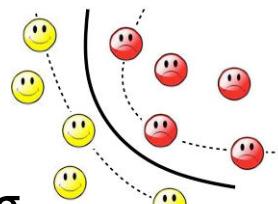


Machine Learning and Data Mining (COMP 5318)



Deep learning

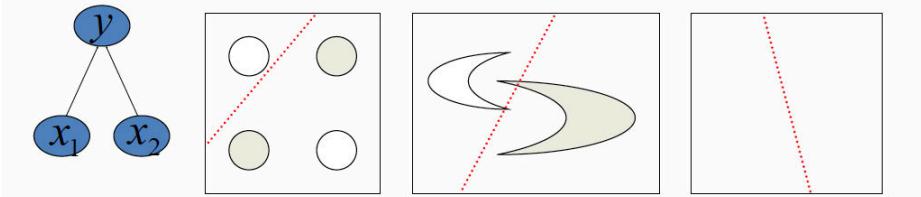
Nguyen Hoang Tran

1

Feed Forward Neural Networks

Neural networks can be very expressive, especially as you add more layers (i.e., 'deep' neural networks)

0 hidden layers: linear classifier



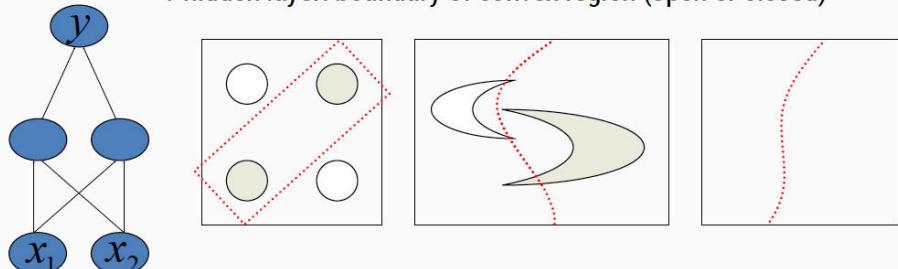
2

Feed Forward Neural Networks

Feed Forward Neural Networks

Neural networks can be very expressive, especially as you add more layers (i.e., 'deep' neural networks)

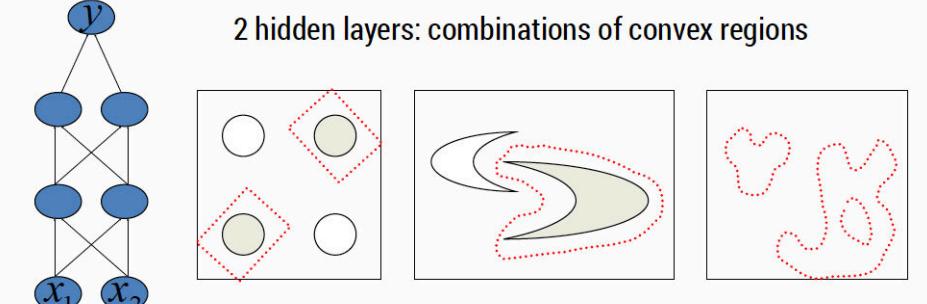
1 hidden layer: boundary of convex region (open or closed)



3

Neural networks can be very expressive, especially as you add more layers (i.e., 'deep' neural networks)

2 hidden layers: combinations of convex regions



4

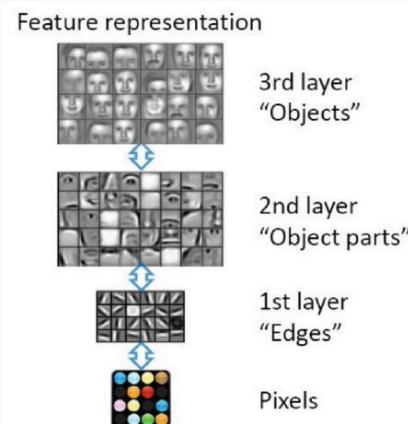
Feed Forward Neural Networks



Neural networks can be very expressive, especially as you add more layers (i.e., 'deep' neural networks)

Pro: Can allow the model to learn a feature representation and the appropriate levels of abstraction from your data

Challenge: this can make DNNs expensive ...



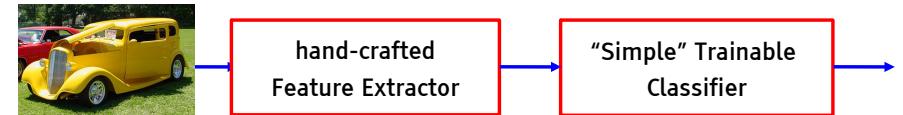
5

Deep Learning = Learning Features



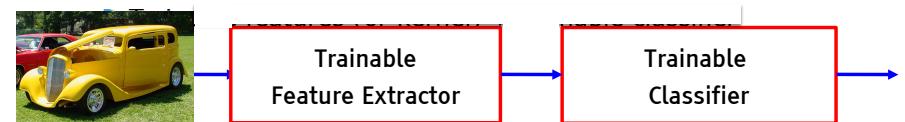
■ The traditional model of pattern recognition (since the late 50's)

▶ Fixed/engineered features (or fixed kernel) + trainable classifier



■ End-to-end learning / Feature learning / Deep learning

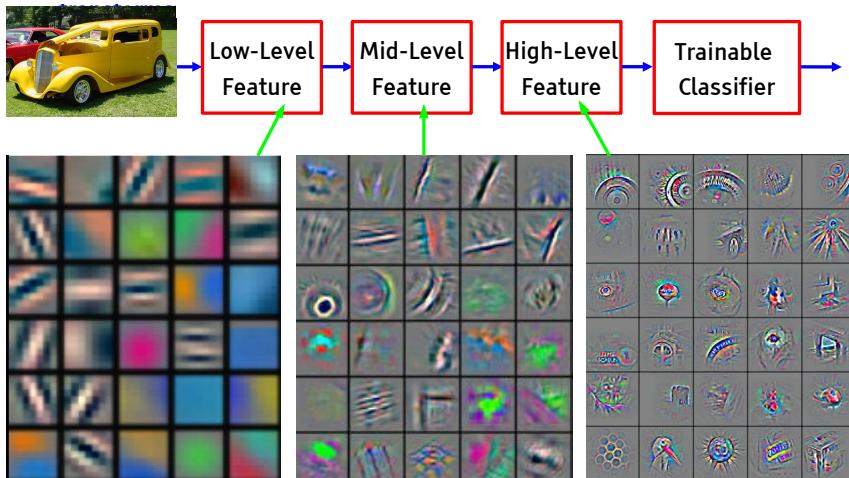
▶ Trainable features (or kernel) + classifier



