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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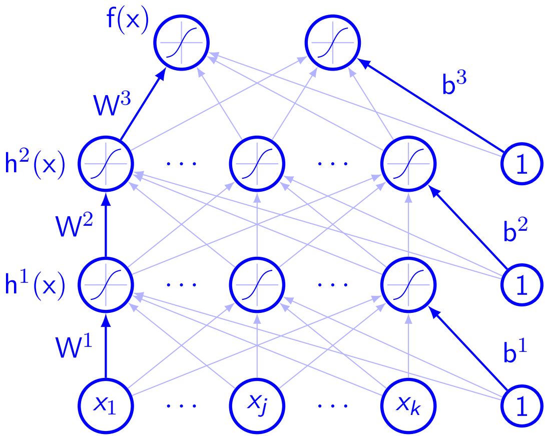
- Goal of NN is not to model brain accurately!

Multilayer neural network



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

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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 $y = f(\mathrm{x}; \boldsymbol{\theta}, \mathrm{w}) = \phi(\mathrm{x}; \boldsymbol{\theta})^T \mathrm{w}$
- We use $\boldsymbol{\theta}$ to learn ϕ
- 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 $\phi(\mathrm{x}, \boldsymbol{\theta})$
  - $\boldsymbol{\theta}$ can be determined by solving optimization problem
- Advantages
  - ϕ can be very generic
  - Human practitioner can encode their knowledge to designing $\phi(\mathrm{x}; \boldsymbol{\theta})$

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

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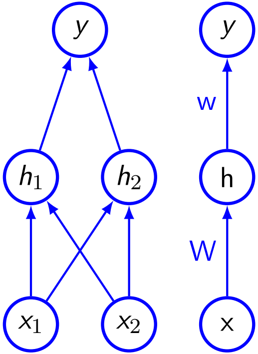
- Solving these, we get $\mathrm{w} = 0$ and $b = \frac{1}{2}$

Simple FFN with hidden layer

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



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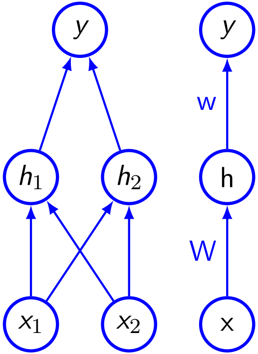

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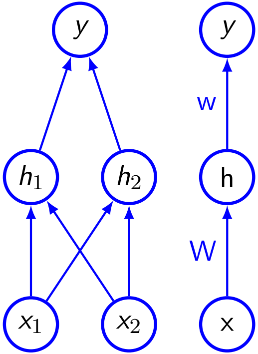

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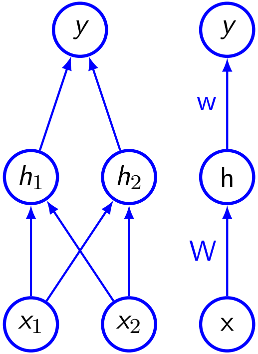

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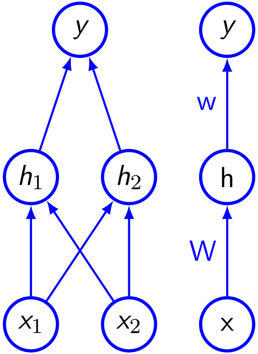
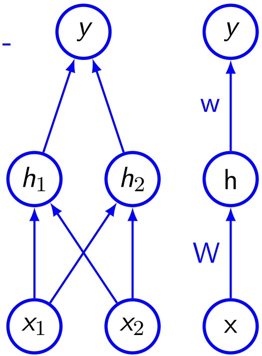


Simple FFN with hidden layer (contd.)

- 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 $\mathbf{h} = g(\mathbf{W}^T\mathbf{x} + \mathbf{c})$
- Let us use ReLU as activation function $g(z) = \max\{0, z\}$
- g is chosen element wise $h_i = g(\mathbf{x}^T\mathbf{W}_{:,i} + c_i)$



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  - $\mathsf{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, $\mathsf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$, $\mathsf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$, $b = 0$

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  - $\mathbf{X}$

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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

- For 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. $\frac{\partial}{\partial \mathrm{x}_i} f(\mathrm{x})$
- Gradient vector is represented as $\nabla_{\mathrm{x}} f(\mathrm{x})$
- Gradient descent proposes a new point as $\mathrm{x}' = \mathrm{x} - \epsilon \nabla_{\mathrm{x}} f(x)$ where ϵ is the learning rate

Stochastic gradient descent

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

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

SGD example

- Consider the following pair (x, y) of points - $(1, 2)$, $(2, 4)$, $(3, 6)$, $(4, 8)$
- Let us try to fit a curve as follows $y = w \times x$ where w is initialized with 4, learning rate as 0.1
- MSE as cost function. Derivative will be $x(w \times x - y)$

