Introduction to Deep Learning

8. Model Selection, Weight Decay, Dropout

MGMT 735

Slides from Alex Smola and Mu Li

courses.d2l.ai/berkeley-stat-157

Predict Who Will Repay Their Loans

- A lender hires you to investigate who will repay their loans
  - You are given complete files on 100 applicants
  - 5 defaulted within 3 years

Image credit debt.org

A Surprising Finding

- All 5 people who defaulted wore blue shirts during interviews
- Your model may find this strong signal as well

Image credit: rumble.com

Model Evaluation

Training Error and Generalization Error

- Training error: model error on the training data
- Generalization error: model error on new data
- Example: practice a future exam with past exams
  - Doing well on past exams (training error) doesn't guarantee a good score on the future exam (generalization error)
  - Student A gets 0 errors on past exams by rote learning
  - Student B understands the reasons for the given answers

Validation Dataset and Test Dataset

- Validation dataset: a dataset used to evaluate/choose the model
  - E.g. Take out 50% of the training data
  - Should not be mixed with the training data (#1 mistake)
- Test dataset: a dataset can be used once, e.g.
  - A future exam
  - The house sale price I bided
  - Dataset used in private leaderboard in Kaggle

K-fold Cross Validation

- Useful when not sufficient data
- Algorithm:
  - Partition the training data into *K* parts
  - For *i = 1, …, K*
    - Use the *i*-th part as the validation set, the rest for training
  - Report the averaged the *K* validation errors
- Popular choices: *K = 5 or 10*

Underfitting
Overfitting

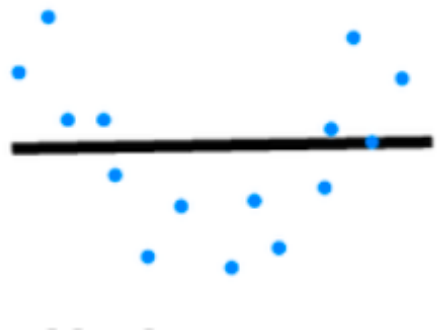
Image credit: hackernoon.com

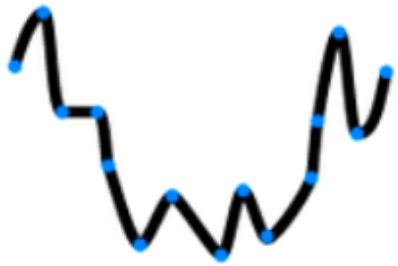
Underfitting and Overfitting

		Data complexity	
		Simple	Complex
Model capacity	Low	Normal	Underfitting
	High	Overfitting	Normal

