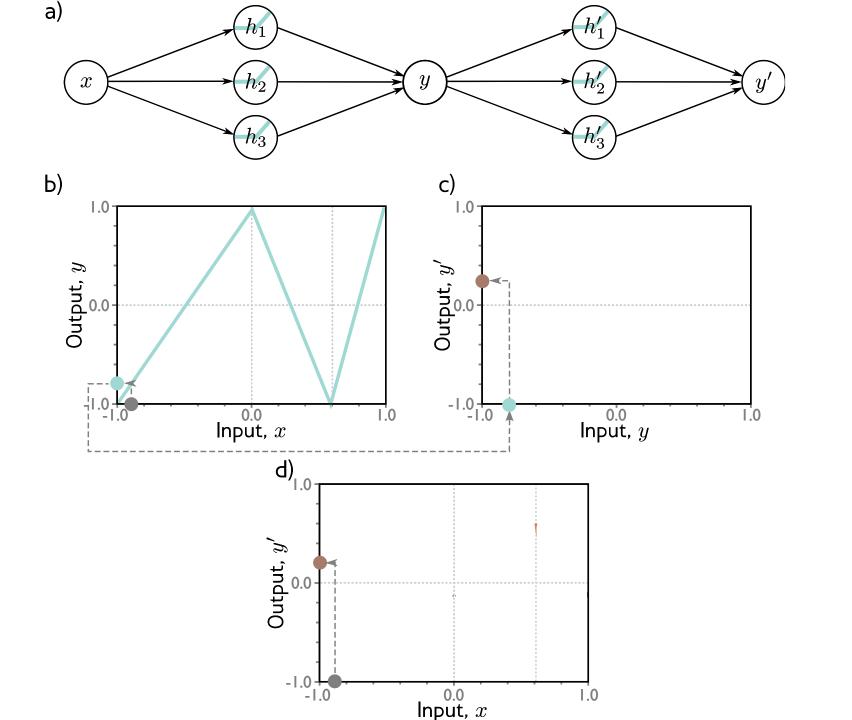
$$h_3' = a[\theta_{30}' + \theta_{31}'y]$$

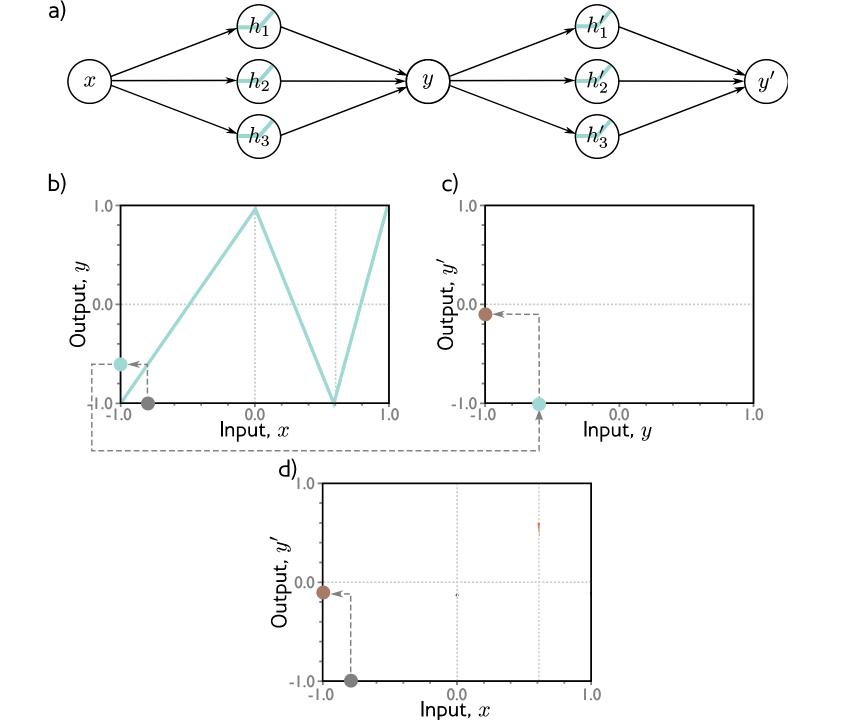
$$h'_2 = a[\theta'_{20} + \theta'_{21}y]$$
 $y' = \phi'_0 + \phi'_1h'_1 + \phi'_2h'_2 + \phi'_3h'_3$

