Training Neural Networks

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Deep Learning
Course Structure
8. Natural Language
Processing Applications
7. Recurrent
Neural Networks
9. Unsupervised
Learning
6. Computer Vision
Applications
2. Neural
Networks
3. Optimizing
5. Convolutional
Neural Networks
4. Debugging
N
1. Introduction

Bibliography

Textbooks:

- Deisenroth, Mathematics for Machine Learning, [Ch. 5 - Vector Calculus]
- Goodfellow, Deep Learning
- Prince, Understanding Deep Learning

Courses:

- Stanford, CS231n
- NYU Deep Learning

Recap++

Goals

1. Optimize large, deep neural networks...

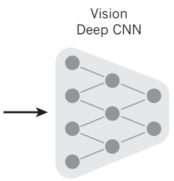
Goals

1. Optimize large, deep neural networks...
2. ...for learning *useful* representations.

Terminology

- **Supervised learning:** labeled data points of the correct behaviour.
- **Reinforcement learning:** receive some reward signal and try to maximize it by improving the model's behaviour
- **Unsupervised learning:** no labels - the aim is discovering interesing patterns in the data and usefull representations

Supervised Learning[1]: Caption generation[2]



A group of people shopping at an outdoor market.

There are many vegetables at the fruit stand.

A woman is throwing a **frisbee** in a park.

A **dog** is standing on a hardwood floor.

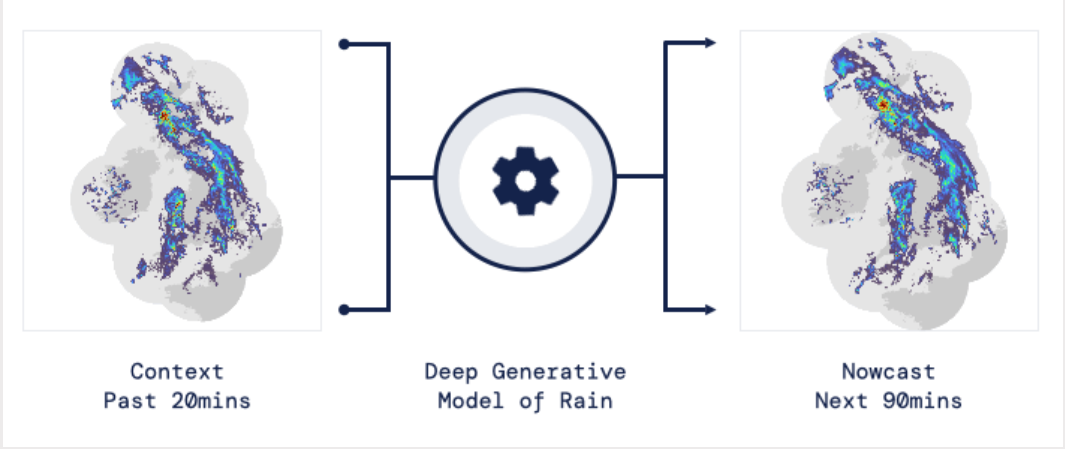
A **stop** sign is on a road with a mountain in the background

[1]from Grosse, Ba, 2019
[2]Xu et al., 2015

Unsupervised Learning[1]: Image compression[2]

[1]from CS294-158, 2019
[2]Rippel, Bourdev, 2017

Unsupervised Learning: Nowcasting the next hour of rain [1]



[1] DeepMind, 2022

Linear regression

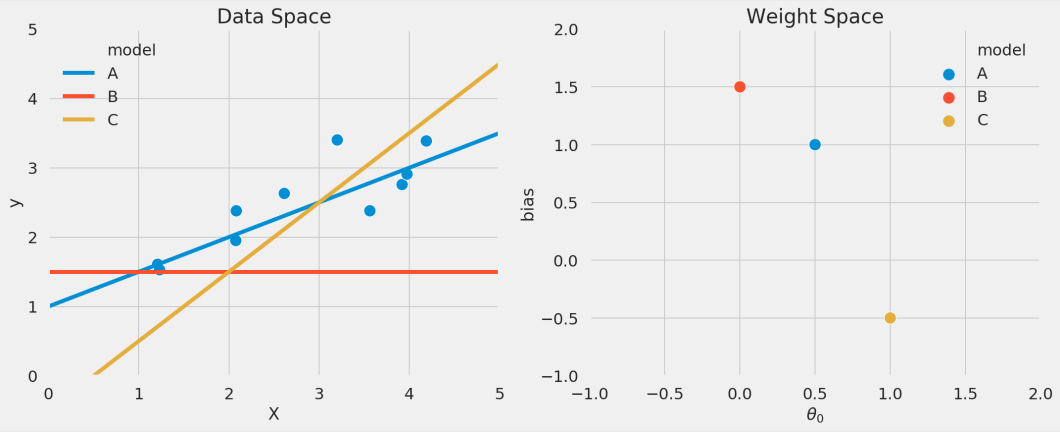


Figure: Three different linear models in the data and weight space [1].

$$y = \boldsymbol{\theta}^T \mathbf{x} + b$$

[1] following Grosse, Ba - CS421, 2019

Linear models

- Linear model $y = \boldsymbol{\theta}^T \boldsymbol{\phi}(\mathbf{x})$, with `Mean Squared Error` objective function $L(\boldsymbol{\theta}) = (t - y)^2$

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  - Perform gradient descent:

$$\boldsymbol{\theta}_{j+1} \leftarrow \boldsymbol{\theta}_j - \alpha\nabla_{\boldsymbol{\theta}_j} L$$

- Why do gradient descent if we can find the minimum analytically?

Linear models

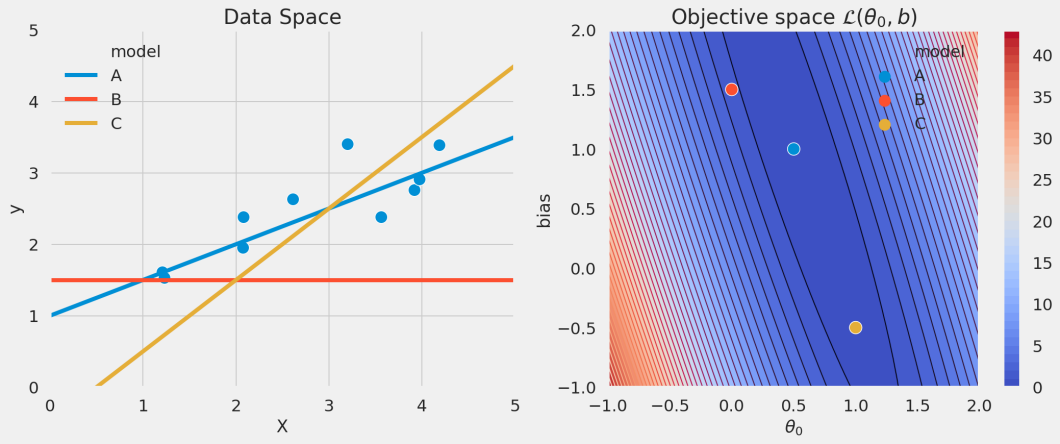


Figure: Three different linear models in the data and objective $L(\theta_0, b) = [t - f(x; \theta_0, b)]^2$ space.

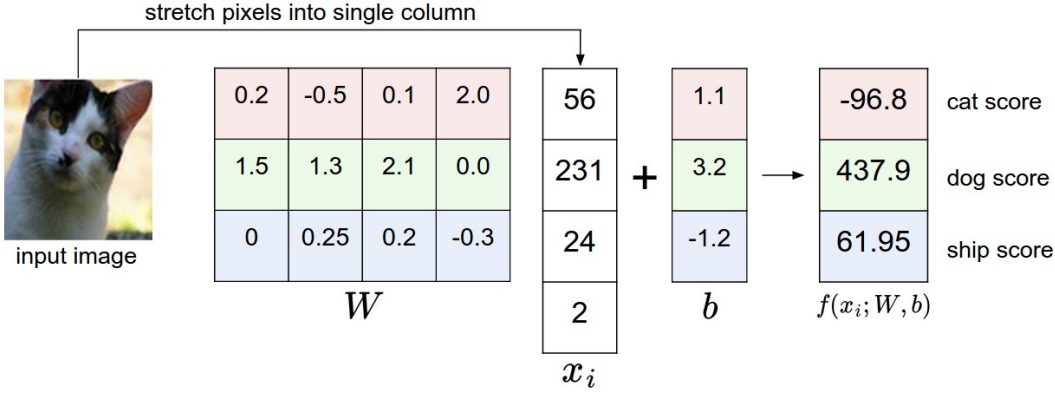
[1] following Grosse, Ba - CS421, 2019

Also discussed

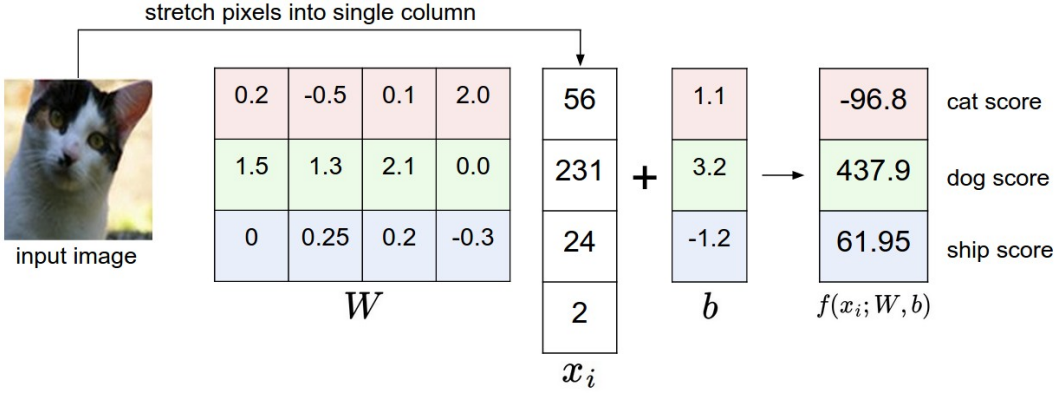
- Model complexity
- Regularization
- Bias / Variance trade-off
- Over-fitting / Under-fitting

Understanding Neural Networks

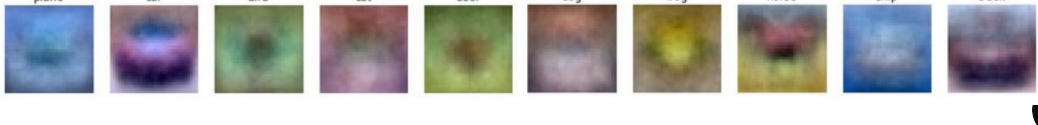
Linear classification



Linear classification



Learned weights:



A simple transformation

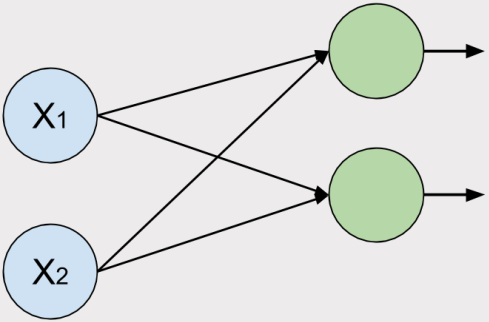
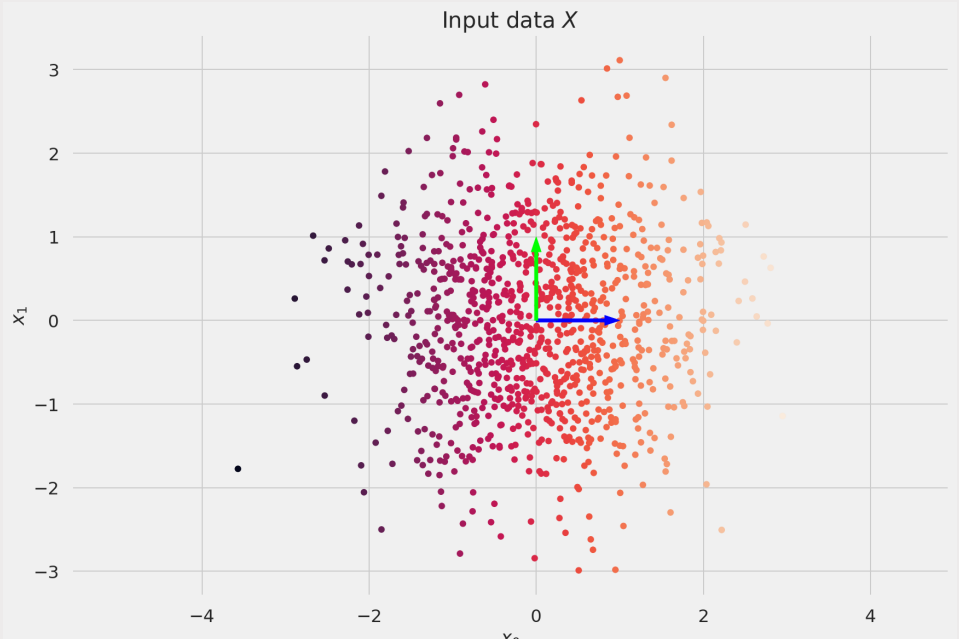


Figure: A linear model with four weights. Also can be seen as two stacked "neurons" without activation functions.

Linear case: **y** = **Wx**

A simple transformation



A simple transformation

- $\mathbf{y} = \mathbf{W}\mathbf{x}$
- What is $\mathbf{W}$ actually doing to $\mathbf{x}$?

[1] Mathematics for Machine Learning, ch. 4

A simple transformation

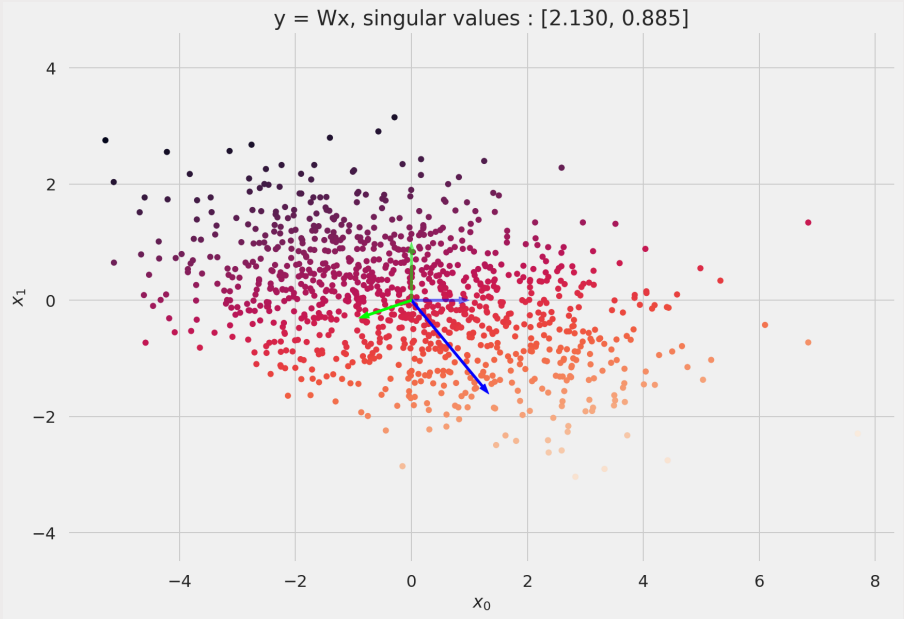
- $\mathbf{y} = \mathbf{W}\mathbf{x}$
- What is $\mathbf{W}$ actually doing to $\mathbf{x}$?
- Let's perform singular value decomposition[2] for some intuition:

$$\mathbf{W} = \mathbf{U} \times \mathbf{S} \times \mathbf{V}^T$$

$$\begin{bmatrix} 0.19 & 1.84 \\ -0.97 & -0.93 \end{bmatrix} = \underbrace{\begin{bmatrix} 0.83 & -0.55 \\ -0.55 & -0.83 \end{bmatrix}}_{\text{rotation}} \times \underbrace{\begin{bmatrix} 2.17 & 0.00 \\ 0.00 & 0.74 \end{bmatrix}}_{\text{scale}} \times \underbrace{\begin{bmatrix} 0.32 & 0.94 \\ 0.94 & -0.32 \end{bmatrix}}_{\text{reflection}}$$

[1] Mathematics for Machine Learning, ch. 4

A simple transformation



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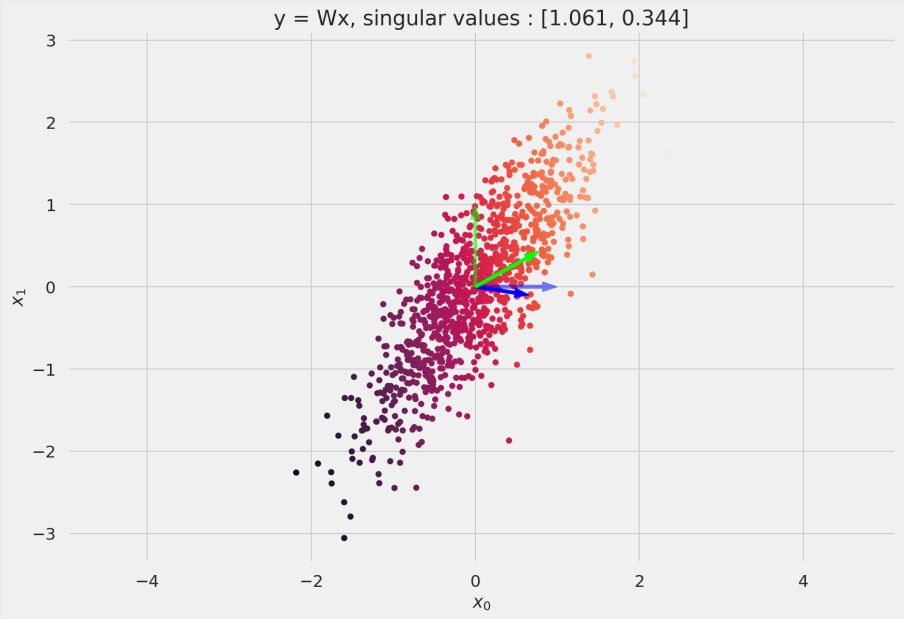


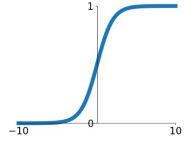
A simple transformation

We can **scale**, **rotate** and **reflect** data. Can we do more?

Non-linear functions[1]

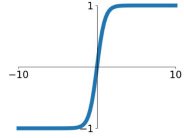
Sigmoid

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



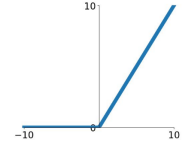
tanh

$\tanh(x)$



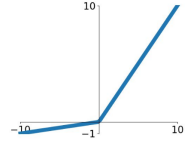
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

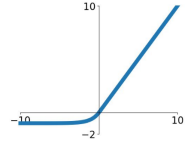


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



[1] from CS231n, lecture 4, 2019

Non-linear transformation

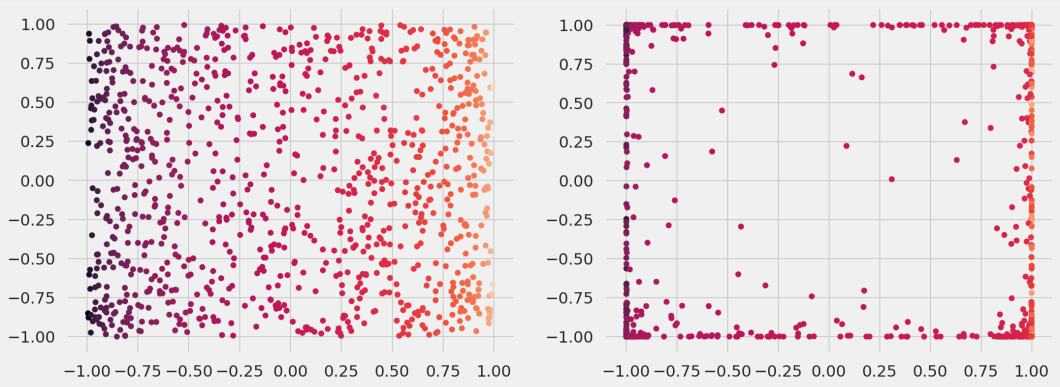


Figure: `tanh(Sx)` activation function with two different scale factors (left=1.0, right=5.0).

Non-linear transformation

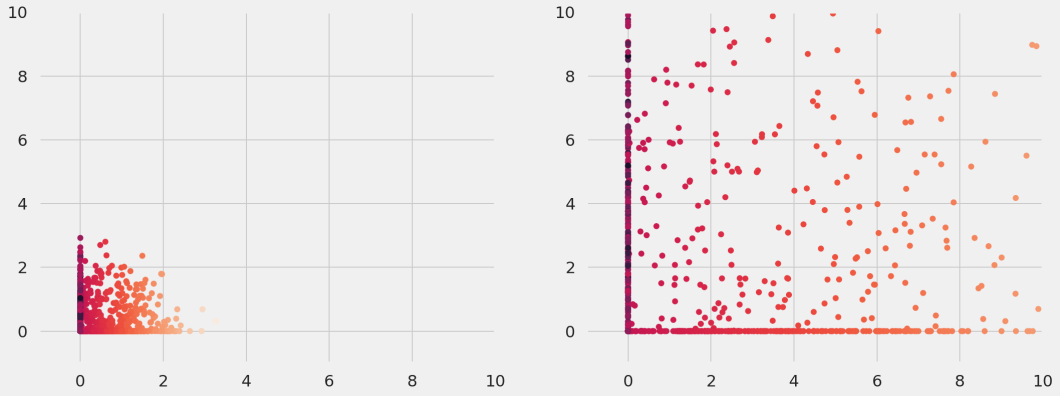


Figure: ReLU(**Sx**) activation function with two different scale factors (left=1.0, right=5.0).