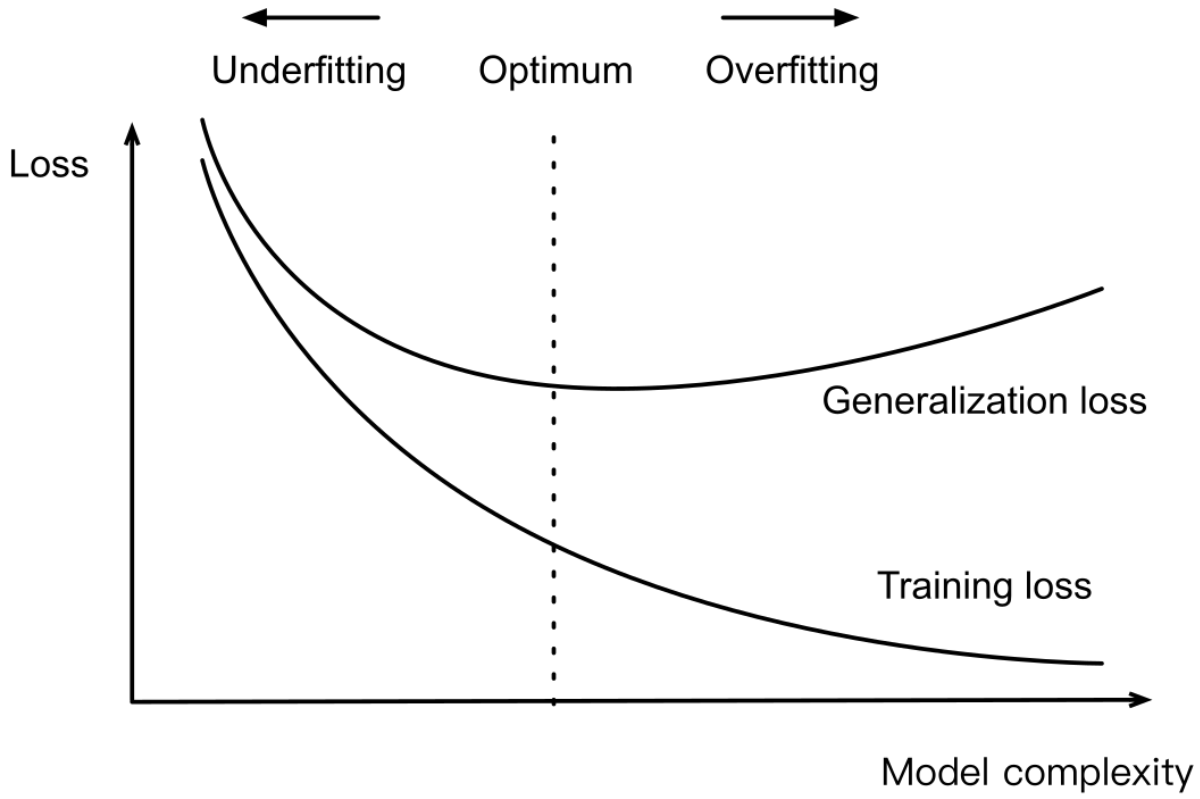
Model Capacity

- The ability to fit variety of functions
- Low capacity models struggles to fit training set
  - Underfitting
- High capacity models can memorize the training set
  - Overfitting





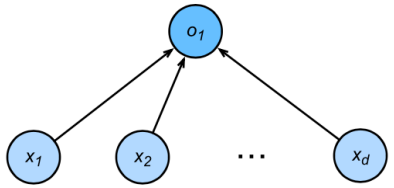
Influence of Model Complexity



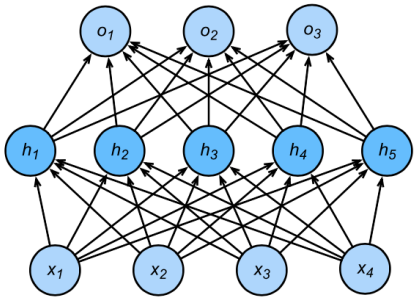
Estimate Model Capacity

- It's hard to compare complexity between different algorithms
  - e.g. tree vs neural network
- Given an algorithm family, two main factors matter:
  - The number of parameters
  - The values taken by each parameter

$d + 1$



$(d + 1)m + (m + 1)k$



VC Dimension

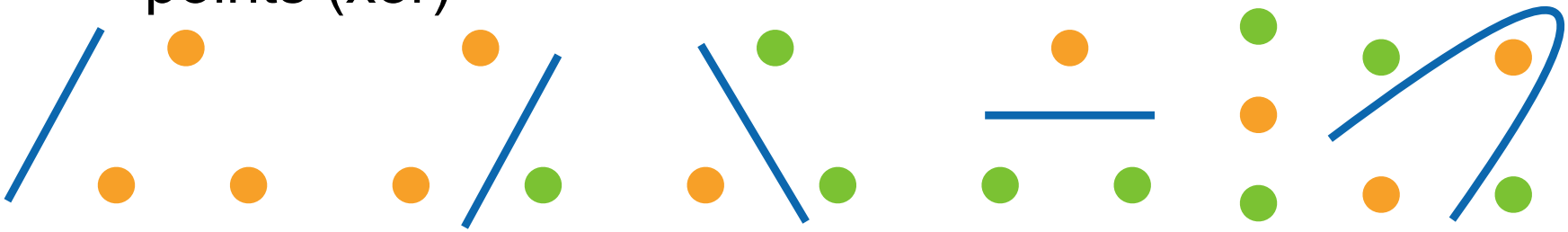
- A center topic in Statistic Learning Theory
- Measure the model capacity
- For a classification model, it's the size of the largest dataset, no matter how we assign labels, there exist a model to classify them perfectly

Vladimir **V**apnik

Alexey **C**hervonenkis

VC-Dimension for Linear Classifier

- 2-D perceptron: VCdim = 3
  - Can classify any 3 points (not co-linear), but not 4 points (xor)



- Perceptron with *N* parameters: VCdim = N
- Some Multilayer Perceptrons: VCdim = $O(N \log_2(N))$

