# Google Cloud for Scientific Infrastructure

Karan Bhatia, PhD

ESGF Annual Meeting, Dec 2017

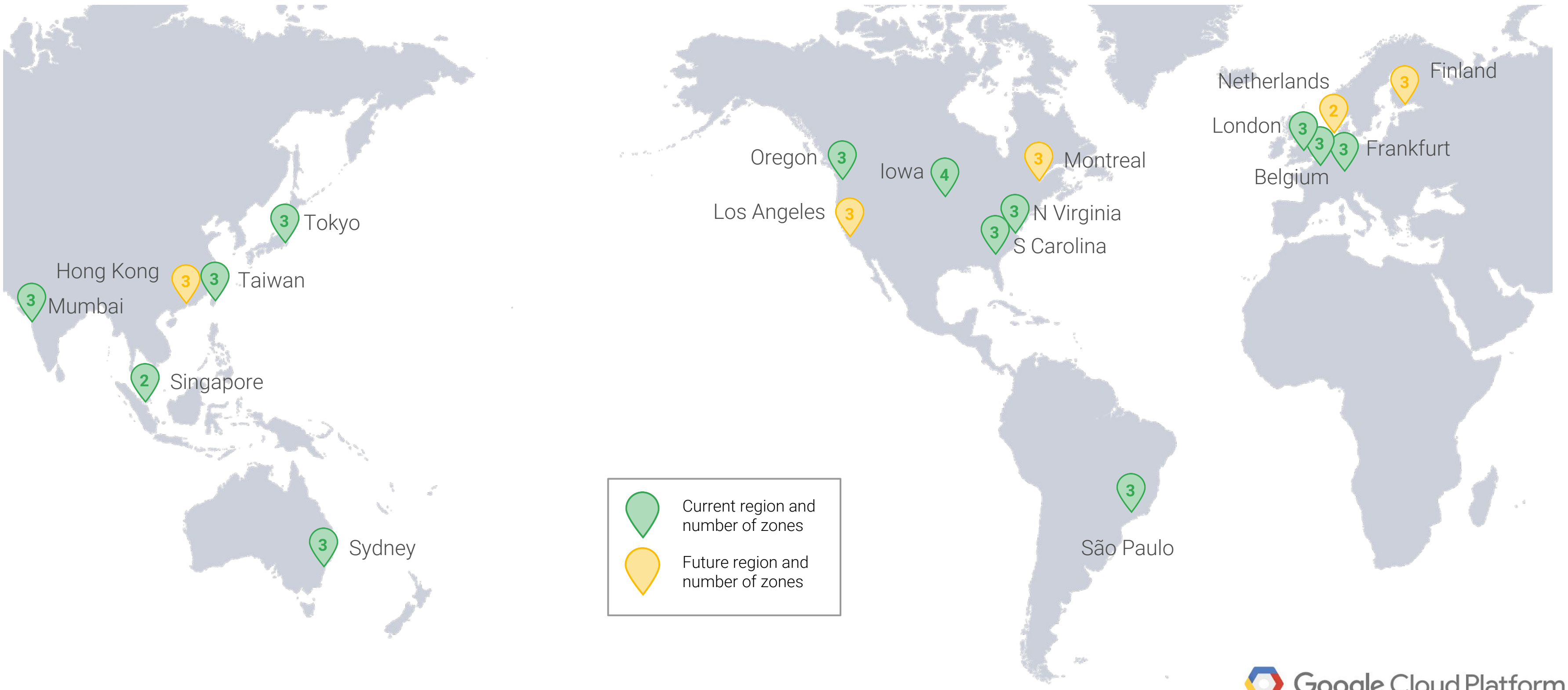

Google Cloud Platform

# $29.4 Billion

3 year trailing Google
CAPEX investment

# Google Cloud Platform Regions

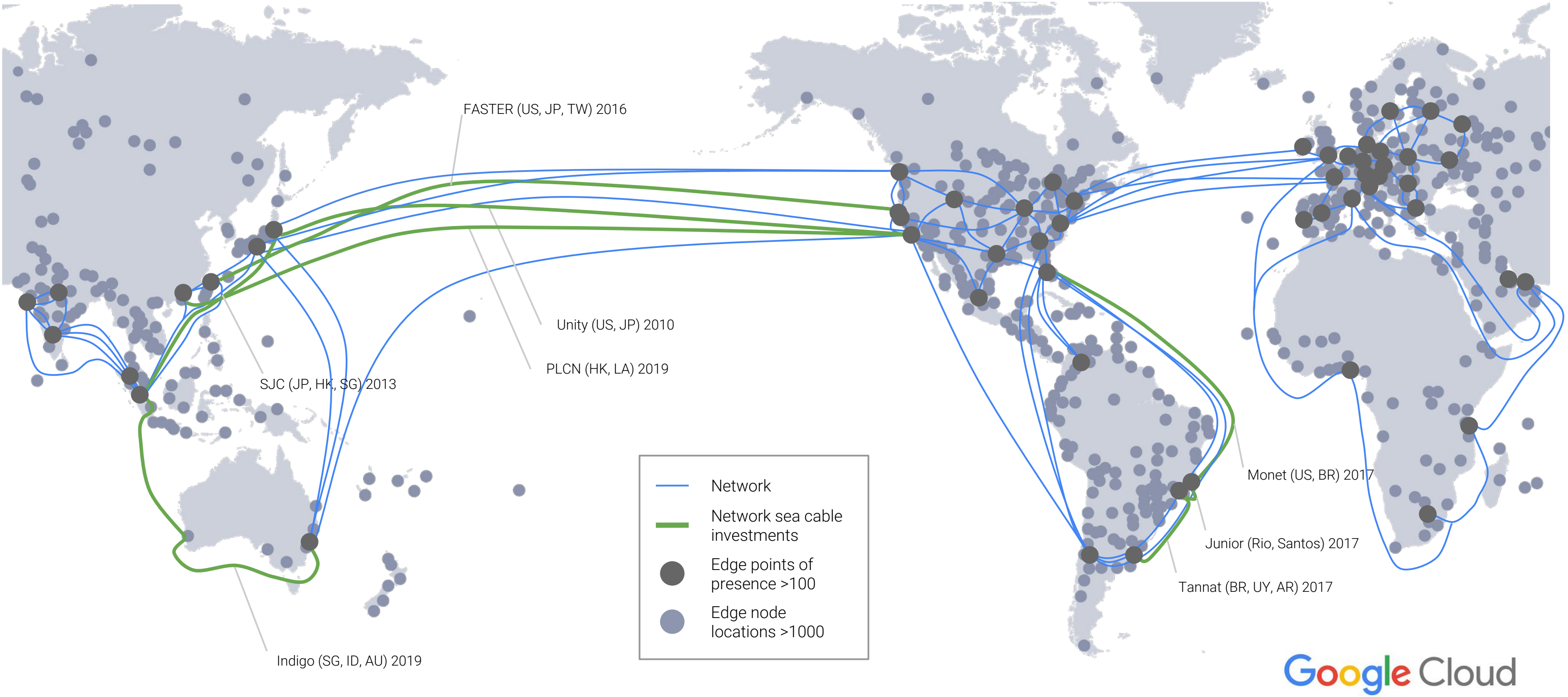
Select from 13 regions. 5 new regions coming in 2018.

