Deep Learning: Towards Deeper Understanding

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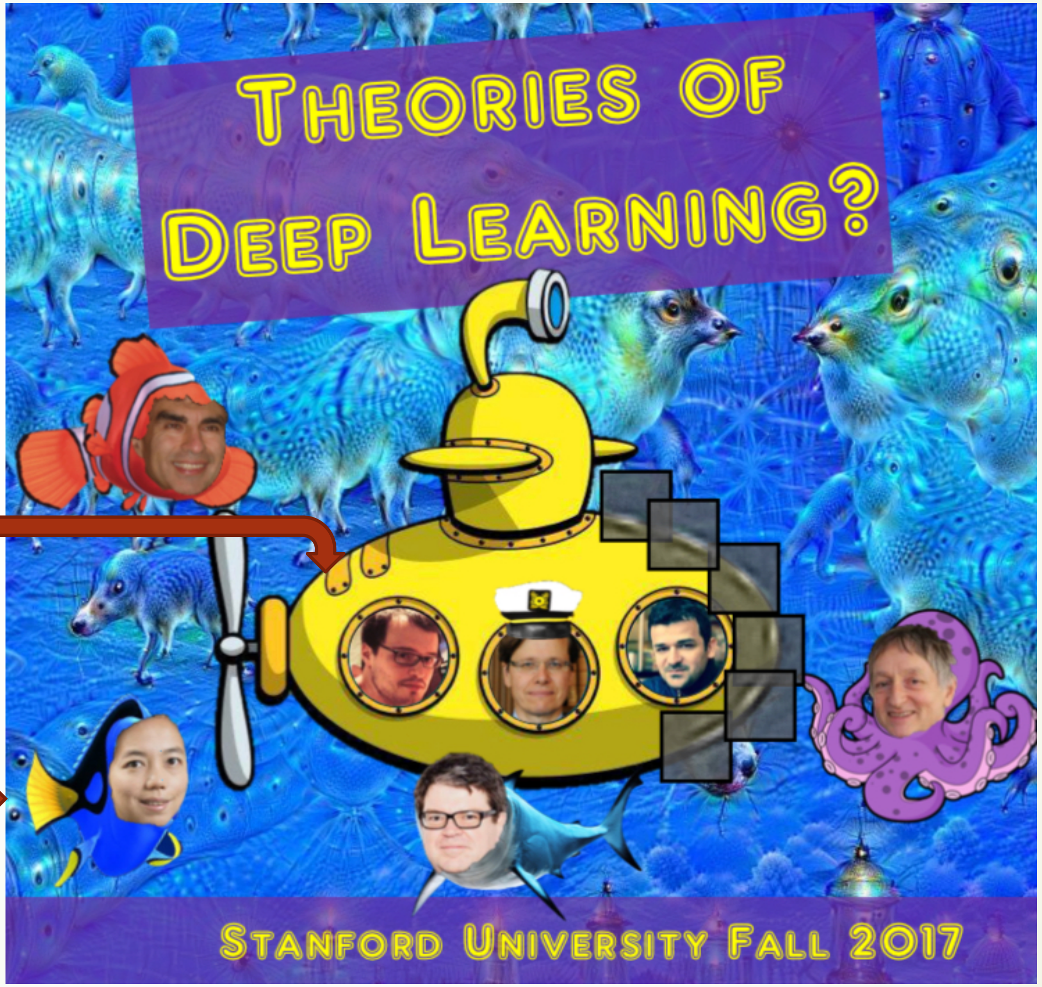
HKUST

Acknowledgement



https://stats385.github.io/

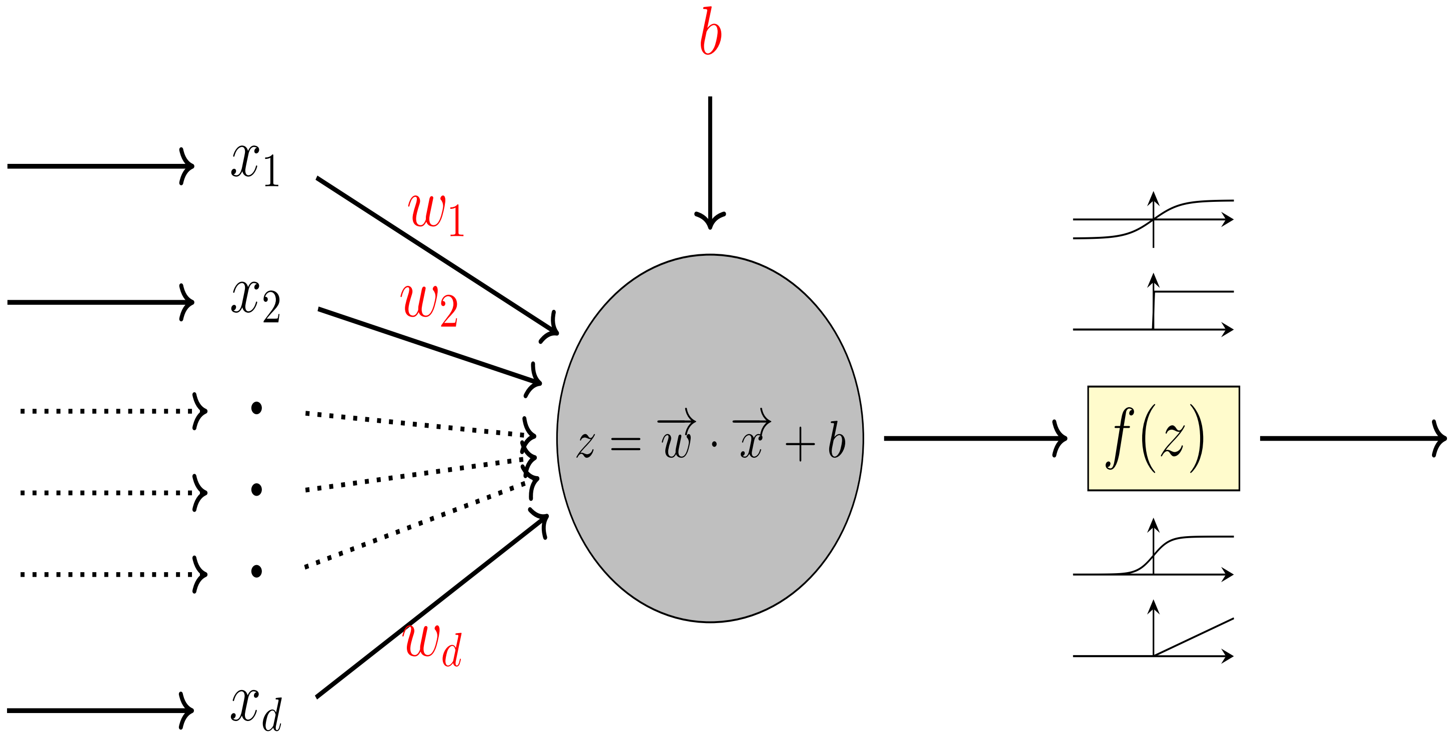
http://cs231n.github.io/

A following-up course at HKUST that evolves every year:
https://deeplearning-math.github.io/

A Brief History of Neural Networks

Perceptron: single-layer

- Invented by Frank Rosenblatt (1957)



Hilbert's 13th Problem

Algebraic equations (under a suitable transformation) of degree up to 6 can be solved by functions of two variables. What about

$$x^7 + ax^3 + bx^2 + cx + 1 = 0?$$

Hilbert's conjecture: $x(a, b, c)$ cannot be expressed by a superposition (sums and compositions) of bivariate functions.

Question: can every continuous (analytic, C^∞, etc) function of n variables be represented as a superposition of continuous (analytic, C^∞, etc) functions of $n-1$ variables?

Theorem (D. Hilbert)

There is an analytic function of three variables that cannot be expressed as a superposition of bivariate ones.

Kolmogorov's Superposition Theorem

Theorem (A. Kolmogorov, 1956; V. Arnold, 1957)

Given $n \in \mathbb{Z}^+$, every $f_0 \in C([0,1]^n)$ can be reprensented as

$$f_0(x_1, x_2, \cdots, x_n) = \sum_{q=1}^{2n+1} g_q \left(\sum_{p=1}^{n} \phi_{pq}(x_p) \right),$$

where $\phi_{pq} \in C[0,1]$ are increasing functions independent of f_0 and $g_q \in C[0,1]$ depend on f_0.

