DDA5001 Machine Learning

Neural Networks (Part I): Model

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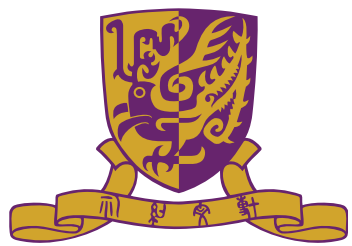


Neural Network Model

Training Two Layer Neural Networks

The Linear Models We Studied and Limitations

We have mainly studied linear regression and linear classification.

- Least squares, perception, logistic regression, and SVM. They are all linear supervised machine learning models.
- Linear model does not perform well on highly non-linearly separable / regressible data.

Many challenging objectives consist of non-linear structures. One way to deal with non-linear case is through nonlinear transformation of data, making the data to be linearly separable in higher dimension.

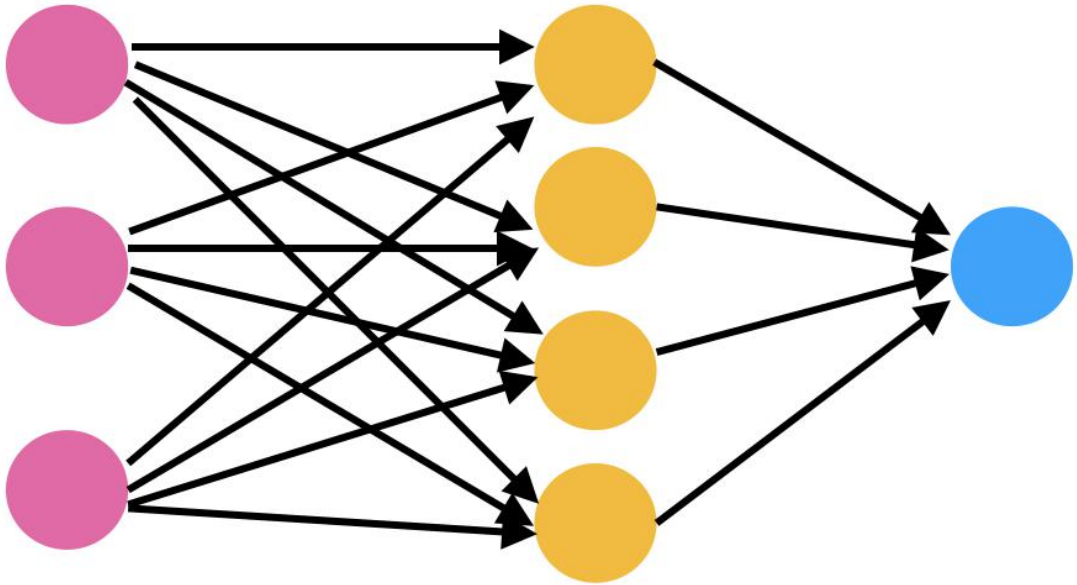
- Kernel method. However, this method needs to choose the right κ.

Another way is to impose non-linearity in our model $f_{\boldsymbol{\theta}}(\boldsymbol{x})$ (nonlinear in $\boldsymbol{\theta}$), leading to nonlinear supervised learning model.

- Note that supervised learning model is to use $f_{\boldsymbol{\theta}}(\boldsymbol{x})$ to approximate the underlying (nonlinear) pattern g.
- One most noticeable model is neural networks due to its universal approximation power.