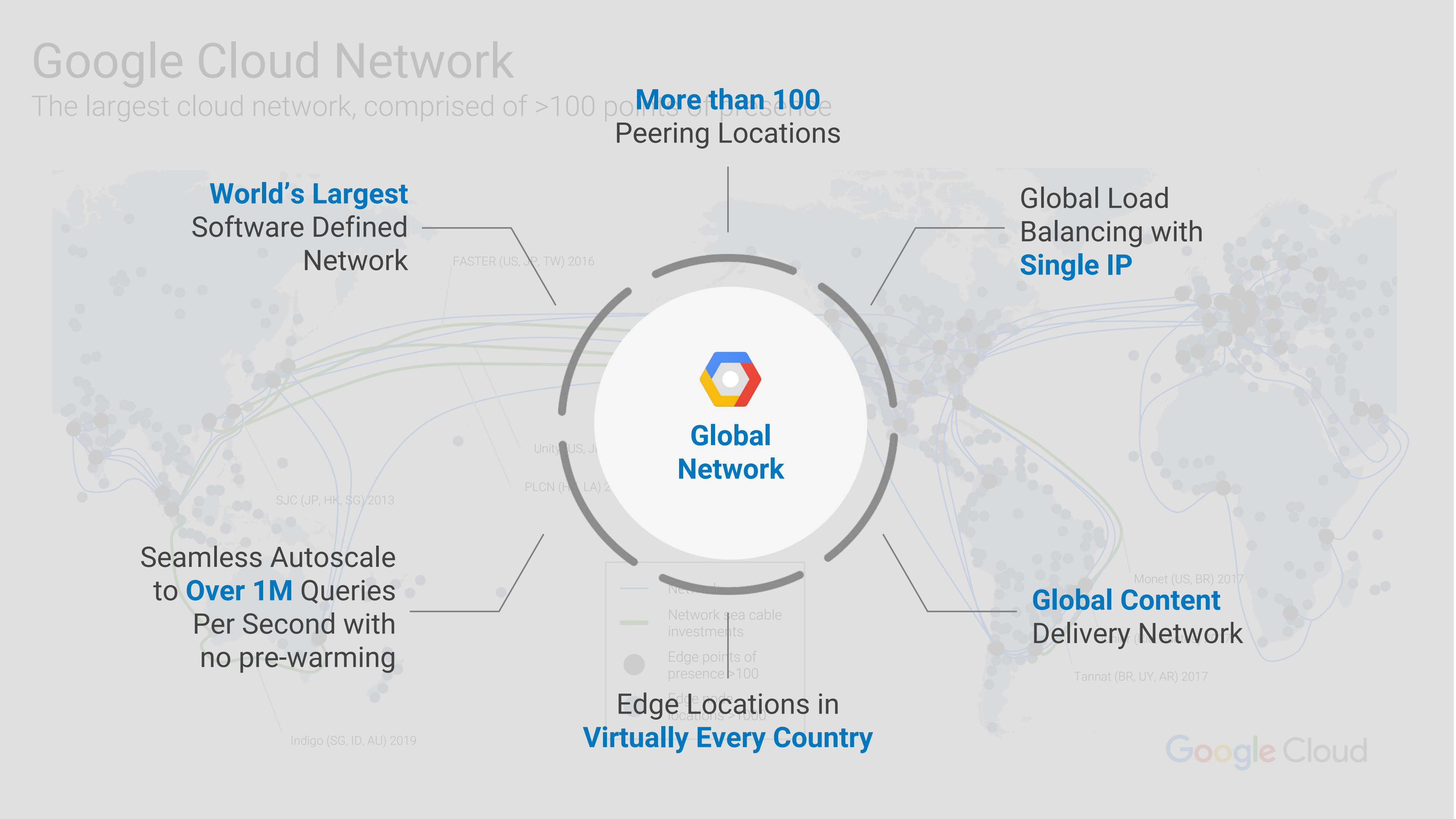



Google Cloud Platform

# Google Cloud Network

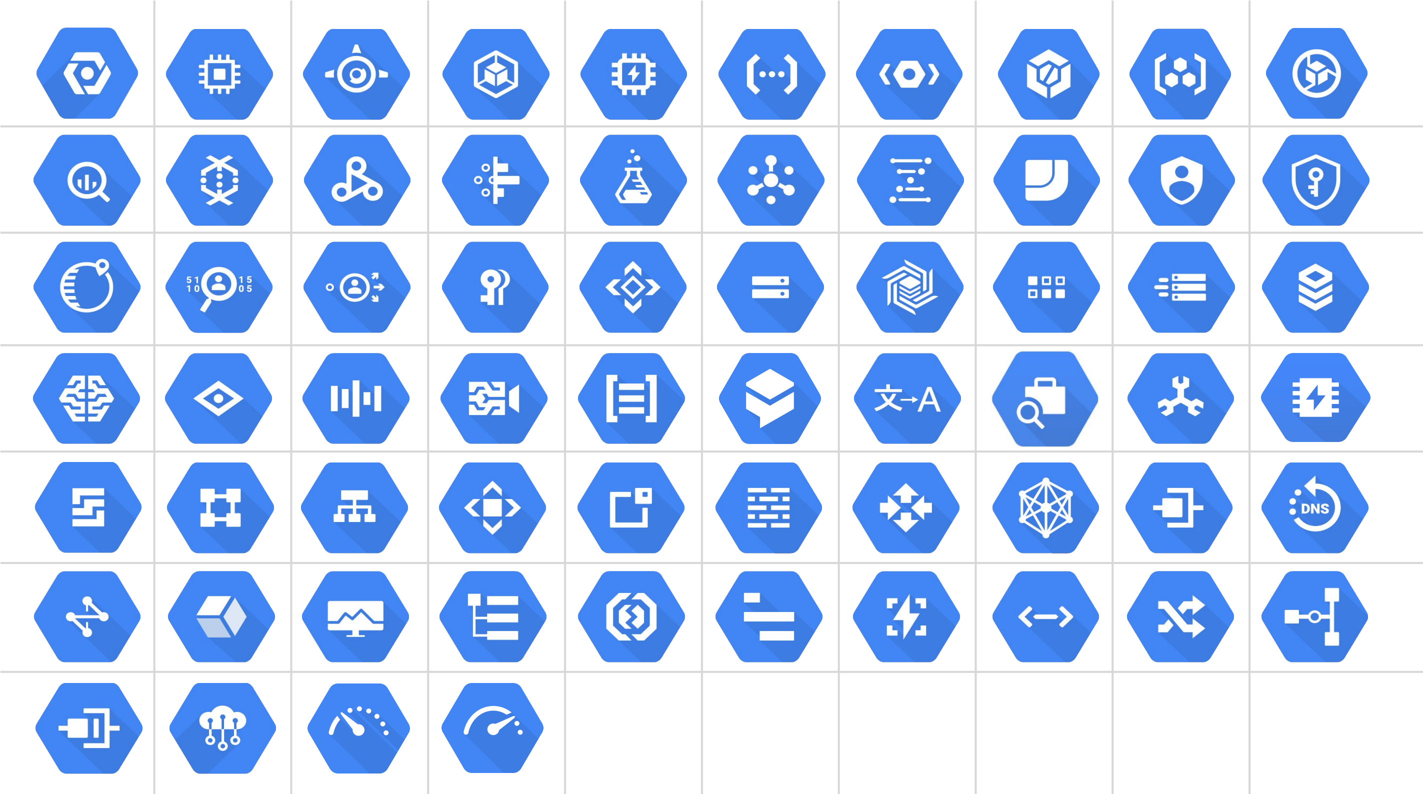
## The largest cloud network, comprised of >100 points of presence





Google Cloud Network
More than 100
Peering Locations
World's Largest
Software Defined
Network
Global Load
Balancing with
Single IP
Global
Network
Seamless Autoscale
to Over 1M Queries
Per Second with
no pre-warming
Global Content
Delivery Network
Edge Locations in
Virtually Every Country
Google Cloud