- Can choose g_q to be all the same $g_q \equiv g$ (Lorentz, 1966).
- Can choose ϕ_{pq} to be Hölder or Lipschitz continuous, but not C^1 (Fridman, 1967).
- Can choose $\phi_{pq} = \lambda_p \phi_q$ where $\lambda_1, \cdots, \lambda_n > 0$ and $\sum_p \lambda_p = 1$ (Sprecher, 1972).

If *f* is a multivariate continuous function, then *f* can be written as a superposition of composite functions of mixtures of continuous functions of single variables:
finite **composition** of continuous functions of a **single variable** and the **addition**.

Kolmogorov's Exact Representation is Irrelavant

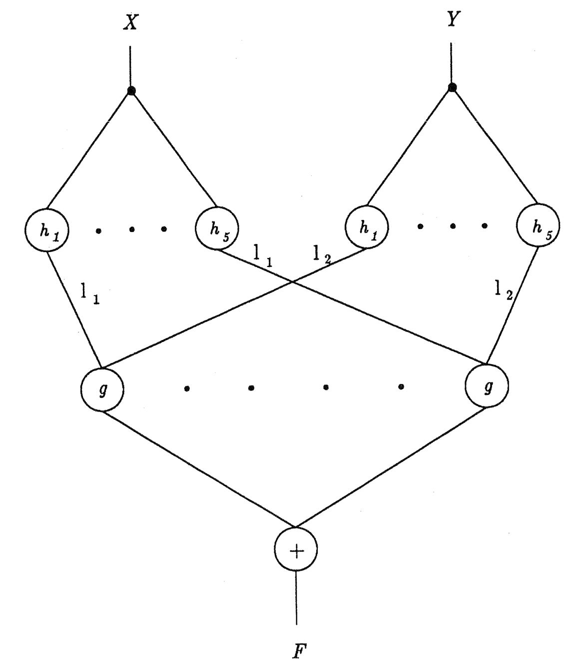


Figure 1: The network representation of an improved version of Kolmogorov's theorem, due to Kahane (1975). The figure shows the case of a bivariate function. The Kahane's representation formula is $f(x_1, \ldots, x_n) = \sum_{q=1}^{2n+1} g[\sum_{p=1}^{n} l_p h_q(x_p)]$ where h_q are strictly monotonic functions and l_p are strictly positive constants smaller than 1.

- [Girosi-Poggio'1989] Representation Properties of Networks: Kolmogorov's Theorem Is Irrelevant, https://www.mitpressjournals.org/doi/pdf/10.1162/neco.1989.1.4.465
- Lacking smoothness in *h* and *g* [Vitushkin'1964] fails to guarantee the **generalization ability (stability)** against noise and perturbations
- The representation is **not universal** in the sense that *g* and *h* both depend on the function F to be represented.

A Simplified illustration by David McAllester

A Simpler, Similar Theorem

For (possibly discontinuous) $f : [0,1]^N \to \mathbb{R}$ there exists (possibly discontinuous) $g, h_i : \mathbb{R} \to \mathbb{R}$.

$$f(x_1, \ldots, x_N) = g\left(\sum_i h_i(x_i)\right)$$

Proof: Select h_i to spread out the digits of its argument so that $\sum_i h_i(x_i)$ contains all the digits of all the x_i.

Universal Approximate Representation

[Cybenko'1989, Hornik et al. 1989, Poggio-Girosi'1989, ...]

For continuous $f : [0,1]^N \to \mathbb{R}$ and $\varepsilon > 0$ there exists

$$\begin{aligned} F(x) &= \alpha^\top \sigma(Wx + \beta) \\ &= \sum_i \alpha_i \sigma \left(\sum_j W_{i,j}\, x_j + \beta_i \right) \end{aligned}$$

such that for all x in $[0,1]^N$ we have $|F(x) - f(x)| < \varepsilon$.

Complexity (regularity, smoothness) thereafter becomes the central pursuit in Approximation Theory.

The Perceptron Algorithm for classification

$$\ell(w) = -\sum_{i \in \mathcal{M}_w} y_i \langle w, \mathbf{x}_i \rangle , \quad \mathcal{M}_w = \{i : y_i \langle \mathbf{x}_i, w \rangle < 0, y_i \in \{-1, 1\}\}.$$

The Perceptron Algorithm is a *Stochastic Gradient Descent* method (**Robbins-Monro 1951**):

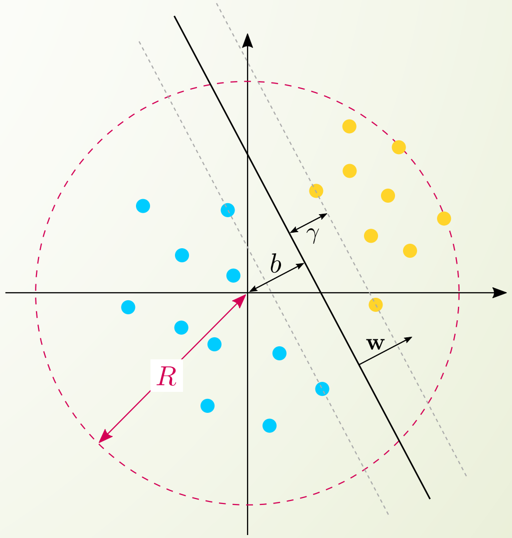
$$\begin{aligned} w_{t+1} &= w_t - \eta_t \nabla_i \ell(w) \\ &= \begin{cases} w_t - \eta_t y_i \mathbf{x}_i, & \text{if } y_i w_t^T \mathbf{x}_i < 0, \\ w_t, & \text{otherwise.} \end{cases} \end{aligned}$$

Finiteness of Stopping Time and Margin

The perceptron convergence theorem was proved by Block (1962) and Novikoff (1962). The following version is based on that in Cristianini and Shawe-Taylor (2000).

Theorem 1 (Block, Novikoff). *Let the training set $S = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$ be contained in a sphere of radius R about the origin. Assume the dataset to be linearly separable, and let $\mathbf{w}_{\text{opt}}$, $\|\mathbf{w}_{\text{opt}}\| = 1$, define the hyperplane separating the samples, having functional margin $\gamma > 0$. We initialise the normal vector as $\mathbf{w}_0 = \mathbf{0}$. The number of updates, k, of the perceptron algorithms is then bounded by*

$$k \leq \left(\frac{2R}{\gamma}\right)^2 . \tag{10}$$



Input ball: $R = \max_i \|\mathbf{x}_i\|$.

Margin: $\gamma := \min_i y_i f(x_i)$

Locality or Sparsity of Computation

Minsky and Papert, 1969

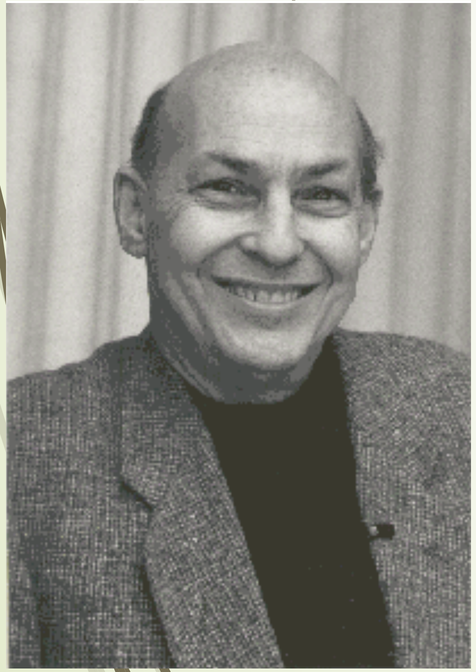
Perceptron can't do **XOR** classification

