Foundations of Machine Learning
AI2000 and AI5000

FoML-22
Neural Networks - learning the basis functions

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భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
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DiL
Data-driven Intelligence
& Learning Lab

So far in FoML

- Intro to ML and Probability refresher
- MLE, MAP, and fully Bayesian treatment
- Supervised learning
    a. Linear Regression with basis functions (regularization, model selection)
    b. Bias-Variance Decomposition (Bayesian Regression)
    c. Decision Theory - three broad classification strategies
        - Probabilistic Generative Models - Continuous & discrete data
        - (Linear) Discriminant Functions - least squares solution, Perceptron
        - Probabilistic Discriminative Models - Logistic Regression

Neural Networks - I

So far in the supervised learning

- We have seen models that are linear combinations of fixed basis functions

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

So far in the supervised learning

- Fixed basis functions
    - Don’t scale easily to complex settings (e.g., curse of dimensionality)
    - Need to adapt the basis functions to the data - e.g., SVM

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

An alternative

- Fix the number of basis functions
- But, allow them to be adaptive
- → parametric form and learn them during the training

(Artificial) Neural Networks

Feed-forward Neural networks

- The linear models we have seen so far = linear combination of fixed nonlinear basis functions
  - What is f for regression and classification?

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_j(\mathbf{x})\right)$$

Feed-forward Neural networks

- Let's extend this model
- Make the basis functions depend on 'learnable' parameters

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_j(\mathbf{x})\right)$$

Feed-forward Neural networks

- Neural networks - each basis function is a nonlinear function of a linear combination of inputs
  - Coefficients in the combination are adaptive parameters

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_j(\mathbf{x})\right)$$

Feed-forward Neural networks

- Basic neural network model as a series of transformations
    - M linear combinations of the i/p variables x_1, x_2, ...x_D

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

j = 1, . . . , M, and the superscript 1 indicates the first transformation or 'layer'

Feed-forward Neural networks

- a_j are referred to as the 'activations'
- Then passed through a differentiable, nonlinear activation function h(.)

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

$$z_j = h(a_j)$$

Feed-forward Neural networks

- z_j are the o/ps of the basis functions
  - referred to as the 'hidden units'
  - General nonlinear functions - sigmoid/tanh/ReLU

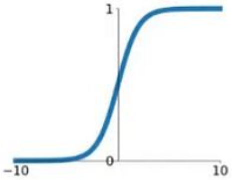
$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

$$z_j = h(a_j)$$

Activation Fucntions

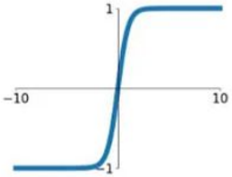
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



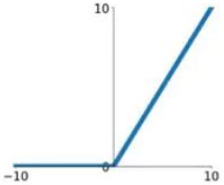
tanh

$\tanh(x)$



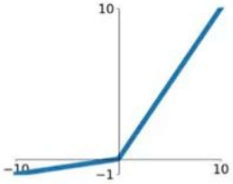
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

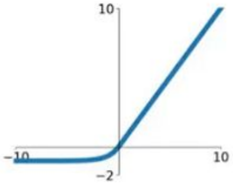


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Feed-forward Neural networks

- These values are again linearly combined to give o/p units
  - This transformation - second layer of the NN

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$

Feed-forward Neural networks

- Finally, the o/p unit activations are transformed through an appropriate activation function → y_k

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$

Feed-forward Neural networks

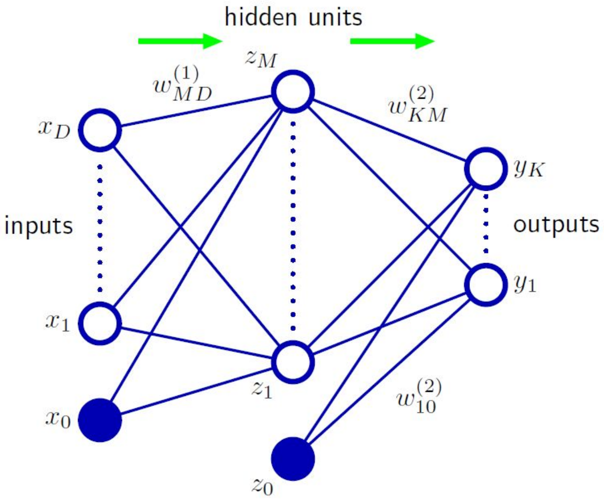
- Regression - identity ($y_k = a_k$)
- Binary classification - sigmoid ($y_k = \sigma(a_k)$)
- Multiclass classification - softmax

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$

Feed-forward Neural networks

- Overall

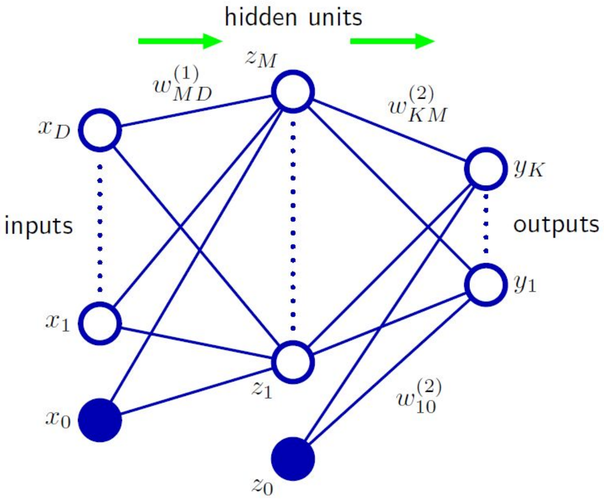
$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right) + w_{k0}^{(2)}\right)$$