# Google Cloud Platform



# Agenda

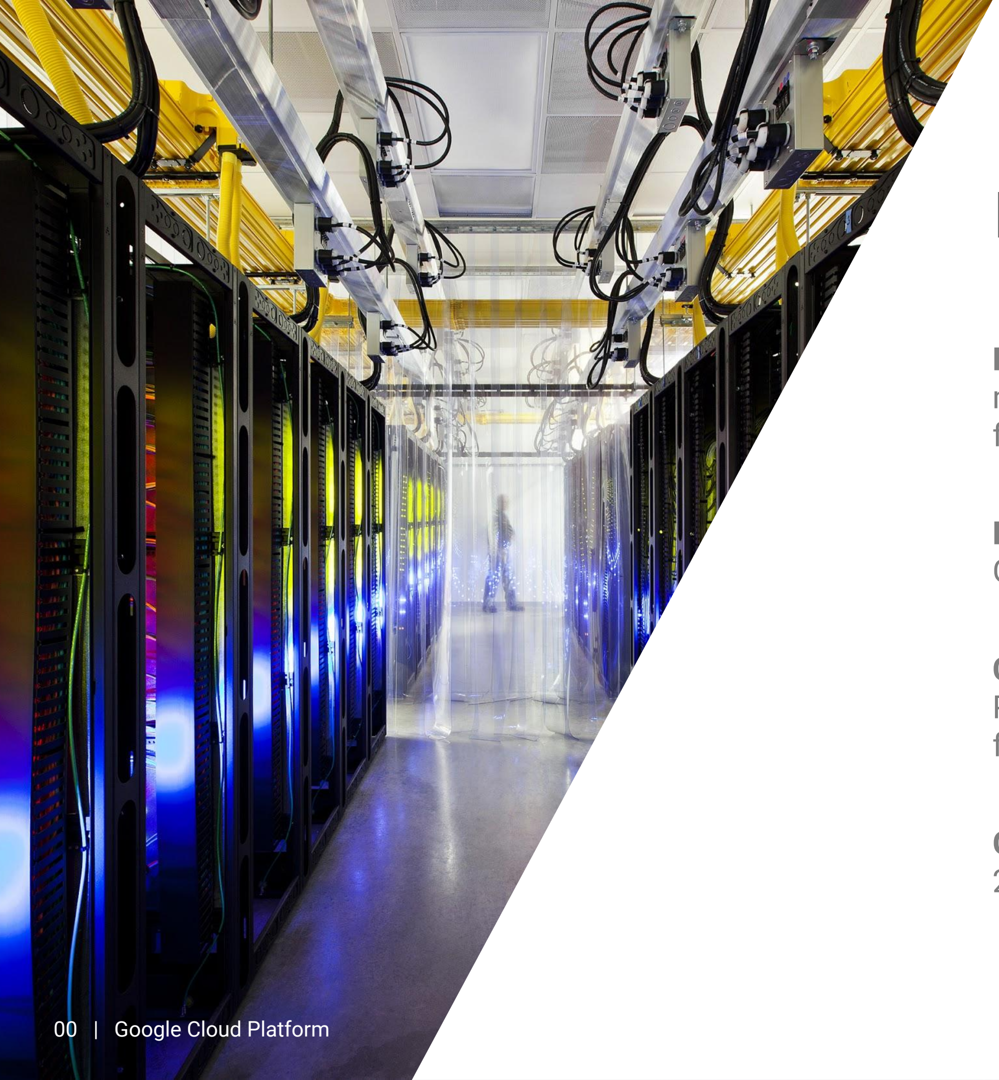
Compute

Data

Machine Learning

Academic / Research Programs

# Compute



# Infrastructure

**Lightning fast & scalable:** Fast VM startup time, millisecond access for all storage classes, high IOPS for VCPUs,  high bandwidth global networking

**Reliable**: Built-in redundancy and scale, live Migration, Google Site Reliability Engineering for your workload.

**Customer friendly pricing:** simple and efficient: Pay-per-second, custom VMs, automatic discounts, flexible buy-in-bulk discounts

**Geographic coverage:**  11 new regions in 2017-18 for a total of 17, HA in each region

- Significant “per core” performance improvements
- Intel® Advanced Vector Extension 51 (Intel® AVX-512)
    - 2x flops/second
- Accelerated IO with Intel® Omni-Path Architecture (Fabric)
- Integrated Intel® QuickAssist Technology (crypto & compression offload)
- Intel® Resource Director Technology (Intel® RDT) for Efficiency & TCO

Google Cloud Platform Blog

Product updates, customer stories, and tips and tricks on Google Cloud Platform

## Google Cloud Platform is the first cloud provider to offer Intel Skylake

Friday, February 24, 2017

By Urs Hölzle, Senior Vice President, Google Cloud Infrastructure

I’m excited to announce that Google Cloud Platform (GCP) is the first cloud provider to offer the next generation Intel Xeon processor, codenamed Skylake.

# Hardware Accelerated

- Available Today: **NVIDIA K80 GPU, P100s**
- Coming Soon: **Tensor Processing Unit (TPU)**
- Custom ASIC built and optimized for TensorFlow
- Used in production at Google for over 16 months
- 7 years ahead of GPU performance per watt

