

Why your machine learning code is slow

Designing algorithms for modern hardware
(disclaimer - this isn't a deep learning talk)

Alexander Smola, Amazon AWS

alex@smola.org

Most important slide - free AWS credits

- Register at AWS Educate for credit
<http://www.awseducate.com>
- Use **PEK_DEEPLARNING** for extra \$25 credits
- **Use the AWS account option**

Do **not** use the capped AWS Educate Starter Account.

- To apply for a position email CV/GitHub/short intro to
aws-ai-event-recruiting@amazon.com

Thanks

- **Amazon**

Mu Li, Anima Anandkumar, Vishy Vishwanathan

- **CMU**

Yu-Xiang Wang (+Amazon), Manzil Zaheer (+Amazon),
Dave Andersen, Zichao Yang, Ziqi Liu

- **Google**

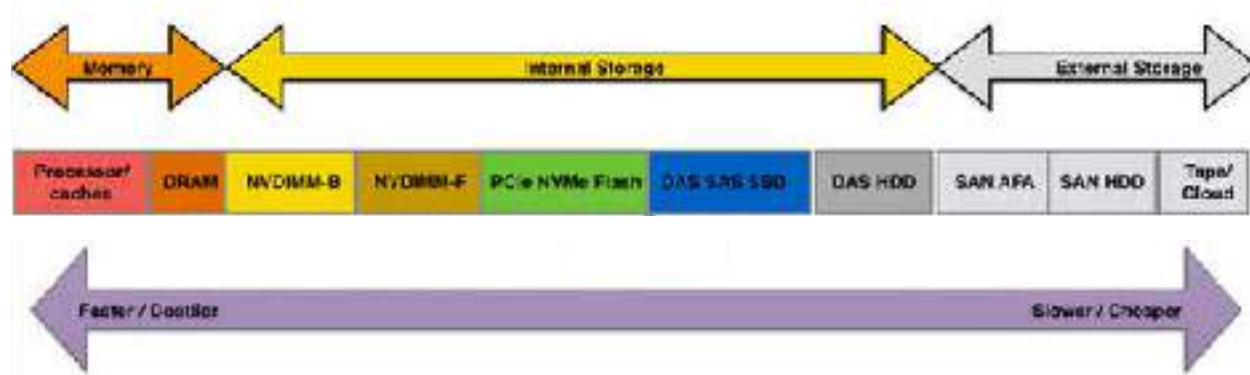
Amr Ahmed, Vanja Josifovski, Steffen Rendle, Sujith Ravi

Outline

- **Memory**
Cache, RAM, SSD, Harddisk, Network
- **Computation**
vectorization, multicore
- **MxNet**
language, parallelization, AWS Templates

Memory

Memory



http://www.theregister.co.uk/2016/04/04/memory_and_storage_boundary_changes/



10MB
1ns



10GB
100ns



500GB
10 μ s



5TB
10ms



100TB
100s

Numbers you should know

	Nanoseconds (ns)	Microseconds (us)	Milliseconds (msec)	If L1 access is 1 second
L1 cache reference	0.5			1 sec
L2 cache reference	7			14 secs
DRAM access	200			6 mins 40 secs
NVDIMM-N	5,000	5		2 hours 46 mins 40 secs
NVMe PCIe SSD write	30,000	30		18 hours 40 mins
Mangstor NX NVMe-F array write	30,000	30		18 hours 40 mins
Zstor NVMe-F SSD array read	30,000	30		18 hours 40 mins
D3GD D5 NVMe-F array				55 hours 33 mins 20 secs
Mangstor NX NVMe-F array read				61 hours 6 mins 40 secs
NVMe PCIe SSD read				61 hours 6 mins 40 secs
Zstor NVMe-F SSD array write				61 hours 6 mins 40 secs
Random 4K read from SSD				3 days, 11 hours, 20 mins
Sequential Read 1MB from DRAM	250,000	250		5 days, 10 hours, 50 mins, 20 secs
Round trip datacenter	500,000	500	0.5	11 days, 12 hours, 46 mins, 40 secs
Sequential read 1MB from SSD	1,000,000	1,000	1	23 days, 3 hours, 33 mins, 20 secs
Disk seek	10,000,000	10,000	10	231 days, 11 hours, 33 mins, 20 secs
Sequential read 1MB from disk	20,000,000	20,000	20	1 year, 97 days, 23 hours, 6 mins, 40 secs
DAS disk access	100,000,000	100,000	100	5 years, 119 days, 19 hours, 33 mins, 20 secs
Send packet CA->Netherlands->CA	150,000,000	150,000	150	9 years, 185 days, 5 hours, 20 mins, 0 secs
SAN array access	300,000,000	300,000	300	19 years, 5 days, 10 hours, 40 mins, 0 secs

ignorant code can
kill performance

Use Case: Recommender Systems

- Users u , movies m (or projects)
- Function class

$$r_{um} = \langle v_u, w_m \rangle + b_u + b_m$$

- Loss function for recommendation (Yelp, Netflix)

$$\sum_{u \sim m} (\langle v_u, w_m \rangle + b_u + b_m - y_{um})^2$$



Use Case: Recommender Systems

Regularized Objective

$$\sum_{u \sim m} (\langle v_u, w_m \rangle + b_u + b_m + b_0 - r_{um})^2 + \frac{\lambda}{2} [\|U\|_{\text{Frob}}^2 + \|V\|_{\text{Frob}}^2]$$

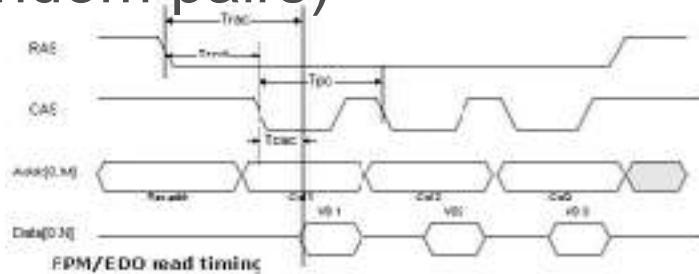
Update operations

$$v_u \leftarrow (1 - \eta_t \lambda) v_u - \eta_t w_m (\langle v_u, w_m \rangle + b_u + b_m + b_0 - r_{um})$$
$$w_m \leftarrow (1 - \eta_t \lambda) w_m - \eta_t v_u (\langle v_u, w_m \rangle + b_u + b_m + b_0 - r_{um})$$

Very simple SGD algorithm (random pairs)

This should be cheap ...

memory subsystem



Not so cheap ...

Netflix contest

- 100M samples, 2048 dimensions, 30 steps
- $100\text{M} \times 2048 \times 30 \times 4 \times 8\text{byte}$ burst reads
- $100\text{M} \times 30 \times 4$ random reads

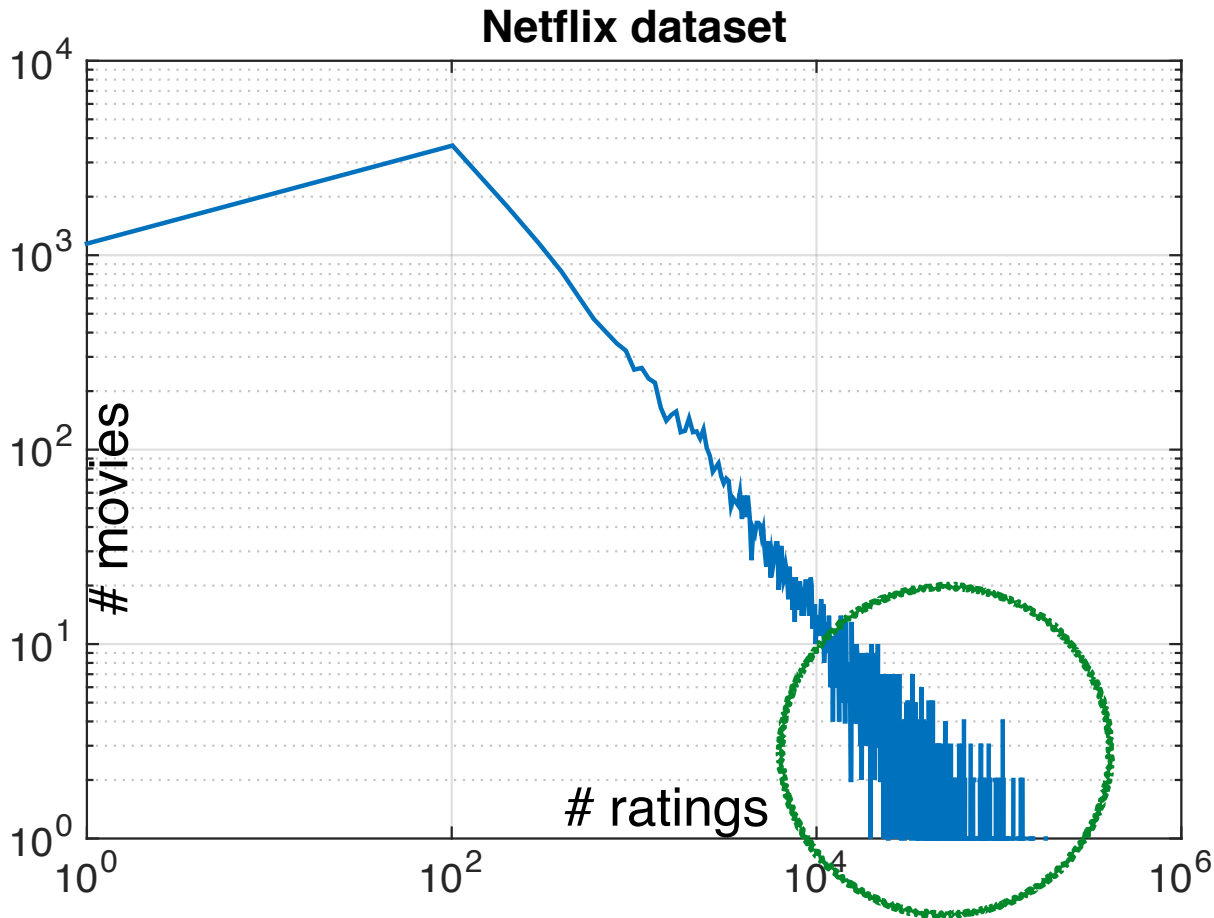
Runtime (1h 15 min)

- 3300s for burst reads (@60GB/s)
- 1200s for random reads (@10ns/read)

Better engineering gets 9.5 min. How?

Liu, Wang, Smola, RecSys 2015

Power law in Collaborative Filtering



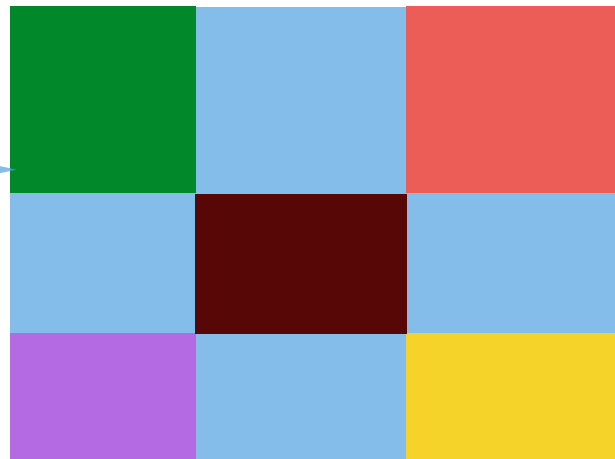
Key Ideas

- **Stratify ratings by users**
(only 1 cache miss / read per user / out of core)
- **Keep frequent movies in cache**
(stratify by blocks of movie popularity)
- **Avoid false sharing between sockets**
(key cached in the wrong CPU causes miss)

K	SC-SGD		GraphChi	
	L1 Cache	L3 Cache	L1 Cache	L3 Cache
16	2.84%	0.43%	12.77%	2.21%
256	2.85%	0.50%	12.89%	2.34%
2048	3.3%	1.7%	15%	9.8%

