

## Deep Learning and Applications in Medicine and Science

Jeff Dean Google Brain team g.co/brain

Presenting the work of **many** people at Google Mostly the work of Google Brain and Google Applied Sciences teams

## Intro to machine learning and deep learning Artificial Intelligence



Observation: programming a computer to <u>be</u> clever is harder than programming a computer <u>to learn to be</u> clever.

## Deep learning is causing a machine learning revolution



### **Deep Learning**

#### **Modern Reincarnation of Artificial Neural Networks**

Collection of simple trainable mathematical units, organized in layers, that work together to solve complicated tasks

## What's New

layered network architecture, new training math, \*scale\*

## **Key Benefit**

Learns features from raw, heterogeneous data No explicit feature engineering required



### CAT DOG





Pixels:

"lion"

Pixels:



Audio:

5354	Ture	-	m	-	

"lion"

"How cold is it outside?"

Pixels:



Audio:



"Hello, how are you?"

"lion"

"How cold is it outside?"

"Bonjour, comment allez-vous?"

Pixels:



Audio:

"Hello, how are you?"

Pixels:



"lion"

"How cold is it outside?"

"Bonjour, comment allez-vous?"

"A blue and yellow train travelling down the tracks"

## But why now?





# Now more compute Accuracy neural networks other approaches Scale (data size, model size)



humans



**5% errors** 



2016

3% errors

#### humans



**5% errors** 

Google Brain Team Mission: Make Machines Intelligent. Improve People's Lives.

### How do we do this?

- Conduct long-term research (>200 papers, see g.co/brain & g.co/brain/papers)
  - Unsupervised learning of cats, Inception, word2vec, seq2seq, DeepDream, image captioning, neural translation, Magenta, ML for robotics control, ...
- Build and open-source systems like **TensorFlow** (see tensorflow.org and https://github.com/tensorflow/tensorflow)
- Collaborate with others at Google and Alphabet to **get our work into the hands of billions of people** (e.g., Google Translate, RankBrain for Google Search, GMail Smart Reply, Google Photos, Google speech recognition, Waymo, ...)
- Train new researchers: internships, Google Brain Residency program
- Conduct **applied ML research** in emerging areas where new ML methods will make a big difference like **healthcare** and **robotics**

#### Main Research Areas

- General Machine Learning Algorithms and Techniques
- Computer Systems for Machine Learning
- Natural Language Understanding
- Perception
- Healthcare
- Robotics
- Music and Art Generation



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### Growing Use of Deep Learning at Google



#### Experiment Turnaround Time and Research Productivity

- Minutes, Hours:
  - Interactive research! Instant gratification!
- 1-4 days
  - Tolerable
  - Interactivity replaced by running many experiments in parallel

### • 1-4 weeks

- High value experiments only
- Progress stalls

#### • >1 month

• Don't even try



### Build the right tools



http://tensorflow.org/

and

https://github.com/tensorflow/tensorflow

Open, standard software for general machine learning

Great for Deep Learning in particular

First released Nov 2015

Apache 2.0 license

#### **TensorFlow Goals**

Establish **common platform** for expressing machine learning ideas and systems

Make this platform the **best in the world** for both research and production use

Open source it so that it becomes a **platform for everyone**, not just Google



#### TensorFlow: A Vibrant Open-Source Community

- Rapid development, many outside contributors
  - 475+ non-Google contributors to TensorFlow 1.0
  - 15,000+ commits in 15 months
  - Many community created tutorials, models, translations, and projects
    - ~7,000 GitHub repositories with 'TensorFlow' in the title
- Direct engagement between community and TensorFlow team
  - 5000+ Stack Overflow questions answered
  - 80+ community-submitted GitHub issues responded to weekly
- Growing use in ML classes: Toronto, Berkeley, Stanford, ...