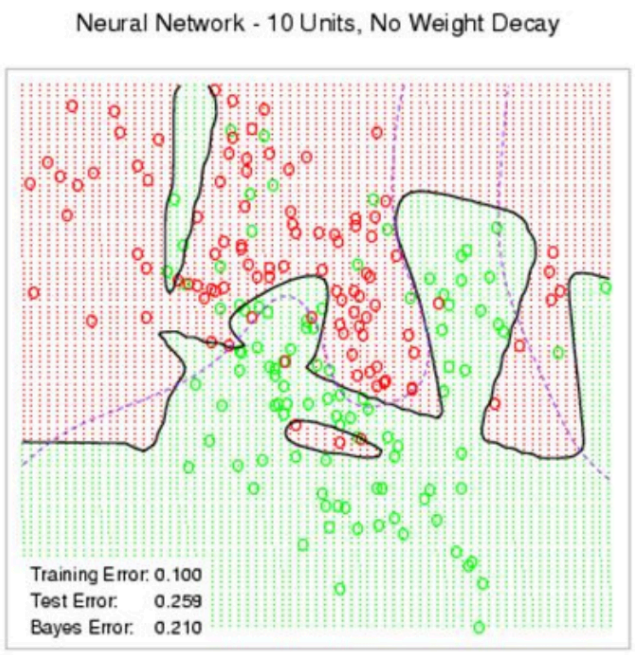
Usefulness of VC-Dimension

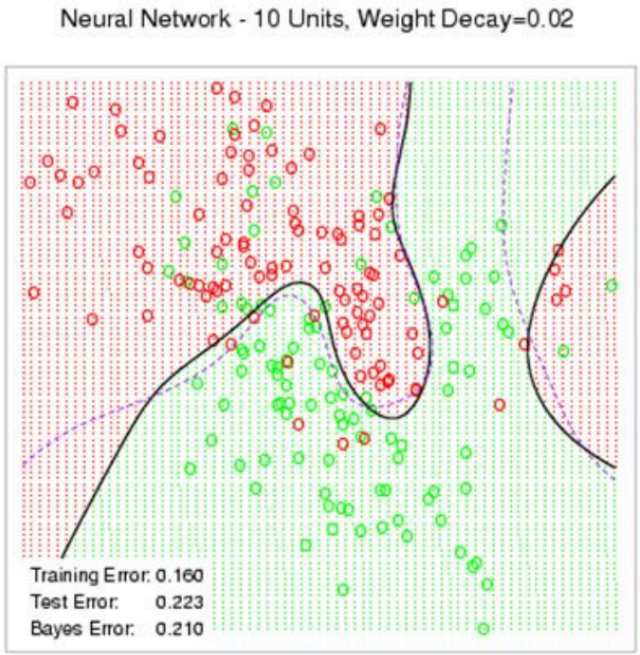
- Provides theory insights why a model works
  - Bound the gap between training error and generalization error
- Rarely used in practice with deep learning
  - The bounds are too loose
  - Difficulty to compute VC-dimension for deep neural networks
- Same for other statistic learning theory tools

Data Complexity

- Multiple factors matters
  - # of examples
  - # of elements in each example
  - time/space structure
  - diversity (golden retriever, pit bull)

Weight Decay



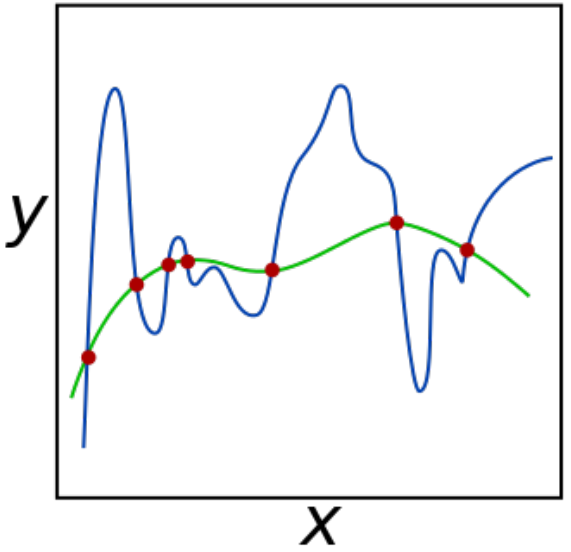


Squared Norm Regularization as Hard Constraint

- Reduce model complexity by limiting value range

$$\min \ \ell(\mathbf{w}, b) \quad \text{subject to} \quad \|\mathbf{w}\|^2 \leq \theta$$

  - Often do not regularize bias b
    - Doing or not doing has little difference in practice
  - A small θ means more regularization



