# Training neural network

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## **Neural Network**

# Machine Learning as Optimization

Supervised learning

 $\min_{ heta} d(y, \hat{y})$ 

where  $\hat{y} = f(X, \theta)$ 

- $\circ$   $\theta$  is the parameter
- $\circ$   $\hat{y}$  is output, X is input
- y is ground truth
- d is the objective function
- Unsupervised learning some oracle function r: low rank, sparse, K
- where  $\hat{y} = f(X, \theta)$  $\min_{ heta} r(\hat{y})$

# Machine Learning as Optimization

Regularized supervised learning

$$\min_{ heta} d(y,\hat{y}) + r(\hat{y}) \ ext{where } \hat{y} = f(X, heta)$$

- Probabilistic interpretation
- r measures prior probability

 $\Rightarrow d(y,\hat{y}) + r(\hat{y}) = -\log p(y)$ 

 $r(\hat{y}) = -\log p(\hat{y})$ 

 $d(y,\hat{y}) = -\log p(y|\hat{y})$ 

d measures conditional probability

- Probability approach is more constrained than the optimization-approach due to normalization problem
- Not easy to represent uniform distribution over [0, \infty]

## Gradient descent

$$\min_{ heta} d(y, \hat{y}) + r(\hat{y})$$
 $ext{where } \hat{y} = f(X, heta)$ 

- Can be solved by an ODE:  $\theta = -\frac{\partial}{\partial t}$  $\partial C(\theta(t))$  $\theta\theta$
- Discretizing with step length λ we get gradient descent with learning rate \(\lambda\)

$$\dot{ heta} pprox rac{ heta_{t+\lambda} - heta_t}{\lambda} \hspace{0.5cm} \stackrel{ ext{Derive}}{=} \hspace{0.5cm} rac{ heta_{t+\lambda}}{ heta_t} = heta_t - \lambda rac{\partial C( heta)}{\partial heta}$$

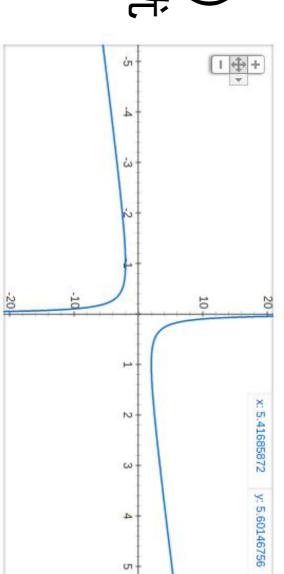
Convergence proof

$$\frac{\mathrm{d}C(\theta)}{\mathrm{d}t} = \frac{\partial C(\theta)}{\partial \theta} \frac{\mathrm{d}\theta}{\mathrm{d}t} = -(\frac{\partial C(\theta)}{\partial \theta})^2 \leq 0$$

# Trapping in Local Minimum

"x+1/x"的图表

$$f(x) = (x + 1/x - 1)^2$$
  
 $g(x) = 2(x+1/x-1)(1-x^2)$   
 $g(-1) = 0$ ,而 $f(-1)$ 非最优  
 $g(-1/2) = 21$   
 $g(-3/2) = -3.52$ 



### converge Discretized Gradient Descent may not

- Let learning rate be 1,  $f(x) = x^2$
- $\circ f'(1) = 2, f'(-1) = -2$

- Diverges if lr > 1:  $x_{t+1} = -(2 lr 1) x_t$
- No matter how small is the learning rate
- If learning rate is  $10^{-6}$ , i.e.  $x_{t+1} = x_t 10^{-6}$  f'(x\_t) When  $f(x) = 10^6$   $x^2$ , x will oscillate between  $10^{-6}$  and

## method Beyond Gradient Descent: second-order

- $f(x) = 10^6 x^2$
- Can be solved by Newton's method trivially

- Get to optimum in one-step
- We should use second-order method for A little regularization will stop divergence last-round tuning?

= 1500+(2)+(2-1)+(2-1)+(2-1)+(2-1)+00)-1-100+ 3 (10+10) (10) + 10-10+10) (10-10) (10) = 75 116-x1111/arta-1(+(R-X)+R)+B)+411 0/5 (R-X) (MHO-(A)+-(M)+ = B 11x-3112 Jo of(出ナインーがはかくナイルーメントル) イルフトルン (triangle mequality) ( Cauchy - Schwartz)

112x-113x11 = + (1x-113x) (3x) + (1x) + (1x) + = 11x+1-x1/2 = 11c40+011 = + 11c4x+4/10 - (+x) == = +(xt) - 2012-0) 110+(xt)112

只要月二十十分如何最多

when bound is most tight:

$$f(x_{t+1}) \le f(x_t) - \frac{\eta}{2} ||\nabla f(x_t)||^2$$

This inequality is still scale-invariant, as \eta \beta = 1

## Geometry perspective **Newton's method from Differential**

First order method does not  $X_{t+1} = X_t - \lambda \frac{\partial f(X)}{\partial X}$ respect tensor variance

adding pseudo-vector to vector

Hessian corresponds to metric tensor

$$X_{t+1} = X_t - H^{-1} \frac{\partial f(X)}{\partial X}$$

Gauss-Newton algorithm

$$H pprox rac{\partial f(X)}{\partial X} \mid rac{\partial f(X)}{\partial X}$$

But Hessian need not be positive-semidefinite.

$$X_{t+1} = X_t - \frac{\partial f(X)}{\partial X}^+$$

## Linear Regression

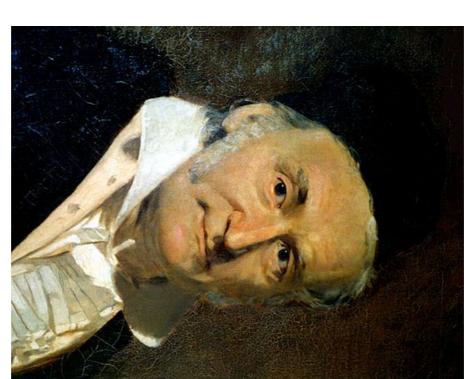
$$\min_{W} \|y - Wx\|^2$$

$$\hat{y} = f(X, \theta) = WX$$

$$\circ \quad d(y,\hat{y}) = \|y - \hat{y}\|^2$$

- x is input, \hat{y} is prediction, y is ground truth.
- W with dimension (m,n)
- "param = m n, "OPs = m n

$$ypprox\hat{y}=Wx$$



## Linear Regression

- Least square solution
- For A x = b, we have:  $x = A^+b + [I A^+A]w$
- Hence  $W = \hat{y} x^{+} + c (I x x^{+})$ x^{+} is pseudo-inverse.
- c is free variable. Using regularization can suppress it.

