

Deep Feedforward Network

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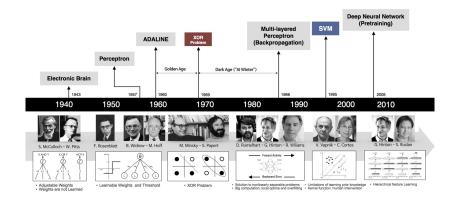
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A bit about Jie...

- Jie Tang, Full Professor, Associate Chair of Dept. of Computer Science of Tsinghua University. Interests include social network, data mining, machine learning, knowledge graph
- I have been visiting scholar at Cornell U. (working with John Hopcroft, Jon Kleinberg), UIUC (working with Jiawei Han), CUHK (with Jeffrey Yu), and HKUST (with Qiong Luo)
- I was awarded with the NSFC for Distinguished Young Scholars, NSFC for Excellent Young Scholars, CCF Young Scientist Award, Newton Advanced Fellowships Award, IBM Innovation Faculty Award, and New Star of Beijing S&T
- Have published more than 300+ paper on international conf/journals, including KDD (20+), IJCAI/AAAI (20+), NIPS/ICML, ACM/IEEE Trans. (27)
- #Citation: 13,503 and h-index: 59
- Have a notable system, AMiner.org for academic researcher network analysis. The system has attracted 10 million users from 220 countries/regions
- Homepage: http://keg.cs.tsinghua.edu.cn/jietang/

Overview

- 1 What is Deep Feedforward Network?
- IntroductionExample: Learning XOR
- 3 Backpropagation Algorithm
- 4 Activation Functions
- 5 Advanced Architecture
- 6 Summary



Deep Feedforward Networks

- A deep feedforward network (DFN), also referred to as Multi-layer Perceptron and Feedforward Neural Network, is an artificial neural network wherein connections between the units do not form a cycle. It is the first and also the simplest type of ANN.
- When extended to include feedback connections, they are called Recurrent Neural Networks (RNN).

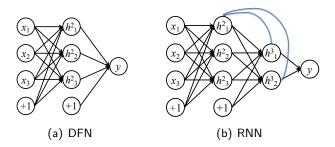
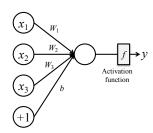


Figure 1: Deep Forward Network (DFN) v.s. Recurrent Neural Network (RNN).

Perceptron

- in 1957, perceptron was first invented at the Cornell Aeronautical Laboratory by Frank Rosenblatt.
- in 1940s, a similar neuron was actually described by McCulloch and Pitts;
- in 1958, Rosenblatt made statements that Perceptron will grow up to be a computer that is "able to walk, talk, see, write, reproduce itself and be conscious of its existence.";
- in 1960s, people recognized that multilayer perceptron had far greater processing power than perceptrons with one layer (Minsky and Papert; Grossberg);
- in 1964, kernel perceptron (Aizerman);
- in 1998, Margin bounds guarantees were given in the general non-separable case first by Freund and Schapire;
- in 1999, voted percepton giving comparable generalization bounds to the kernel SVM.



Single-layer Perceptron

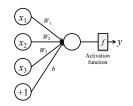
$$y = f(W^T x) = f(\sum_{i=1}^{3} W_i x_i + 1 \times b)$$

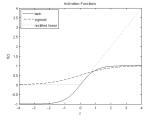
where f is the activation function:

- sigmoid function $f(z) = \frac{1}{1 + \exp(-z)}$
- hyperbolic tangent $tanh(z) = \frac{e^z e^{-z}}{e^z + e^{-z}}$
- rectified linear function f(z) = max(0, x)

remember, it is useful

- sigmoid function f'(z) = f(z)(1 f(z))
- hyperbolic tangent $f'(z) = 1 (f(z))^2$
- rectified linear function f'(z) = 0, if $z \le 0$; and 1 otherwise



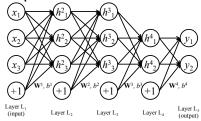


Softmax Units for Multinomial Output Distributions

A softmax output unit is defined by:

- $softmax(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$
- Softmax units naturally represent a probability distribution over a discrete variable with k possible values.
- A linear layer predicts unnormalized log probabilities $z = W^{\mathsf{T}} h + b$. where $z_i = \log \tilde{P}(y = i|x)$
- This can be seen as a generalization of the sigmoid function which was used to represent a probability distribution over a binary variable.
- Softmax functions are most often used as the output of a classifier.
- The log in the log-likelihood can undo the exp of the softmax: $\log softmax(z)_i = z_i \log \sum_j \exp(z_j)$.