Squared Norm Regularization as Soft Constraint

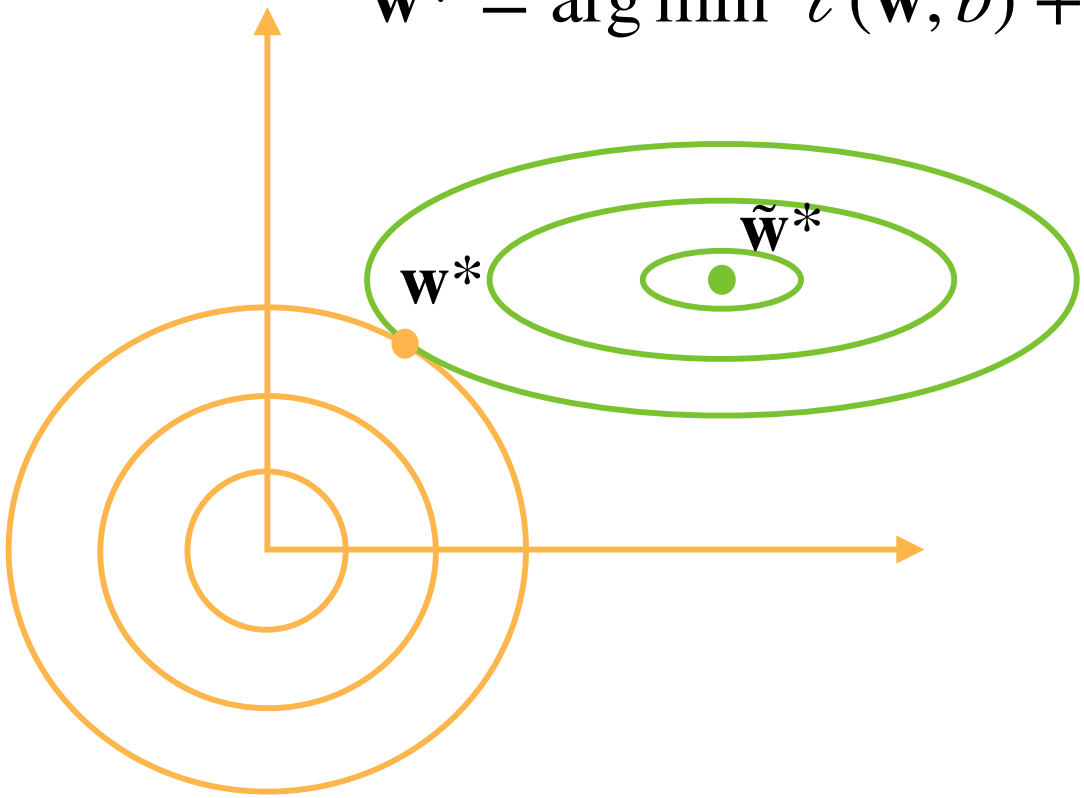
- For each θ , we can find λ to rewrite the hard constraint version as

$$\min \ \ell(\mathbf{w}, b) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

  - Can prove by Lagrangian multiplier method
  - Hyper-parameter λ controls regularization importance
  - $\lambda = 0$: no effect
  - $\lambda \to \infty, \mathbf{w}^* \to \mathbf{0}$

Illustrate the Effect on Optimal Solutions

$$\mathbf{w}^* = \arg\min \ \ell(\mathbf{w}, b) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$



$$\tilde{\mathbf{w}}^* = \arg\min \ \ell(\mathbf{w}, b)$$

Update Rule

- Compute the gradient

$$\frac{\partial}{\partial \mathbf{w}} \left(\ell(\mathbf{w}, b) + \frac{\lambda}{2} \|\mathbf{w}\|^2 \right) = \frac{\partial \ell(\mathbf{w}, b)}{\partial \mathbf{w}} + \lambda \mathbf{w}$$

- Update weight at time *t*

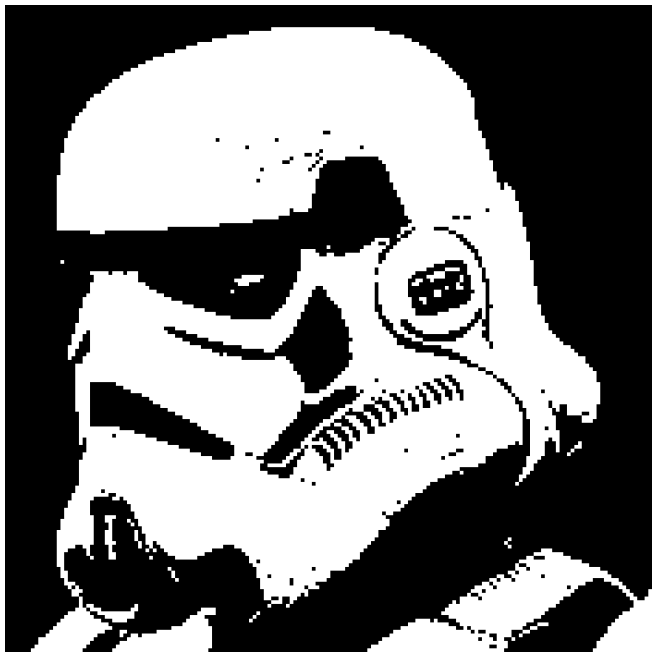
$$\mathbf{w}_{t+1} = (1 - \eta\lambda)\mathbf{w}_t - \eta \frac{\partial \ell(\mathbf{w}_t, b_t)}{\partial \mathbf{w}_t}$$

  - Often $\eta\lambda < 1$, so also called weight decay in deep learning

Dropout

Motivation

- A good model should be robust under modest changes in the input
  - Training with input noise equals to Tikhonov Regularization $=\lambda \|\Gamma W\|_F^2$
  - Dropout: inject noises into internal layers