### Fully-connected

$$y \approx W_2 f(W_1(x))$$

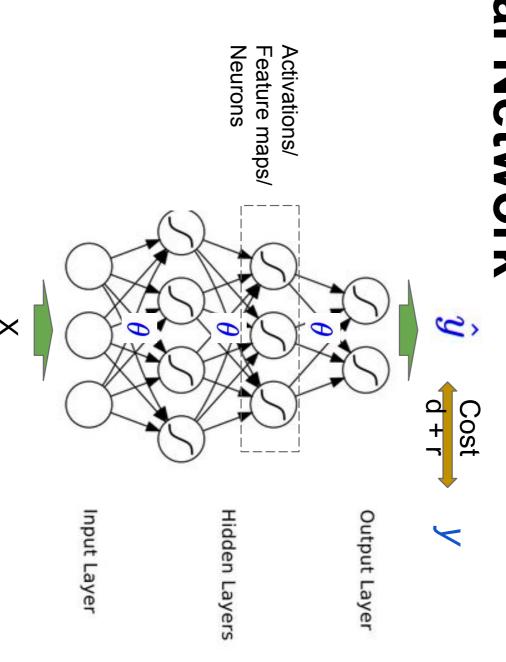
- In general, will use nonlinearity to increase "model capacity".
- Make sense if f is identity? I.e.

$$f(x) = x$$
?

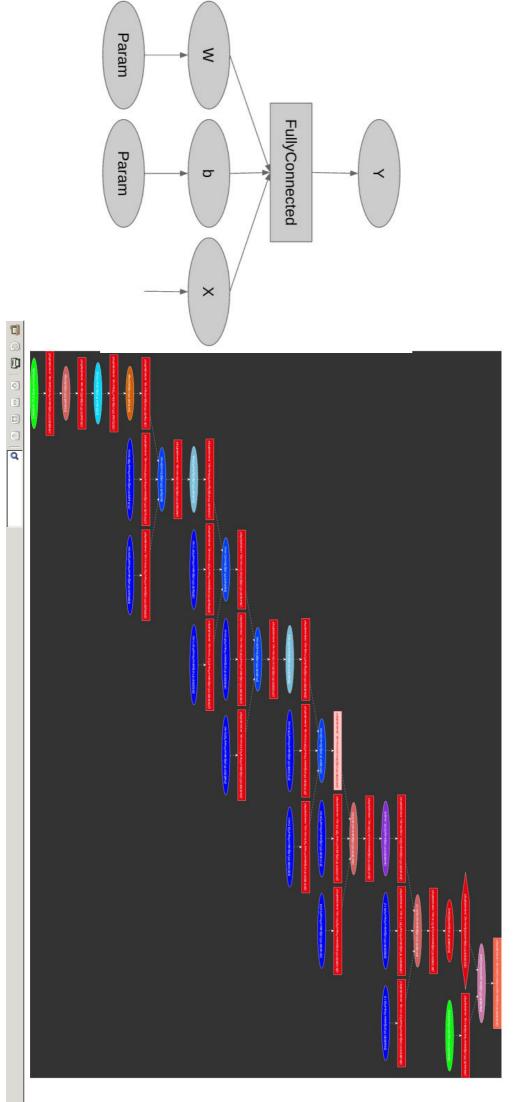
Sometimes, if W\_2 is m by r and W\_1 is r by n, then W\_2 W\_1 is a matrix of rank r, which is different from a m by n matrix.

- $ypprox W_3(f(W_2f(W_1(x))))$
- Deep learning!

### **Neural Network**



## **Computation Graph**



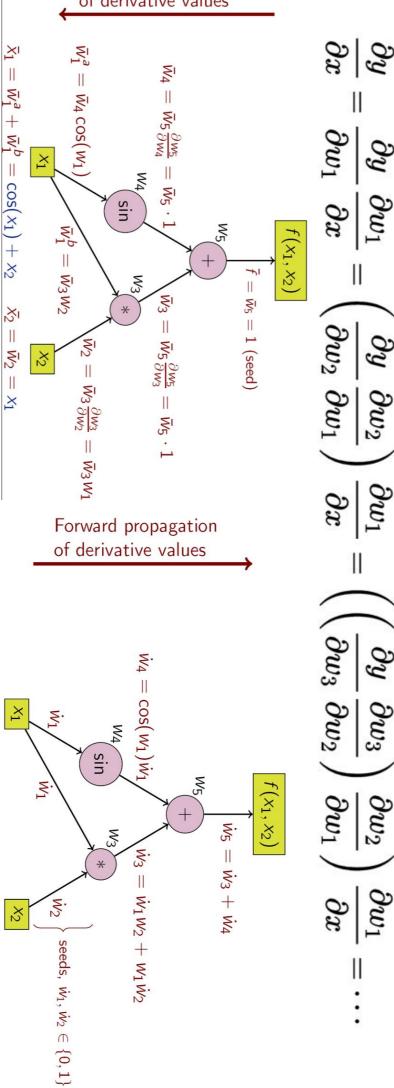
#### Chain rule

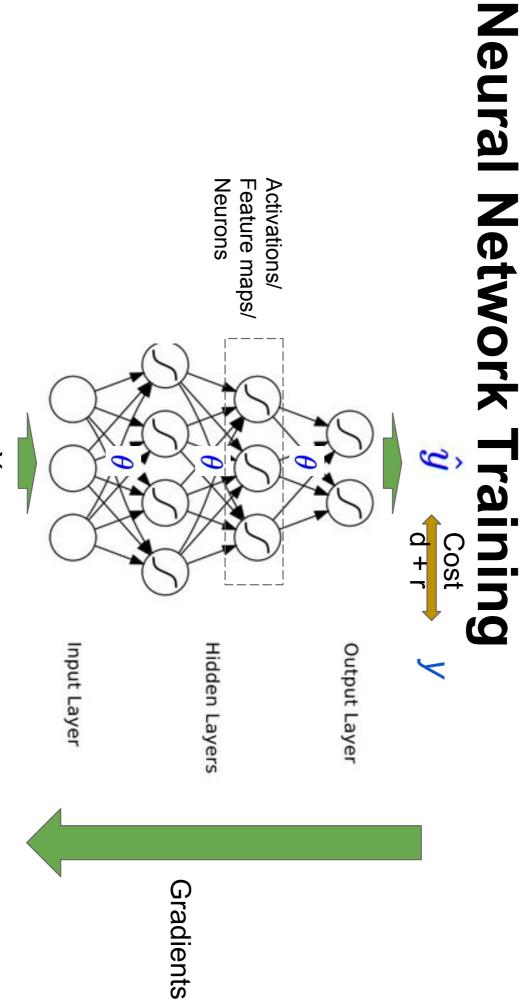
- For training, need to save all intermediate feature maps.
- Can compute from scratch instead of saving, especially for deep nets.