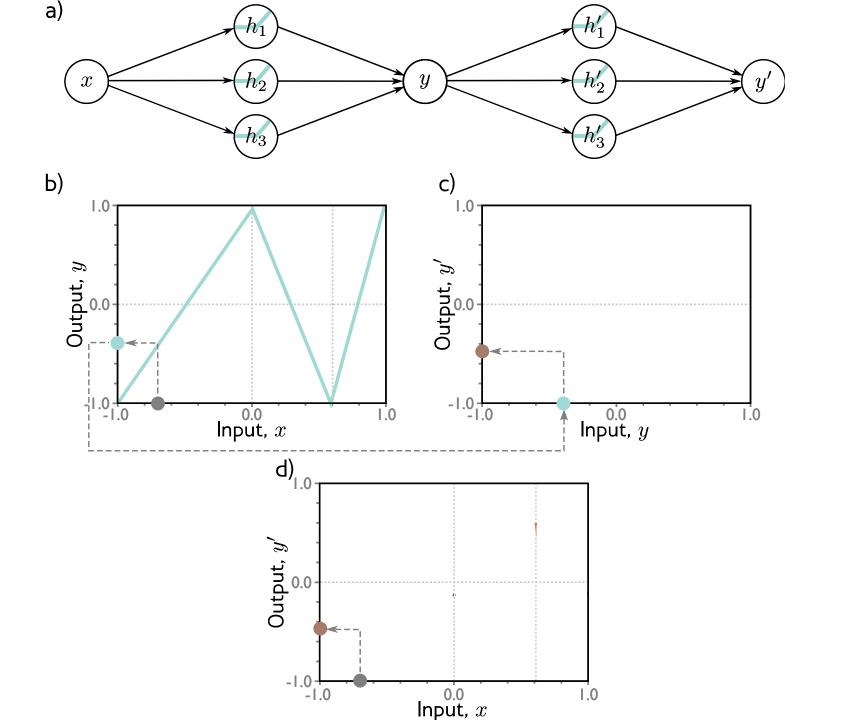


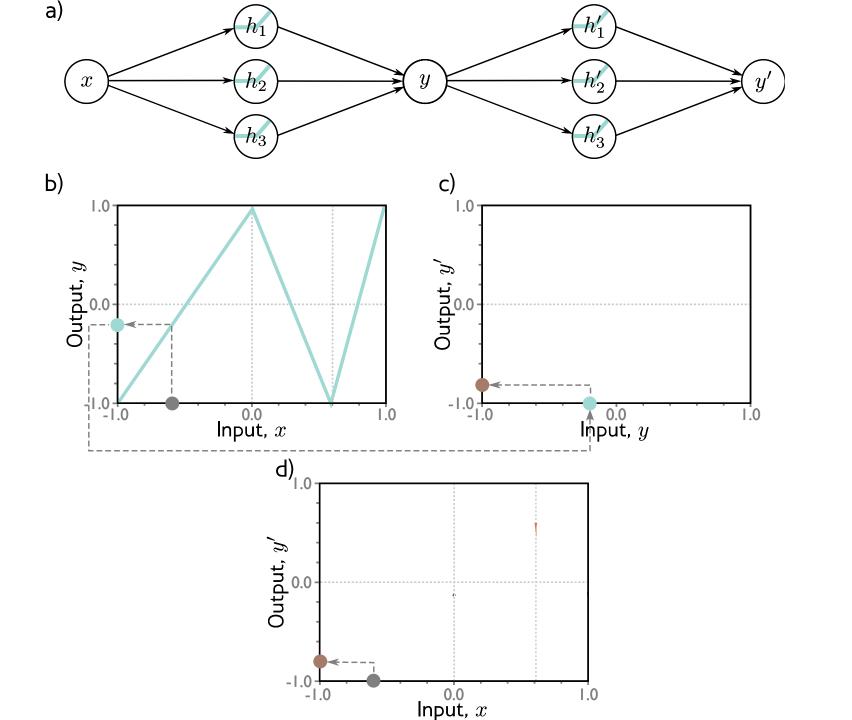


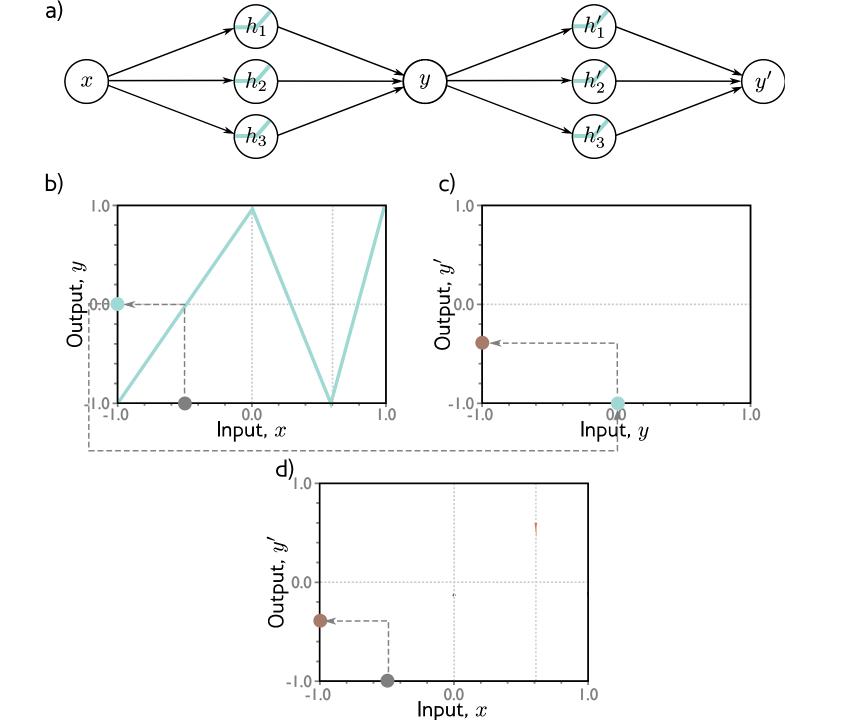


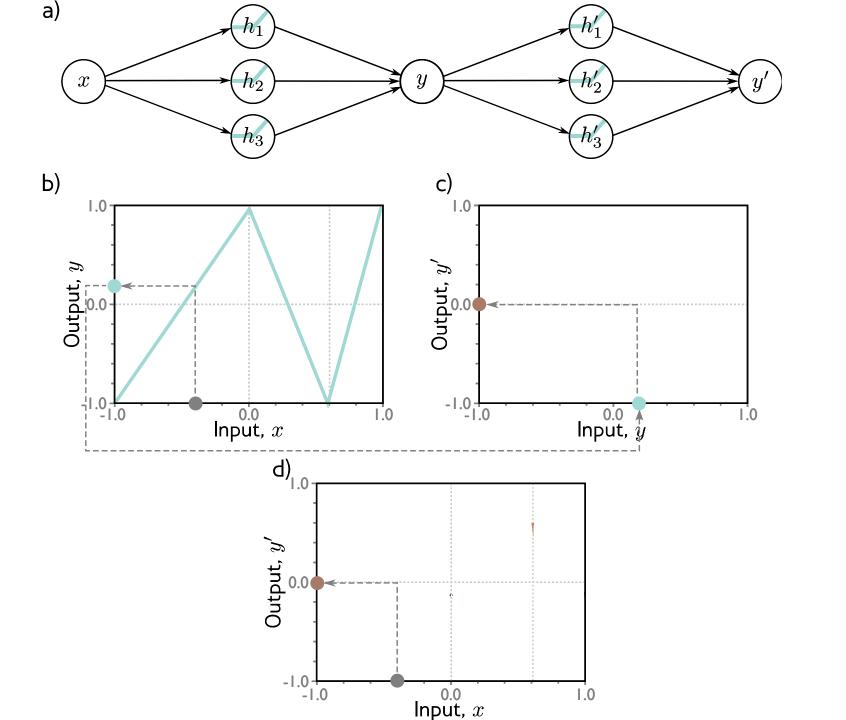


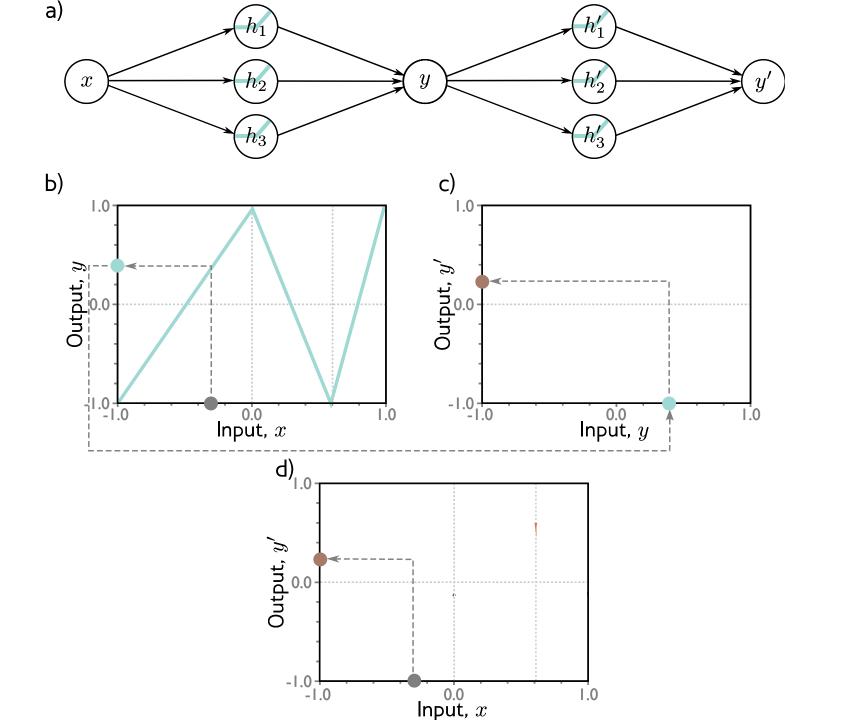


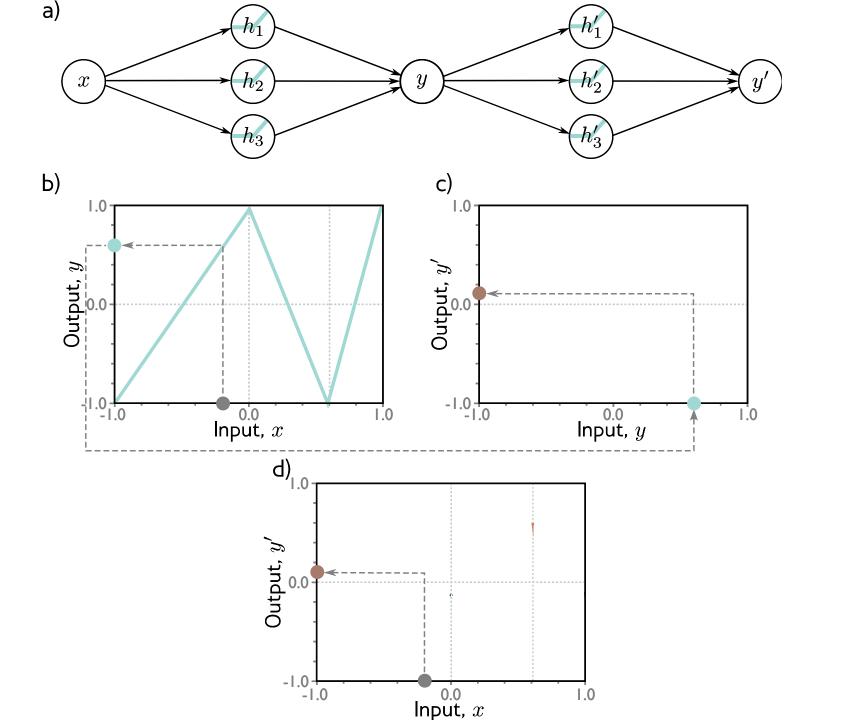


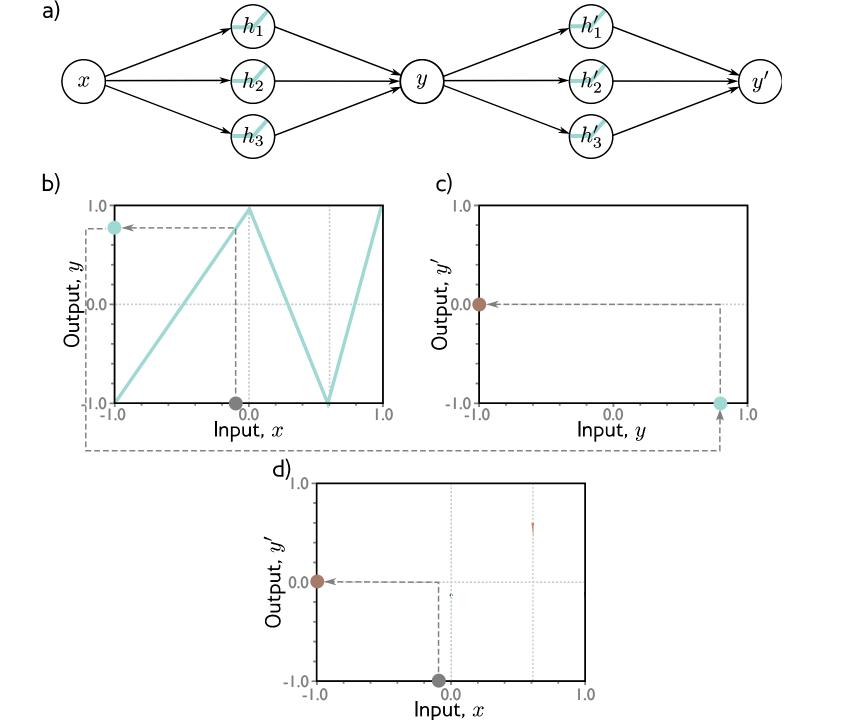