A simple, non-linear function

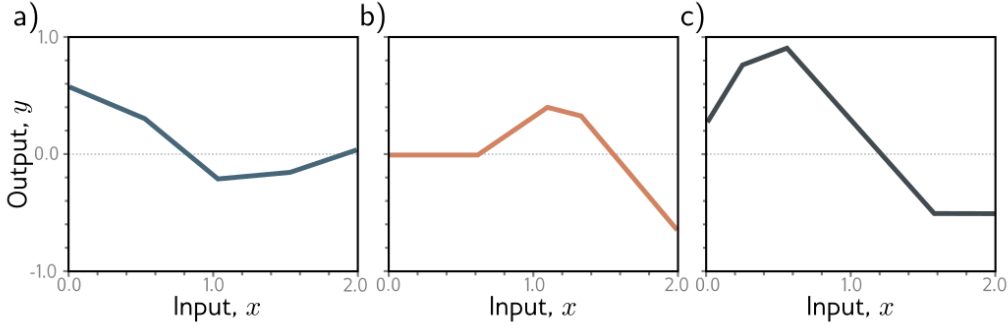


Figure: Functions defined by $y = \phi_0 + \phi_1 \sigma[\theta_{10} + \theta_{11}x] + [\theta_{20} + \theta_{21}x] + [\theta_{30} + \theta_{31}x]$

Neural Networks, finally

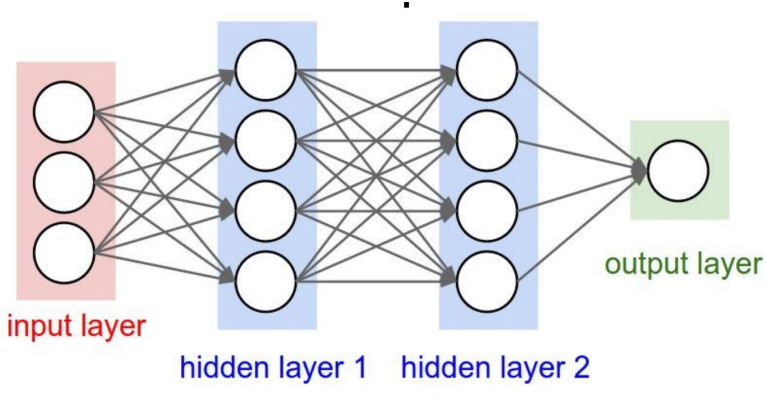


Figure: Typical "three-layer" or "two-hidden-layer" neural network

- Linear case: $f(\mathbf{x}) = \mathbf{W}\mathbf{x}$
- Neural Net: $f(\mathbf{x}) = \mathbf{W}_3\, \sigma(\mathbf{W}_2\, \sigma(\mathbf{W}_1 \mathbf{x}))$

NN transformation

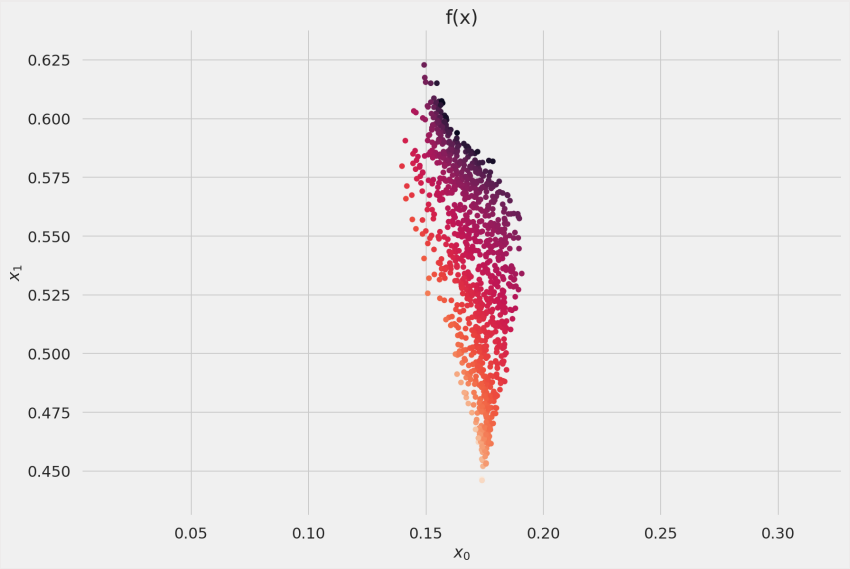


Figure: Transformation performed by a 5-layer **random** neural network

NN transformation

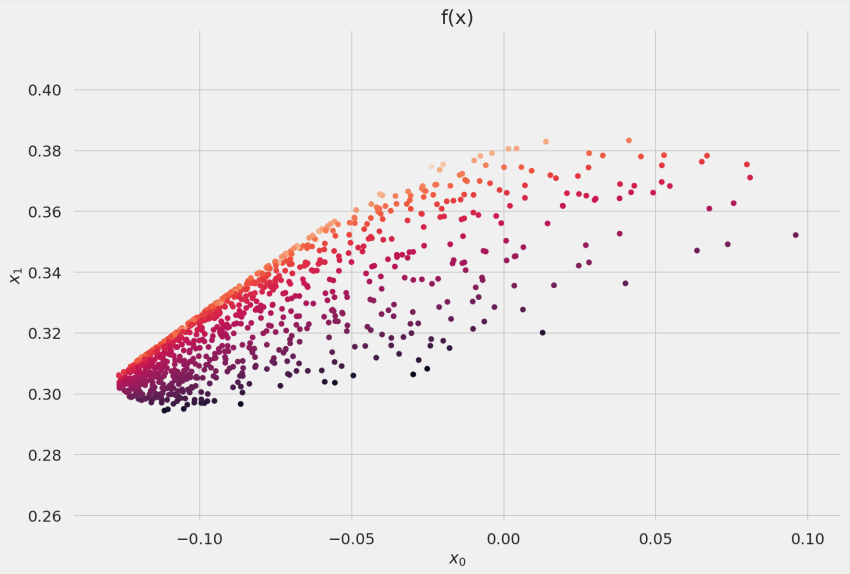


Figure: Transformation performed by a 5-layer **random** neural network

Warping space. Why is it useful

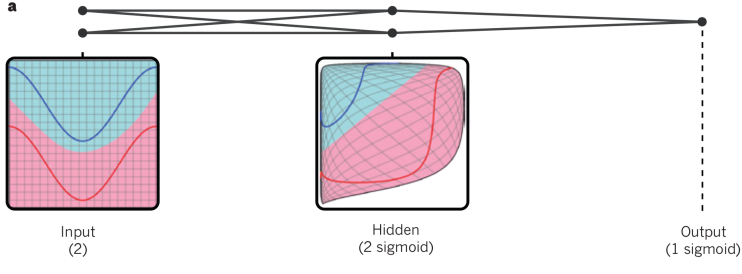
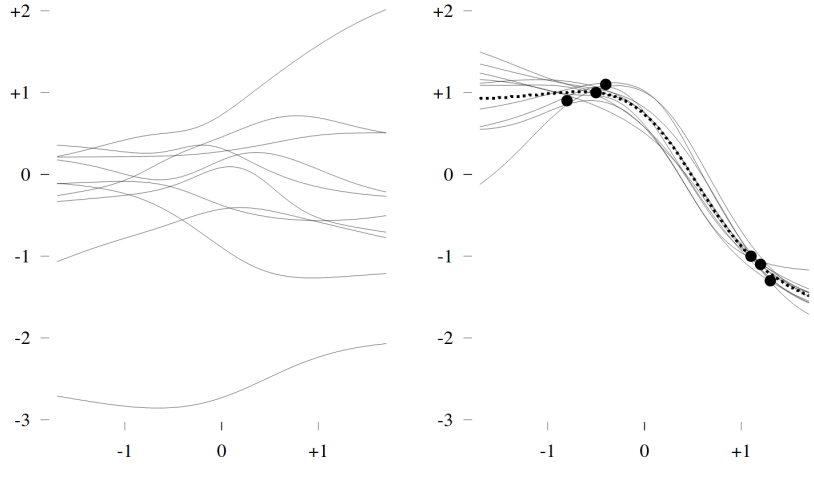


Figure: Space warping by a one hidden layer neural network for learning a linearized representation of the decision boundary[1].

[1] from LeCun 2015, Nature.

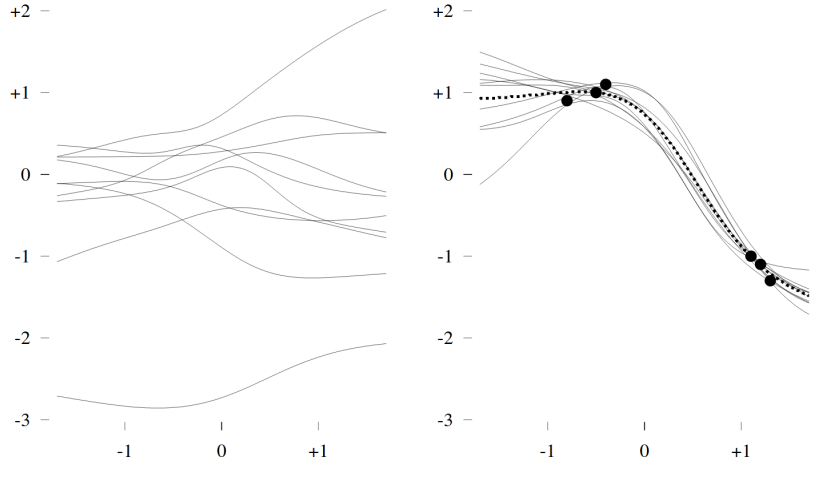
Optimizing Neural Networks

How to learn θ?



[1] Radford M. Neal, Bayesian Learning for Neural Networks

How to learn θ?



Sample 2.6 million networks and you're done!

[1] Radford M. Neal, Bayesian Learning for Neural Networks

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- Can we do better?

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- Find the weights using gradient descent.

How to learn θ?

- Can we do better?
- Use the lesson from the iterative linear regression
- Compute the gradient of $L(\Theta)$ w.r.t. Θ,
- Find the weights using gradient descent.
- It can get tedious and inflexible:
  - Additional cost functions, regularization loss, etc...
  - We would want to quickly experiment with different layers and activations.