$$rac{\partial Wx}{\partial x} = W^{ op} \ rac{\partial f}{\partial x} = rac{\partial Wx}{\partial x} rac{\partial f}{\partial Wx} = W^{ op} rac{\partial f}{\partial Wx} \ rac{\partial Wx}{\partial W} = (rac{\partial Wx}{x})^{ op} x$$

#### Backward propagation of derivative values

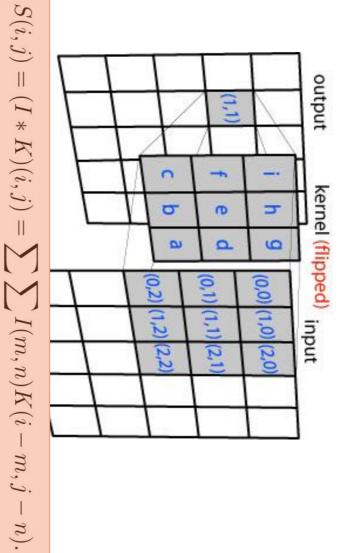
### Accumulation **Backpropagation: Reverse**





### Convolutional Neural Network

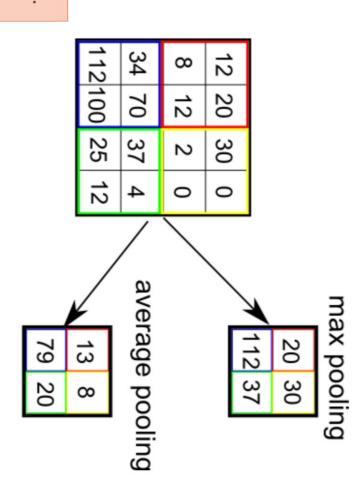
# 2D Convolution, Pooling, MaxOut



2D Convolution

Convolution mode: flip kernel

Correlation mode: don't flip kernel



Pooling is channel-wise nonlinear convolution with fixed params

# Method 1: Convolution as Sparse Matrix

#### Product

Laplacian } = A \vect{M}

 Because convolution is linear, it can be represented by a matrix

A is the sparse Poisson Matrix

```
A =
```

# Side note: Poisson Matrix

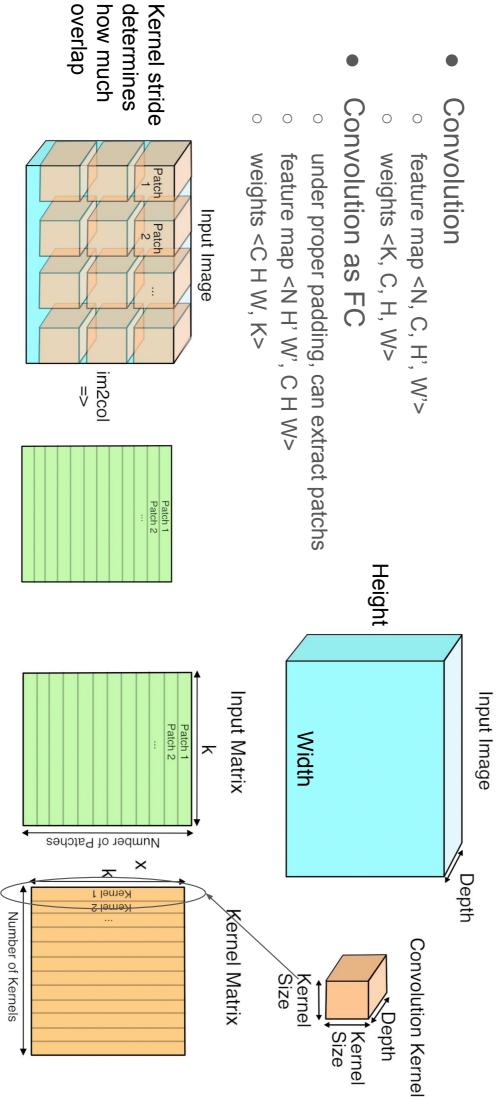
- $\mathcal{P}(m,n) = \mathcal{L}(n) \oplus \mathcal{L}(m)$
- \oplus is <u>Kronecker sum</u>
- \vect{M} P = L\_1 M + M L\_2
- Another way of saying 2D Laplacian is separable to x-axis Laplacian and y-axis Laplacian
- Laplacian matrix is

## Convolutional layer

- Translation-invariance
- Less free #param than Fully-Connected
- Will have worse global minimum
- But empirically can find better local minimum
- architecture engineering The most important reason behind network

# Method 2: Convolution as matrix product





### Locally-Connected

- Convolution is a block triband sparse matrix with shared parameters
- LC layers have unshared parameters, though the same nnz's as Convolutions
- Same amount of computation
- H' W' more parameters
- Useful for Algined Objects (faces)

#### Pooling

- Can use stride-2 conv to replace pooling for reducing #OP
- Neupack requires special combination, like kernel\_shape=4, padding=(1,1), stride=2
- Completely no-overlap seems bad: kernel\_shape=4, stride=4

### Nonlinearity

- fin  $y \approx W_2 f(W_1(x))$
- some extent work Tanh/ReLU/MaxOut/Sin/Abs/AbsTanh all to
- ReLU has point-wise scale invariance:
- max(0, k x) = k max(0, x)
- W and k W are both local minima
- MaxOut has point-wise affine invariance:
- $max(k \times 1 + b, k \times 2 + b) = k max(x 1, x 2) + b$ W and k W + b are both local minima