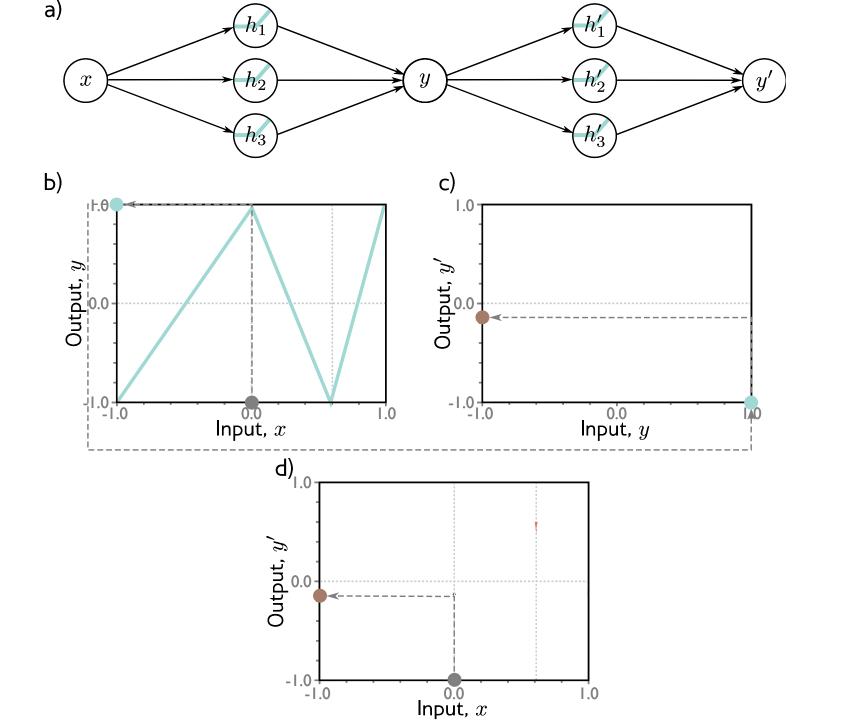


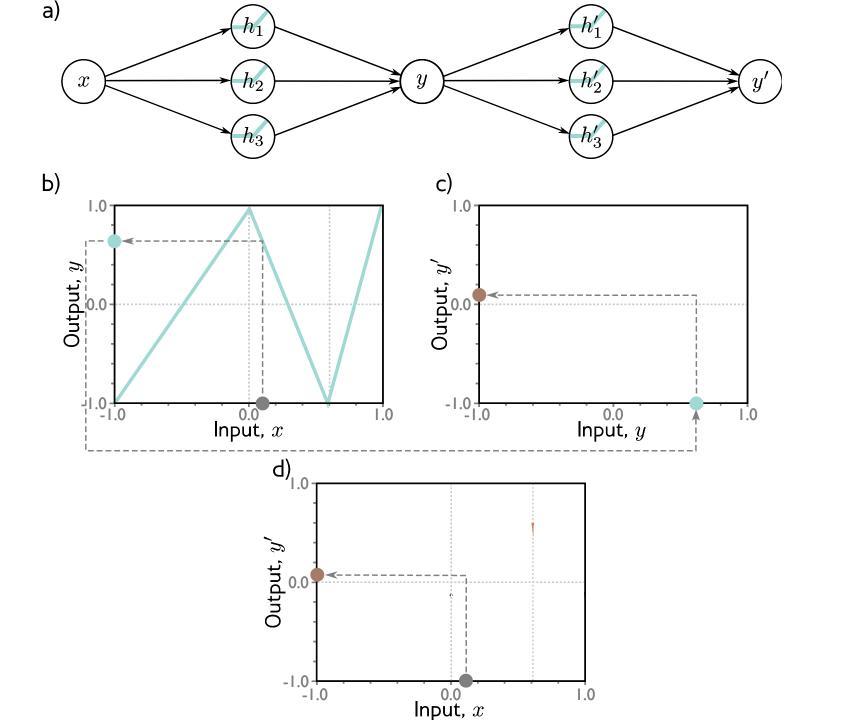


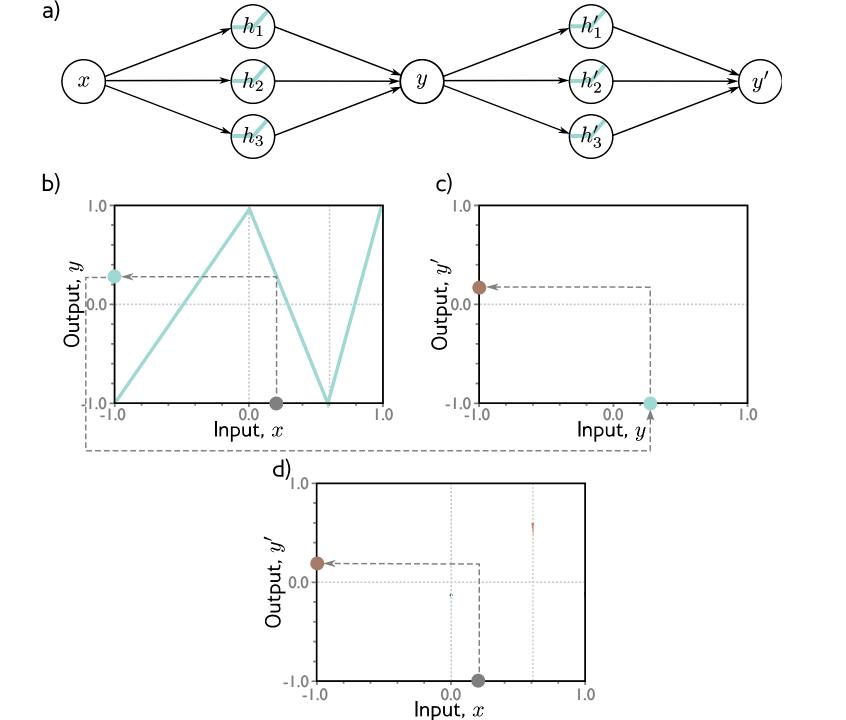


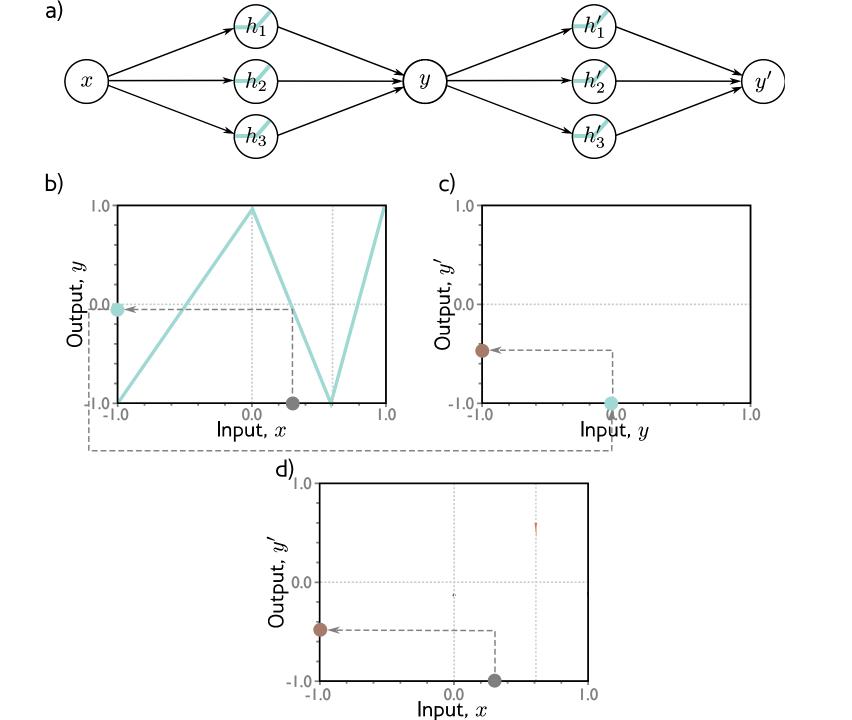


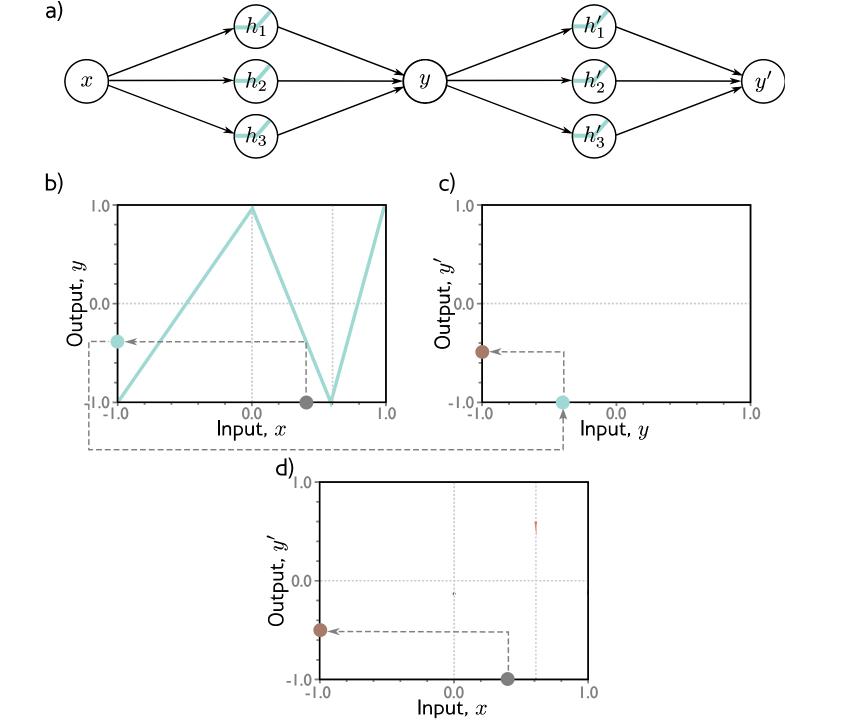


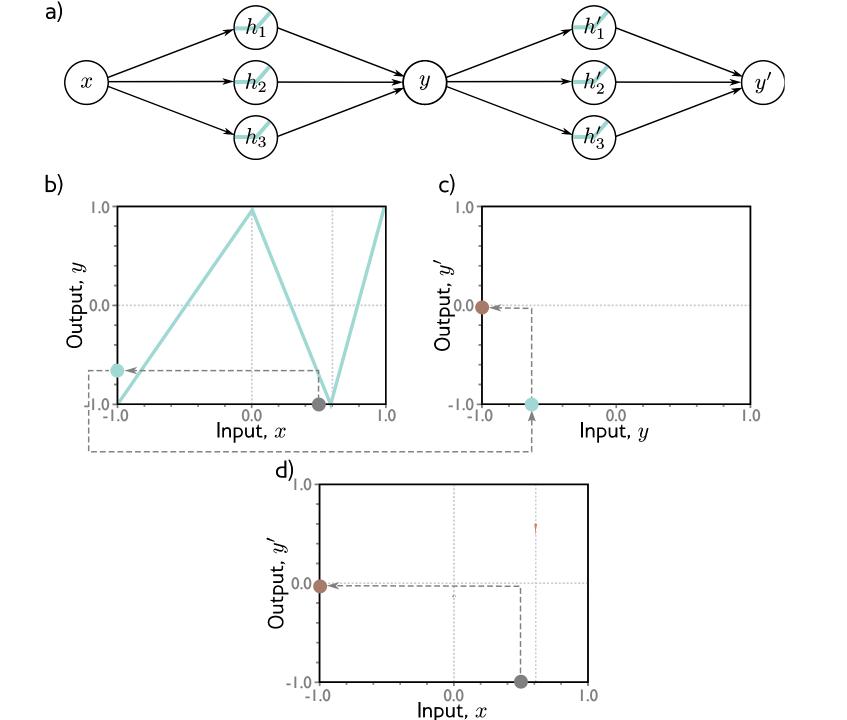


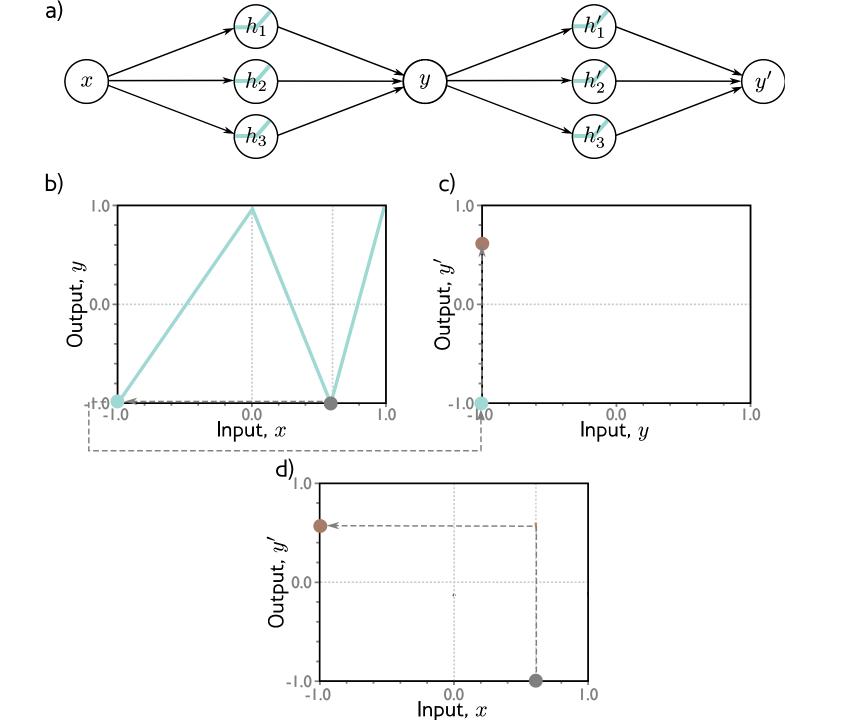


