Optimization



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Last time ...

Optimization: Is it possible to find f^* in the function space.



Optimization

Optimization ≠ Learning

Network: $f_{\theta}(x)$

Training data:

$$L(\theta) = \sum_{r=1}^{R} l(f_{\theta}(x^r) - \hat{y}^r)$$

$$(x^{1}, \hat{y}^{1}) \qquad \theta^{*}$$

 $(x^{2}, \hat{y}^{2}) \qquad \ln |$

 $\theta^* = \arg\min_{\theta} L(\theta)$

In Deep Learning, $L(\theta)$ is not convex.

 (x^R, \hat{y}^R) Non-convex optimization is NP-hard.

Why can we solve the problem by gradient descent?

Loss of Deep Learning is not convex

There are at least exponentially many global minima for a neural net.

Permutating the neurons in one layer does not change the loss.





Non-convex \neq Difficult



Outline

Review: Hessian

Deep Linear Model

Deep Non-linear Model

Conjecture about Deep Learning

Empirical Observation about Error Surface

Hessian Matrix: When Gradient is Zero

Some examples in this part are from: https://www.math.upenn.edu/~kazdan/312F12/Notes/ max-min-notesJan09/max-min.pdf

Training stops

critical point: gradient is zero



When Gradient is Zero

$$f(\theta) = f(\theta^0) + (\theta - \theta^0)^T g + \frac{1}{2} (\theta - \theta^0)^T H(\theta - \theta^0) + \cdots$$

Gradient g is a *vector*

$$g_i = \frac{\partial f(\theta^0)}{\partial \theta_i} \qquad \nabla f(\theta^0)$$

Hessian H is a *matrix*

$$H_{ij} = \frac{\partial^2}{\partial \theta_i \partial \theta_j} f(\theta^0)$$
$$= \frac{\partial^2}{\partial \theta_j \partial \theta_i} f(\theta^0) = H_{ji}$$

symmetric

Source of image: http://www.deeplearningbook.org /contents/numerical.html

Hessian

 $f(\theta) = f(\theta^0) + (\theta - \theta^0)^T g + \frac{1}{2} (\theta - \theta^0)^T H(\theta - \theta^0) + \cdots$



Hessian

$$f(\theta) = f(\theta^{0}) + (\theta - \theta^{0})^{T}g + \frac{1}{2}(\theta - \theta^{0})^{T}H(\theta - \theta^{0}) + \cdots$$
Newton's method Find the space such that $\nabla f(\theta) = 0$
 $\nabla f(\theta) \approx \underline{\nabla [(\theta - \theta^{0})^{T}g]} + \underline{\nabla [\frac{1}{2}(\theta - \theta^{0})^{T}H(\theta - \theta^{0})]}_{H(\theta - \theta^{0})}$
 $\frac{\partial [(\theta - \theta^{0})^{T}g]}{\partial \theta_{i}} = g_{i}$
 $\frac{\partial [\frac{1}{2}(\theta - \theta^{0})^{T}H(\theta - \theta^{0})]}{\partial \theta_{i}}$



Newton's method

$$\nabla f(\theta) \approx \frac{\nabla [(\theta - \theta^0)^T g]}{= g} + \frac{\nabla \left[\frac{1}{2}(\theta - \theta^0)^T H(\theta - \theta^0)\right]}{H(\theta - \theta^0)}$$
$$\nabla f(\theta) \approx g + H(\theta - \theta^0) = 0$$
$$H(\theta - \theta^0) = -g \qquad \theta = \theta^0 - \frac{H^{-1}g}{H^{-1}g} \quad \text{V.s.} \quad \theta = \theta^0 - \eta g$$
$$\theta - \theta^0 = -H^{-1}g \qquad \text{Change the direction, determine step size}$$

Hessian

Source of image: https://math.stackexchange.com/questions/60 9680/newtons-method-intuition

$$f(\theta) = f(\theta^0) + (\theta - \theta^0)^T g + \frac{1}{2} (\theta - \theta^0)^T H(\theta - \theta^0) + \cdots$$



If f(x) is a quadratic function, obtain critical point in one step. What is the problem? Source of image: http://www.offconvex.org/2016/03/22/saddlepoints/

Hessian

$$f(\theta) = f(\theta^0) + (\theta - \theta^0)^T g + \frac{1}{2} (\theta - \theta^0)^T H(\theta - \theta^0) + \cdots$$

At critical point (g = 0)

H tells us the properties of critical points.