6

Deep Learning = Learning Hierarchies

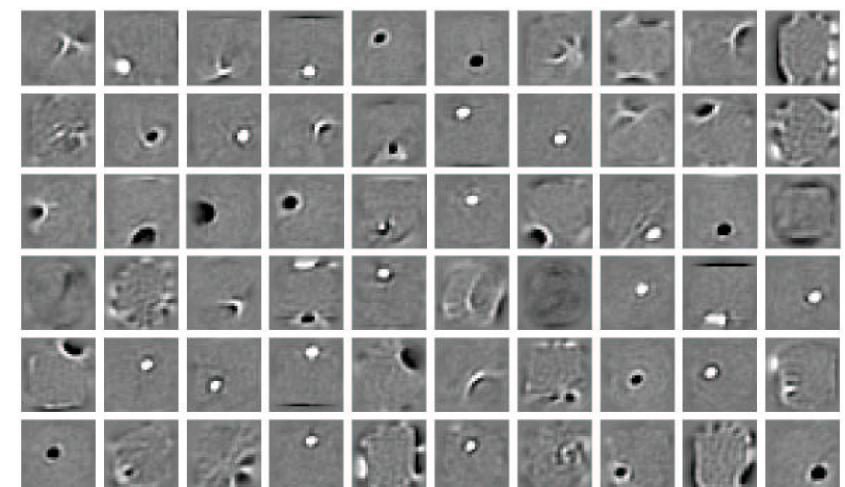
- It's **deep** if it has **more than one stage** of nonlinear feature transformation



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

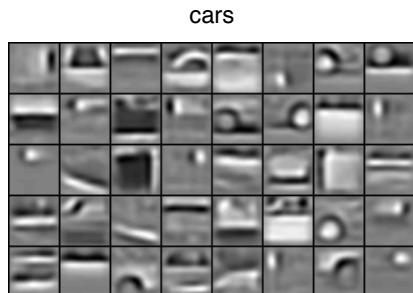
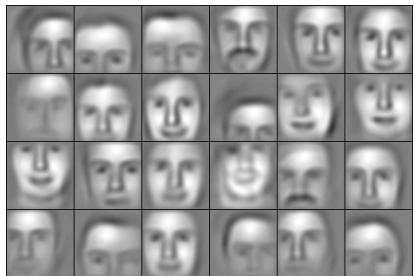
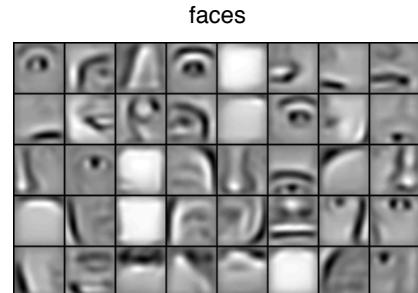
7

First Layer

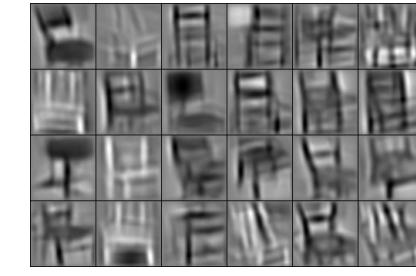
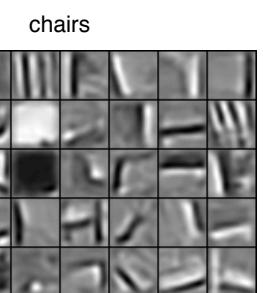
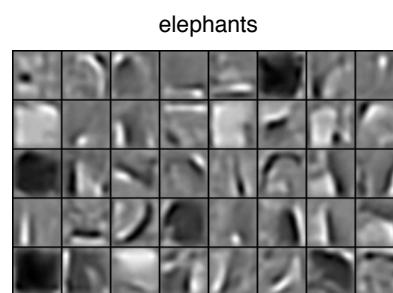


8

Other Layers



Other Layers

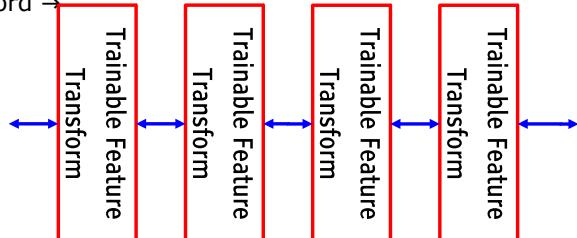


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Trainable Feature Hierarchy

- Hierarchy of representations with increasing level of abstraction
- Each stage is a kind of trainable feature transform
- Image recognition
 - ▶ Pixel → edge → texton → motif → part → object
- Text
 - ▶ Character → word → word group → clause → sentence → story
- Speech
 - ▶ Sample → spectral band → sound → ... → phone → phoneme → word



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Deep architectures

- Feed-Forward: multilayer neural nets, convolutional nets
- Feed-Back: Stacked Sparse Coding, Deconvolutional Nets
- Bi-Directional: Deep Boltzmann Machines, Stacked Auto-Encoders

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12

Let's try DL in playground



Iterations: 000,000 Learning rate: 0.03 Activation: ReLU Regularization: L2 Regularization rate: 0.001 Problem type: Regression

DATA
Which dataset do you want to use?
 Ratio of training to test data: 40%
Noise: 20
Batch size: 10
REGENERATE

FEATURES
Which properties do you want to feed in?
 X_1 , X_2 , X_1^2 , X_2^2 , $X_1 X_2$, $\sin(X_1)$, $\sin(X_2)$

3 HIDDEN LAYERS
+ - 4 neurons
+ - 4 neurons
+ - 2 neurons

OUTPUT
Test loss 0.121
Training loss 0.134

This is the output from one neuron. Hover to see it larger.
The outputs are mixed with varying weights, shown by the thickness of the lines.
Colors shows data, neuron and weight values.