Deep Feedforward Networks

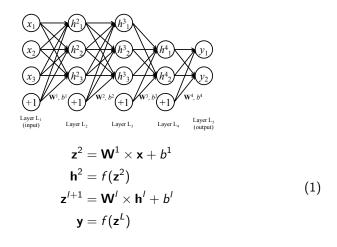


- bias units $\{+1\}$, input layer $\{x_i\}$, hidden layer(s) h_i^I , output layer y_i ;
- Goal: approximate some map function f^*
 - e.g., a classifier $y = f^*(x)$ to map an input x onto a category y
 - Feedforward Network defines a mapping

$$y = f^*(x; \theta)$$

– and learns parameters $\theta = (\mathbf{W}^I, \mathbf{b}^I)$ that result in the best approximation.

Deep Feedforward Networks

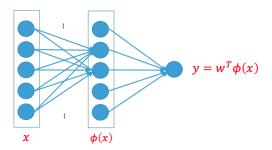


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Extending Linear Models

• Linear functions $\phi(x) = W^T x$ do not work in some cases: need some nonlinearity $\phi(x)$.



Extending Linear Models

- To represent non-linear functions of x, by transforming x using a non-linear function $\phi(x)$
 - Similar "kernel" trick obtains a nonlinearity
 - SVM: $f(x) = w^T x + b \rightarrow f(x) = b + \sum_i \alpha_i \phi(x) \phi(x^i)$
 - where $\phi(x)\phi(x^i) = K(x, x^i)$

Then how to **choose** the mapping ϕ .

- Use a very **generic** ϕ , such as infinite-dimensional ϕ , but the generalization is poor.
- Manually engineer ϕ , but with little transfer between domains.
- The strategy of deep learning is to learn ϕ . We parametrize the **representation** as $\phi(x;\theta)$ and use the optimization algorithm to find the θ .
 - capture the benefit of the first approach by being highly generic by using a very broad family $\phi(x; \theta)$.
 - the human designer only needs to find the right general function family rather than precisely the right function.

Example: Learning XOR

- We will not be concerned with statistical generalization.
 - Perform correctly on the four points

•
$$X = \{[0,0]^T, [0,1]^T, [1,0]^T, [1,1]^T\}$$

- The only challenge is to fit the training set.
- The XOR function provides the target function $y = f^*(x)$ that we want to learn. Our model provides a function $y = f(x; \theta)$ and our learning algorithm will adapt the parameters θ to make f as similar as possible to f^* .

Linear model doesn't fit

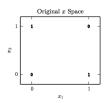
- Treat this problem as a regression problem and use a mean squared error
 - The MSE loss function is

$$J(\theta) = \frac{1}{4} \sum_{x \in \mathbb{X}} (f^*(x) - f(x; \theta))^2$$

- Usually not used for binary data, but math is simple.
- We now choose the form of model, consider a linear model.
 - $f(x; \mathbf{w}, b) = x^T \mathbf{w} + b$
 - Minimizing the $J(\theta)$, we obtain $\mathbf{w} = 0$ and $b = \frac{1}{2}$
 - Then the linear model simply outputs $\frac{1}{2}$ everywhere.