Structure of Neural Network

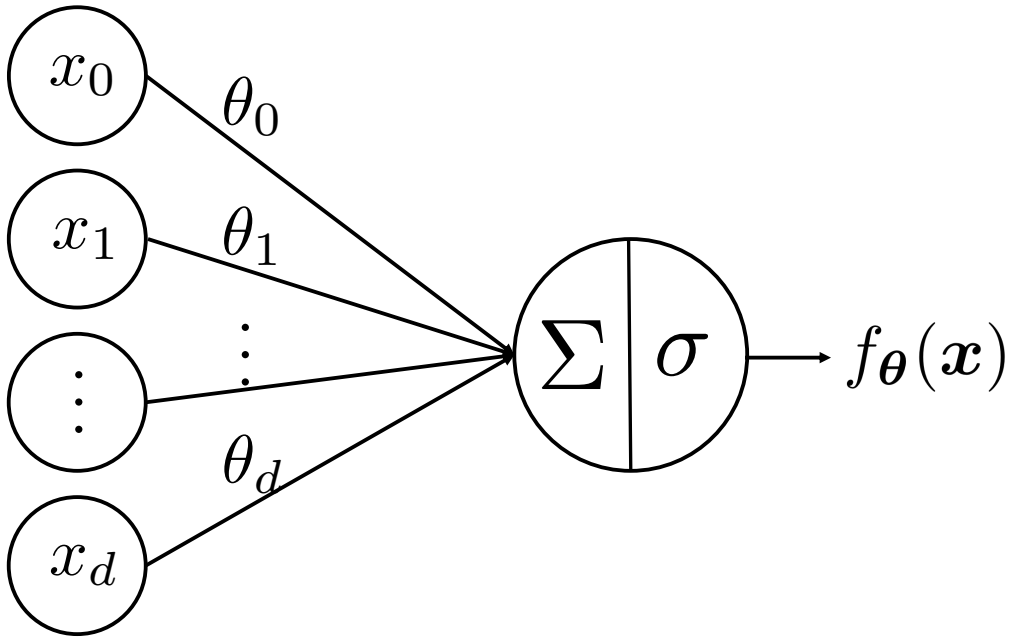
Neural network structure:



- Originally conceived as models for the brain.
  - Nodes are neurons.
  - Edges are synapses.

Let's start with the simplest single layer neural net.

Single Layer Neural Network

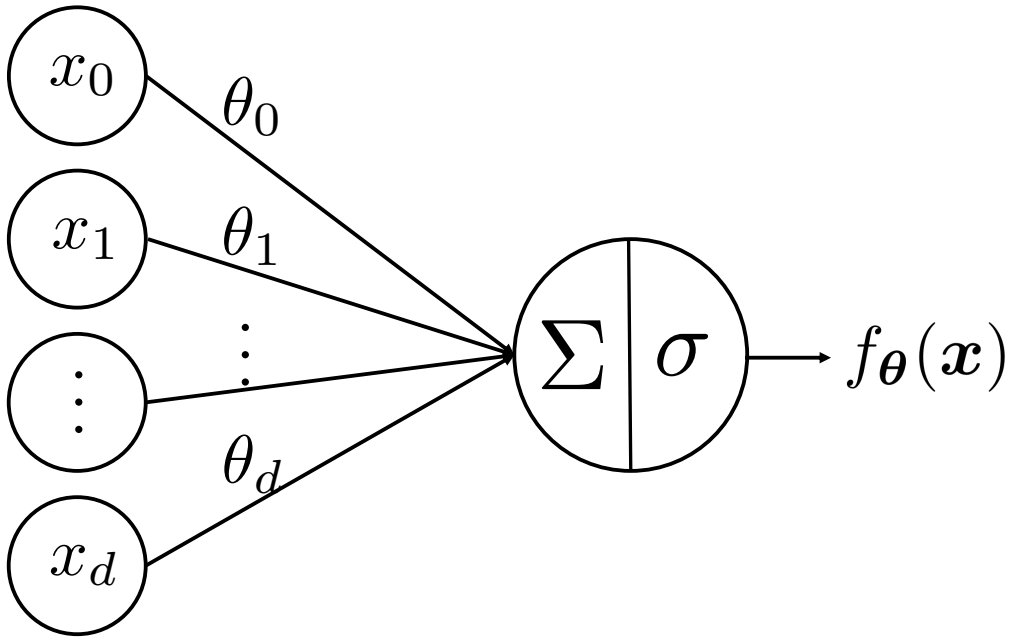


- Sample $\boldsymbol{x} = (x_0, \ldots, x_d)$ with $x_0 = 1$.
- Parameters $\boldsymbol{\theta} = (\theta_0, \ldots, \theta_d)$, called weights.
- σ is called activation function.

This neural network (NN) structure means

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma\left(\sum_{i=0}^{d} \theta_i x_i\right) = \sigma(\boldsymbol{\theta}^\top \boldsymbol{x}).$$

Neural Network As A Generalized Linear Model



This single layer neural network covers linear models.