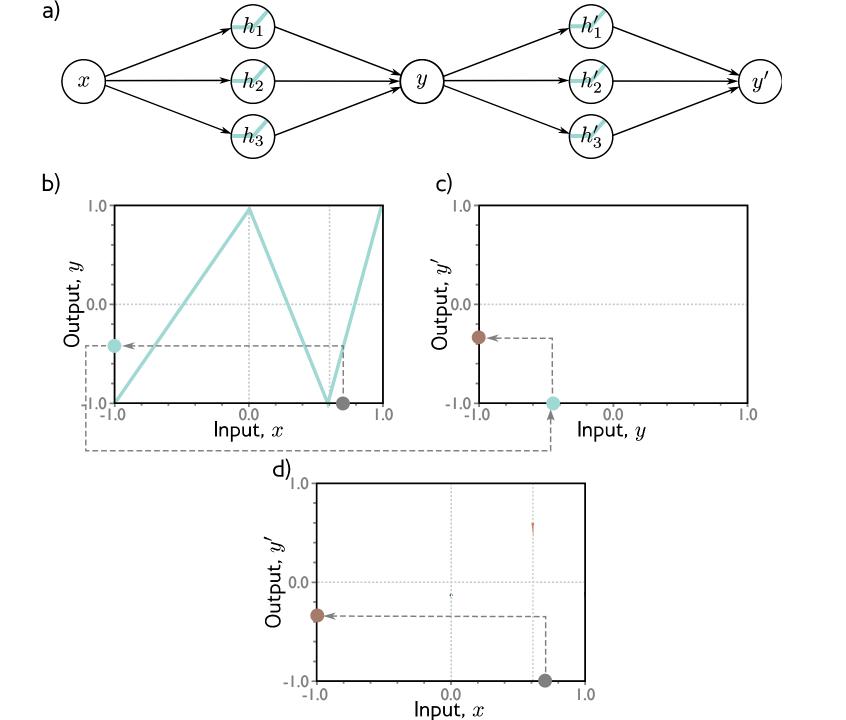


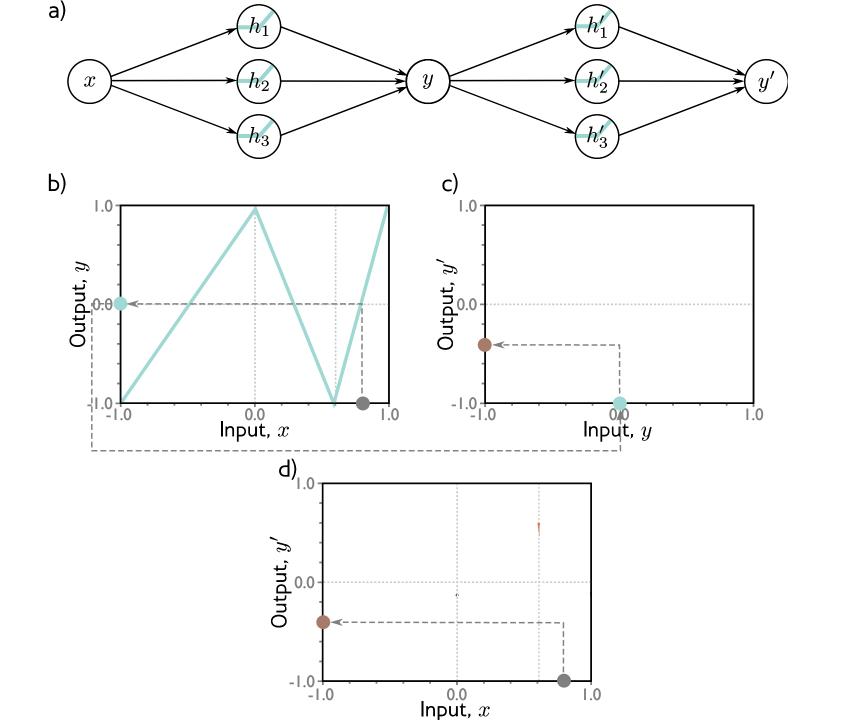


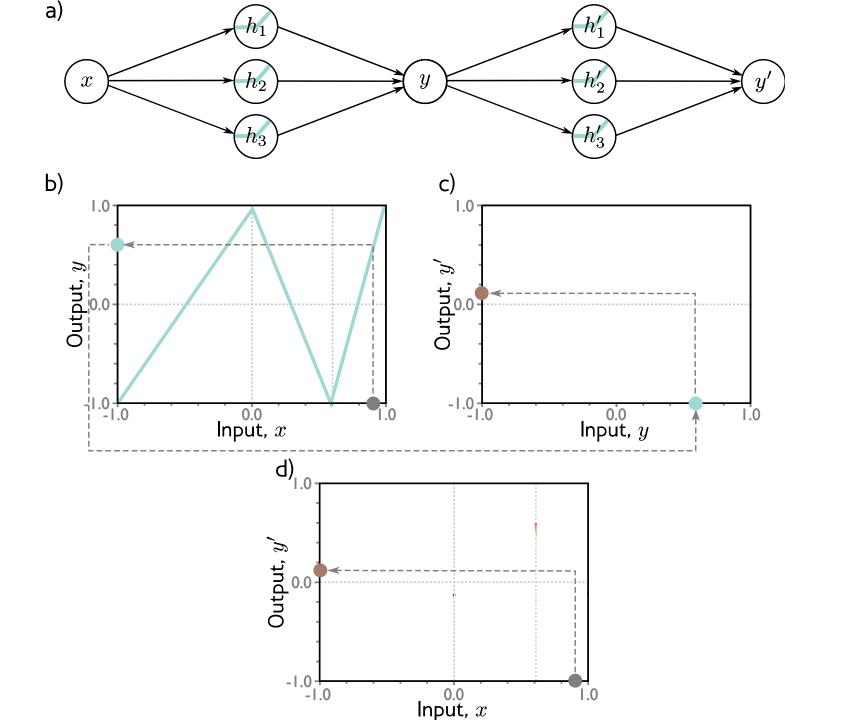




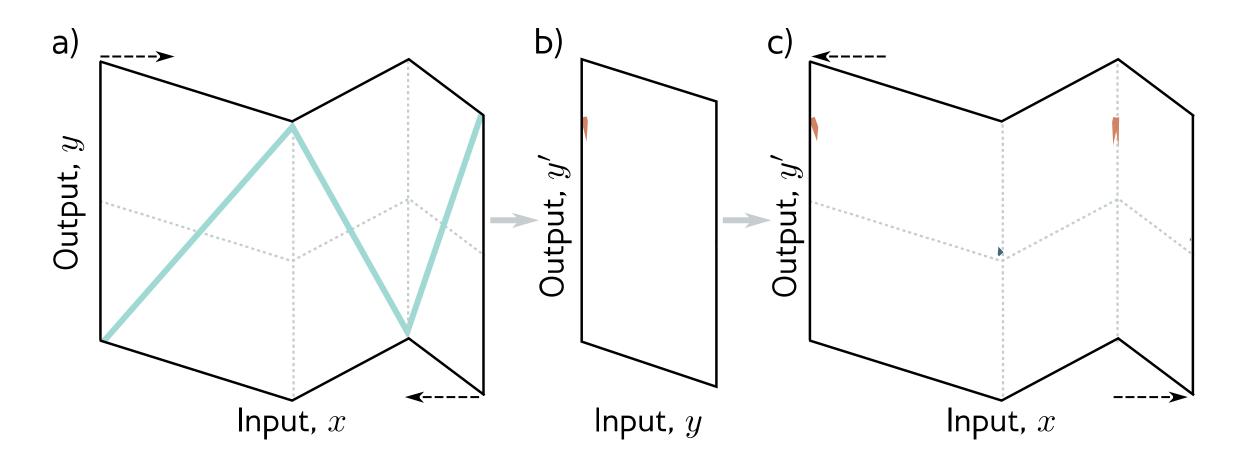




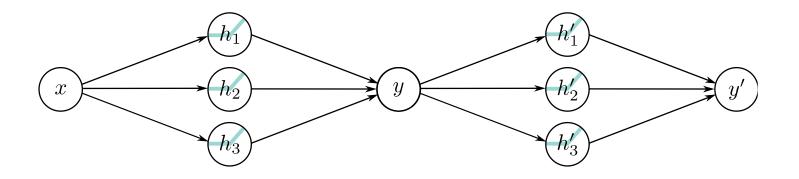




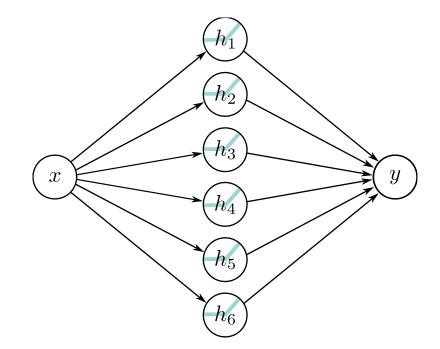
"Folding analogy"