Linear model doesn't fit

- Solving the XOR problem by learning a representation.
 - When $x_1 = 0$, output has to increase with x_2
 - When x₁ = 1, output has to decrease with x₂
 - Linear model $f(x, w, b) = x_1w_1 + x_2w_2 + b$ has to assign a single weight to x_2 so it **cannot** solve the problem.
- A better solution.
 - We user a simple feedforward network.
 - one hidden layer containing two hidden units
 - the nonlinear features have mapped both $x = [1, 0]^T$ and $x = [0, 1]^T$ to a single point in feature space, $h = [1, 0]^T$.
 - A linear model can now solve the problem.



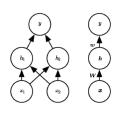


Feedforward Network for XOR

Layer 1 (hidden layer):

$$h_i = f(\mathbf{x}^{\mathsf{T}} \mathbf{W}_{:,i} + c_i)$$

- c are bias variables.
- g is typically chosen to be an element-wise activation function.
- the default activation function is the rectified linear unit or ReLU defined by g(z) = max{0, z}



The complete network:

$$f(\mathbf{x}; \mathbf{W}, \mathbf{c}, \mathbf{w}, b) = \mathbf{w}^T f(\mathbf{W}^T \mathbf{x} + \mathbf{c}) + b$$

Feedforward Network for XOR

• Let
$$\mathbf{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$
, $\mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$, $\mathbf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$, and $b = 0$. We get correct answers on all points.

- Now walk through how models processes.
 - Design matrix X of all four points.
 - XW.
 - Adding c.
 - Applying ReLU.
 - Multipying by w.

$$\mathbf{X} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}, \\ \mathbf{XW} = \begin{bmatrix} 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 2 & 2 \end{bmatrix}, \\ \mathbf{XW+c} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}, \\ \mathbf{g}(\mathbf{XW+c}) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}, \\ \mathbf{w}g(\mathbf{XW+c}) + b = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

Feedforward Network for XOR

- We simply specified the solution by defining
 - It achieves zero error.

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

- In real situations there might be billions of parameters and billions of training examples.
 - So one cannot simply guess the solution.
- Instead gradient descent optimization can find parameters that produce very little error.

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Loss Function

• Support we are given a set of **training data** $\{(x^1, y^1), \dots, (x^n, y^n)\}$ of n training examples. To learning our **parameters** $\theta = (\mathbf{W}, \mathbf{b})$, we can define the following **loss function**:

$$\mathcal{J}(W, b; x, y) = \frac{1}{2} ||\hat{y} - y||^2$$

where \hat{y} is the value predicted by the learned neural network.

To avoid overfitting, we could add a regularization term

$$\mathcal{J}(W,b) = \frac{1}{n} \left[\sum_{i=1}^{n} \frac{1}{2} ||\hat{y} - y||^{2} \right] + \frac{\lambda}{2} \sum_{l=1}^{L} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{l=1}} (W_{ji}^{l})^{2}$$

* please note that we do not regularize *b*, as it makes little difference.

Model Learning

- Our goal is to minimize $\mathcal{J}(W, b)$ as a function of W and b.
- We first initialize each parameter $W_{ij}^{(I)}$ and each $b_i^{(I)}$ to a small random value near zero (say according to a Normal $(0, \epsilon^2)$ distribution for some small ϵ).
 - all-zero initialization will be very bad;
 - W'_{ij} will be the same for all h and z, $h_1^{l+1} = h_2^{l+1} = \cdots$ for any input.
- We then apply an optimization algorithm such as batch gradient descent.
- Since $\mathcal{J}(W,b)$ is a non-convex function, gradient descent is susceptible to local optima; however, in practice gradient descent usually works fairly well.

Backpropagation

• One iteration of gradient descent updates the parameters W, b as follows:

$$W_{ij}^{(I)} = W_{ij}^{(I)} - \alpha \frac{\partial}{\partial W_{ij}^{(I)}} J(W, b)$$
 (2)

$$b_i^{(I)} = b_i^{(I)} - \alpha \frac{\partial}{\partial b_i^{(I)}} J(W, b)$$
 (3)

- ullet where lpha is the learning rate.
- The key step is computing the partial derivatives above.
- We next describe the backpropagation algorithm, which gives an efficient way to compute these partial derivatives.

