



# MATHEMATICAL FRONTIERS

*The National  
Academies of* | SCIENCES  
ENGINEERING  
MEDICINE

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Board on  
Mathematical Sciences & Analytics

# MATHEMATICAL FRONTIERS

## 2018 Monthly Webinar Series, 2-3pm ET

**February 13\*:**

*Mathematics of the Electric Grid*

**March 13\*:**

*Probability for People and Places*

**April 10\*:**

*Social and Biological Networks*

**May 8\*:**

*Mathematics of Redistricting*

**June 12\*:** *Number Theory: The Riemann Hypothesis*

**\* Recording posted**

**July 10\*:** *Topology*

**August 14\*:** *Algorithms for Threat Detection*

**September 11\*:** *Mathematical Analysis*

**October 9\*:** *Combinatorics*

**November 13:**

*Why Machine Learning Works*

**December 11:**

*Mathematics of Epidemics*

Made possible by support for BMSA from the  
National Science Foundation Division of Mathematical Sciences and the  
Department of Energy Advanced Scientific Computing Research

# MATHEMATICAL FRONTIERS

## Why Machine Learning Works



**Aarti Singh,**  
Carnegie Mellon University



**David Donoho,**  
Stanford University



**Mark Green,**  
UCLA (moderator)

# MATHEMATICAL FRONTIERS

## Why Machine Learning Works



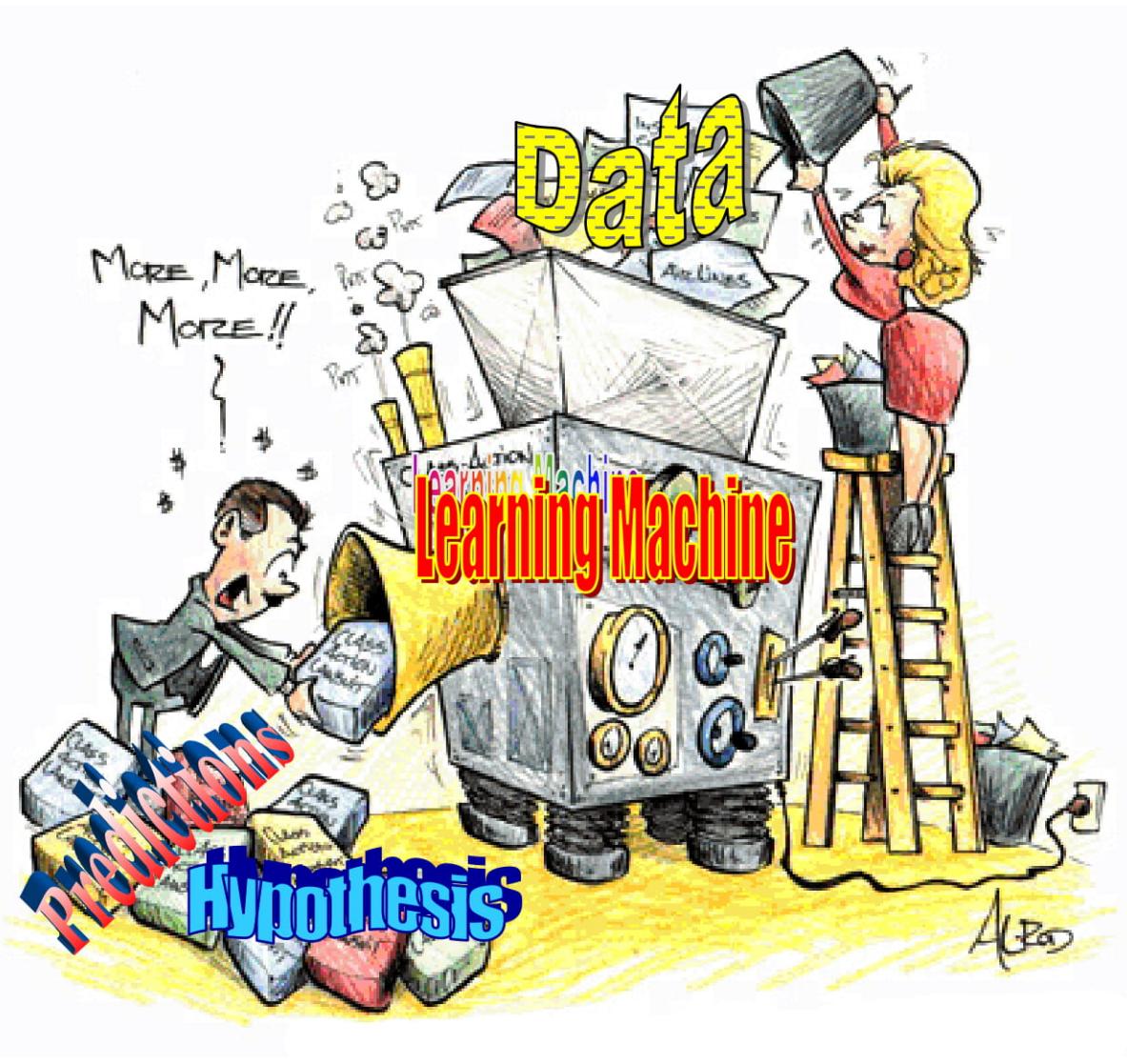
*Associate Professor,  
Machine Learning Department*

## Why Machine Learning Works

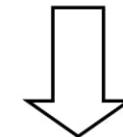
**Aarti Singh,**  
Carnegie Mellon University

*View webinar videos and learn more about BMSA at [www.nas.edu/MathFrontiers](http://www.nas.edu/MathFrontiers)*

# What is Machine Learning?



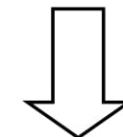
Data



584146951941511609455057270  
6115021911161401111909  
618801194190377a887406  
190702179860945702770859217

Learning algorithm

Knowledge



# What is Machine Learning?

Design and Analysis of algorithms that

- improve their performance
- at some task
- with experience



Tom Mitchell  
Carnegie Mellon Univ.

