MLDS HW1-3

TAs
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Outline

- Timeline
- Task Descriptions
- Q&A

Timeline

Three Parts in HW1

- (1-1) Deep vs Shallow:
  - Simulate a funtion.
  - Train on actual task using shallow and deep models.
- (1-2) Optimization
  - Visualize the optimization process.
  - Observe gradient norm during training.
  - What happens when gradient is almost zero?
- (1-3) Generalization
  - Can network fit random labels?
  - Number of parameters v.s. Generalization
  - Flatness v.s. Generalization

Schedule

- 3/9 :
    - Release HW1-1
- 3/16 :
    - Release HW1-2
- 3/23:
    - Deadline to team-up by yourselves
    - Release HW1-3
- 3/30:
    - Deadline to team-up by TAs
- 4/6:
    - All HW1 due (including HW1-1, HW1-2 and HW1-3)

Task Descriptions

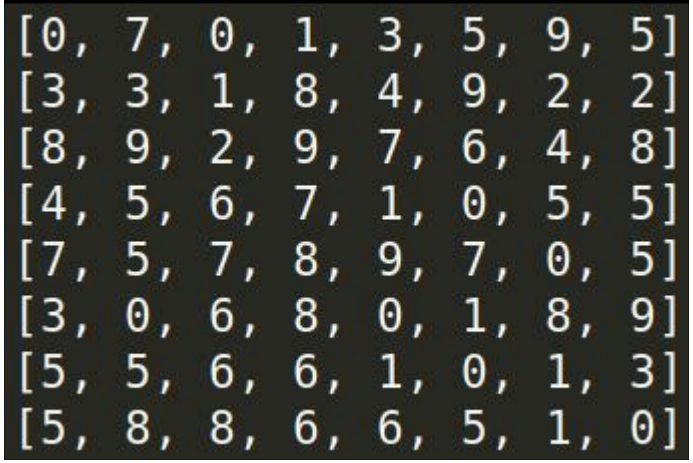
HW1-3: Generalization

- Three subtask
  - Can network fit random labels?
  - Number of parameters v.s. Generalization
  - Flatness v.s. Generalization
- Train on MNIST or CIFAR-10...

Can network fit random labels? 1/2

- Requirement
  - Train on MNIST or CIFAR-10
  - Randomly shuffle the label before training.
  - Try to fit the network with these random labels.

Can network fit random labels? 2/2



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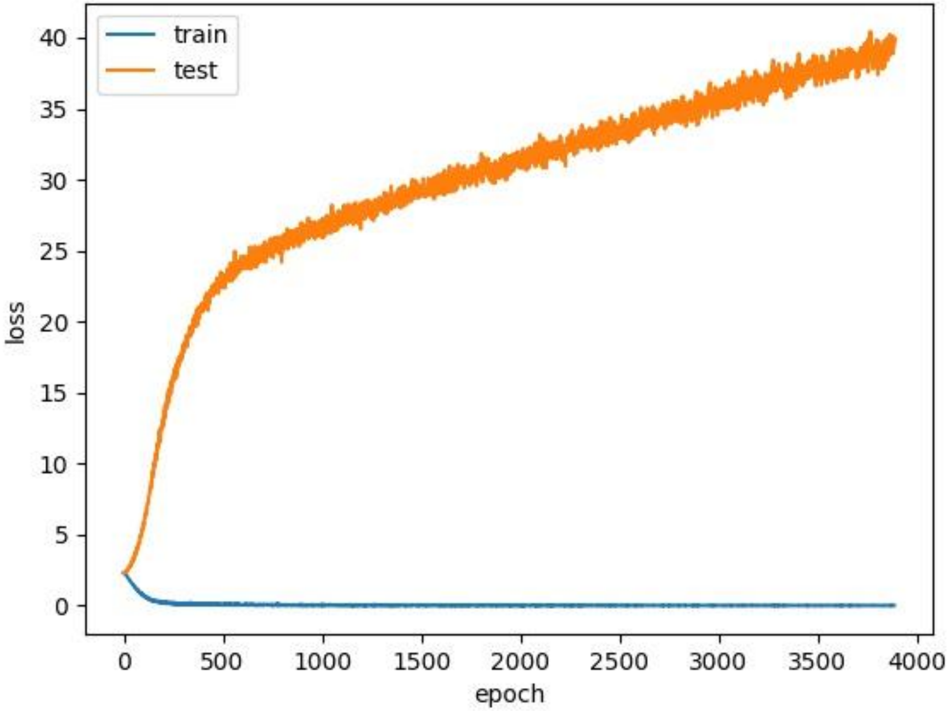
[0, 7, 0, 1, 3, 5, 9, 5]
[3, 3, 1, 8, 4, 9, 2, 2]
[8, 9, 2, 9, 7, 6, 4, 8]
[4, 5, 6, 7, 1, 0, 5, 5]
[7, 5, 7, 8, 9, 7, 0, 5]
[3, 0, 6, 8, 0, 1, 8, 9]
[5, 5, 6, 6, 1, 0, 1, 3]
[5, 8, 8, 6, 6, 5, 1, 0]
```

- MNIST
  - 3 hidden layers with 256 nodes.