Comparing to shallow with six hidden units

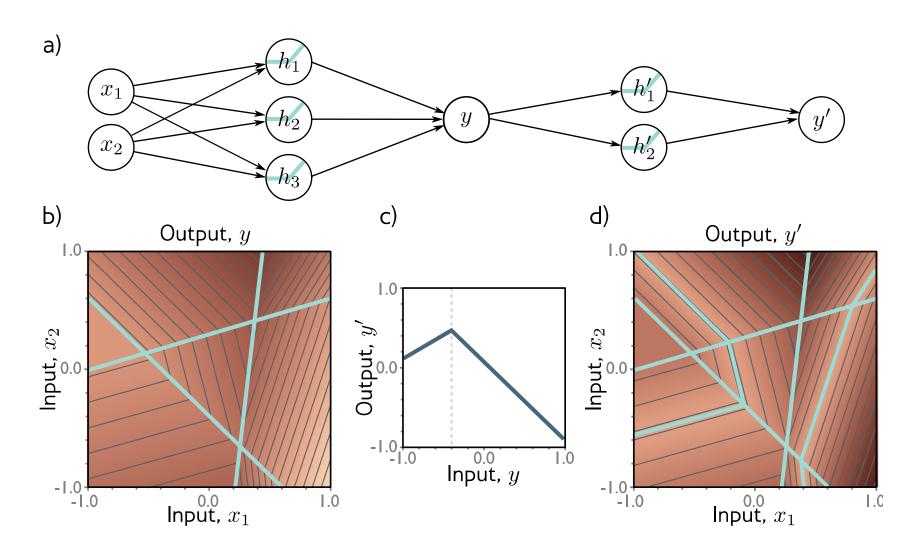


- 20 parameters
- (at least) 9 regions



- 19 parameters
- Max 7 regions

Composing networks in 2D



Deep neural networks

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- Combining the two networks into one
- Hyperparameters
- Notation change and general case
- Shallow vs. deep networks

Combine two networks into one

$$h_1 = a[\theta_{10} + \theta_{11}x]$$

 $h_2 = a[\theta_{20} + \theta_{21}x]$ $y = \phi_0 + \phi_1h_1 + \phi_2h_2 + \phi_3h_3$ Network 1:

$$h_3 = \mathbf{a}[\theta_{30} + \theta_{31}x]$$

$$h_1' = a[\theta_{10}' + \theta_{11}'y]$$

Network 2:

$$h_2' = a[\theta_{20}' + \theta_{21}'y]$$

$$h_3' = a[\theta_{30}' + \theta_{31}'y]$$

$$h'_2 = a[\theta'_{20} + \theta'_{21}y]$$
 $y' = \phi'_0 + \phi'_1h'_1 + \phi'_2h'_2 + \phi'_3h'_3$

Hidden units of second network in terms of first:

$$h'_{1} = a[\theta'_{10} + \theta'_{11}y] = a[\theta'_{10} + \theta'_{11}\phi_{0} + \theta'_{11}\phi_{1}h_{1} + \theta'_{11}\phi_{2}h_{2} + \theta'_{11}\phi_{3}h_{3}]$$

$$h'_{2} = a[\theta'_{20} + \theta'_{21}y] = a[\theta'_{20} + \theta'_{21}\phi_{0} + \theta'_{21}\phi_{1}h_{1} + \theta'_{21}\phi_{2}h_{2} + \theta'_{21}\phi_{3}h_{3}]$$

$$h'_{3} = a[\theta'_{30} + \theta'_{31}y] = a[\theta'_{30} + \theta'_{31}\phi_{0} + \theta'_{31}\phi_{1}h_{1} + \theta'_{31}\phi_{2}h_{2} + \theta'_{31}\phi_{3}h_{3}]$$

Create new variables

$$h'_{1} = a[\theta'_{10} + \theta'_{11}y] = a[\theta'_{10} + \theta'_{11}\phi_{0} + \theta'_{11}\phi_{1}h_{1} + \theta'_{11}\phi_{2}h_{2} + \theta'_{11}\phi_{3}h_{3}]$$

$$h'_{2} = a[\theta'_{20} + \theta'_{21}y] = a[\theta'_{20} + \theta'_{21}\phi_{0} + \theta'_{21}\phi_{1}h_{1} + \theta'_{21}\phi_{2}h_{2} + \theta'_{21}\phi_{3}h_{3}]$$

$$h'_{3} = a[\theta'_{30} + \theta'_{31}y] = a[\theta'_{30} + \theta'_{31}\phi_{0} + \theta'_{31}\phi_{1}h_{1} + \theta'_{31}\phi_{2}h_{2} + \theta'_{31}\phi_{3}h_{3}]$$

$$h'_{1} = a[\psi_{10} + \psi_{11}h_{1} + \psi_{12}h_{2} + \psi_{13}h_{3}]$$

$$h'_{2} = a[\psi_{20} + \psi_{21}h_{1} + \psi_{22}h_{2} + \psi_{23}h_{3}]$$

$$h'_{3} = a[\psi_{30} + \psi_{31}h_{1} + \psi_{32}h_{2} + \psi_{33}h_{3}]$$

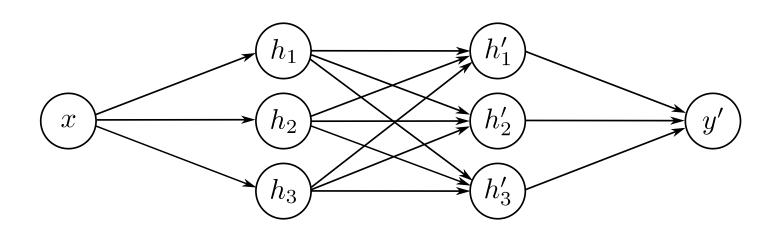
Two-layer network

$$h_1 = a[\theta_{10} + \theta_{11}x] \qquad h'_1 = a[\psi_{10} + \psi_{11}h_1 + \psi_{12}h_2 + \psi_{13}h_3]$$

$$h_2 = a[\theta_{20} + \theta_{21}x] \qquad h'_2 = a[\psi_{20} + \psi_{21}h_2 + \psi_{22}h_2 + \psi_{23}h_3]$$

$$h_3 = a[\theta_{30} + \theta_{31}x] \qquad h'_3 = a[\psi_{30} + \psi_{31}h_2 + \psi_{32}h_2 + \psi_{33}h_3]$$

$$y' = \phi_0' + \phi_1' h_1' + \phi_2' h_2' + \phi_3' h_3'$$



Two-layer network as one equation

$$h_1 = a[\theta_{10} + \theta_{11}x] \qquad h'_1 = a[\psi_{10} + \psi_{11}h_1 + \psi_{12}h_2 + \psi_{13}h_3]$$

$$h_2 = a[\theta_{20} + \theta_{21}x] \qquad h'_2 = a[\psi_{20} + \psi_{21}h_1 + \psi_{22}h_2 + \psi_{23}h_3]$$

$$h_3 = a[\theta_{30} + \theta_{31}x] \qquad h'_3 = a[\psi_{30} + \psi_{31}h_1 + \psi_{32}h_2 + \psi_{33}h_3]$$

$$y' = \phi_0' + \phi_1' h_1' + \phi_2' h_2' + \phi_3' h_3'$$

$$y' = \phi'_0 + \phi'_1 a \left[\psi_{10} + \psi_{11} a \left[\theta_{10} + \theta_{11} x \right] + \psi_{12} a \left[\theta_{20} + \theta_{21} x \right] + \psi_{13} a \left[\theta_{30} + \theta_{31} x \right] \right]$$

$$+ \phi'_2 a \left[\psi_{20} + \psi_{21} a \left[\theta_{10} + \theta_{11} x \right] + \psi_{22} a \left[\theta_{20} + \theta_{21} x \right] + \psi_{23} a \left[\theta_{30} + \theta_{31} x \right] \right]$$

$$+ \phi'_3 a \left[\psi_{30} + \psi_{31} a \left[\theta_{10} + \theta_{11} x \right] + \psi_{32} a \left[\theta_{20} + \theta_{21} x \right] + \psi_{33} a \left[\theta_{30} + \theta_{31} x \right] \right]$$

Remember shallow network with two outputs?