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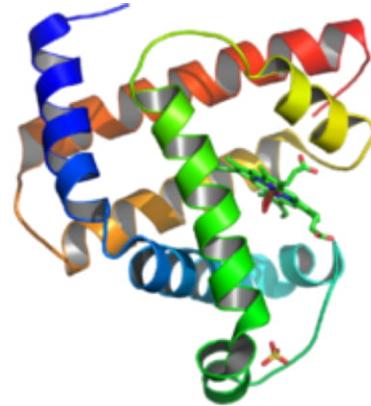
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# Understanding ML ingredients

<http://phillips-lab.biochem.wisc.edu/>

**Task:** Learning stage of protein crystallization



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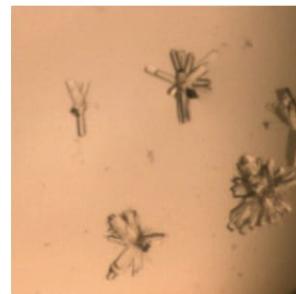
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Crystal



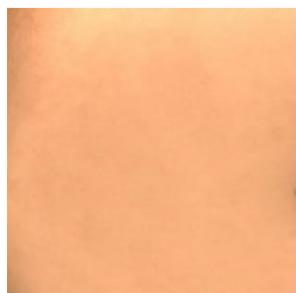
Needle



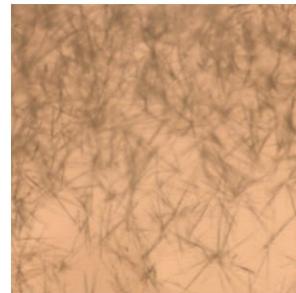
Tree



Tree

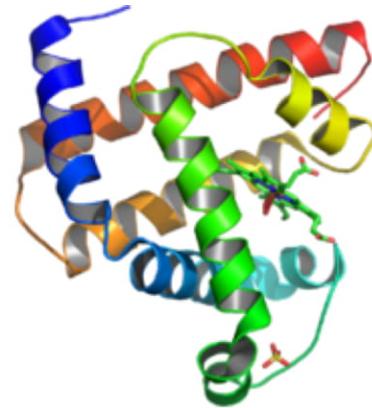


Empty



Needle

**Experience**



# Understanding ML ingredients

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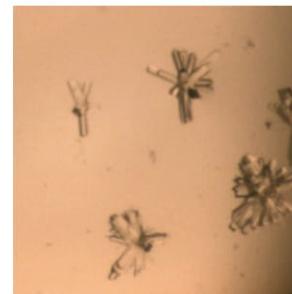
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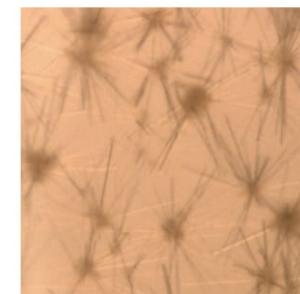


Empty



Needle

**Experience**

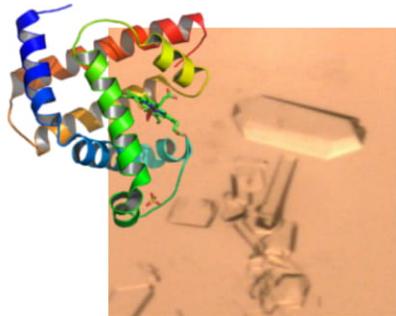


?

**Performance**

# Why learn from data (experience)?

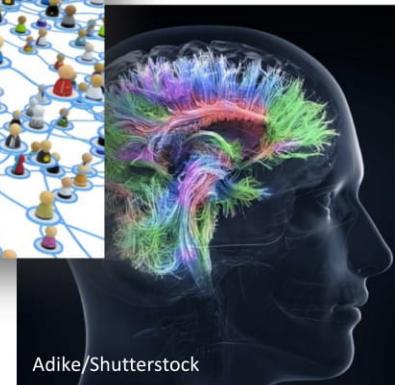
## Understanding large-scale complex systems



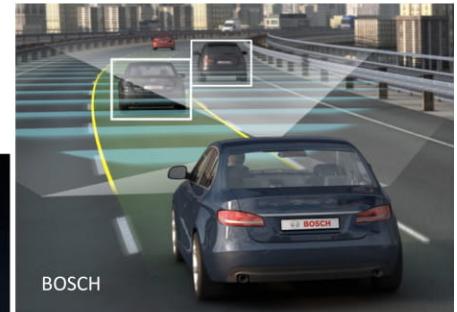
Bio-chemical  
molecules



Social  
networks



Brain

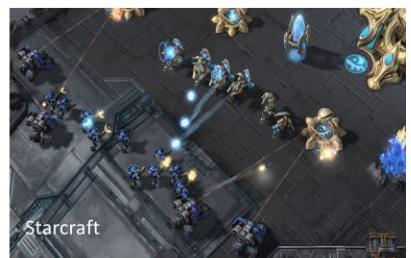


Self-driving vehicles



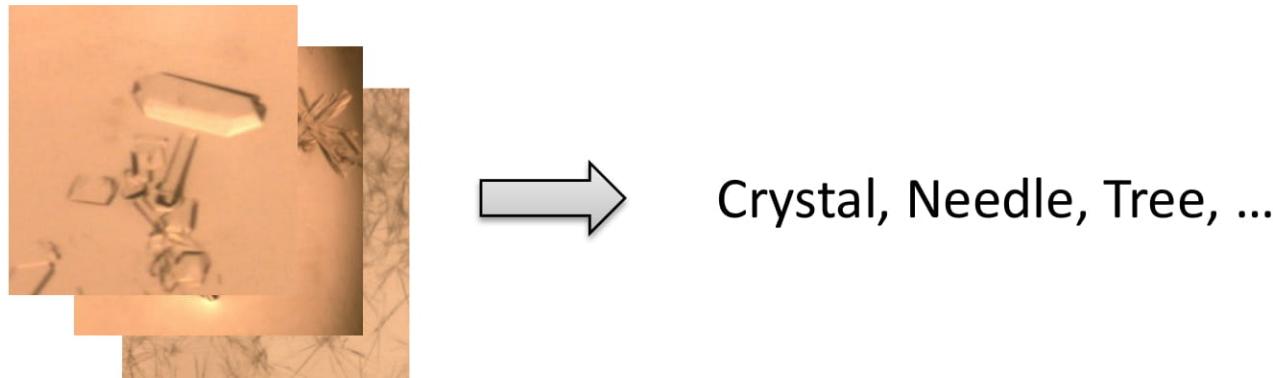
Cosmos

rules and governing equations  
are hard to discover  
involve too many variables  
are computationally too expensive  
are typically stochastic