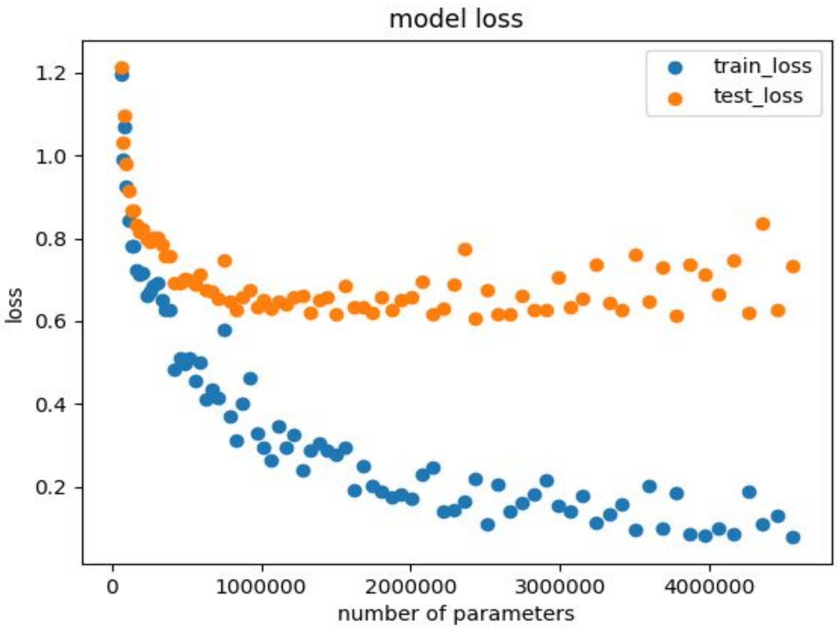


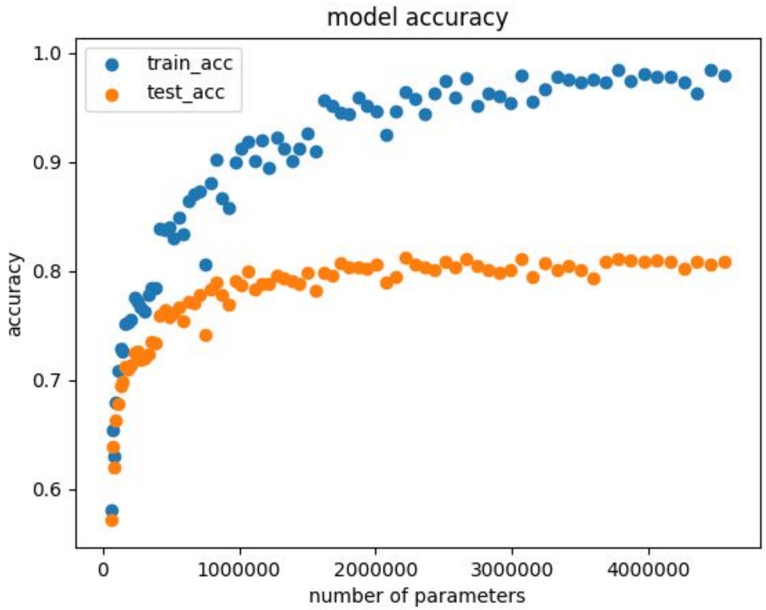
Number of parameters v.s. Generalization 1/2

- Requirement
  - Train on MNIST or CIFAR-10
  - At least 10 similar-structured models with different amount of parameters
  - Record both training and testing, loss and accuracy

Number of parameters v.s. Generalization 2/2

- CIFAR-10



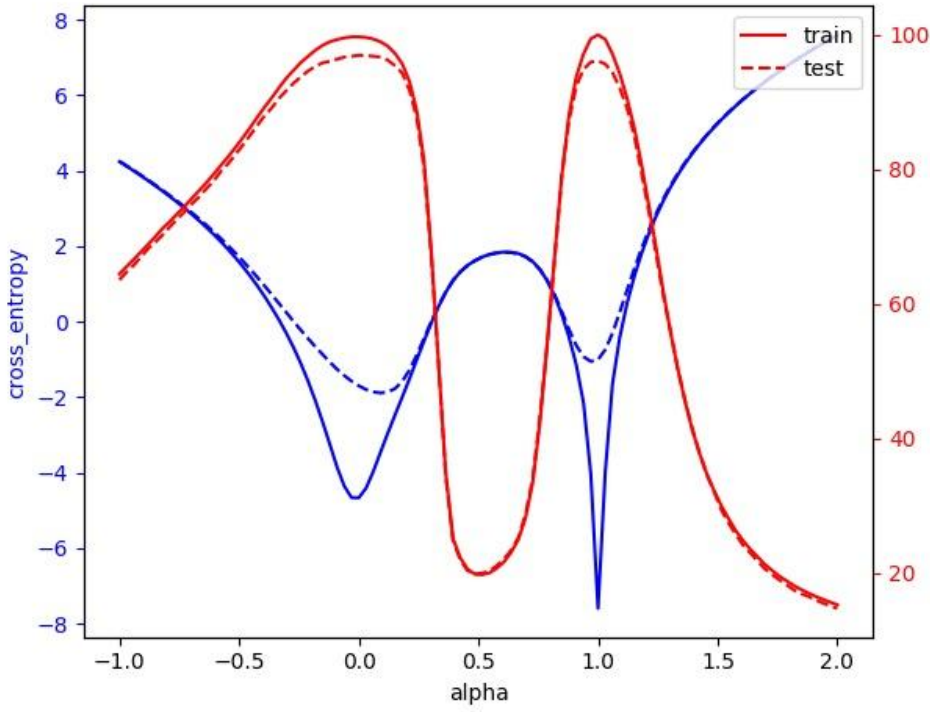


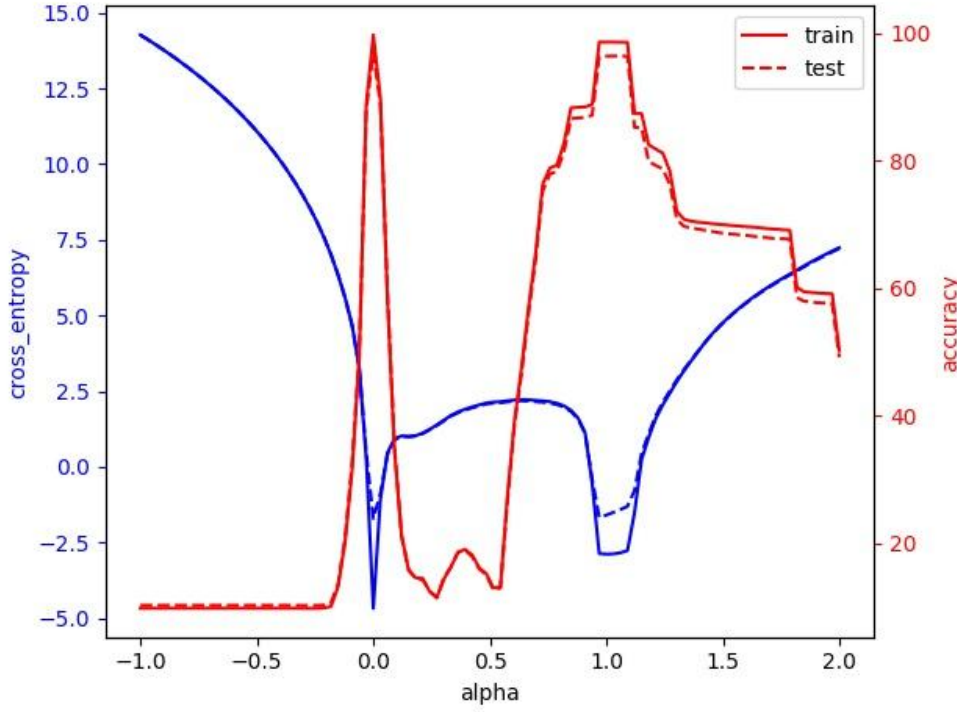
Flatness v.s. Generalization - part1 1/2

- Visualize the line between two trained models
- Requirement:
  - Train two models (m1 and m2) with different training approach. (e.g. batch size 64 and 1024)
  - Record the loss and accuracy of the model which is linear interpolation between m1 and m2.
  - $\boldsymbol{\theta_\alpha} = (1 - \alpha)\boldsymbol{\theta_1} + \alpha\boldsymbol{\theta_2}$, where α is the interpolation ratio, $\boldsymbol{\theta}$ is the parameter of the model.

