4. Deep learning

Outline

Non-linear models

Neural networks

Layers in neural networks

From linear to non-linear models

▶ In linear regression, the prediction

$$h(x;\theta) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n,$$

is a linear (strictly speaking, affine) function of the feature vector x.

► In logistic regression,

$$\log \frac{P(y=1|x;\theta)}{1 - P(y=1|x;\theta)} = h(x;\theta)$$

- ► Such linear models are simple and easy to interpret, but not flexible enough to capture complex patterns in various applications.
- lt is desirable to make $h(x; \theta)$ a non-linear function of x.

Non-linear models

- ▶ Many choices of non-linear functions for $h(x; \theta)$, e.g.:
 - Polynomial regression
 - Kernel methods
 - Decision trees, random forests, boosting
 - Neural networks
- ▶ Models based on neural networks have proven to be very effective.
- ▶ Besides neural network architectures, various computing techniques are developed to train them.
- ► The combinations of neural network architectures and computing techniques are often referred to as **deep learning**.

Outline

Non-linear models

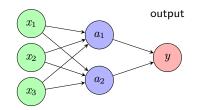
Neural networks

Layers in neural networks

Neural networks

input

hidden



values of hidden units

$$\begin{split} a_1 &= \text{ReLU}(w_{11}^{[1]}x_1 + w_{12}^{[1]}x_2 + w_{13}^{[1]}x_3 + b_1^{[1]}) \\ a_2 &= \text{ReLU}(w_{21}^{[1]}x_1 + w_{22}^{[1]}x_2 + w_{23}^{[1]}x_3 + b_2^{[1]}) \end{split}$$

- value of output unit
 - regression:

$$y = w_1^{[2]} a_1 + w_2^{[2]} a_2 + b^{[2]}$$

- classification:

$$y = \text{Sigmoid}(w_1^{[2]}a_1 + w_2^{[2]}a_2 + b^{[2]})$$

Neural networks in matrix notation

hidden output

values of hidden units

$$a = \text{ReLU}(W^{[1]}x + b^{[1]})_1$$

- value of output unit
 - regression:

$$y = W^{[2]}a + b^{[2]}$$

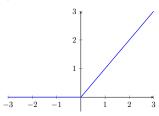
- classification:

$$y = \operatorname{Sigmoid}(W^{[2]}a + b^{[2]})$$

Activation functions

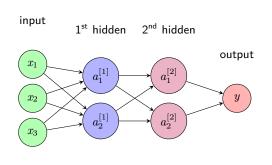
Used to introduce non-linearity to the neural network

 $ightharpoonup \operatorname{ReLU}(x) = \max(0, x)$



- ▶ Other activation functions: sigmoid, tanh, leaky ReLU, ELU, etc
- See https://pytorch.org/docs/stable/nn.functional.html# non-linear-activation-functions for more

Neural networks with multiple hidden layers



values of hidden units

$$\begin{split} &a^{[1]} = \operatorname{ReLU}(\,W^{[1]}x + b^{[1]}) \\ &a^{[2]} = \operatorname{ReLU}(\,W^{[2]}a^{[1]} + b^{[2]}) \end{split}$$

- ▶ value of output unit
 - regression:

$$y = W^{[2]}a^{[2]} + b^{[2]}$$

classification:

$$y = \operatorname{Sigmoid}(\,W^{[2]}a^{[2]} \!+\! b^{[2]})$$

Neural networks with multiple hidden layers

- ▶ input layer: *x*
- ► hidden layers:

$$\begin{split} a^{[1]} &= \text{ReLU}(\,W^{[1]}x + b^{[1]}) \\ a^{[2]} &= \text{ReLU}(\,W^{[2]}a^{[1]} + b^{[2]}) \\ &\vdots \\ a^{[L]} &= \text{ReLU}(\,W^{[L]}a^{[L-1]} + b^{[L]}) \end{split}$$

- output layer:
 - regression:

$$y = W^{[L+1]}a^{[L]} + b^{[L+1]}$$

- classification:

$$y = \text{Sigmoid}(W^{[L+1]}a^{[L]} + b^{[L+1]})$$

Multi-layer perceptrons

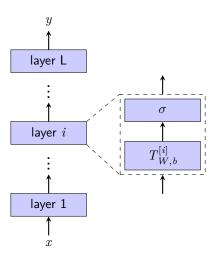
- Such neural network architectures are often referred to as multi-layer perceptrons (MLPs).
- ▶ A layer corresponds to the transformation of

$$z_{\text{out}} = \sigma(Wz_{\text{in}} + b) = \sigma(T_{W,b}(z))$$

where σ is an activation function, W and b are the weight and bias parameters, respectively, and $T_{W,b}$ is the affine transformation $T_{W,b}(z)=Wz+b$.

Each layer has its own weight and bias parameters.

Multi-layer perceptrons



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Residue connections

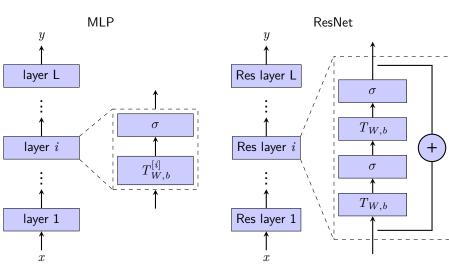
- ► An influential architecture that makes it easier to train networks with many layers
- ► A residue layer

$$\operatorname{Res}(z) = z + \sigma(T(\sigma(T(z))))$$

► A residue network is a sequence of residue layers

$$ResNet(z) = T(Res(...Res(z)))$$

MLP and Residue network



 $(ML \cup MD) \cap Biophysics$

Ding

4.14