Key Ideas

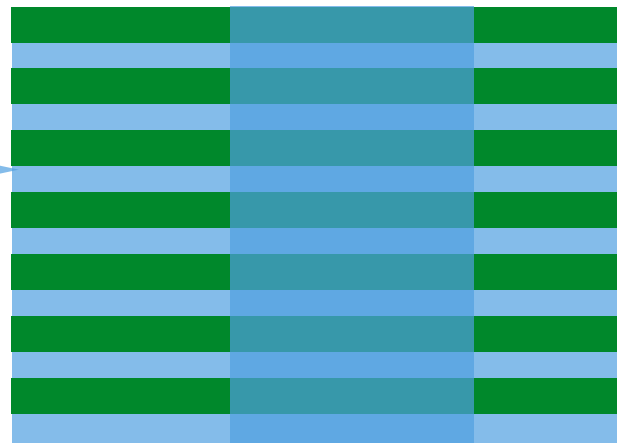
GraphChi
Partitioning



K	SC-SGD		GraphChi	
	L1 Cache	L3 Cache	L1 Cache	L3 Cache
16	2.84%	0.43%	12.77%	2.21%
256	2.85%	0.50%	12.89%	2.34%
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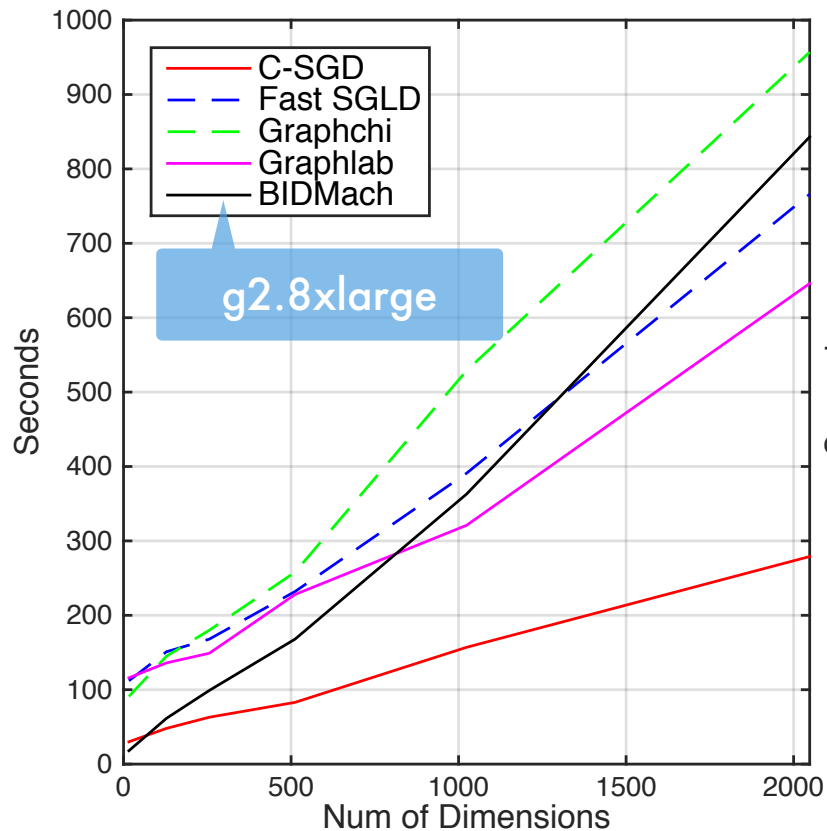
Key Ideas

SC-SGD
partitioning

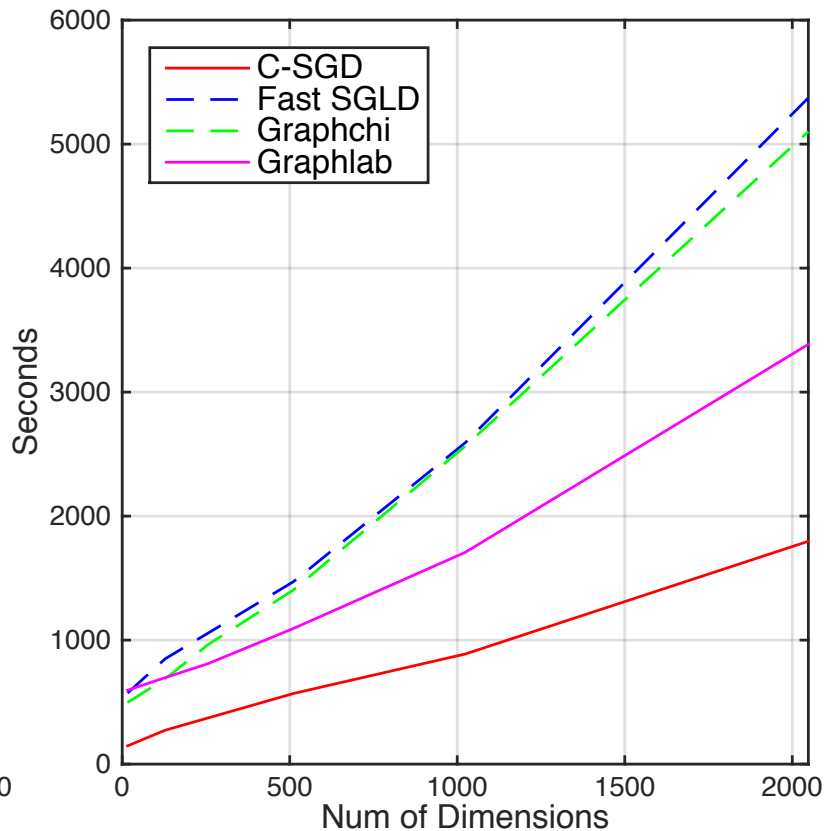


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Speed (c4.8xlarge)

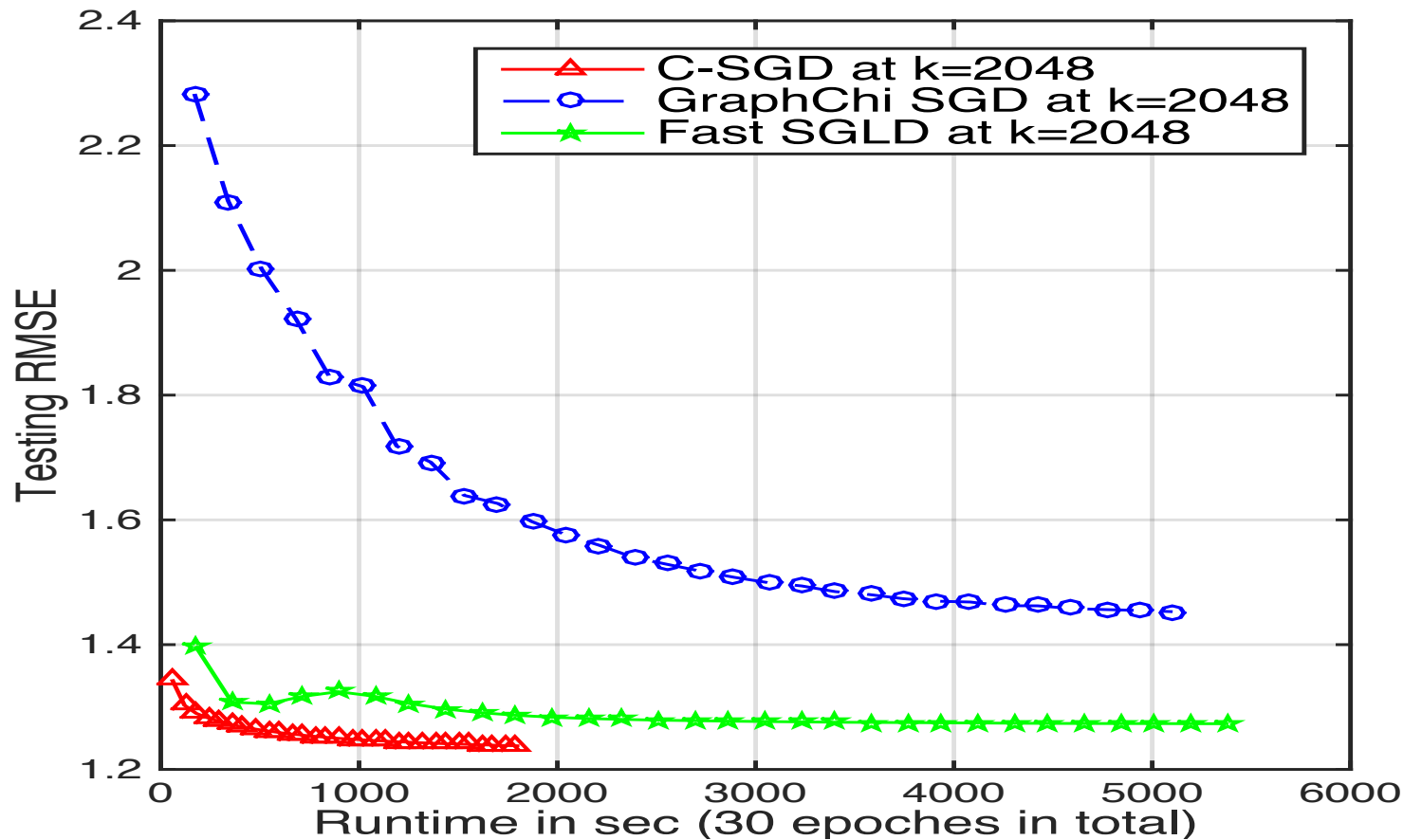


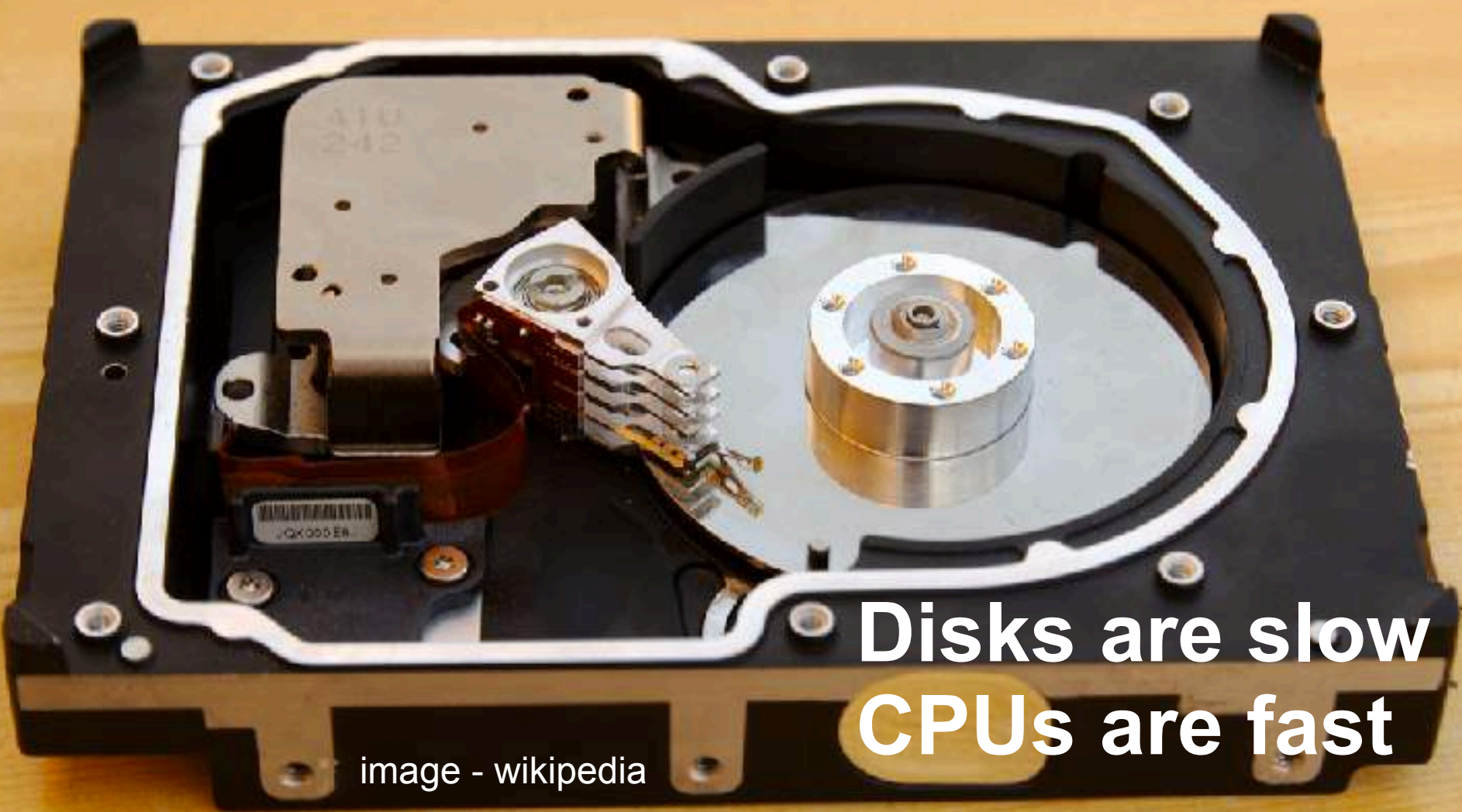
Netflix - 100M, 15 iterations



Yahoo - 250M, 30 iterations

Convergence





Disks are slow
CPU's are fast

image - wikipedia

Use Case: SVM Optimization

- LibLinear / SMO style optimization
 - Read data from disk
 - Update parameters w in memory (soft margin, logistic)
- CPU is much faster than HDD