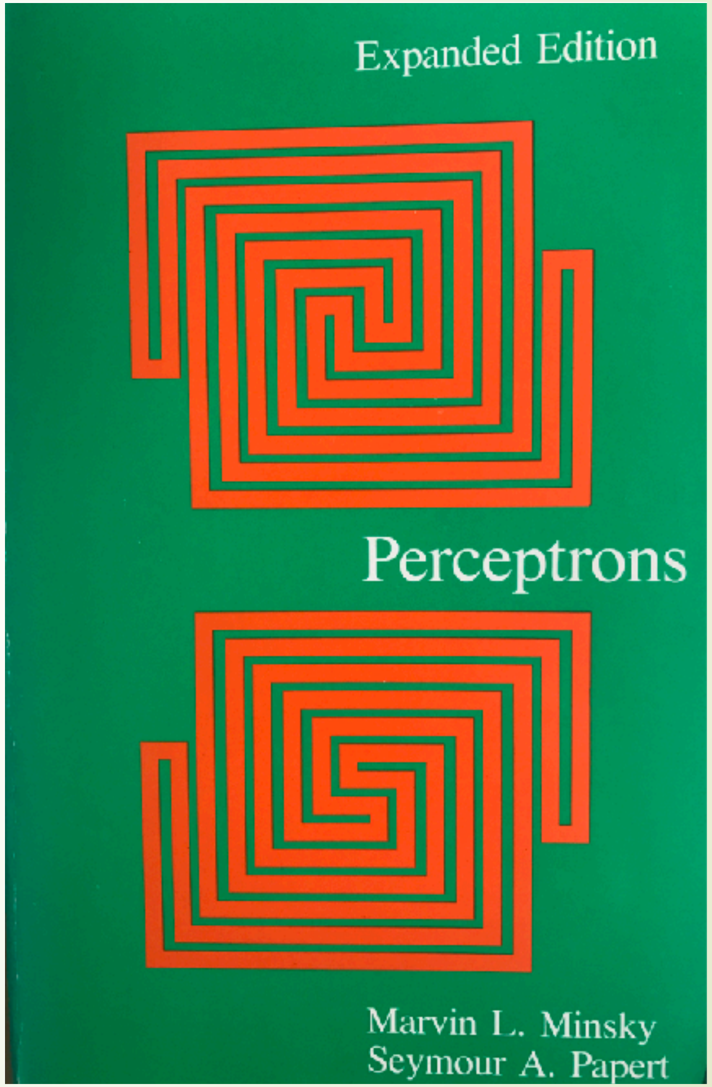
Perceptron needs infinite global information to compute **connectivity**

Locality or **Sparsity** is important:

Locality in time?

Locality in space?



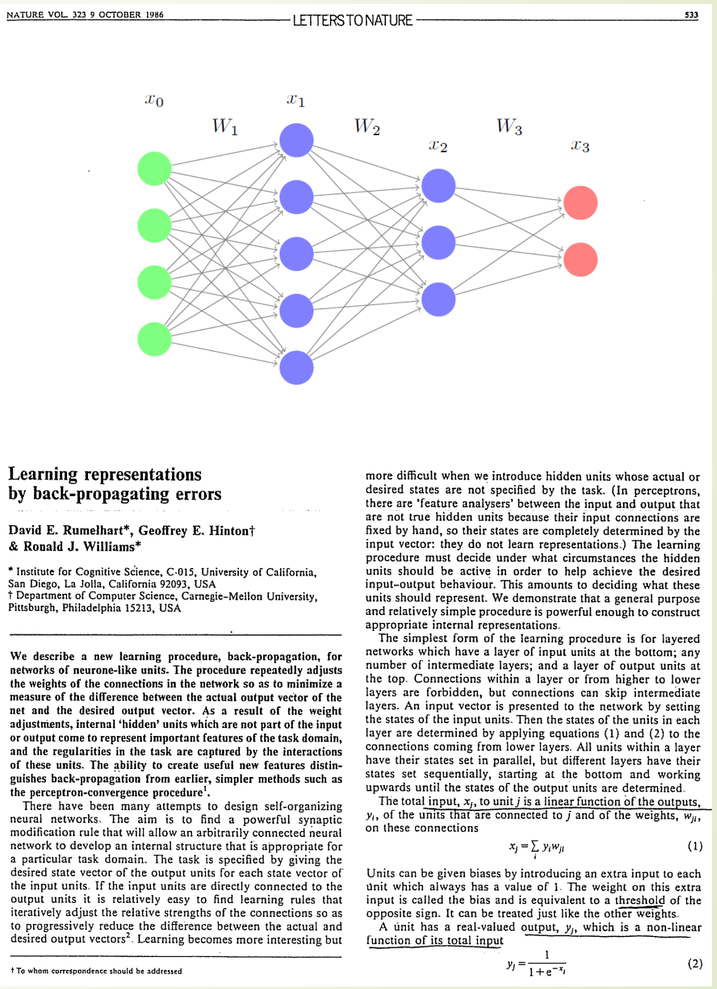


Multilayer Perceptrons (MLP) and Back-Propagation (BP) Algorithms

Rumelhart, Hinton, Williams (1986)
Learning representations by back-propagating errors, Nature, 323(9): 533-536

BP algorithms as **stochastic gradient descent** algorithms (**Robbins–Monro 1950; Kiefer-Wolfowitz 1951**) with Chain rules of Gradient maps

MLP classifies **XOR**, but the global hurdle on topology (connectivity) computation still exists: condition number in **Blum-Shub-Smale** real computation models helps.



Learning representations by back-propagating errors

David E. Rumelhart*, Geoffrey E. Hinton† & Ronald J. Williams*

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† Department of Computer Science, Carnegie-Mellon University, Pittsburgh, Philadelphia 15213, USA

We describe a new learning procedure, back-propagation, for networks of neurone-like units. The procedure repeatedly adjusts the weights of the connections in the network so as to minimize a measure of the difference between the actual output vector of the net and the desired output vector. As a result of the weight adjustments, internal 'hidden' units which are not part of the input or output come to represent important features of the task domain, and the regularities in the task are captured by the interactions of these units. The ability to create useful new features distinguishes back-propagation from earlier, simpler methods such as the perceptron-convergence procedure[1].

There have been many attempts to design self-organizing neural networks. The aim is to find a powerful synaptic modification rule that will allow an arbitrarily connected neural network to develop an internal structure that is appropriate for a particular task domain. The task is specified by giving the desired state vector of the output units for each state vector of the input units. If the input units are directly connected to the output units it is relatively easy to find learning rules that iteratively adjust the relative strengths of the connections so as to progressively reduce the difference between the actual and desired output vectors[2]. Learning becomes more interesting but more difficult when we introduce hidden units whose actual or desired states are not specified by the task. (In perceptrons, there are 'feature analysers' between the input and output that are not true hidden units because their input connections are fixed by hand, so their states are completely determined by the input vector: they do not learn representations.) The learning procedure must decide under what circumstances the hidden units should be active in order to help achieve the desired input–output behaviour. This amounts to deciding what these units should represent. We demonstrate that a general purpose and relatively simple procedure is powerful enough to construct appropriate internal representations.

The simplest form of the learning procedure is for layered networks which have a layer of input units at the bottom; any number of intermediate layers; and a layer of output units at the top. Connections within a layer or from higher to lower layers are forbidden, but connections can skip intermediate layers. An input vector is presented to the network by setting the states of the input units. Then the states of the units in each layer are determined by applying equations (1) and (2) to the connections coming from lower layers. All units within a layer have their states set in parallel, but different layers have their states set sequentially, starting at the bottom and working upwards until the states of the output units are determined.

The total input, x_j, to unit j is a linear function of the outputs, y_i, of the units that are connected to j and of the weights, w_{ji}, on these connections

$$x_j = \sum_i y_i w_{ji} \tag{1}$$

Units can be given biases by introducing an extra input to each unit which always has a value of 1. The weight on this extra input is called the bias and is equivalent to a threshold of the opposite sign. It can be treated just like the other weights.

A unit has a real-valued output, y_j, which is a non-linear function of its total input

$$y_j = \frac{1}{1+e^{-x_j}} \tag{2}$$

† To whom correspondence should be addressed.

BP Algorithm: Forward Pass

- Cascade of repeated [linear operation followed by coordinatewise nonlinearity]'s
- Nonlinearities: sigmoid, hyperbolic tangent, (recently) ReLU.