• 1 input, 4 hidden units, 2 outputs

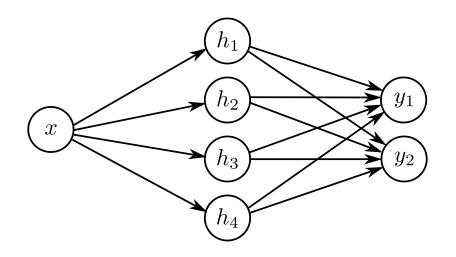
$$h_1 = a[\theta_{10} + \theta_{11}x]$$

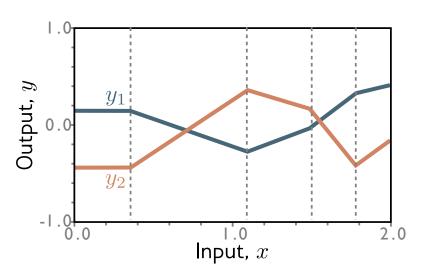
$$h_2 = a[\theta_{20} + \theta_{21}x]$$

$$h_3 = a[\theta_{30} + \theta_{31}x]$$

$$h_4 = a[\theta_{40} + \theta_{41}x]$$

$$y_1 = \phi_{10} + \phi_{11}h_1 + \phi_{12}h_2 + \phi_{13}h_3 + \phi_{14}h_4$$
$$y_2 = \phi_{20} + \phi_{21}h_1 + \phi_{22}h_2 + \phi_{23}h_3 + \phi_{24}h_4$$





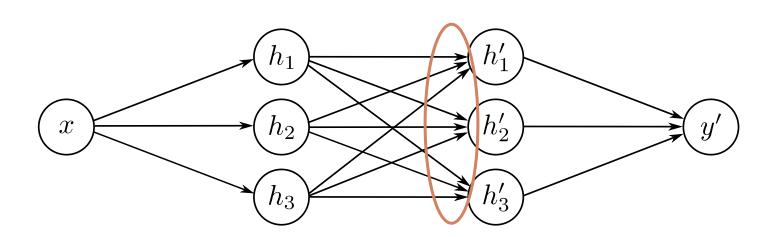
Networks as composing functions

$$h_1 = a[\theta_{10} + \theta_{11}x] \qquad h'_1 = a[\psi_{10} + \psi_{11}h_1 + \psi_{12}h_2 + \psi_{13}h_3]$$

$$h_2 = a[\theta_{20} + \theta_{21}x] \qquad h'_2 = a[\psi_{20} + \psi_{21}h_1 + \psi_{22}h_2 + \psi_{23}h_3]$$

$$h_3 = a[\theta_{30} + \theta_{31}x] \qquad h'_3 = a[\psi_{30} + \psi_{31}h_1 + \psi_{32}h_2 + \psi_{33}h_3]$$

Consider the pre-activations at the second hidden units At this point, it's a one--layer network with three outputs



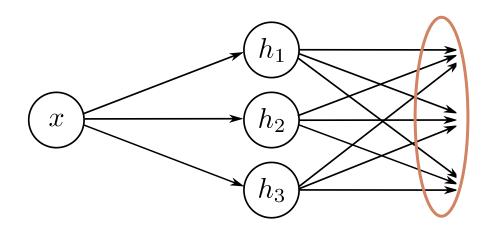
Networks as composing functions

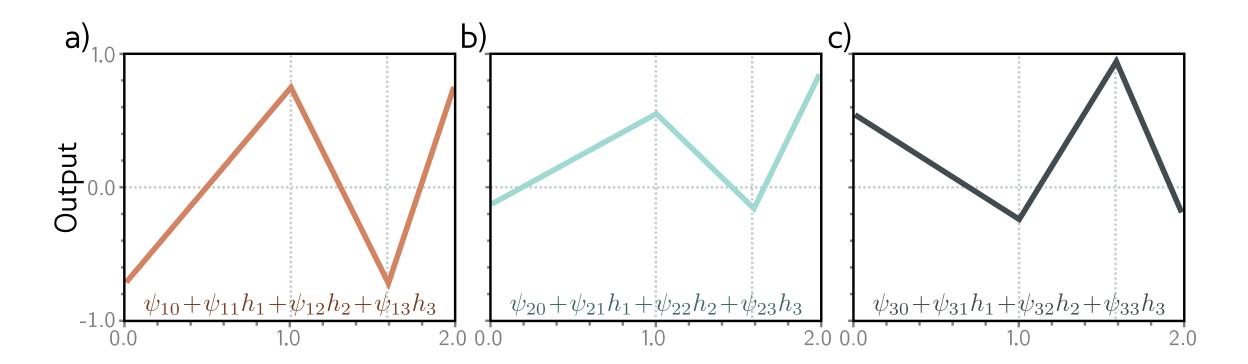
$$h_1 = a[\theta_{10} + \theta_{11}x] \qquad h'_1 = a[\psi_{10} + \psi_{11}h_1 + \psi_{12}h_2 + \psi_{13}h_3]$$

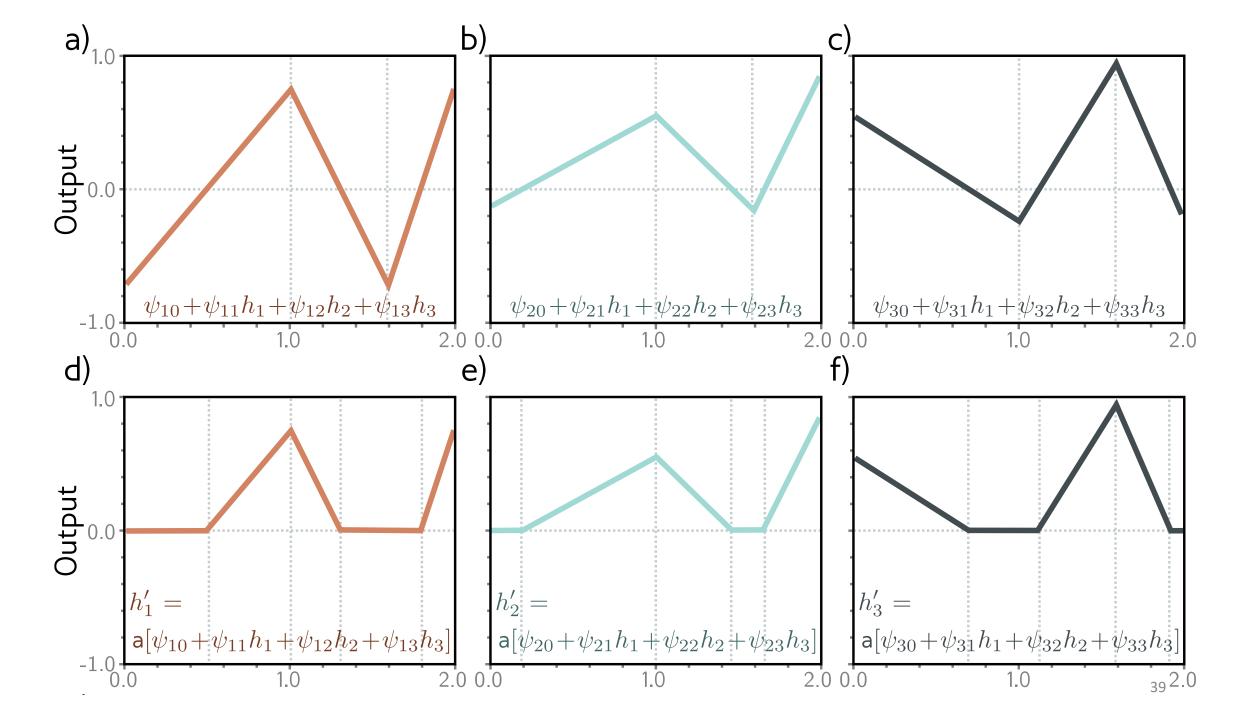
$$h_2 = a[\theta_{20} + \theta_{21}x] \qquad h'_2 = a[\psi_{20} + \psi_{21}h_1 + \psi_{22}h_2 + \psi_{23}h_3]$$

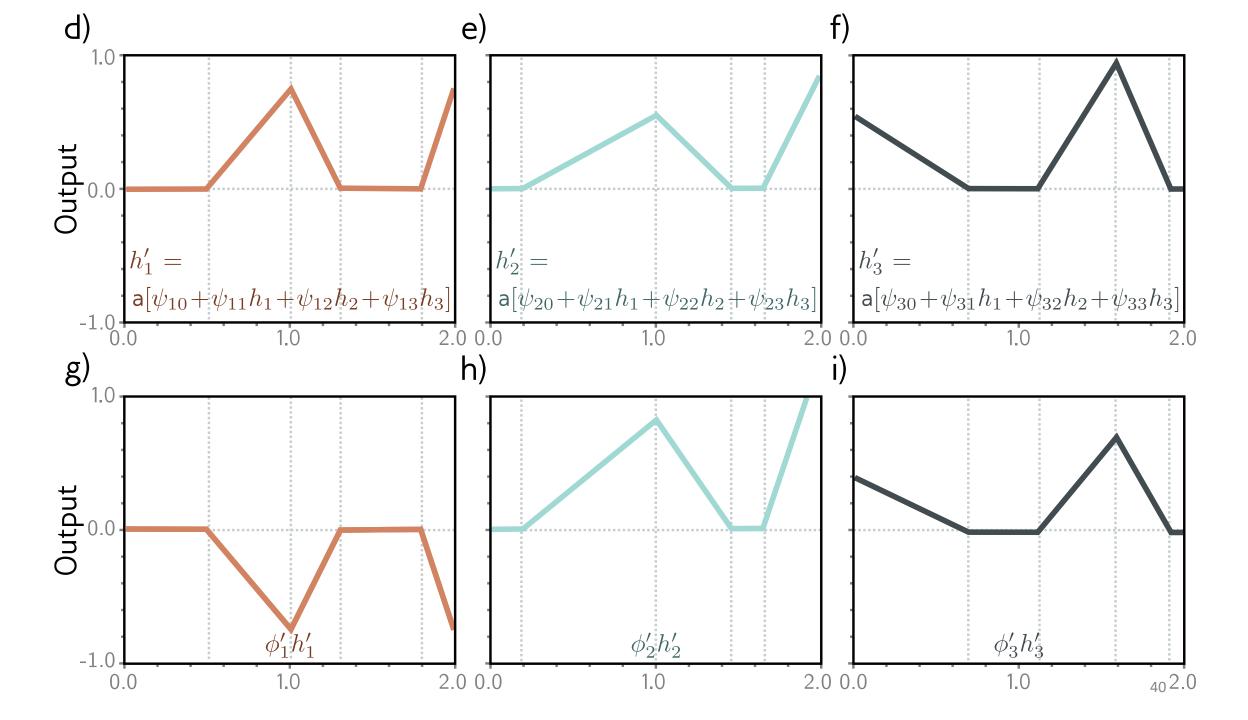
$$h_3 = a[\theta_{30} + \theta_{31}x] \qquad h'_3 = a[\psi_{30} + \psi_{31}h_1 + \psi_{32}h_2 + \psi_{33}h_3]$$