Flatness v.s. Generalization - part1 2/2

- MNIST (The cross_entropy is log scale)
  - batch size 64 vs. batch size 1024
  - learning rate 1e-3 vs. 1e-2





Flatness v.s. Generalization - part2 1/

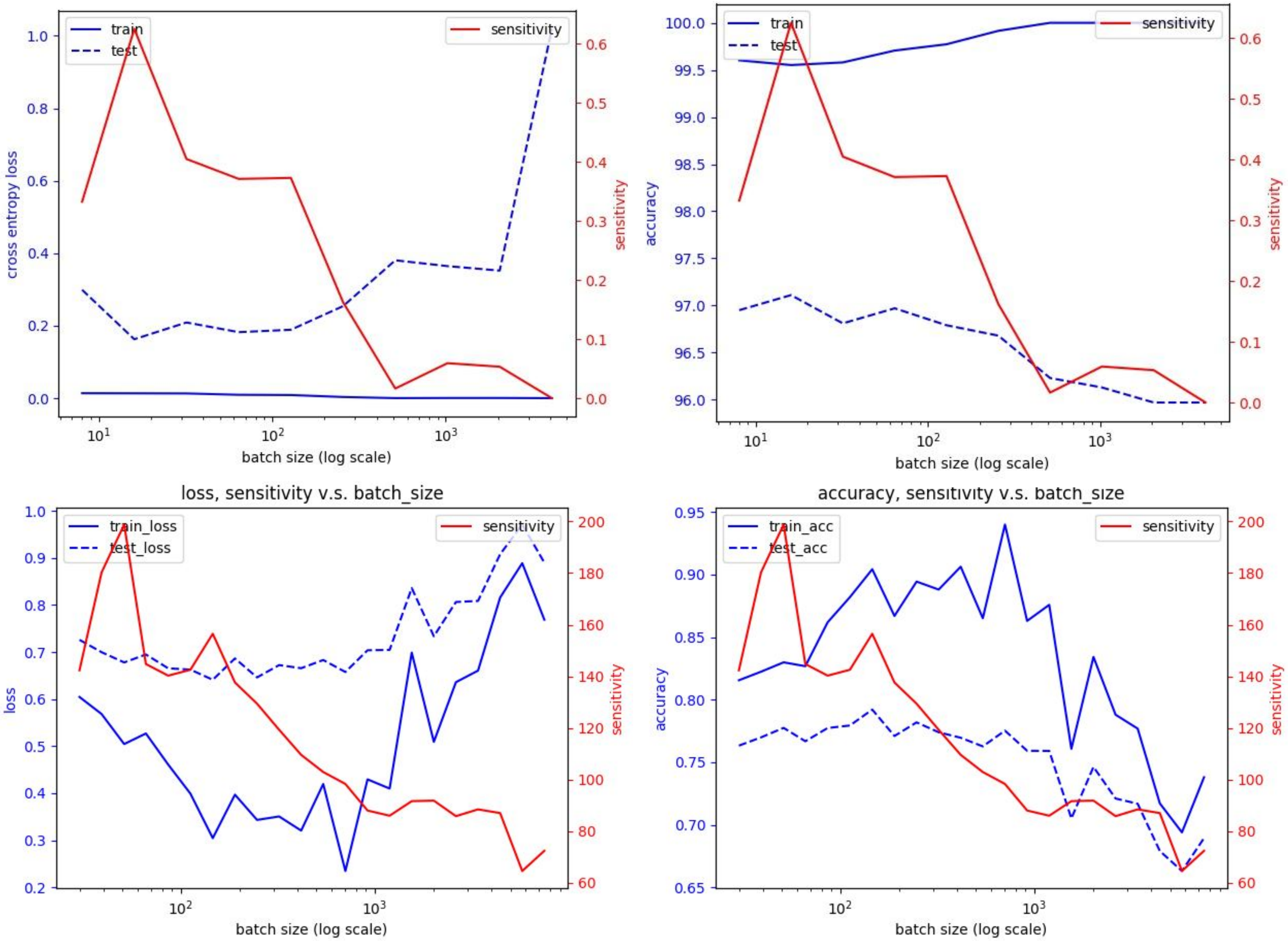
- Requirement:
    - Train at least 5 models with different training approach.
    - Record the loss and accuracy of all models.
    - Record the sensitivity of all models.

Flatness v.s. Generalization - part2 2/

- What is sensitivity:
    - Reference: https://arxiv.org/pdf/1802.08760.pdf
    - Original definition:
        - Frobenius norm of Jacobian matrix of model output (class probability) to input
        - Computationally expensive for us
    - Our definition:
        - Frobenius norm of gradients of loss to input

Flatness v.s. Generalization - part2 3/

- MNIST :
- CIFAR10 :



loss, sensitivity v.s. batch_size

accuracy, sensitivity v.s. batch_size

HW1-3 Report Questions (10%)

- Can network fit random variables?