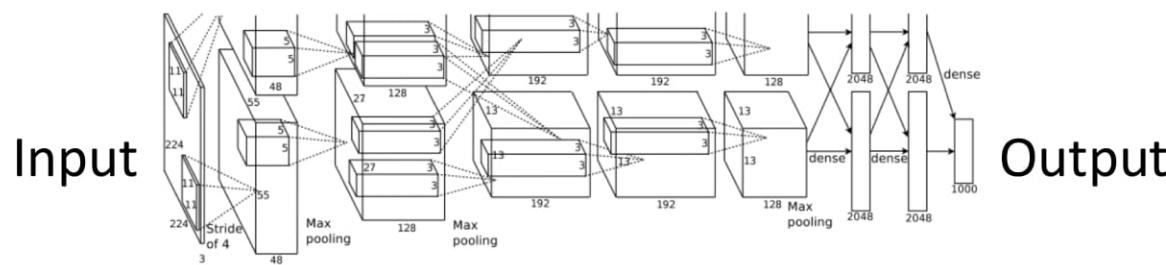


Games

# How ML works



- Model  $f$ : mapping between input and output  
linear, nonlinear, deep model



- Algorithm: fits model to data  
Optimize Performance(Model  $f$ , Data)  
 $f$

# Why ML works

- Lots of data due to improved high-throughput technologies
- Improved machine learning algorithms
- Enhanced computing power

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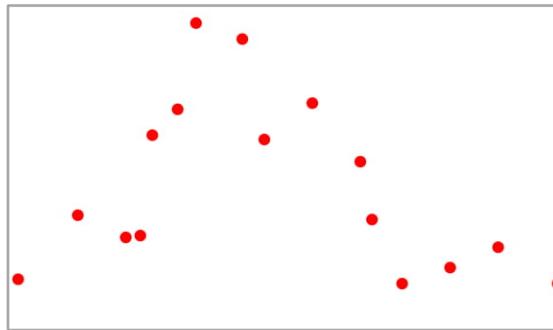
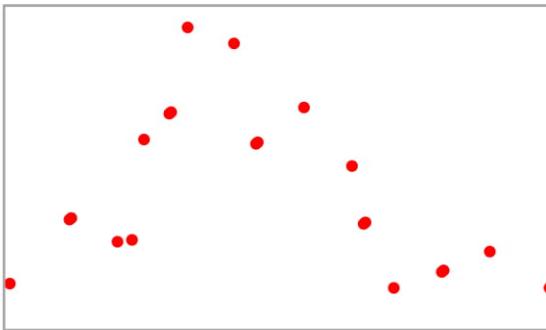
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e.g. Social media and web data (Petabytes/min), Large Synoptic Survey Telescope (20 TB/night)
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  - Generalize well to unseen data
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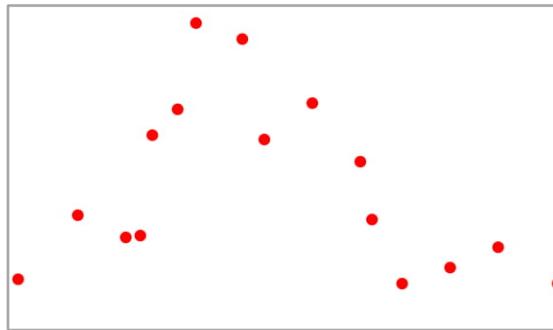
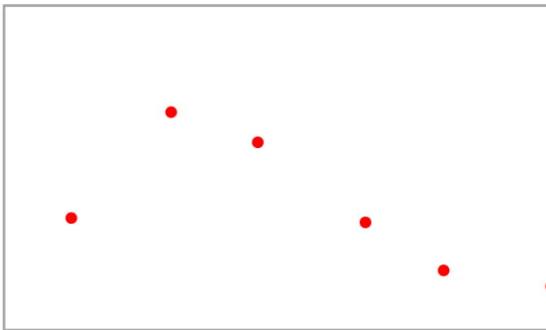
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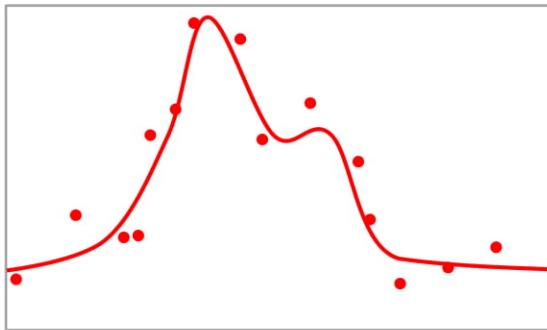
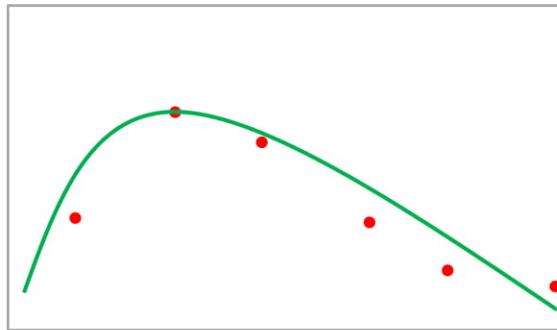
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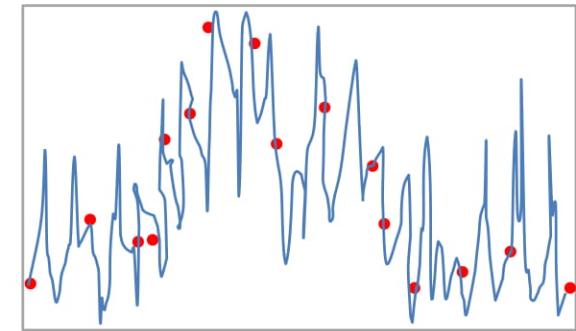
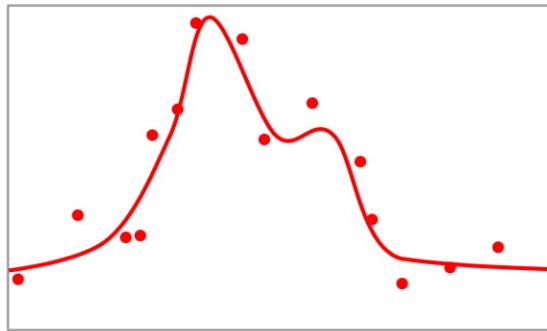
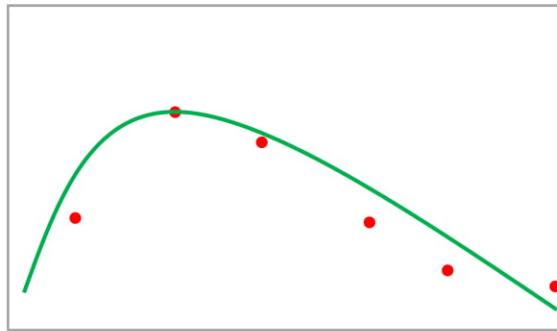
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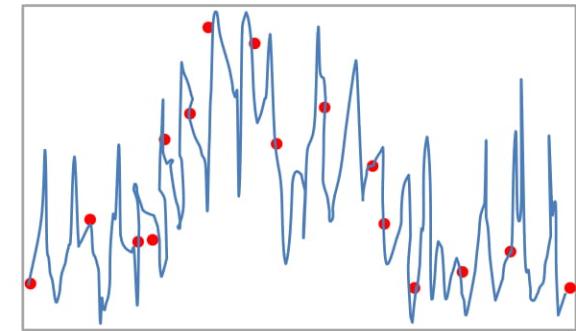
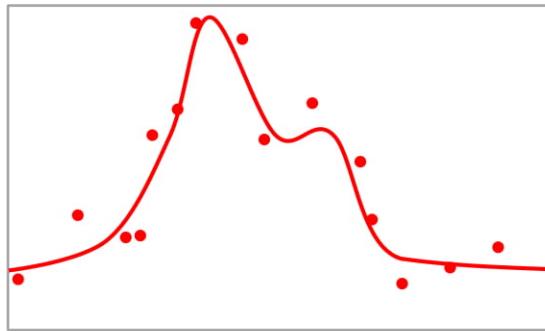
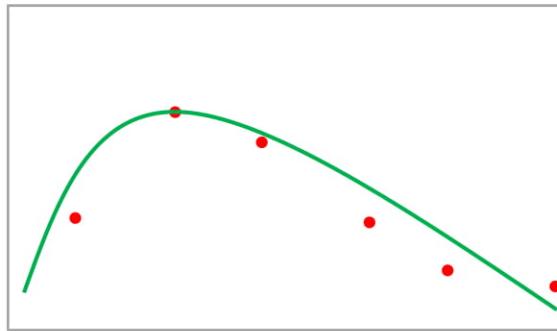
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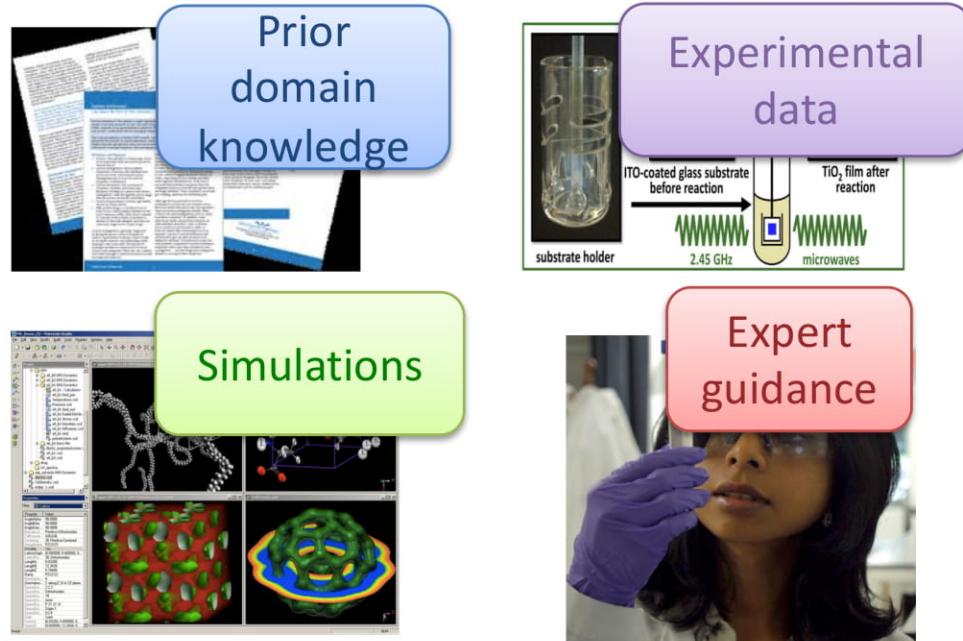