## New-found computer vision prowess.

Often can develop a model to solve one problem, reuse it for other problems







#### Google Project Sunroof

#### www.google.com/sunroof



## Medical Imaging



#### **Diabetic Retinopathy as a Classification Problem**



#### Moderate

#### Proliferative



#### Humans are inconsistent



Ophthalmologist Graders

Google

**Consistency:** intergrader ~60%, intragrader ~65%



December 13, 2016

#### Development and Validation of a Deep Learning Algorithm for Detection of Diabetic Retinopathy in Retinal Fundus Photographs

Varun Gulshan, PhD<sup>1</sup>; Lily Peng, MD, PhD<sup>1</sup>; Marc Coram, PhD<sup>1</sup>; et al

> Author Affiliations

JAMA. 2016;316(22):2402-2410. doi:10.1001/jama.2016.17216



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Performance **on par or slightly better** than the median of 8 U.S. board-certified ophthalmologists (F-score of 0.95 vs. 0.91). http://research.googleblog.com/2016/11/deep-learning-for-detection-of-diabetic.html

#### Detecting Cancer Metastases on Gigapixel Pathology Images

 Yun Liu<sup>1\*</sup>, Krishna Gadepalli<sup>1</sup>, Mohammad Norouzi<sup>1</sup>, George E. Dahl<sup>1</sup>, Timo Kohlberger<sup>1</sup>, Aleksey Boyko<sup>1</sup>, Subhashini Venugopalan<sup>2\*\*</sup>,
Aleksei Timofeev<sup>2</sup>, Philip Q. Nelson<sup>2</sup>, Greg S. Corrado<sup>1</sup>, Jason D. Hipp<sup>3</sup>, Lily Peng<sup>1</sup>, and Martin C. Stumpe<sup>1</sup>

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Blog: <u>https://research.googleblog.com/2017/03/assisting-pathologists-in-detecting.html</u> Paper: <u>https://arxiv.org/abs/1703.02442</u>
### **ML Challenges in Pathology**

- □ Extremely large images (> 100k x 100k pixels)
- Multiscale problem need detail as well as context



150k pixels (15 Gigapixel image)









5x





20x



### **Detecting breast cancer metastases in lymph nodes**

biopsy image





ground truth (from pathologist)



model prediction (early results) model prediction (current results)



reduced noise in normal regions (everywhere else)

tumor (in ground truth)

### Model performance compared to pathologist

	our model	pathologist*
Tumor localization score (FROC)	0.89	0.73
Sensitivity at 8 FP	0.92	0.73
Slide classification (AUC)	0.97	0.96

\* pathologist given infinite time per image (reaching 0 FPs)

Evaluated using Camelyon16 dataset (just 270 training examples!)

# nature

THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE



Artificial intelligence powers detection of skin cancer from images PAGES 36 & 115

> O NATURE.COM/NATURE 2 February 2017 £10 Vol. 542. No. 7639

### LETTER

#### Dermatologist-level classification of skin cancer with deep neural networks

Andre Esteva<sup>1\*</sup>, Brett Kuprel<sup>1\*</sup>, Roberto A. Novoa<sup>2,3</sup>, Justin Ko<sup>2</sup>, Susan M. Swetter<sup>2,4</sup>, Helen M. Blau<sup>5</sup> & Sebastian Thrun<sup>6</sup>



#### Work on dermatology from Stanford University

Measuring live cells with image to image regression

"Seeing More"



### **Enabling technology: Image to image regression**



Google

### **Depth prediction on portrait data**



Google

### **Applications for camera effects**

Input





Defocus









### Predict cellular markers from transmission microscopy?

brightfield z-stack



two fluorescence channels



Google

# Human cancer cells / DIC / nuclei (blue) and cell mask (green)

# Human cancer cells / DIC / nuclei (blue) and cell mask (green)

# Human iPSC neurons / phase contrast / nuclei (blue), dendrites (green), and axons (red)

# Human iPSC neurons / phase contrast / nuclei (blue), dendrites (green), and axons (red)

# Rat neurons / phase contrast / nuclei (blue), dendrites (green), and axons (red)

### **Many applications**

- Measure live cells that can't be modified
- Impute labels on live cells in longitudinal studies to build predictors of ultimate fate
- Map the entire cellular neighborhood for experiments coupled to partial transfection
- Impute unlimited number of labels; no longer limited by microscope's channels



### Deep learning for genomics



### **Recasting variant calling for deep learning**



#### Use inception-v3 to call variant genotype



### Train on Genome in a Bottle sample using their genotype labels

Each germline WGS dataset provides e.g., ~3.7M labeled varaints for training:

- 215K false positives candidates
- 2.1M true heterozygotes
- 1.3M true homozygous alternates

Google

Encoding is roughly red = {A,C,G,T}; green = {quality score}; blue = {read strand}; alpha = {matches ref genome}

### DeepVariant won an award at the 2016 **PrecisionFDA competition**



F-measure is the harmonic mean of precision and recall.