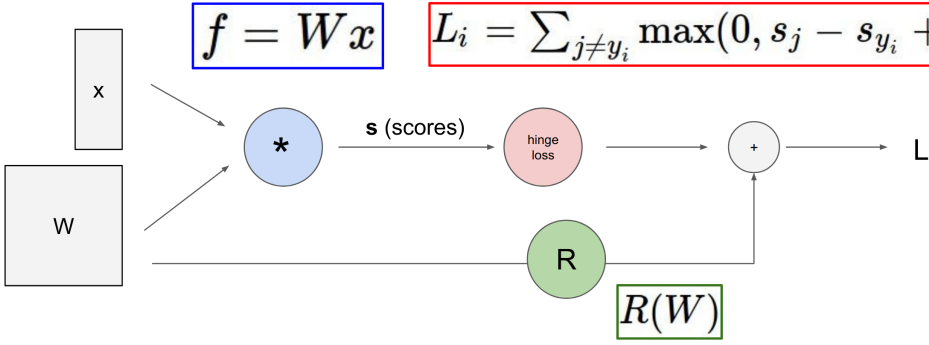
But it's not that complicated[1]

```python
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

[1] from CS231n, lecture 4, 2019

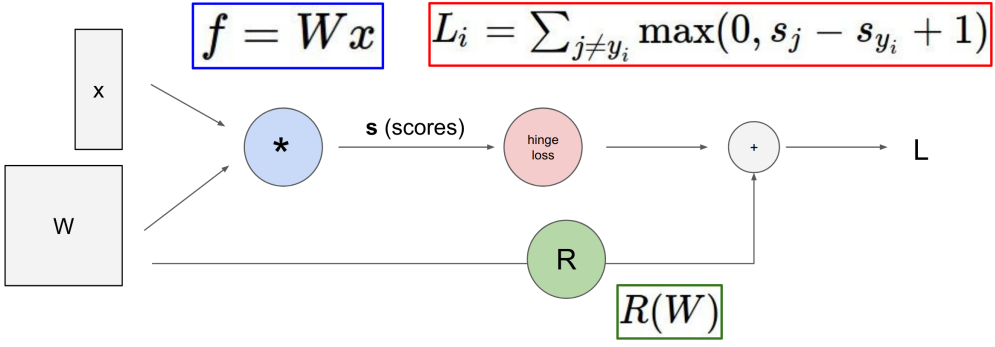
Computational Graphs

Computation graphs + automatic differentation



[1]Grosse, Ba, CS421

Computation graphs + automatic differentation



Automatic differentiation: takes a program which computes a value, and automatically constructs a procedure for computing derivatives of that value[1].

[1] Grosse, Ba, CS421

Simple example[1]

$$f(x, y, z) = (x + y)z$$

[1] from CS231n, lecture 4, 2019

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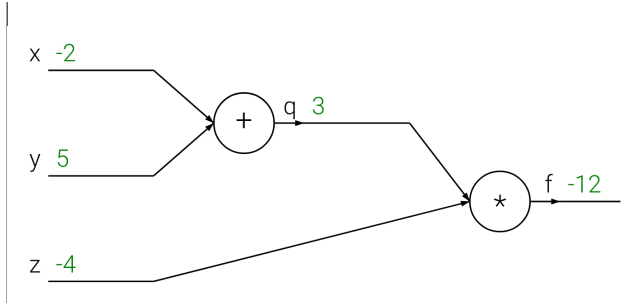

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Simple example[1]

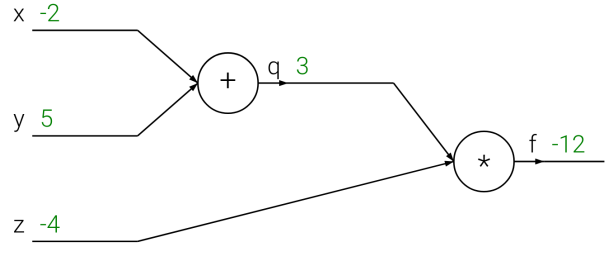
$$f(x, y, z) = (x + y)z$$

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

We want:

$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



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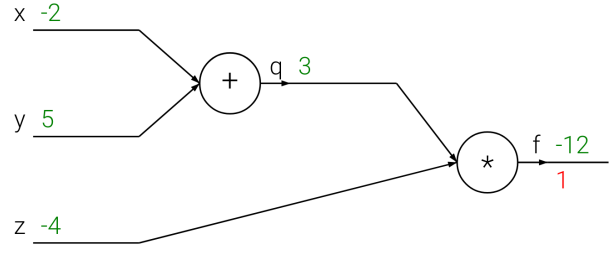

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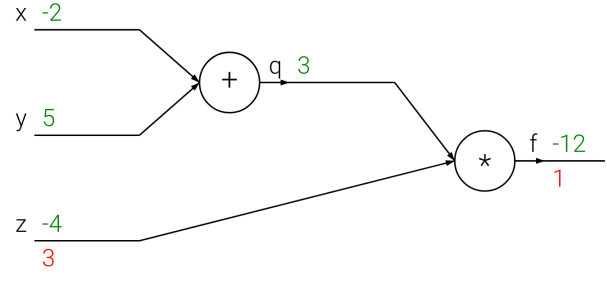

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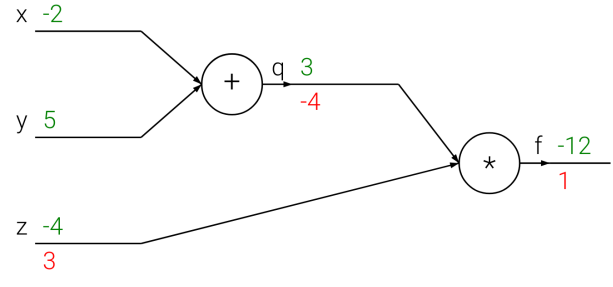

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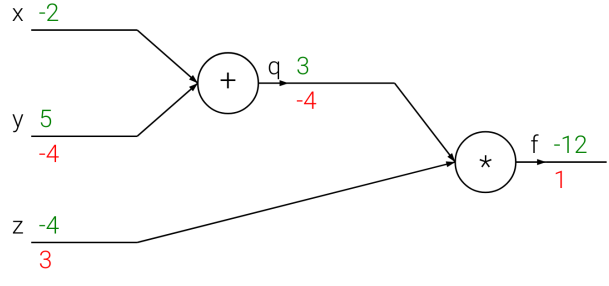
$$f(x, y, z) = (x + y)z$$

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

We want:

$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y}$$

[1] from CS231n, lecture 4, 2019

Simple example[1]

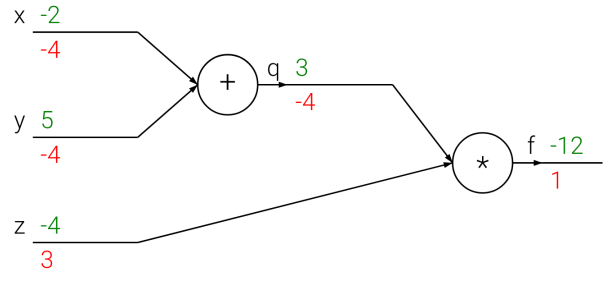
$$f(x, y, z) = (x + y)z$$

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

We want:

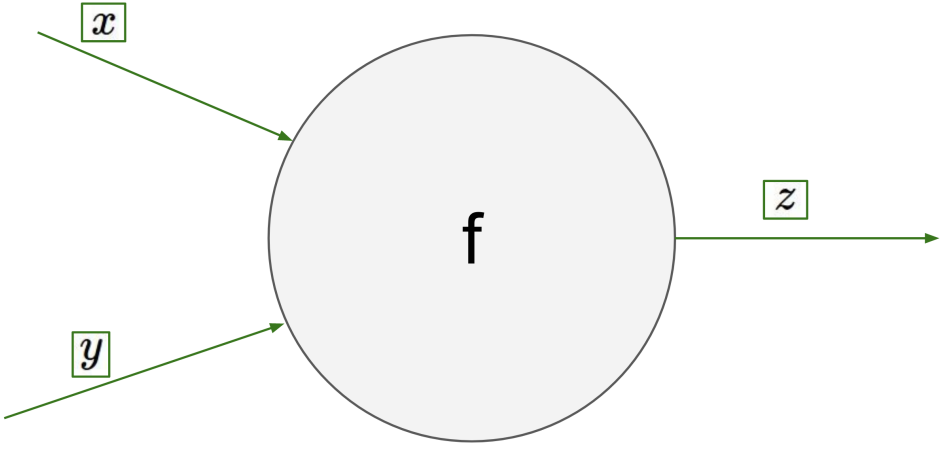
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}$$

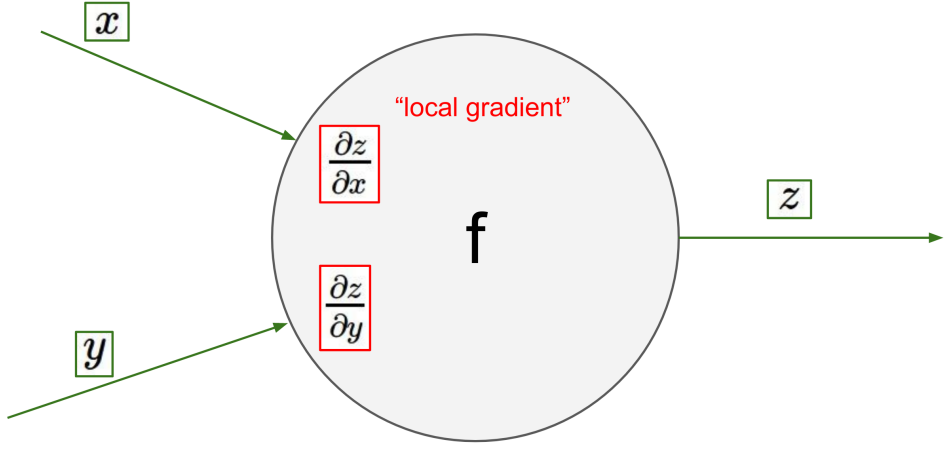
[1] from CS231n, lecture 4, 2019

Backprop[1]



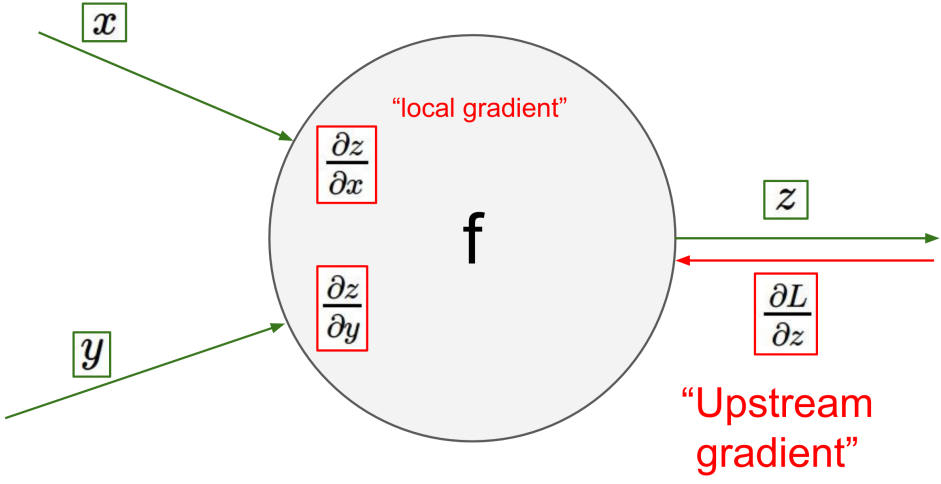
[1] from CS231n, lecture 4, 2019

Backprop[1]



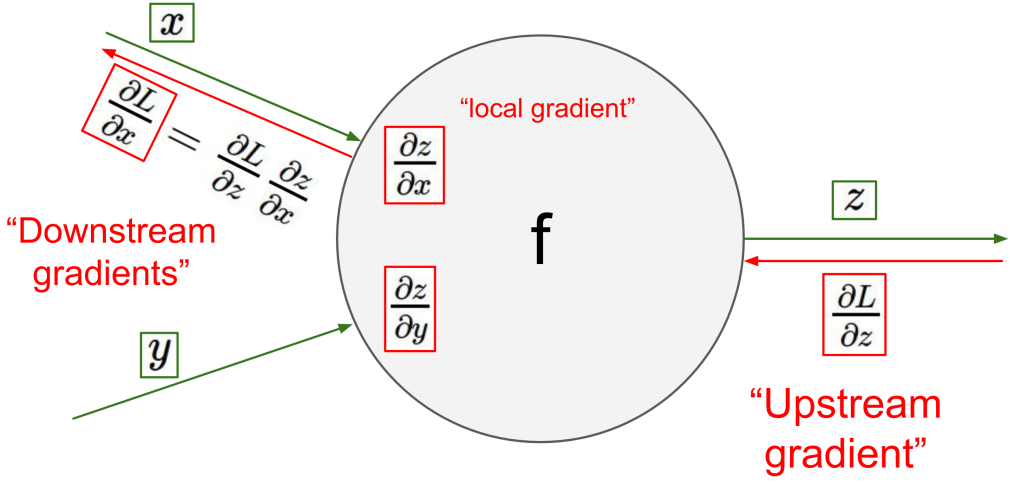
[1] from CS231n, lecture 4, 2019