  - Describe your settings of the experiments. (e.g. which task, learning rate, optimizer) (1%)
  - Plot the figure of the relationship between training and testing, loss and epochs. (1%)
- Number of parameters v.s. Generalization
  - Describe your settings of the experiments. (e.g. which task, the 10 or more structures you choose) (1%)
  - Plot the figures of both training and testing, loss and accuracy to the number of parameters. (1%)
  - Comment your result. (1%)
- Flatness v.s. Generalization
  - Part 1:
    - Describe the settings of the experiments (e.g. which task, what training approaches) (0.5%)
    - Plot the figures of both training and testing, loss and accuracy to the number of interpolation ratio. (1%)
    - Comment your result. (1%)
  - Part 2 :
    - Describe the settings of the experiments (e.g. which task, what training approaches) (0.5%)
    - Plot the figures of both training and testing, loss and accuracy, sensitivity to your chosen variable. (1%)
    - Comment your result. (1%)
  - Bonus : Use other metrics or methods to evaluate a model's ability to generalize and concretely describe it and comment your results.
- Check TA's examples to know what to plot !

Flatness v.s. Generalization - bonus example 1/8

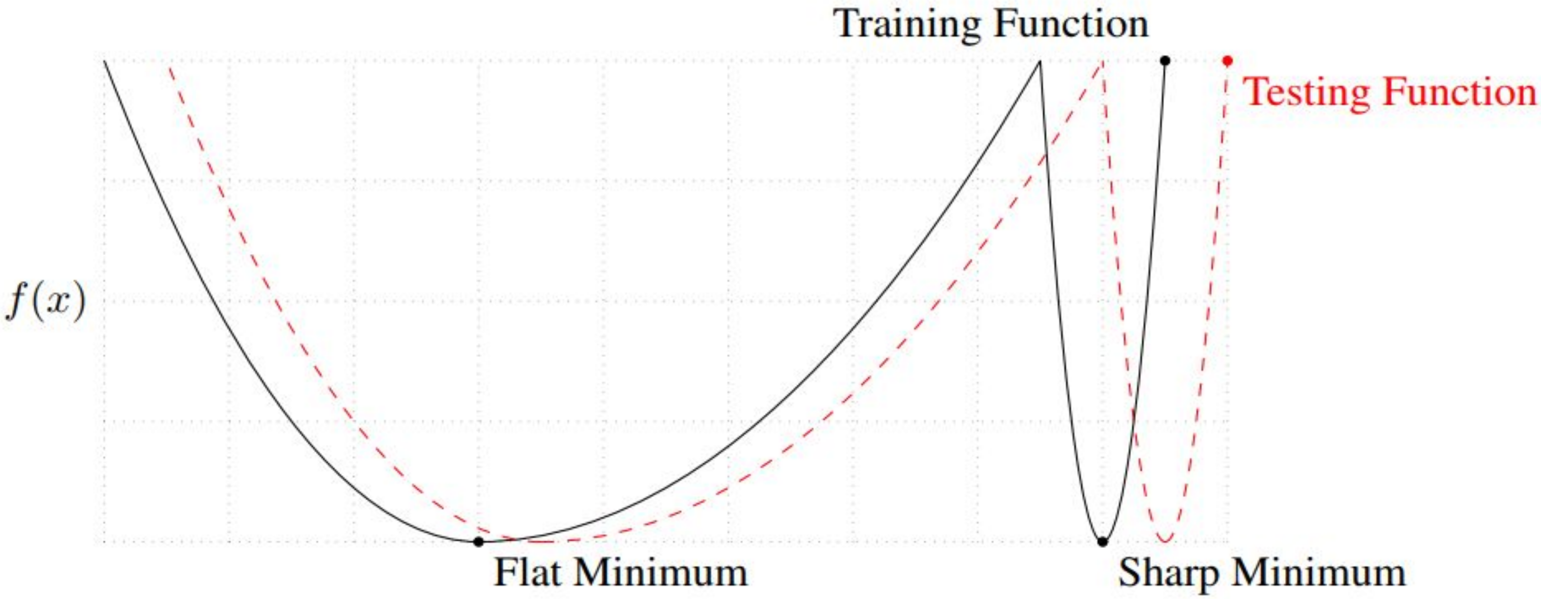
- Reference : https://arxiv.org/pdf/1609.04836.pdf
- Requirement
  - Train on MNIST or CIFAR-10
  - Use at least ten different approaches to train the same model
  - Calculate the sharpness of trained models
- Tips
  - Train on MNIST
  - Train with different batch size

Flatness v.s. Generalization - bonus example 2/8

- There is a generalization gap when using large-batch (LB) methods (instead of small-batch (SB) methods) for training deep learning models.