- Enhanced computing power (advanced GPUs, cloud platforms)  
e.g. accelerated training from 6 days to 18 mins in 5 years

# Data Challenges

## Heterogeneous types of data

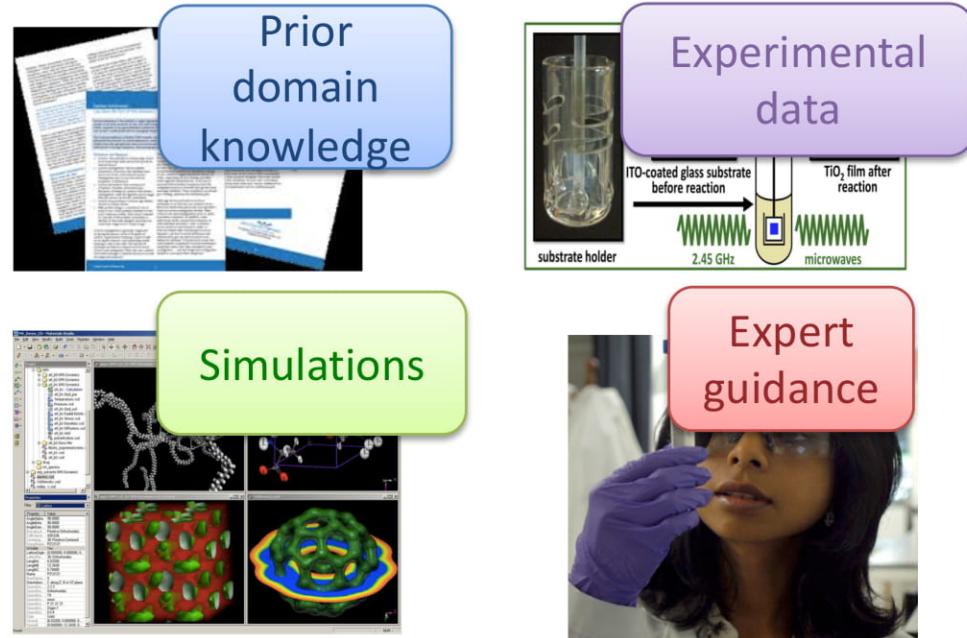
- Multi-modal
- Direct vs indirect
- Missing, incorrect
- Biased