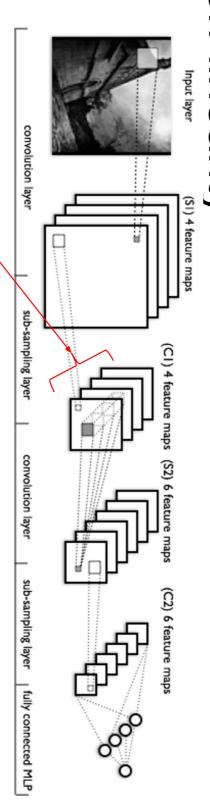
### Nonlinearity

- Avoid tanh family as costly on CPU
- CappedReLU, CappedAbs: seems better

ELU

#### **MaxOut**

- Simply max pooling over the channels
- Can effective reduce #output channels
- (?) In general don't mix maxout with other non-linearity



MaxOut is Max pooling over channels

#### **MaxOut**

- Maxout before softmax to boost quality
- FC to 4\*nr\_class -> Maxout(4) ->Softmax
- or 2\*nr\_class

#### Softmax

Make anything like a probability  $y_i = \sum_{j \ exp(x_j)}$ 

 $exp(x_i)$ 

- **Boltzmann distribution**
- beta is reciprocal of temperature

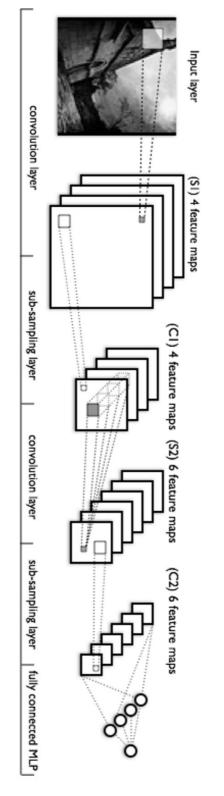
$$y_i = rac{exp(-eta x_i)}{\sum_j exp(-eta x_j)}$$

#### Softmax

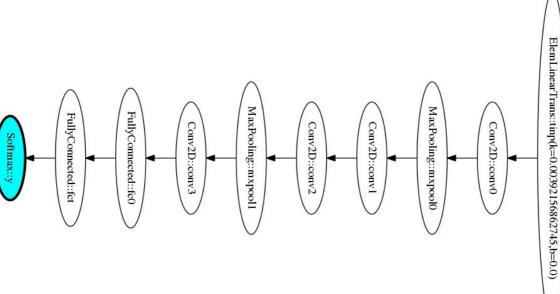
Partition
training
corpus and
limits to
smaller set
of positive
classes.

|                      |                    |  | ט פֿ   |                                       | 5   |           |   |
|----------------------|--------------------|--|--|---------------------------------------|---|-----------|---|
| Sampled<br>Softmax   | Full<br>Softmax    | Full Logistic  | Sampled<br>Logistic                                      | Negative<br>Sampling                  | Noise<br>Contrastive<br>Estimation<br>(NCE) |           |   |
| ${T}_i = \{t_i\}$    | $T_i = \{t_i\}$    | $T_{i}$  | $T_{i}$  | $T_{i}$                               | $T_{i}$                                     | $POS_i =$ | Positive training classes associated with training example $(x_i, T_i)$ : |
| $(S_i - T_i)$        | $(L-T_i)$          | $(L-T_i)$  | $(S_i - T_i)$  | $S_i$                                 | $S_i$                                       | $NEG_i =$ | Negative training classes associated with training example $(x_i, T_i)$ : |
| F(x,y) - log(Q(y x)) | F(x,y)             | F(x,y)   | F(x,y) - log(Q(y x))                                     | F(x,y)                                | F(x,y)<br>-log(Q(y x))                      |           | Input to Training Loss $G(x, y) =$  |
| Softmax              | Softmax            | Logistic   | Logistic   | Logistic                              | Logistic                                    |           | Training<br>Loss  |
| log(P(y x)) + K(x)   | log(P(y x)) + K(x) | $log(odds(y x)) = log\left(\frac{P(y x)}{1-P(y x)}\right)$ | $logodds(y x) = log\left(\frac{P(y x)}{1-P(y x)}\right)$ | $log\left(rac{P(y x)}{Q(y x)} ight)$ | log(P(y x))                                 |           | F(x,y) gets trained to approximate:                                       |

## **CNN: Alexnet-like**







# Importance of Convolutions and FC

| Neupack: inspect_model.py NeuPeak: npk-model-manip XXX info NeuPeak: npk-model-manip XXX info NeuPeak: npk-model-manip XXX info NeuPeak: npk-model-manip XXX info NeuPeak: npk-model.py  Most storage  Size ature map size  0.00% 32.43% #################################### |
|---|
|---|

# The Matrix View of Neural Network

- Weights of FullyConnected and Convolutions layers
- take up most computation and storage size
- are representable as matrices
- Approximating the matrices approximates the network
- The approximation error accumulates.

$$W_a \approx W \Rightarrow f(X, W_a) \approx f(X, W)$$

## **BatchNormalization**

$$v \frac{X - \operatorname{mean}(X)}{\operatorname{std}(X)} + \beta$$

#### Mechanism

- Standardization of data by computing mean and std of mini-batch (In Megbrain, if multiple card, only the part on first-card is computed.)
- recompute stats for inference: using moving-average or plain average over samples (latter more stable)
- 0 Followed by an affine layer to deal with nonlinearites that are not scale-invariant. alpha, beta are learnt.

#### Effect

- Stabilizer of model training
- Faster convergence as we can use larger Ir
- npk-sanitize-batch-normalization
- Fine-tuning
- BN有freezed

# Tweaking learning rate

- Learning rate are "step lengths"
- Sum of step length need be infinity, to be independent of initial value.

Good initial value saves

distance.

It helps to have learning rate "decay" to do local search.