Algorithm 1 Forward pass

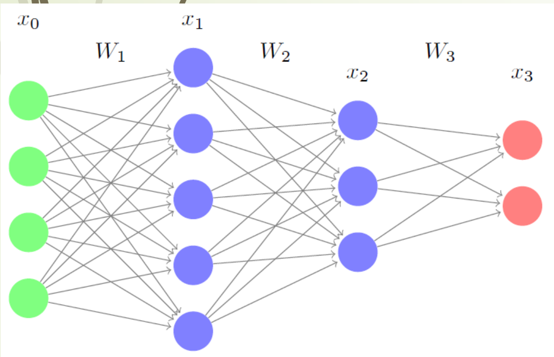
Input: x_0

Output: x_L

1: **for** $\ell = 1$ to L **do**

2: $\quad x_\ell = f_\ell(W_\ell x_{\ell-1} + b_\ell)$

3: **end for**



BP algorithm = Gradient Descent Method

- Training examples $\{x_0^i\}_{i=1}^n$ and labels $\{y^i\}_{i=1}^n$
- Output of the network $\{x_L^i\}_{i=1}^m$
- Objective Square loss, cross-entropy loss, etc.

$$J(\{W_l\}, \{b_l\}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{2}\|y^i - x_L^i\|_2^2 \tag{1}$$

- Gradient descent

$$W_l = W_l - \eta\frac{\partial J}{\partial W_l}$$
$$b_l = b_l - \eta\frac{\partial J}{\partial b_l}$$

In practice: use Stochastic Gradient Descent (SGD)

Derivation of BP: Lagrangian Multiplier

LeCun et al. 1988

Given n training examples $(I_i, y_i) \equiv$ (input,target) and L layers

- Constrained optimization

$$\min_{W,x} \quad \sum_{i=1}^{n} \|x_i(L) - y_i\|_2$$

$$\text{subject to} \quad x_i(\ell) = f_\ell\Big[W_\ell x_i\,(\ell - 1)\Big],$$

$$i = 1, \ldots, n, \quad \ell = 1, \ldots, L, \; x_i(0) = I_i$$

- Lagrangian formulation (Unconstrained)

$$\min_{W,x,B} \mathcal{L}(W, x, B)$$

$$\mathcal{L}(W, x, B) = \sum_{i=1}^{n} \Bigg\{ \|x_i(L) - y_i\|_2^2 + \sum_{\ell=1}^{L} B_i(\ell)^T \Big(x_i(\ell) - f_\ell\Big[W_\ell x_i\,(\ell - 1)\Big] \Big) \Bigg\}$$

http://yann.lecun.com/exdb/publis/pdf/lecun-88.pdf

back-propagation – derivation

- $\frac{\partial \mathcal{L}}{\partial B}$

Forward pass

$$x_i(\ell) = f_\ell\Big[\underbrace{W_\ell x_i\,(\ell-1)}_{A_i(\ell)}\Big] \quad \ell = 1,\ldots,L, \quad i = 1,\ldots,n$$

- $\frac{\partial \mathcal{L}}{\partial x}$, $z_\ell = [\nabla f_\ell] B(\ell)$

Backward (adjoint) pass

$$z(L) = 2\nabla f_L\Big[A_i(L)\Big]\,(y_i - x_i(L))$$

$$z_i(\ell) = \nabla f_\ell\Big[A_i(\ell)\Big] W_{\ell+1}^T z_i(\ell+1) \quad \ell = 0,\ldots,L-1$$

- $W \leftarrow W + \lambda \frac{\partial \mathcal{L}}{\partial W}$

Weight update

$$W_\ell \leftarrow W_\ell + \lambda \sum_{i=1}^n z_i(\ell) x_i^T(\ell-1)$$

Convolutional Neural Networks: shift invariances and locality

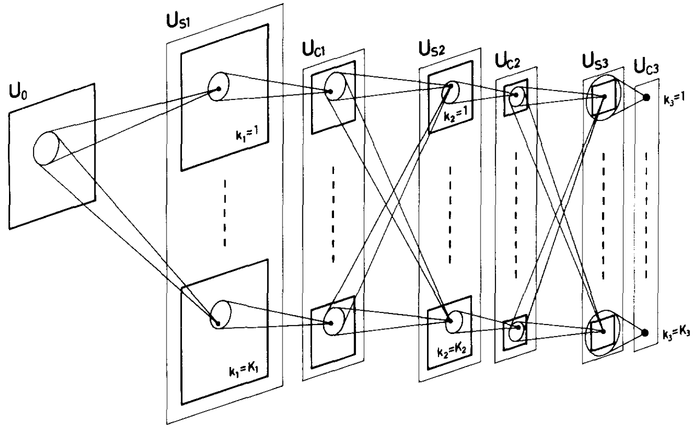
- Can be traced to *Neocognitron* of Kunihiko Fukushima (1979)
- Yann LeCun combined convolutional neural networks with back propagation (1989)
- Imposes **shift invariance** and **locality** on the weights
- Forward pass remains similar
- Backpropagation slightly changes – need to sum over the gradients from all spatial positions

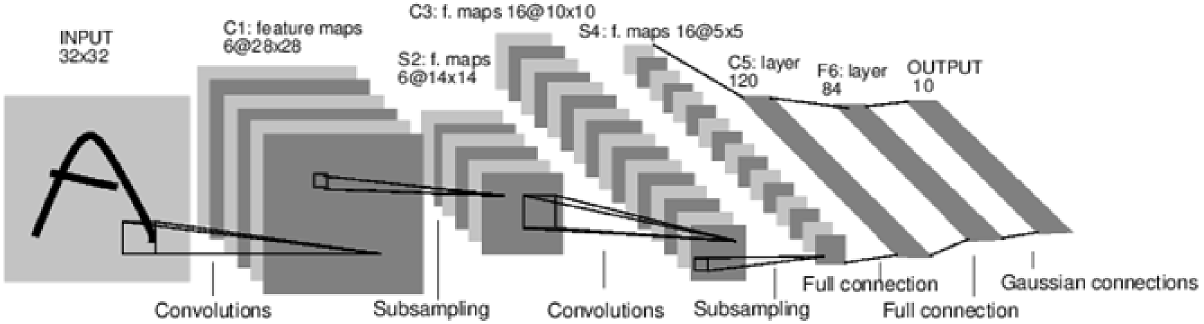
Biol. Cybernetics 36, 193–202 (1980)

Neocognitron: A Self-organizing Neural Network Model for a Mechanism of Pattern Recognition Unaffected by Shift in Position

