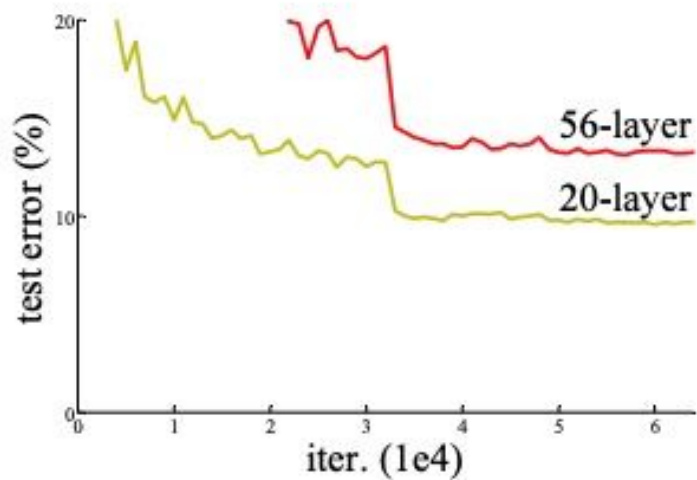


Applied Machine Learning for Business Analytics

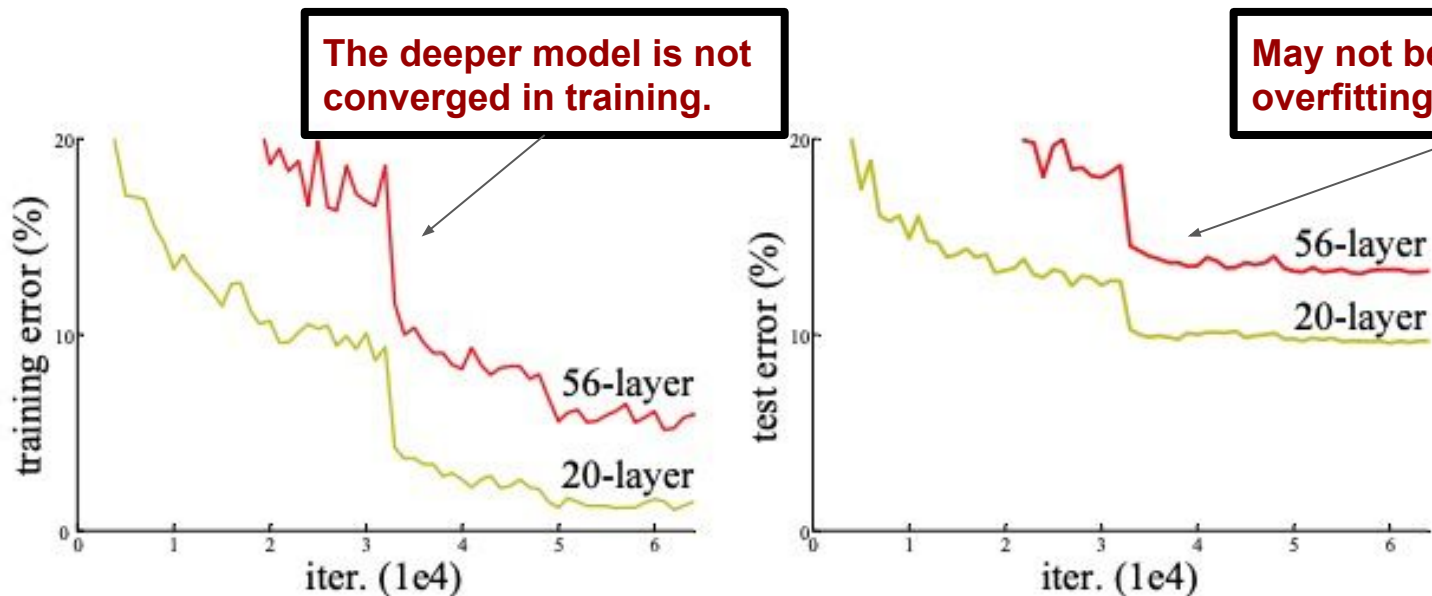
Lecture 4: Deep Learning Practices

Overfitting?



<https://arxiv.org/abs/1512.03385>

Training a deep model is challenging



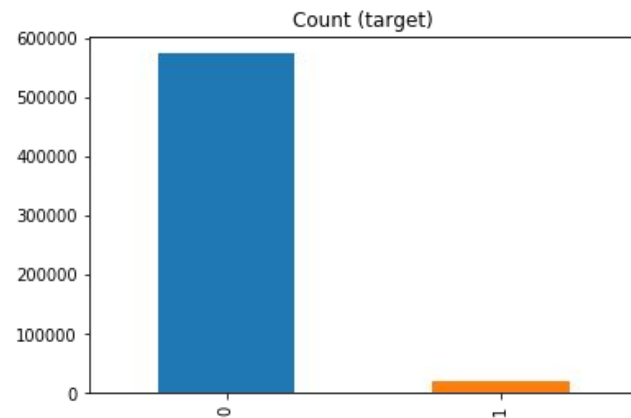
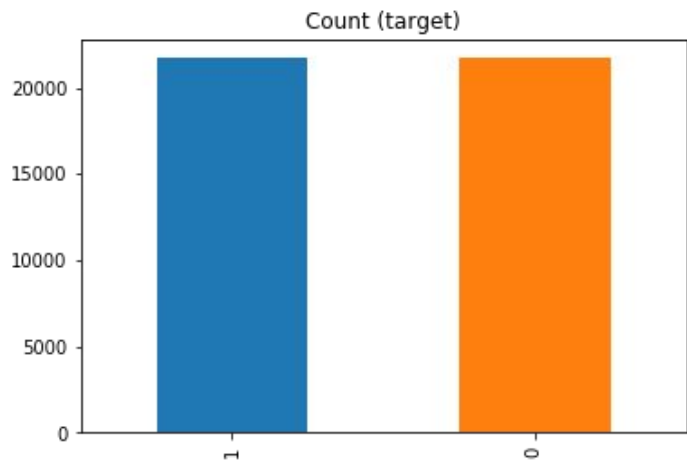
Source: <https://arxiv.org/abs/1512.03385>

Agenda

1. Class Imbalance
2. Data Augmentation
3. Network Configuration
4. Parameters Initialization
5. Optimizers
6. Regularization Techniques
7. Deep learning vs Tree-based Methods on Tabular Data

1. Class Imbalance

Small data in some categories



Class imbalance is the norm

- Bridge Structural Fault Detection
- Fraud Detection
- Disease Diagnosis
- Spam Detection

Class Imbalance is challenging

- Not enough knowledge to learn about rare classes
- Imbalanced problem: the number of fraud cases are much less than the one of normal cases.
- Rare classes are usually with high cost of wrong predictions.



Computer Facts
@computerfact



concerned parent: if all your friends jumped off a bridge
would you follow them?
machine learning algorithm: yes.