10MB
1ns
1TB/s

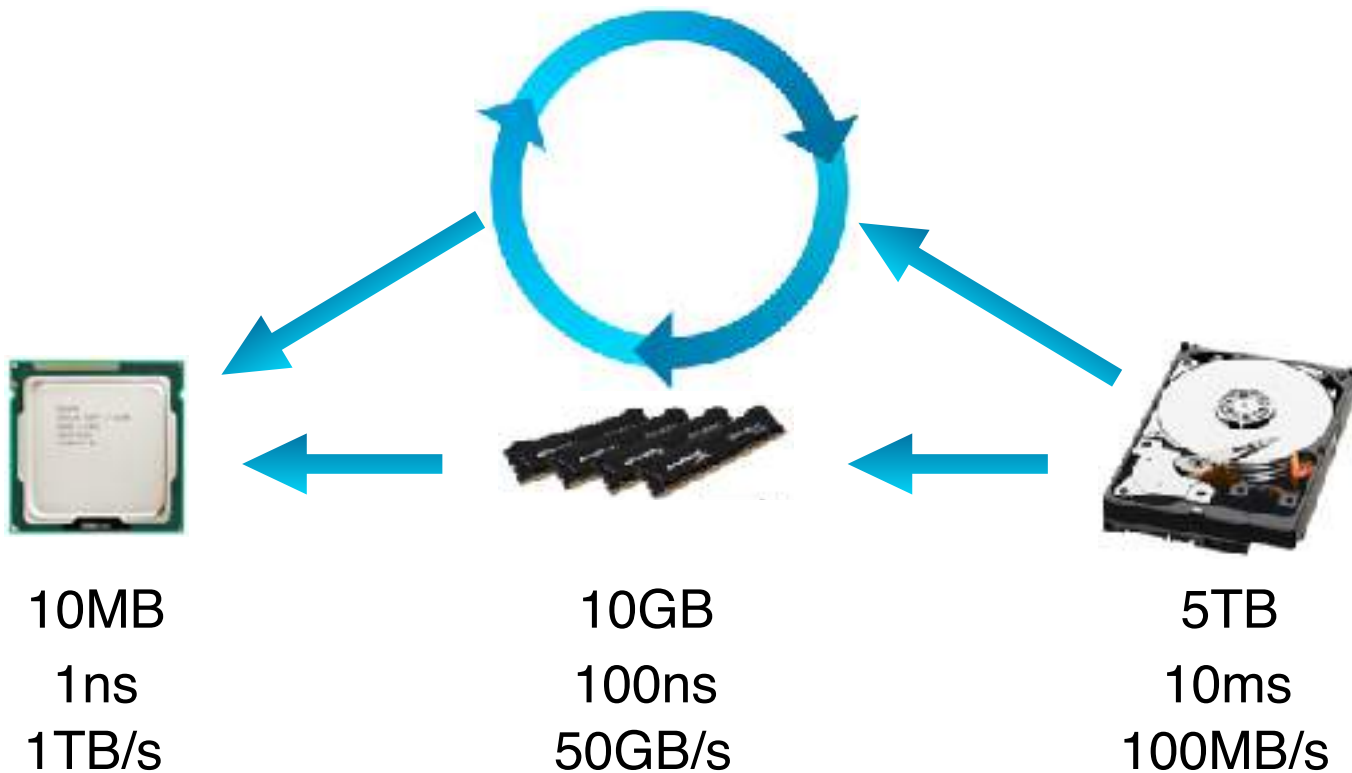


10GB
100ns
50GB/s



5TB
10ms
100MB/s

Use Case: SVM Optimization

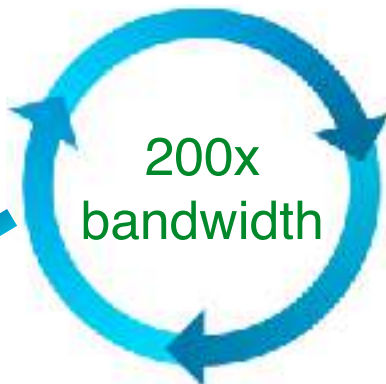


Use Case: SVM Optimization

trainer - read data
repeatedly from RAM
update model



10MB
1ns
1TB/s



10GB
100ns
50GB/s

reader - get data
from disk and
write to memory



5TB
10ms
100MB/s

Technical challenge

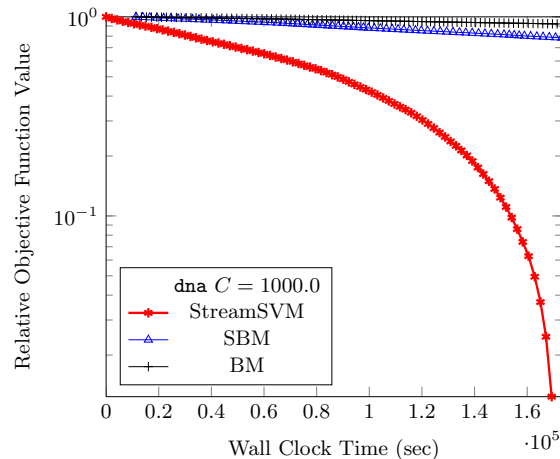
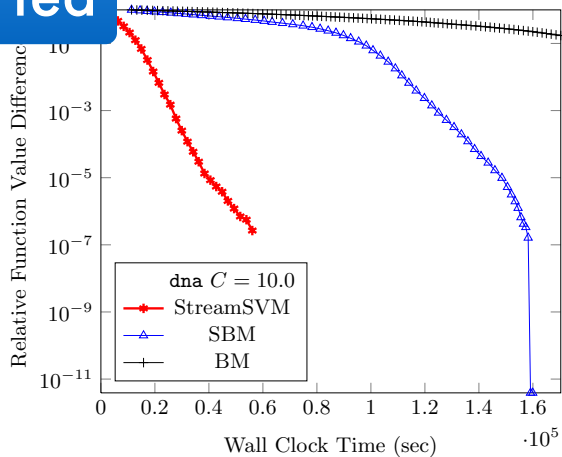
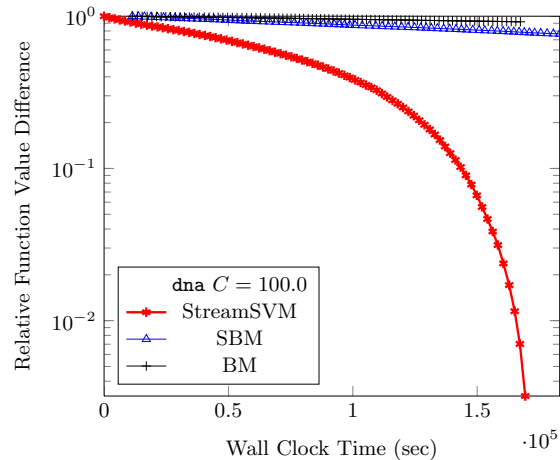
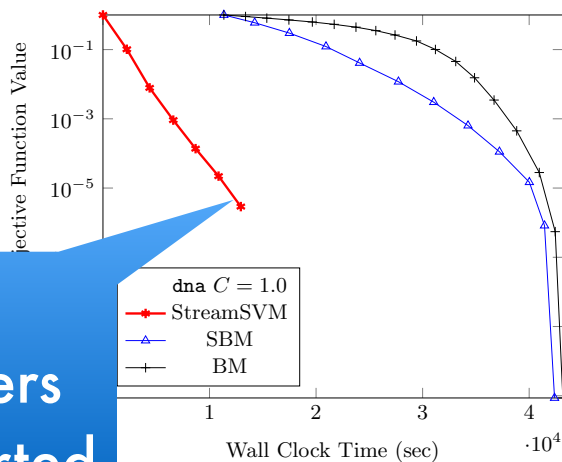
- If we just reuse observations we might overweight some data relative to the rest

$$\sum_i l(x_i, y_i, f(x_i)) \longrightarrow \sum_j \sum_{i \in S_j} l(x_i, y_i, f(x_i))$$

- Primal descent impossible (without bookkeeping)
- Dual ascent is accurate (leaves objective unchanged)

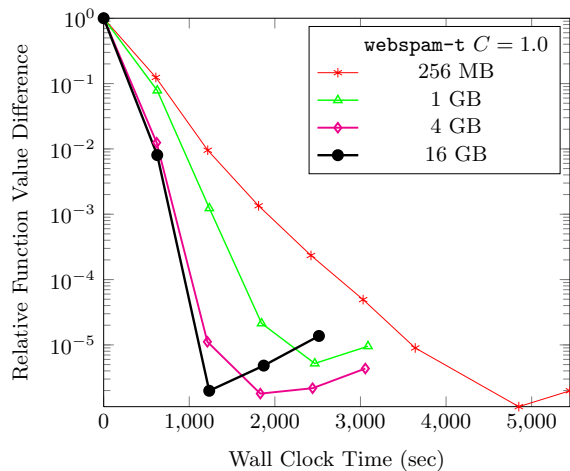
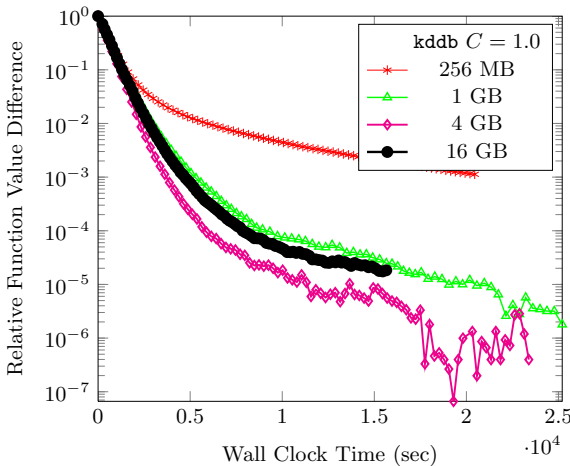
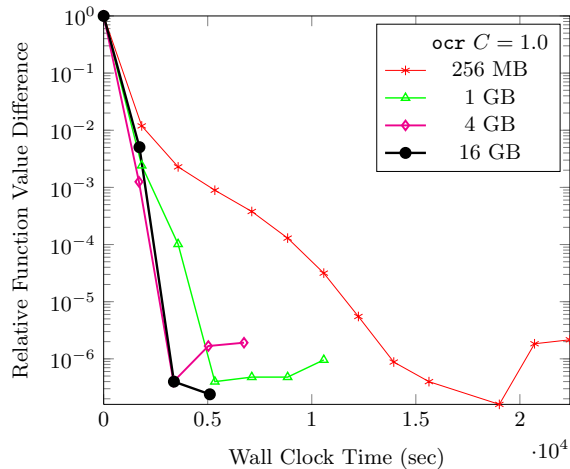
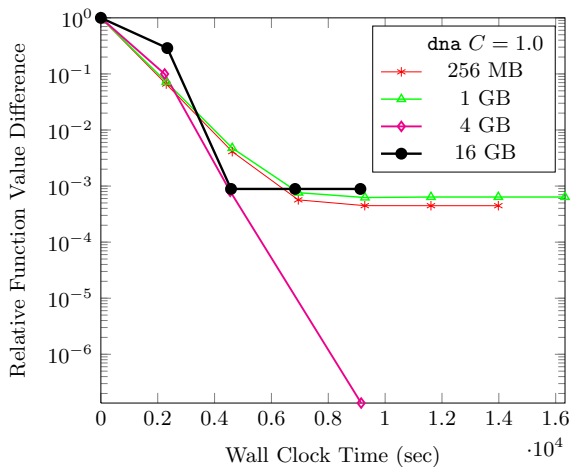
Speed (DNA dataset, different C)

