Neural Network

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Learning problem

- Input data: $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}^k$.
- Approximator: $f_w : \mathbb{R}^d \to \mathbb{R}^k$ where w is the parameters of f. Find w such that f predicts exactly the labels of unseen data, i.e., $f_w(x_t) = y_t$ for unseen data point x_t.
- Loss function $\ell : \mathbb{R}^d \times \mathbb{R}^k \to \mathbb{R}$. $\ell(f_w(x_t), y_t)$ is small if $f_w(x_t)$ is close to y_t.
- Test data and train data are supposed to be drawn from the same distribution $\to$ find w such that $f_w(x)$ and y are close on the training data.

- We solve the optimization problem:

$$\min_w \frac{1}{n} \sum_{i=1}^{n} \ell(f_w(x_i), y_i) + \lambda \Omega(w),$$

  where $\Omega(w)$ is a regularization term on w and its weight λ. Functions ℓ, f_w and Ω are usually chosen convex to ease the optimization.
- Different models have different loss functions ℓ and/or approximators (f).

Linear models

Linear Regression (LinReg)

- $w = (w_0, w_1, ..., w_d)^T$ and $f_w(x) = \langle w, [1; x] \rangle$[a].
- $l(y, y') = \|y - y'\|^2$.
- $\Omega(w) = \|w\|^2_{L_2}, \|w\|_{L_1}, \ldots$

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[a] $[1; x]$ is the Matlab notation for $\begin{pmatrix} 1 \\ x \end{pmatrix}$

Logistic Regression (LogReg)

- $w = (w_0, w_1, ..., w_d)^T$ and $f_w(x) = \sigma(\langle w, [1; x] \rangle)$ where $\sigma(x) = \frac{1}{1+\exp(-x)}$.
- $l(y, y') = -y' \log(y) - (1 - y') \log(1 - y)$.
- .. or in another way: $f_w(x) = \langle w, [1; x] \rangle$ and $l(y, y') = -y' \log(\sigma(y)) - (1 - y') \log(1 - \sigma(y))$.
- $\Omega(w) = \|w\|^2_{L_2}, \|w\|_{L_1}, \ldots$

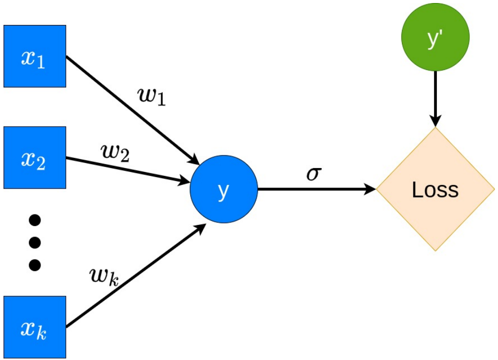
Linear models

Support Vector Machine (SVM)

- $w = (w_0, w_1, ..., w_d)$ and $f_w(x) = w_1x_1 + w_2x_2 + ... + w_0$.
- $l(y, y') = \max(0, 1 - yy')$.

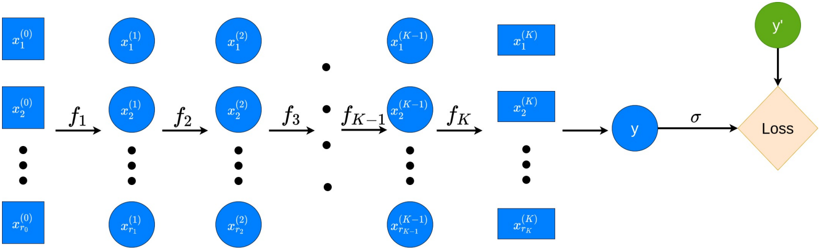
- Linear regression, logistic regression, SVM use linear approximators $\rightarrow$ They are **linear models**.
- Linear models:
  - Pros: Simple, easy to optimize, guaranteed to have a unique solution.
  - Cons: Cannot approximate complex data distribution.
- Non-linearity can be obtained with feature engineering or kernel trick but they require domain specific knowledge. Even so, that is not enough in some complex domain (images, text, sound, ...).

Graphical representation of linear models



- Input data are transformed once.
- $y = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_k x_k$.

Input data are transformed multiple times.



In this lecture

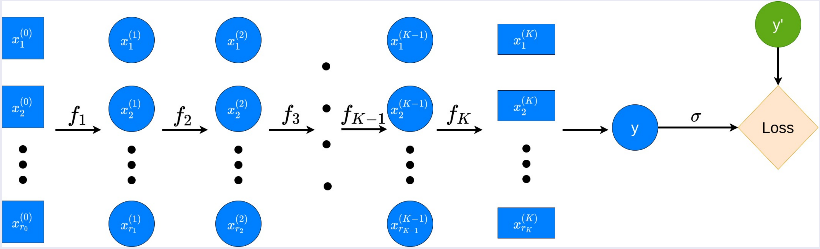
- A basic neural network architecture (Multi-layer perceptron).
- Back-propagation.