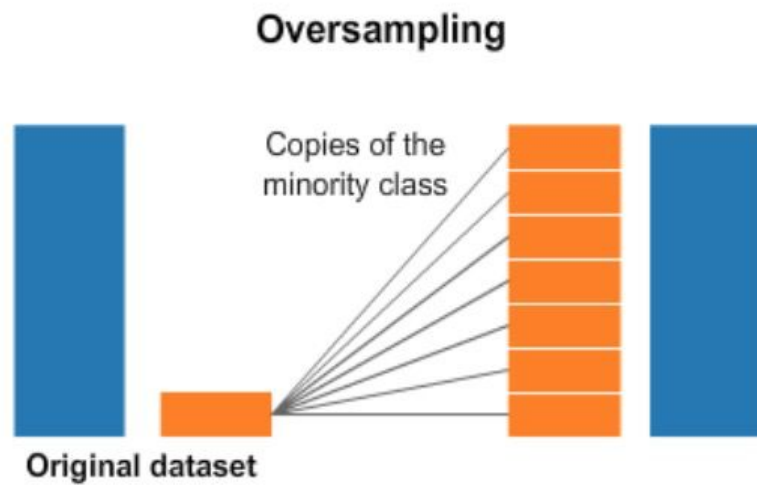
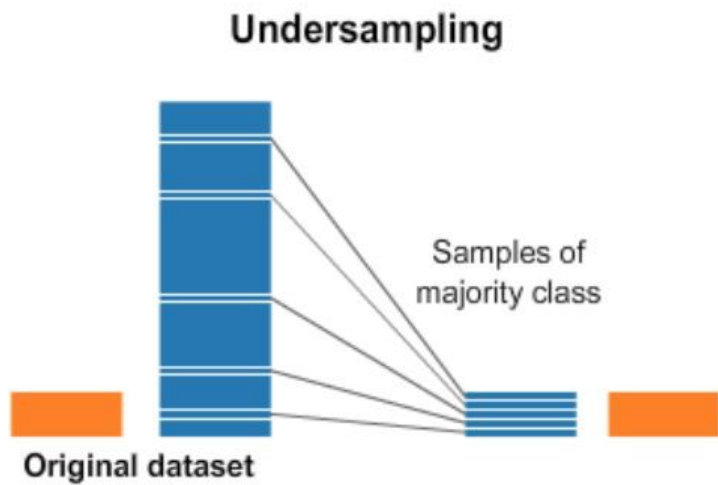
3:20 AM · Mar 16, 2018 · Twitter Web Client

7.1K Retweets **292** Quote Tweets **14.6K** Likes

How to deal with class imbalance

- Resampling
 - Add more minority samples
 - Remove majority samples
- Weights Balancing
 - Tweak the loss function
- Choose robust algorithms to class imbalance

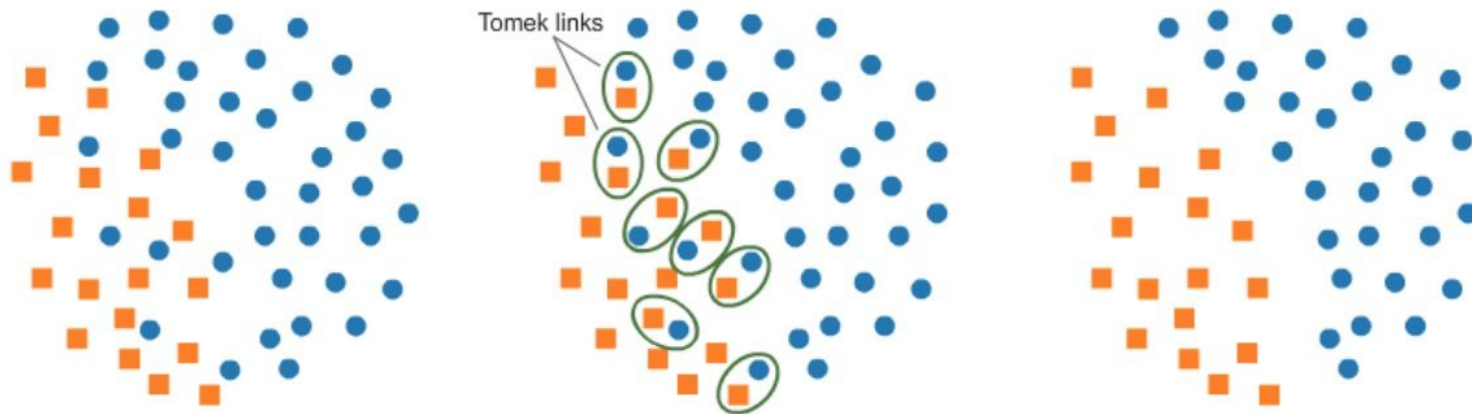
Resampling



<https://www.kaggle.com/rafjaa/resampling-strategies-for-imbalanced-datasets#t1>

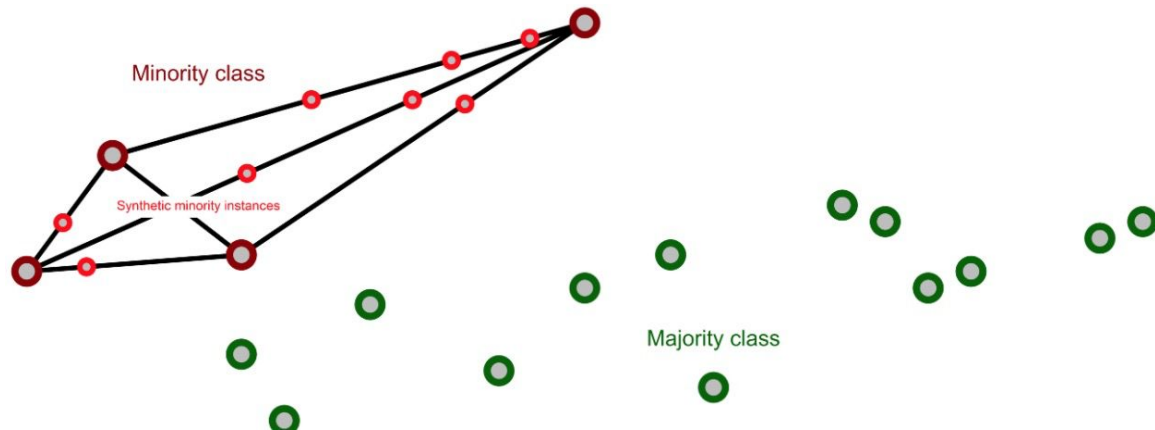
Undersampling: Tomek Links

- Find pairs of close samples of opposite classes
- Remove the sample of majority class in each pair



Oversampling: SMOTE

- Synthesize samples of minority class are convex(\sim linear) combinations of existing points and their nearest neighbors of same class.



Weight balancing

- Normal Loss

$$L_{\theta} = \sum_i L_{\theta}(x_i)$$

- Weighted Loss

$$L_{\theta} = \sum_i w_{y_i} L_{\theta}(x_i)$$

$$w_c = \frac{N}{N_{y=c}}$$

the number of training samples

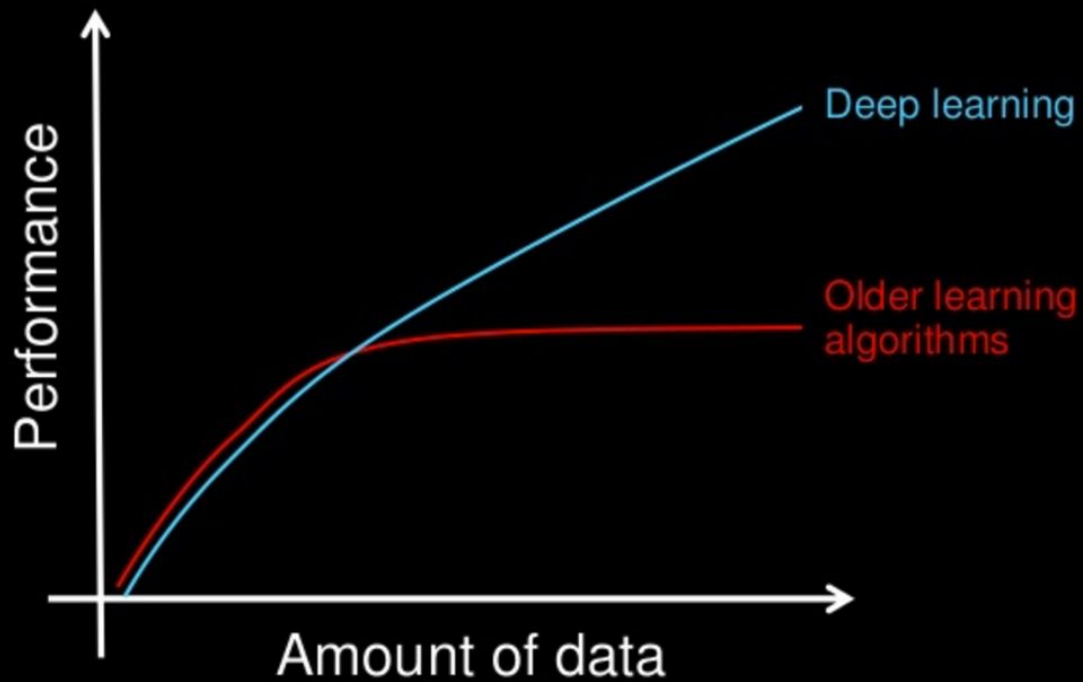
the number of training samples in the category: c