Feed-forward Neural networks

- All the weights & biases are grouped into w
    - Adjustable parameters
- Model is a nonlinear function from x to y
    - Figure: 2-layered MLP (Multilayer Perceptron)

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right) + w_{k0}^{(2)}\right)$$

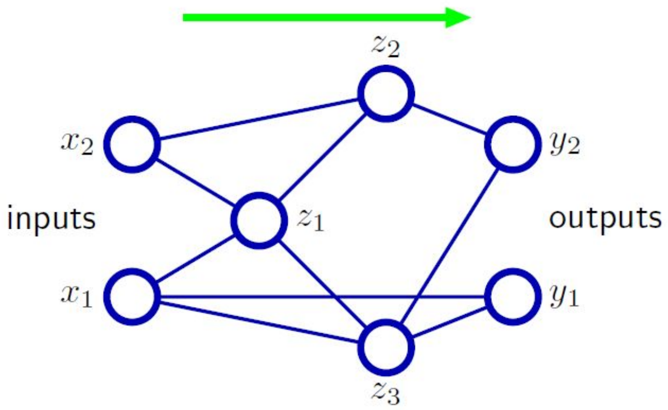


Feed-forward Neural networks

- What if the activation function on all the hidden units are linear?
    - An equivalent network without any hidden units can be found
    - Why?
    - Rare - e.g., PCA

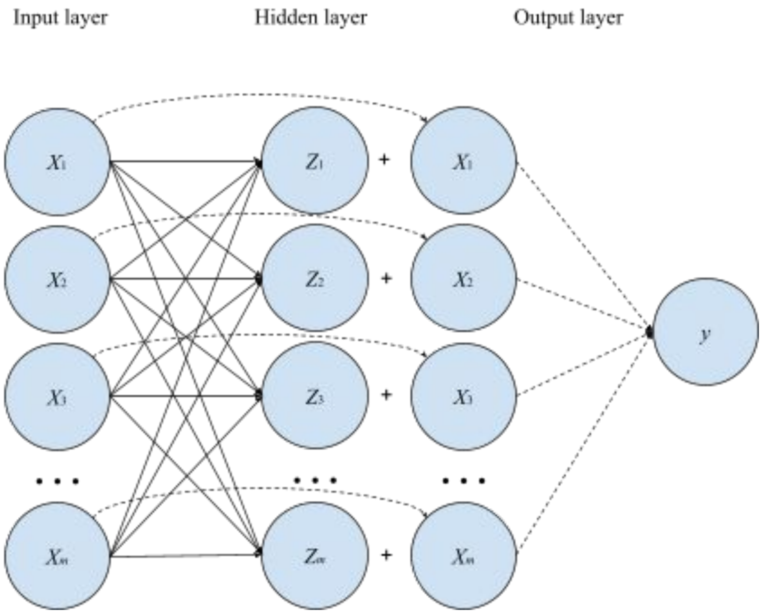
Feed-forward Neural networks

- Networks can be sparse
  - Not all weights may be present



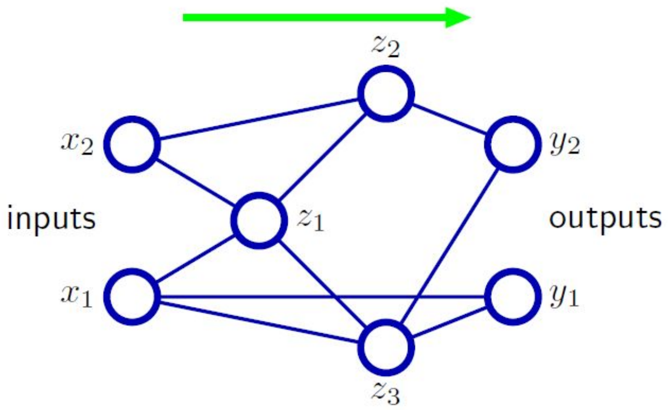
Feed-forward Neural networks

- Skip connects may be added



Feed-forward Neural networks

- FFNN - no closed directed cycles
  - o/p are deterministic functions of i/ps

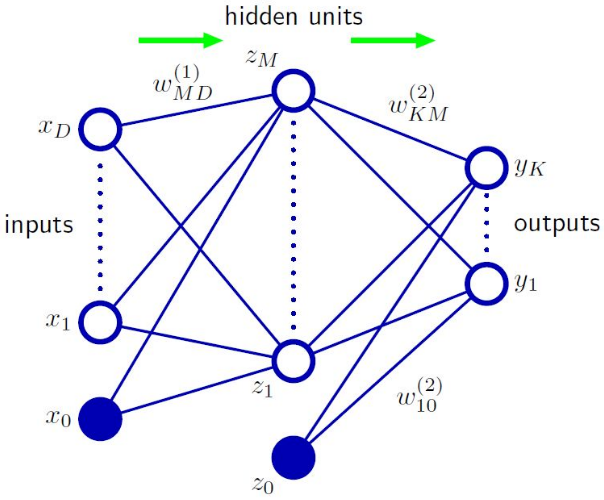


Feed-forward Neural networks

- Approximation capabilities of these networks have been well-studied
    - These networks are very general

Weight space symmetries

- Multiple weights lead to the same i/p-o/p mapping function



Next
Training the Neural Networks