Backprop[1]



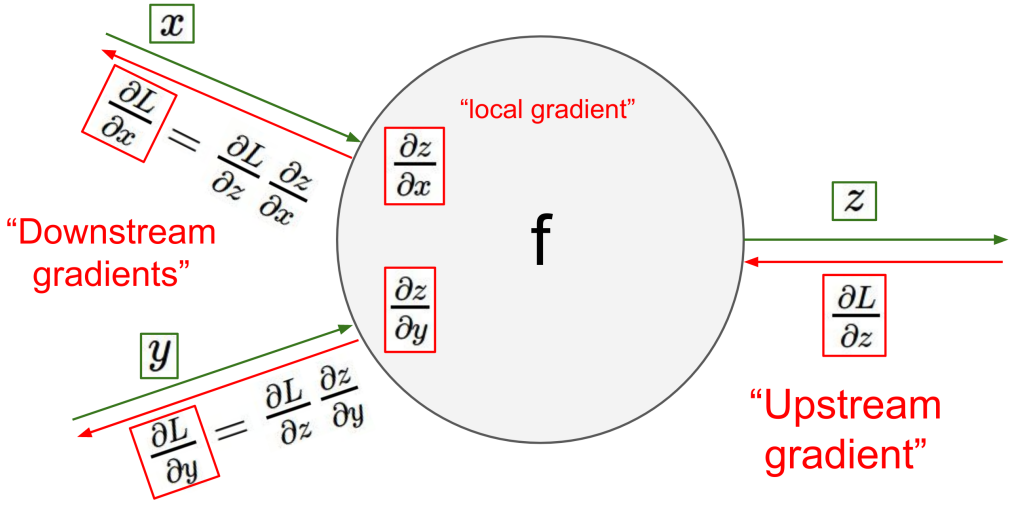
[1]from CS231n, lecture 4, 2019

Backprop[1]



[1]from CS231n, lecture 4, 2019

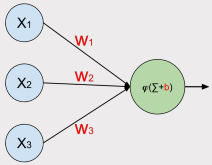
Backprop[1]



[1]from CS231n, lecture 4, 2019

Forward pass

NN = Tensor Operations



Perceptron

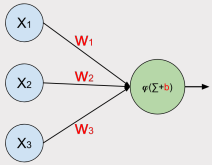
X1	X2	X3

•

W1
W2
W3

+ B = P

NN = Tensor Operations



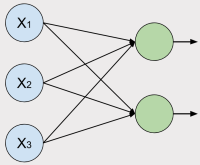
Perceptron

X1	X2	X3

•

W1
W2
W3

+ | B | = | P |



Linear Layer

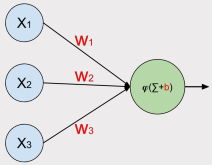
X1	X2	X3

•

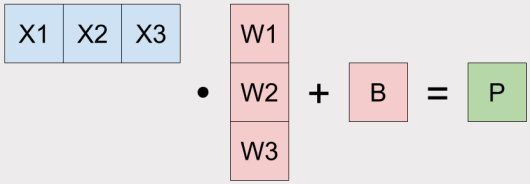
W11	W12
W21	W22
W31	W32

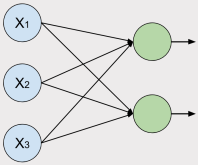
B1	B2	=	P1	P2

NN = Tensor Operations

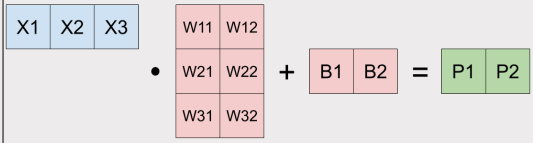


Perceptron





Linear Layer



How about the case with multiple input tensors?

Softmax

$$S(y_i) = e^{y_i} \; / \; \sum_j e^{y_j}$$

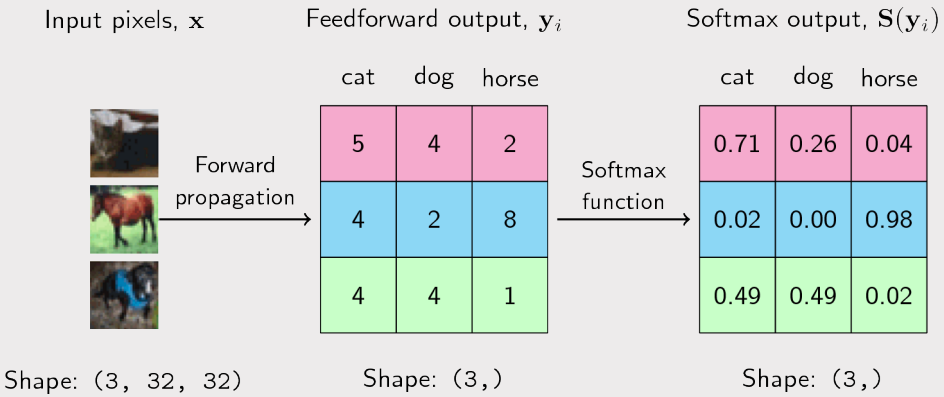
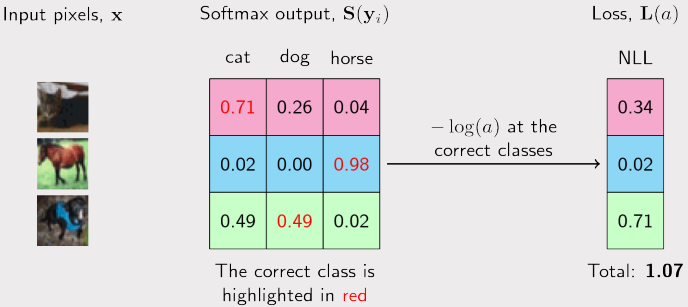


Figure: Softmax [1]

Loss Function

$\frac{1}{n}\sum_i (h_\theta(x_i) - y_i)^2$

$\frac{1}{n}\sum_i -log(h_\theta(x_i)_{y_i})$



Correct classes are known because we are training

Predictor confidence of **horse** is high. *Lower unhappiness.*

Predictor confidence of **dog** is low. *Higher unhappiness.*

Figure: NLL [1]

[1] ljvmiranda921.github.io

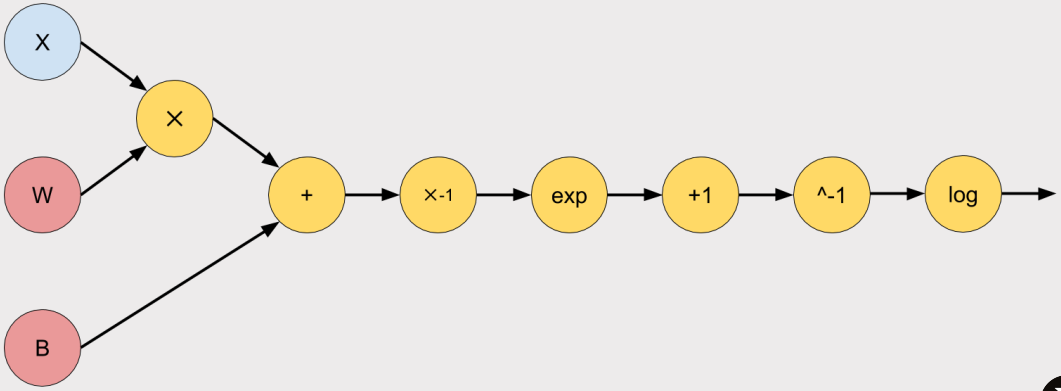
Backward pass

Computation Graph

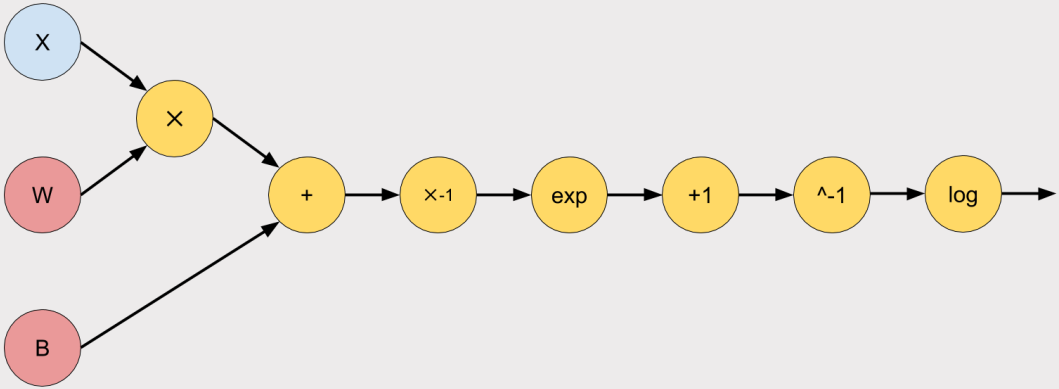
$$L(x, w, b) = log\left(\frac{1}{e^{-(xw+b)} + 1}\right)$$

Computation Graph

$$L(x, w, b) = log\left(\frac{1}{e^{-(xw+b)} + 1}\right)$$

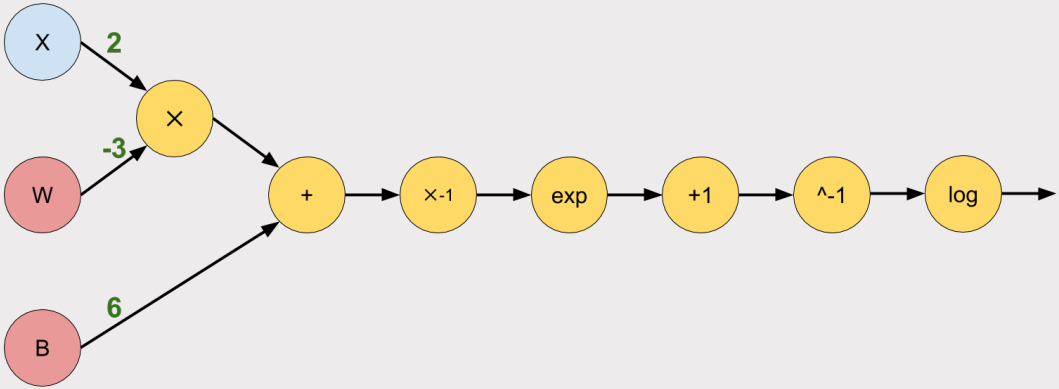


Forward



Task: Compute $L(x, w, b)$

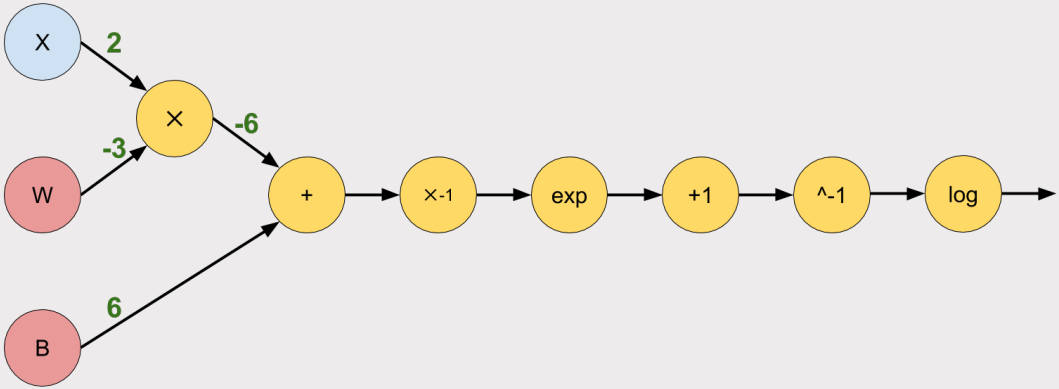
Forward



Task: Compute $L(x, w, b)$

$$x = 2, w = -3, b = 6$$

Forward



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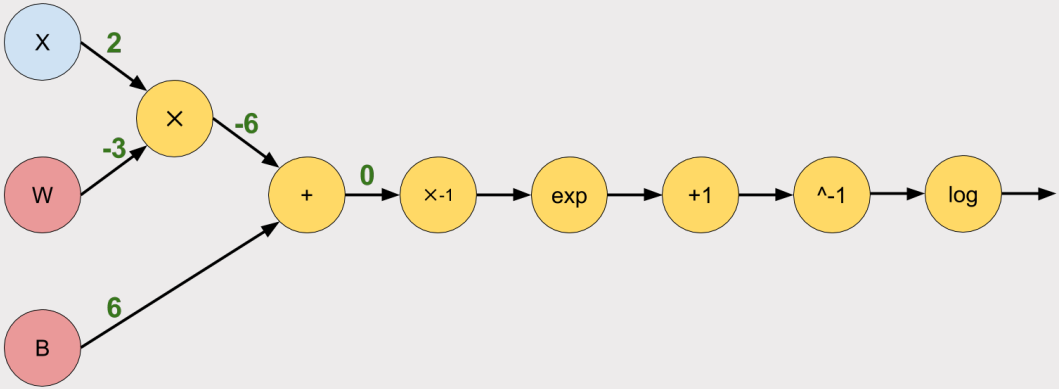

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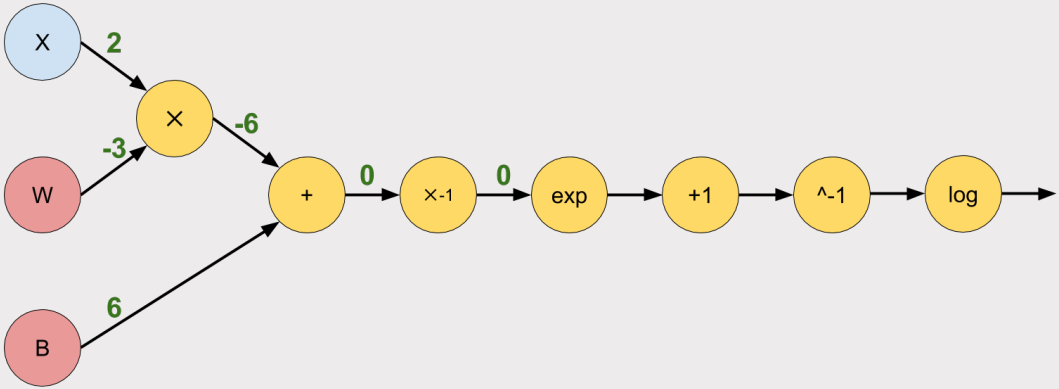
Forward



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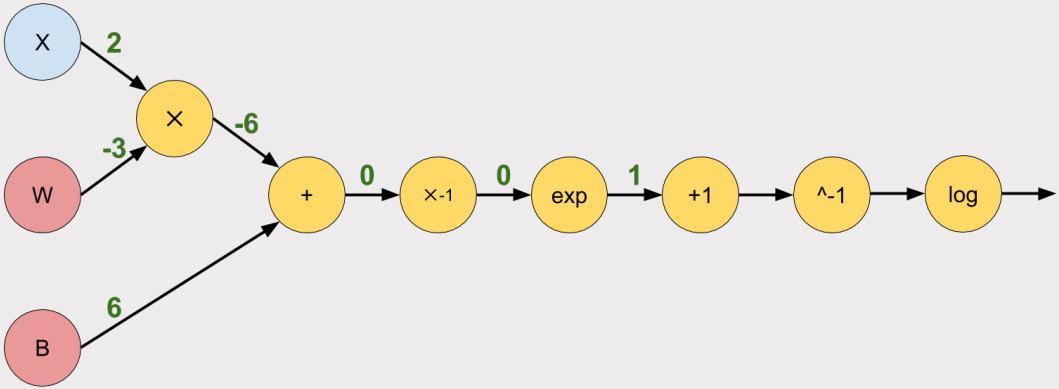