fit method

```
Model.fit(  
    x=None,  
    y=None,  
    batch_size=None,  
    epochs=1,  
    verbose=1,  
    callbacks=None,  
    validation_split=0.0,  
    validation_data=None,  
    shuffle=True,  
    class_weight=None,  
    sample_weight=None,  
    initial_epoch=0,  
    steps_per_epoch=None,  
    validation_steps=None,  
    validation_batch_size=None,  
    validation_freq=1,  
    max_queue_size=10,  
    workers=1,  
    use_multiprocessing=False,  
)
```

From Keras

2. Data Augmentation











From Andrew Ng

Data augmentation

- Deep learning models usually have billions of parameters and then require massive labeled training data
- To improve the generalization capability

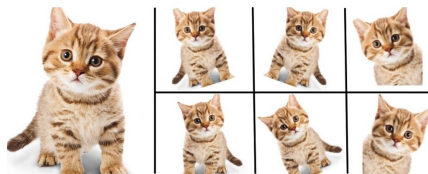
Data Augmentation: create artificially labeled training datasets

Image augmentation

| Original | Flip | Rotation | Random crop |
|--|---|--|---|
|  |  |  |  |
| <ul style="list-style-type: none">• Image without any modification | <ul style="list-style-type: none">• Flipped with respect to an axis for which the meaning of the image is preserved | <ul style="list-style-type: none">• Rotation with a slight angle• Simulates incorrect horizon calibration | <ul style="list-style-type: none">• Random focus on one part of the image• Several random crops can be done in a row |
| Color shift | Noise addition | Information loss | Contrast change |
|  |  |  |  |
| <ul style="list-style-type: none">• Nuances of RGB is slightly changed• Captures noise that can occur with light exposure | <ul style="list-style-type: none">• Addition of noise• More tolerance to quality variation of inputs | <ul style="list-style-type: none">• Parts of image ignored• Mimics potential loss of parts of image | <ul style="list-style-type: none">• Luminosity changes• Controls difference in exposition due to time of day |

How about text data

- In computer vision, data augmentation is quite common.



Enlarge your Dataset

Rotating an image a few degrees does not change its semantics

<https://blog.keras.io/building-powerful-image-classification-models-using-very-little-data.html>

- In NLP or text mining, data augmentation is challenging.

This is simple

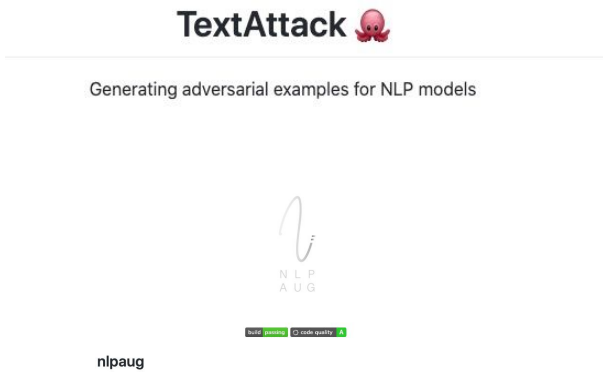


Is this simple

Semantics changed

Text augmentation

- Most of methods are very task-specific
 - Lexical Replacement
 - Back Translation
 - Text Surface Transformation
 - Random Noise Injection
 - Instance Crossover Augmentation
 - Generative Methods



3. Network Configuration

Last-Layer configuration

Depends on the task type

Last-layer activation

Loss function

Binary Classification

sigmoid

binary_crossentropy

```
model.add(layers.Dense(1, activation='sigmoid'))  
model.compile(loss='binary_crossentropy',  
              optimizer=optimizers.RMSprop(lr=1e-4),  
              metrics=['acc'])
```

Multi-class Classification

softmax

categorical_crossentropy

```
model.add(layers.Dense(10, activation='softmax'))  
model.compile(optimizer='rmsprop',  
              loss='categorical_crossentropy',  
              metrics=['accuracy'])
```

Number of unique labels in the task

Last-Layer configuration

Depends on the task type

Last-layer activation

Loss function

Multi-label Classification

Sigmoid

binary_crossentropy

```
model.add(layers.Dense(10, activation='sigmoid'))  
model.compile(loss="binary_crossentropy", optimizer='rmsprop')
```

Three Type of Classification Tasks

Binary
Classification



- Spam
- Not spam

Multiclass
Classification



- Dog
- Cat
- Horse
- Fish
- Bird
- ...

Multi-label
Classification



- Dog
- Cat
- Horse
- Fish
- Bird
- ...

<https://www.microsoft.com/en-us/research/uploads/prod/2017/12/40250.jpg>

Last-Layer configuration

Depends on the task type

Last-layer activation

Loss function

Regression to arbitrary values

Linear

mse

```
model.add(layers.Dense(1))  
model.compile(optimizer='rmsprop', loss='mse', metrics=['mae'])
```

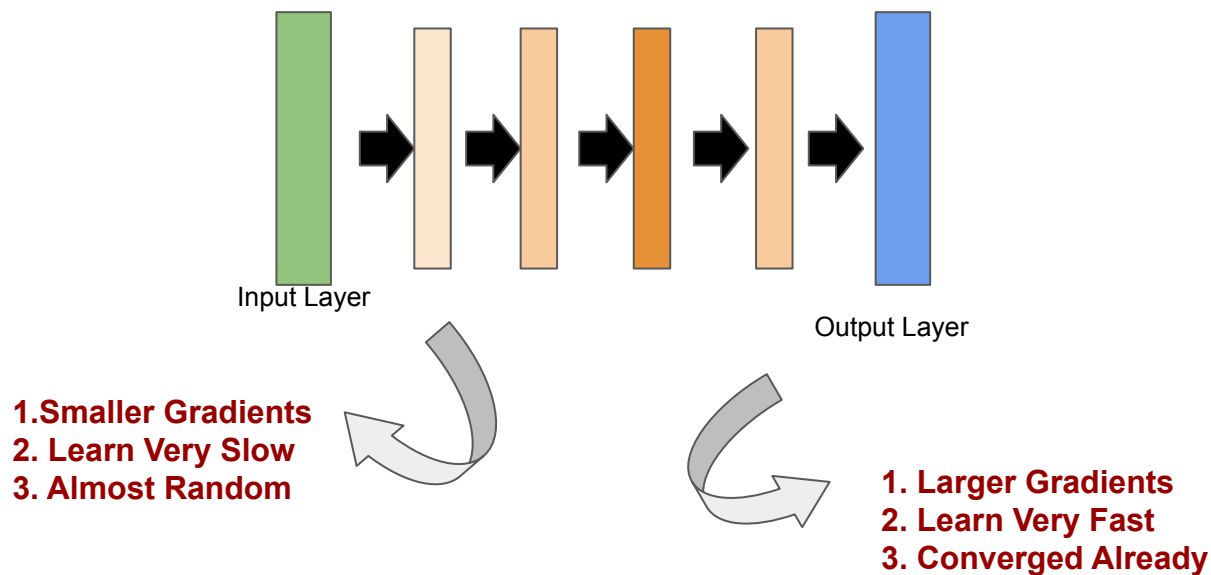
Regression to scaled values
ranging from 0 to 1

sigmoid

mse

```
model.add(layers.Dense(1, activation='sigmoid'))  
model.compile(optimizer='rmsprop', loss='mse', metrics=['mae'])
```