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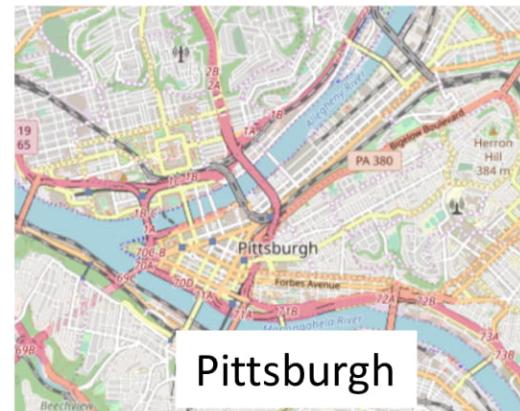
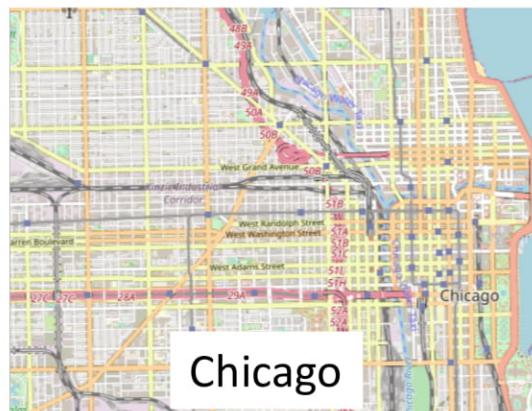
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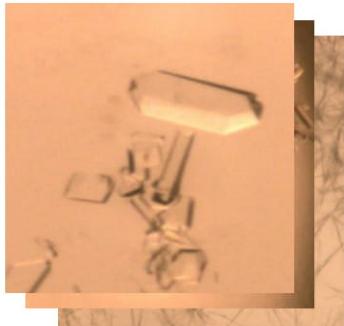
## Handle unseen data from related domain

Self-driving car  
trained in  
Chicago vs  
Pittsburgh

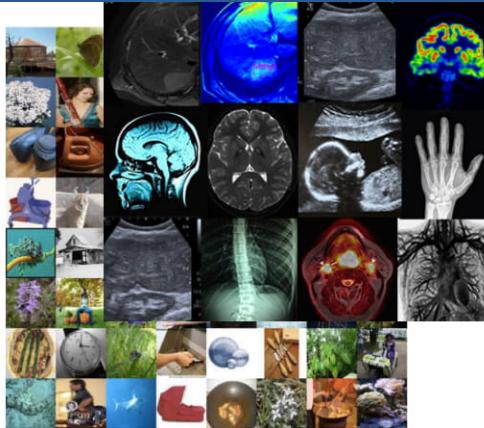


# ML tasks: ubiquitous across domains

## Prediction



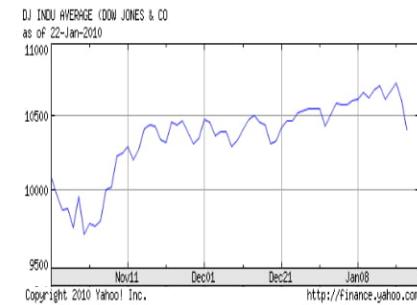
Stage of crystal formation



Object category,  
Medical diagnosis



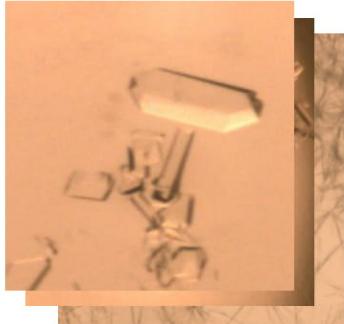
Spam/Fraud identification



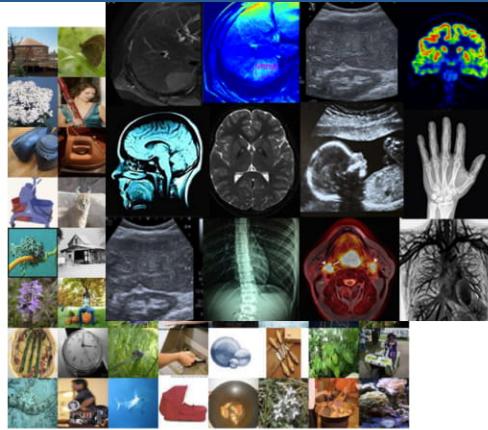
Stock price,  
weather  
forecasting

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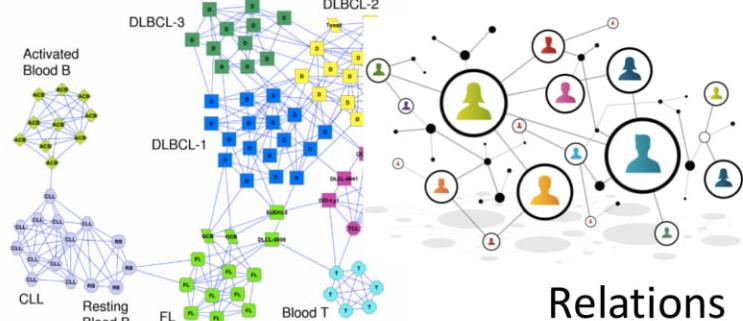


Spam/Fraud  
identification



Stock price,  
weather  
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## Unsupervised learning



Relations  
between people,  
proteins, ...

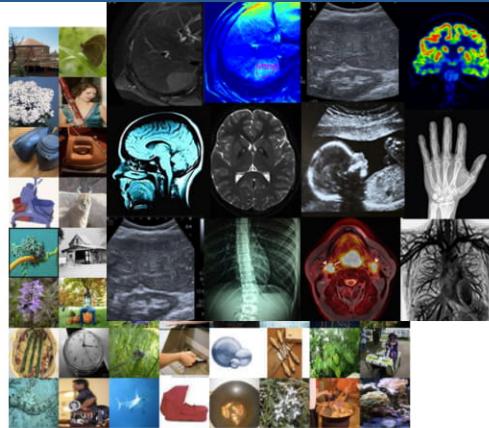
Grouping genes,  
commodities, ...