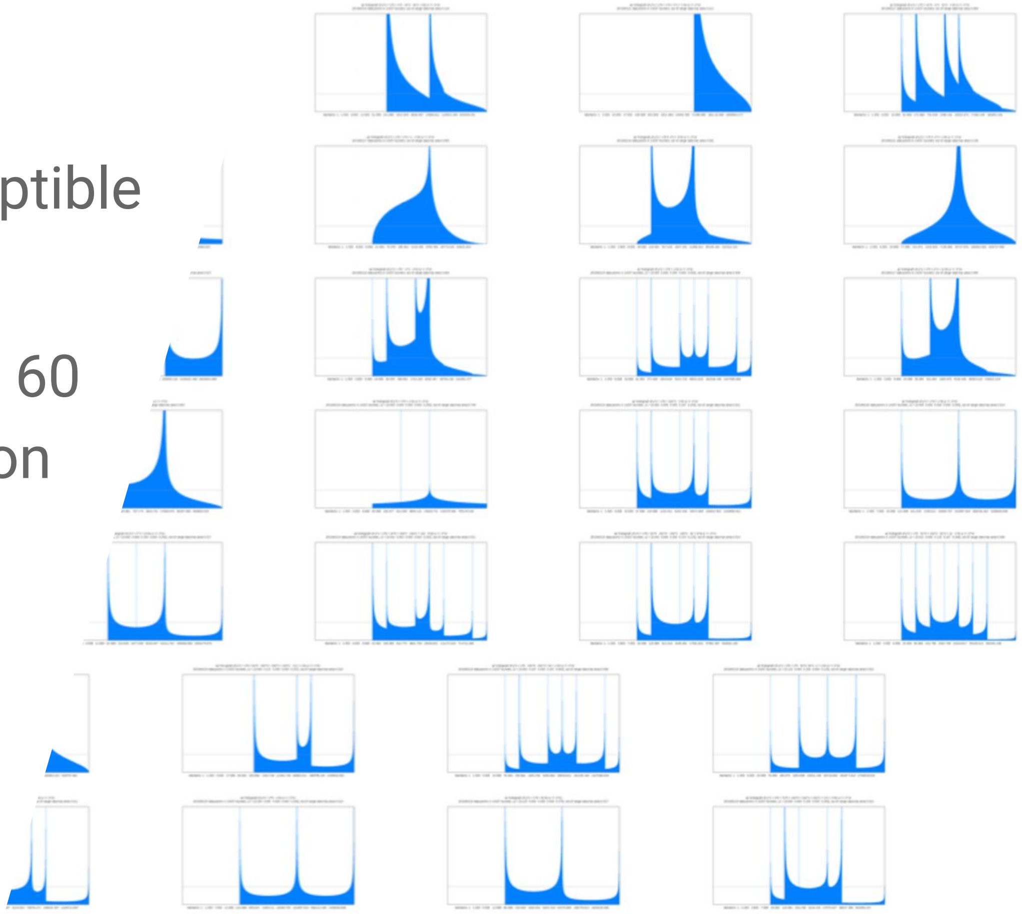
# MIT Research w/ VMs

580,000 cores

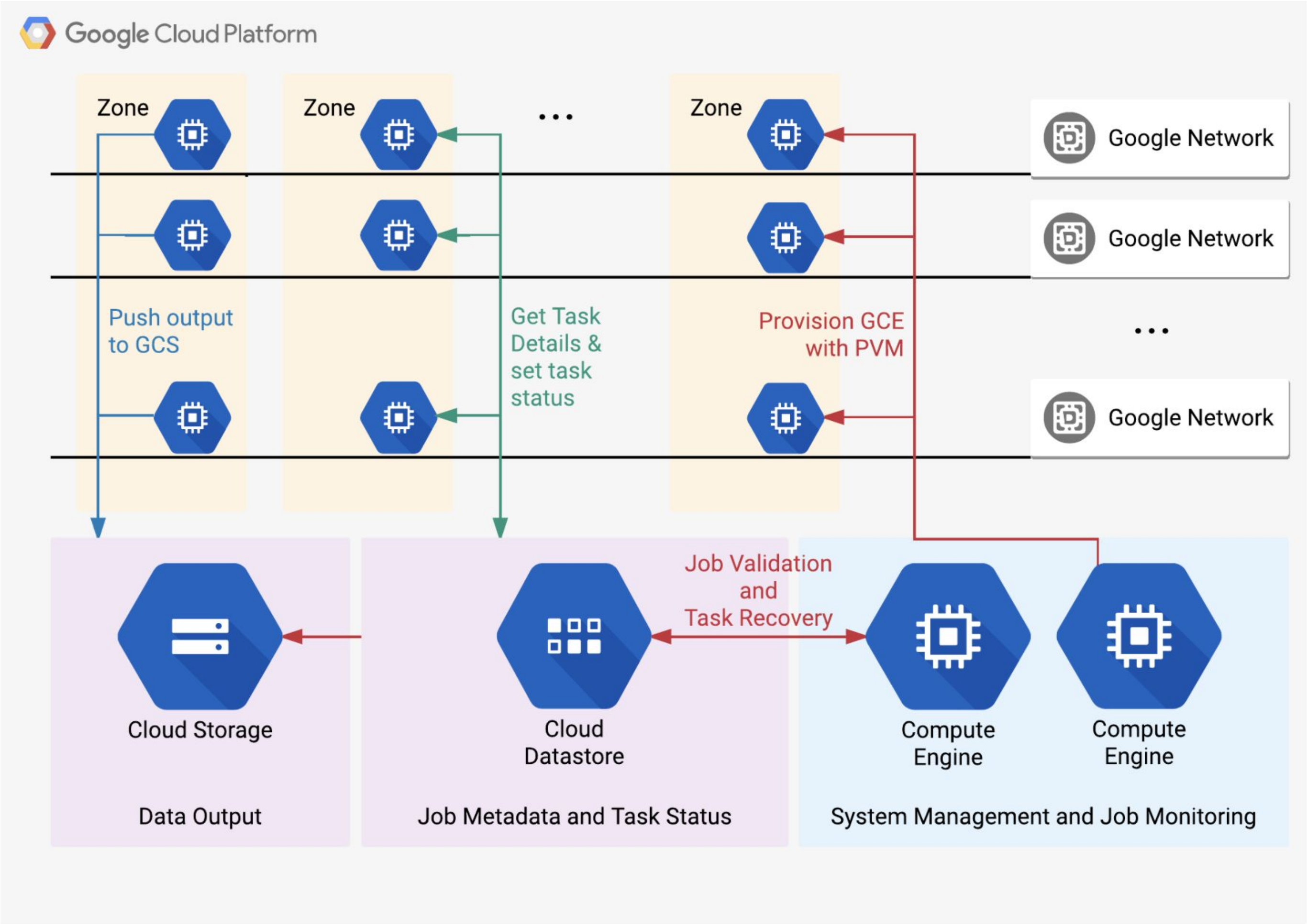
~~220,000~~ cores on preemptible VMs

2,250 32-core instances, 60 CPU-years of computation in a single afternoon

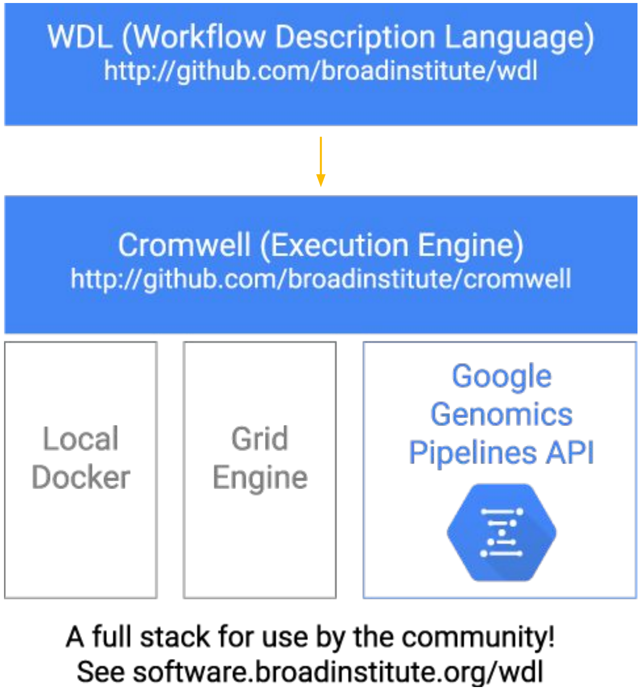
Answers in hours v. months



Products used: Google Compute Engine, Cloud Storage, DataStore


Google Cloud Platform
Zone
Zone
Zone
Google Network
Google Network
Google Network
Push output to GCS
Get Task Details & set task status
Provision GCE with PVM
Job Validation and Task Recovery
Cloud Storage
Cloud Datastore
Compute Engine
Compute Engine
Data Output
Job Metadata and Task Status
System Management and Job Monitoring

Broad Firecloud:
WDL, Cromwell and Google Genomics




WDL: an external DSL used by computational biologists to express the analytical pipelines

Cromwell: a scalable, robust engine for executing WDL against pluggable backends including local, Docker, Grid Engine or …

Google Genomics Pipelines API: co-developed by Broad and Google Genomics, a scalable Docker-as-a-Service with data scheduling

# Pipeline definition


```
{
  "name": "samtools index",
  "description": "Run samtools index to generate a BAM index file",
  "inputParameters": [
    {"name": "inputFile",
      "localCopy": {
        "disk": "data",
        "path": "input.bam"
      }
    },
    {"name": "outputFile",
      "localCopy": {
        "disk": "data",
        "path": "output.bam.bai"
      }
    },
  ],
  "resources": {
    "minimumCpuCores": 1,
    "minimumRamGb": 1,
    "disks": [{
      "name": "data",
      "type": "PERSISTENT_HDD"
      "sizeGb": 200,
      "mountPoint": "/mnt/data",
    }]
  },
  "docker": {
    "imageName": "quay.io/cancercollaboratory/dockstore-tool-samtools-index",
    "cmd": "samtools index /mnt/data/input.bam /mnt/data/output.bam.bai"
  }
}
```

# Create, run, monitor, and kill pipelines

## Create

```
$ gcloud alpha genomics pipelines create --pipeline-json-file PIPELINE-FILE.json --pipeline-json-file samtools_index.json
Created samtools index, id: PIPELINE-ID
```

