Introduction to Deep Learning

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Deep Feedforward Networks

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  - Three functions $f^{(1)}, f^{(2)}, f^{(3)}$ are connected in chain
  - Overall function realized is $f(x) = f^{(3)}(f^{(2)}(f^{(1)}(x)))$
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- Goal of NN is not to accurately model brain!

Multilayer neural network

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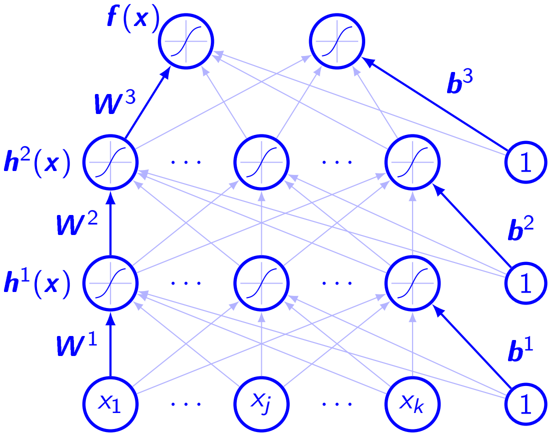

Issues with linear FFN

- Fit well for linear and logistic regression
- Convex optimization technique may be used
- Capacity of such function is limited
- Model cannot understand interaction between any two variables

Overcome issues of linear FFN

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  - Manually design ϕ
    - Require domain knowledge
  - Strategy of deep learning is to learn ϕ

Goal of deep learning

- We have a model $y = f(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{w}) = \phi(\boldsymbol{x}; \boldsymbol{\theta})^T \boldsymbol{w}$
- We use $\boldsymbol{\theta}$ to learn ϕ
- $\boldsymbol{w}$ and ϕ determines the output. ϕ defines the hidden layer
- It looses the convexity of the training problem but benefits a lot
- Representation is parameterized as $\phi(\boldsymbol{x}, \boldsymbol{\theta})$
  - $\boldsymbol{\theta}$ can be determined by solving optimization problem
- Advantages
  - ϕ can be very generic
  - Human practitioner can encode their knowledge to designing $\phi(\boldsymbol{x}; \boldsymbol{\theta})$

Design issues of feedforward network

- Choice of optimizer
- Cost function
- The form of output unit
- Choice of activation function
- Design of architecture - number of layers, number of units in each layer
- Computation of gradients

Example

- Let us choose XOR function
- Target function is $y = f^*(\boldsymbol{x})$ and our model provides $y = f(\boldsymbol{x}; \boldsymbol{\theta})$
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- Target is to fit output for $\boldsymbol{X} = \{[0,0]^T, [0,1]^T, [1,0]^T, [1,1]^T\}$
- This can be treated as regression problem and MSE error can be chosen as loss function
- MSE loss function $J(\boldsymbol{\theta}) = \frac{1}{4}\sum_{\boldsymbol{x} \in \boldsymbol{X}} (f^*(\boldsymbol{x}) - f(\boldsymbol{x}; \boldsymbol{\theta}))^2$
- We need to choose $f(\boldsymbol{x}; \boldsymbol{\theta})$ where $\boldsymbol{\theta}$ depends on $\boldsymbol{w}$ and b
- Let us consider a linear model $f(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{x}^T \boldsymbol{w} + b$

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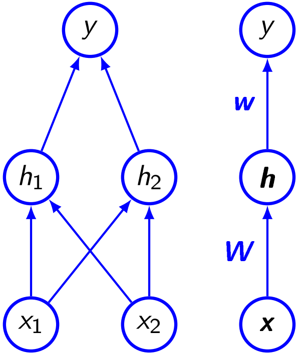
- Solving these, we get $\boldsymbol{w} = 0$ and $b = \frac{1}{2}$

Simple feedforward network with hidden layer

- Let us assume that the hidden unit $\boldsymbol{h}$ computes $f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c})$



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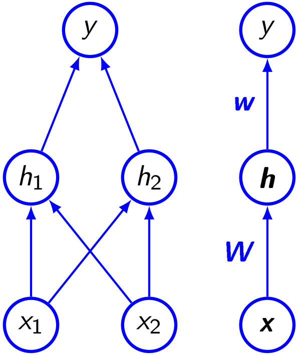

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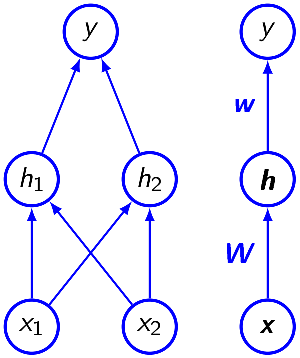

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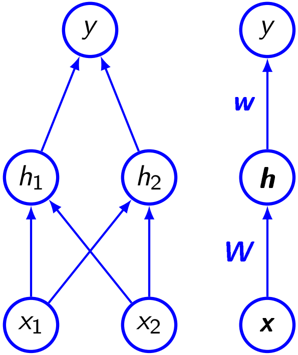