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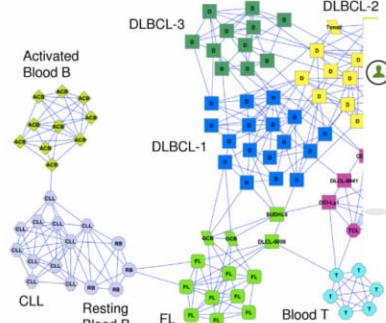


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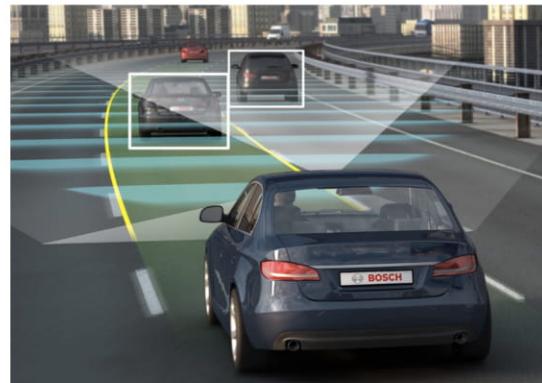


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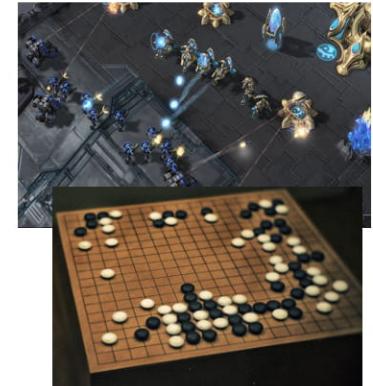
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## Decision making



Automated Navigation

Games



# ML Task Challenges

- + Input-Output mapping tasks with given representations, lots of data and clearly defined performance metric

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- + Input-Output mapping tasks with given representations, lots of data and clearly defined performance metric
- Higher level tasks beyond input-output mapping (e.g. learn representations; guide data collection; design, test and refine hypothesis; interact with humans and environment)
- Multiple heterogeneous tasks
- High-stake decision making with very little tolerance for errors (e.g. criminal justice, medical decisions, etc.)

# ML Performance Challenges

Current focus:

Accuracy/error

ImageNet error: 30% to 3% (since 2010)

runtime, memory, ...

Google speech recognition: 8.4% to 4.9% (since 2016)

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Robustness [Szegedy et al'14]



dog



ostrich

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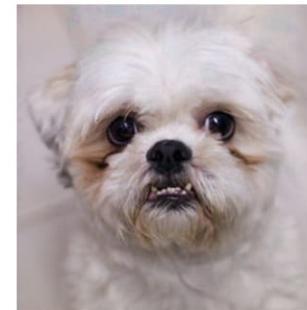
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Interpretability and Transparency

dog

ostrich

Trust and Accountability

# ML Performance Challenges

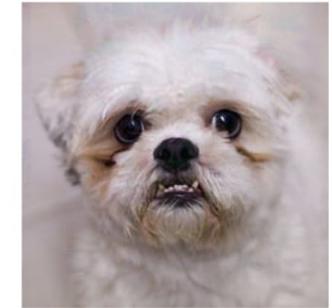
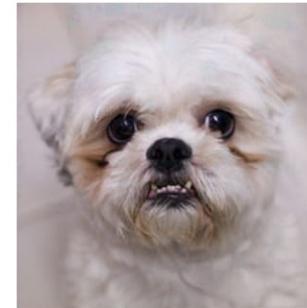
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Robustness [Szegedy et al'14]

Interpretability and Transparency

dog

ostrich

Trust and Accountability

Fairness and Ethics

[Buolamwini-Gebru'18]



1% error

35% error

# MATHEMATICAL FRONTIERS

## Why Machine Learning Works



David Donoho,  
Stanford University

*Anne T. and Robert M. Bass Professor of  
Humanities and Sciences  
Professor of Statistics*

**What Makes  
Machine Learning  
Work?**

# Outline

Overview

Empirical Revolution

Deepnet Emergence

A Role for Math

Speed up Training

Improve Learning

Improve Embeddings

Improve Understanding

# Themes

In a longer talk, I would situate the current moment as follows:

- (a) Smartphone Revolution
- (b) Computing Disocntinuity
- (c) Empirical Science Revolution
- (d) Deepnet emergence
- (c) Role for Math

# Themes

For reasons of time, I emphasize **only**

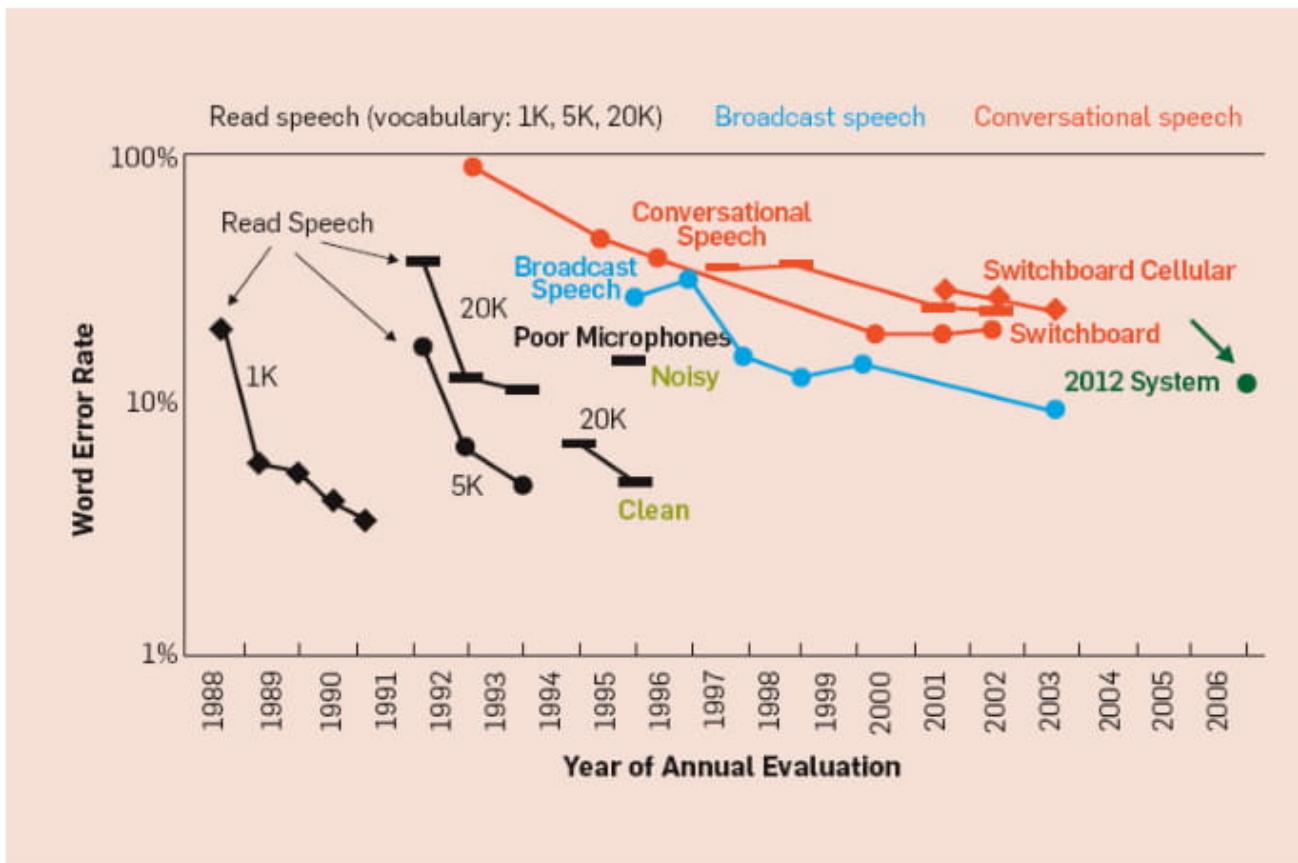
- (a) Smartphone Revolution
- (b) Computing Discontinuity
- (c) **Empirical Science Revolution**
- (d) Deepnet emergence
- (e) **Role for Math**