we finish
before others
even get started



Effect of caching

Matsushima, Vishwanathan, Smola, KDD'12

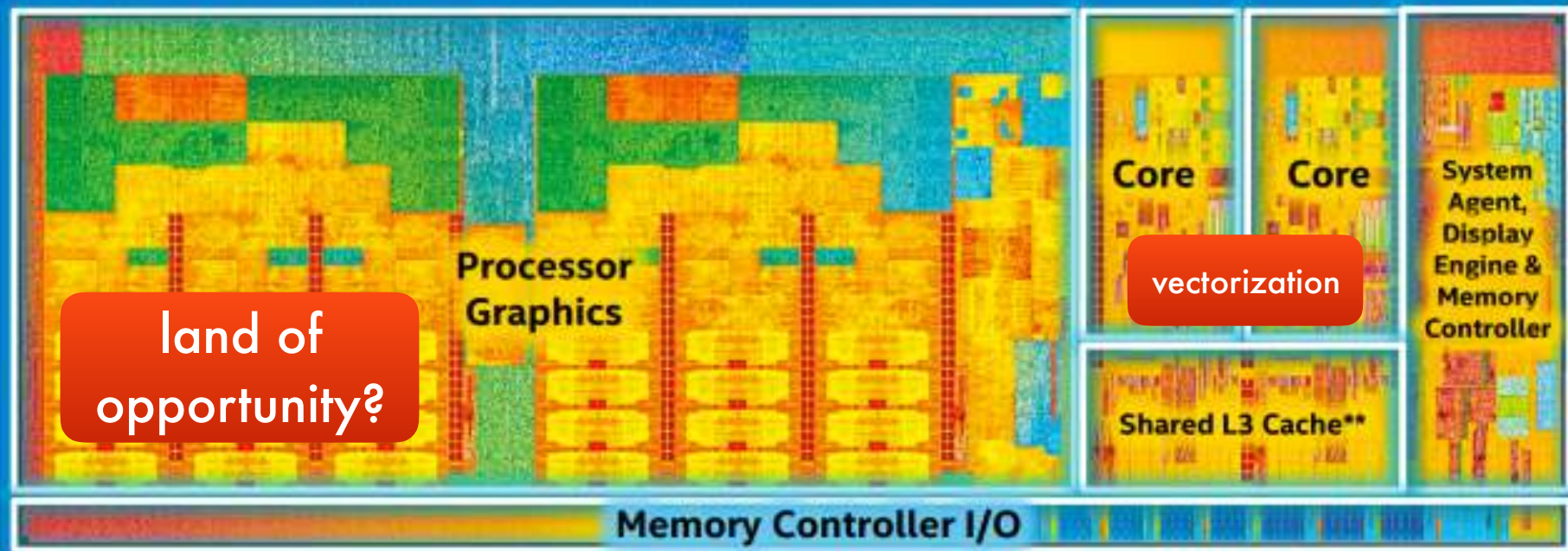


A black and white photograph of a large, industrial-style room, likely a data processing center or office from the mid-20th century. The room is filled with rows of women, mostly young to middle-aged, seated at long wooden desks. They are working on typewriters and handling large stacks of papers and files. The room has high ceilings with exposed wooden beams and large windows on the right side, letting in natural light. The overall atmosphere is one of busy, organized labor.

Computation

5th Gen Intel® Core™ Processor Die Map

Intel® HD Graphics 6000 or Intel® Iris™ Graphics 6100



Dual Core Die Shown Above

Transistor Count: 1.9 Billion

Die Size: 133 mm²

4th Gen Core Processor (U series): 1.3B

4th Gen Core Processor (U series): 181mm²

** Cache is shared across both cores and processor graphics

Vectorization

Per Core (up to 18 per chip - Xeon E5)

- Multiple integer and FP units
(each one needs to be fed with data)
- Naive calculation (i7-5960X)
 $8 \times 3 \text{ GHz} = 24 \text{ GFlops}$ but benchmark has **183 GFlops**

AVX Instructions (256 bit or 512 bit wide on Xeon)

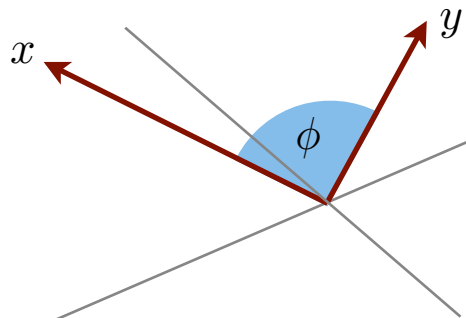
- Works on arrays of numbers (8 floats = 256 bit)
- **In one clock cycle**
- Improved calculation (i7-5960X)
 $8 \times 3 \times 8 \text{ GHz} = 192 \text{ GFlops}$ (much better)

BLAS/LAPACK/EISPACK/whateverPACK libraries

highly optimized - don't write your own code **needlessly**

Use Case: SimHash

- Basic Idea

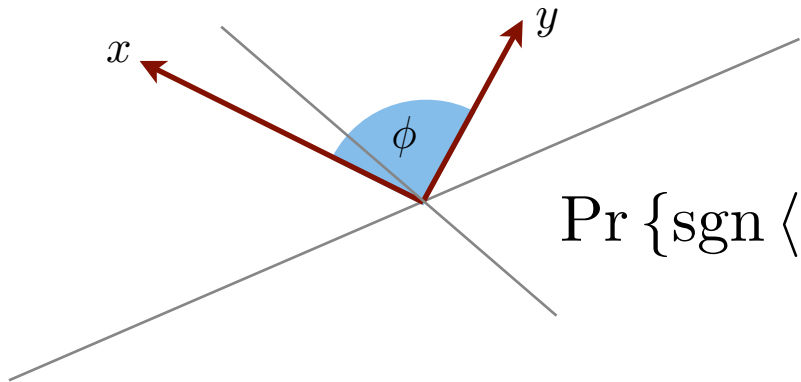


$$\Pr \{ \text{sgn} \langle x, w \rangle \neq \text{sgn} \langle y, w \rangle \} = \frac{\phi}{\pi}$$

- Goemans & Williamson, 1995
Use this for an SDP relaxation of graph cut
- Charikar, 2003
Use this for hashing angles between vectors

Use Case: SimHash

- Basic Idea



$$\Pr \{ \text{sgn} \langle x, w \rangle \neq \text{sgn} \langle y, w \rangle \} = \frac{\phi}{\pi}$$

- Hash map is very memory efficient (n bits)

$$x \rightarrow h(x) = (\text{sgn} \langle x, w_1 \rangle, \dots, \text{sgn} \langle x, w_n \rangle)$$

Compute with matrix-vector product

- Inner product estimation

$$\langle x, y \rangle \approx \|x\| \|y\| \cos n^{-1} \|h(x) - h(y)\|_1$$

Cosine similarity

- Similarity measure for many problems (search, retrieval, recommendation)
- Very expensive if we need to compute it many times for high dimensional data
- Good enough approximation for first step

$$\langle x, y \rangle \approx \|x\| \|y\| \cos n^{-1} \|h(x) - h(y)\|_1$$

compute
once

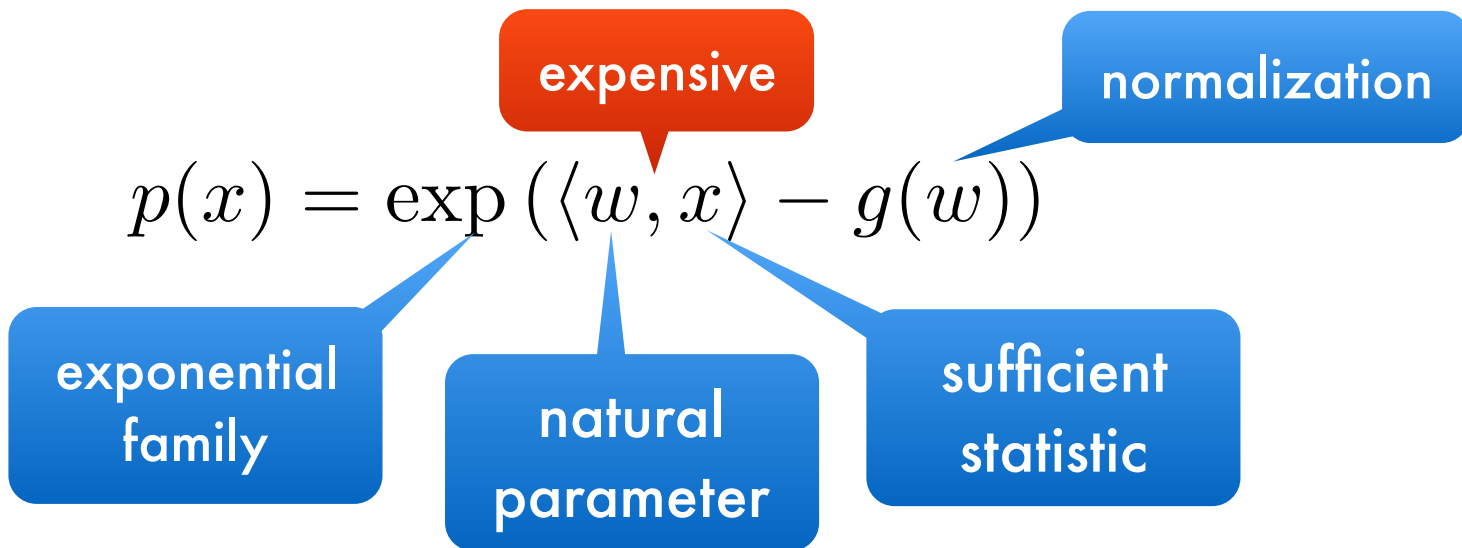
negligible

vectorize with AVX

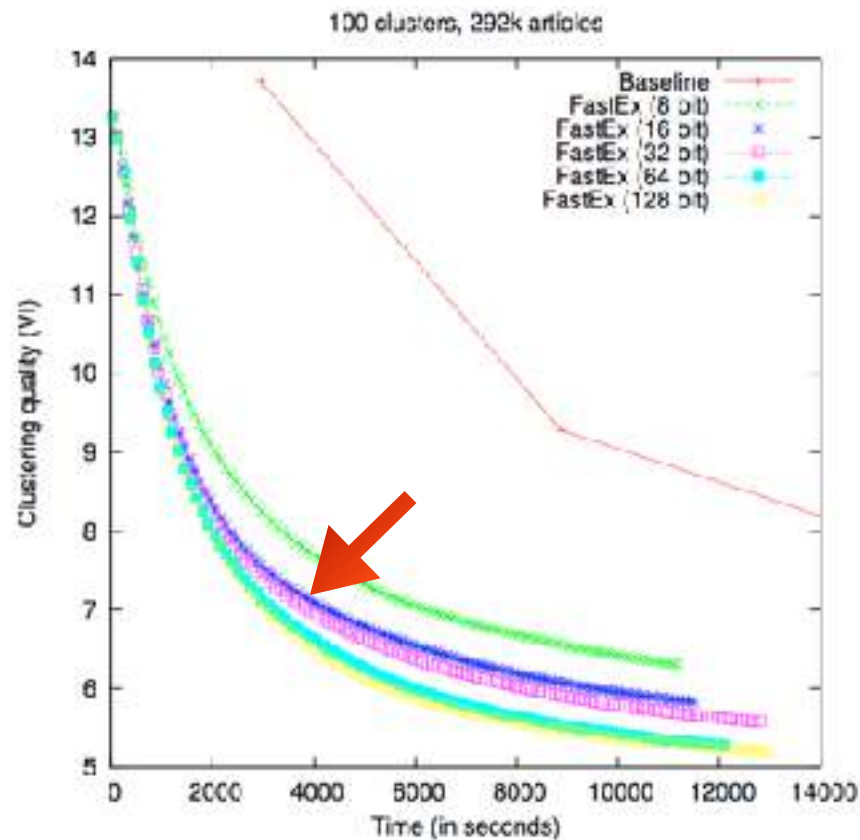
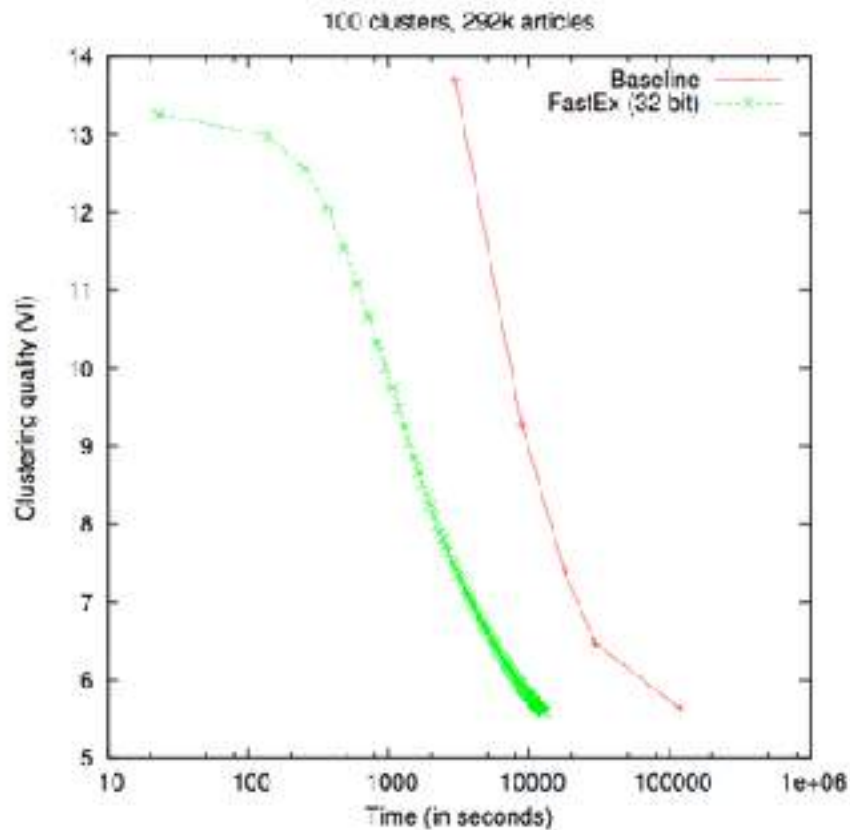
Clustering