Step	Point	Derivative	New w

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3	(3,6)	3*(3.1*3-6)=9.7	2.11
4	(4,8)	4*(2.1*4-8)=1.7	1.94
5	(1,2)	1*(1.9*1-2)=-0.1	1.94
6	(2,4)	2*(1.9*2-4)=-0.2	1.97
7	(3,6)	3*(2.0*3-6)=-0.3	1.99
8	(4,8)	4*(2.0*4-8)=-0.1	2.00
9	(4,8)	1*(2.0*1-2)=0.0	2.00

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2	3.75	2.13

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- Consider the following pair (x, y) of points - $(1, 2)$, $(2, 4)$, $(3, 6)$, $(4, 8)$
- Let us try to fit a curve as follows $y = w \times x$ where w is initialized with 4, learning rate as 0.1
- MSE as cost function. Derivative will be $\frac{1}{4}\sum_i x_i(w \times x_i - y_i)$

Step	Derivative	New w
1	15	2.5
2	3.75	2.13
3	0.94	2.03
4	0.23	2.01
5	0.06	2.00

Cost function

- Similar to other parametric model like linear models
- Parametric model defines distribution $p(\mathrm{y}|\mathrm{x};\boldsymbol{\theta})$
- Principle of maximum likelihood is used (cross entropy between training data and model prediction)
- Instead of predicting the whole distribution of y, some statistic of y conditioned on 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 $p_{data}(\mathrm{x})$
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- By dividing m we get $\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\mathrm{x} \sim p_{data}} \log p_{model}(\mathrm{x}; \boldsymbol{\theta})$

Maximum likelihood estimation (cont.)

- Minimizing dissimilarity between the empirical $\hat{p}_{data}$ and model distribution p_{model} and it is measured by KL divergence

$$D_{KL}(\hat{p}_{data} \| p_{model}) = \arg\min_{\boldsymbol{\theta}} \mathbb{E}_{\mathsf{x} \sim \hat{p}_{data}} \left[\log \hat{p}_{data}(\mathsf{x}) - \log p_{model}(\mathsf{x}; \boldsymbol{\theta})\right]$$

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- We need to minimize $-\arg\min_{\boldsymbol{\theta}} \mathbb{E}_{\mathrm{x} \sim \hat{p}_{data}} \log p_{model}(\mathrm{x}; \boldsymbol{\theta})$

Conditional log-likelihood

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

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

Linear regression as maximum likelihood

- Instead of producing single prediction $\hat{y}$ for a given x, we assume the model produces conditional distribution $p(y|\mathrm{x})$
- 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 $p(y|\mathrm{x})$

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

Learning conditional distributions

- 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 $J(\boldsymbol{\theta}) = -\mathbb{E}_{\mathsf{X},\mathsf{Y}\sim\hat{p}_{data}} \log p_{model}(\mathsf{y}|\mathsf{x}, \boldsymbol{\theta})$
- 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 $p(\mathrm{y}|\mathrm{x};\boldsymbol{\theta})$, we want to learn one conditional statistics of y given x
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- Range of function is limited by features like continuity, boundedness, etc.
- Cost function becomes functional rather than a function

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- Need to solve the optimization problem

$$f^* = \arg\min_f \mathbb{E}_{\mathsf{X},\mathsf{Y}\sim p_{data}} \|\mathsf{y} - f(\mathsf{x})\|^2$$

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Calculus of variations (contd.)

- Now we have

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

Calculus of variations (contd.)

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- Hence $\displaystyle\int_{x_1}^{x_2} \eta\left(\frac{\partial L}{\partial f} - \frac{d}{dx}\frac{\partial L}{\partial f'}\right) dx = 0$

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$$= \int_{x_1}^{x_2} \left(\frac{\partial L}{\partial f}\eta - \eta\frac{d}{dx}\frac{\partial L}{\partial f'}\right) dx + \left.\frac{\partial L}{\partial f'}\eta\right|_{x_1}^{x_2}$$

- Hence $\int_{x_1}^{x_2} \eta \left(\frac{\partial L}{\partial f} - \frac{d}{dx}\frac{\partial L}{\partial f'}\right) dx = 0$
- 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 $A[y] = \int_{x_1}^{x_2} \sqrt{1 + [y'(x)]^2}\, dx$
  - $y'(x) = \dfrac{dy}{dx}\,, \quad y_1 = f(x_1)\,, \quad y_2 = f(x_2)$

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- Now we have, $\dfrac{d}{dx}\dfrac{f'(x)}{\sqrt{1 + [f'(x)]^2}} = 0$