Backpropagation

Forward propagation

The inputs x provide the initial information that then propagates up to the hidden units at each layer and finally produces \hat{y} .

Backward propagation

simply called **backprop**, allows the information from the cost to then flow backwards through the network, in order to compute the gradient.

Training

• One iteration of gradient descent updates the parameters W,b as follows:

$$W_{ij}^{(I)} = W_{ij}^{(I)} - \alpha \frac{\partial}{\partial W_{ii}^{(I)}} \mathcal{J}(W, b)$$
 (4)

$$b_i^{(I)} = b_i^{(I)} - \alpha \frac{\partial}{\partial b_i^{(I)}} \mathcal{J}(W, b)$$
 (5)

 \bullet where α is the learning rate.

$$\frac{\partial}{\partial W_{ij}^{(l)}} \mathcal{J}(W, b) = \left[\frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial W_{ij}^{l}} \mathcal{J}(W, b; x, y) \right] + \lambda W_{ij}^{l}
\frac{\partial}{\partial b_{i}^{(l)}} \mathcal{J}(W, b) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial b_{i}^{l}} \mathcal{J}(W, b; x, y)$$
(6)

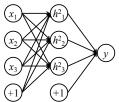
• Now, our problem becomes how to compute $\frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial W_{ii}^{l}} \mathcal{J}(W, b; x, y)$ with backpropagation.

Backpropagation: Intuition

- Given a training example (x, y), we will first run a "forward pass" to compute all the activations throughout the network, including the output value of the hypothesis \hat{y} .
- Then, for each node i in layer I, we would like to compute an "error term" $\delta_i^{(I)}$ that measures how much that node was "responsible" for any errors in our output.
- For an output node, we can directly measure the difference between the network's activation and the true target value, and use that to define $\delta_i^{(L)}$.
- For hidden units, we will compute $\delta_i^{(l)}$ based on a weighted average of the error terms of the nodes that uses $z_i^{(l)}$ as an input.

Backpropagation: forward

• Given a training example (x, y), we will first run a "forward pass" to compute all the activations throughout the network, including the output value of the hypothesis \hat{y} .



$$z_1^{(2)} = f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)})$$
 (7)

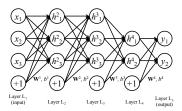
$$z_2^{(2)} = f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)})$$
 (8)

$$z_3^{(2)} = f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)})$$
 (9)

$$\hat{y} = z_1^{(3)} = f(W_{11}^{(2)}z_1^{(2)} + W_{12}^{(2)}z_2^{(2)} + W_{13}^{(2)}z_3^{(2)} + b^{(2)})(10)$$

Backpropagation: error in the output layer

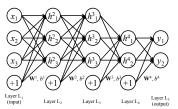
- Then, for each node i in layer l, we would like to compute an "error term" $\delta_i^{(l)}$ that measures how much that node was "responsible" for any errors in our output.
- For an output node, we can directly measure the difference between the network's activation and the true target value, and use that to define $\delta_i^{(L)}$.



$$\delta_i^L = \frac{\partial}{\partial z_i^L} \frac{1}{2} \|y - \hat{y}\|^2 = -(y_i - f(z_i^L)) \cdot f'(z_i^L) \tag{11}$$

Backpropagation: error backpropagation

- For an output node, we can directly measure the difference between the network's activation and the true target value, and use that to define $\delta_i^{(L)}$.
- For hidden units, we will compute $\delta_i^{(l)}$ based on a weighted average of the error terms of the nodes that uses $z_i^{(l)}$ as an input.

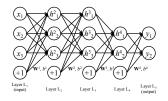


For $l = L - 1, L - 2, \dots, 2$ and each node i in layer l, set

$$\delta_i^{(l)} = (\sum_{i=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)}) f'(z_i^{(l)})$$
 (12)

Backpropagation: error backpropagation (2)

• For hidden units, we will compute $\delta_i^{(I)}$ based on a weighted average of the error terms of the nodes that uses $z_i^{(I)}$ as an input.