### Learning rule

$$w:=w-\eta 
abla Q(w)=w-\eta \sum_{i=1}^n 
abla Q_i(w),$$

Momentum

$$\Delta w := -\eta 
abla Q_i(w) + lpha \Delta w$$

$$w := w + \Delta w$$

AdaGrad

$$w:=w-\eta\operatorname{diag}(G)^{-rac{1}{2}}\circ g$$

RMSProp

$$v(w,t) := \gamma v(w,t-1) + (1-\gamma)(\nabla Q_i(w))^2$$
 $w := w - \frac{\eta}{\sqrt{v(w,t)}} \nabla Q_i(w)$ 

# ADAM Learning rule

while  $\theta_t$  not converged do

$$t \leftarrow t+1$$
 $g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})$  (Get gradients w.r.t. stochastic objective at timestep  $t$ )
 $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1-\beta_1) \cdot g_t$  (Update biased first moment estimate)
 $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1-\beta_2) \cdot g_t^2$  (Update biased second raw moment estimate)
 $\widehat{m}_t \leftarrow m_t/(1-\beta_1^t)$  (Compute bias-corrected first moment estimate)
 $\widehat{v}_t \leftarrow v_t/(1-\beta_2^t)$  (Compute bias-corrected second raw moment estimate)
 $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t/(\sqrt{\widehat{v}_t} + \epsilon)$  (Update parameters)

# Model & Training

### CNN: Alexnet-like

# Works for almost-square Image

- 28x28, 1 or 3 channel
- Conv (5x5), 32 channel, nonlinearity
- 24x24, 32 channel
- pool(2x2)
- 12x12, 32 channel
- Conv (3x3), 32 channel, nonlinearity
- often speed bottleneck as input also 32 channel

In fact a 5x5 conv without zero

- 10x10, 32 channel
- pool(2x2)
- 5x5: should not be too small padding
- FC (512) + nonlinearity: often speed bottle neck and most #param
- FC(10) + softmax

# Model design rule-of-thumb

| Neupack: inspect_model.py NeuPeak: npk-model-manip XXX info NeuPeak: npk-model.py  ature map size  0.00% 32.43% #################################### |
|--|
|--|

### **CNN: Alexnet**

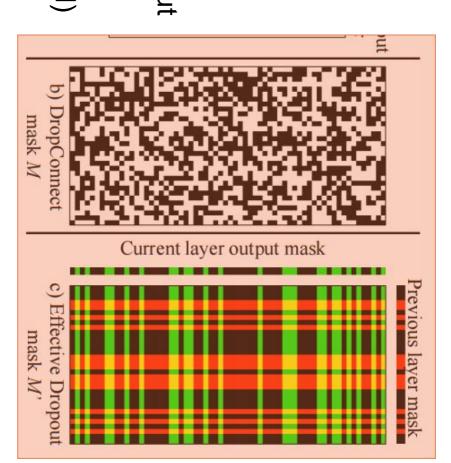
- SGD
- Momentum
- AdamV8(1e-4) seems fine
- Pooling: max/meanpooling

shape 3 stride 2(better on SVHN-cropped)

#### Dropout

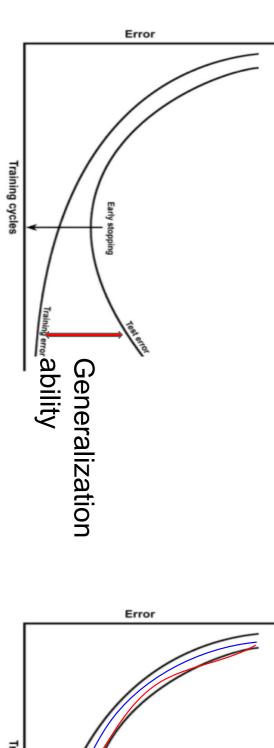
#### Dropout

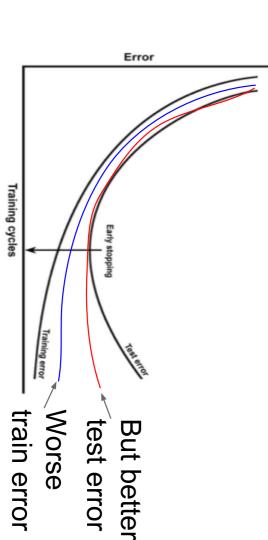
- Multiple W element-wise with Bernoulli distribution.
- 0 p=0.5: Good on FC, but never on output
- maybe good on input or p=0.7 (better on SVHN-cropped)



# **Generalization Ability**

Wisdom: torture NN, but don't kill it, and it will have better generalizability.





### CNN: Maxout

# Works for square like object, and faster

- 28x28, 1 or 3 channel
- Conv (5x5), 32 channel + Identity + Maxout(2)
- 24x24, **16** channel
- pool(2x2)
- Feature map 12x12, 16 channel
- Conv (3x3), 32 channel + Identity + Maxout(2)
- faster as input only also 16 channel
- Feature map 10x10, 16 channel
- pool(2x2)
- Feature map 5x5
- FC (512) + nonlinear: often most #param
- FC(10) + softmax

# **CNN: word recognition**

- Softmax replacement:
- MultiSoftmax: 0010 0100 0001
- Use epsilon to encode var-length labels: (label | epsilon)<sup>n</sup>

### Non-square pooling

- Final feature map size should not be too small, but height may be much smaller than width
- 0 MaxPooling('pool2', pool\_shape=(2, 3), padding=(0,2), pool\_stride=(2,2)))
- out\_shape = (in\_shape + padding pool\_shape) / pool\_stride + 1 4,13 => 2,7

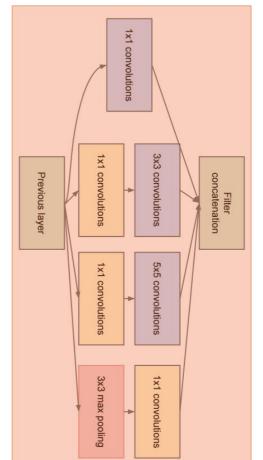
# **CNN: word recognition**

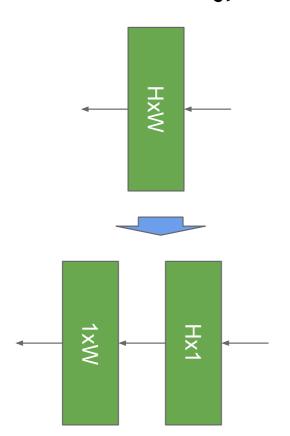
- Fully-Connected
- X = #instance, #channel\_in
- W = #channel\_in, #channel\_out
- Columwise Fully-Connected
- Less #param and invarint to X-dimension translation
- X = #instance, width, #channel\_in
- W = #channel\_in, #channel\_out
- Faster than Recurrent NN