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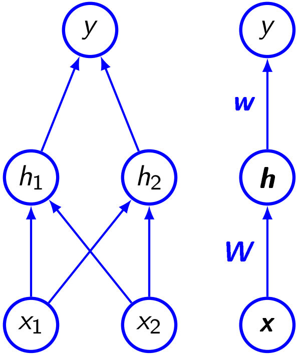

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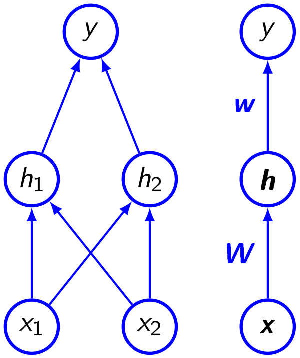
- We need to have nonlinear function to describe the features
- Usually NN have affine transformation of learned parameters followed by nonlinear activation function
- Let us use $\boldsymbol{h} = g(\boldsymbol{W}^T\boldsymbol{x} + \boldsymbol{c})$
- Let us use ReLU as activation function $g(z) = \max\{0, z\}$
- g is chosen element wise $h_i = g(\boldsymbol{x}^T\boldsymbol{W}_{:,i} + c_i)$



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Gradient based learning

- Similar to machine learning tasks, gradient descent based learning is used
  - Need to specify optimization procedure, cost function and model family
- For NN, model is nonlinear and function becomes nonconvex
  - Usually trained by iterative, gradient based optimizer
- Solved by using gradient descent or stochastic gradient descent (SGD)

Gradient descent

- Suppose we have a function $y = f(x)$, derivative (slope at point x) of it is $f'(x) = \frac{dy}{dx}$
- A small change in the input can cause output to move to a value given by $f(x+\epsilon) \approx f(x) + \epsilon f'(x)$
- We need to take a jump so that y reduces (assuming minimization problem)
- We can say that $f(x - \epsilon \text{sign}(f'(x)))$ is less than $f(x)$
- For multiple inputs partial derivatives are used ie. $\frac{\partial}{\partial x_i} f(\boldsymbol{x})$
- Gradient vector is represented as $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$
- Gradient descent proposes a new point as $\boldsymbol{x}' = \boldsymbol{x} - \epsilon \nabla_{\boldsymbol{x}} f(x)$ where ϵ is the learning rate

Stochastic gradient descent

- Large training set are necessary for good generalization
- Typical cost function used for optimization is $J(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} L(x^{(i)}, y^{(i)}, \boldsymbol{\theta})$
- Gradient descent requires computing of $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} \nabla_{\boldsymbol{\theta}} L(x^{(i)}, y^{(i)}, \boldsymbol{\theta})$

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  - Computation cost is $O(m)$
- For SGD, gradient is an expectation estimated from a small sample known as mini-batch ($\mathbb{B} = \{x^{(1)}, \ldots, x^{(m')}\}$)
- Estimated gradient is $\boldsymbol{g} = \frac{1}{m'}\sum_{i=1}^{m'} \nabla_{\boldsymbol{\theta}} L(x^{(i)}, y^{(i)}, \boldsymbol{\theta})$
- New point will be $\boldsymbol{\theta} = \boldsymbol{\theta} - \epsilon \boldsymbol{g}$

Cost function

- Similar to other parametric model like linear models
- Parametric model defines distribution $p(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})$
- Principle of maximum likelihood is used (cross entropy between training data and model prediction)
- Instead of predicting the whole distribution of $\boldsymbol{y}$, some statistic of $\boldsymbol{y}$ conditioned on $\boldsymbol{x}$ is predicted
- It can also contain regularization term

Maximum likelihood estimation

- Consider a set of m examples $\mathbb{X} = \{x^{(1)}, \ldots, x^{(m)}\}$ drawn independently from the true but unknown data generating distribution $p_{data}(\boldsymbol{x})$
- Let $p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$ be a parametric family of probability distribution

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- By dividing m we get $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x} \sim \hat{p}_{data}} \log p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$

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- Let $p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$ be a parametric family of probability distribution
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$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} p_{model}(\mathbb{X}; \boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{m} p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

- It can be written as $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$
- By dividing m we get $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x} \sim \hat{p}_{data}} \log p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$
- We need to minimize $-\arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x} \sim \hat{p}_{data}} \log p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$

Conditional log-likelihood

- In most of the supervised learning we estimate $P(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})$
- If $\boldsymbol{X}$ be the all inputs and $\boldsymbol{Y}$ be observed targets then conditional maximum likelihood estimator is $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} P(\boldsymbol{Y}|\boldsymbol{X};\boldsymbol{\theta})$
- If the examples are assumed to be i.i.d then we can say

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log P(\boldsymbol{y}^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{\theta})$$