Neural network

- A high-capacity model for machine learning
  - Can contain millions or billions of parameters.
  - Can approximate complicated data distribution.
  - Yielding state-of-the-art performances in many important problems.
  - Many variants: Multi-Layer Perceptron, Convolutional Neural Network, Recurrent Neural Network, Transformers, ...
  - Deep learning: Branch of machine learning that studies neural network and its applications.
- Training with Stochastic Gradient Descent using back-propagation.
- Applications: Image perception/generation, machine translation, speech recognition, autonomous driving, ...
- We investigate the simplest type of neural network, Multi-Layer Perceptron, in the next slides.

Multi-Layer Perceptron (MLP)

Graphical representation

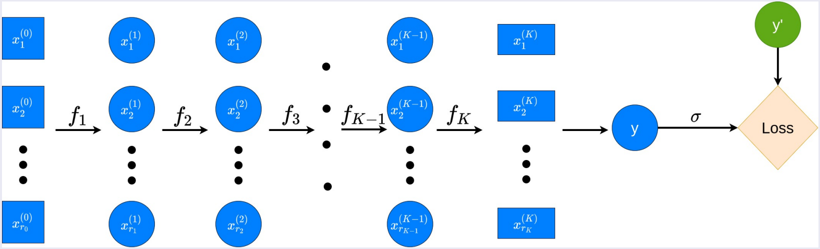


Functional representation

- $f = f_K \circ f_{K-1} \circ \ldots \circ f_1$ or $f(x) = f_K(f_{K-1}(\ldots(f_1(x))))$.
- Denote $x^{(k)} = f_k(f_{k-1}(\ldots(f_1(x))))$. We have: $x_k = f_k(x_{k-1})$.
- x_0 is the input layer, x_K is the output layer, x_k is the layer k of the neural network. x_k with $1 \leq k \leq K-1$ are **hidden layers**.

Multi-Layer Perceptron (MLP)

Graphical representation

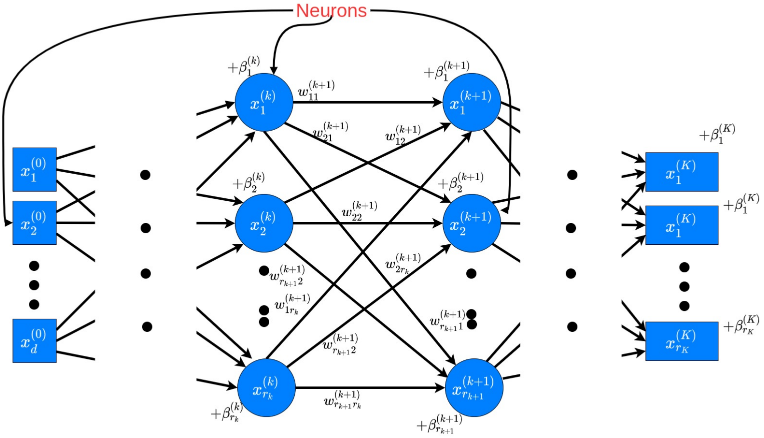


Functional representation

- Usually $f_k(x) = \sigma_k(W^{(k)}x + \beta^{(k)})$ where $W^{(k)} \in \mathbb{R}^{r_k \times c_k}$ and $\beta^{(k)} \in \mathbb{R}^{r_k}$ and σ_k **is a point-wise non-linear activation function**. So:$x^{(k)} = \sigma(W^{(k)}x^{(k-1)} + \beta^{(k)})$.
- $W^{(k)}$ and $\beta^{(k)}$, $1 \leq k \leq K$, are the parameters of the neural network. K and r_k, $1 \leq k \leq K$ are hyper-parameters.
- We must have $c_{k+1} = r_k$ for all $k \in [1..K-1]$ and $x^{(0)} \in \mathbb{R}^{c_1}$?

Multi-Layer Perceptron (MLP)

- Graphical representation: A closer look.