- Text clustering via exponential family distributions
- Discrete distribution (approximate with SimHash)

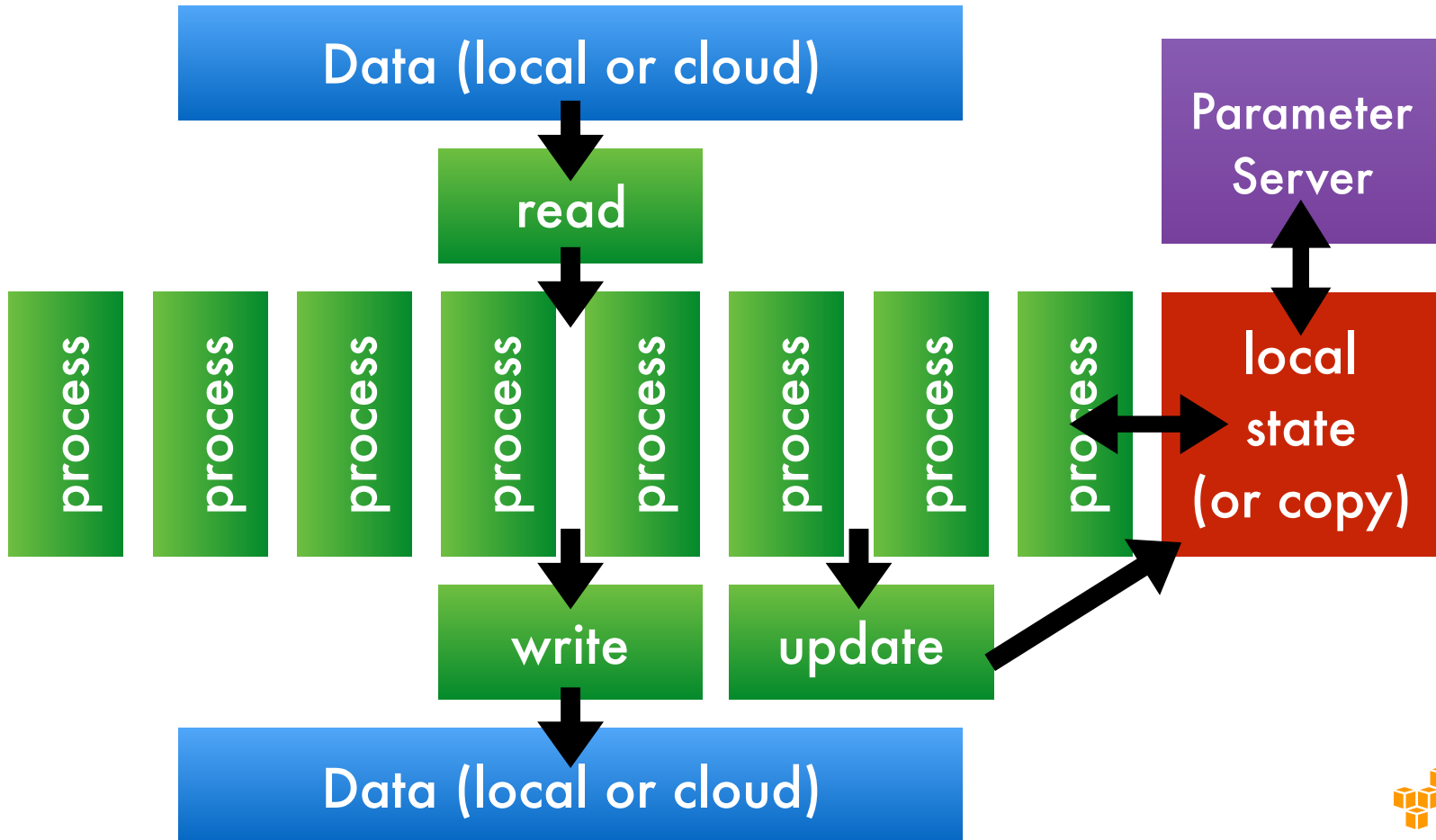
Once per cluster is expensive for 10k clusters



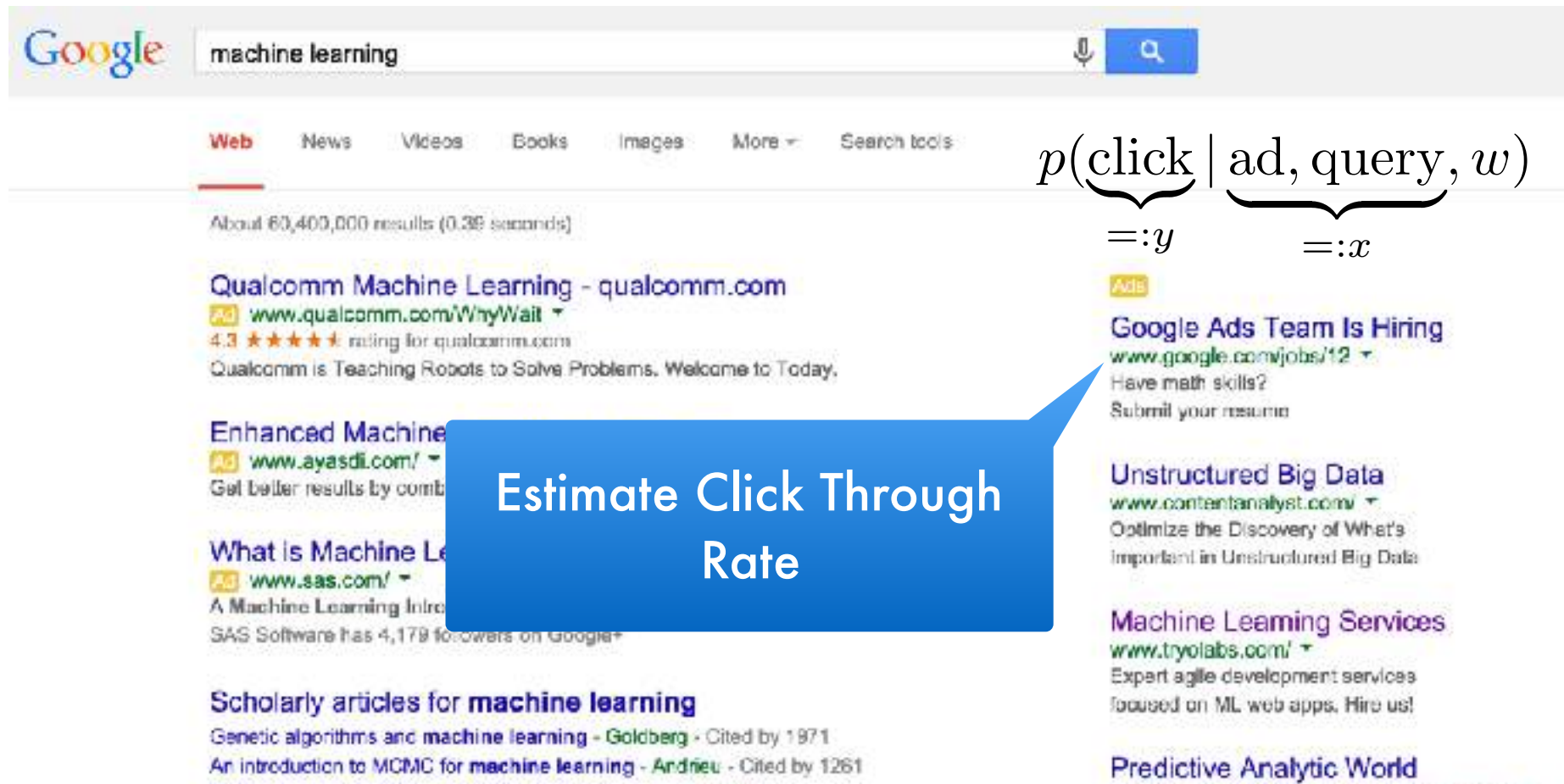
Results



No Locks for Multicore



A boring problem (worth \$100B)



The image shows a Google search interface for the query "machine learning". The search results include organic links and several advertisements. A blue callout box with the text "Estimate Click Through Rate" points to an advertisement for "Google Ads Team Is Hiring".

Google

machine learning

Web News Videos Books Images More Search tools

About 60,400,000 results (0.39 seconds)

Qualcomm Machine Learning - qualcomm.com
Ad www.qualcomm.com/WhyWait
4.3 ★★★★★ rating for qualcomm.com
Qualcomm is Teaching Robots to Solve Problems. Welcome to Today.

Enhanced Machine Learning - ayasdi.com
Ad www.ayasdi.com/
Get better results by combining machine learning with your data.

What is Machine Learning - sas.com
Ad www.sas.com/
A Machine Learning Introduction
SAS Software has 4,179 followers on Google+

Scholarly articles for machine learning
Genetic algorithms and machine learning - Goldberg - Cited by 1971
An introduction to MCMC for machine learning - Andrieu - Cited by 1261

Google Ads Team Is Hiring
Ad www.google.com/jobs/12
Have math skills?
Submit your resume

Unstructured Big Data
Ad www.contentanalyst.com/
Optimize the Discovery of What's Important in Unstructured Big Data

Machine Learning Services
Ad www.tryolabs.com/
Expert agile development services focused on ML web apps. Hire us!

Predictive Analytic World

Estimate Click Through Rate

$$p(\underbrace{\text{click}}_{=:y} \mid \underbrace{\text{ad, query, } w}_{=:x})$$

Logistic Regression

- Linear function class

$$f(x) = \langle w, x \rangle$$

- Logistic regression

$$p(y|x, w) = \frac{1}{1 + \exp(-y \langle w, x \rangle)}$$

- Optimization Problem

$$\underset{w}{\text{minimize}} \sum_{i=1}^m \log(1 + \exp(-y_i \langle w, x_i \rangle)) + \lambda \|w\|_1$$

sparse models
for advertising

- Small network

100M users, 10 days = 1B examples, 1 big server

Stochastic gradient descent

- **Compute gradient on data**

$$g_i = \partial_w l(x_i, y_i, w) \text{ e.g. } \partial_w \log(1 + \exp(-y_i \langle x_i, w \rangle))$$

- Update parameter with gradient (for l_2 penalty)