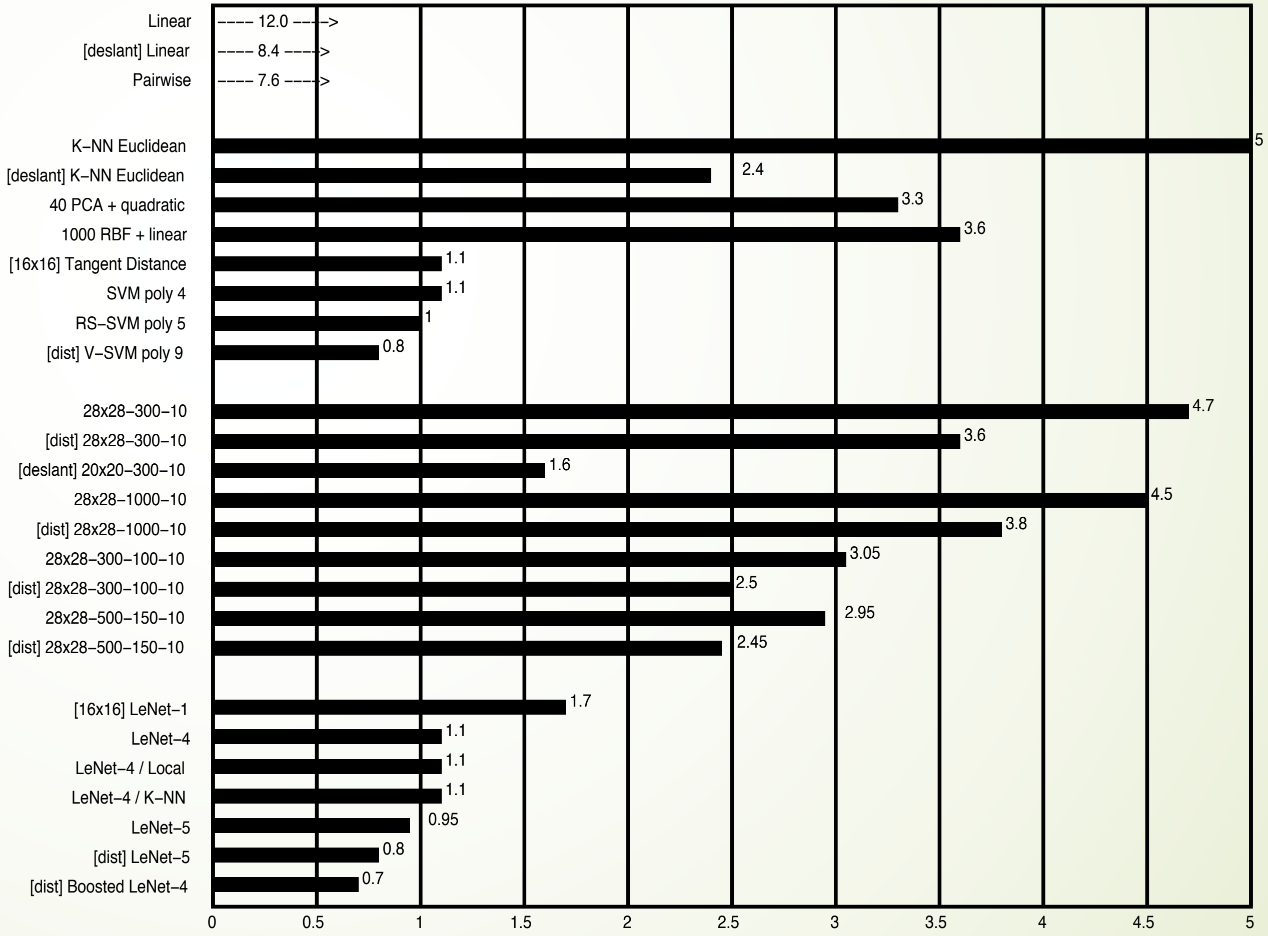
Kunihiko Fukushima

NHK Broadcasting Science Research Laboratories, Kinuta, Setagaya, Tokyo, Japan





MNIST Dataset Test Error LeCun et al. 1998

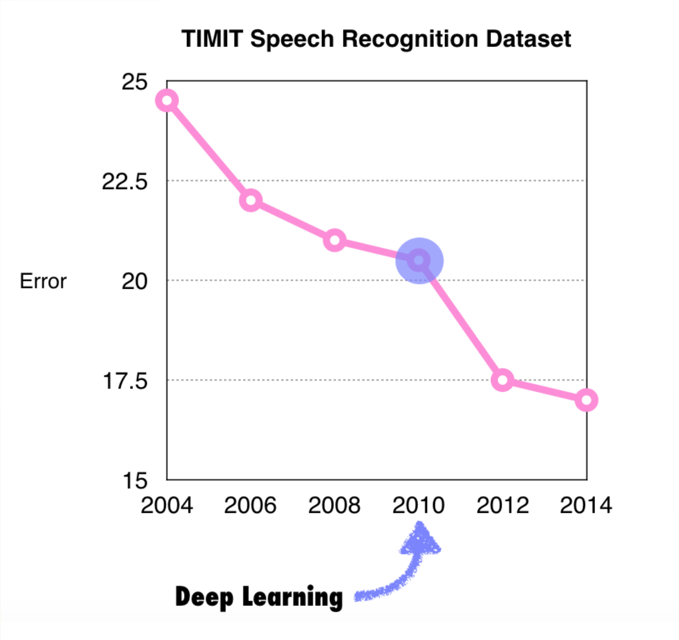


Simple SVM performs as well as Multilayer Convolutional Neural Networks which need careful tuning (LeNets)

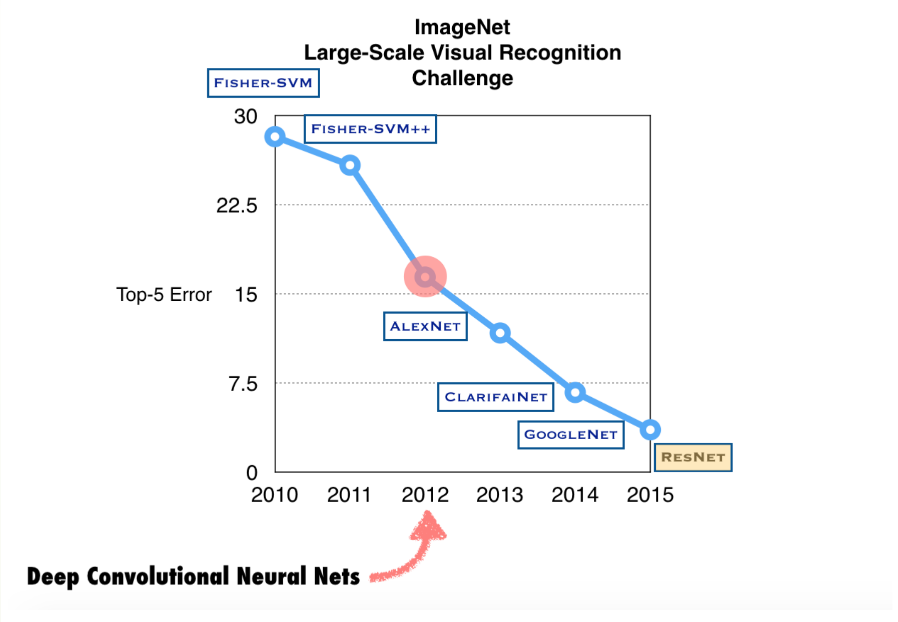
Dark era for NN: 1998-2012

Around the year of 2012: return of NN as `deep learning’

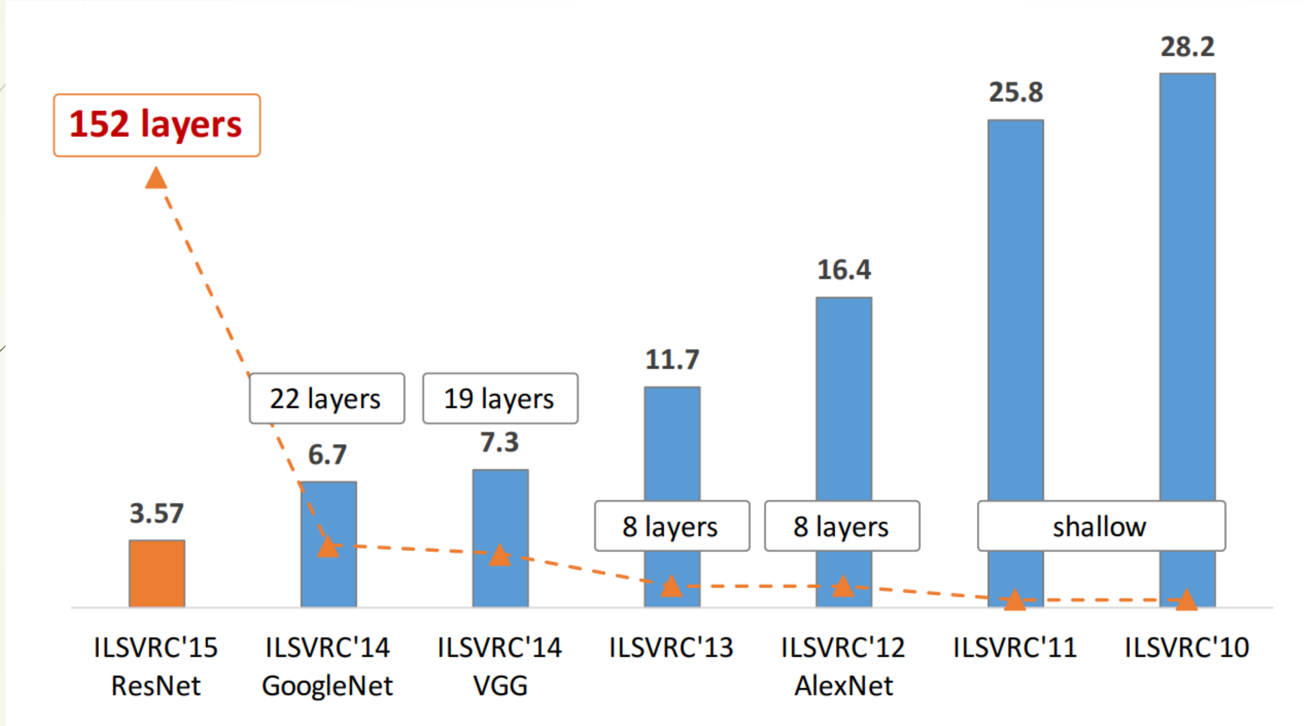
Speech Recognition: TIMIT



Computer Vision: ImageNet



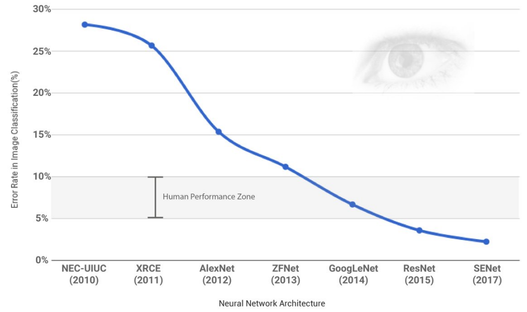
Depth as function of year



[He et al., 2016]

ILSVRC ImageNet Top 5 errors

- ImageNet (subset):
  - 1.2 million training images
  - 100,000 test images
  - 1000 classes
- ImageNet large-scale visual recognition Challenge