Show test data Discretize output

Source: <http://playground.tensorflow.org/>



Training protocols

Purely Supervised

- ▶ Initialize parameters randomly
- ▶ Train in supervised mode
 - ▶ typically with SGD, using backprop to compute gradients
- ▶ Used in most practical systems for speech and image recognition

Unsupervised, layerwise + supervised classifier on top

- ▶ Train each layer unsupervised, one after the other
- ▶ Train a supervised classifier on top, keeping the other layers fixed
- ▶ Good when very few labeled samples are available

Unsupervised, layerwise + global supervised fine-tuning

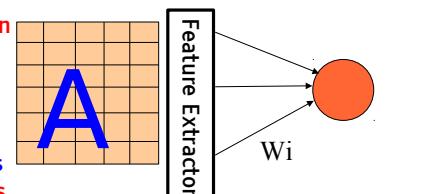
- ▶ Train each layer unsupervised, one after the other
- ▶ Add a classifier layer, and retrain the whole thing supervised
- ▶ Good when label set is poor (e.g. pedestrian detection)

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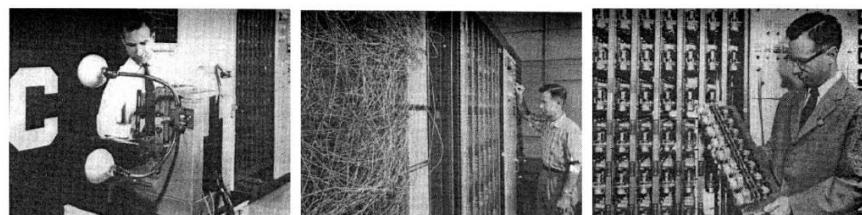
Basic element



- The first learning machine: the Perceptron
 - ▶ Built at Cornell in 1960
- The Perceptron was a linear classifier on top of a simple feature extractor
- The vast majority of practical applications of ML today use glorified linear classifiers or glorified template matching.
- Designing a feature extractor requires considerable efforts by experts.



$$y = \text{sign} \left(\sum_{i=1}^N W_i F_i(X) + b \right)$$



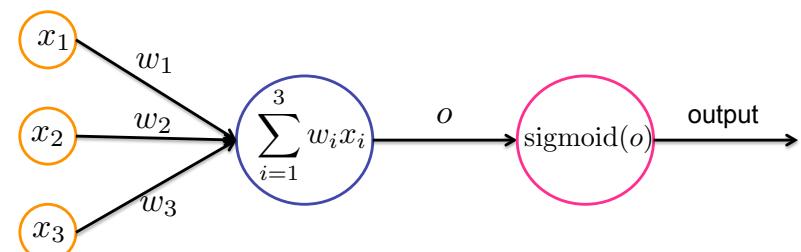
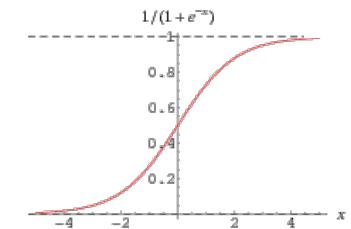
15

Basic element



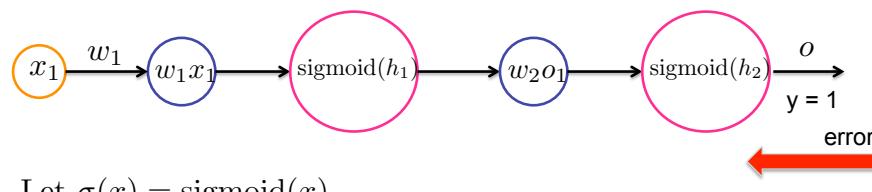
Sigmoid function

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$



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Training



Let $\sigma(x) = \text{sigmoid}(x)$

Forward propagation : $o = \sigma(w_2 \sigma(w_1 x_1))$

Loss : $L(w_1, w_2) = -\log o$

$$\frac{\partial}{\partial w_2} L(w_1, w_2) = \frac{\partial L}{\partial o} \frac{\partial o}{\partial h_2} \frac{\partial h_2}{\partial w_2}$$

$$\frac{\partial}{\partial w_1} L(w_1, w_2) = \frac{\partial L}{\partial o} \frac{\partial o}{\partial h_2} \frac{\partial h_2}{\partial o_1} \frac{\partial o_1}{\partial h_1} \frac{\partial h_1}{\partial w_1}$$



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Back-prop in practice



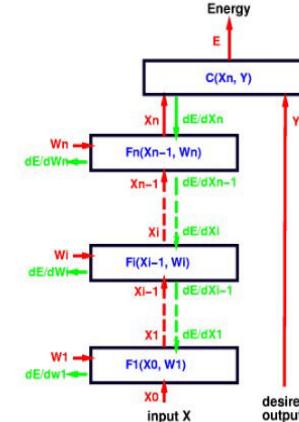
- Use ReLU non-linearities (tanh and logistic are falling out of favor)
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination)
 - ▶ But it's best to turn it on after a couple of epochs
- Use "dropout" for regularization
 - ▶ Hinton et al 2012 <http://arxiv.org/abs/1207.0580>
- Lots more in [LeCun et al. "Efficient Backprop" 1998]
- Lots, lots more in "Neural Networks, Tricks of the Trade" (2012 edition) edited by G. Montavon, G. B. Orr, and K-R Müller (Springer)