Forward



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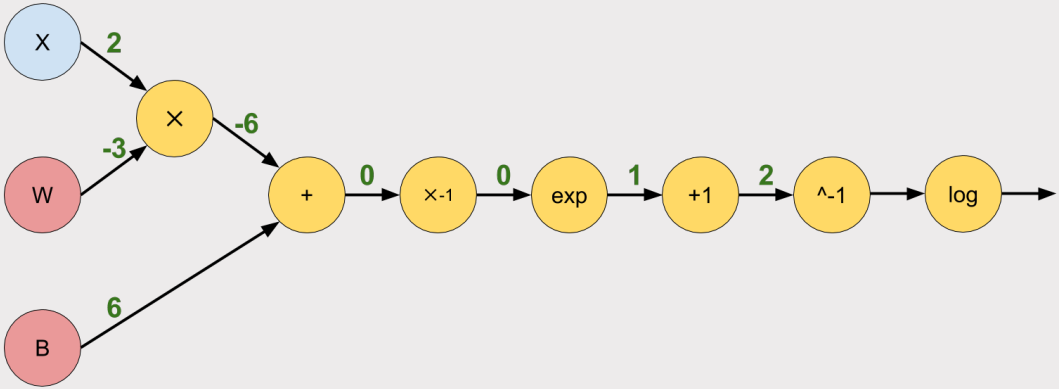
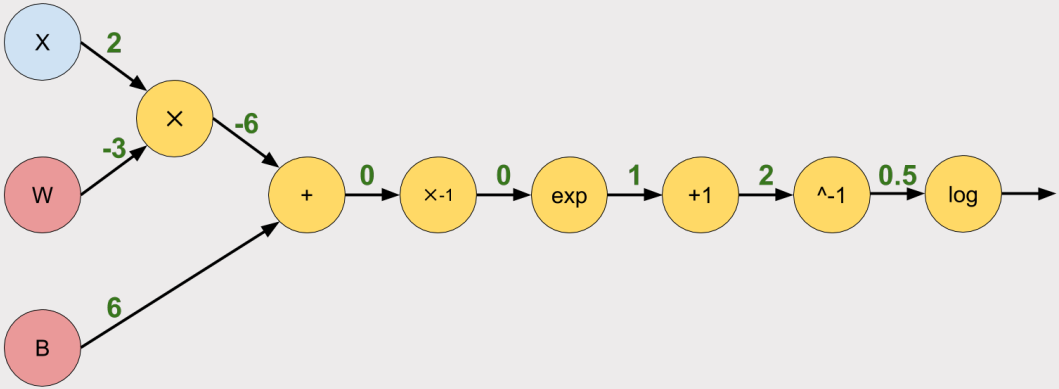
Forward



Task: Compute $L(x, w, b)$

$$x = 2, w = -3, b = 6$$

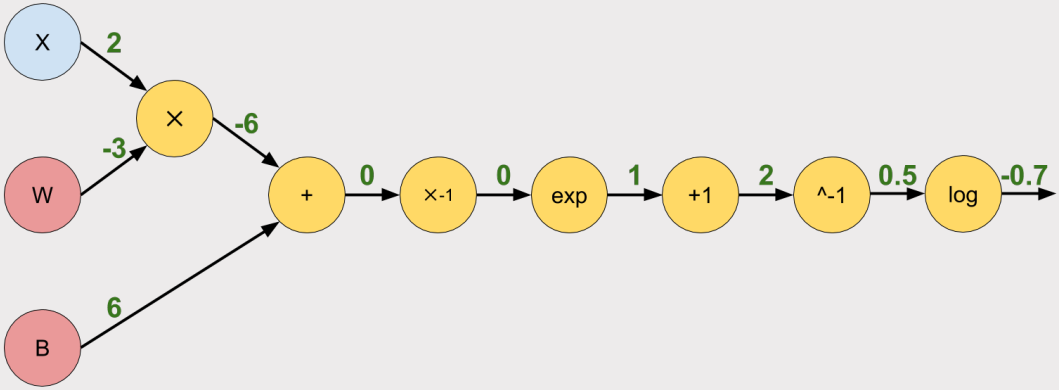
Forward



Task: Compute $L(x, w, b)$

$$x = 2, w = -3, b = 6$$

Forward

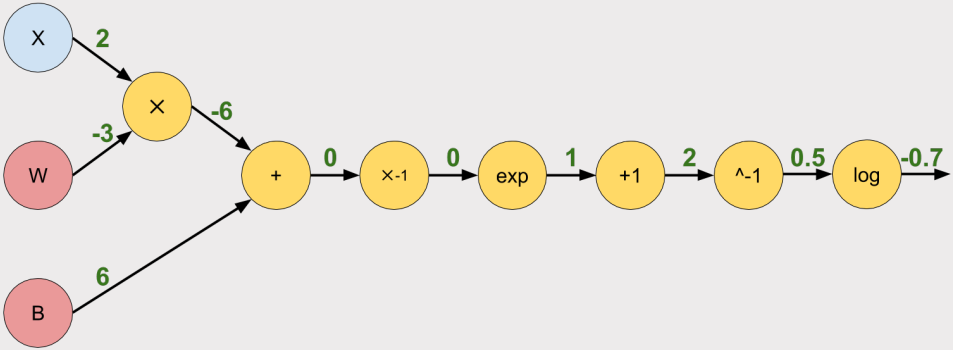


Task: Compute $L(x, w, b)$

$$x = 2, w = -3, b = 6$$

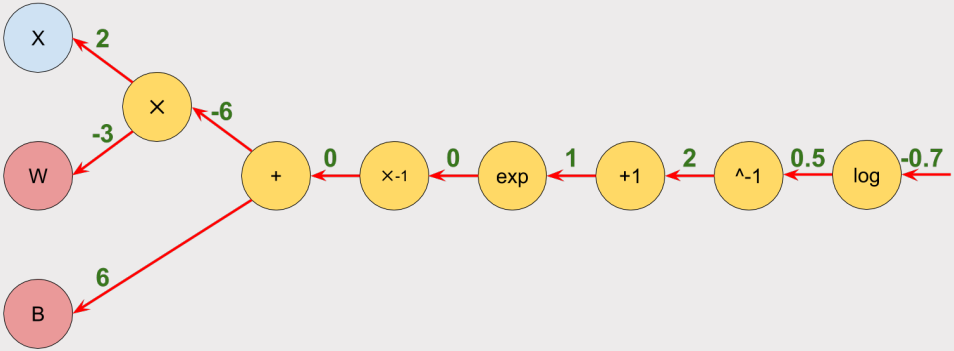
$$L(2, -3, 6) \approx 0.7$$

Backward



Task: Compute $\nabla L = \left[\frac{\partial L}{\partial x}, \frac{\partial L}{\partial w}, \frac{\partial L}{\partial b}\right]$

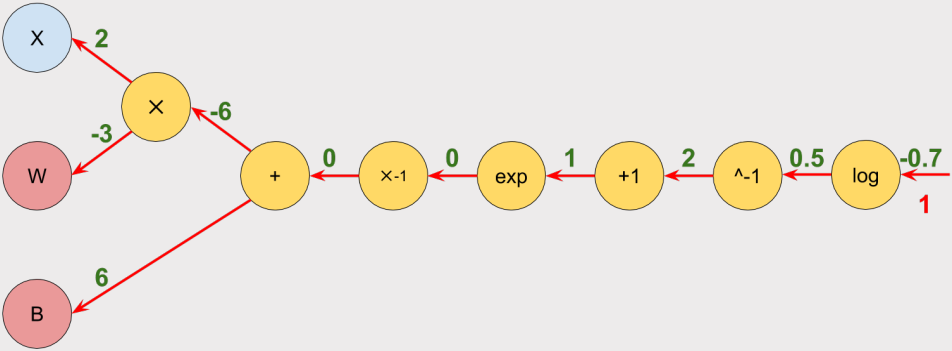
Backward



Task: Compute $\nabla L = \left[\frac{\partial L}{\partial x}, \frac{\partial L}{\partial w}, \frac{\partial L}{\partial b}\right]$
Chain-rule $\Longrightarrow$ each sub-module M:

- receives $\frac{\partial L}{\partial M(in)}$
- computes $\frac{\partial M(in)}{\partial in_k}$
- returns $\frac{\partial L}{\partial in_k} = \frac{\partial L}{\partial M(in)} \frac{\partial M(in)}{\partial in_k}$

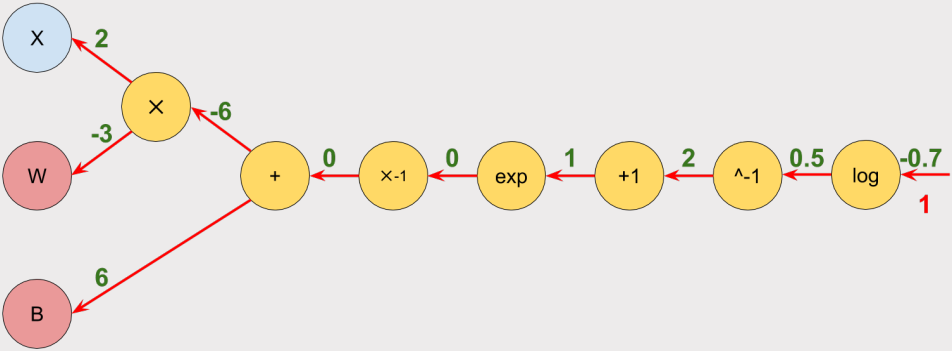
Backward



log:

- receives $\frac{\partial L}{\partial log(in)} = 1$

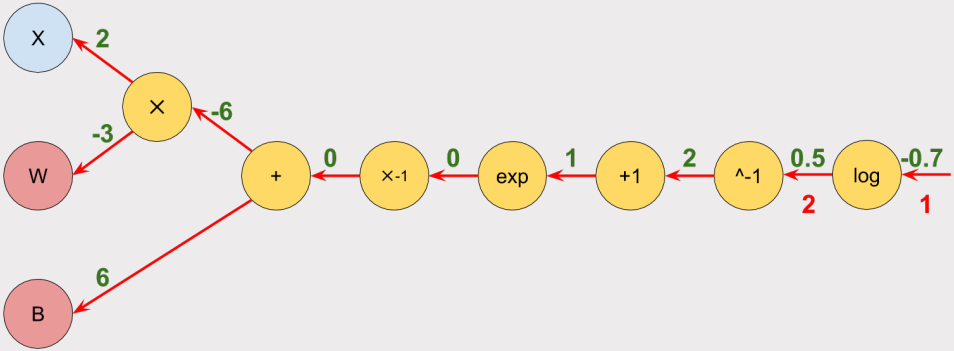
Backward



log:

- receives $\frac{\partial L}{\partial log(in)} = 1$
- computes $\frac{\partial log(in)}{\partial in} = \frac{1}{in} = 2$

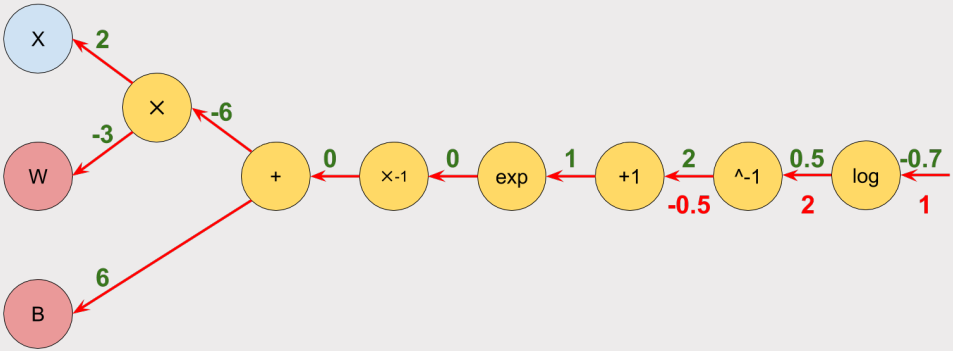
Backward



log:

- receives $\frac{\partial L}{\partial log(in)} = 1$
- computes $\frac{\partial log(in)}{\partial in} = \frac{1}{in} = 2$
- returns $\frac{\partial L}{\partial in} = 1 * 2$

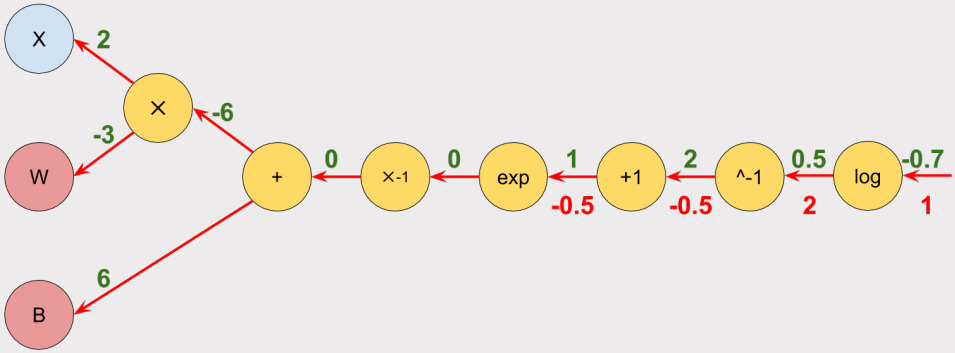
Backward



ˆ− 1:

- receives $\frac{\partial L}{\partial (in)^{-1}} = 2$
- computes $\frac{\partial (in)^{-1}}{\partial in} = -(in)^{-2} = -0.25$
- returns $\frac{\partial L}{\partial in} = 2 * -0.25 = -0.5$

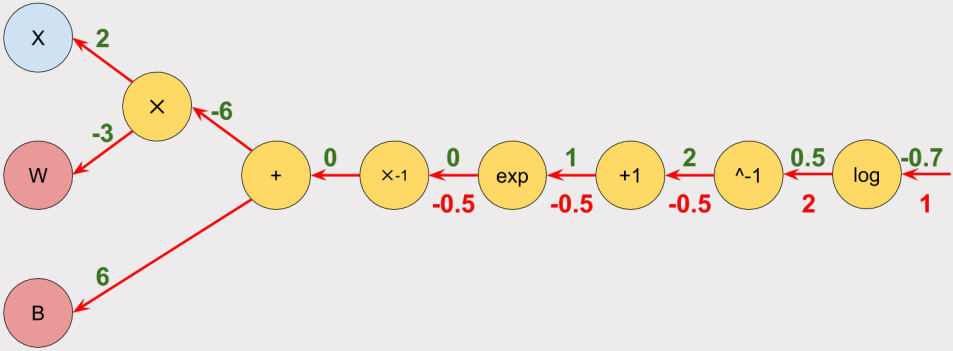
Backward



+1:

- receives $\frac{\partial L}{\partial (in+1)} = -0.5$