For $l = L - 1, L - 2, \dots, 2$ and each node i in layer l, set

$$\delta_i^{(l)} = (\sum_{i=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)}) f'(z_i^{(l)})$$

Recall **chain rule**: if y = g(x) and z = f(y), then

$$\frac{\partial z}{\partial x_i} = \sum_{j} \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

Backpropagation: derivations

Compute the desired partial derivatives, which are given as:

$$\frac{\partial}{\partial W_{ij}^{(l)}}J(W,b;x,y) = z_j^{(l)}\delta_i^{(l+1)}$$
 (13)

$$\frac{\partial}{\partial b_i^{(l)}} J(W, b; x, y) = \delta_i^{(l+1)}$$
 (14)

• Plug it back into:

$$\frac{\partial}{\partial W_{ij}^{(I)}} \mathcal{J}(W, b) = \left[\frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial W_{ij}^{I}} \mathcal{J}(W, b; x, y) \right] + \lambda W_{ij}^{I}$$

$$\frac{\partial}{\partial b_{i}^{(I)}} \mathcal{J}(W, b) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial b_{i}^{I}} \mathcal{J}(W, b; x, y)$$
(15)

Backpropagation: summary (pseudo-code)

- repeat
 - $\Delta \mathbf{W}^{I} := 0$, $\Delta \mathbf{b}^{I} := 0$ for all I;
 - for i = 1 to n,
 - perform forward propagation;
 - use backpropagation to computer errors at each layer;
 - compute partial derivatives $\nabla_{\mathbf{W}^l} \mathcal{J}(W,b;x,y)$ and $\nabla_{\mathbf{b}^l} \mathcal{J}(W,b;x,y)$
 - update the parameters

$$\mathbf{W}' = \mathbf{W}' - \alpha \left[\left(\frac{1}{n} \Delta \mathbf{W}' \right) + \lambda \mathbf{W}' \right]$$
$$\mathbf{b}' = \mathbf{b}' - \alpha \left[\left(\frac{1}{n} \Delta \mathbf{b}' \right) \right]$$

until convergence.

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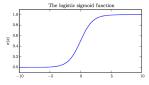
Activation functions

The design of activation functions for hidden units is an extremely active area of research.

- Logistic Sigmoid
- Hyperbolic Tangent
- Rectified Linear Units
- Generalized Rectified Linear Units
- Maxout Units

Logistic Sigmoid

- $g(z) = \sigma(z)$. It's also used in output units.
- Logistic sigmoid activation function, sigmoidal units saturate across most of their domain and can make gradient-based

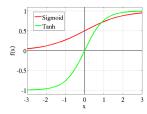


learning very difficult.

 Recurrent networks, many probabilistic models, and some autoencoders have additional requirements that rule out the use of piecewise linear activation functions and make sigmoidal units more appealing despite the drawbacks of saturation.

Hyperbolic Tangent

- $g(z) = tanh(z) = 2\sigma(2z)-1$.
- The hyperbolic tangent activation function typically performs

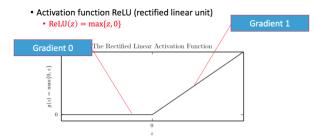


better than the logistic sigmoid.

• Because tanh is similar to the identity function near 0, $\hat{y} = w^T \tanh(U^T \tanh(V^T x))$ resembles training a linear model $\hat{y} = w^T U^T V^T x$ so long as the activations of the network can be kept small. This makes training the tanh network easier.

Rectified Linear Units

Rectified linear units are an excellent default choice of hidden unit (Nair&Hinton, 2010).



- The second derivative of the rectifying is 0 almost everywhere and the derivative is 1.
- So the gradient direction is far more useful for learning than it would be with activation functions that introduce second-order effects. Rectified linear units and its generalizations are based on the principle that models are easier to optimize if their behavior is closer to linear.