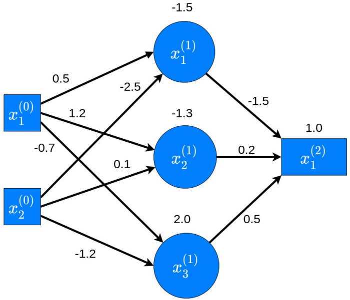


$$x^{(k+1)} = \sigma(W^{(k)}x^{(k)} + \beta^{(k+1)})$$

$$\Rightarrow x_i^{(k+1)} = \sigma(W_{i1}^{(k+1)}x_1^{(k)} + W_{i2}^{(k+1)}x_2^{(k)} + \ldots + W_{ir_k}^{(k+1)}x_{r_k}^{(k)} + \beta^{(k+1)}).$$

Multi-Layer Perceptron (MLP)

- Example: MLP with one hidden layer.



Compute the hidden layer and the output layer with $x^{(0)} = [0.5, -0.5]^T$ and $\sigma : x \mapsto \frac{1}{1+\exp(-x)}$.

Multi-Layer Perceptron (MLP)

- Example: MLP with one hidden layer.

$x_1^{(1)} = \sigma(0.5 \times 0.5 + (-2.5) \times (-0.5) - 1.5) = 0.5$
$x_2^{(1)} = \sigma(1.2 \times 0.5 + 0.1 \times (-0.5) - 1.3) = 0.3208$
$x_3^{(1)} = \sigma((-0.7) \times 0.5 + (-1.2) \times (-0.5) + 2.0) = 0.9047$
$x_1^{(2)} = \sigma((-1.5) \times 0.5 + 0.2 \times 0.3208 + 0.5 \times 0.9047 + 1.0) = 0.6828$
Or

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{bmatrix} = \sigma\left(\begin{bmatrix} 0.5 & -2.5 \\ 1.2 & 0.1 \\ -0.7 & -1.2 \end{bmatrix} \begin{bmatrix} 0.5 \\ -0.5 \end{bmatrix} + \begin{bmatrix} -1.5 \\ -1.3 \\ 2.0 \end{bmatrix}\right) = \begin{bmatrix} 0.5 \\ 0.3208 \\ 0.9047 \end{bmatrix}$$

and

$$x_1^{(2)} = \sigma\left(\begin{bmatrix} -1.5 & 0.2 & 0.5 \end{bmatrix} \begin{bmatrix} 0.5 \\ 0.3208 \\ 0.9047 \end{bmatrix} + 1.0\right) = 0.6828.$$

Multi-Layer Perceptron (MLP)

Training MLP

- Gradient descent: At iteration t, update parameters $W^{(k)}$ and $\beta^{(k)}$ with $W^{(k)} \longleftarrow W^{(k)} - \eta_w \frac{1}{n} \sum_{i=1}^{n} \nabla_{W^{(k)}} l_i$ and $\beta^{(k)} \longleftarrow \beta^{(k)} - \eta_b \frac{1}{n} \sum_{i=1}^{n} \nabla_{\beta^{(k)}} l_i$.
- Stochastic gradient descent: At iteration t, select a small set of indices I from $\{1, 2, \dots, n\}$ and update parameters $W^{(k)}$ and $\beta^{(k)}$ with $W^{(k)} \longleftarrow W^{(k)} - \eta_w \frac{1}{n} \sum_{i \in I} \nabla_{W^{(k)}} l_i$ and $\beta^{(k)} \longleftarrow \beta^{(k)} - \eta_b \frac{1}{n} \sum_{i \in I} \nabla_{\beta^{(k)}} l_i$.
- How to compute the gradients? $\longrightarrow$ Chain rule.
- How to compute the gradients efficiently? $\longrightarrow$ Back-propagation.

Multi-Layer Perceptron (MLP)

Chain rule

- Chain rule: $\dfrac{dz}{dx} = \dfrac{dz}{dy}\dfrac{dy}{dx}$.

$$\frac{\partial l}{\partial W^{(k)}} = \frac{dl}{dx_K}\frac{dx_K}{dx_{K-1}}\cdots\frac{\partial x_k}{\partial W^{(k)}} = \frac{dl}{dx_K}\frac{df_k(x_{K-1})}{dx_{K-1}}\cdots\frac{\partial f_k(x_{k-1})}{\partial W^{(k)}},$$

$$\frac{\partial l}{\partial \beta^{(k)}} = \frac{dl}{dx_K}\frac{dx_K}{dx_{K-1}}\cdots\frac{\partial x_k}{\partial \beta^{(k)}} = \frac{dl}{dx_K}\frac{df_k(x_{K-1})}{dx_{K-1}}\cdots\frac{\partial f_k(x_{k-1})}{\partial \beta^{(k)}},$$