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Training with back-propagation



To compute all the derivatives, we use a backward sweep called the **back-propagation algorithm** that uses the recurrence equation for $\frac{\partial E}{\partial X_i}$



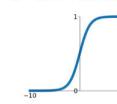
- $\frac{\partial E}{\partial X_n} = \frac{\partial C(X_n, Y)}{\partial X_n}$
- $\frac{\partial E}{\partial X_{n-1}} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial X_{n-1}}$
- $\frac{\partial E}{\partial W_n} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial W_n}$
- $\frac{\partial E}{\partial X_{n-2}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial X_{n-2}}$
- $\frac{\partial E}{\partial W_{n-1}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial W_{n-1}}$
-etc, until we reach the first module.
- we now have all the $\frac{\partial E}{\partial W_i}$ for $i \in [1, n]$.

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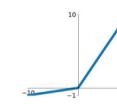
Rectified Linear Units

Activation Functions

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



Leaky ReLU
 $\max(0.1x, x)$



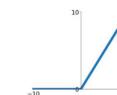
tanh
 $\tanh(x)$



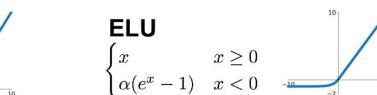
Maxout
 $\max(w_1^T x + b_1, w_2^T x + b_2)$



ReLU
 $\max(0, x)$



ELU
 $\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$



- $f(x) = \max(0, x)$ More efficient gradient propagation, derivative is 0 or constant, just fold into learning rate
 - Helps $f'(net)$ issue, but still left with other unstable gradient issues
- More efficient computation: Only comparison, addition and multiplication.
 - Leaky ReLU $f(x) = x$ if $x > 0$ else ax , where $0 \leq a \leq 1$, so that derivative is not 0 and can do some learning for net < 0 (does not "die").
 - Lots of other variations
- Sparse activation: For example, in a randomly initialised networks, only about 50% of hidden units are activated (having a non-zero output)
- Learning in linear range easier for most learning models

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Problems where DL is the best



- Handwriting recognition MNIST (many), Arabic HWX (IDSIA)
- OCR in the Wild [2011]: StreetView House Numbers (NYU and others)
- Traffic sign recognition [2011] GTSRB competition (IDSIA, NYU)
- Pedestrian Detection [2013]: INRIA datasets and others (NYU)
- Volumetric brain image segmentation [2009] connectomics (IDSIA, MIT)
- Human Action Recognition [2011] Hollywood II dataset (Stanford)
- Object Recognition [2012] ImageNet competition
- Scene Parsing [2012] Stanford bgd, SiftFlow, Barcelona (NYU)
- Scene parsing from depth images [2013] NYU RGB-D dataset (NYU)
- Speech Recognition [2012] Acoustic modeling (IBM and Google)
- Breast cancer cell mitosis detection [2011] MITOS (IDSIA)

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Why Deep?



- **Theoretician's dilemma:** "We can approximate any function as close as we want with shallow architecture. Why would we need deep ones?"

$$y = \sum_{i=1}^P \alpha_i K(X, X^i) \quad y = F(W^1.F(W^0.X))$$

► kernel machines (and 2-layer neural nets) are "universal".

- **Deep learning machines**

$$y = F(W^K.F(W^{K-1}.F(\dots.F(W^0.X)\dots)))$$

- **Deep machines are more efficient for representing certain classes of functions, particularly those involved in visual recognition**

► they can represent more complex functions with less "hardware"

- **We need an efficient parameterization of the class of functions that are useful for "AI" tasks (vision, audition, NLP...)**

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Is there any theory?



- **Deep Learning involves non-convex loss functions**
 - With non-convex losses, all bets are off
 - Then again, every speech recognition system ever deployed has used non-convex optimization (GMMs are non convex).
- **But to some of us all "interesting" learning is non convex**
 - Convex learning is invariant to the order in which sample are presented (only depends on asymptotic sample frequencies).
 - Human learning isn't like that: we learn simple concepts before complex ones. The order in which we learn things matter.

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Is there any theory?



intuitively: generalization error = |training error - test error|

- **No generalization bounds?**

► Actually, the usual VC bounds apply: most deep learning systems have an infinite VC dimension.
► We don't have tighter bounds than that.
► But then again, how many bounds are tight enough to be useful for model selection?

- **It's hard to prove anything about deep learning systems**

► Then again, if we only study models for which we can prove things, we wouldn't have speech, handwriting, and visual object recognition systems today.

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Some theory emerging



Deep Learning is about representing high-dimensional data

- ▶ There has to be interesting theoretical questions there
- ▶ What is the geometry of natural signals?
- ▶ Is there an equivalent of statistical learning theory for unsupervised learning?
- ▶ What are good criteria on which to base unsupervised learning?

Deep Learning Systems are a form of latent variable factor graph

- ▶ Internal representations can be viewed as latent variables to be inferred, and deep belief networks are a particular type of latent variable models.
- ▶ The most interesting deep belief nets have intractable loss functions: how do we get around that problem?

Lots of theory at the 2012 IPAM summer school on deep learning

- ▶ Wright's parallel SGD methods, Mallat's "scattering transform", Osher's "split Bregman" methods for sparse modeling, Morton's "algebraic geometry of DBN",....

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An intuitive understanding



Recall that: intuitively, Generalisation error = |training error - test error|

Intuitively, a learning algorithm is said to be stable if slight perturbations in the training data result in small changes in the output of the algorithm, and these changes vanish as the data set grows bigger and bigger.

Good algorithmic stability implies small generalisation error. (we can gradually change the training examples to the test ones while the output hypotheses will not change much.)