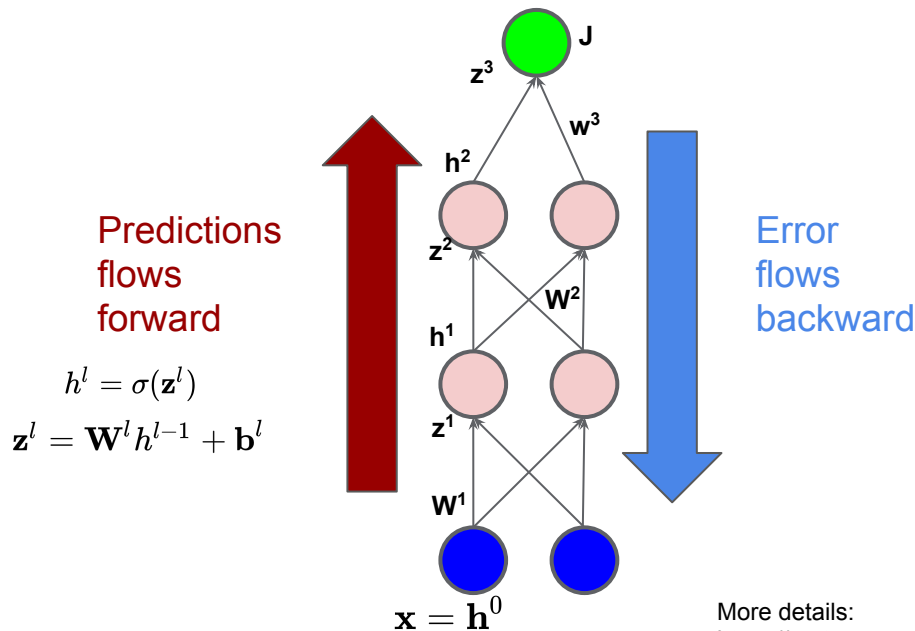
Vanishing gradient problem



Backpropagation (From Last Lecture)

Definition (from wiki):

By computing the gradient of the loss function with respect to each weight by the **chain rule**, computing the gradient one layer at a time, iterating backward from the last layer to avoid redundant calculations of intermediate terms in the chain rule



$$\frac{\partial J}{\partial \mathbf{w}^3} = \frac{\partial J}{\partial \mathbf{z}^3} \frac{\partial \mathbf{z}^3}{\partial \mathbf{w}^3}$$

$$\frac{\partial J}{\partial \mathbf{W}^2} = \frac{\partial J}{\partial \mathbf{z}^3} \frac{\partial \mathbf{z}^3}{\partial \mathbf{h}^2} \frac{\partial \mathbf{h}^2}{\partial \mathbf{z}^2} \frac{\partial \mathbf{z}^2}{\partial \mathbf{W}^2}$$

From \mathbf{w}^3

$$\frac{\partial J}{\partial \mathbf{W}^1} = \frac{\partial J}{\partial \mathbf{z}^3} \frac{\partial \mathbf{z}^3}{\partial \mathbf{h}^2} \frac{\partial \mathbf{h}^2}{\partial \mathbf{z}^2} \frac{\partial \mathbf{z}^2}{\partial \mathbf{h}^1} \frac{\partial \mathbf{h}^1}{\partial \mathbf{z}^1} \frac{\partial \mathbf{z}^1}{\partial \mathbf{W}^1}$$

From \mathbf{w}^3 From \mathbf{W}^2

More details:

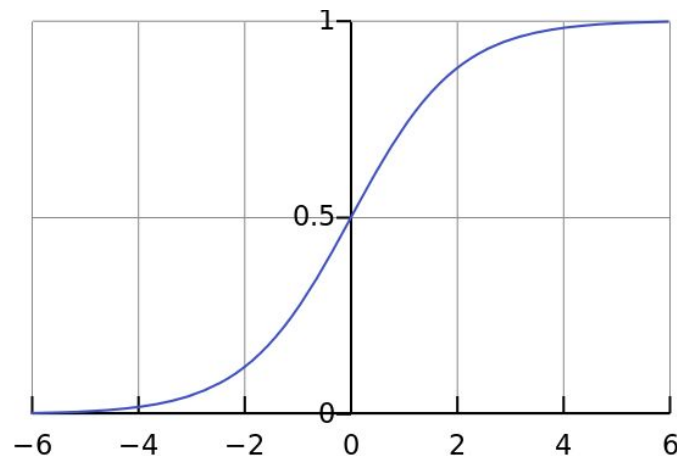
<https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/>

Sigmoid function

Equation:

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

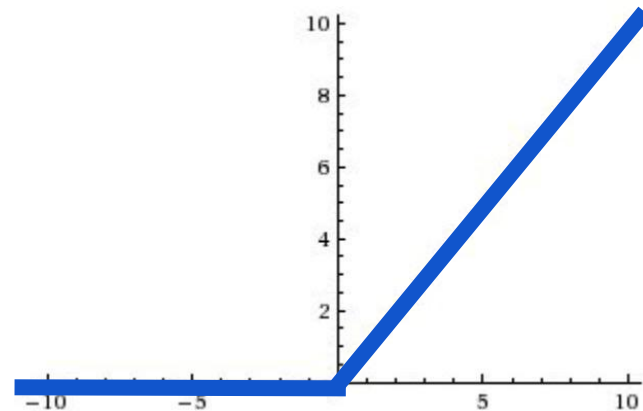
- Vanishing Gradient Problem



How about gradient curve ?

ReLU function

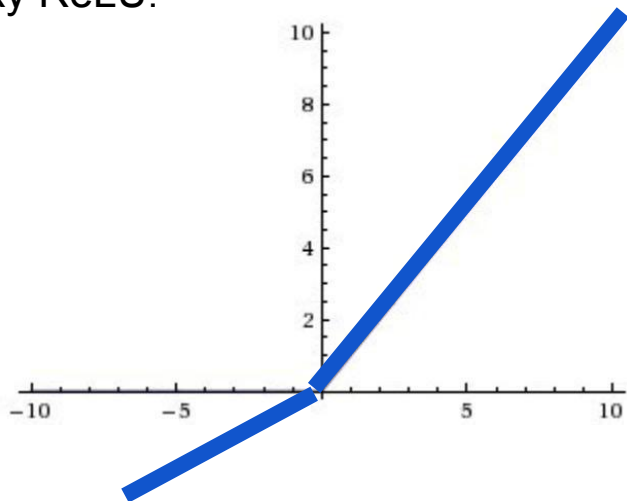
- Fast Compute
- Still have vanishing gradient problem



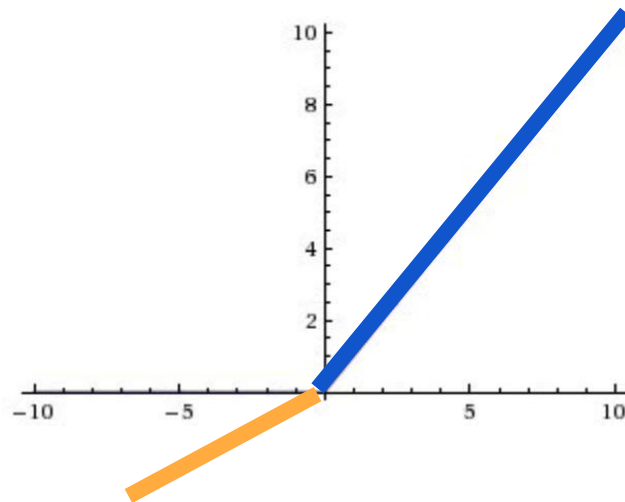
How about gradient curve ?