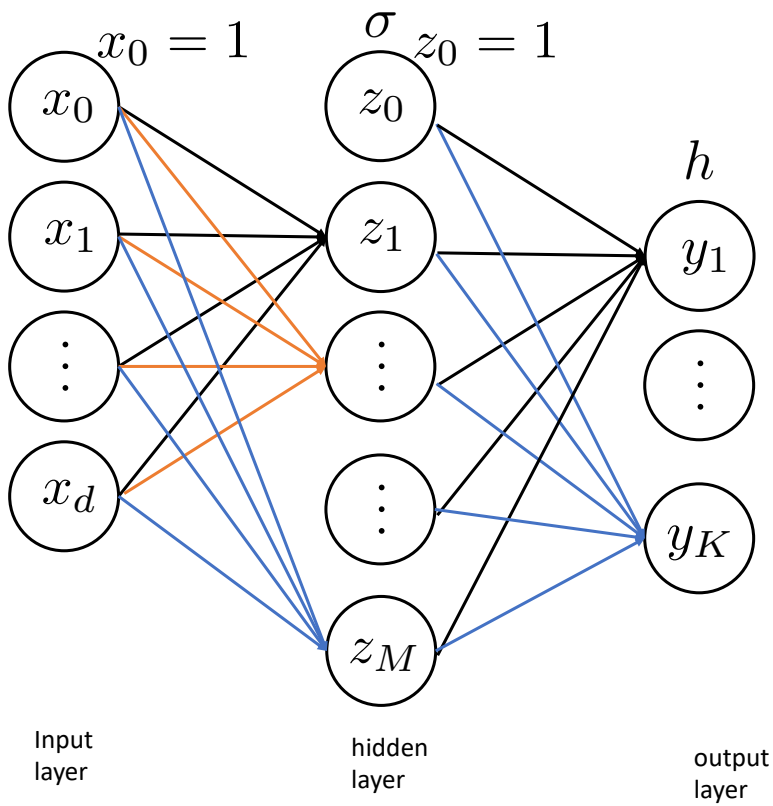
- Vanilla linear regression model if $\sigma(t) = t$.
- Logistic regression (binary case) if

$$\sigma(t) = \frac{1}{1 + e^{-y \cdot t}}$$

More generally, neural network can have more than one layer.

One Hidden Layer (Two-Layer) Neural Network

We generalize neural network to two-layer:



Model:

$$z_m = \sigma(\boldsymbol{v}_m^\top \boldsymbol{x}), \quad m = 1, \ldots, M$$
$$y_k = h(\boldsymbol{w}_k^\top \boldsymbol{z}), \quad k = 1, \ldots, K$$

One Hidden Layer Neural Network

Mathematically, this one hidden layer neural network is presented as

$$z_m = \sigma(\boldsymbol{v}_m^\top \boldsymbol{x}), \quad m = 1, \ldots, M$$
$$y_k = h(\boldsymbol{w}_k^\top \boldsymbol{z}), \quad k = 1, \ldots, K$$

The main idea: Use the output of M linear models + possibly nonlinear transformation σ as the input to another linear model.

- σ is fixed activation function, h depends on tasks.
- What are the unknown parameters?

$$\boldsymbol{v}_m, \quad \boldsymbol{w}_k, \qquad m = 1, \ldots, M \quad \text{and} \quad k = 1, \ldots, K$$

- What are the dimension of $\boldsymbol{v}_m$ and $\boldsymbol{w}_k$?
- How many extra parameters compared to vanilla linear model?

Neural Network Model in Matrix Form

$$z_m = \sigma(\boldsymbol{v}_m^\top \boldsymbol{x}), \quad m = 1, \ldots, M.$$
$$y_k = h(\boldsymbol{w}_k^\top \boldsymbol{z}), \quad k = 1, \ldots, K.$$

Let us omit the bias term for simplicity and without loss of generality. Letting $\boldsymbol{V} \in \mathbb{R}^{M \times d}$ denote the matrix having rows $\boldsymbol{v}_m^\top$ and $\boldsymbol{W} \in \mathbb{R}^{K \times M}$ denote the matrix having rows $\boldsymbol{w}_k^\top$, we can write this neural net as

$$\boldsymbol{z} = \sigma(\boldsymbol{V}\boldsymbol{x}).$$
$$\boldsymbol{y} = h(\boldsymbol{W}\boldsymbol{z}).$$