Linear regression as maximum likelihood

- Instead of producing single prediction $\hat{y}$ for a given x, we assume the model produces conditional distribution $p(y|x)$
- For infinitely large training set, we can observe multiple examples having the same x but different values of y
- Goal is to fit the distribution $p(y|x)$

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$$\sum_{i=1}^{m} \log p(\boldsymbol{y}^{(i)}|\boldsymbol{x}^{(i)}; \boldsymbol{\theta}) = -m \log \sigma - \frac{m}{2} \log(2\pi) - \sum_{i=1}^{m} \frac{\|\hat{y}^{(i)} - y^{(i)}\|^2}{2\sigma^2}$$

Learning conditional distributions with max likelihood

- Usually neural networks are trained using maximum likelihood. Therefore the cost function is negative log-likelihood. Also known as cross entropy between training data and model distribution
- Cost function $J(\boldsymbol{\theta}) = -\mathbb{E}_{\boldsymbol{X},\boldsymbol{Y}\sim\hat{p}_{data}} \log p_{model}(\boldsymbol{y}|\boldsymbol{x})$
- Uniform across different models
- Gradient of cost function is very much crucial
  - Large and predictable gradient can serve good guide for learning process
  - Function that saturates will have small gradient
    - Activation function usually produces values in a bounded zone (saturates)
  - Negative log-likelihood can overcome some of the problems
    - Output unit having exp function can saturate for high negative value
    - Log-likelihood cost function undoes the exp of some output functions

Learning conditional statistics

- Instead of learning the whole distribution $p(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})$, we want to learn one conditional statistics of $\boldsymbol{y}$ given $\boldsymbol{x}$
  - For a predicting function $f(\boldsymbol{x};\boldsymbol{\theta})$, we would like to predict the mean of $\boldsymbol{y}$

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- Need to solve the optimization problem $f^* = \arg\min_f \mathbb{E}_{\boldsymbol{X},\boldsymbol{Y}\sim p_{data}} \|\boldsymbol{y} - f(\boldsymbol{x})\|^2$
- Using calculus of variation, it gives $f^*(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{Y}\sim p_{data}(\boldsymbol{y}|\boldsymbol{x})}[y]$
  - Mean of $\boldsymbol{y}$ for each value of $\boldsymbol{x}$
- Using a different cost function $f^* = \arg\min_f \mathbb{E}_{\boldsymbol{X},\boldsymbol{Y}\sim p_{data}} \|\boldsymbol{y} - f(\boldsymbol{x})\|_1$
  - Median of $\boldsymbol{y}$ for each value of $\boldsymbol{x}$

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- As we have $y = f + \varepsilon\eta$ and $y' = f' + \varepsilon\eta'$, therefore, $\frac{dL}{d\varepsilon} = \frac{\partial L}{\partial y}\eta + \frac{\partial L}{\partial y'}\eta'$

Calculus of variation

- Now we have

$$\int_{x_1}^{x_2} \frac{dL}{d\varepsilon}\bigg|_{\varepsilon=0} dx \quad = \int_{x_1}^{x_2} \left(\frac{\partial L}{\partial f}\eta + \frac{\partial L}{\partial f'}\eta' \right) dx$$

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- Euler-Lagrange equation

$$\frac{\partial L}{\partial f} - \frac{d}{dx}\frac{\partial L}{\partial f'} = 0$$

Example

- Let us consider distance between two points $A[y] = \int_{x_1}^{x_2} \sqrt{1 + [y'(x)]^2}\, dx$
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- Therefore we have, $\frac{d^2 f}{dx^2} = 0$
- Hence we have $f(x) = mx + b$ with $m = \frac{y_2 - y_1}{x_2 - x_1}$ and $b = \frac{x_2 y_1 - x_1 y_2}{x_2 - x_1}$

Output units

- Choice of cost function is directly related with the choice of output function
- In most cases cost function is determined by cross entropy between data and model distribution
- Any kind of output unit can be used as hidden unit

Linear units

- Suited for Gaussian output distribution
- Given features $\boldsymbol{h}$, linear output unit produces $\hat{\boldsymbol{y}} = \boldsymbol{W}^T\boldsymbol{h} + \boldsymbol{b}$
- This can be treated as conditional probablity $p(\boldsymbol{y}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{y}; \hat{\boldsymbol{y}}, \boldsymbol{I})$
- Maximizing log-likelihood is equivalent to minimizing mean square error

Sigmoid unit

- Mostly suited for binary classification problem that is Bernoulli output distribution
- The neural networks need to predict $p(y = 1|\boldsymbol{x})$
  - If linear unit has been chosen, $p(y = 1|\boldsymbol{x}) = \max\left\{1, \min\{0, \boldsymbol{W}^T\boldsymbol{h} + \boldsymbol{b}\}\right\}$
  - Gradient?
- Model should have strong gradient whenever the answer is wrong
- Hence, logistic sigmoid function is preferred $\sigma(x) = \dfrac{1}{1 + \exp(-x)}$