- The reasons (maybe more than these):
    - LB methods lack the explorative properties of SB methods and tend to zoom-in on the minimizer closest to the initial point.
    - SB and LB methods converge to qualitatively different minimizers with differing generalization properties (i.e. SB converges to flat minimizer, LB converges to sharp minimizer)
- We will focus on the second reason.

Flatness v.s. Generalization - bonus example 3/8

- Visually, it means that :



- How to measure sharpness (or flatness) ?

Flatness v.s. Generalization - bonus example 4/8

- Many methods can measure sharpness, but we will only utilize one in this assignment.
- Notations:
  - θ : vector of all parameters
  - $L(\theta)$: loss of the model given the paramters
  - $B_2(\epsilon, \theta)$: a Euclidean ball centers at θ with radius ϵ
- Sharpness:

$$\frac{\max_{\theta' \in B_2(\epsilon,\theta)} (L(\theta') - L(\theta))}{1 + L(\theta)}$$

Flatness v.s. Generalization - bonus example 5/8

- How to calculate this : $\frac{\max_{\theta' \in B_2(\epsilon,\theta)}(L(\theta')-L(\theta))}{1+L(\theta)}$
- Original paper : Use L-BFGS-B to maximize $L(\theta')$
- Around a critical point :

$$L(\theta') = L(\theta) + \frac{1}{2}(\theta' - \theta)^T(\nabla^2 L)(\theta)(\theta' - \theta) + o(\|\theta' - \theta\|_2^2)$$

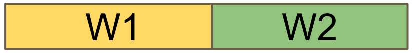
- Then :

$$\frac{\max_{\theta' \in B_2(\epsilon,\theta)}(L(\theta')-L(\theta))}{1+L(\theta)} \longrightarrow \frac{\|(\nabla^2 L)(\theta)\|_2 \epsilon^2}{2(1+L(\theta))}$$

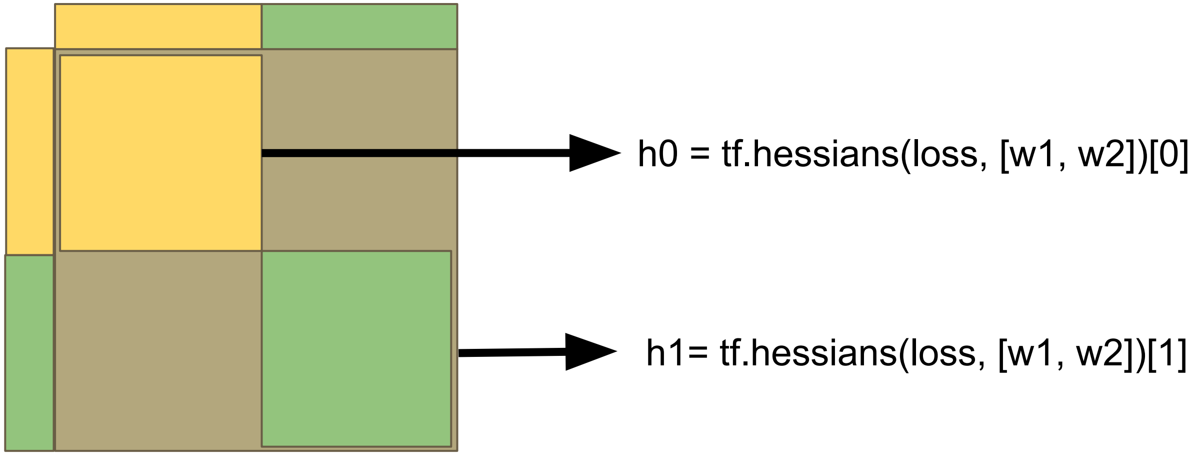
- Since 2-norm of a matrix is defined as :

$$\|A\|_2 = \max\{\|Ax\|_2 : x \in R^n \text{with} \|x\|_2 = 1\} = \sqrt{\lambda_{\max}(A^T A)}$$

Flatness v.s. Generalization - bonus example 6/8

- How to calculate Hessian matrices efficiently:
  - Use GPU : tf.hessians
  - Calculate only 500 out of 60000 examples in MNIST