# DeepVariant can learn to call variants in many sequencing technologies

	10× GENOMICS-			
Dataset	<u>10X Chromium</u> <u>75x WGS</u>	PacBio raw reads 40x WGS	SOLID SE 85x WGS	<u>Illumina</u> TruSeq exome
DeepVariant (F1 metric)	99.3%	92.7%	86.4%	96.1%
-				
Comparator (F1 metric)	98.2%	56.1% <sup>1</sup>	78.8% <sup>2</sup>	95.4%

<sup>1</sup>No standard caller exists for this technology for human samples; <sup>2</sup>Old technology without any maintained variant callers.

Gooale

## Machine learning for Predictive Tasks in Healthcare



### Predictive tasks for healthcare

Given a patient's EMR data, can we predict the future?

Deep learning methods for sequential prediction are becoming extremely good e.g. recent improvements in Google Translation

### **Neural Machine Translation**



### Predictive tasks for healthcare

Given a large corpus of training data of de-identified medical records, can we predict interesting aspects of the future for a patient not in the training set?

- will patient be readmitted to hospital in next N days?
- what is the likely length of hospital stay for patient checking in?
- what are the most likely diagnoses for the patient right now? and why?
- what medications should a doctor consider prescribing?
- what tests should be considered for this patient?
- which patients are at highest risk for X in next month?

Collaborating with several healthcare organizations, including UCSF, Stanford, and Univ. of Chicago. Have early very promising results (no public paper yet)

If your org might be interested in working with us, see contact link at bottom of: <u>g.co/brain/healthcare</u>

### Machine learning for Quantum Chemistry



### Levels of quantum theory

Paul Dirac: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the **exact application of these laws leads to equations much too complicated to be soluble**.

The community has spent years developing approximations that can be practically applied

#### Electronic structure methods

Valence bond theory

Generalized valence bond Modern valence bond Resonance

#### Molecular orbital theory

Hartree–Fock method Semi-empirical quantum chemistry methods Møller–Plesset perturbation theory Configuration interaction Coupled cluster Multi-configurational self-consistent field Quantum chemistry composite methods Quantum Monte Carlo Linear combination of atomic orbitals Electronic band structure

Nearly free electron model Tight binding Muffin-tin approximation Density functional theory k-p perturbation theory Empty lattice approximation



#### Google Research Blog

Predicting Properties of Molecules with Machine Learning

Friday, April 07, 2017

https://research.googleblog.com/2017/04/predicting-properties-of-molecules-with.html

Fast machine learning models of electronic and energetic properties consistently reach approximation errors better than DFT accuracy

Felix A. Faber,<sup>1,2</sup> Luke Hutchison,<sup>3,2</sup> Bing Huang,<sup>1</sup> Justin Gilmer,<sup>4,\*</sup> Samuel S. Schoenholz,<sup>4,\*</sup> George E. Dahl,<sup>4</sup> Oriol Vinyals,<sup>5</sup> Steven Kearnes,<sup>3</sup> Patrick F. Riley,<sup>3</sup> and O. Anatole von Lilienfeld<sup>1,†</sup>
<sup>1</sup>Institute of Physical Chemistry and National Center for Computational Design and Discovery of Novel Materials, Department of Chemistry, University of Basel, Switzerland.
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<sup>4</sup>Google Brain, CA, USA.
<sup>5</sup>Google DeepMind, London, UK. (Dated: February 21, 2017)

**Neural Message Passing for Quantum Chemistry** 

To appear in ICML 2017

Justin Gilmer<sup>1</sup> Samuel S. Schoenholz<sup>1</sup> Patrick F. Riley<sup>2</sup> Oriol Vinyals<sup>3</sup> George E. Dahl<sup>4</sup>

https://arxiv.org/abs/1702.05532 and https://arxiv.org/abs/1704.01212

Basic Idea: Use New Kind of Neural Net Model to Approximate Really Expensive Computation



Figure 1. A Message Passing Neural Network predicts quantum properties of an organic molecule by modeling a computationally expensive DFT calculation.