ReLU variants

Leaky ReLU:



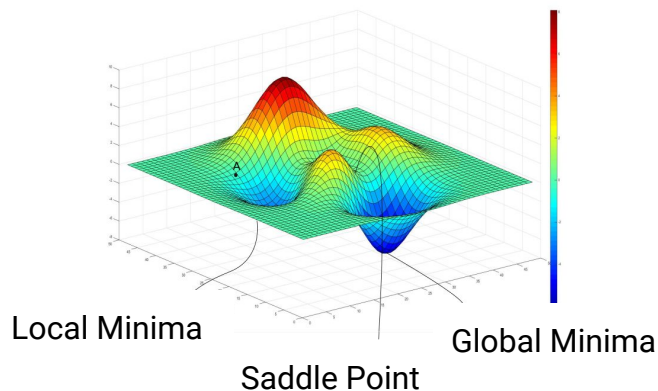
Parametric ReLU::



4. Parameters Initializations

Initialization

- Optimization for neural network in nature is a iterative method, which requires initialization



- Some general rules for initialization of model parameters:
 - Can not initialize all weights to the same value
 - Randomness should be incorporated

Normal distribution

- Initialize weights randomly, following standard normal distribution
 - The normal distribution should take into account characteristics that are unique to the architecture

For Layers with ReLu

$$\sqrt{\frac{2}{\text{size}^{[l-1]}}}$$

$$W^{[l]} = \text{np.random.randn}(\text{size_l}, \text{size_l-1}) * \text{np.sqrt}(2/\text{size_l-1})$$

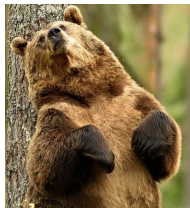
For Layers with Tanh/Sigmoid

$$\sqrt{\frac{1}{\text{size}^{[l-1]}}}$$

$$W^{[l]} = \text{np.random.randn}(\text{size_l}, \text{size_l-1}) * \text{np.sqrt}(1/\text{size_l-1})$$

Transfer learning

Task: Build a bear/cat classifier



bear

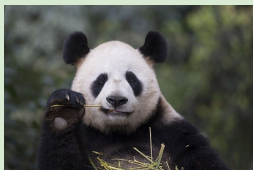


cat

Available Data: not **directly** related



dog



panda

similar domain, different tasks



bear



cat

Different domains, similar task

Applications

- Sentiment Analysis
 - Available data: IMDB reviews



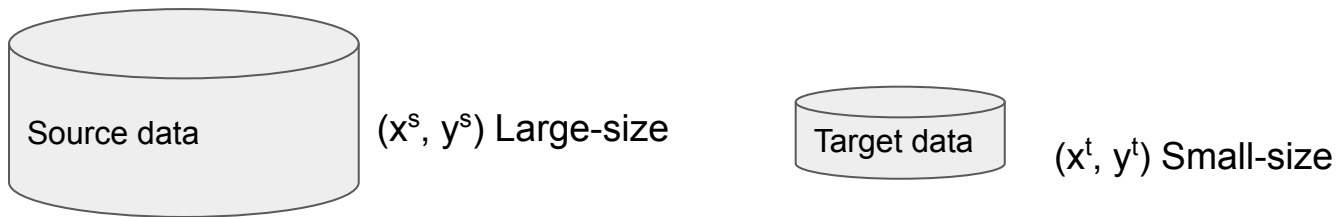
- Target tasks: Teaching feedback analysis
- Image Classification:
 - Available data: Imagenet Dataset



- Target Task: Cancer Diagnostic (Medial Image)

How to transfer knowledge

- Task Definition:

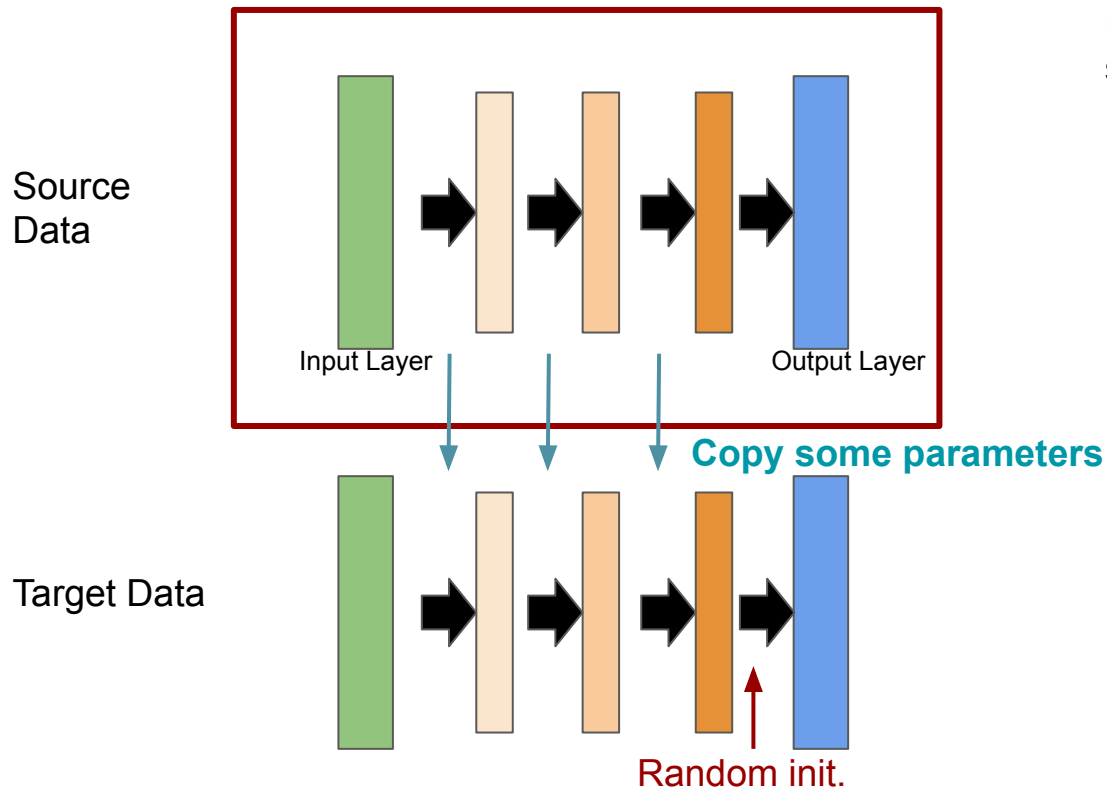


- Steps:

- Train a model using the source data
- Transfer layer from the model trained in source domain to the model in target domain
- Fine-tune the model using the target data

Any concerns?