### CNN: GoogLeNet

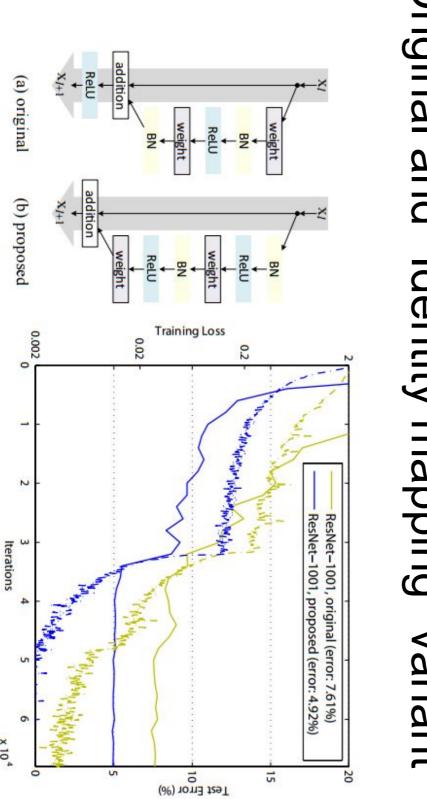
- Inception layer
- Less #OP does not necessarily mean faster
- especially on GPU as GPU loves regularity. CPU suffers less as has less #parallelism.
- A final large average pooling turns teature map size to 1x1
- eliminates large FC, significantly reduce storage size and #OP
- But may hurt performance
- Two rank-1 conv's may be better





### CNN: ResNet

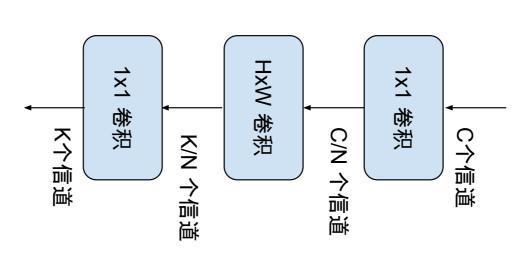
Original and "Identity mapping" variant



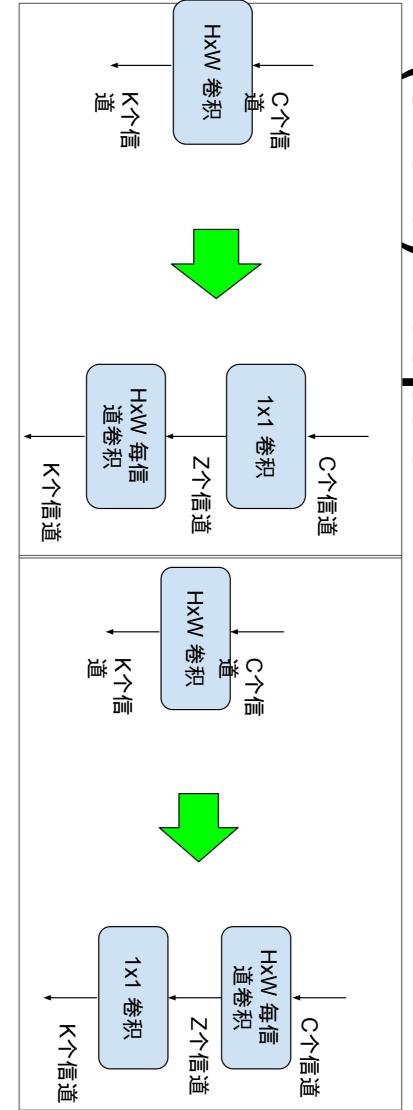
× 104

# **Bottleneck Structure**

- ResNet-50 and above
- CP decomposition If channels-wise HxW conv



### (Shard) Xception



计算量极小,Receptive-field担当

## Training Model

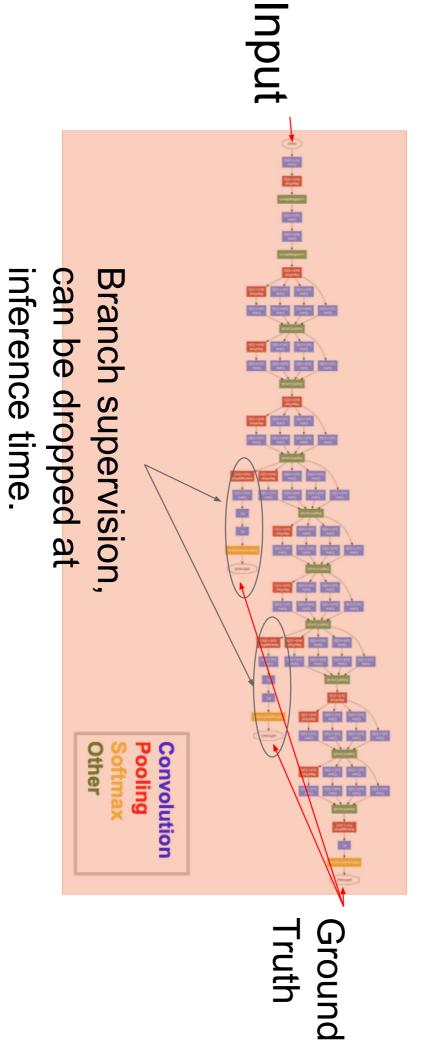
### Before training

- Check list
- data must be shuffled
- Stochastic Gradient Descent relies on unordered order of data.
- color images are not in BGR
- The human face should not be blue
- read the work log if there is one make sure have not mixed training/validation/test
- check #OP and learnable params in your model
- If your model is big, don't save too often.

# Model Death (misclassify 0.9748)

- Tweak learning rate (larger or smaller)
- May add Batch normalization layers
- May try branch supervisions
- Check value range of parameters
- If strange, change initial value range.
- Lower dropout
- Try wider & deeper model
- but too wide & deep also may cause death