## Run

```
$ gcloud alpha genomics pipelines run --pipeline_id PIPELINE-ID \
--logging gs://YOUR-BUCKET/YOUR-DIRECTORY/logs \
--inputs inputFile=gs://genomics-public-data/gatk-examples/example1/NA12878_chr22.bam \
--outputs outputFile=gs://YOUR-BUCKET/YOUR-DIRECTORY/output/NA12878_chr22.bam.bai
Running: operations/OPERATION-ID
```

## Status

```
$ gcloud alpha genomics operations describe OPERATION-ID
```

## Kill

```
$ gcloud alpha genomics operations cancel OPERATION-ID
```

# DSUB (google genomics pipelines)

Features Business Explore Pricing This repository Search Sign in or Sign up

googlegenomics / dsub

Watch 14 Star 16 Fork 4

Code Issues 11 Pull requests 0 Projects 0 Pulse Graphs

Branch: master dsub / README.md Find file Copy path

```
./dsub \
    --project my-cloud-project \
    --zones "us-*" \
    --logging gs://my-bucket/logs \
    --input BAM=gs://genomics-public-data/1000-genomes/bam/HG00114.mapped.ILLUMINA.bwa.GBR.low_covera
    --output BAI=gs://my-bucket/HG00114.mapped.ILLUMINA.bwa.GBR.low_coverage.20120522.bam.bai \
    --image quay.io/cancercollaboratory/dockstore-tool-samtools-index \
    --command 'samtools index ${BAM} ${BAI}' \
    --wait
```

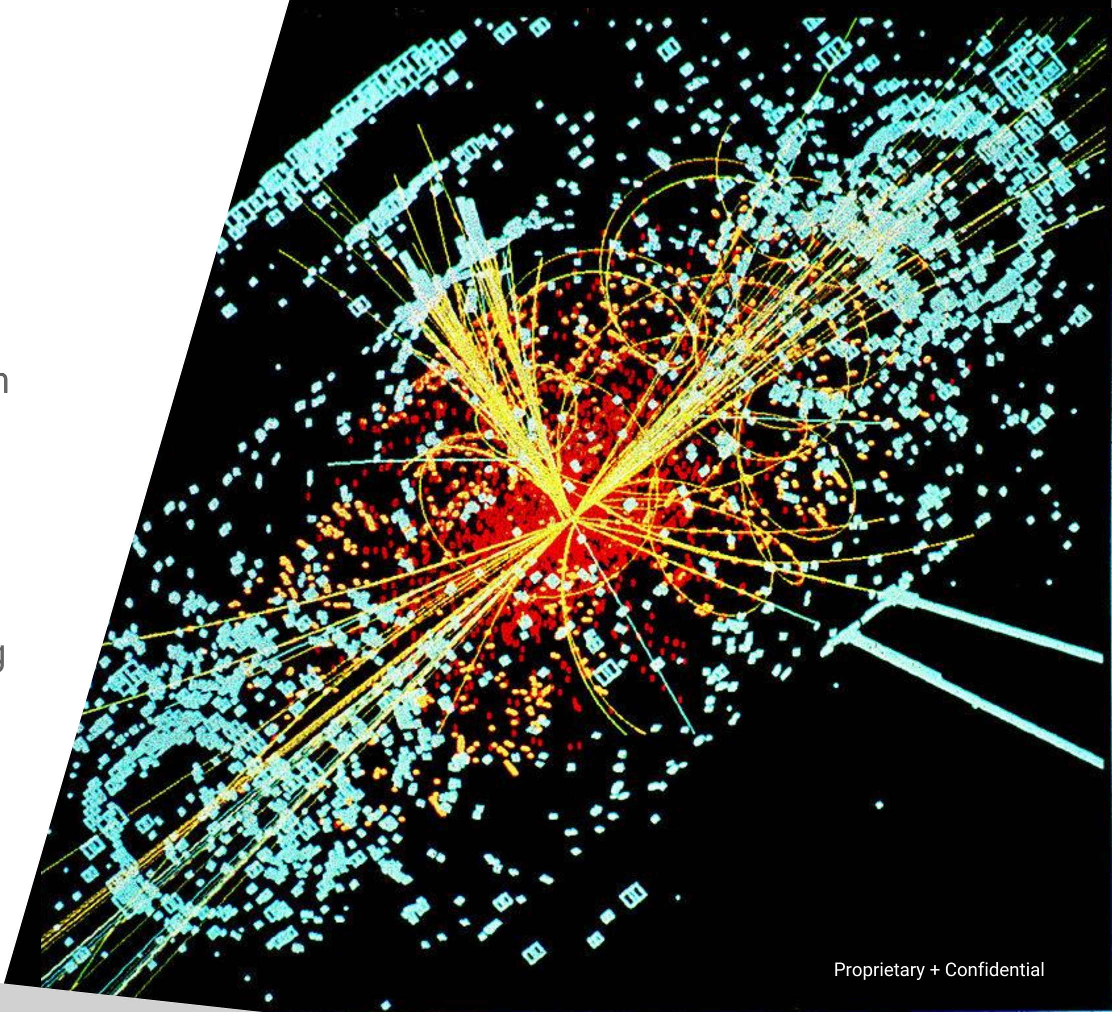
# SC16 CMS Demonstrator

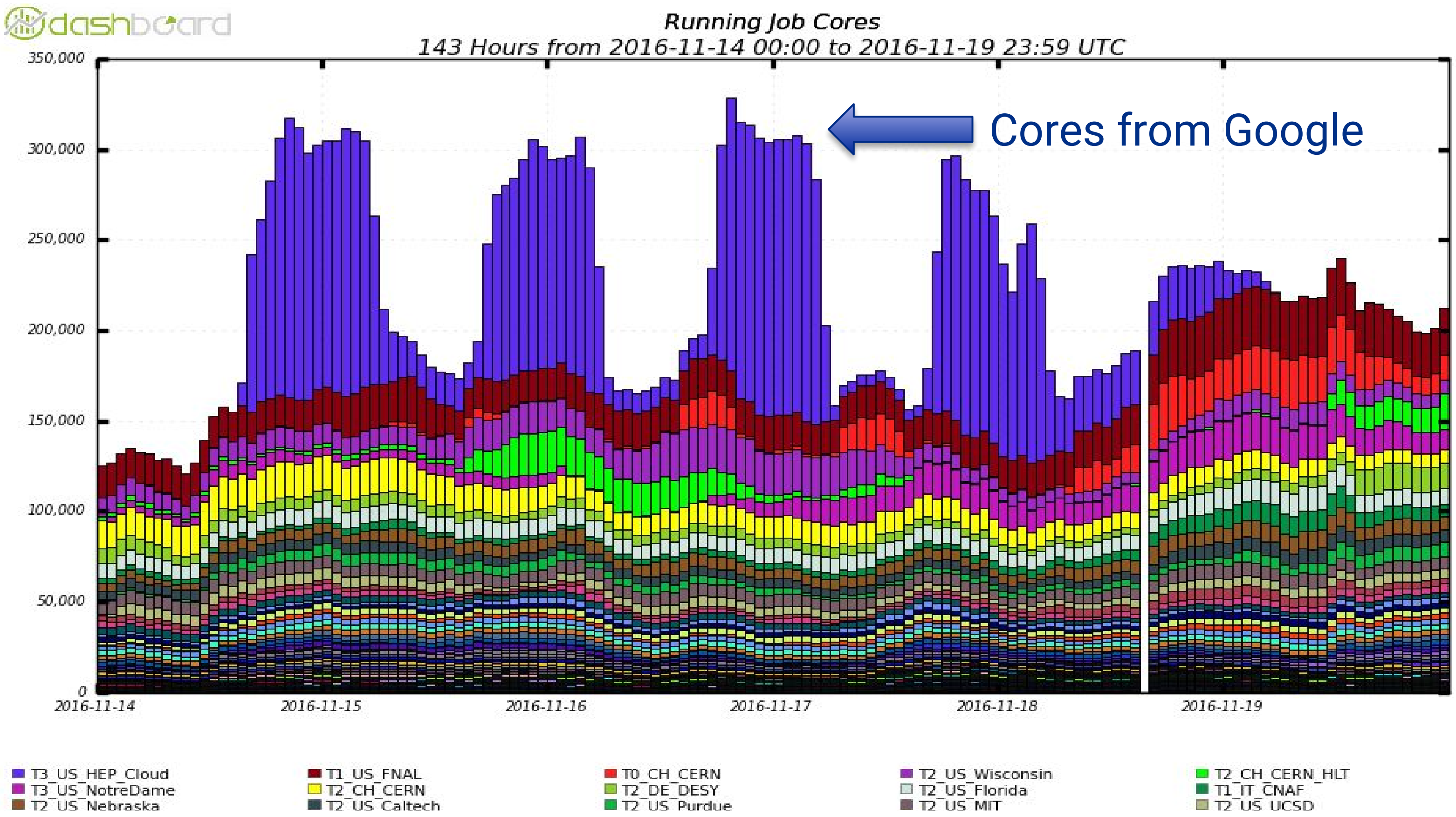
Target: generate 1 Billion events in 48 hours during Supercomputing 2016 on Google Cloud via HEPCloud