One hidden layer NN model can be written compactly

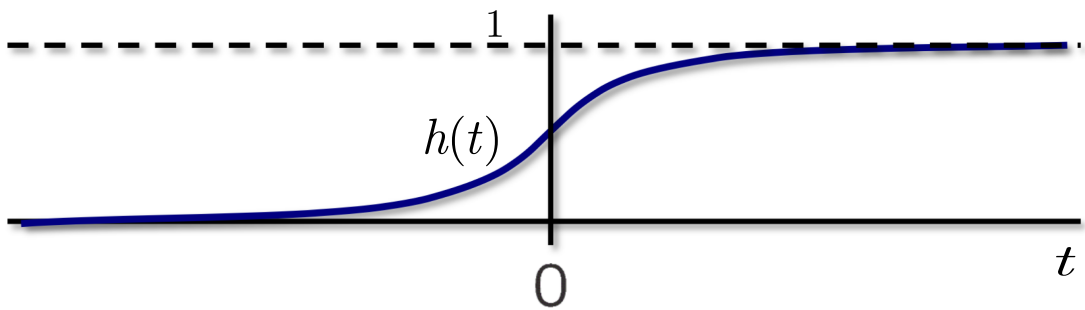
$$\boxed{\boldsymbol{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}) = h(\boldsymbol{W}\sigma(\boldsymbol{V}\boldsymbol{x})).}$$

- $\boldsymbol{\theta} := (\boldsymbol{V}, \boldsymbol{W})$ contains the network parameters, called weights.
- The input of the next layer is the output of the previous layer ($\boldsymbol{z} = \sigma(\boldsymbol{V}\boldsymbol{x})$).

The Ingredients in Typical Neural Networks

- A historically common choice for σ is the logistic / sigmoid function:

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



- A popular activation function design based on sigmoid is SiLU (Sigmoid Linear Unit):

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

- Another popular choice of σ is the ReLU (rectified linear unit):

$$\sigma(t) = \max(0, t).$$

The Ingredients in Typical Neural Networks

The choice of h depends somewhat on the application.

- Regression, we usually use

$$h(t) = t.$$

- Logistic regression for binary classification, where $K = 1, y = \{+1, -1\}$

$$h(t) = \frac{1}{1 + e^{-y \cdot t}}.$$

  One can also use SVM model here.

- Multiclass classification

$$h(t_k) = \frac{e^{t_k}}{\sum_{j=1}^{K} e^{t_j}}, \quad t_k = \boldsymbol{w}_k^\top \boldsymbol{z},$$

  which is to let the last layer to be a multi-class logistic regression classifier.

$\rightsquigarrow$ h is to impose certain linear model ($\boldsymbol{z}$ as input) at the end of NN.

The Representation Power of Neural Networks

One natural question would be why consider neural network model for nonlinear case.

- Supervised learning is to approximate the underlying pattern g. The target function g is nonlinear in general.
- The following theorem shows a universal approximation power of just one hidden layer neural networks, which shows that neural networks can represent any regular function, and thus can approximate any underlying (possibly nonlinear) g.

Theorem: Universal approximation Power

Let g be a continuous function on a bounded subset $\mathcal{K}$ of d-dimensional space. Then, there exists a one hidden layer neural network $f_{\boldsymbol{\theta}}$ with a finite number of hidden neurons that approximates g arbitrarily well. Namely, for all sample $\boldsymbol{x} \in \mathcal{K}$, we have $|f_{\boldsymbol{\theta}}(\boldsymbol{x}) - g(\boldsymbol{x})| < \varepsilon$ for every $\varepsilon > 0$.

Remarks

- Like kernel methods, neural networks fit a linear model in a nonlinear feature space.
- Unlike kernel methods, these nonlinear features are learned — i.e., output of the hidden layer.
- Interpretation of NN: One can think neural network model as extracting features by nonlinear network and finally put the extracted feature z into the last layer for regression or classification. So, the last layer can be viewed as LS, LR, SVM, etc.
  $\rightsquigarrow$ This is also true for deep learning, i.e., deep neural network model (later).
- We will see that the training of neural network model involves nonconvex optimization because of the involved nonlinear structure of $f_{\boldsymbol{\theta}}$.

Training Two Layer Neural Networks

Training Neural Networks

- Training data: $(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{y}_n)$ with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $\boldsymbol{y}_i \in \mathbb{R}^K$
- Neural network model

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = h(\boldsymbol{W}\sigma(\boldsymbol{V}\boldsymbol{x})).$$

- We aim to learn the weight parameters $\boldsymbol{\theta} = (\boldsymbol{V}, \boldsymbol{W})$ such that

$$\boldsymbol{y}_i \leftarrow f_{\boldsymbol{\theta}}(\boldsymbol{x}_i).$$

  Thus, this is a supervised learning problem.