Review: Linear Algebra

- If $Av = \lambda v$ (v is a vector, λ is a scalar)
 - *v* is an eigenvector of A excluding zero vector
 - λ is an eigenvalue of A that corresponds to v



Review: Positive/Negative Definite

- An nxn matrix A is symmetric.
- For every non-zero vector x ($x \neq 0$)

positive definite: $x^T A x > 0$

All eigen values are positive.

 $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

 ≥ 0 \longrightarrow All eigen values are non-negative.

- All eigen values are negative.
- All eigen values are non-positive.

positive semi-definite: $x^T A x \ge 0$

negative definite:
$$x^T A x < 0$$

negative semi-definite: $x^T A x \leq 0$





Because H is an nxn symmetric matrix,

H can have eigen vectors $\{v_1, v_2, ..., v_n\}$ form a orthonormal basis.

At critical point: Hessian $f(\theta) \approx f(\theta^0) + \frac{1}{2}(\theta - \theta^0)^T H(\theta - \theta^0)$

$$v$$
 is an eigen vector $\implies v^T H v = v^T (\lambda v) = \lambda ||v||^2$
Unit vector $= \lambda$

+?
$$u = a_1v_1 + a_2v_2 + \dots + a_nv_n$$

 $u = (a_1)^2 \lambda_1 + (a_2)^2 \lambda_2 + \dots + (a_n)^2 \lambda_n$
 θ^0

Because H is an nxn symmetric matrix,

H can have eigen vectors $\{v_1, v_2, ..., v_n\}$ form a orthonormal basis.

Examples

$$\frac{\partial f(x,y)}{\partial x} = 2x \qquad \frac{\partial f(x,y)}{\partial y} =$$

$$x=0, y=0$$

$$\frac{\partial^2}{\partial x \partial x} f(x, y) = 2$$

$$\frac{\partial^2}{\partial y \partial x} f(x, y) = 0$$

$$\frac{\partial^2}{\partial x \partial y} f(x, y) = 0$$

6*y*

$$\frac{\partial^2}{\partial y \partial y} f(x, y) = 6$$



 $H = \begin{bmatrix} 2 & 0 \\ 0 & 6 \end{bmatrix}$

Positive-definite Local minima

Examples

$$\frac{\partial f(x,y)}{\partial x} = -2x \quad \frac{\partial f(x,y)}{\partial y} = 6y$$

$$x = 0, y = 0$$

$$\frac{\partial^2}{\partial x \partial x} f(x, y)$$
$$= -2$$

$$\frac{\partial^2}{\partial y \partial x} f(x, y) = 0$$

$$\frac{\partial^2}{\partial x \partial y} f(x, y)$$

= 0
$$\frac{\partial^2}{\partial y \partial y} f(x, y)$$

= 6

$$f(x,y) = -x^2 + 3y^2$$



Saddle

Degenerate

• Degenerate Hessian has at least one zero eigen value

$$f(x,y) = x^2 + y^4$$

$$\frac{\partial f(x,y)}{\partial x} = 2x \qquad \frac{\partial f(x,y)}{\partial y} = 4y^3 \qquad \qquad x = y = 0$$

$$\frac{\partial^2}{\partial x \partial x} f(x, y) = 2 \qquad \frac{\partial^2}{\partial x \partial y} f(x, y) = 0 \qquad H = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$$
$$\frac{\partial^2}{\partial y \partial x} f(x, y) = 0 \qquad \frac{\partial^2}{\partial y \partial y} f(x, y) = 12y^2$$

Degenerate

• Degenerate Hessian has at least one zero eigen value

$$f(x,y) = x^{2} + y^{4} \qquad g(x,y) = x^{2} - y^{4}$$
$$x = y = 0$$
$$g = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad x = y = 0$$
$$g = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
$$H = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} \qquad H = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$$