An intuitive understanding



Deep learning: going deeper, generalising better!

"Deeper" implies

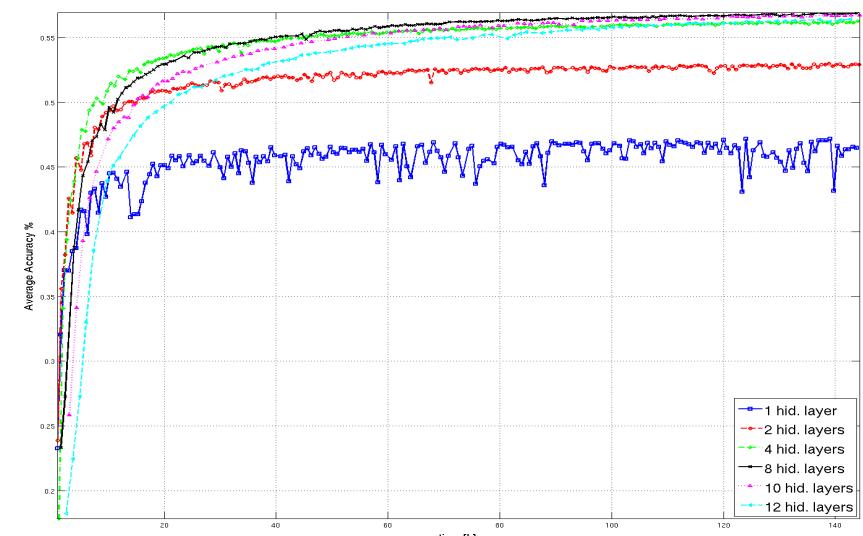
"smaller input and output mutual information" implies

"better" algorithmic stability" implies

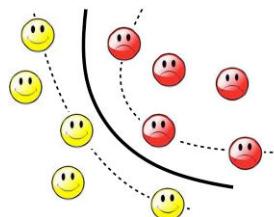
"smaller generalisation error".

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Speech Recog. Example



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Auto-encoders

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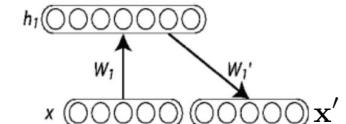
Auto-encoder

- Simple Auto-encoder
 - Encoder maps input into hidden representation.
 - Decoder reconstructs input from hidden representation.
- Minimize reconstruction errors.
 - reconstruction = decoder(encoder (input)).
 - Minimize difference between reconstruction and input.
 - E.g.

$$\mathbf{h} = \tanh(\mathbf{b} + \mathbf{W}_1 \mathbf{x})$$

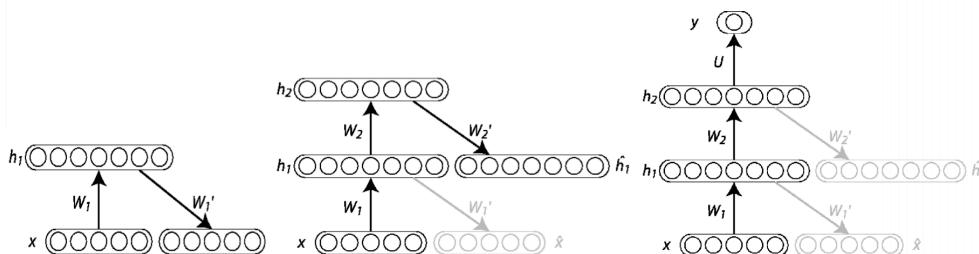
reconstruction $\mathbf{x}' = \tanh(\mathbf{b}' + \mathbf{W}'_1 \mathbf{h})$

$$\text{Loss } L(\mathbf{x}, \mathbf{x}') = 0.5 \|\mathbf{x}' - \mathbf{x}\|^2$$



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Stacked auto-encoders

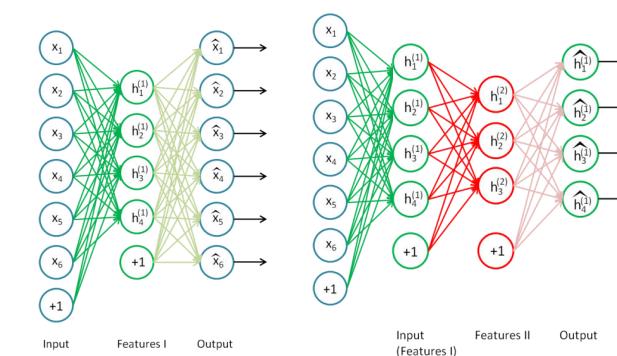


Simple auto-encoders or denoising auto-encoders can be stacked to form deep architectures. The parameters are initialized with unsupervised pre-training. (Bengio et al 2006, Vincent et al 2008)

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Stacked auto-encoders

- Bengio (2007) – After Deep Belief Networks (2006)
- Stack many (sparse) auto-encoders in succession and train them using greedy layer-wise training

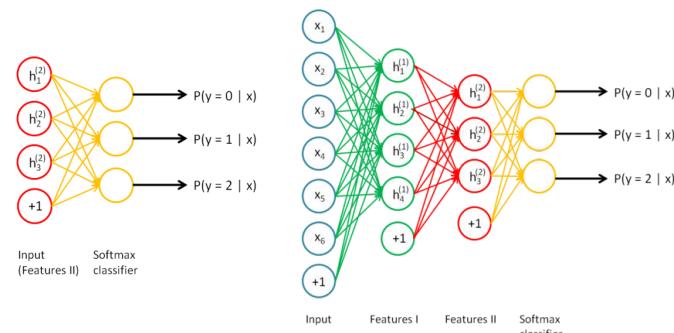


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Stacked auto-encoders



- Do supervised training (can now only used labeled examples) on the last layer using final features
- Then do supervised training on the entire network to fine-tune all weights