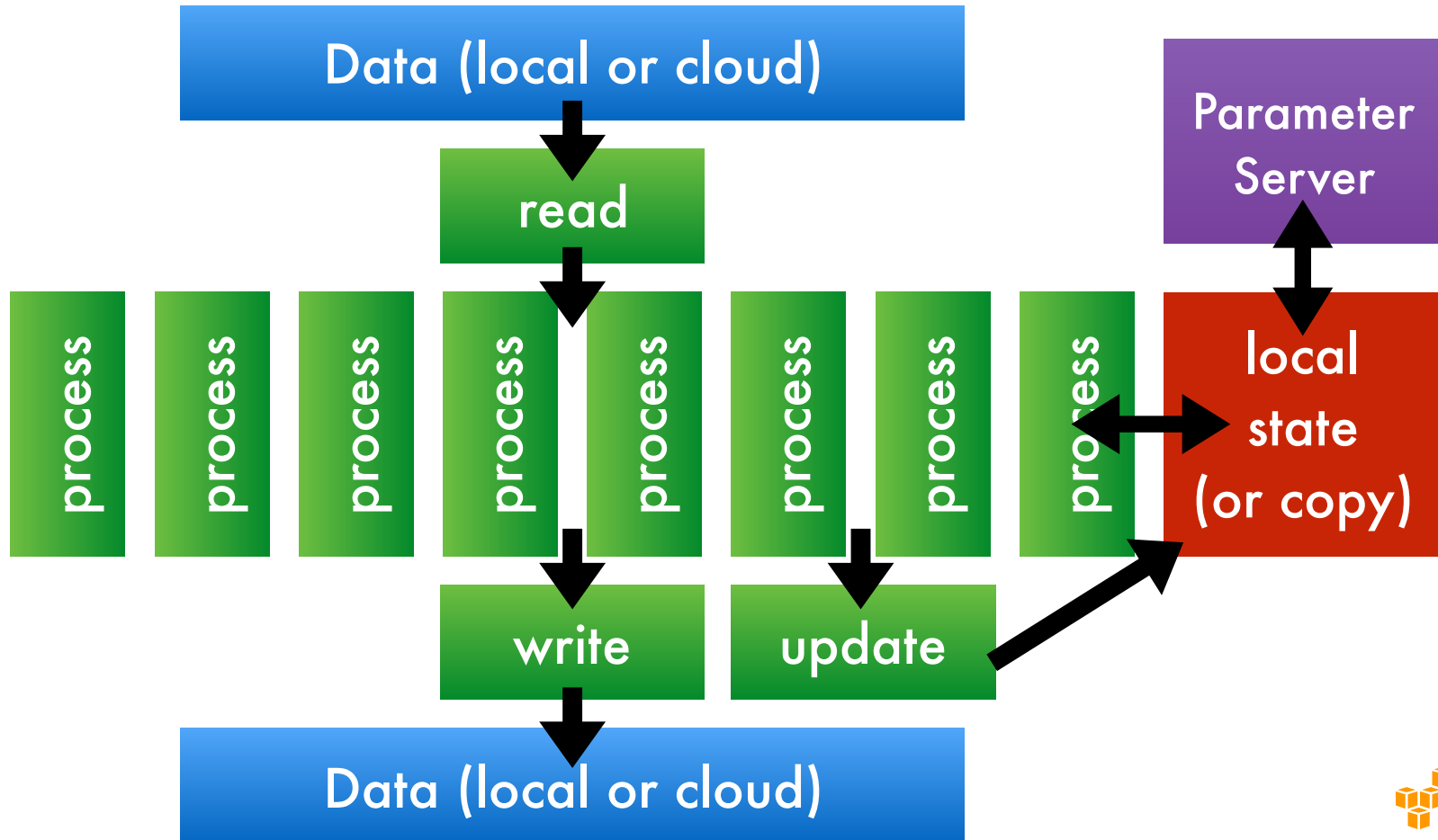
$$w \leftarrow (1 - \lambda\eta)w - \eta g_i$$

- Update parameter with prox operator (l_1 penalty)

$$w \leftarrow \operatorname{argmin}_w \|w\|_1 + \frac{\gamma}{2} \|w - (w_i - \eta g_i)\|^2$$

- This is **sequential**. Most cores will be idle
- But most updates are sparse. **Discard locks!**
(Hogwild - Recht, Re, Wright, 2014)

Dataflow



A red elephant with a gold patterned blanket is the central focus of the image. It is standing in a living room with a brick wall, a lamp, and a painting in the background. The elephant is covered in a red blanket with a gold geometric pattern. The room has a warm, dimly lit atmosphere with a brick wall, a lamp, and a painting in the background.

2. MXNet

- Imperative and Declarative Programming
- Language Support
- Backend and Automatic Parallelization

Caffe(2)
(Py)Torch
Theano
Tensorflow
CNTK
Keras
Paddle
Chainer
SINGA
DL4J

Why yet another deep networks tool?

- **Frugality & resource efficiency**

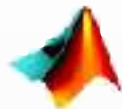
Engineered for cheap GPUs with smaller memory, slow networks

- **Speed**

- Linear scaling with `#machines` and `#GPUs`
- High efficiency on single machine, too (C++ backend)

- **Simplicity**

Mix declarative and imperative code



single implementation of
backend system and
common operators

performance guarantee
regardless which frontend
language is used

frontend

backend



A large elephant is the central focus, covered in a vibrant red blanket with a repeating gold-colored geometric pattern. The elephant is standing in a room with a dark brick wall in the background. To the left, there is a small table with a lamp and some books. To the right, a white picket fence runs along the wall, and a framed picture is visible. The scene is lit with warm, ambient light.

Ease of coding & efficiency (imperative & declarative)

image credit - Banksy/wikipedia

Imperative Programs



```
import numpy as np
a = np.ones(10)
b = np.ones(10) * 2
c = b * a
print c
d = c + 1
```

Easy to tweak
with python
codes

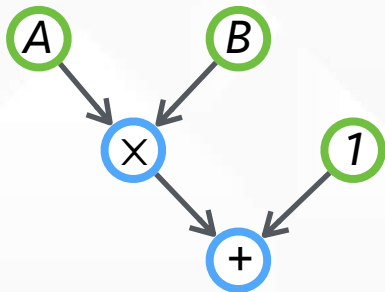
Pro

- Straightforward and flexible.
- Take advantage of language native features (loop, condition, debugger)

Con

- Hard to optimize

Declarative Programs



```
A = Variable('A')
B = Variable('B')
C = B * A
D = C + 1
f = compile(D)
d = f(A=np.ones(10),
      B=np.ones(10)*2)
```

Pro

- More chances for optimization
- Cross different languages

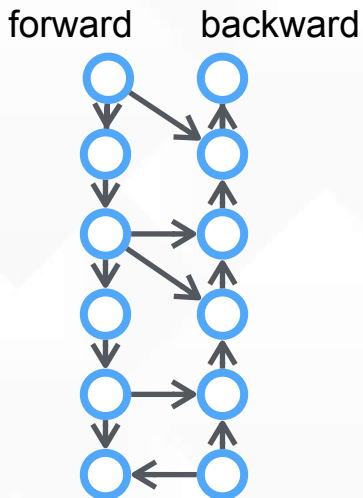
Con

- Less flexible

C can share memory with D,
because C is deleted later

Imperative vs. Declarative for Deep Learning

Computational Graph
of the Deep Architecture



Needs heavy optimization,
fits **declarative** programs

Updates and Interactions
with the graph

- Iteration loops
- Parameter update

$$w \leftarrow w - \eta \partial_w f(w)$$

- Beam search
- Feature extraction ...

Needs mutation and more
language native features, good for
imperative programs

MXNet: Mix the Flavors Together

Imperative
NDArray API

```
import mxnet as mx
a = mx.nd.zeros((100, 50))
b = mx.nd.ones((100, 50))
c = a + b
c += 1
print(c)
```

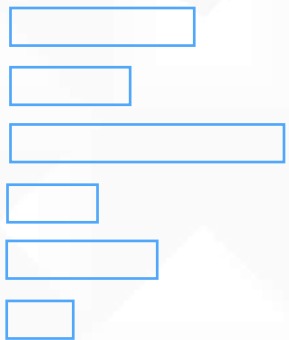
Declarative
Symbolic Executor

```
import mxnet as mx
net = mx.symbol.Variable('data')
net = mx.symbol.FullyConnected(data=net, num_hidden=100)
net = mx.symbol.SoftmaxOutput(data=net)
texec = mx.module.Module(net)
texec.forward(data=c)
texec.backward()
```

Imperative NDArray can be
set as input to the graph

Mixed API for Quick Extensions

Variable length sentences



Bucketing



- Runtime switching between different graphs depending on input
- Useful for sequence modeling and image size reshaping
- Use of imperative code in Python, **10 lines** of additional Python code

3D Image Construction

<https://github.com/piiswrong/deep3d>



Deep3D



100 lines of Python code



A large elephant is the central focus, covered in a vibrant red blanket with a repeating gold geometric pattern. It stands in a dimly lit room with a brick wall. To the left, a small table holds a lamp and a red bag. In the background, a fireplace is visible. To the right, a white picket fence separates the elephant from a fireplace mantel where a framed picture of a person is hanging. A lamp sits on a table next to the fence.

Multiple Languages Multiple Toolkits

image credit - Banksy/wikipedia

What We Heard from Users

Programming Languages:

- Python is nice, but I like R/Julia/Matlab more
- I want Scala to work with the Spark pipeline
- I need C++ interface to run on embedded systems
- I prefer Javascript to run on user browsers

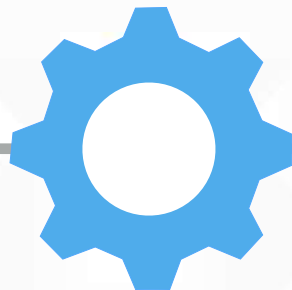
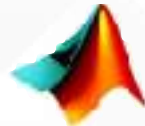
Frameworks:

- I used Torch for 7 years
- All my codes are in Caffe
- I like Keras
- I started deep learning with Tensorflow
- I only used Numpy before, how should I start?

Multiple Programming Languages



Scala



frontend

backend

single implementation
of backend system and
common operators

performance guarantee
regardless of which
frontend language is used

Bringing Caffe to MXNet

Caffe is widely used in computer vision

Call Caffe Operators in MXNet

```
import mxnet as mx
data = mx.symbol.Variable('data')
fc1 = mx.symbol.CaffeOp(data_0=data, num_weight=2, prototxt=
    "layer{type:\"InnerProduct\" inner_product_param{num_output: 128} }")
act1 = mx.symbol.CaffeOp(data_0=fc1, prototxt="layer{type:\"TanH\"}")
fc2 = mx.symbol.CaffeOp(data_0=act1, num_weight=2, prototxt=
    "layer{type:\"InnerProduct\" inner_product_param{num_output: 10}}")
mlp = mx.symbol.SoftmaxOutput(data=fc3)
```

Bringing Torch to MXNet



Torch is a popular Lua framework for both scientific computing and deep learning

Tensor Computation

```
import mxnet as mx
x = mx.th.randn(2, 2, ctx=mx.gpu(0))
y = mx.th.abs(x)
print y.asnumpy()
```

Modules (Layers)

```
import mxnet as mx
data = mx.symbol.Variable('data')
fc = mx.symbol.TorchModule(data_0=data, lua_string='nn.Linear(784, 128)', ...
mlp = mx.symbol.TorchModule(data_0=fc, lua_string='nn.LogSoftMax()', ...
```

MinPy: NumPy in MxNet

Printing & Debugging

```
1 import tensorflow as tf
2 x = tf.zeros((2, 3))
3 with tf.control_dependencies([x]):
4     tf.Print(x, [x])
5 sess = ... # create session.
6 sess.run([x], ...)
```

Tensorflow Program

```
1 import minpy.numpy as np
2 x = np.zeros((2, 3))
3 print x
```

MinPy Program

Data-dependent execution (with AutoGrad)

```
1 import tensorflow as tf
2 x = ... # create x array
3 y = ... # create y array
4 z = tf.cond(x < y,
5             lambda: tf.add(x, y),
6             lambda: tf.square(y))
```

Tensorflow Program

```
1 import minpy.numpy as np
2 x = ... # create x array
3 y = ... # create y array
4 if x < y:
5     z = x + y
6 else:
7     z = y ** 2
```

MinPy Program

... Keras coming very soon ...

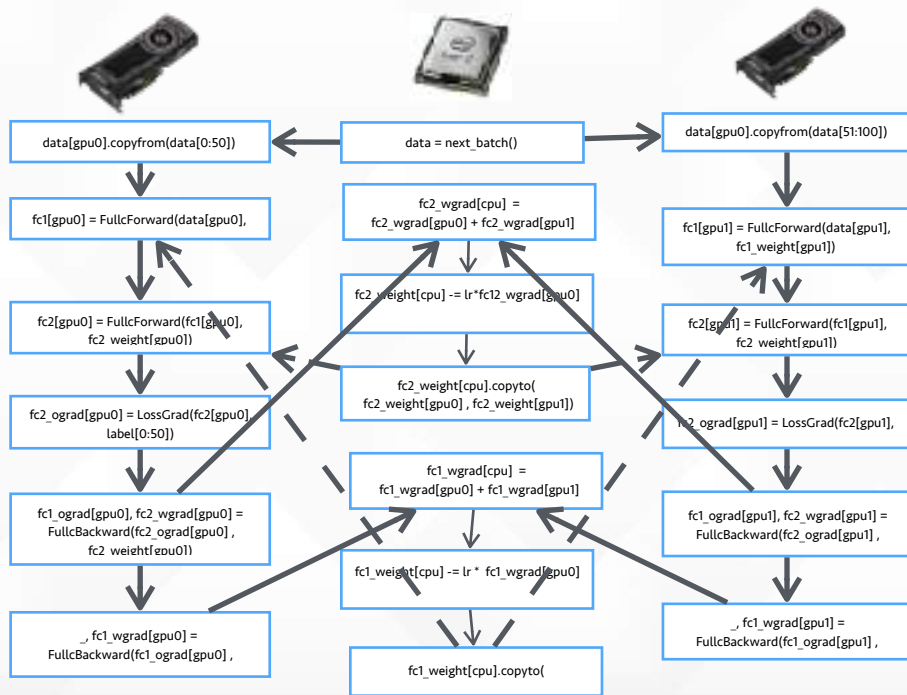
A large elephant is the central focus, covered in a vibrant red blanket with a repeating gold geometric pattern. It stands in a dimly lit room with a brick wall. To the left, a small table holds a lamp and a red cloth. To the right, a fireplace with a patterned screen is visible. The scene is surreal, juxtaposing a wild animal with a domestic interior.