35% filter efficiency = stage out 380 million events → 150 TB output

Double the size of global CMS computing resources

CMS Higgs Event - credit: CERN
https://commons.wikimedia.org/wiki/File:CMS_Higgs-event.jpg




dashboard
Running Job Cores
143 Hours from 2016-11-14 00:00 to 2016-11-19 23:59 UTC
Cores from Google
350,000
300,000
250,000
200,000
150,000
100,000
50,000
0
2016-11-14
2016-11-15
2016-11-16
2016-11-17
2016-11-18
2016-11-19
T3_US_HEP_Cloud
T1_US_FNAL
T0_CH_CERN
T2_US_Wisconsin
T2_CH_CERN_HLT
T3_US_NotreDame
T2_CH_CERN
T2_DE_DESY
T2_US_Florida
T1_IT_CNAF
T2_US_Nebraska
T2_US_Caltech
T2_US_Purdue
T2_US_MIT
T2_US_UCSD

# On-prem vs. Cloud

Average cost per core-hour (~25% error)

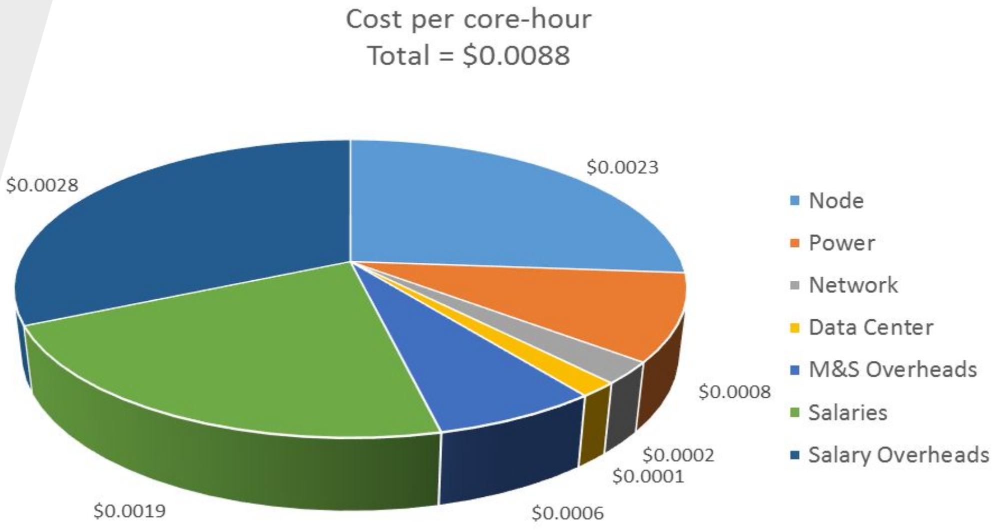
- On-premises Fermilab:
  0.9 cents per core-hour
  (assumes 100% utilization)
- Google Cloud:
  1.6 cents per core-hour
  (comparable to other vendors)

Fermilab has years of experience in optimizing its facility

Cloud costs larger, but approaching equivalence

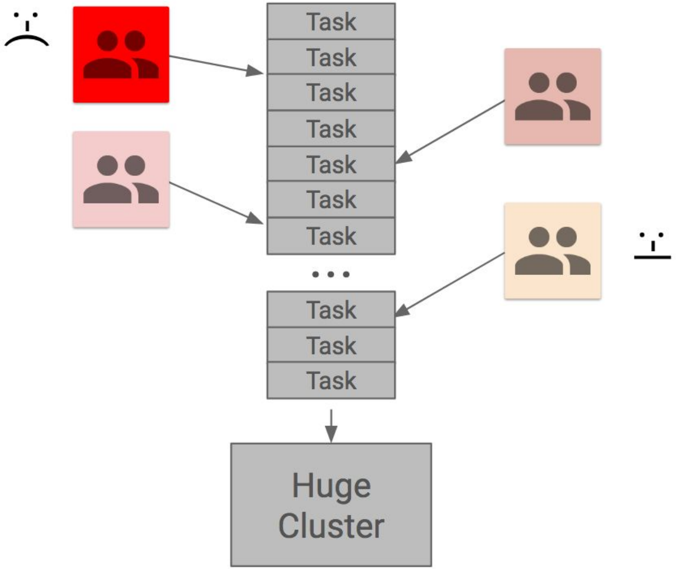
Considered well worth the cost of adding 160,000 core in a few hours

## Fermilab CMS Tier1 Costs

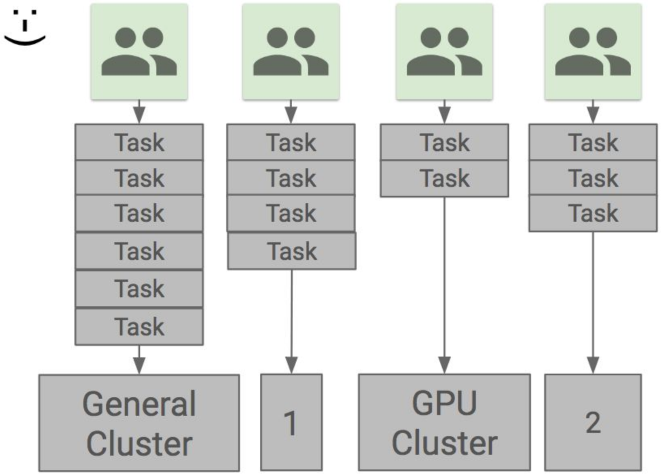


# Task Tailored Resources

**On-prem**: One cluster, one queue, one size fits all hardware, angry users.




**In the cloud**: Tailored clusters, less queue sharing, happy users.




1 - n1-highcpu-16, Preemptible VM Cluster
2 - n1-highmem-32 Cluster

# Preemptible VM Instances

- **What Preemptible VMs are**
  - Up to 80% cheaper than regular VMs. (~$0.01 per core hour)
  - Very easy to use -- just flip one switch in the UI, API or command line
  - Many of our biggest customers run huge clusters (10k+ cores) with great success and savings.