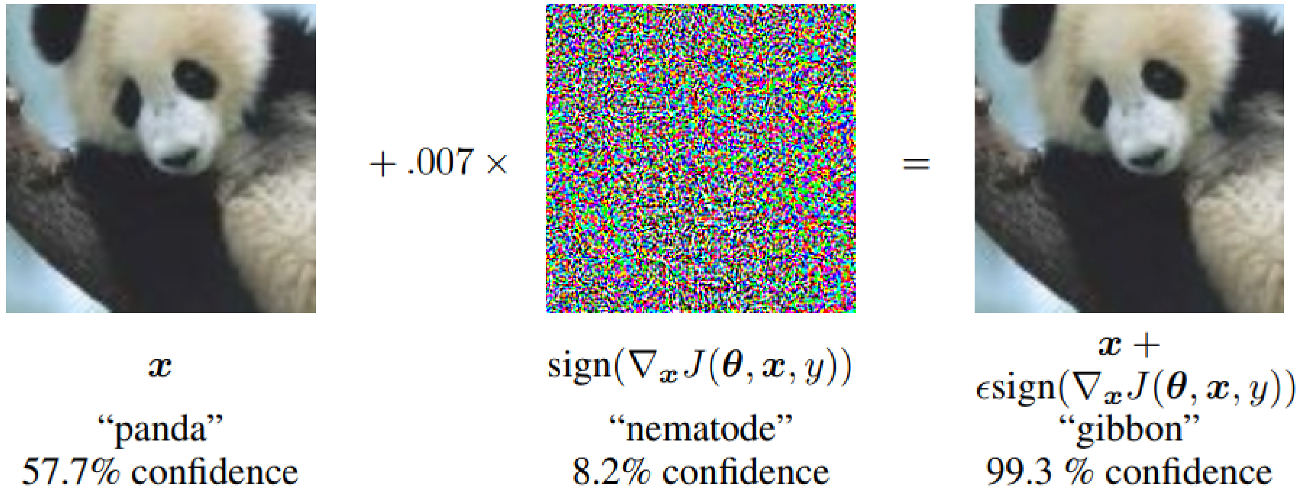


source: https://www.linkedin.com/pulse/must-read-path-breaking-papers-image-classification-muktabh-mayank

Some Cold Water: Tesla Autopilot Misclassifies Truck as Billboard

Problem: Why? How can you trust a blackbox?

Deep Learning may be fragile in generalization against noise!



[Goodfellow et al., 2014]

- Small but malicious perturbations can result in severe misclassification
- Malicious examples generalize across different architectures
- What is source of instability?
- Can we robustify network?

What's wrong with deep learning?

Ali Rahimi NIPS'17: Machine (deep) Learning has become **alchemy**.
https://www.youtube.com/watch?v=ORHFOnaEzPc

Yann LeCun CVPR'15, invited talk: **What's wrong with deep learning?** One important piece: **missing some theory (clarity in understanding)**!

http://techtalks.tv/talks/whats-wrong-with-deep-learning/61639/

Being alchemy is certainly not a shame, not wanting to work on advancing to chemistry is a shame! -- **by Eric Xing**

What’s wrong with deep learning?

In this course, we only raise problems, and leave you to explore answers.

CNN learns texture features, not shapes

(a) Texture image

81.4%	**Indian elephant**
10.3%	indri
8.2%	black swan

(b) Content image

71.1%	**tabby cat**
17.3%	grey fox
3.3%	Siamese cat

(c) Texture-shape cue conflict

63.9%	**Indian elephant**
26.4%	indri
9.6%	black swan

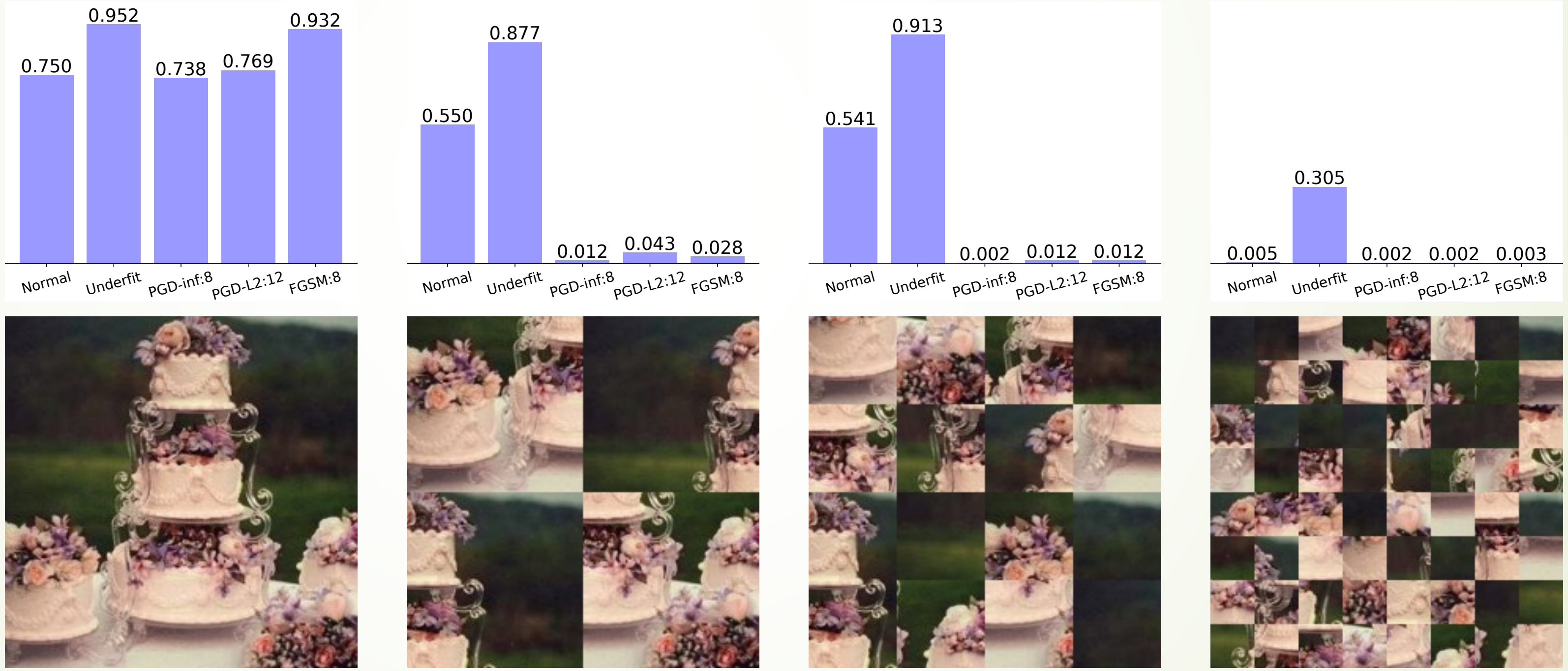
Geirhos et al. ICLR 2019

https://videoken.com/embed/W2HvLBMhCJQ?tocitem=46

1:16:47

Lack of Causality or Interpretability

- ImageNet training learns non-semantic texture features: after random shuffling of patches, shapes information are destroyed which does not affect CNN's performance much.



(a) Original Image (b) Patch-Shuffle 2 (c) Patch-Shuffle 4 (d) Patch-Shuffle 8

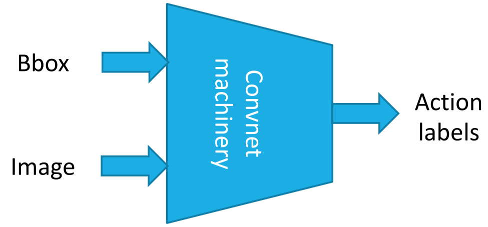
Zhanxing Zhu et al., ICML 2019

Capture spurious correlations and can't do causal inference on counterfactuals

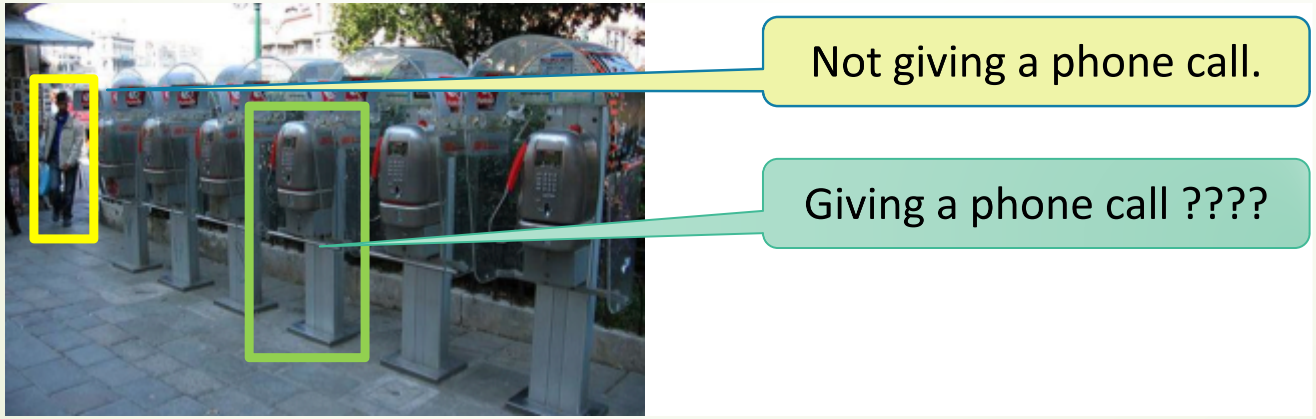
https://videoken.com/embed/8UxS4ls6g1g?tocitem=2