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Example

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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 h, linear output unit produces $\hat{\mathsf{y}} = \mathsf{W}^T\mathsf{h} + \mathsf{b}$
- This can be treated as conditional probability $p(\mathsf{y}|\mathsf{x}) = \mathcal{N}(\mathsf{y}; \hat{\mathsf{y}}, \mathbf{I})$
- 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 $p(y = 1|\mathrm{x})$
  - If linear unit has been chosen, $p(y = 1|\mathrm{x}) = \max\left\{0, \min\{1, \mathrm{W}^T\mathrm{h} + \mathrm{b}\}\right\}$
  - Gradient?
- Model should have strong gradient whenever the answer is wrong
- Let us assume unnormalized log probability is linear with $z = \mathrm{W}^T\mathrm{h} + \mathrm{b}$
- Therefore, $\log \tilde{P}(y) = yz \Rightarrow \tilde{P}(y) = \exp(yz) \Rightarrow P(y) = \frac{\exp(yz)}{\sum_{y' \in \{0,1\}} \exp(y'z)}$
  - It can be written as $P(y) = \sigma((2y - 1)z)$
- The loss function for maximum likelihood is $J(\boldsymbol{\theta}) = -\log P(y|\mathrm{x}) = -\log \sigma((2y - 1)z) = \zeta((1 - 2y)z)$

Softmax unit

- Similar to sigmoid. Mostly suited for multinoulli distribution
- We need to predict a vector $\hat{\mathrm{y}}$ such that $\hat{y}_i = P(Y = i|\mathrm{x})$
- A linear layer predicts unnormalized probabilities $\mathrm{z} = \mathrm{W}^T\mathrm{h} + \mathrm{b}$ that is $z_i = \log \tilde{P}(y = i|\mathrm{x})$
- Formally, $\mathrm{softmax}(\mathrm{z})_i = \dfrac{\exp z_i}{\sum_j \exp(z_j)}$
- Log in log-likelihood can undo exp $\log\ \mathrm{softmax}(\mathrm{z})_i = z_i - \log \sum_j \exp(z_j)$
  - Does it saturate?
  - What about incorrect prediction?
- Invariant to addition of some scalar to all input variables ie. $\mathrm{softmax}(\mathrm{z}) = \mathrm{softmax}(\mathrm{z} + \mathrm{c})$

Hidden units

- Active area of research and does not have good guiding theoretical principle
- Usually rectified linear unit (ReLU) is chosen in most of the cases
- Design process consists of trial and error, then the suitable one is chosen
- Some of the activation functions are not differentiable (eg. ReLU)
  - Still gradient descent performs well
  - Neural network does not converge to local minima but reduces the value of cost function to a very small value

Generalization of ReLU

- ReLU is defined as $g(z) = \max\{0, z\}$
- Using non-zero slope, $h_i = g(\mathbf{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$
  - Absolute value rectification will make $\alpha_i = -1$ and $g(z) = |z|$
- Leaky ReLU assumes very small values for α_i
- Parametric ReLU tries to learn α_i parameters
- Maxout unit $g(\mathbf{z})_i = \max_{j \in \mathbb{G}^{(i)}} z_j$
  - Suitable for learning piecewise linear function

Logistic sigmoid & hyperbolic tangent

- Logistic sigmoid $g(z) = \sigma(z)$
- Hyperbolic tangent $g(z) = tanh(z)$
  - $tanh(z) = 2\sigma(2z) - 1$
- Widespread saturation of sigmoidal unit is an issue for gradient based learning
  - Usually discouraged to use as hidden units
- Usually, hyperbolic tangent function performs better where sigmoidal function must be used
  - Behaves linearly at 0
  - Sigmoidal activation function are more common in settings other than feedforward network

Other hidden units

- Differentiable functions are usually preferred
- Activation function $h = \cos(\mathsf{Wx} + \mathsf{b})$ performs well for MNIST data set
- Sometimes no activation function helps in reducing the number of parameters
- Radial Basis Function - $\phi(\mathsf{x}, \mathsf{c}) = \phi(\|\mathsf{x} - \mathsf{c}\|)$
  - Gaussian - $\exp(-(\varepsilon r)^2)$
- Softplus - $g(x) = \zeta(x) = \log(1 + exp(x))$
- Hard tanh - $g(x) = \max(-1, \min(1, x))$
- Hidden unit design is an active area of research

Architecture design

- Structure of neural network (chain based architecture)
  - Number of layers
  - Number of units in each layer
  - Connectivity of those units
- Single hidden layer is sufficient to fit the training data
- Often deeper networks are preferred
  - Fewer number of units
  - Fewer number of parameters
  - Difficult to optimize