# **Branch Supervisions**



# Model Death (misclassify 0.9748)

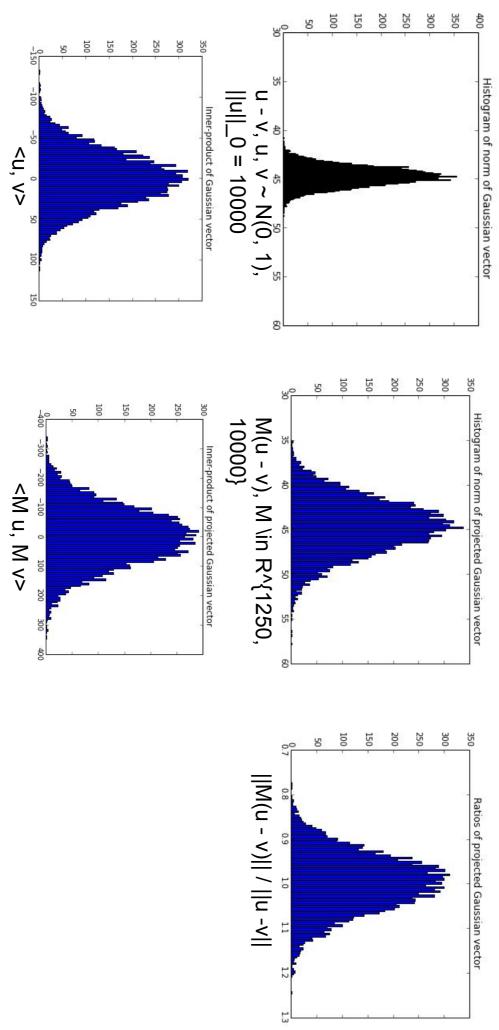
- Init'ing from a working model
- Can steal some layers
- Curriculum learning (<u>Doom</u>)
- Initiating a model on harder data with a model that works on easier data
- w.r.t. number of class
- Train 100-class before training 1000-class.
- w.r.t. noise level
- Reduce level of augmentation

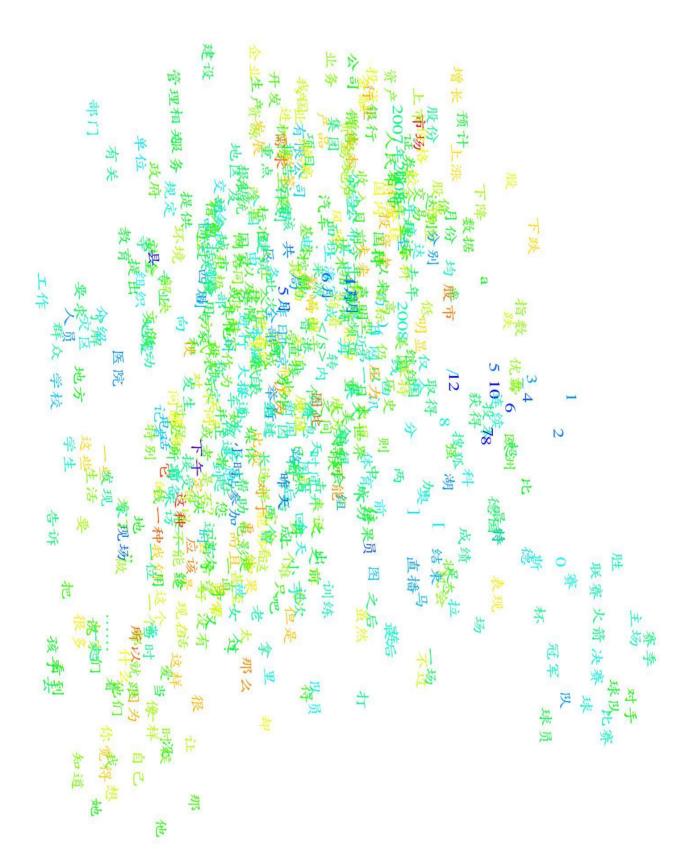
# Working Mechanism

# **Dimension Reduction**

- Symmetric (zero-mean) distribution perserves norm
- whether Gaussian/Bernoulli/ternary
- Even random projection works somehow Good initializers

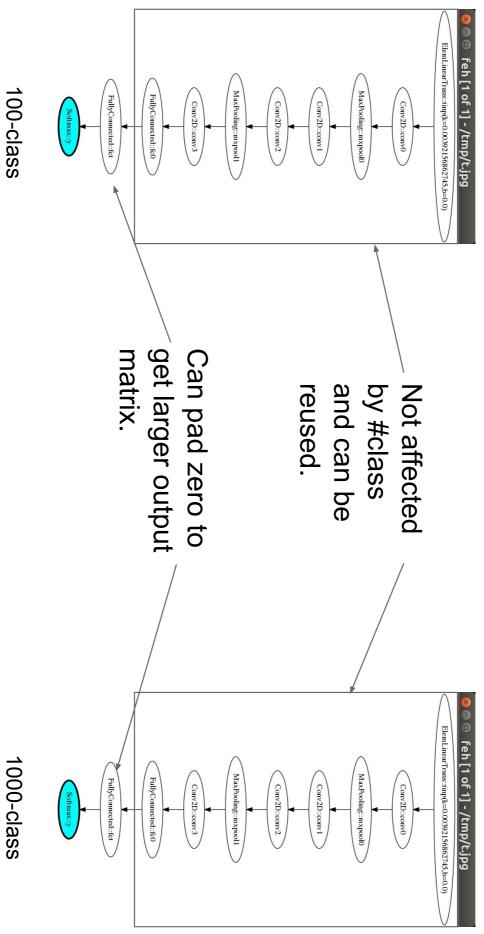
### Norm and Inner-product





# Good practices

# 100-class to 1000-class



### Multi-task learning

- Wisdom: weak supervsion signal may be problematic
- 2-class detection may be harder to train than n-class recognition



Tank classifier, or weather classifier?

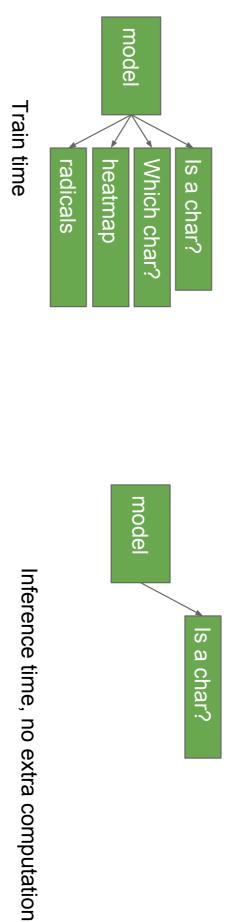


**Z**0

Yes

### Multi-task learning

Can use additional supervision signal for training, but can omit when inference.



Need balancing the order of magnitude of losses, otherwise the smaller losses will be "drowned" in the fluctuations of the larger losses.

# Pairwise Loss, Triplet Loss

 When many classes with few per-class instances, need pairwise loss



Figure 2. **Model structure.** Our network consists of a batch input layer and a deep CNN followed by  $L_2$  normalization, which results in the face embedding. This is followed by the triplet loss during training.

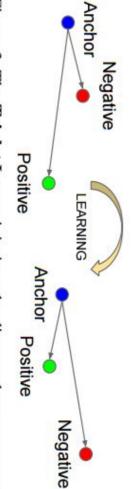


Figure 3. The **Triplet Loss** minimizes the distance between an *an-chor* and a *positive*, both of which have the same identity, and maximizes the distance between the *anchor* and a *negative* of a different identity.