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Auto-encoder in practice

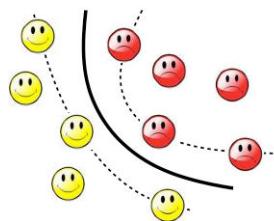


- Use more hidden nodes in the encoder
- Use regularisation techniques which encourage sparseness (e.g. a significant portion of nodes have 0 output for any given input)
 - Penalty in the learning function for non-zero nodes
 - Weight decay
 - etc.
- De-noising Auto-Encoder
 - Stochastically corrupt training instance each time, but still train auto-encoder to decode the uncorrupted instance, forcing it to de-noise and learn conditional dependencies within the instance
 - Improved empirical results, handles missing values well

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Convolutional Neural Nets

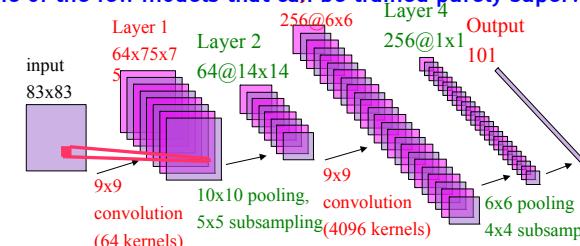


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Convolutional Networks

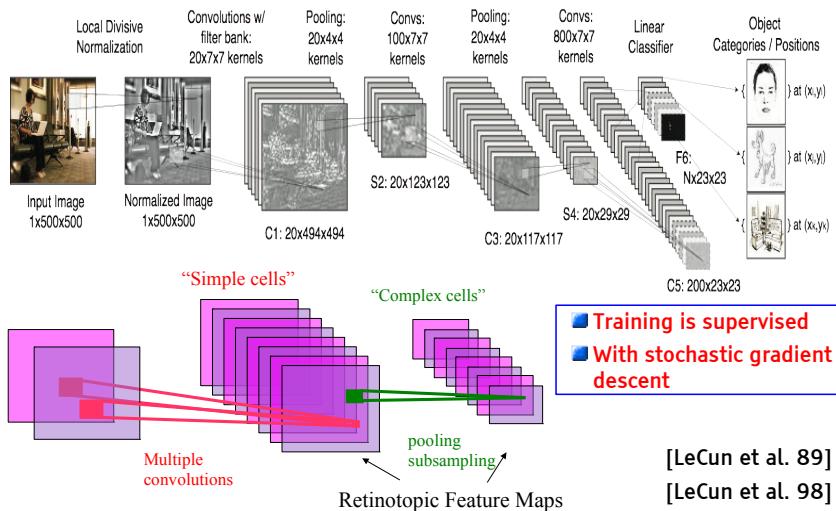


- Are deployed in many practical applications
 - ▶ Image recognition, speech recognition, Google's and Baidu's photo taggers
- Have won several competitions
 - ▶ ImageNet, Kaggle Facial Expression, Kaggle Multimodal Learning, German Traffic Signs, Connectomics, Handwriting....
- Are applicable to array data where nearby values are correlated
 - ▶ Images, sound, time-frequency representations, video, volumetric images, RGB-Depth images,.....
- One of the few models that can be trained purely supervised



;

CNN Structure



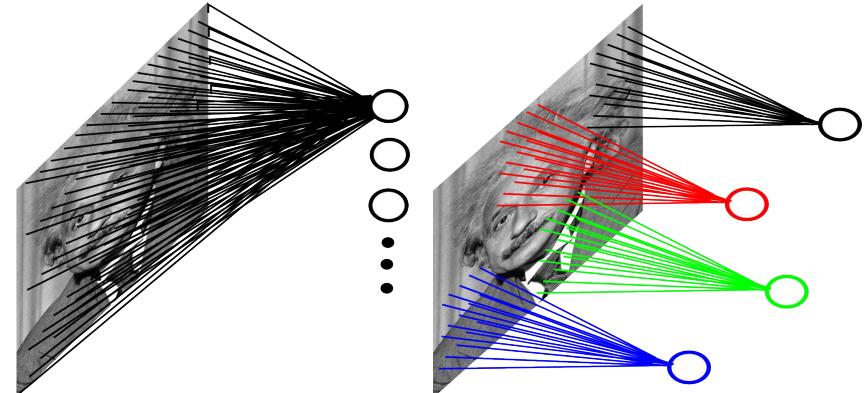
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Fully connected



Example: 200x200 image

- ▶ Fully-connected, 400,000 hidden units = 16 billion parameters
- ▶ Locally-connected, 400,000 hidden units 10x10 fields = 40 million params
- ▶ Local connections capture local dependencies



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Convolution example



1	1	1	0	0
0	1	1	1	0
0	0	1	1	1
0	0	1	1	0
0	1	1	0	0

Image

1	0	1
0	1	0
1	0	1

Convolved Feature

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Shared Weights



Features that are useful on one part of the image and probably useful elsewhere.

All units share the same set of weights

Shift equivariant processing:

- ▶ When the input shifts, the output also shifts but stays otherwise unchanged.

Convolution

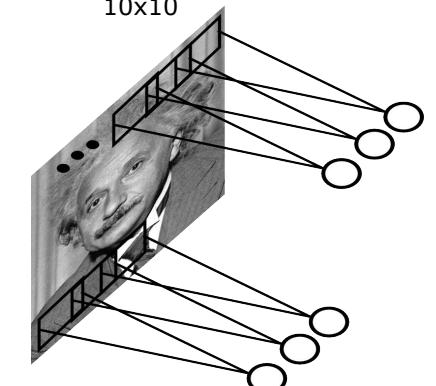
- ▶ with a learned kernel (or filter)
- ▶ Non-linearity: ReLU (rectified linear)

$$A_{ij} = \sum_{kl} W_{kl} X_{i+j, k+l}$$

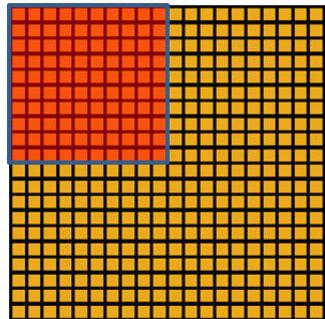
$$Z_{ij} = \max(0, A_{ij})$$

Example: 200x200 image

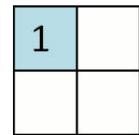
- ▶ 400,000 hidden units with 10x10 fields = 1000 params
- ▶ 10 feature maps of size 200x200, 10 filters of size 10x10