To appear in ICML 2017

https://arxiv.org/abs/1704.01212

### Machine learning approximation error below DFT error

=		11	a	EIIO	ELU	$\Lambda \varepsilon$	$\langle \mathbf{R}^2 \rangle$	ZPVE	Uo	C	(1)1
-		Debve	Bohr <sup>3</sup>	oV		oV	$\frac{10^{10}}{\text{Bohr}^2}$	eV	oV	cal/molK	$cm^{-1}$
-	Mean	2.67	75.3	-6.54	0.322	6.86	1190	4.06	-76.6	31.6	3500
	MAD	1.17	6.29	0.439	1.05	1.07	203	0.717	8.19	3.21	238
	Target	$0.1^{6,41}$	$0.1^{6,41}$	$0.0434^{6}$	$0.0434^{6}$	$0.0434^{6}$	$1.2^{6}$	$0.00124^{6,42}$	$0.0434^{6}$	$0.05^{6}$	$10^{6,42}$
FT/	B3LYP	$0.1^{41}$	$0.1^{41}$	$0.24^{43}$	$0.088^{43}$	$0.22^{43}$	-	$0.0097^{39}$	$0.12^{44}$	$0.34^{45}$	$28^{39}$

#### MAD: mean average deviation

**Target**: Target mean average error values generally accepted as "accurate enough" by chemistry community **DFT/B3LYP**: Mean average error obtained by very computationally expensive density functional theory simulations

#### https://arxiv.org/abs/1702.0553

### Machine learning approximation error below DFT error

-		$\mu$	α	$\varepsilon_{ m HO}$	$arepsilon_{ m LU}$	$\Delta arepsilon$	$\langle \mathrm{R}^2 \rangle$	ZPVE	$U_0$	$C_{\rm v}$	$\omega_1$
		Debye	$\mathrm{Bohr}^3$	eV	eV	eV	$Bohr^2$	eV	eV	cal/molK	$\mathrm{cm}^{-1}$
Mean		2.67	75.3	-6.54	0.322	6.86	1190	4.06	-76.6	31.6	3500
MAD		1.17	6.29	0.439	1.05	1.07	203	0.717	8.19	3.21	238
Target		$0.1^{6,41}$	$0.1^{6,41}$	$0.0434^{6}$	$0.0434^{6}$	$0.0434^{6}$	$1.2^{6}$	$0.00124^{6,42}$	$0.0434^{6}$	$0.05^{6}$	$10^{6,42}$
T/B3LYP		$0.1^{41}$	$0.1^{41}$	$0.24^{43}$	$0.088^{43}$	$0.22^{43}$	-	0.0097 39	$0.12^{44}$	$0.34^{40}$	28 39
GG	MG	0.238	0.151	0.0587	0.0564	0.0835	5.98	0.00291	0.0317	0.0724	6.32

**0.0696** 0.227 **0.0509 0.0471 0.0766** 5.68

GC

MG

https://arxiv.org/abs/1702.0553

0.0892

3.15

0.00975

 $\bigvee \times \checkmark \checkmark \checkmark \checkmark \checkmark \checkmark \checkmark \checkmark$ 

0.13

### Connectomics

# Machine Learning for High-throughput Neuroanatomy





### **Connectomics Timeline**

1970's: c. elegans
 300 neurons; printed photos; MRC in the UK

2013: retina, drosophila visual system
 1000 neurons; O(gigavoxels); Max Planck Institute, MIT, HHMI

• In progress: mouse cortical column, whole drosophila brain, song-bird <100,000 neurons; O(teravoxels); Harvard, HHMI, Allen Institute, MPI

 Machines now being designed & built for whole mouse brain 100,000,000 neurons; O(petavoxels)

Google

### Automated Reconstruction Progress at Google



Google

### Automated Reconstruction Progress at Google



"mean microns between failure" of automated neuron tracing

### **Classical Approach**

- Classical segmentation pipeline:
  - Predict local image boundaries (edge detectors ['70s]  $\rightarrow$  SVMs ['00s]  $\rightarrow$  deep learning [today]).
  - Discrete graph partitioning (watershed, connected components, etc.) without machine learning.
  - Agglomeration of "superpixels" using classifier or heuristics.