Add Noise without Bias

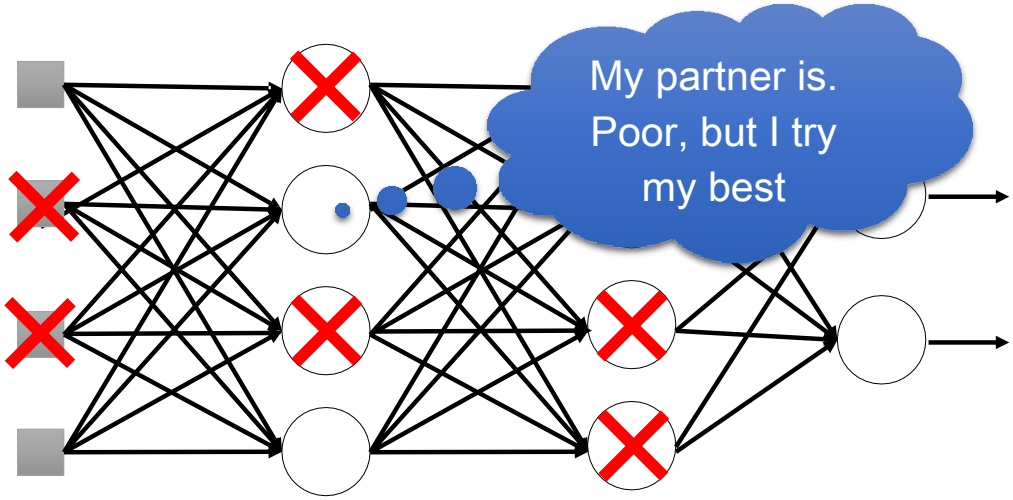
- Add noise into ***x*** to get ***x'***, we hope

$$\mathbf{E}[\mathbf{x}'] = \mathbf{x}$$

- Dropout perturbs each element by

$$x_i' = \begin{cases} 0 & \text{with probablity } p \\ \frac{x_i}{1-p} & \text{otherise} \end{cases}$$

Dropout – Intuitive Reason



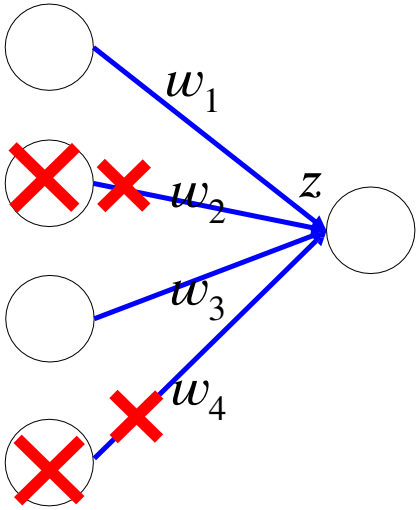
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Dropout - Intuitive Reason

- Why the weights should multiply (1-p)% (dropout rate) when testing?