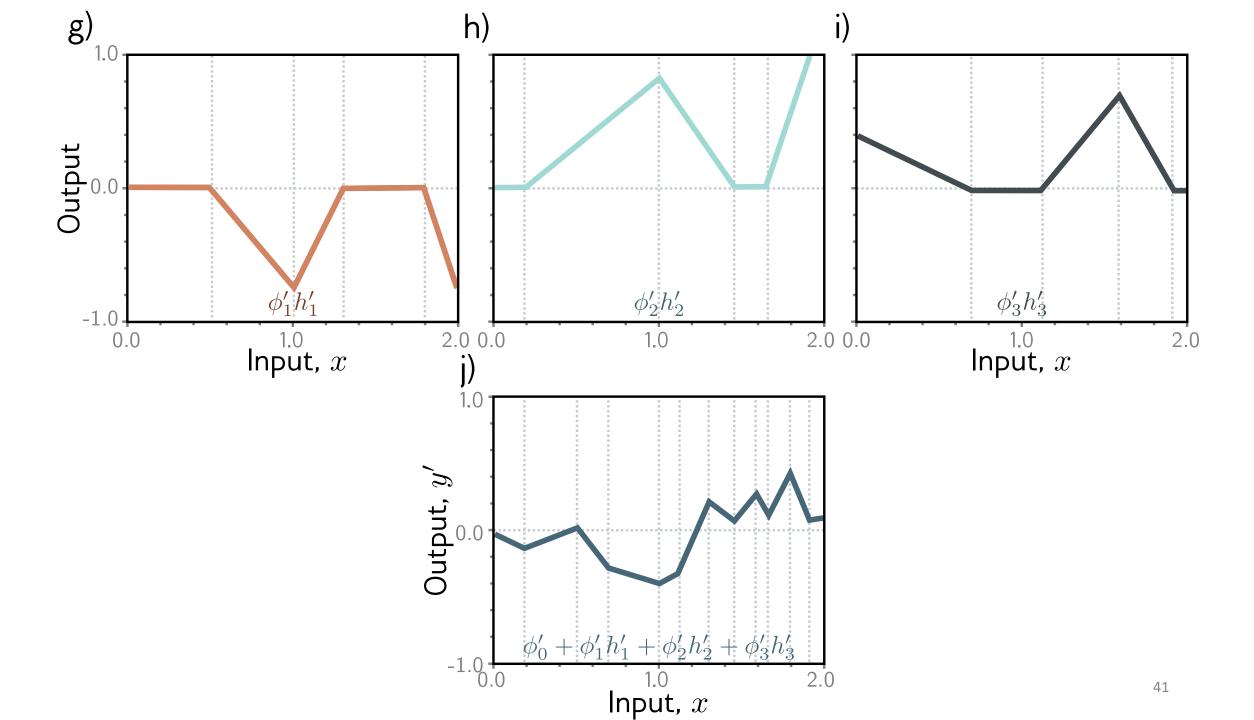
Consider the pre-activations at the second hidden units At this point, it's a one--layer network with three outputs











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Hyperparameters

- K layers = depth of network
- D_k hidden units per layer = width of network

- These are called hyperparameters chosen before training the network
- Can try retraining with different hyperparameters hyperparameter optimization or hyperparameter search

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$$h_1 = a[\theta_{10} + \theta_{11}x]$$

$$h_2 = a[\theta_{20} + \theta_{21}x]$$

$$h_3 = a[\theta_{30} + \theta_{31}x]$$

$$h'_{1} = a[\psi_{10} + \psi_{11}h_{1} + \psi_{12}h_{2} + \psi_{13}h_{3}]$$

$$h'_{2} = a[\psi_{20} + \psi_{21}h_{1} + \psi_{22}h_{2} + \psi_{23}h_{3}]$$

$$h'_{3} = a[\psi_{30} + \psi_{31}h_{1} + \psi_{32}h_{2} + \psi_{33}h_{3}]$$

$$y' = \phi_0' + \phi_1' h_1' + \phi_2' h_2' + \phi_3' h_3'$$

$$h_1 = \mathbf{a}[\theta_{10} + \theta_{11}x]$$

$$h_2 = \mathbf{a}[\theta_{20} + \theta_{21}x]$$

$$h_3 = \mathbf{a}[\theta_{30} + \theta_{31}x]$$

$$\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} = \mathbf{a} \begin{bmatrix} \theta_{10} \\ \theta_{20} \\ \theta_{30} \end{bmatrix} + \begin{bmatrix} \theta_{11} \\ \theta_{21} \\ \theta_{31} \end{bmatrix} x$$

$$h'_{1} = a[\psi_{10} + \psi_{11}h_{1} + \psi_{12}h_{2} + \psi_{13}h_{3}]$$

$$h'_{2} = a[\psi_{20} + \psi_{21}h_{1} + \psi_{22}h_{2} + \psi_{23}h_{3}]$$

$$h'_{3} = a[\psi_{30} + \psi_{31}h_{1} + \psi_{32}h_{2} + \psi_{33}h_{3}]$$

$$y' = \phi_0' + \phi_1' h_1' + \phi_2' h_2' + \phi_3' h_3'$$

$$h_1 = \mathbf{a}[\theta_{10} + \theta_{11}x]$$

$$h_2 = \mathbf{a}[\theta_{20} + \theta_{21}x]$$

$$h_3 = \mathbf{a}[\theta_{30} + \theta_{31}x]$$

$$\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} = \mathbf{a} \begin{bmatrix} \theta_{10} \\ \theta_{20} \\ \theta_{30} \end{bmatrix} + \begin{bmatrix} \theta_{11} \\ \theta_{21} \\ \theta_{31} \end{bmatrix} x$$

$$h'_{1} = \mathbf{a}[\psi_{10} + \psi_{11}h_{1} + \psi_{12}h_{2} + \psi_{13}h_{3}] h'_{2} = \mathbf{a}[\psi_{20} + \psi_{21}h_{1} + \psi_{22}h_{2} + \psi_{23}h_{3}] h'_{3} = \mathbf{a}[\psi_{30} + \psi_{31}h_{1} + \psi_{32}h_{2} + \psi_{33}h_{3}]$$

$$\begin{bmatrix} h'_{1} \\ h'_{2} \\ h'_{3} \end{bmatrix} = \mathbf{a} \begin{bmatrix} \begin{bmatrix} \psi_{10} \\ \psi_{20} \\ \psi_{30} \end{bmatrix} + \begin{bmatrix} \psi_{11} & \psi_{12} & \psi_{13} \\ \psi_{21} & \psi_{22} & \psi_{23} \\ \psi_{31} & \psi_{32} & \psi_{33} \end{bmatrix} \begin{bmatrix} h_{1} \\ h_{2} \\ h_{3} \end{bmatrix}$$

$$h_{1} = a[\theta_{10} + \theta_{11}x] h_{2} = a[\theta_{20} + \theta_{21}x] h_{3} = a[\theta_{30} + \theta_{31}x]$$

$$\begin{bmatrix} h_{1} \\ h_{2} \\ h_{3} \end{bmatrix} =$$

$$h'_{1} = a[\psi_{10} + \psi_{11}h_{1} + \psi_{12}h_{2} + \psi_{13}h_{3}]$$

$$h'_{2} = a[\psi_{20} + \psi_{21}h_{1} + \psi_{22}h_{2} + \psi_{23}h_{3}]$$

$$h'_{3} = a[\psi_{30} + \psi_{31}h_{1} + \psi_{32}h_{2} + \psi_{33}h_{3}]$$

$$\begin{bmatrix} h'_1 \\ h'_2 \\ h'_3 \end{bmatrix} = \mathbf{a} \begin{bmatrix} \begin{bmatrix} \psi_{10} \\ \psi_{20} \\ \psi_{30} \end{bmatrix} + \begin{bmatrix} \psi_{11} & \psi_{12} & \psi_{13} \\ \psi_{21} & \psi_{22} & \psi_{23} \\ \psi_{32} & \psi_{32} & \psi_{33} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} \end{bmatrix}$$

$$y' = \phi_0' + \phi_1' h_1' + \phi_2' h_2' + \phi_3' h_3'$$

$$y' = \phi_0' + \begin{bmatrix} \phi_1' & \phi_2' & \phi_3' \end{bmatrix} \begin{bmatrix} h_1' \\ h_2' \\ h_3' \end{bmatrix}$$

$$\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} = \mathbf{a} \begin{bmatrix} \theta_{10} \\ \theta_{20} \\ \theta_{30} \end{bmatrix} + \begin{bmatrix} \theta_{11} \\ \theta_{21} \\ \theta_{31} \end{bmatrix} x$$

$$\mathbf{h} = \mathbf{a} [\boldsymbol{\theta}_0 + \boldsymbol{\theta} x]$$

$$\begin{bmatrix} h'_1 \\ h'_2 \\ h'_3 \end{bmatrix} = \mathbf{a} \begin{bmatrix} \begin{bmatrix} \psi_{10} \\ \psi_{20} \\ \psi_{30} \end{bmatrix} + \begin{bmatrix} \psi_{11} & \psi_{12} & \psi_{13} \\ \psi_{21} & \psi_{22} & \psi_{23} \\ \psi_{32} & \psi_{32} & \psi_{33} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} \end{bmatrix} \longrightarrow \mathbf{h'} = \mathbf{a} \begin{bmatrix} \boldsymbol{\psi}_0 + \mathbf{\Psi} \mathbf{h} \end{bmatrix}$$

$$y' = \phi'_0 + \begin{bmatrix} \phi'_1 & \phi'_2 & \phi'_3 \end{bmatrix} \begin{vmatrix} h'_1 \\ h'_2 \\ h'_2 \end{vmatrix}$$
 \longrightarrow $y = \boldsymbol{\phi}'_0 + \boldsymbol{\phi}' \mathbf{h}'$

$$\mathbf{h} = \mathbf{a} \left[\boldsymbol{\theta}_0 + \boldsymbol{\theta} x \right]$$

$$\mathbf{h}_1 = \mathbf{a}[oldsymbol{eta}_0 + oldsymbol{\Omega}_0 \mathbf{x}]$$

$$\mathbf{h}' = \mathbf{a} \left[\boldsymbol{\psi}_0 + \mathbf{\Psi} \mathbf{h} \right]$$

$$\mathbf{h}_2 = \mathbf{a}[oldsymbol{eta}_1 + oldsymbol{\Omega}_1 \mathbf{h}_1]$$

$$y = \phi_0' + \phi' \mathbf{h}'$$

$$\mathbf{y} = oldsymbol{eta}_2 + oldsymbol{\Omega}_2 \mathbf{h}_2$$

$$\mathbf{h} = \mathbf{a} \left[\boldsymbol{\theta}_0 + \boldsymbol{\theta} x \right]$$