$$\frac{df_k(x_{k-1})}{dx_{k-1}} = \frac{d\sigma(W^{(k)}x_{k-1}+\beta^{(k)}))}{dx_{k-1}} = \mathrm{diag}(\sigma'(z_k))W^{(k)},$$

$$\frac{\partial f_k(x_{k-1})}{\partial W^{(k)}} = \frac{\partial\sigma(W^{(k)}x_{k-1}+\beta^{(k)}))}{\partial W^{(k)}} = \mathrm{diag}(\sigma'(z_k))\mathbb{1}_{r_k}x_{k-1}^T,$$

$$\frac{\partial f_k(x_{k-1})}{\partial \beta^{(k)}} = \frac{\partial\sigma(W^{(k)}x_{k-1}+\beta^{(k)}))}{\partial \beta^{(k)}} = \mathrm{diag}(\sigma'(z_k))\mathbb{1}_{r_k}.$$

where $z_k = W^{(k)}x_{k-1} + \beta^{(k)}$ and σ' is the derivative of the activation function σ.

Multi-Layer Perceptron (MLP)

Back-propagation

- Compute the gradients separately is expensive $\Rightarrow$ compute from the last layer to the first layer, save intermediate results (memoization, dynamic programming).

$$
\begin{aligned}
\frac{\partial l}{\partial W^{(k)}} &= \frac{dl}{dx_k}\frac{\partial x_k}{\partial W^{(k)}} = \frac{dl}{dx_k}\frac{\partial f_k(x_{k-1})}{\partial W^{(k)}}, \\
\frac{\partial l}{\partial \beta^{(k)}} &= \frac{dl}{dx_k}\dots\frac{\partial x_k}{\partial \beta^{(k)}} = \frac{dl}{dx_k}\dots\frac{\partial f_k(x_{k-1})}{\partial \beta^{(k)}}, \\
\frac{dl}{dx_k} &= \frac{dl}{dx_K}\frac{dx_K}{dx_{K-1}}\dots\frac{dx_{k+1}}{dx_k} = \frac{dl}{dx_{k+1}}\frac{dx_{k+1}}{dx_k}.
\end{aligned}
$$

  We save $\dfrac{dl}{dx_k}$ for all $k, 1 \leq k \leq K$.

- Back-propagation: A fancy name for memoization and dynamique programming in neural network's gradient computation.

Multi-Layer Perceptron (MLP)

Back-propagation

Example with one hidden MLP:

- $l(x^{(2)}, y') = y' \log(x^{(2)}) + (1 - y') \log(1 - x^{(2)})$.
- Let $y' = 1$, we have:

$$\frac{dl}{dx^{(2)}} = \frac{y'}{x^{(2)}} = \frac{1}{0.6828} = 1.4646.$$

$$\frac{dx^{(2)}}{dx^{(1)}} = \mathrm{diag}(\sigma'(W^{(2)}x_1 + \beta^{(2)}))W^{(2)} = [0.3249, -0.0433, -0.1083]$$

$$\frac{dx^{(1)}}{dx^{(0)}} = \mathrm{diag}(\sigma'(W^{(1)}x_0 + \beta^{(1)}))W^{(1)} = \begin{bmatrix} -0.125 & 0.625 \\ -0.2615 & -0.0218 \\ 0.0604 & 0.1035 \end{bmatrix}$$

Back-propagation

Back-propagation

Example with one hidden MLP:

$$\frac{dl}{dx^{(1)}} = [-0.4759, 0.0634, 0.1586], \quad \frac{dl}{dx^{(0)}} = [-0.0525, 0.2824]$$

$$\frac{dl}{dW^{(2)}} = [0.1083, 0.0695, 0.1959]$$

$$\frac{dl}{dW^{(2)}} = [0.1083, 0.0695, 0.1959], \quad \frac{dl}{d\beta^{(2)}} = 0.2166$$

$$\frac{dl}{dW^{(1)}} = \begin{pmatrix} 0.125 & -0.125 \\ 0.1089 & -0.1089 \\ 0.0431 & -0.0431 \end{pmatrix}, \quad \frac{dl}{d\beta^{(1)}} = \begin{pmatrix} 0.25 \\ 0.2179 \\ 0.0863 \end{pmatrix}$$

Exercise

- Write code to reproduce the gradient computation above.
- Compute the gradients with $\sigma : x \mapsto \max(x, 0)$.

Neural Network Applications

- State-of-the-art performance in many tasks.
- Computer Vision: image classification, object detection, image/video synthesis, autonomous driving, surveillance system, robotics, ...
- Natural Language/Audio Processing: Machine translation, speech synthesis, virtual assistance, ...
- More in the next lecture (Convolutional Neural Network).