Layer transfer



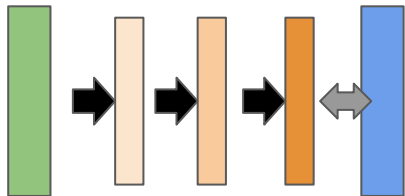
Neural Network: Layer-wise self-contained

1. **Same Task:**
Copy all layers' parameters
2. **Different Tasks:**
Random initialize the softmax/last layer and copy the rest layers' parameters

Fine-tune

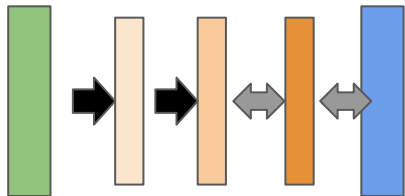
Target Data Size

Small



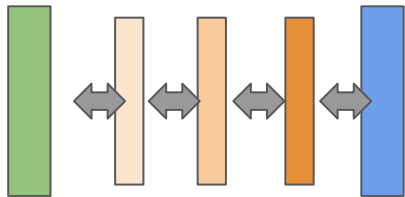
Freeze all layers, train weights on softmax/regression layer

Medium



Freeze most layers, train weights on last layers and softmax/regression layer

Large



Fine-tune all layers

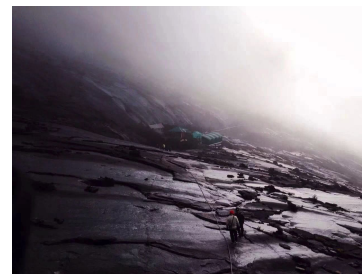
5. Optimizers for Neural Network

SGD

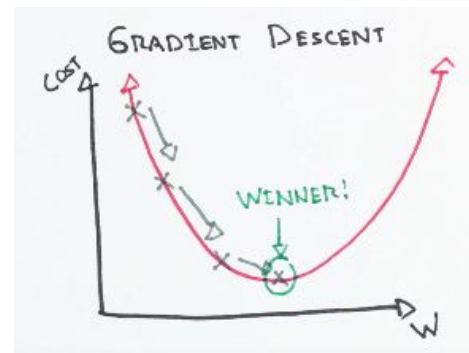
Gradient for loss function f
over parameters, which
computed by BP algorithm

$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

New Parameters Guess Current Parameters Guess Learning Rate

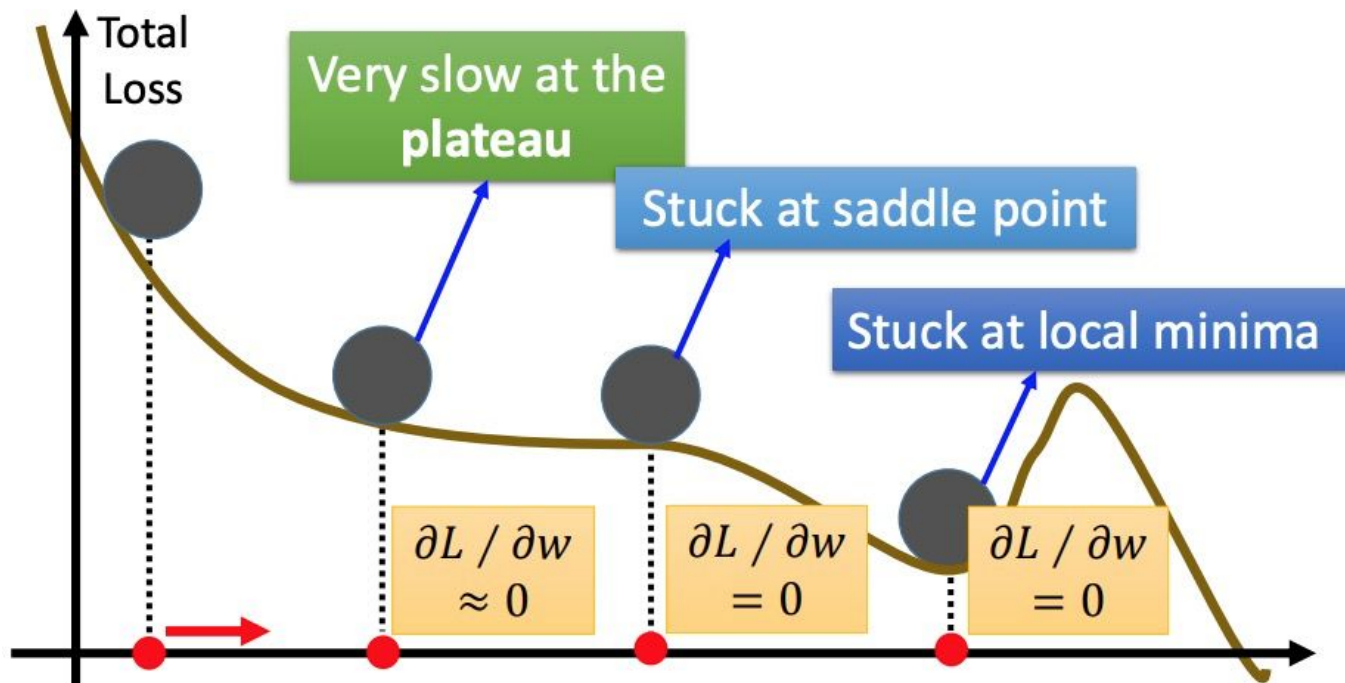


Like hiking down a mountain



Credit: https://ml-cheatsheet.readthedocs.io/en/latest/gradient_descent.html

Hard to find optimal network parameters




Source: <https://speech.ee.ntu.edu.tw/~tlkagk/>

Momentum

- Core idea: the current gradient computation will keep the direction as the previous gradient computation

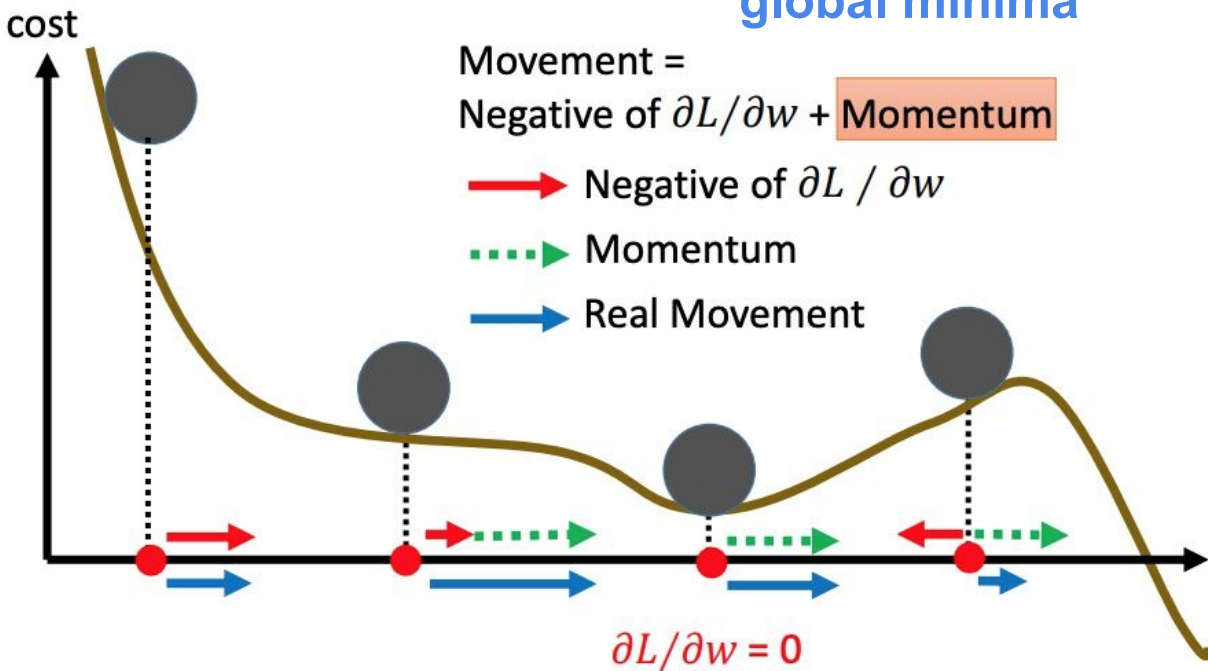
Updated vector of the previous time step


$$v_t = \beta v_{t-1} + \alpha \nabla J(\theta_t)$$
$$\theta_{t+1} = \theta_t - v_t$$