- But tf.hessians only return block-diagonal part:
  - vector of all paramters : 

  - Hessian matrix :



h0 = tf.hessians(loss, [w1, w2])[0]

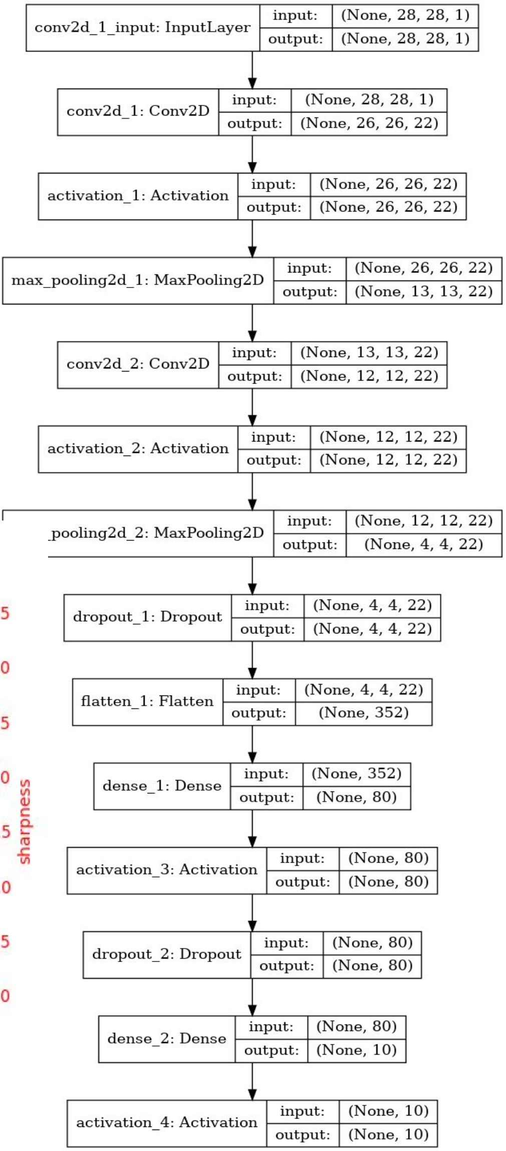
h1= tf.hessians(loss, [w1, w2])[1]

Flatness v.s. Generalization - bonus example 7/8

- If we assume off-block-diagonal elements is negligable:
    - Square of block-diagonal matrix is also block-diagonal.
    - Eigenvalues of a block-diagonal matrix is the list of all eigenvalues of each block submatrix.
    - Since we only want the largest eigenvalue, we can conclude that the 2-norm of a block-diagonal matrix is the 2-norm of block submatrix that contains the largest eigenvalue itself.
    - 2-norm of matrix A in tensorflow : tf.norm(A, 2)
    - 2-norm of matrix A in numpy : np.linalg.norm(A, 2)

Flatness v.s. Generalization - bonus example 8/8

- MNIST :
  - 20000~30000 parameters (in order to calculate hessian matrices while maintaining enough model capacity)
  - Calculate hessian matrices as mentioned in previous slide
  - epsilon : 1e-4


conv2d_1_input: InputLayer | input: (None, 28, 28, 1) | output: (None, 28, 28, 1)

conv2d_1: Conv2D | input: (None, 28, 28, 1) | output: (None, 26, 26, 22)

activation_1: Activation | input: (None, 26, 26, 22) | output: (None, 26, 26, 22)

max_pooling2d_1: MaxPooling2D | input: (None, 26, 26, 22) | output: (None, 13, 13, 22)

conv2d_2: Conv2D | input: (None, 13, 13, 22) | output: (None, 12, 12, 22)

activation_2: Activation | input: (None, 12, 12, 22) | output: (None, 12, 12, 22)

pooling2d_2: MaxPooling2D | input: (None, 12, 12, 22) | output: (None, 4, 4, 22)

dropout_1: Dropout | input: (None, 4, 4, 22) | output: (None, 4, 4, 22)

flatten_1: Flatten | input: (None, 4, 4, 22) | output: (None, 352)

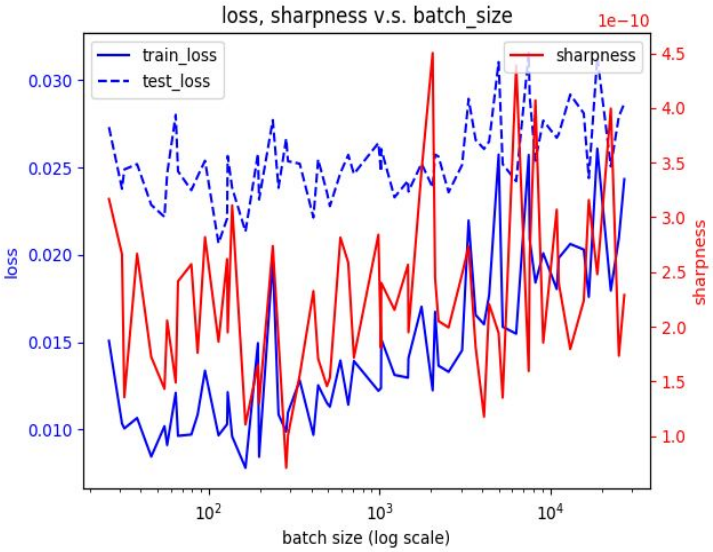
dense_1: Dense | input: (None, 352) | output: (None, 80)