# Common Task Framework (1980's)

Under CTF we have the following ingredients

- (a) A **publicly available training dataset** involving, for each observation, a list of (possibly many) feature measurements, and a class label for that observation.
- (b) A set of **enrolled competitors** whose **common task** is to **infer** a class **prediction rule from the training data**.
- (c) A **scoring referee**, to which competitors can submit their prediction rule. The referee runs the prediction rule against a testing dataset which is sequestered behind a Chinese wall. The referee objectively and automatically reports the score achieved by the submitted rule.

See Mark Liberman's description (Liberman, 2009).



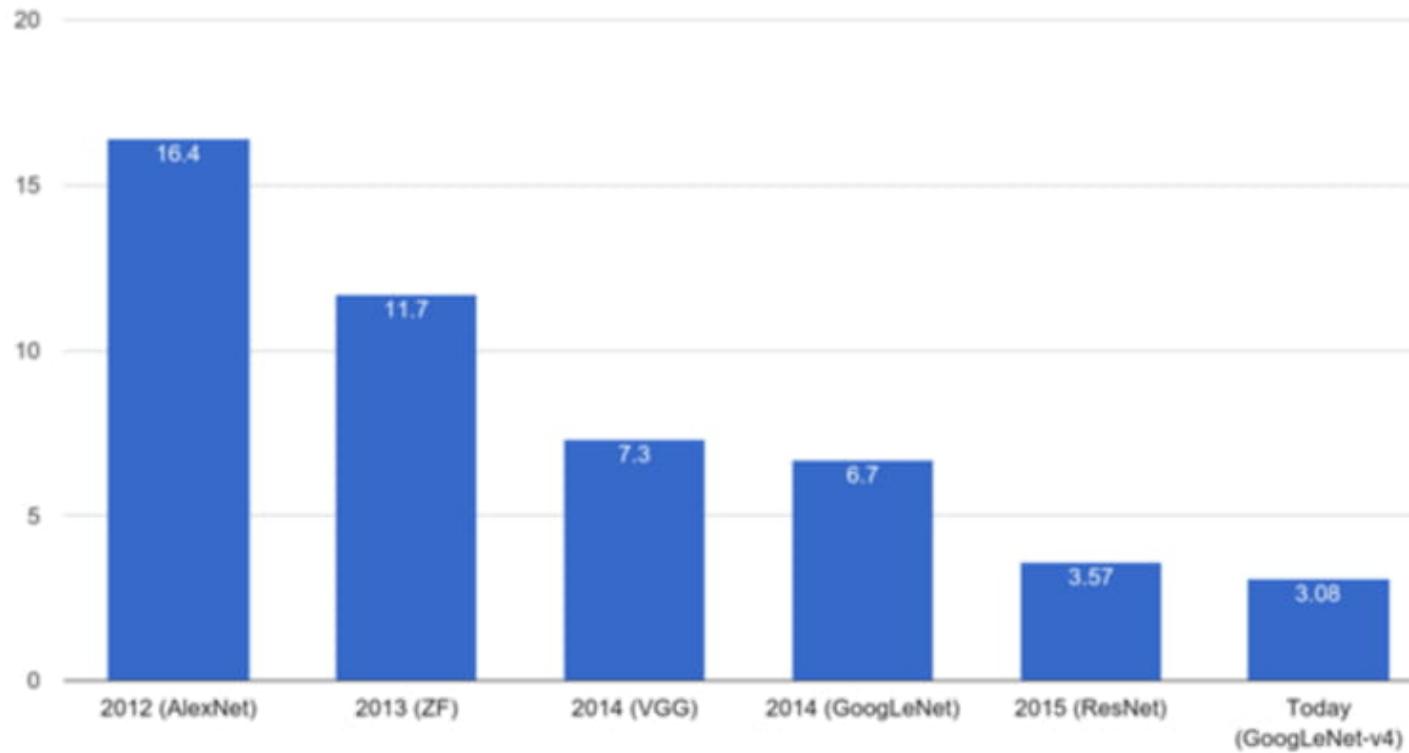
# Emergence of Deep Learning Research

- (a) The success of deep nets is an *entirely* empirical success.  
All basic ideas were around for 30 years  
Nothing beyond high school required
- (b) Deep learning is a new *laboratory science*

Lab Science Term	↔	Deep Learning Term
Laboratory	↔	compute cluster Software Stack
Lab Equipment	↔	Elasticcluster/ClusterJob TensorFlow/Pytorch
Testube/Culture	↔	train/test deepnet modify architecture
Experiment	↔	modify dataset modify training algorithm
High Throughput	↔	Run Hyperparameter Grid

- (c) Today **1000's PhD researchers** developing/studying deepnets **fulltime**  
Factoid: Google has hired  $\approx$  1500 PhD researchers over 5 years.  
 $\approx$  *all CS faculty in USA!*  
Major commitment to deep learning  
Major effects on scholarship, conferences, *younger generation*