Bias Weight wector
$$\mathbf{h}_1 = \mathbf{a}[oldsymbol{eta}_0 + oldsymbol{\Omega}_0 \mathbf{x}]$$

$$\mathbf{h}' = \mathbf{a} \left[\boldsymbol{\psi}_0 + \mathbf{\Psi} \mathbf{h} \right]$$

$$\mathbf{h}_2 = \mathbf{a}[oldsymbol{eta}_1 + oldsymbol{\Omega}_1 \mathbf{h}_1]$$

$$y = \phi_0' + \phi' \mathbf{h}'$$

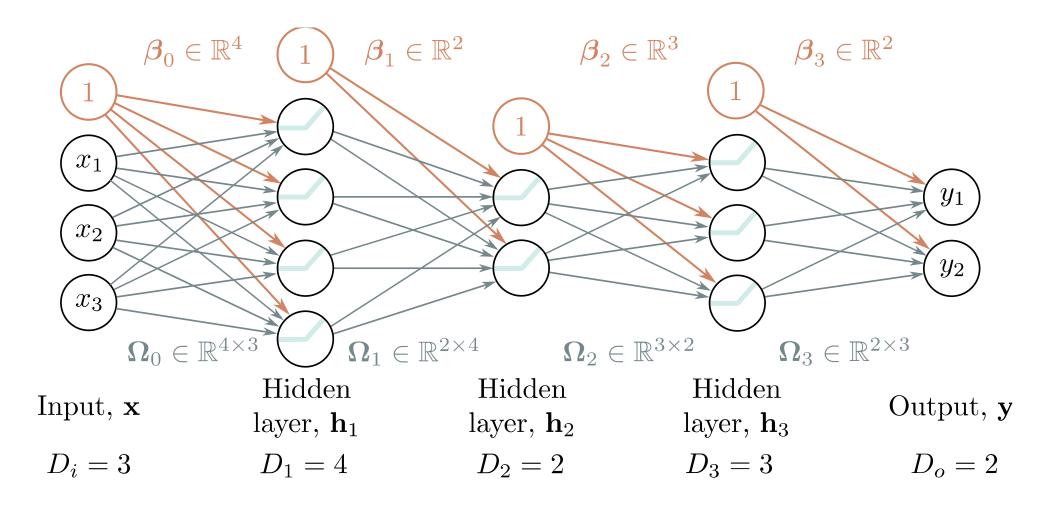
$$\mathbf{y} = \boldsymbol{eta}_2 + \mathbf{\Omega}_2 \mathbf{h}_2$$

General equations for deep network

$$egin{aligned} \mathbf{h}_1 &= \mathbf{a}[oldsymbol{eta}_0 + oldsymbol{\Omega}_0 \mathbf{x}] \ \mathbf{h}_2 &= \mathbf{a}[oldsymbol{eta}_1 + oldsymbol{\Omega}_1 \mathbf{h}_1] \ \mathbf{h}_3 &= \mathbf{a}[oldsymbol{eta}_2 + oldsymbol{\Omega}_2 \mathbf{h}_2] \ &dots \ \mathbf{h}_K &= \mathbf{a}[oldsymbol{eta}_{K-1} + oldsymbol{\Omega}_{K-1} \mathbf{h}_{K-1}] \ \mathbf{y} &= oldsymbol{eta}_K + oldsymbol{\Omega}_K \mathbf{h}_K, \end{aligned}$$

$$\mathbf{y} = oldsymbol{eta}_K + oldsymbol{\Omega}_K \mathbf{a} \left[oldsymbol{eta}_{K-1} + oldsymbol{\Omega}_{K-1} \mathbf{a} \left[\dots oldsymbol{eta}_2 + oldsymbol{\Omega}_2 \mathbf{a} \left[oldsymbol{eta}_1 + oldsymbol{\Omega}_1 \mathbf{a} \left[oldsymbol{eta}_0 + oldsymbol{\Omega}_0 \mathbf{x}
ight]
ight] \dots
ight]$$

Example



Deep neural networks

- Composing two networks
- Combining the two networks into one
- Hyperparameters
- Notation change and general case
- Shallow vs. deep networks

The best results are created by deep networks with many layers.

- 50-1000 layers for most applications
- Best results in
 - Computer vision
 - Natural language processing
 - Graph neural networks
 - Generative models
 - Reinforcement learning

All use deep networks. But why?

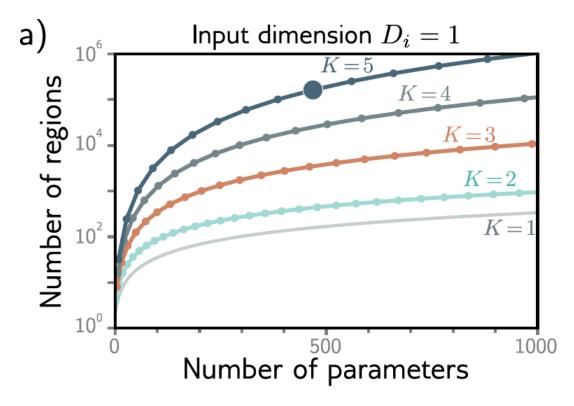
1. Ability to approximate different functions?

Both obey the universal approximation theorem.

Argument: One layer is enough, and for deep networks could arrange for the other layers to compute the identity function.

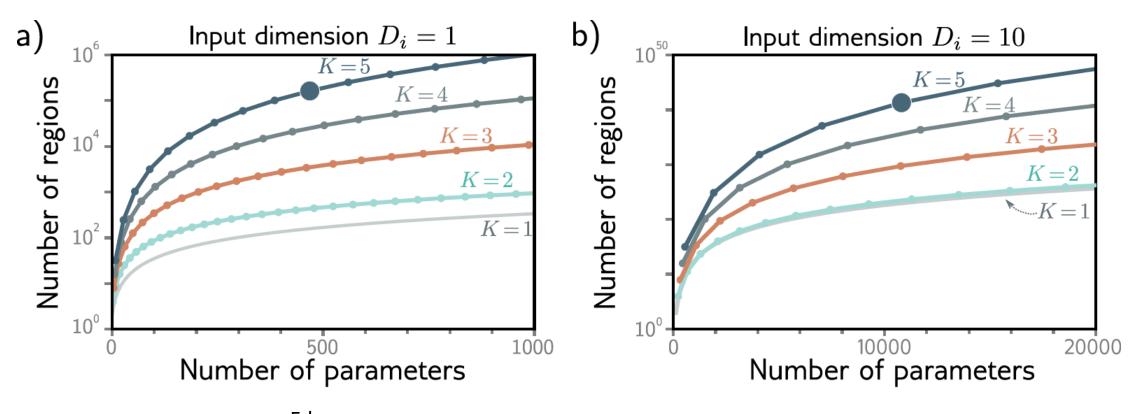
2. Number of linear regions per parameter

Number of linear regions per parameter



5 layers 10 hidden units per layer 471 parameters 161,501 linear regions

Number of linear regions per parameter



5 layers 10 hidden units per layer 471 parameters 161,501 linear regions

5 layers
50 hidden units per layer
10,801 parameters
>10⁴⁰ linear regions

2. Number of linear regions per parameter

- Deep networks create many more regions per parameters
- But there are dependencies between them
 - Think of folding example
 - Perhaps similar symmetries in real-world functions? Unknown

3. Depth efficiency

- There are some functions that require a shallow network with exponentially more hidden units than a deep network to achieve an equivalent approximation
- This is known as the depth efficiency of deep networks
- But do the real-world functions we want to approximate have this property? Unknown.

4. Large structured networks

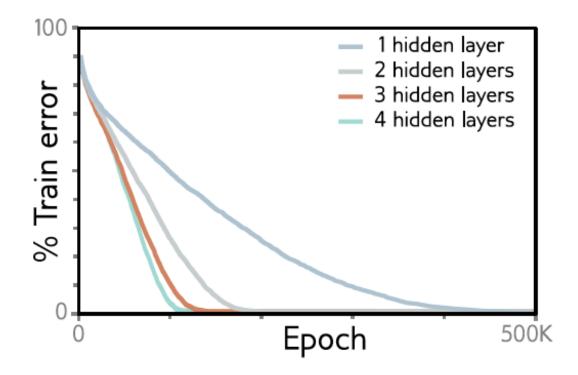
- Think about images as input might be 1M pixels
- Fully connected works not practical
- Answer is to have weights that only operate locally, and share across image
- This leads to convolutional networks
- Gradually integrate information from across the image needs multiple layers

5. Fitting and generalization

- Fitting of deep models seems to be easier up to about 20 layers
- Then needs various tricks to train deeper networks, so (in vanilla form), fitting becomes harder
- Generalization is good in deep networks. Why?

5. Fitting and generalization

Figure 20.2 MNIST-1D training. Four fully connected networks were fit to 4000 MNIST-1D examples with random labels using full batch gradient descent, He initialization, no momentum or regularization, and learning rate 0.0025. Models with 1,2,3,4 layers had 298, 100, 75, and 63 hidden units per layer and 15208, 15210, 15235, and 15139 parameters, respectively. All models train successfully, but deeper models require fewer epochs.



Where are we going?

- We have defined families of very flexible networks that map multiple inputs to multiple outputs
- Now we need to train them
 - How to choose loss functions
 - How to find minima of the loss function
 - How to do this in particular for deep networks
- Then we need to test them