- computes $\frac{\partial (in+1)}{\partial in} = 1$
- returns $\frac{\partial L}{\partial in} = -0.5 * 1 = -0.5$

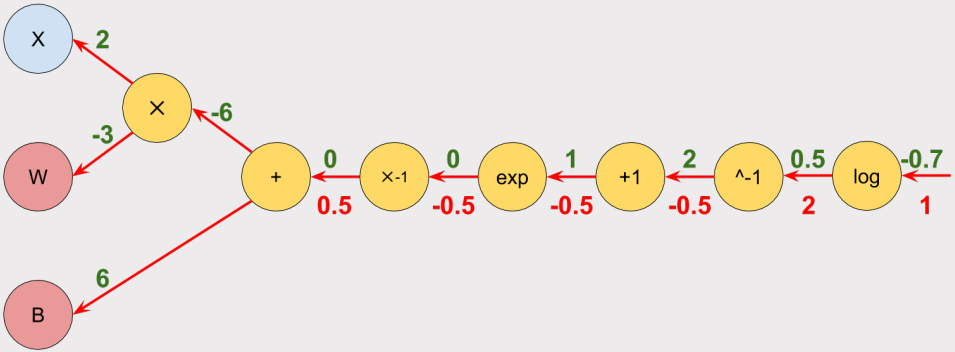
Backward



exp:

- receives $\frac{\partial L}{\partial e^{in}} = -0.5$
- computes $\frac{\partial e^{in}}{\partial in} = e^{in} = 1$
- returns $\frac{\partial L}{\partial in} = -0.5 * 1 = -0.5$

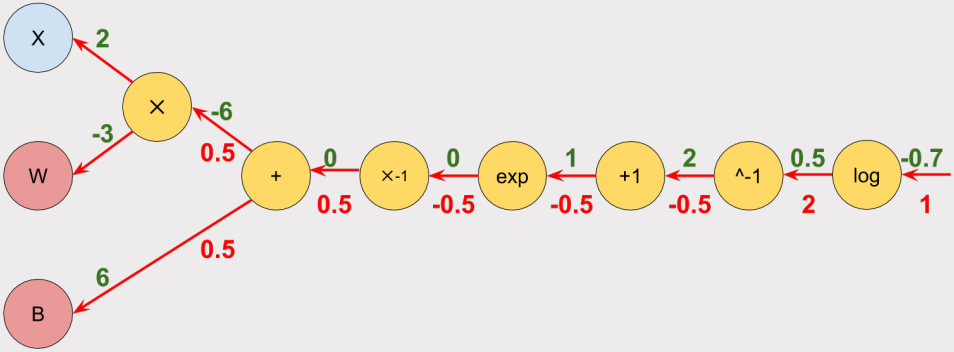
Backward



× − 1:

- receives $\frac{\partial L}{\partial(-in)} = -0.5$
- computes $\frac{\partial(-in)}{\partial in} = -1$
- returns $\frac{\partial L}{\partial in} = -0.5 * -1 = 0.5$

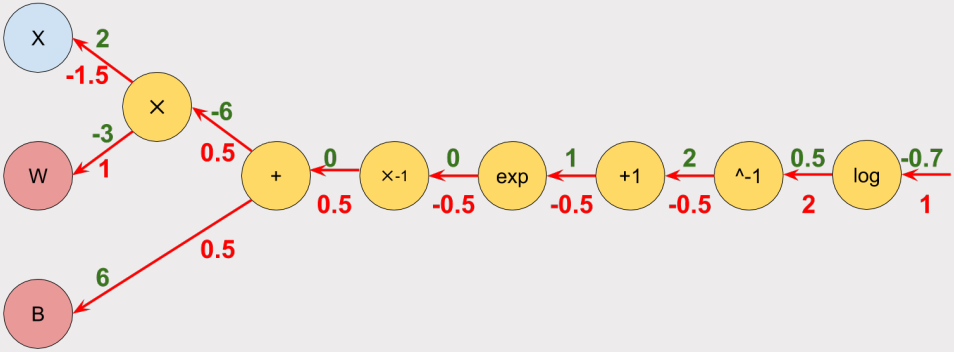
Backward



+:

- receives $\frac{\partial L}{\partial (in_1 + in_2)} = 0.5$
- computes $(\frac{\partial (in_1 + in_2)}{\partial in_1}, \frac{\partial (in_1 + in_2)}{\partial in_2} = (1, 1)$
- returns $(\frac{\partial L}{\partial in_1}, \frac{\partial L}{\partial in_2}) = (0.5, 0.5)$

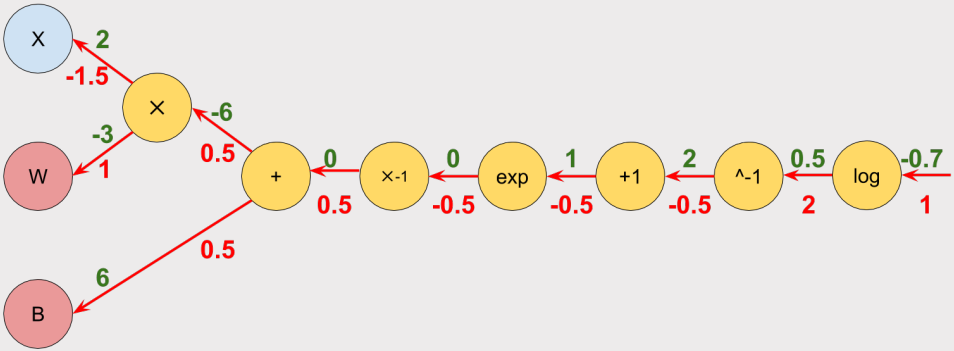
Backward



×:

- receives $\frac{\partial L}{\partial (in_1 \times in_2)} = 0.5$
- computes $(\frac{\partial (in_1 \times in_2)}{\partial in_1}, \frac{\partial (in_1 \times in_2)}{\partial in_2} = (in_2, in_1) = (-3, 2)$
- returns $(\frac{\partial L}{\partial in_1}, \frac{\partial L}{\partial in_2}) = 0.5 * (-3, 2) = (-1.5, 1)$

Backward



$$\nabla L = \left[\frac{\partial L}{\partial x}, \frac{\partial L}{\partial w}, \frac{\partial L}{\partial b}\right] = [-1.5, 1, 0.5]$$

Parameter updating

- Measure data fitting performance: loss function $L(D, \theta)$,

[1] dsdeepdive.blogspot.com

Parameter updating

- Measure data fitting performance: loss function $L(D, \theta)$,
- Compute the gradient of the loss function with respect to weights,

[1] dsdeepdive.blogspot.com

Parameter updating

- Measure data fitting performance: loss function $L(D, \theta)$,
- Compute the gradient of the loss function with respect to weights,
- Find incremental solutions that better explain the data.

using:

$$\theta_{j+1} \leftarrow \theta_j - \alpha \nabla_{\theta_j} L$$

sequentially find:

$$\theta_0, \theta_1, ..., \theta_k$$

such that $L(D, \theta)$decreases.

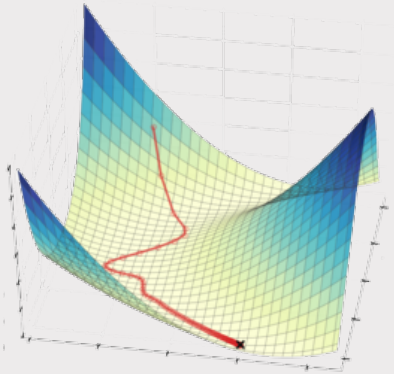


Figure: Sequential minimizing $L(D, \theta)$ [1]

[1] dsdeepdive.blogspot.com

Wild beasts and how to tame them?

Universal Approximation Theorem

A fully connected network with one hidden layer followed by a non-linear function can approximate any function from one finite-dimensional space to another in the limit of the **width** of the hidden layer (Hornik et al., 1990).

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Potentially the hidden layer can get exponentially large. Eg.: no of possible binary functions on vectors $\mathbf{v} \in \{0, 1\}^n$ is 2^{2^n}, requiring $O(2^n)$ units, each responding to a single input.

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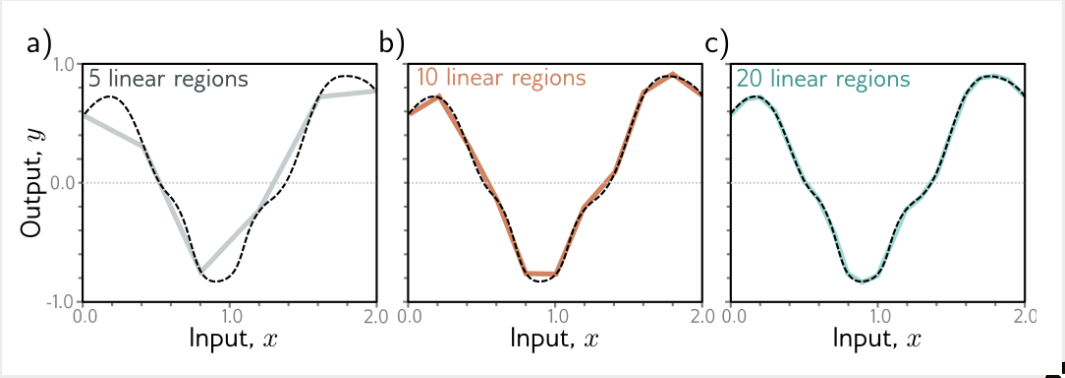

UAT and depth

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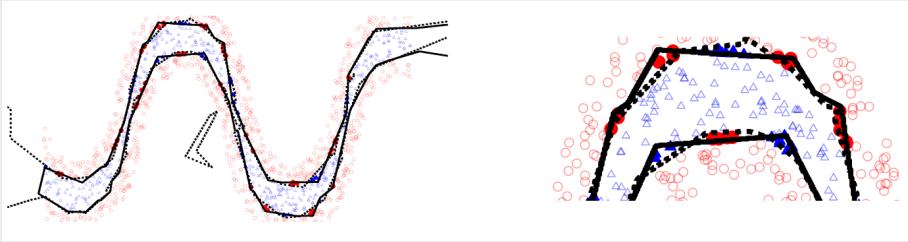

Figure: A network with ReLU units learns piece-wise linear functions at each layer and deep networks reuse these computations exponentially more often than shallow networks. Solid line is a 20 units, one layer NN and dotted line is a 2 layers, 10 units each NN.

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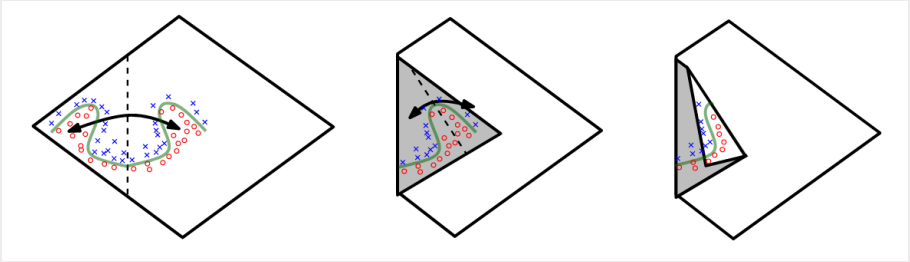

Figure: A network with ReLU units creates mirror images of the function computed at the input of some hidden unit resulting in increasingly expressive networks

UAT and depth

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- There exist families of functions which can be approximated efficiently (in numbers of parameters) by **deep** networks.
- Goodfellow et al. 2014:

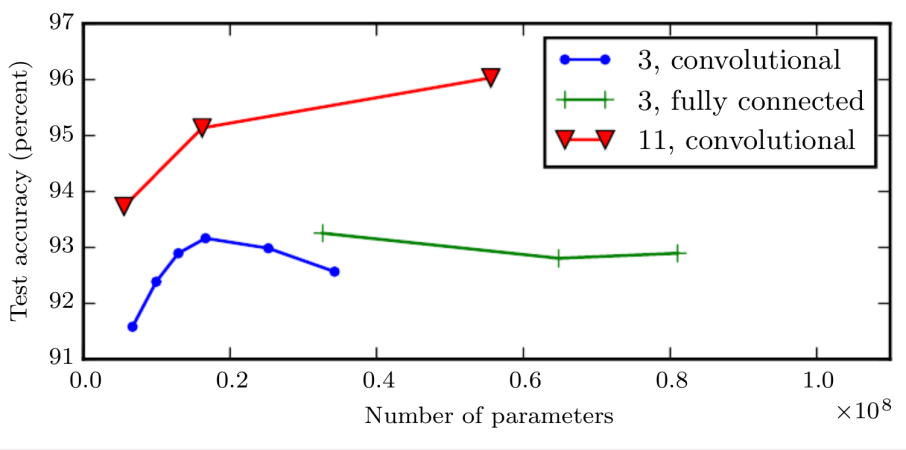


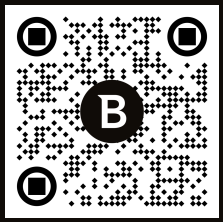
Figure: Generalization correlates with depth, not number of parameters.

The new generalization theory

Figure: Is the classic generalization theory still valid?

Thank you!

florin.gogianu@gmail.com



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