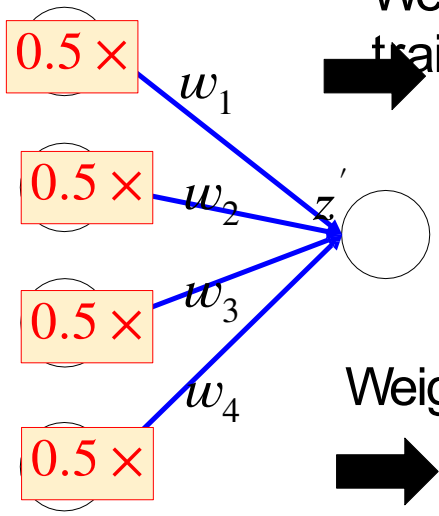
Training of Dropout

Assume dropout rate is 50%



Testing of Dropout

No dropout



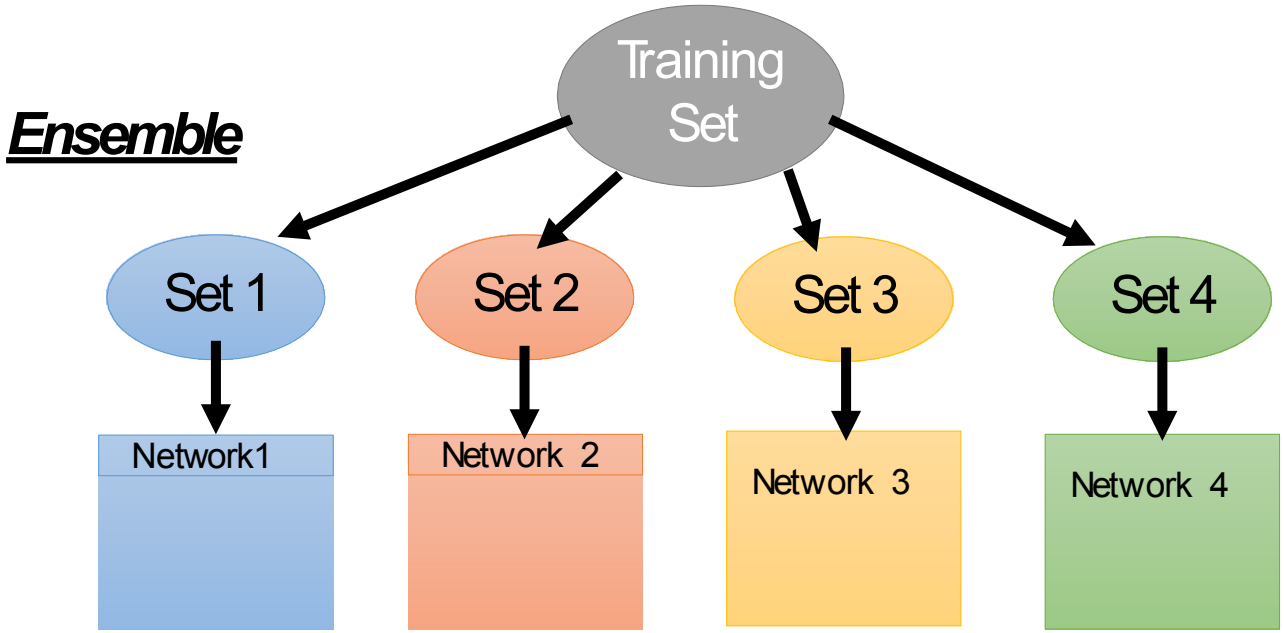
Weights from training

$z' \approx z/(1\text{-p})\%$

Weights do nothings.

$z' \approx z$

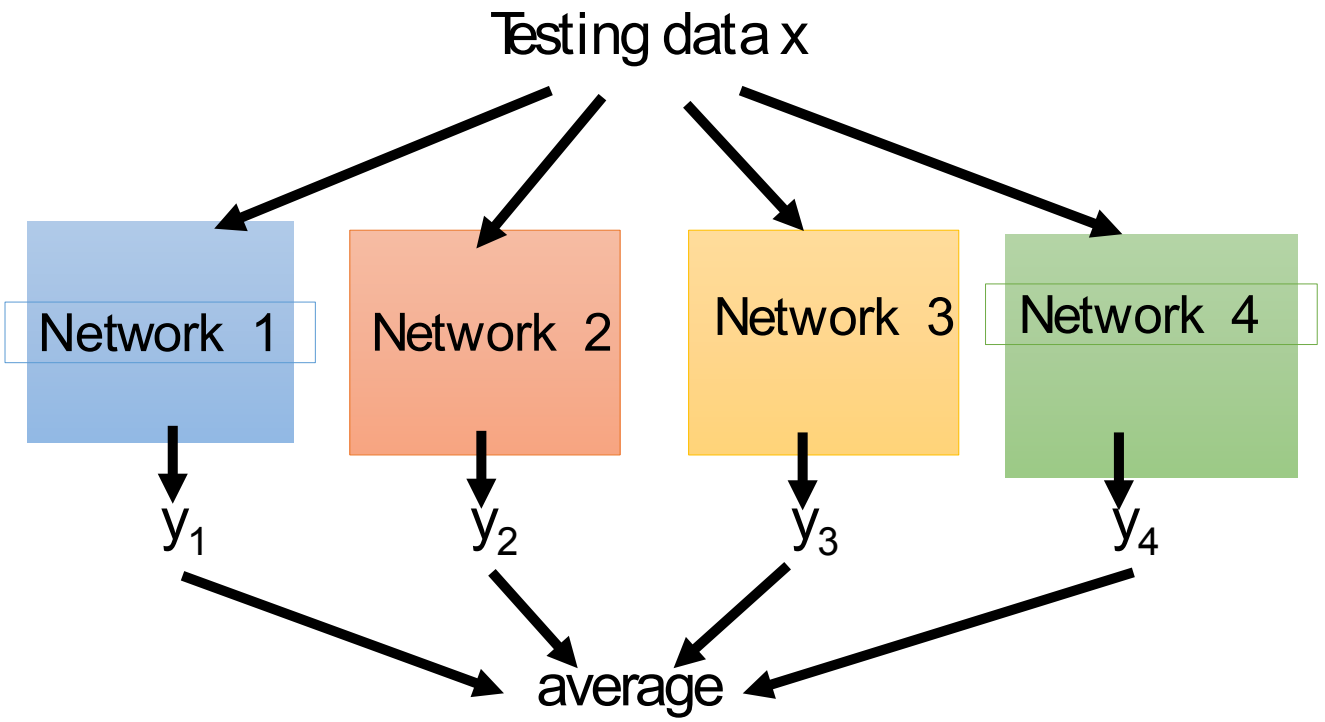
Dropout is a kind of ensemble.