- We can quantify this approximation by choosing a loss function which we will seek to minimize by picking $\boldsymbol{\theta}$ appropriately

The Learning Problem for Training Neural Networks

Regression: $h(t) = t$ and use squared ℓ_2 loss, resulting in

- $K = 1$

$$\min_{\boldsymbol{\theta}} \left\{ \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i))^2 \right\}$$

- $K > 1$

$$\min_{\boldsymbol{\theta}} \left\{ \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{y}_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)\|_2^2 \right\}$$

The Learning Problem for Training Neural Networks

Classification (Binary): $K = 1, y = \{+1, -1\}$ and h is logistic function, and use logistic loss, resulting in

$$\min_{\boldsymbol{\theta}} \left\{ \mathcal{L}(\boldsymbol{\theta}) = -\frac{1}{n} \sum_{i=1}^{n} \log(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)) \right\}$$

Classification (Multi-class): $K > 1$, $\boldsymbol{y} = (0, \ldots, 1, \ldots, 0)$, h is softmax and use multiple-class logistic loss, resulting in

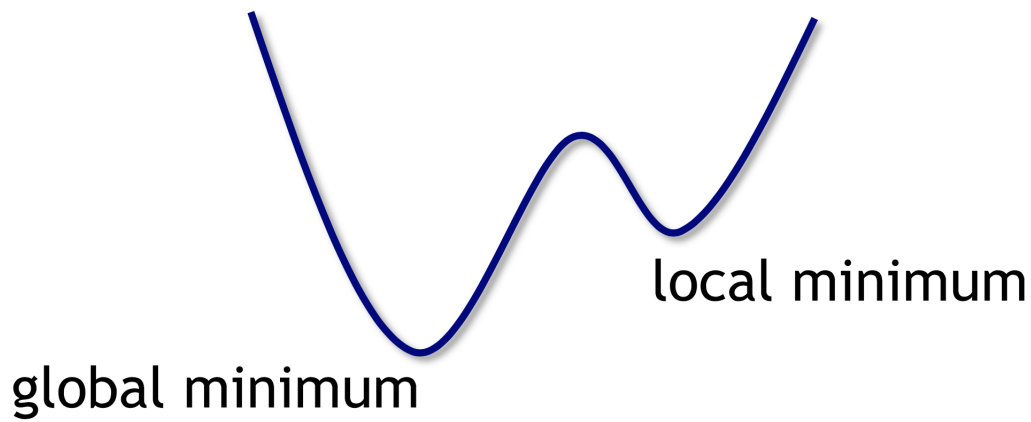
$$\min_{\boldsymbol{\theta}} \left\{ \mathcal{L}(\boldsymbol{\theta}) = -\frac{1}{n} \sum_{i=1}^{n} \boldsymbol{y}_i^\top \log(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)) \right\}$$

Training Neural Networks is Nonconvex Optimization

For example, regression training problem can be written as:

$$\min_{\boldsymbol{\theta}=(\boldsymbol{V},\boldsymbol{W})} \left\{ \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{y}_i - h(\boldsymbol{W}\sigma(\boldsymbol{V}\boldsymbol{x}_i))\|^2 \right\}.$$

This is a highly nonconvex optimization problem.



Training Neural Networks

We put an abstract form of the former learning problems:

$$\min_{\boldsymbol{\theta}} \left\{ \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \ell_i(\boldsymbol{\theta}) \right\}$$

For different applications (regression or classification), ℓ_i has its own form.

- One can apply a gradient-based training algorithm.
- One needs to compute the gradient

$$\nabla \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \ell_i(\boldsymbol{\theta}).$$

- Apply gradient-based training algorithm:

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \mu_k \nabla \mathcal{L}(\boldsymbol{\theta}_k).$$

However... The gradient is not easy to compute and GD training algorithm might be too optimistic.

Next: Training Algorithm and its Ingredients

Next lectures will dive into the depth of neural network training:

- How to compute the gradient?
  $\rightsquigarrow$ The well-known backpropagation (BP).
- In contemporary applications, n is so large. Applying GD is not feasible.
  $\rightsquigarrow$ Stochastic gradient descent, Adagrad, and Adam family.