No Difference

$$h(x,y) = 0$$

$$x = y = 0$$

$$g = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad f(x,y) = -x^{4} - y^{4}$$

$$H = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\frac{\partial f(x,y)}{\partial x} = -4x^{3} \quad \frac{\partial f(x,y)}{\partial y} = -4y^{3}$$

$$\frac{\partial^{2}}{\partial x \partial x} f(x,y) = -12x^{2} \quad \frac{\partial^{2}}{\partial x \partial y} f(x,y) = 0$$

$$\frac{\partial^{2}}{\partial y \partial x} f(x,y) = 0 \quad \frac{\partial^{2}}{\partial y \partial y} f(x,y) = -12y^{2}$$

$$H = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$



http://homepages.math.uic.edu/~juliu s/monkeysaddle.html

Monkey Saddle

$$\frac{\partial f(x,y)}{\partial x} = 3x^2 - 3y^2$$

$$\frac{\partial f(x,y)}{\partial y} = -6xy$$

$$\frac{\partial^2}{\partial x \partial x} f(x, y) = 6x \qquad \frac{\partial^2}{\partial x \partial y} f(x, y) = -6y$$
$$\frac{\partial^2}{\partial y \partial x} f(x, y) = -6y \qquad \frac{\partial^2}{\partial y \partial y} f(x, y) = -6x$$

Training stuck ≠ Zero Gradient

• People believe training stuck because the parameters are around a critical point



Training stuck ≠ Zero Gradient



http://videolectures.net/deeplearning2015_bengio_theoretical_motivations/

Deep Linear Network





$$x \xrightarrow{w_1} \overbrace{\longrightarrow}^{w_2} \overbrace{\longrightarrow}^{w_2} y \iff \hat{y} = 1$$

$$L = (\hat{y} - w_1 w_2 x)^2 = (1 - w_1 w_2)^2$$

$$\frac{\partial L}{\partial w_1} = 2(1 - w_1 w_2)(-w_2)$$

$$\frac{\partial L}{\partial w_2} = 2(1 - w_1 w_2)(-w_1)$$

The probability of stuck as saddle point is almost zero.

-0.5

w1

Easy to escape

0.5

1.5

- 2.5

$$\frac{\partial^2 L}{\partial w_1^2} = 2(-w_2)(-w_2)$$
$$\frac{\partial^2 L}{\partial w_2 \partial w_1} = -2 + 4w_1 w_2$$

$$\frac{\partial^2 L}{\partial w_1 \partial w_2} = -2 + 4w_1 w_2$$
$$\frac{\partial^2 L}{\partial w_2^2} = 2(-w_1)(-w_1)$$

Gradient Manifold of global minima Saddle point Gradient descent path Linear path Interpolation between minin

0.

-0.5

-1

-1.5

-1

22

$\frac{2\text{-hidden layers}}{L = (1 - w_1 w_2 w_3)^2} \quad x \xrightarrow{w_1} \swarrow \xrightarrow{w_2} \checkmark \xrightarrow{w_3} \checkmark \longrightarrow y \nleftrightarrow \hat{y}$

 $w_1 w_2 w_3 = 1$ global minima $\frac{\partial L}{\partial w_1} = 2(1 - w_1 w_2 w_3)(-w_2 w_3)$ $w_1 = w_2 = w_3 = 0$ $\frac{\partial L}{\partial w_2} = 2(1 - w_1 w_2 w_3)(-w_1 w_3)$ $H = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ $\frac{\partial L}{\partial w_3} = 2(1 - w_1 w_2 w_3)(-w_1 w_2)$ So flat $\frac{\partial^2 L}{\partial w_1^2} = 2(-w_2 w_3)^2$ $w_1 = w_2 = 0, w_3 = k$ $\frac{\partial^2 L}{\partial w_2 \partial w_1} = -2w_3 + 4w_1 w_2 (w_3)^2$ $H = \begin{bmatrix} 0 & -2 & 0 \\ -2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ All minima are global, some Saddle point critical points are "bad".