Pooling example



Convolved
feature



Pooled
feature

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Examples

Traffic Sign Recognition (GTSRB)

- ▶ German Traffic Sign Reco Bench
- ▶ 99.2% accuracy



House Number Recognition (Google)

- ▶ Street View House Numbers
- ▶ 94.3 % accuracy

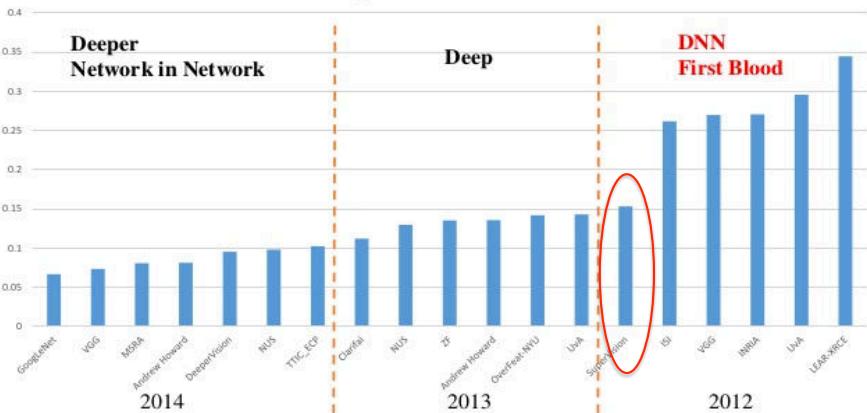


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ILSVRC



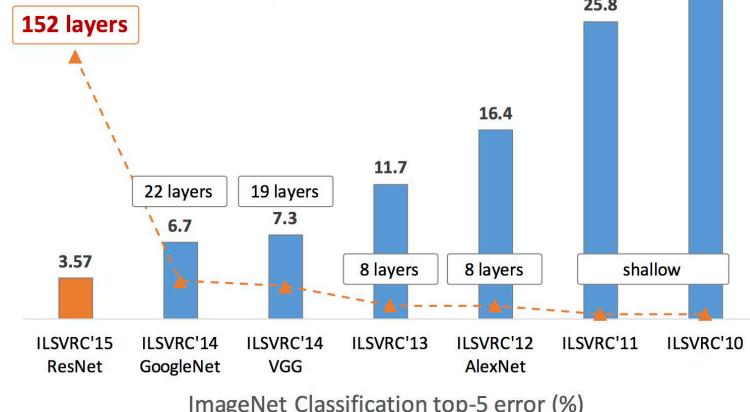
ImageNet Classification error throughout years and groups



Li Fei-Fei: ImageNet Large Scale Visual Recognition Challenge, 2014 <http://image-net.org/>

Depth vs Error

Revolution of Depth



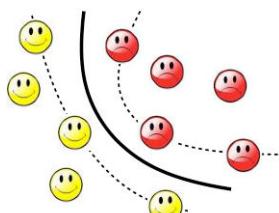
Kaiming He, Xiangyu Zhang, Shaoqing Ren, & Jian Sun. "Deep Residual Learning for Image Recognition". CVPR

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Making DL work

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Dropout

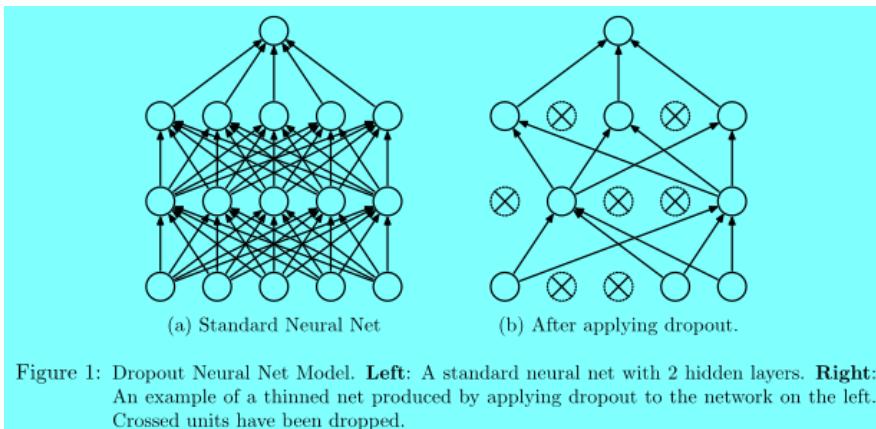


Figure 1: Dropout Neural Net Model. **Left:** A standard neural net with 2 hidden layers. **Right:** An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

- For each instance drop a node (hidden or input) and its connections with probability p and train
- Final net just has all averaged weights (actually scaled by $1-p$)
- As if ensembling 2^n different network substructures

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Vanishing gradients

- Analyzing the norms of the Jacobians, yields:

$$\left\| \frac{\partial h_j}{\partial h_{j-1}} \right\| \leq \|W^T\| \|\text{diag}[f'(h_{j-1})]\| \leq \beta_W \beta_h$$

- Where we defined β 's as upper bounds of the norms
- The gradient is a product of Jacobian matrices, each associated with a step in the forward computation.

$$\left\| \frac{\partial h_t}{\partial h_k} \right\| = \left\| \prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} \right\| \leq (\beta_W \beta_h)^{t-k}$$

- This can become very small or very large quickly [Bengio et al 1994], and the locality assumption of gradient descent breaks down. → **Vanishing or exploding gradient**