Efficiency & Parallelization

image credit - Banksy/wikipedia

Writing Parallel Programs is Painful

Dependency graph for 2-layer neural networks with 2 GPUs



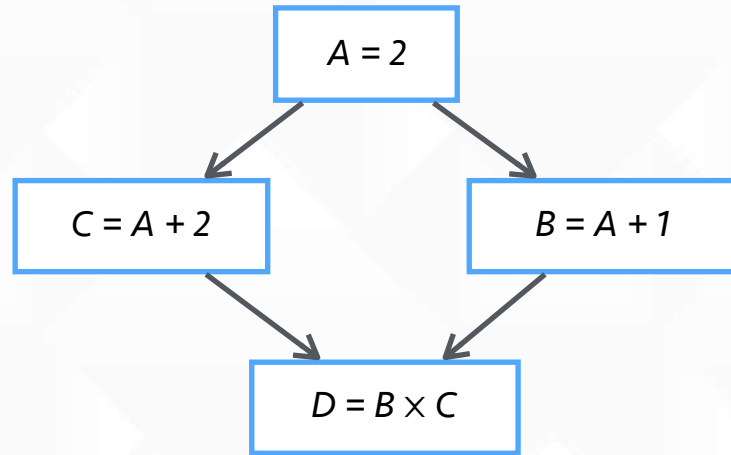
Each forward-backward-update involves $O(\text{num_layer})$, which is often 100–1,000, tensor computations and communications

Auto Parallelization

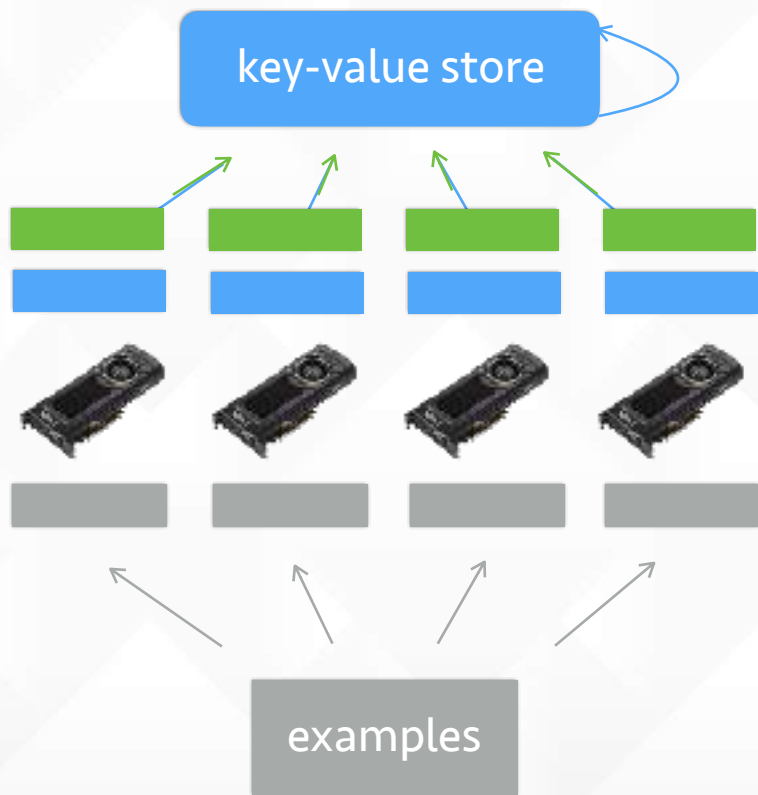
Write **serial** programs

```
import mxnet as mx
A = mx.nd.ones((2,2)) * 2
C = A + 2
B = A + 1
D = B * C
```

Run in **parallel**



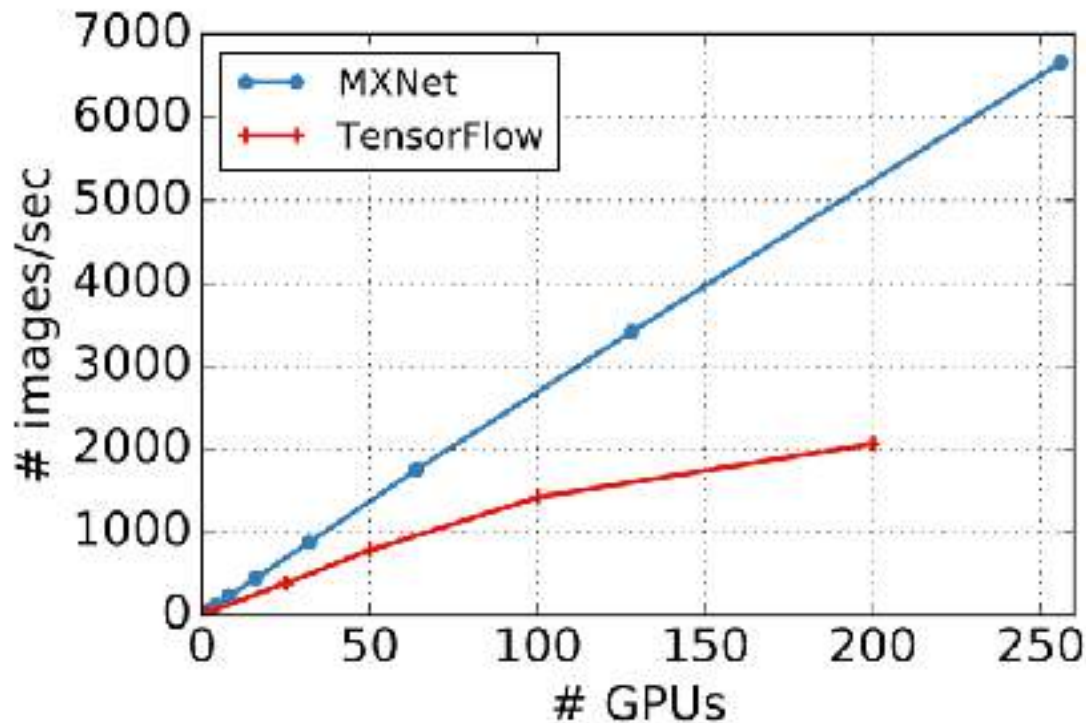
Data Parallelism



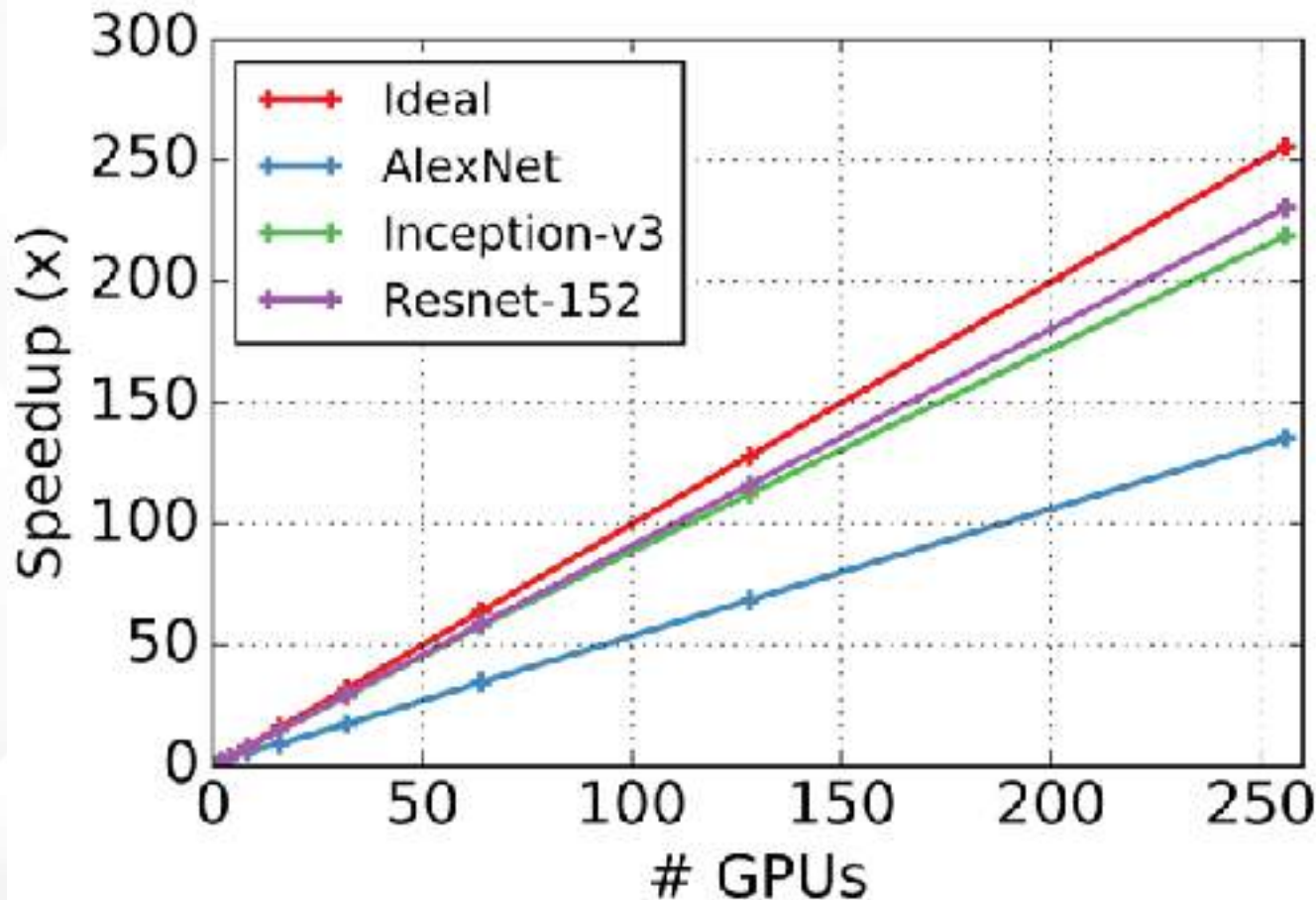
1. Read a data partition
2. Pull the parameters
3. Compute the gradient
4. Push the gradient
5. Update the parameters

Distributed Experiments

- Google Inception v3
- Increasing machines from 1 to 47
- 2x faster than TensorFlow if using more than 10 machines