10-hidden layers

Demo

Deep Linear Network

$$\hat{y} \longleftrightarrow y \longleftrightarrow W^{K} \longleftrightarrow W^{2} \longleftrightarrow W^{1} \bigstar x$$

$$y = W^{K}W^{K-1} \cdots W^{2}W^{1}x \quad L = \sum_{n=1}^{N} (x^{n} - \hat{y}^{n})^{2}$$

Hidden layer size \geq Input dim, output dim

More than two hidden layers can produce saddle point without negative eigenvalues.

Reference

- Kenji Kawaguchi, Deep Learning without Poor Local Minima, NIPS, 2016
- Haihao Lu, Kenji Kawaguchi, Depth Creates No Bad Local Minima, arXiv, 2017
- Thomas Laurent, James von Brecht, Deep linear neural networks with arbitrary loss: All local minima are global, arXiv, 2017
- Maher Nouiehed, Meisam Razaviyayn, Learning Deep Models: Critical Points and Local Openness, arXiv, 2018

Non-linear Deep Network

Does it have local minima?

證明事情不存在很難,證明事情存在相對容易

感謝曾子家同學發現投影片上的錯字
Even Simple Task can be Difficult

h		XOR ReLU	XOR Sigmoid	Jellyfish ReLU	Jellyfish Sigmoid		XOR ReLU	XOR Sigmoid	Jellyfish ReLU	Jellyfish Sigmoid
2	Adam	28%	79%	7%	0%	GD	23%	90%	16%	62%
3	Adam	52%	98%	34%	0%	GD	47%	100%	33%	100%
4	Adam	68%	100%	50%	2%	GD	70%	100%	66%	100%
5	Adam	81%	100%	51%	27%	GD	80%	100%	68%	100%
6	Adam	91%	100%	61%	17%	GD	89%	100%	69%	100%
7	Adam	97%	100%	69%	58%	GD	89%	100%	86%	100%



(a) Optimally converged net for Jellyfish.



(b) Stuck net for Jellyfish.







This relu network has local minima.

"Blind Spot" of ReLU



It is pretty easy to make this happens

"Blind Spot" of ReLU

Consider your initialization





Considering Data

Table 1: Spurious local minima found for n = k

k	n	% of runs	Average	Average	
		converging to	minimal	objective	
		local minima	eigenvalue	value	
6	6	0.3%	0.0047	0.025	
7	7	5.5%	0.014	0.023	
8	8	12.6%	0.021	0.021	
9	9	21.8%	0.027	0.02	
10	10	34.6%	0.03	0.022	
11	11	45.5%	0.034	0.022	
12	12	58.5%	0.035	0.021	
13	13	73%	0.037	0.022	
14	14	73.6%	0.038	0.023	
15	15	80.3%	0.038	0.024	
16	16	85.1%	0.038	0.027	
17	17	89.7%	0.039	0.027	
18	18	90%	0.039	0.029	
19	19	93.4%	0.038	0.031	
20	20	94%	0.038	0.033	

Table 2: Spurious local minima found for $n \neq k$

k	n	% of runs	Average	Average	
		converging to	minimal	objective	
		local minima	eigenvalue	value	
8	9	0.1%	0.0059	0.021	
10	11	0.1%	0.0057	0.018	
11	12	0.1%	0.0056	0.017	
12	13	0.3%	0.0054	0.016	
13	14	1.5%	0.0015	0.038	
14	15	5.5%	0.002	0.033	
15	16	10.1%	0.004	0.032	
16	17	18%	0.0055	0.031	
17	18	20.9%	0.007	0.031	
18	19	36.9%	0.0064	0.028	
19	20	49.1%	0.0077	0.027	
	I	1	1	1	

No local for $n \ge k + 2$





Pr. of Converging to Minimum Below Objective

Reference

- Grzegorz Swirszcz, Wojciech Marian Czarnecki, Razvan Pascanu, "Local minima in training of neural networks", arXiv, 2016
- Itay Safran, Ohad Shamir, "Spurious Local Minima are Common in Two-Layer ReLU Neural Networks", arXiv, 2017
- Yi Zhou, Yingbin Liang, "Critical Points of Neural Networks: Analytical Forms and Landscape Properties", arXiv, 2017
- Shai Shalev-Shwartz, Ohad Shamir, Shaked Shammah, "Failures of Gradient-Based Deep Learning", arXiv, 2017

The theory should looks like ...