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Batch normalisation (I)

- Rather than just guess initial parameters to maintain learning balance, why not renormalise activations at each layer to maintain balance
- Since we like 0-mean and unit variance inputs (standard 1st layer normalisation), we can just re-normalise the activation/net values at each input dimension k at each layer

$$\hat{x}^{(k)} = \frac{x^{(k)} - \mathbb{E}[x^{(k)}]}{\sqrt{\text{Var}[x^{(k)}]}}$$

- Want mean and variance of that activation for the entire data set. Approximate the empirical mean and variance over a mini-batch of instances and then normalise the activation
- Then scale and shift the normalised activation with 2 learnable weights per input, γ and β , to attain the final batch normalisation for that activation

$$y^{(k)} = \gamma^{(k)} \hat{x}^{(k)} + \beta^{(k)}$$

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Batch normalisation (2)



Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\dots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\begin{aligned}\mu_{\mathcal{B}} &\leftarrow \frac{1}{m} \sum_{i=1}^m x_i && // \text{mini-batch mean} \\ \sigma_{\mathcal{B}}^2 &\leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 && // \text{mini-batch variance} \\ \hat{x}_i &\leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} && // \text{normalize} \\ y_i &\leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) && // \text{scale and shift}\end{aligned}$$

Note: at test time
BatchNorm layer
functions differently:

The mean/std are not
computed based on
the batch. Instead, a
single fixed empirical
mean of activations
during training is used.

(e.g. can be estimated
during training with
running averages)

Allows larger LR,
improves gradient flow
and reduces
dependence on
initialisation

[Ioffe and Szegedy, 2015]

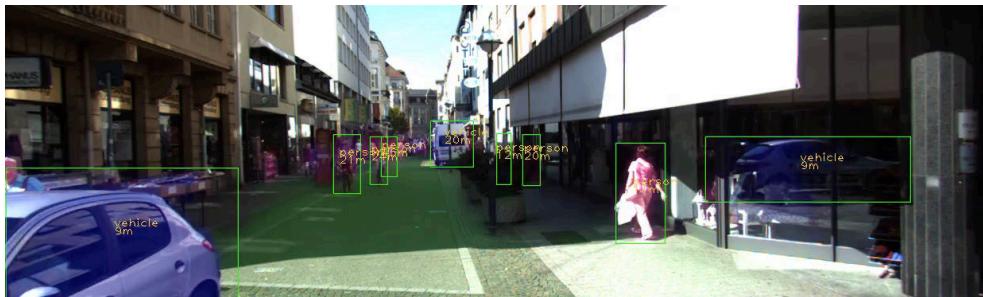
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When to try deep learning

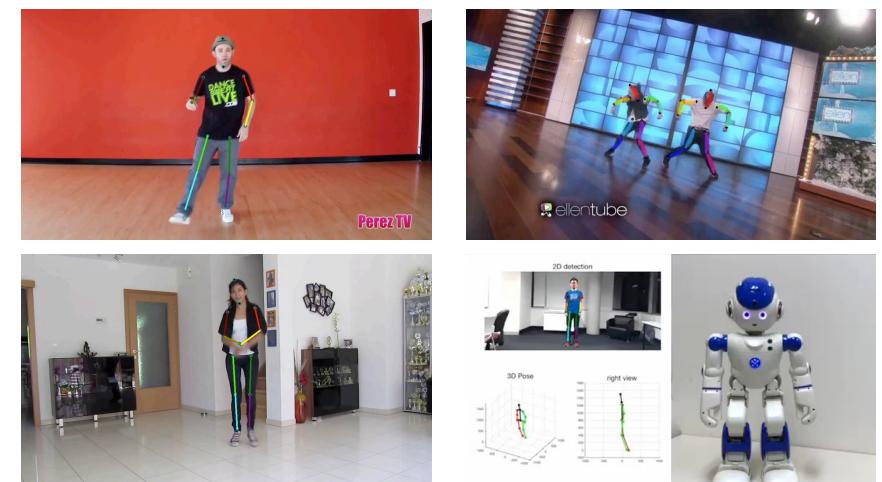


- There is lots of data
- The data is high dimensional
- The data has an underlying structure
- You have good GPUs

Real-time object recognition



Deep pose estimation



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Beyond Autoencoders and CNNs



- Deep Belief Networks
- Restricted Boltzman Machines
- Variational Bayesian Autoencoders
- Convolutional Autoencoders
- Recurrent Neural Nets
- Variational Bayesian CNNs
- Convolutional Kernel Networks
- Residual networks (ResNets)
- Inception networks
- Generative adversarial networks (GANs)

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Software



- TensorFlow
- PyTorch
- Theano
- Keras
- Caffe
- Lasagne

http://deeplearning.net/software_links/

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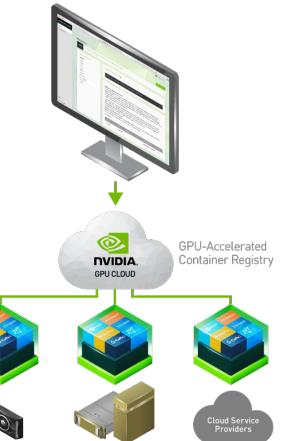
Very powerful GPUs

NVIDIA TESLA V100 FOR NVLINK

Ultimate performance for deep learning.



Workload: ResNet-50 | CPU: 2X Xeon E5-2660 v4, 2GHz | GPU: add 1X Tesla P100 or V100 at 150W | V100 measured on pre-production hardware.



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Resources



- Deep learning website:
<http://deeplearning.net>
- Deep learning book:
<http://www.deeplearningbook.org/>
- Deep learning for NLP tutorial:
<http://www.socher.org/index.php/DeepLearningTutorial/DeepLearningTutorial>
- Neural networks tutorials:
<http://www.coursera.org/course/neuralnets>

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