- Accelerate SGD
- Dampens Oscillations
- Two Parameters to tune

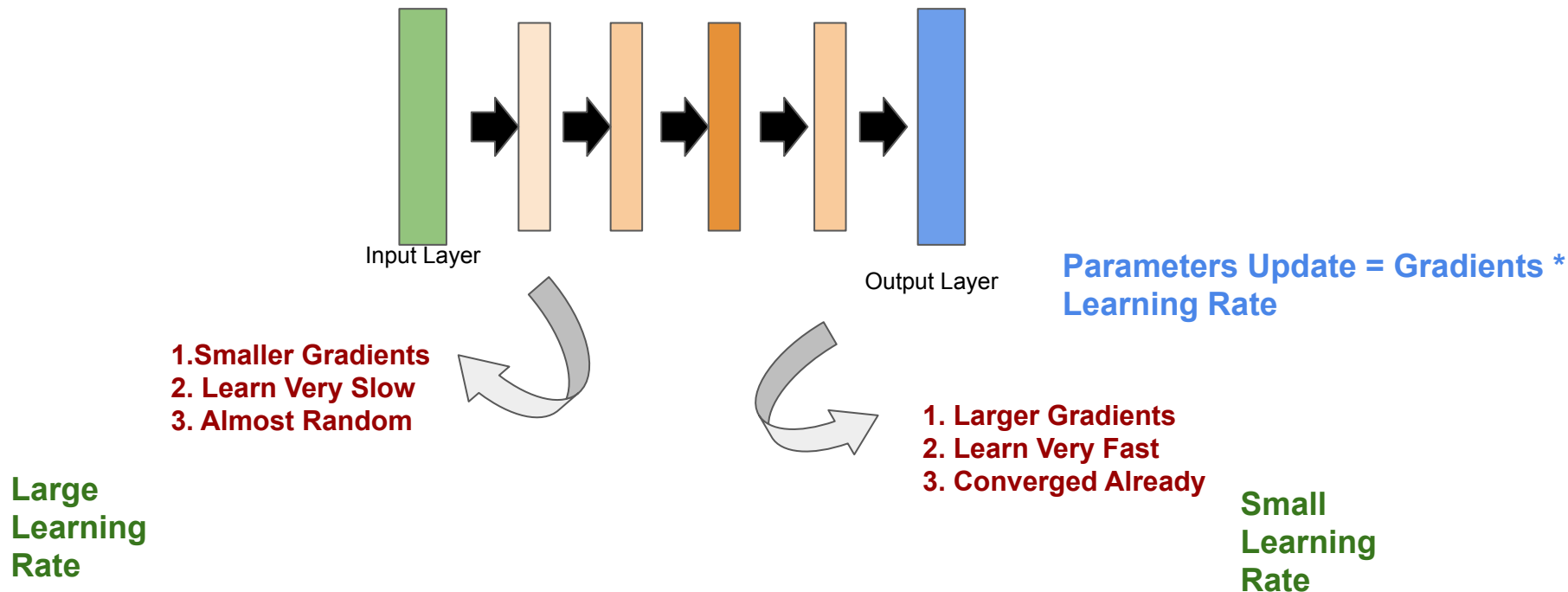
Momentum

Improve the chance to find the global minima



Source: <https://speech.ee.ntu.edu.tw/~tlkagk/>

Separated adaptive learning rate



Keep a moving average of the squared gradient for each parameter to change the learning rate.

How to select the optimizer

- Except SGD, Momentum, RMSprop and Adam, other popular methods include Adadelta and Adagrad.
- It is hard to find a general answer
- Adam is the most commonly used technique
- If you want to train a deep or complex neural networks with fast converge, do not just use SGD.

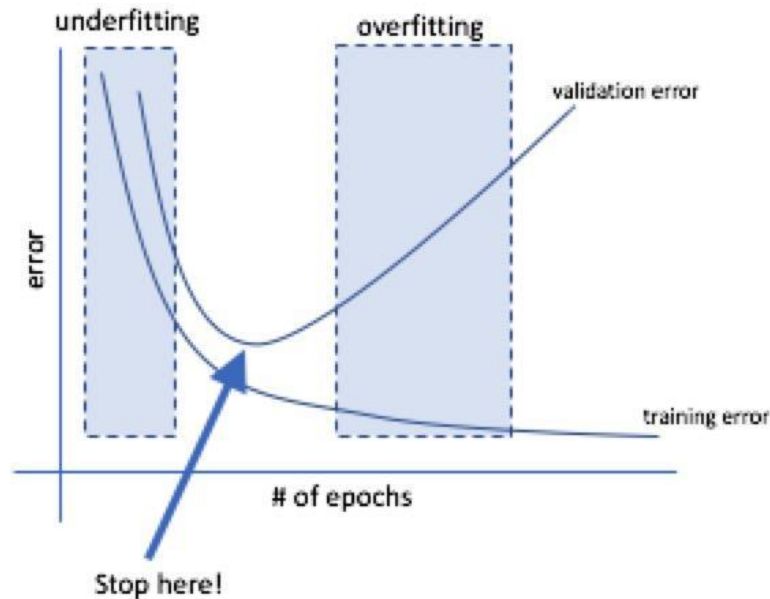
6. Regularization Techniques

Overfitting for NN

- Neural Network with a deep structure easily get overfitted
 - Early stopping
 - Parameters Regularization
 - Dropout
 - Most effective: Train with more data.

Early stopping

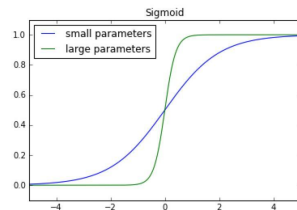
- Watch the validation curve
- Stop updating the weights once validation errors starts increasing



In Keras: https://keras.io/api/callbacks/early_stopping/

Parameter regularization

- Why large model parameters should be penalized:
 - In NN, inputs are linearly combined with parameters. Therefore, large parameters can amplify small changes in the input.
 - Large parameters may **arbitrarily** increase the confidence in our predictions.



To make sure that parameters are not too large and then the model is not overfitting
Add regularization terms to the loss function

$$\dots + \lambda g(\theta)$$



Control the degree to which we select to penalize large parameters

Regularization terms

- L1 Regularization:

$$g(\theta) = ||\theta||_1$$

L1-norm is commonly used for feature selection as it tends to produce sparse parameter vectors where only the important features take on non-zero values

- L2 Regularization:

$$g(\theta) = ||\theta||_2^2$$

L2-Norm does not tend to push less important weights to zero and typically produces better results when training a model.

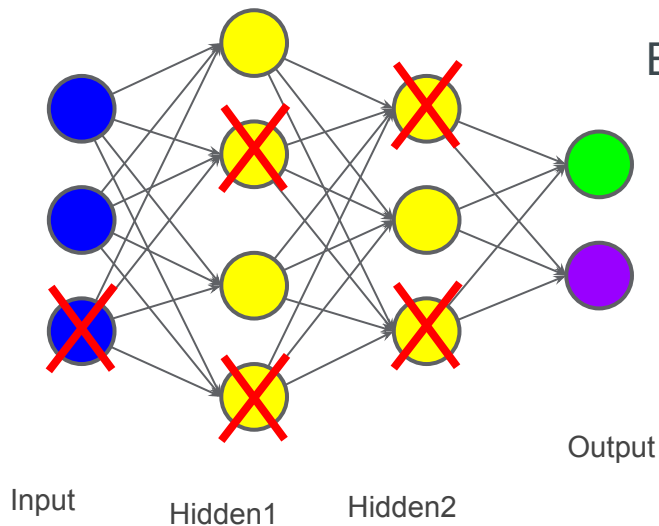
- Elastic Net:

$$g(\theta) = \alpha ||\theta||_1 + (1 - \alpha) ||\theta||_2^2$$

Trade-off between L1 and L2 Regularization techniques

Dropout

Training:

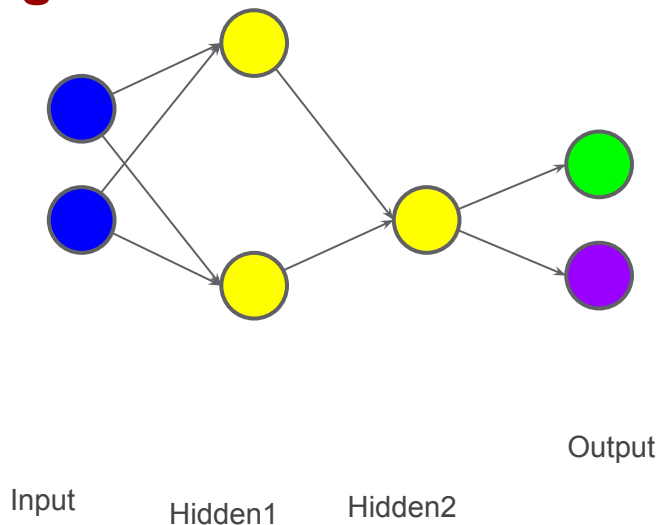


Each mini-batch before updating the parameters

1. Each neuron has **%p** to dropout(mask)

Dropout

Training:



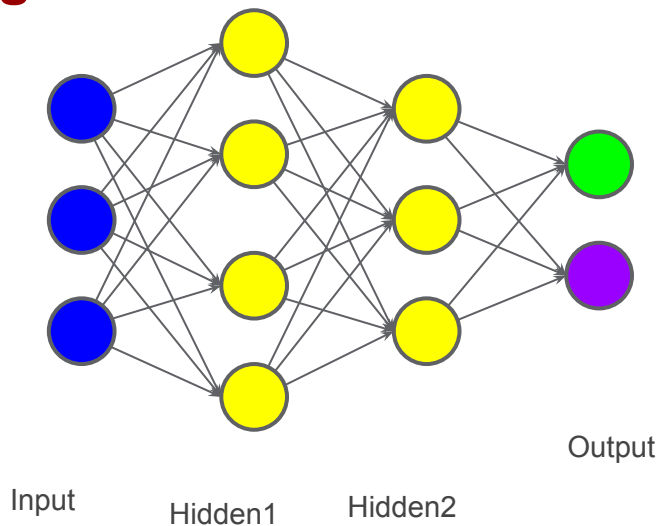
Each mini-batch before updating the parameters

1. Each neuron has **%p** to dropout(mask)
2. The network structure is changed (More Thinner!)
3. Using the updated network structure for training

For each mini-batch, we resample the dropout neurons.

Dropout

Testing:



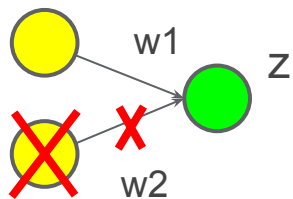
No dropout, but shrink weights following the rule:

If the dropout rate during training is $p\%$, all the weights will time $1-p\%$.

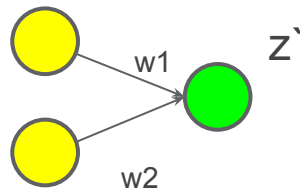
When many people work together, they usually rely on others to do more of the work and share the same results.

Dropout

Training: Assume dropout rate is 50%



Testing: No dropout



Directly Copy:

$$z' = 2z$$

Weight multiply $1-p\%$:

$$z' \sim z$$

Dropout effects

Experimental Studies on MNIST dataset:

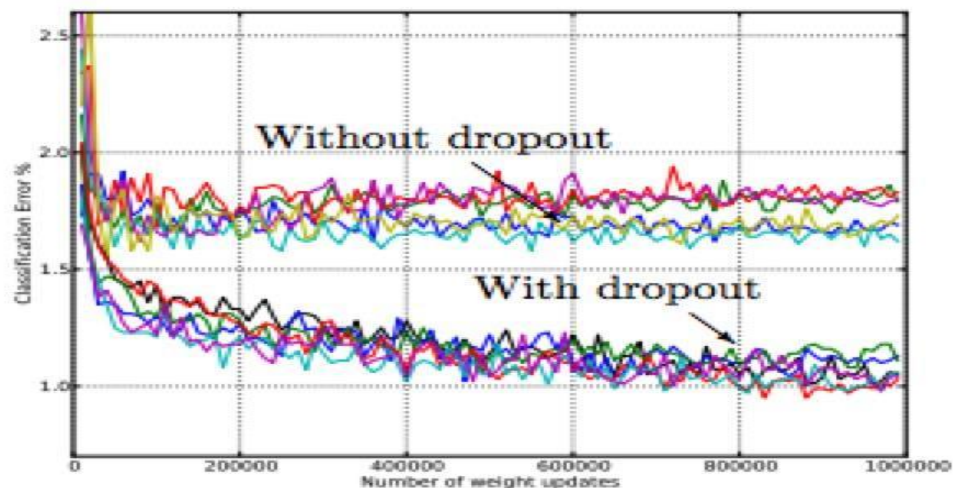


Figure 4: Test error for different architectures with and without dropout. The networks have 2 to 4 hidden layers each with 1024 to 2048 units.

7. Deep Learning vs Tree-based Methods on Tabular Data

Why do tree-based models still outperform deep learning on tabular data?

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ISIR, CNRS, Sorbonne University

Gaël Varoquaux
Soda, Inria Saclay

Abstract

Model comparison

Tree-based Models outperform deep learning on tabular data

Based on 45 middle-sized datasets
(10, 000 samples)

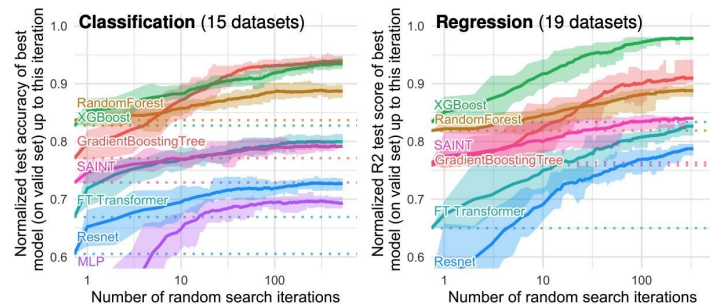


Figure 1: **Benchmark on medium-sized datasets, with only numerical features.** Dotted lines correspond to the score of the default hyperparameters, which is also the first random search iteration. Each value corresponds to the test score of the best model (on the validation set) after a specific number of random search iterations, averaged on 15 shuffles of the random search order. The ribbon corresponds to the minimum and maximum scores on these 15 shuffles.

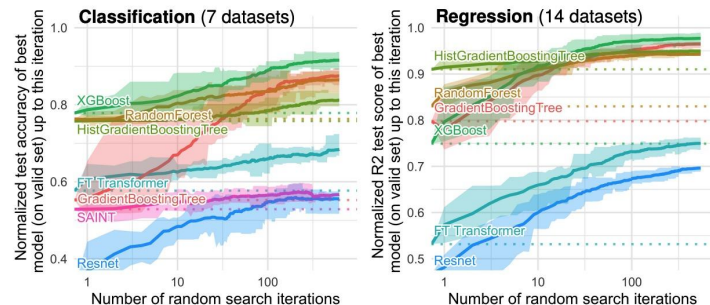


Figure 2: **Benchmark on medium-sized datasets, with both numerical and categorical features.** Dotted lines correspond to the score of the default hyperparameters, which is also the first random search iteration. Each value corresponds to the test score of the best model (on the validation set) after a specific number of random search iterations, averaged on 15 shuffles of the random search order. The ribbon corresponds to the minimum and maximum scores on these 15 shuffles.

Why?

- Deep learning bias to the overly smooth solution, while tree-based models are able to generate irregular decision boundaries
- Deep learning are very sensitive to uninformative features which could be easily spotted in tabular data, while tree-based models are more robust

Deep Learning for unstructured data

- Deep learning are good at capturing high dimensional and spatial patterns/interactions among data
- Therefore, for image, video, text and even audio, deep learning is still the first choice especially enough data are present

Next Class: Auto-encoders