- **Things to keep in mind**
  - Same great disk, OS images and network
  - Google Compute Engine can *preempt* (i.e. shutdown/take-away) the VM with 30 seconds of notice
  - Maximum 24 hours of uptime
  - No SLAs or guarantees of any kind but we historically see preemption rates of 5-15%

# Data

# Fully Managed Storage & Database Services

| Object | Key-value | Non-relational | | Relational | | Warehouse |
|---|---|---|---|---|---|---|
| **Cloud Storage** | **App Engine Memcache** | **Cloud Datastore** | **Cloud Bigtable** | **Cloud SQL** | **Cloud Spanner** | **BigQuery** |
| Binary or object data | Web/mobile applications, gaming | Hierarchical, mobile, web | Heavy read + write, events | Web frameworks | RDBMS+scale, HA, HTAP | Enterprise Data Warehouse |
| Images, Media serving, backups | Game state, user sessions | User profiles, Game State | AdTech, Financial, IoT | CMS, eCommerce | Transactions, Ad/Fin/MarTech | Analytics, Dashboards |

# Block storage

Reliable, high-performance block storage for any GCE VM instance

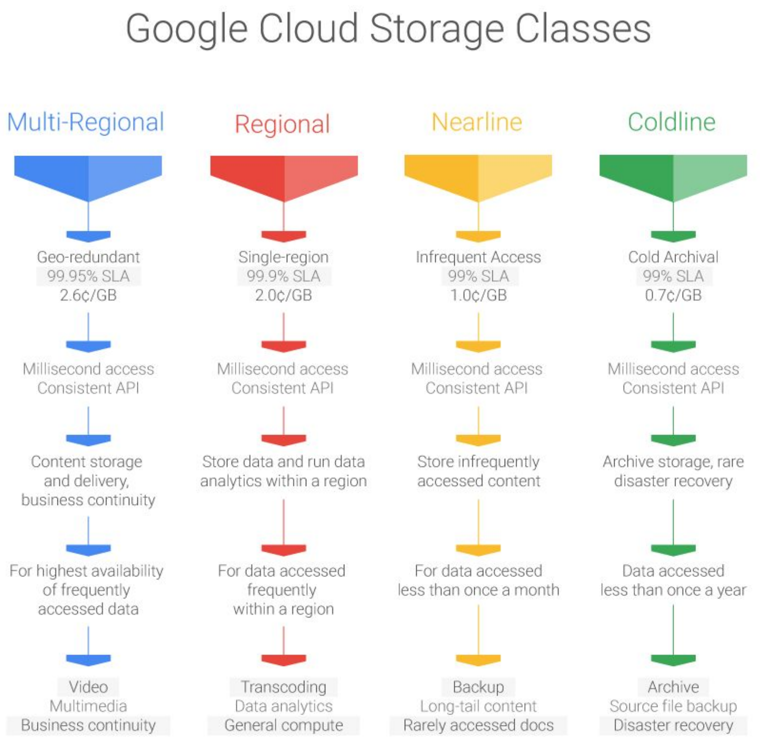
| | **Local SSD**<br>Fastest, Attached, Ephemeral | **Persistent Disk: SSD**<br>Fast, Persistent, Durable, Remote | **Persistent Disk: HDD**<br>Cheapest, Persistent, Durable, Remote |
|---|---|---|---|
| **Target scenarios** | - High-performance scratch space. Frequently accessed data.<br>- Excellent for scientific workloads, especially when combined with fast compute VMs like GPU instances | - Latency sensitive applications and files.<br>- High performance database and enterprise applications<br>- Databases | - Large data processing workloads<br>- Latency incentive tasks with lots of data: Genomics processing, video transcoding in GCE |
| **Features** | - Ephemeral storage<br>- Highest-performance ($0.218 GB)<br>- **IOPS:** 680k read / 360k write | - Persistent storage<br>- Performance sensitive ($0.17GB)<br>- **IOPS:** up to 40k read / 30k write | - Persistent storage<br>- Cost sensitive ($.04 GB)<br>- **IOPS:** 3k read / 15k write |
| | Encryption<br>3TB - 375 GB per partition, up to 8 partitions | Encryption, Snapshots<br>64 TB, Disk Size sets performance<br>(Attach larger VMs for max SSD performance) | |

# GCS: Object/Blob store

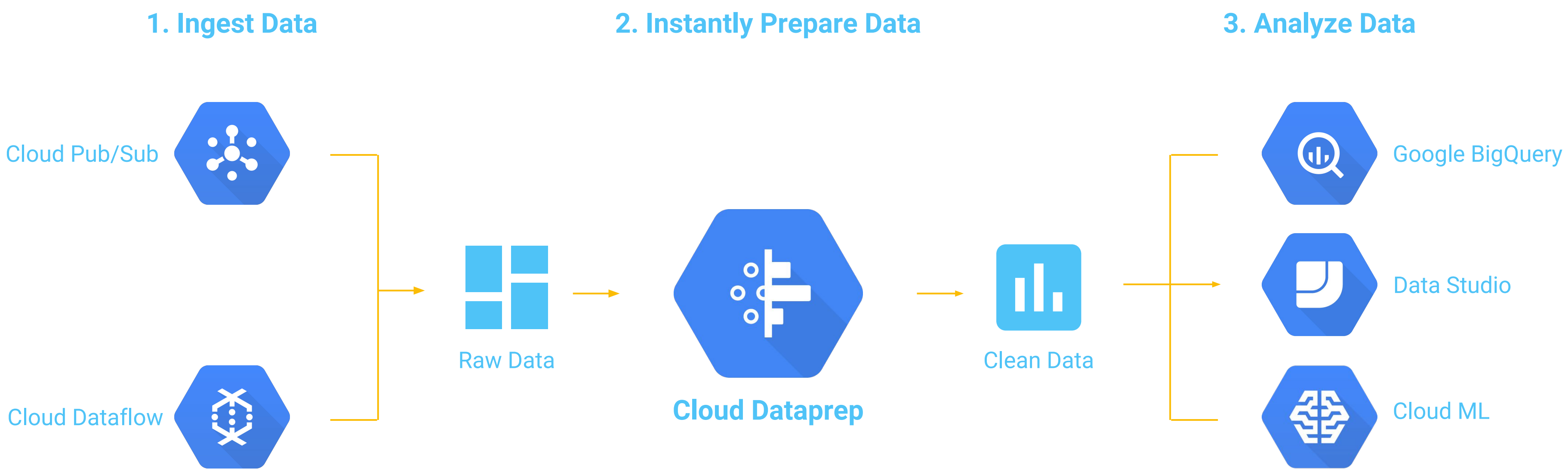
- Google Cloud Storage is a scalable object storage service suitable for all kinds of unstructured data

- **Cloud Storage vs Perst. Disk:**
    - Scales to exabytes
    - Accessible from anywhere; REST interface
    - Higher latency than PD
    - Write semantics include insert and overwrite file only
    - Offers versioning
    - Cheaper - put your data here until you need it

- Lots of guidelines on picking storage on our site



# Data Prep


1. Ingest Data
2. Instantly Prepare Data
3. Analyze Data
Cloud Pub/Sub
Cloud Dataflow
Raw Data
Cloud Dataprep
Clean Data
Google BigQuery
Data Studio
Cloud ML