Leon Bottou, ICLR 2019

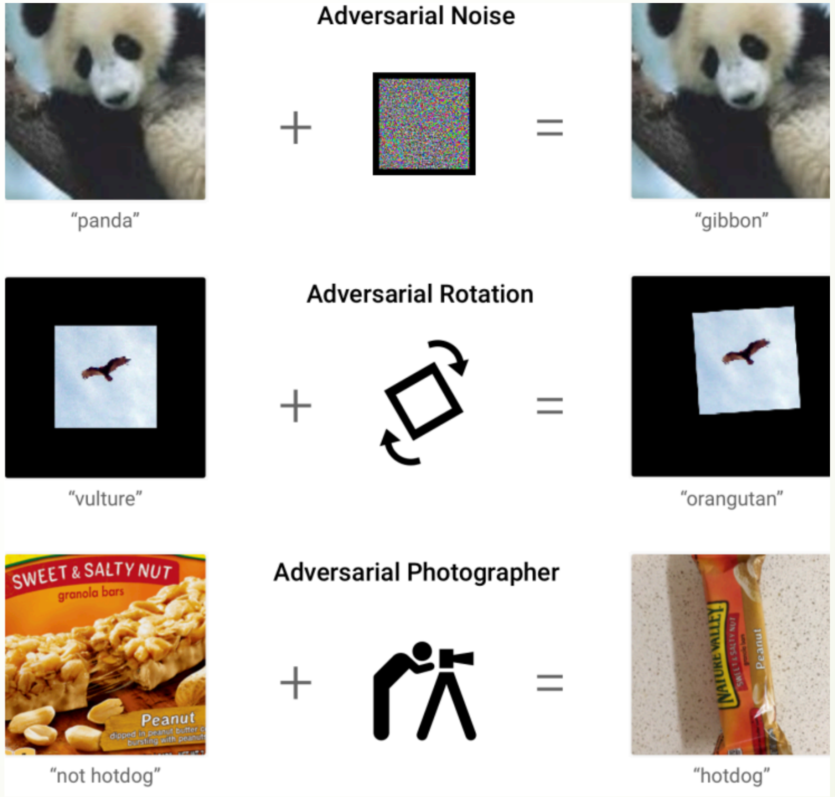
Example: detection of the action "*giving a phone call*"



(Oquab et al., CVPR 2014)
~70% correct (SOTA in 2014)



Deep learning is not robust
-- adversarials are ubiquitous



[BCZOCG'18] Unrestricted Adversarial Example.

Overfitting causes privacy leakage

- Model inversion attack leaks privacy

Figure: Recovered (Left), Original (Right)

Fredrikson et al. Proc. CCS, 2016

Towards a deeper understanding of deep learning

- How to achieve robustness?
  - Madry's adversarial training, random smoothing, ensemble methods, stability regularization, etc.
- How to guarantee privacy?
  - Differential privacy, model inversion privacy, membership privacy, etc.
- How to improve interpretability or causality?
  - Invariance (learning), disentanglement of representation, etc.

Some Theories are limited but help:

- *Approximation Theory and Harmonic Analysis* : **What functions are represented well by deep neural networks, without suffering the curse of dimensionality and better than shallow networks?**
  - Sparse (local), hierarchical (multiscale), compositional functions avoid the curse dimensionality
  - Group (translation, rotational, scaling, deformation) invariances achieved as depth grows
- *Statistics learning:* **How can deep learning generalize well without overfitting the noise?**
  - "Benign overfitting"? …
- *Optimization:* **What is the landscape of the empirical risk and how to optimize it efficiently?**
  - Wide networks may have simple landscape for GD/SGD algorithms …

Thank you!

Generalization Ability

Why over-parameterized models may generalize well without overfitting?

Generalization Error

- Consider the empirical risk minimization under i.i.d. samples

$$\hat{R}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i;\theta)) + \mathcal{R}(\theta)$$

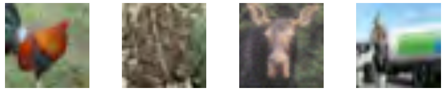
- The population risk with respect to unknown distribution

$$R(\theta) = \mathbf{E}_{x,y\sim P}\ell(y, f(x;\theta))$$

- Fundamental Theorem of Machine Learning (for 0-1 misclassification loss, called 'errors' below)

$$R(\theta) = \underbrace{\hat{R}_n(\theta)}_{\text{training loss/error}} + \underbrace{R(\theta) - \hat{R}_n(\theta)}_{\text{generalization loss/error}}$$

Why big models generalize well?



CIFAR10

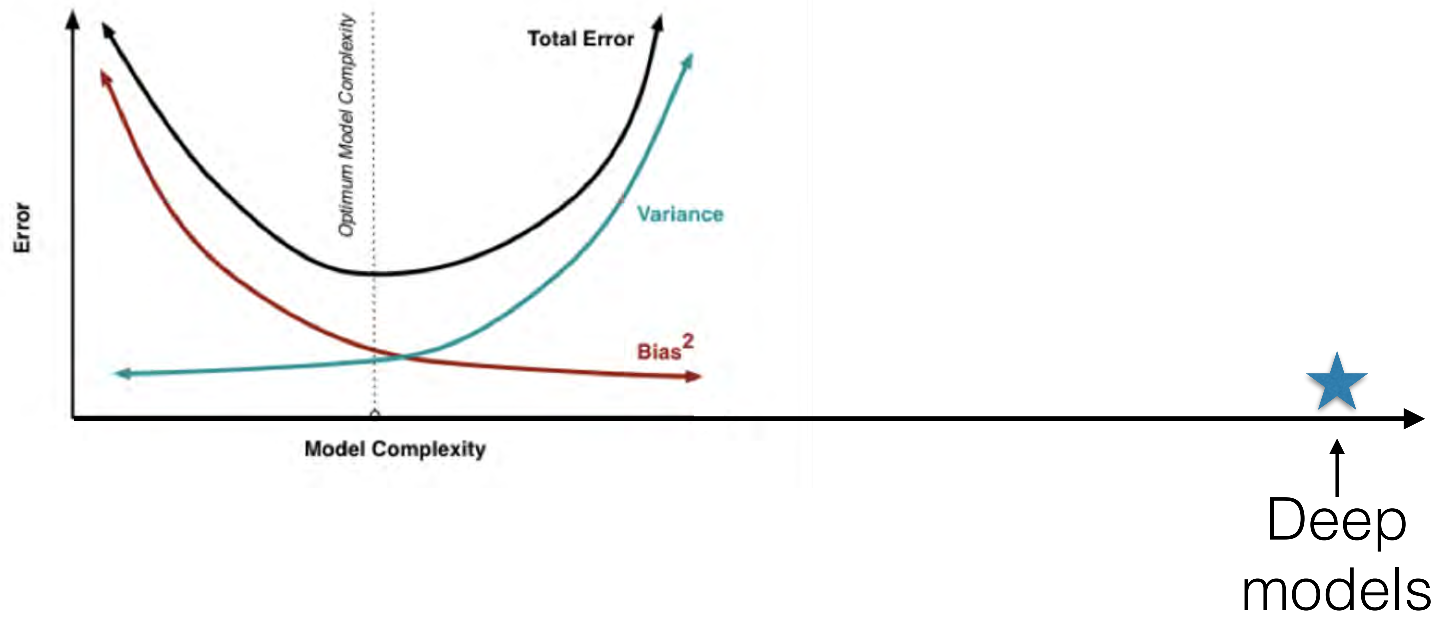
n=50,000
d=3,072
k=10

What happens when I turn off the regularizers?