## ImageNet Classification Error (Top 5)



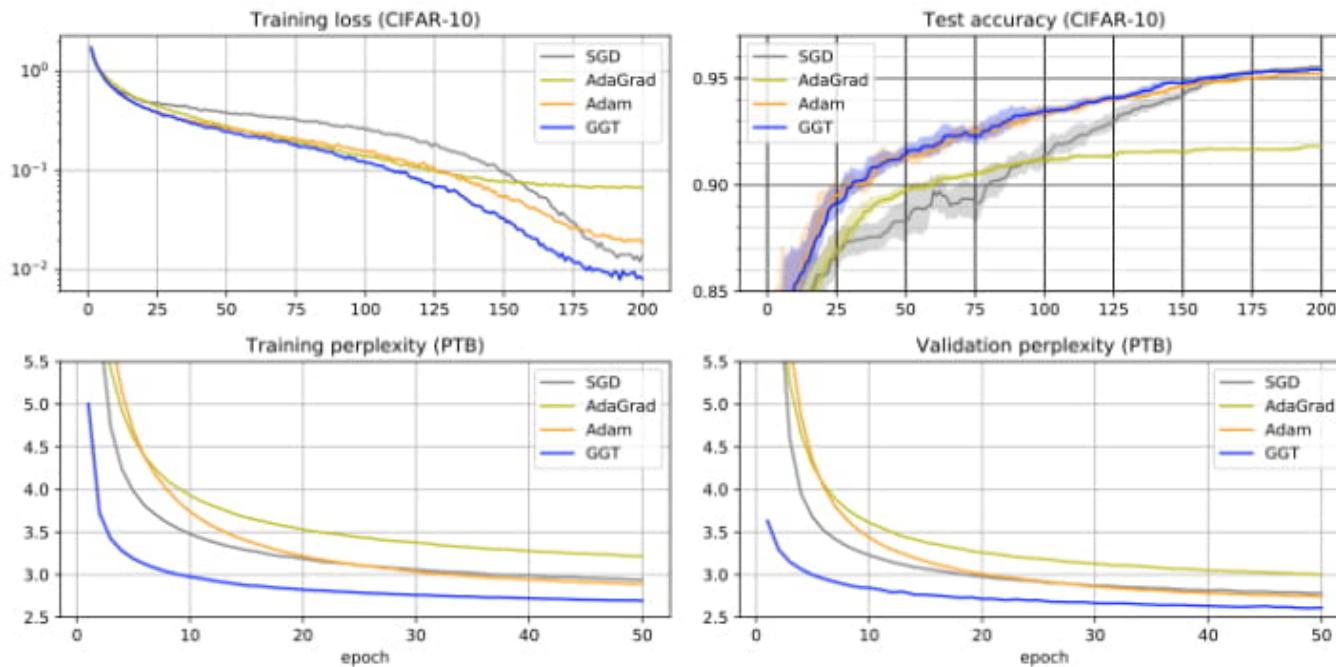


Figure 3: Results of CNN and RNN experiments. GGT dominates in training loss across both tasks, and generalizes better on the RNN task. *Top:* CIFAR-10 classification with a 3-branch ResNet. *Bottom:* PTB character-level language modeling with a 3-layer LSTM.



Sebastiao Salgado, *Work*

# Speed up Training

- ▶ A 6-page conference paper may burn  $> \$100K$  (retail) computer time.
- ▶ State of the Art Deepnet training *extremely slow*:  
Stochastic Gradient Descent
- ▶ State of the Art hyperparameter search *extremely slow*:  
Exhaustive evaluation
- ▶ Traditional mathematical sciences attacked both problems
  - ▶ Second-order methods (Newton's Method and successors)  
much better than First-order
  - ▶ Experimental design much better than exhaustive evaluation
- ▶ Adapt/Extend traditionally successful optimization ideas in mathematical sciences to Deepnet setting  
Save \$100's M in research costs annually. *Forever.*

# Improve Learning

- ▶ State of the Art results often use gigantic datasets (e.g. Laurens van der Maaten, FB, 700M images).
- ▶ Hopes for perfection: driving force for even larger data
- ▶ Scaling relation of errors vs. dataset size *very unfavorable*
- ▶ Training practices *very doubtful* (train to zero error).
- ▶ Traditional mathematical sciences attacked both problems
  - ▶ Most accurate estimates possible for a given sample size (RA Fisher etc.)
  - ▶ Regularization to defeat curse of dimensionality (Tikhonov Regularization, Stein Shrinkage, Lasso etc.)
- ▶ Adapt/Extend traditionally successful estimation ideas in mathematical sciences to Deepnet setting  
Deepnets achieve current performance specs at much smaller dataset size  $N$

# Improve Embeddings

- ▶ State of the Art results often use special embeddings to make Deepnets applicable.
  - ▶ Word2Vec (Glove, etc)
  - ▶ TSNE
- ▶ Successful but poorly understood.  
Possibly can be much improved
- ▶ Traditional mathematical sciences attacked embeddings, but without invariances:
  - ▶ PCA
  - ▶ ISOMAP
  - ▶ LLE
- ▶ Recent mathematical sciences attacked embeddings, *with invariances*  
S. Mallat, Scattering Networks
- ▶ Adapt/Extend traditionally successful embedding ideas in mathematical sciences to Deepnet setting  
Deepnets applicable to many other problems.

# Historic Challenge to the Mathematical Sciences

- ▶ Ingrid Daubechies' *dictum*  
*When a **mathematical** object has interesting behavior, there's a **mathematical** reason.*
- ▶ Great deal of historical success
- ▶ But does it continue to work here?
  - ▶ Deepnets involve *mathematically-definable* entities
  - ▶ Superhuman performance is *interesting*
- ▶ Daubechies' *dictum* seems to apply.
- ▶ Encounter with Ian Goodfellow suggests difficulties with mathematical mindset:
  - ▶ Must there be a reason?
  - ▶ Should we care about the reason?

# Historic Challenge to the Mathematical Sciences, 2

If we care about 'understanding' and 'reasons' here are some challenges:

- ▶ Deepnets in practice are *high-dimensional interpolation scheme*.  
Almost nothing known about the classes of functions well approximated by *actual deepnets* using *actual training algorithms typical in practice*.  
Learning more can lead to better training and better nets.
- ▶ High-dimensional training uses high-dimensional Hessian and gradient.  
We have limited window on such objects, learning more enables speed ups optimization.

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**May 8\*:**

*Mathematics of Redistricting*

**June 12\*:** *Number Theory: The Riemann Hypothesis*

**\* Recording posted**

**July 10\*:** *Topology*

**August 14\*:** *Algorithms for Threat Detection*

**September 11\*:** *Mathematical Analysis*

**October 9\*:** *Combinatorics*

**November 13:**

*Why Machine Learning Works*

**December 11:**

*Mathematics of Epidemics*

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