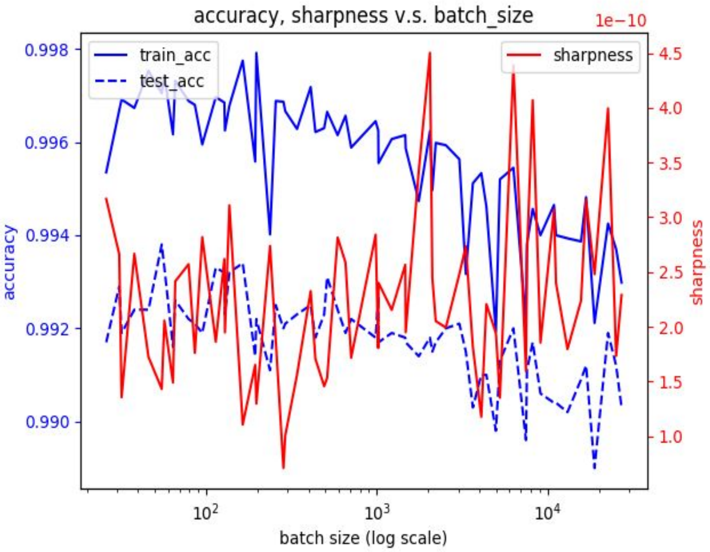
activation_3: Activation | input: (None, 80) | output: (None, 80)

dropout_2: Dropout | input: (None, 80) | output: (None, 80)

dense_2: Dense | input: (None, 80) | output: (None, 10)

activation_4: Activation | input: (None, 10) | output: (None, 10)





Flatness v.s. Generalization - more possible bonus 1/2

- Reference: https://arxiv.org/pdf/1703.04933.pdf
- This paper shows that several metrics (including sharpness) do not indicates ability of generalization for any RELU-based deep models.
- Reparametrize:
  - $\text{relu}(x \cdot (\alpha\theta_1)) \cdot \theta_2 = \text{relu}(x \cdot \theta_1) \cdot (\alpha\theta_2)$

    if $\alpha > 0$

Allow Packages

- python 3.6
- TensorFlow r1.6
- PyTorch 0.3 / torchvision
- Keras 2.0.7 (TensorFlow backend only)
- MXNet 1.1.0
- CNTK 2.4
- matplotlib
- scikit-learn 0.19.1
- Python Standard Library
- Pandas
- If you want to use other packages, please ask TAs for permission first!

Submission

- Deadline: **2018/4/6 23:59 (GMT+8)**
- Write the questions of HW1-1, HW1-2 and HW1-3 in **one** report.
- Chinese unless you are not familiar with Chinese
- At most 10 pages for HW1-1, HW1-2 and HW1-3
- Your github must have several files under directory hw1/
  - Readme.*
  - Report.pdf
  - other code
- In your Readme, state clearly how to run your program to generate the results in your report.
- Files for training is required.
- Check github collaborator. If you still not receive the confirmation, please invite TA's account (mldsta) again.

Q&A

ntu.mldsta@gmail.com

組隊

1.組隊結果公布在
https://docs.google.com/spreadsheets/d/1zcbUvkgjbVV4ghG0EbHfEZ2uvxWdcDmN2ddvsaAkk7o/edit?usp=sharing
請大家確認, 之後助教幫忙組隊的名單也會公佈在這裡。

2.自行組隊將於3/23 23:59 UTC +8 (今天)截止，之後助教將會以盡量每組湊到三個人為原則幫大家組隊

3.如果你們有兩個人已經一隊，希望找到第三個人一組，但是找不到，**請不要填表單並於3/23 23:59 UTC +8(今天)前寄信到助教信箱**。助教會盡量從尚未組隊的名單中找人跟你們一隊(不保證找得到，且不保證找到的是強者)，不會把你們拆散。