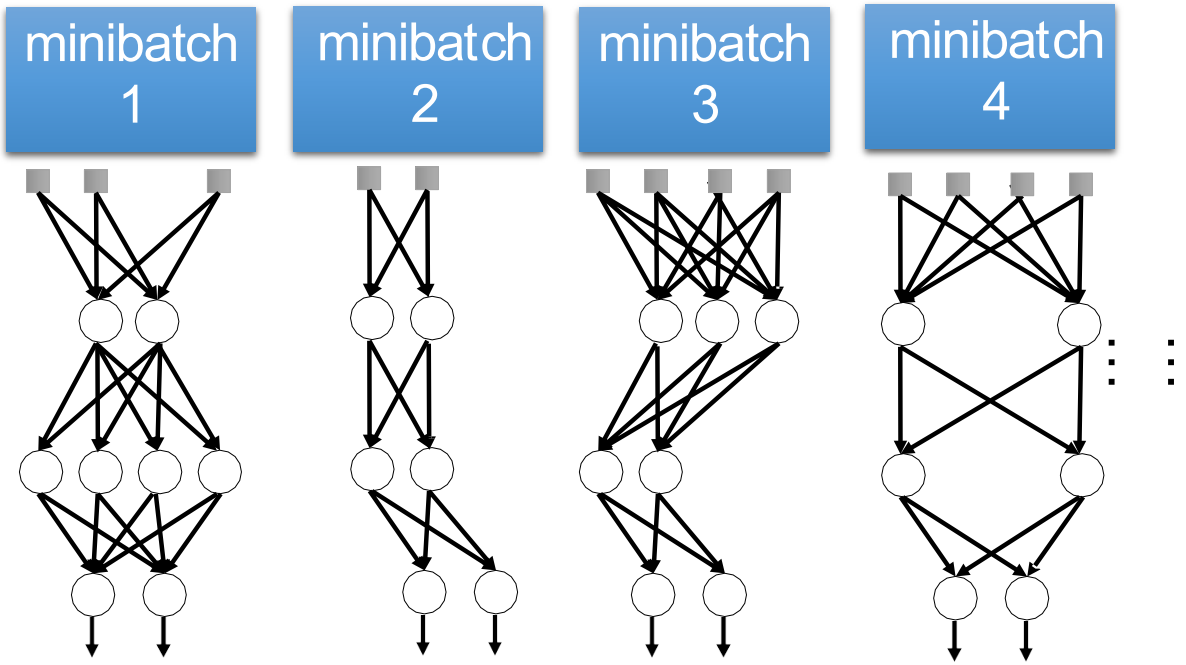
Train a bunch of networks with different structures

Dropout is a kind of ensemble.

Ensemble



Dropout is a kind of ensemble.



Training of Dropout M neurons

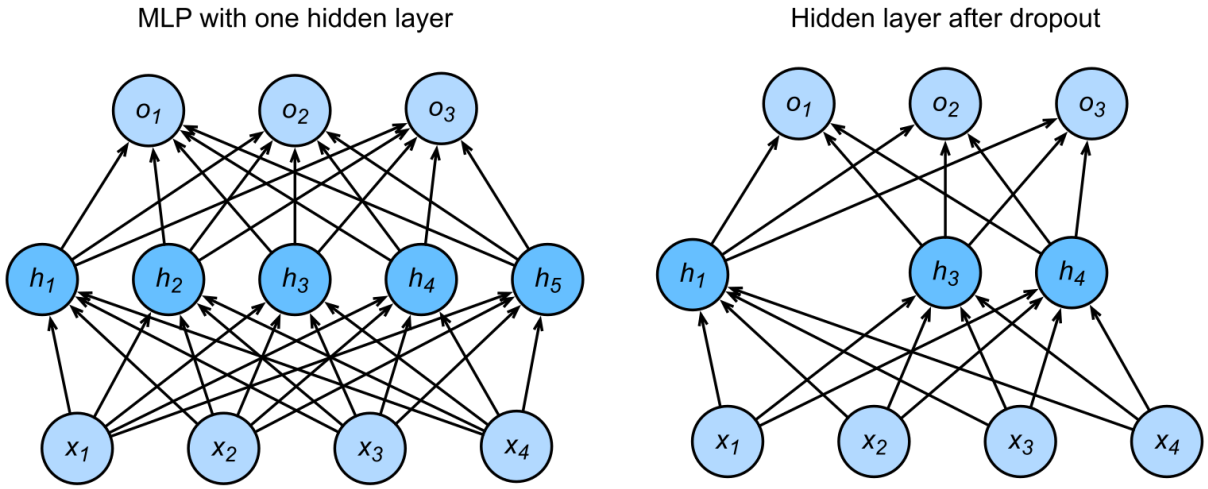
2^M ***Possible Networks***

- Using one mini-batch to train one network
- Some parameters in the network are shared