- Issues with classical approach:
  - Lack of end-to-end training; certain steps not differentiable.
  - Pipeline complexity.
  - Graph partitioning procedure is very brittle and impoverished.
#### New Technology: Flood Filling Networks

#### **Flood-Filling Networks**

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Viren Jain Google viren@google.com

- Start with a seed point
- Recurrent neural network iteratively fills out an object based on image content and its own previous predictions

### 2d Inference



https://arxiv.org/abs/1611.00421

#### Flood Filling Networks: 3d Inference



Q

- Application: songbird brain imaged by Max Planck Institute for Neurobiology using serial block face scanning electron microscopy
- 10,600 × 10,800 × 5,700 voxels = ~600 billion voxels
- Successful reconstruction of the wiring diagram will test specific hypotheses related to how biological nervous systems produce precise, sequential motor behaviors and perform reinforcement learning.



Courtesy Jorgen Kornfeld & Winfried Denk, MPI



Google







# Automated machine learning ("learning to learn")



#### Current: Solution = ML expertise + data + computation

#### Current: Solution = ML expertise + data + computation

### Can we turn this into: Solution = data + 100X computation

???

Early encouraging signs

Trying multiple different approaches:

Reinforcement learning-based architecture search
 Model architecture evolution

#### NEURAL ARCHITECTURE SEARCH WITH REINFORCEMENT LEARNING

Barret Zoph; Quoc V. Le Google Brain {barretzoph, qvl}@google.com Appeared earlier this year at ICLR 2017 in France

#### Idea: model-generating model trained via RL

- (1) Generate ten models
- (2) Train them for a few hours
- (3) Use loss of the generated models as reinforcement learning signal

arxiv.org/abs/1611.01578

#### CIFAR-10 Image Recognition Task



Figure 7: Convolutional architecture discovered by our method, when the search space does not have strides or pooling layers. FH is filter height, FW is filter width and N is number of filters.

Model	Depth	Parameters	Error rate (%)
Network in Network (Lin et al., 2013)	-	-	8.81
All-CNN (Springenberg et al., 2014)	( <b>-</b> )	-	7.25
Deeply Supervised Net (Lee et al., 2015)	3 <b>-</b> 0	-	7.97
Highway Network (Srivastava et al., 2015)	25-27	-	7.72
Scalable Bayesian Optimization (Snoek et al., 2015)	1020	-	6.37
FractalNet (Larsson et al., 2016)	21	38.6M	5.22
with Dropout/Drop-path	21	38.6M	4.60
ResNet (He et al., 2016a)	110	1.7M	6.61
ResNet (reported by Huang et al. (2016b))	110	1.7M	6.41
ResNet with Stochastic Depth (Huang et al., 2016b)	110	1.7M	5.23
	1202	10.2M	4.91
Wide ResNet (Zagoruyko & Komodakis, 2016)	16	11.0M	4.81
	28	36.5M	4.17
ResNet (pre-activation) (He et al., 2016b)	164	1.7M	5.46
	1001	10.2M	4.62
DenseNet $(L = 40, k = 12)$ Huang et al. (2016a)	40	1.0M	5.24
DenseNet $(L = 100, k = 12)$ Huang et al. (2016a)	100	7.0M	4.10
DenseNet $(L = 100, k = 24)$ Huang et al. (2016a)	100	27.2M	3.74
Neural Architecture Search v1 no stride or pooling	15	4.2M	5.50
Neural Architecture Search v2 predicting strides	20	2.5M	6.01
Neural Architecture Search v3 max pooling	39	7.1M	4.47
Neural Architecture Search v3 max pooling + more filters	39	32.0M	3.84

Table 1: Performance of Neural Architecture Search and other state-of-the-art models on CIFAR-10.