Generalized Rectified Linear Units

 One drawback to RLU is that they cannot learn via gradient-based methods on examples for which their activation is zero.

```
• Generalizations of ReLU gReLU(z) = \max\{z,0\} + \alpha \min\{z,0\}

• Leaky-ReLU(z) = \max\{z,0\} + 0.01 \min\{z,0\}

• Parametric-ReLU(z): \alpha learnable gReLU(z)
```

 It is used for object recognition from images, where it makes sense to seek features that are invariant under a polarity reversal of the input illumination.

Maxout Units

• Maxout units generalizes rectified linear units further. Instead of applying an element-wise function g(z), maxout units divide z into groups of k values. One of these groups:

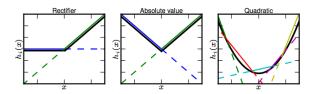
$$g(z)_i = \max_{j \in G^{(i)}} z_j \tag{16}$$

where $G^{(i)}$ is the set of indices into the inputs for group i, $\{(i-1)k+1,...,ik\}$.

 A maxout unit can learn a piecewise linear, convex function with up to k pieces. Maxout units can thus be seen as learning the activation function itself rather than just the relationship between units.

Maxout Units

- In a convolutional network, a maxout feature map can be constructed by taking the maximum across k affine feature maps (i.e., pool across channels).
- A single maxout unit can approximate arbitrary convex functions. The figure shows how maxout behaves with a 1D

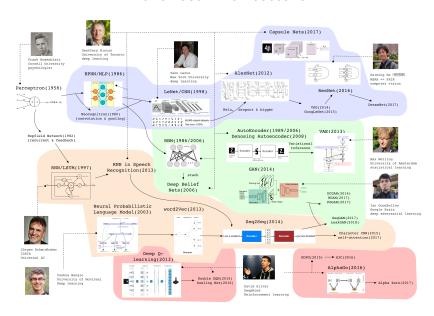


input.

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Advanced Architecture



Residual Neural Networks

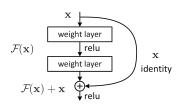


Figure 2: A Residual block in ResNet.

- Residual Neural Networks (He et al. 2015) sums up low level hidden representation and high level hidden representation in a neural network.
- The high level representation tries to learn the residual between the low level representations and the targeted labeling manifold.

Residual Neural Networks

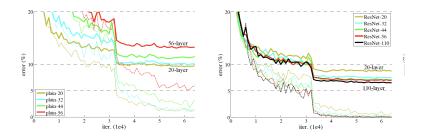
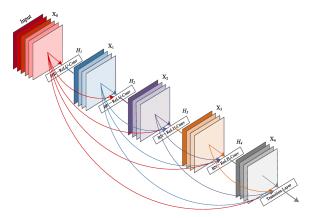


Figure 3: Error rate for plain CNN and Resnet.

- Residual Neural Networks performs slightly better than normal CNNs with the same depth.
- Residual Neural Network structure learns the residual while keeping lower level representations, thus more stable to be expanded very deeply.

Densely Connected Neural Networks



- Every layer is connected with all lower level layers, instead of only the previous one.
- It is also able to be expanded very deeply, since it also keeps the low level representations. (Huang et al. 2017)

Densely Connected Neural Networks

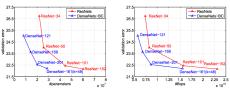


Figure 3. Comparison of the DenseNet and ResNet Top-1 (single model and single-crop) error rates on the ImageNet classification dataset as a function of learned parameters (left) and flops during test-time (right).

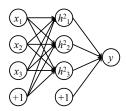
- DenseNet performs better than ResNet using same number of parameters/ same amount of flops.
- However, the densely connected property leads to less parallel computational efficiency. A Tradeoff!
- Both the ResNet and DenseNet authors graduate from Tsinghua!

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- 5 Advanced Architecture
- 6 Summary

Summary

- Our first deep neural network—deep forward network.
- Model learning with forward and backpropagation algorithm.
- We also discuss the most popular non-linear activation functions used in hidden units.
- Finally, we discuss two most commonly-used neural network architectures.



Thanks.

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