Apply Dropout

- Often apply dropout on the output of hidden fully-connected layers in each mini batch

$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{h}' = \text{dropout}(\mathbf{h})$$
$$\mathbf{o} = \mathbf{W}_2\mathbf{h}' + \mathbf{b}_2$$
$$\mathbf{y} = \text{softmax}(o)$$



Dropout in Inference

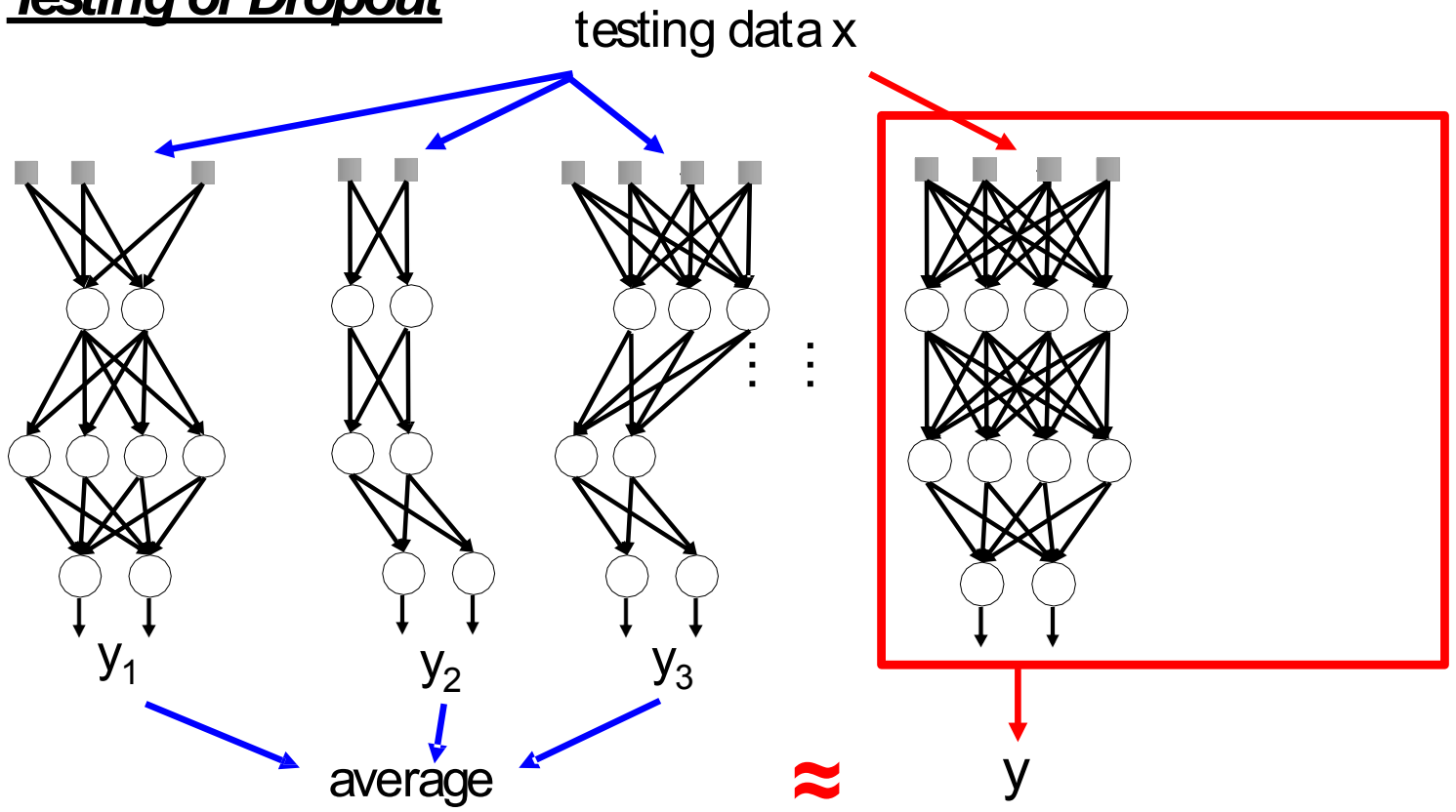
- Regularization is only used in training
- The dropout layer for inference is

$$\mathbf{h}' = \text{dropout}(\mathbf{h})$$

  - Guarantee deterministic results

Dropout is a kind of ensemble.

Testing of Dropout



Homework

- Kaggle competition
- Works with your project teammates
- Start earlier
- If you have more interests, we will access to proprietary datasets and study causality models