Model	parameters	p/n	Train **loss**	Test **error**
CudaConvNet	145,578	2.9	0	23%
CudaConvNet (with regularization)	145,578	2.9	0.34	18%
MicroInception	1,649,402	33	0	14%
ResNet	2,401,440	48	0	13%

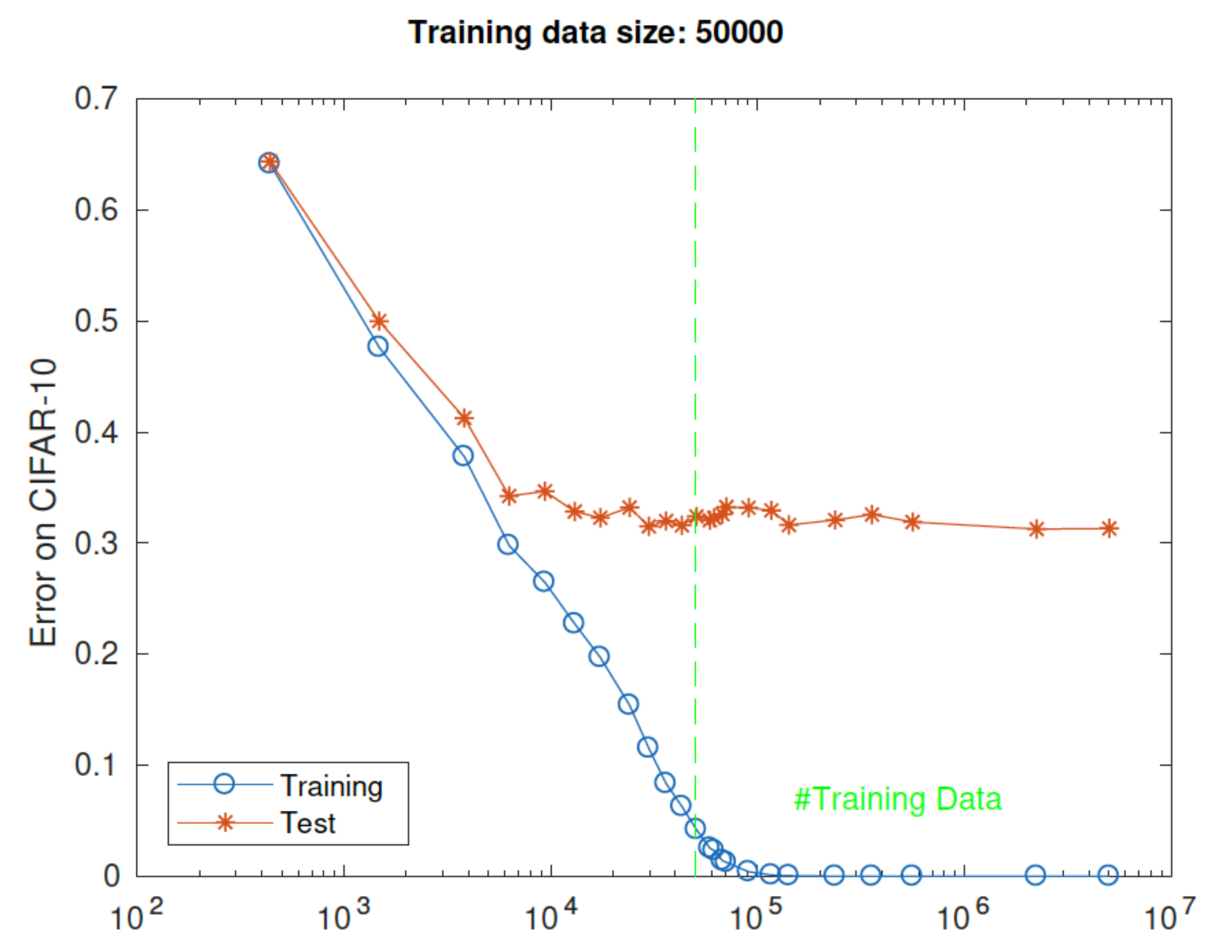
Ben Recht et al. 2016

The Bias-Variance Tradeoff?



Models where p>20n are common

Over-parameterized models



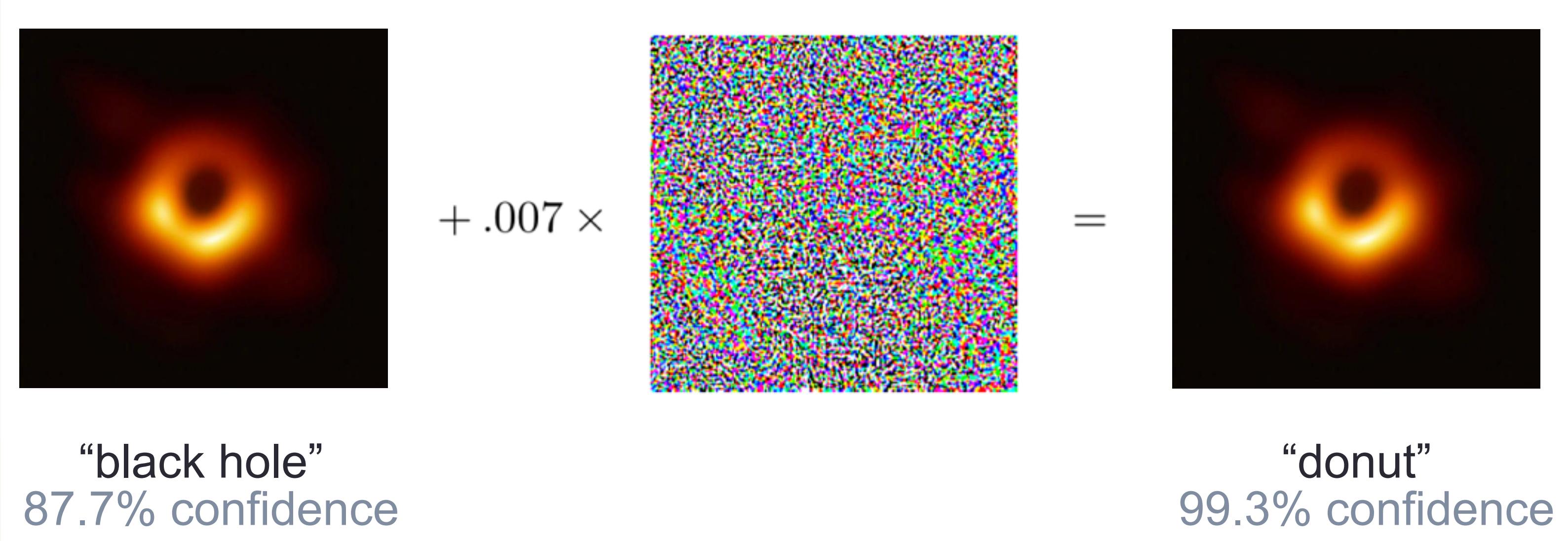
As model complexity grows (p>n), training error goes down to zero, but test error does not increase. Why overparameterized models do not overfit here? -- Tommy Poggio, 2018

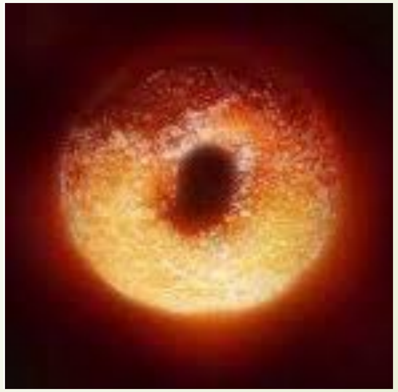
Some tentative answers:

- **Belkin** et al.: Interplolation (overfitting) has a low generalization error in overparameterization regime
  - https://simons.berkeley.edu/talks/tbd-65
- For overparameterized linear regression models:
  - **Peter Bartlett** et al. https://simons.berkeley.edu/talks/tbd-51
  - **Trevor Hastie** et al. asymptotic theory based on random matrix theory
- For logistic regressions:
  - **Telgarsky, Srebro**, et al. GD converges to max margin solution
- Nonlinear neural networks: ???
- Some warnings on “interpolations”:
  - Ben Recht: https://simons.berkeley.edu/talks/tbd-63

Yet, Overfitting indeed hurts…

- Lack of Robustness





Courtesy of Dr. Hongyang ZHANG.