Under some conditions (initialization, data,), We can find global optimal.

Conjecture about Deep Learning

Almost all local minimum have very similar loss to the global optimum, and hence finding a local minimum is good enough.

Analyzing Hessian

- When we meet a critical point, it can be saddle point or local minima.
- Analyzing H

If the network has N parameters

We assume λ has 1/2 (?) to be positive, 1/2 (?) to be negative.

Analyzing Hessian

• If N=1: v_1 1/2 local minima, 1/2 local maxima, λ_1 Saddle point is almost impossible ++• If N=2: v_1 v_2 1/4 local minima, 1/4 local maxima, $\lambda_1 \lambda_2$ 1/2 Saddle points + -, - + 1/1024 local minima, 1/1024 local maxima, • If N=10: Almost every critical point is saddle point

When a network is very large,

It is almost impossible to meet a local minima. Saddle point is what you need to worry about.

Error v.s. Eigenvalues



http://proceedings.mlr.press/v70/pennington17a/pennington17a.pdf

Guess about Error Surface



https://stats385.github.io/assets/lectures/Understanding_and_improving_deep_lea ring_with_random_matrix_theory.pdf

Training Error v.s. Eigenvalues



Training Error v.s. Eigenvalues

Portion of positive eigenvalues

[•] "Degree of Local Minima"





1 - "degree of local minima"(portion of negative eigen values)

 $\alpha \propto \left(\frac{\varepsilon}{c} - 1\right)^{3/2}$

Spin Glass v.s. Deep Learning

 Deep learning is the same as spin glass model with *7 assumptions*.



More Theory

- If the size of network is large enough, we can find global optimal by gradient descent
 - Independent to initialization





Reference

- Razvan Pascanu, Yann N. Dauphin, Surya Ganguli, Yoshua Bengio, On the saddle point problem for non-convex optimization, arXiv, 2014
- Yann Dauphin, Razvan Pascanu, Caglar Gulcehre, Kyunghyun Cho, Surya Ganguli, Yoshua Bengio, "Identifying and attacking the saddle point problem in high-dimensional non-convex optimization", NIPS, 2014
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- Jeffrey Pennington, Yasaman Bahri, "Geometry of Neural Network Loss Surfaces via Random Matrix Theory", PMLR, 2017
- Benjamin D. Haeffele, Rene Vidal, "Global Optimality in Neural Network Training", CVPR, 2017

What does the Error Surface look like?

Error Surface





Profile



Profile







Profile - LSTM





Training Processing

Different initialization / different strategies usually lead to similar loss (there are some exceptions).



Training Processing

• Different strategies (the same initialization)





(c) VGG, CIFAR10

http://mypaper.pchome.com.tw /ccschoolgeo/post/1311484084

水系與流域

Training Processing



何時分道揚鑣?

Different training strategies

分水嶺



Different basins

Training Processing

Training strategies make difference at all stages of training



(b) NIN: Switching from SGD (S, $\eta = .1$) to Adam (A, $\eta = .0001$).



Batch Normalization



Skip Connection



Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The vertical axis is logarithmic to show dynamic range. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

Reference

- Ian J. Goodfellow, Oriol Vinyals, Andrew M. Saxe, "Qualitatively characterizing neural network optimization problems", ICLR 2015
- Daniel Jiwoong Im, Michael Tao, Kristin Branson, "An Empirical Analysis of Deep Network Loss Surfaces", arXiv 2016
- Qianli Liao, Tomaso Poggio, "Theory II: Landscape of the Empirical Risk in Deep Learning", arXiv 2017
- Hao Li, Zheng Xu, Gavin Taylor, Christoph Studer, Tom Goldstein, "Visualizing the Loss Landscape of Neural Nets", arXiv 2017
Concluding Remarks

Concluding Remarks

- Deep linear network is not convex, but all the local minima are global minima.
 - There are saddle points which are hard to escape
- Deep network has local minima.
 - We need more theory in the future
- Conjecture:
 - When training a larger network, it is rare to meet local minima.
 - All local minima are almost as good as global
- We can try to understand the error surface by visualization.
 - The error surface is not as complexed as imagined.