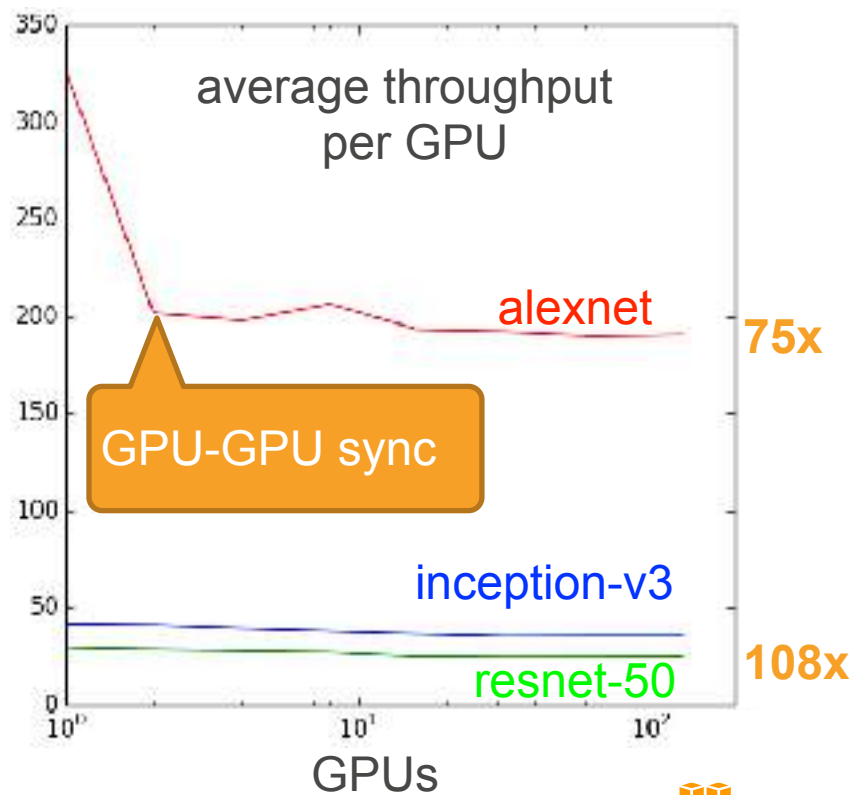
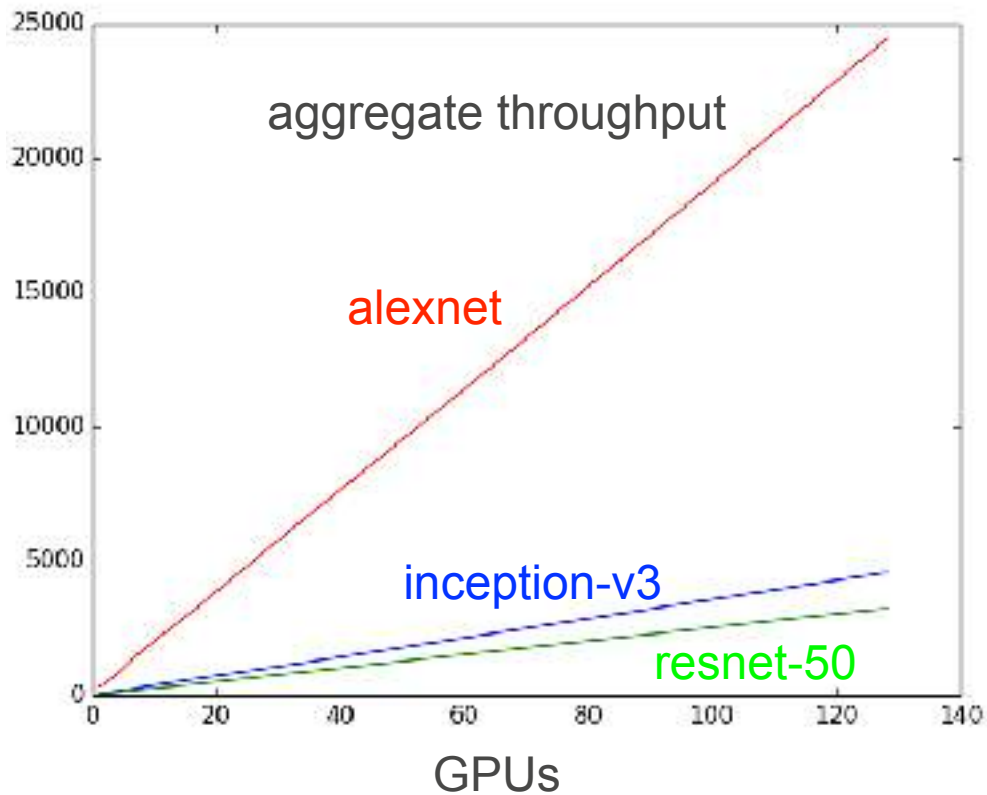


Distributed Training Speedup

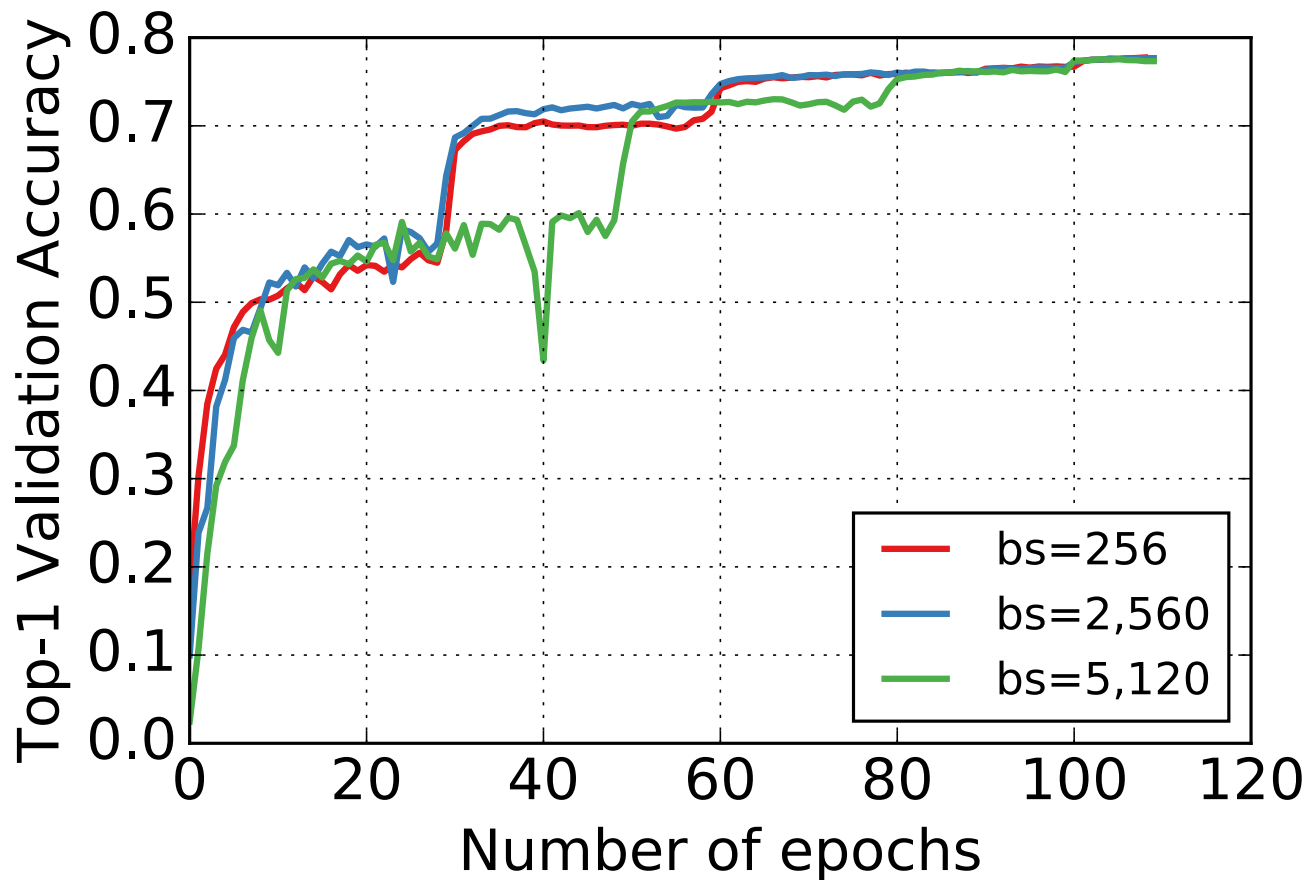


- Cloud formation with Deep Learning AMI
- 16x P2.16xlarge
- Mounted on EFS
- ImageNet
1.2M images
1K classes
- 152-layer ResNet
5.4d on 4x K80s
(1.2h per epoch)
0.22 top-1 error

Scaling on p2.16xlarge



Distributed Training Convergence



3. AMIs and Cloud Formation Templates

- Amazon Machine Images (AMI)
- Deep Learning Frameworks
- Cloud Formation Templates

Amazon Machine Image for Deep Learning

bit.ly/deepami bit.ly/deepubuntu

- Tool for data scientists and developers
- Setting up a DL system takes (install) time & skill
 - Keep packages up to date and compiled (MXNet, TensorFlow, Caffe, Torch, Theano, Keras)
 - Anaconda, Jupyter, Python 2 and 3
 - **NVIDIA** Drivers for G2 and P2 instances
 - **Intel MKL** Drivers for all other instances (C4, M4, ...)

Getting started

```
acbc32cf4de3:image-classification smola$ ssh ec2-user@54.210.246.140
```

Last login: Fri Nov 11 05:58:58 2016 from 72-21-196-69.amazon.com

Deep Learning AMI for Amazon Linux

This is beta version of the Deep Learning AMI for Amazon Linux.

The README file for the AMI →→→→→→→→→→→→→→→→ /home/ec2-user/src/README.md

Tests for deep learning frameworks →→→→→→→→→→ /home/ec2-user/src/bin

7 package(s) needed for security, out of 75 available

Run "sudo yum update" to apply all updates.

Amazon Linux version 2016.09 is available.

```
[ec2-user@ip-172-31-55-21 ~]$ cd src/
```

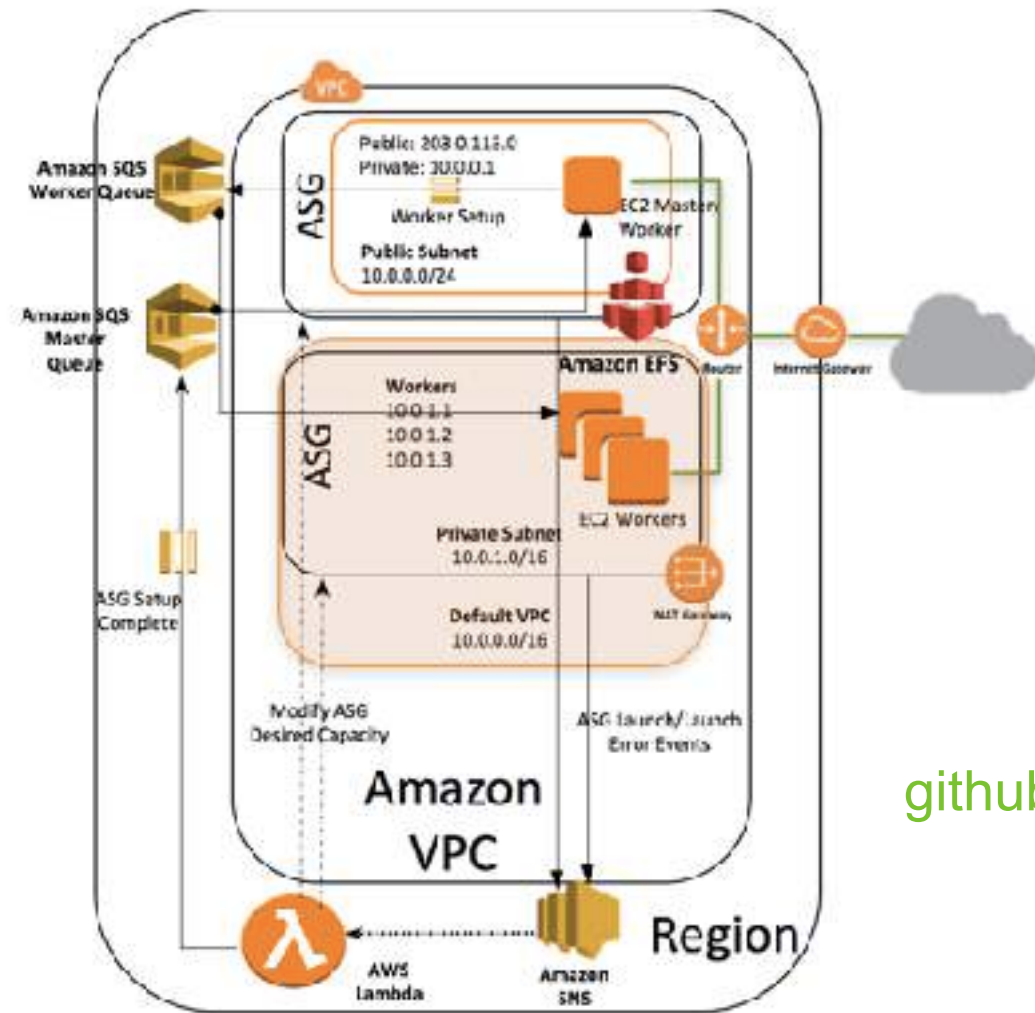
```
[ec2-user@ip-172-31-55-21 src]$ ls
```

anaconda2	bazel	caffe	cntk	keras	mxnet	OpenBLAS	README.md	Theano
anaconda3	bin	caffe3	demos	logs	Nvidia_Cloud_EULA.pdf	opencv	tensorflow	torch



AWS CloudFormation Template for Deep Learning

github.com/aws-labs/deeplearning-cfn



AWS CloudFormation Components

- **VPC** in the customer account.
- The requested number of **worker instances** in an Auto Scaling group within the VPC. Workers are launched in a **private subnet**.
- **Master instance** in a separate Auto Scaling group that acts as a proxy to enable connectivity to the cluster via **SSH**.
- Two security groups that open ports on the **private subnet** for communication between the master and workers.
- **IAM role** that allows users to access and query Auto Scaling groups and the private IP addresses of the EC2 instances.
- **NAT gateway** used by instances within the VPC to talk to the outside.

Summary

- **Memory**
 - Recommender Systems
 - SVM optimization
- **Computation**
 - Hashing and samplers
 - Lock free optimization
- **MxNet**
language, parallelization, AWS Templates

We are hiring!

aws-ai-event-recruiting@amazon.com