# Hard Example Mining

- With pairwise/triplet loss, random sampling will become less efficient
- Both of below work
- recent network checkpoint and computing the argmin and argmax on a subset of the data.
- Generate triplets online. This can be done by selecting the hard positive/negative exemplars from within a mini-batch.

Selecting the hardest negatives can in practice lead to bad local minima early on in training, specifically it can result in a collapsed model (i.e. f(x) = 0). In order to mitigate this, it helps to select  $x_i^n$  such that

$$||f(x_i^a) - f(x_i^p)||_2^2 < ||f(x_i^a) - f(x_i^n)||_2^2$$
.

4

We call these negative exemplars semi-hard, as they are fur-



### **CNN:** further

- Quality-speed tick-tock
- speed: smaller input (O(n^2)), less channels, shallower, maxout
- quality: more data, larger input, more channels, deeper, more dropout
- synthesizing, multitask
- Be prepared for strong unpredicability in convergence/quality

# Model design rule-of-thumb

- Determine input image size
- Roughly compute #layer and #channel
- Don't concentrate your #OP in one layer Figure out how many #OP you can afford
- Feature map should be gradually smaller
- Don't create a bottleneck
- Determine #pooling layers
- Start with a fatter-than-requirement model
- #OP should be at the same order of magnitude
- Later reduce model by cutting #channel
- If no idea, just create a model. It will change a lot anyway.

# Searching for good model

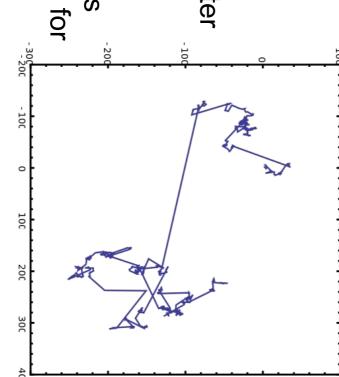
- Analyze the property of the problem
- translation invariance? More conv and less FC.
- sensitive to scale? Sprite like model.
- sequence? Multi-softmax, colfc, RNN

Boostrap by modifying a proven-to-work model

Most models don't work. Better reuse old wisdom.

# Searching for good model

- Repeat: big-step, many baby-step's
- space Big steps helps you explore design
- Make wild changes and hope to get better
- 0 Baby step locally search for local optimum
- Mostly in the form of control experiments where only one factor changes, to allow for later combination of factors
- Should be densely logged



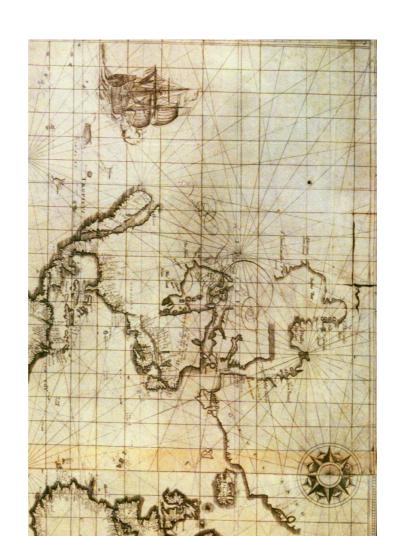
Lévy flight, one way animals find food.

# Systematic naming of experiments

- Naming
- 中浙优8号
- 中稻, 浙江产, 优, 8号
- 隆平稻 (reserved for exceptional good ones) serve to shorten name
- config/quarter\_fc\_noepsilon\_nodupe/model.py
- quarter\_fc: FC only has quarter size of the original
- noepsilon + nodupe: remove epsilon and dupes in labels before matching

### Work log for record

- The way Colombus discovers America
- Scripts:
- Monitoring progress
- watch "python neupeak/scripts/gen\_work\_log.sh train\_log/log.txt|tail"
- Producing record
- neupeak/scripts/gen\_work\_log.py train\_log/log.txt



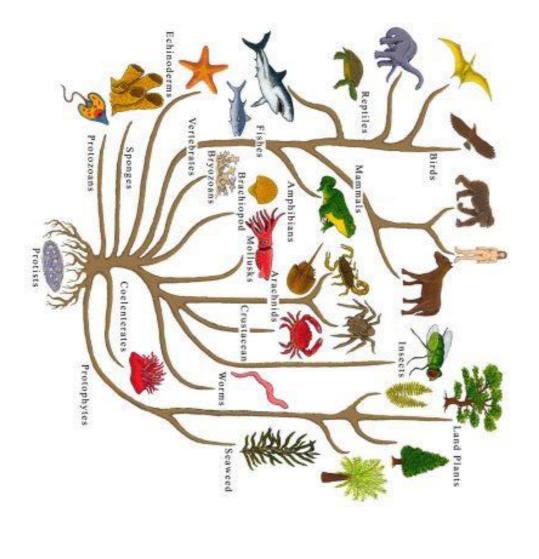
### Work philosophy

- Never stare at training process unless for MNIST
- doing training asynchronously
- Find a quick numeric way to check result
- a bad metric is better than no metric
- or define a tiny representative set (that can be human-eval'ed in <1minute)
- Check before sleep whether the job is alive
- Check if consuming too much memory
- Check deadlock

### 每天工作时间安排

| 16:00 ~ 17:00      | 15:00 ~ 16:00 | 09:00~15:00          | 08:30 ~ 09:00 | 野间   |
|--------------------|---------------|----------------------|---------------|------|
| 制定次日反应方案,准备反应所需材料。 | 开过夜反应B (关键)   | 反应后处理和产品纯化(过夜反应和反应A) | 开新反应A (黄金30分) | 工作安排 |

# Parallel experiments





# Evolution of a NN'ist

- 我一直在搞NN, 开始是Nearest Neighbor,然后是Nuclear Norm,现在的 Neural Network.
- Evolution
- Beginner: read Kevin Murphy's book and anxiously watch MNIST training. Loves trying different nonlinearity. Uses Mathematica for NN.
- 0 Junior: Finds Inception Layer to be great. Discovers Neural Turing coffee is a misspelled word. Machine. Loves making everything differentiable in Theano. Thinks
- Senior: Doing tensor decomposition on convolution weights. Building up bit NN runtime. Trains VGG-16 in proprietry NN framework
- Master: If anything, send an E-mail to zxy@.