#### Penn Tree Bank Language Modeling Task

# "Normal" LSTM cell

#### identity elem\_mult identity add elem\_mult tanh sigmoid elem\_mult sigmoid elem\_mult

# Cell discovered by architecture search



Model	Parameters	Test Perplexity
Mikolov & Zweig (2012) - KN-5	2M <sup>‡</sup>	141.2
Mikolov & Zweig (2012) - KN5 + cache	2M <sup>‡</sup>	125.7
Mikolov & Zweig (2012) - RNN	6M <sup>‡</sup>	124.7
Mikolov & Zweig (2012) - RNN-LDA	7M <sup>‡</sup>	113.7
Mikolov & Zweig (2012) - RNN-LDA + KN-5 + cache	9M <sup>‡</sup>	92.0
Pascanu et al. (2013) - Deep RNN	6M	107.5
Cheng et al. (2014) - Sum-Prod Net	5M <sup>‡</sup>	100.0
Zaremba et al. (2014) - LSTM (medium)	20M	82.7
Zaremba et al. (2014) - LSTM (large)	66M	78.4
Gal (2015) - Variational LSTM (medium, untied)	20M	79.7
Gal (2015) - Variational LSTM (medium, untied, MC)	20M	78.6
Gal (2015) - Variational LSTM (large, untied)	66M	75.2
Gal (2015) - Variational LSTM (large, untied, MC)	66M	73.4
Kim et al. (2015) - CharCNN	19M	78.9
Press & Wolf (2016) - Variational LSTM, shared embeddings	24M	73.2
Merity et al. (2016) - Zoneout + Variational LSTM (medium)	20M	80.6
Merity et al. (2016) - Pointer Sentinel-LSTM (medium)	21M	70.9
Zilly et al. (2016) - Variational RHN, shared embeddings	24M	66.0
Neural Architecture Search with base 8	32M	67.9
Neural Architecture Search with base 8 and shared embeddings	25M	64.0
Neural Architecture Search with base 8 and shared embeddings	54M	62.4

Table 2: Single model perplexity on the test set of the Penn Treebank language modeling task. Parameter numbers with <sup>‡</sup> are estimates with reference to Merity et al. (2016).

# More computational power is needed

# Deep learning is transforming how we design computers



### Special computation properties



## Special computation properties







## **Tensor Processing Unit**

Custom Google-designed chip for neural net computations



In production use for >24 months: used on every search query, for neural machine translation, for AlphaGo match, ...



### Tensor Processing Unit v2



#### Revealed last month at Google I/O



Google-designed device for neural net training and inference

# Google's 2nd-gen TPU:

 $\Theta \Theta \Theta \Theta \Theta$ 

180 teraflops
64 GB of ultra-high-bandwidth memory
Designed for training and inference
Designed to be connected together

 $\Theta \Theta \Theta \Theta \Theta$ 



TPU Pod 64 2nd-gen TPUs 11.5 petaflops 4 terabytes of memory 2-D toroidal mesh network

S-tranking

- 21

# 8 devices (32 chips, 1/8th of a 64-TPU-pod) trains one of our machine translation models 4x faster

than 32 of the best commercially-available GPUs

Programmed via TensorFlow New Estimator interface being added to TF 1.2 Same program will run with only minor modifications on CPUs, GPUs, & TPUs

#### Will be Available through Google Cloud

Cloud VM with TPU - virtual machine w/180 TFLOPS TPUv2 device attached





## TensorFlow Research Cloud (TFRC)



Making 1000 Cloud VMs with TPUs available for free to top researchers who are committed to open machine learning research

Total of 180 PFLOPS: More raw FLOPS than #1 supercomputer in the world <u>g.co/tpusignup</u>

### Conclusions

Deep neural networks and machine learning are starting to produce significant breakthroughs in healthcare and basic science

If you're not considering how to use deep neural nets to solve your problems, **you almost certainly should be** 



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#### More info:

g.co/brain and g.co/brain/healthcare and research.google.com



### Conclusions

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# Thank you! Questions?