# Cloud Dataprep

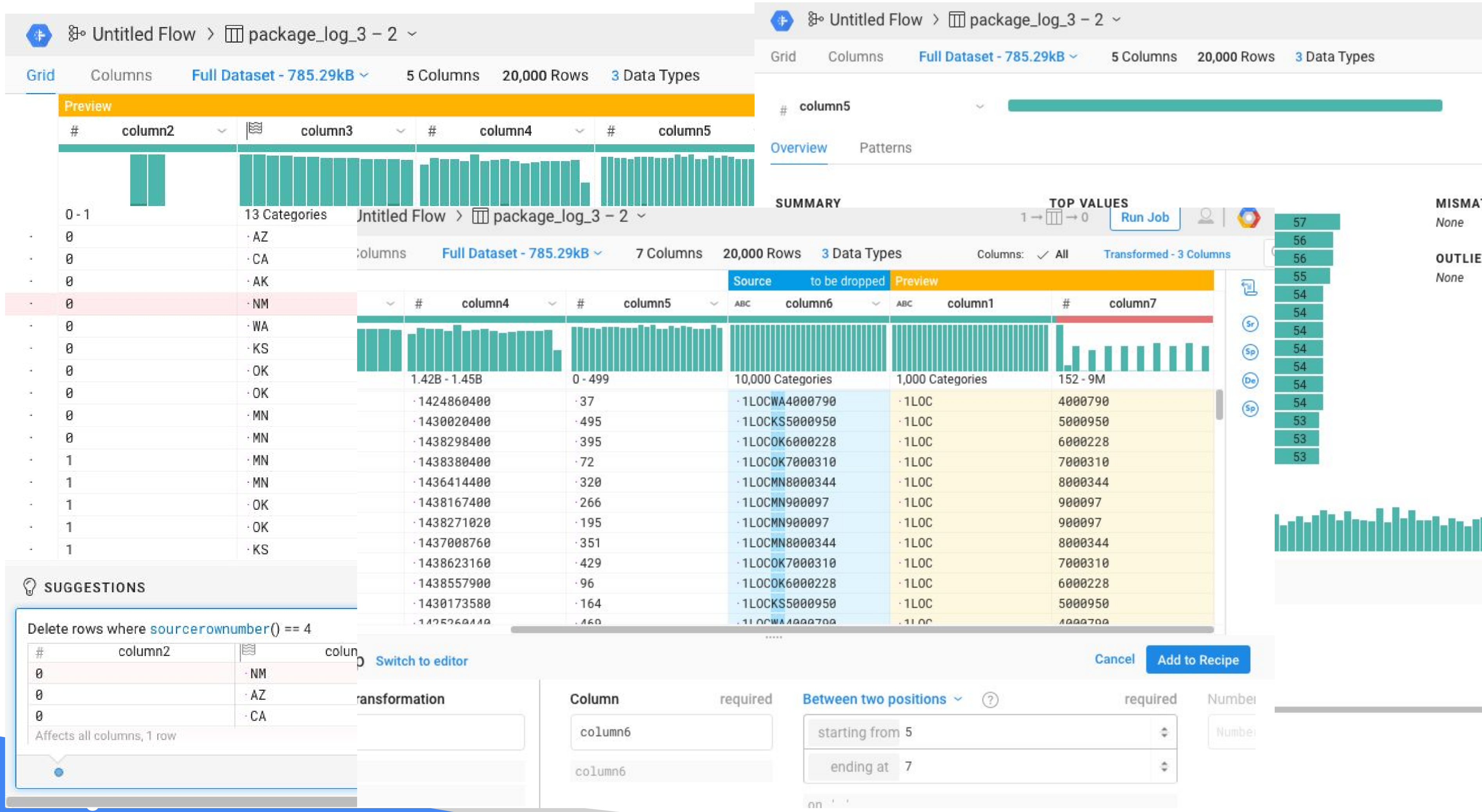
**Instant Data Exploration**
Visually explore and interact with data in seconds. Instantly understand data distribution and patterns. There is no need for one to write code. You can prepare data with a few clicks.

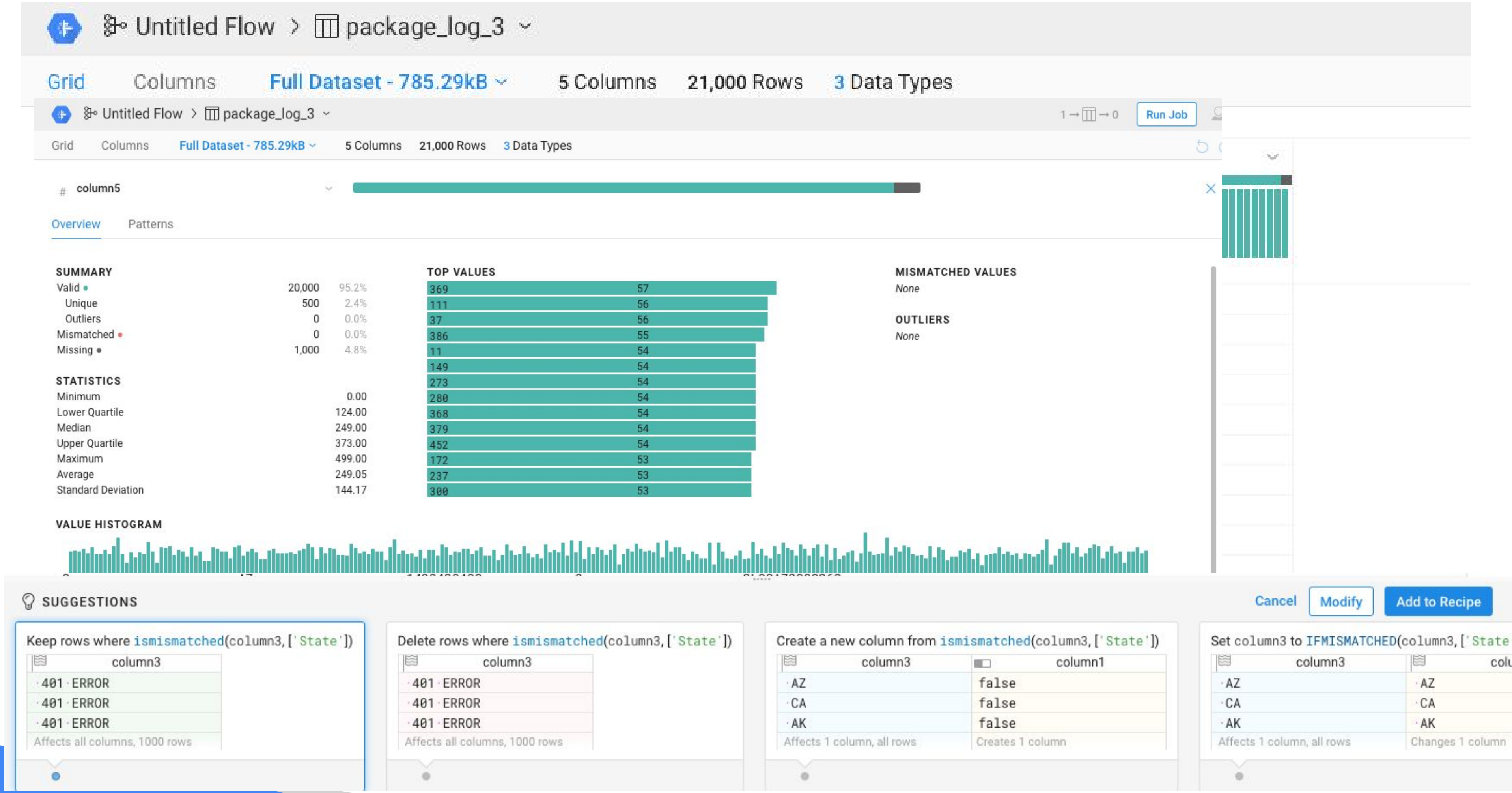
**Intelligent Data Cleansing**
Cloud Dataprep automatically identifies data anomalies and helps you to take corrective actions fast. Get data transformation suggestions based on your usage pattern. Standardize, structure, and join datasets easily with a guided approach.

**Serverless**
Cloud Dataprep is a serverless service, so you do not need to create or manage infrastructure.

**Seriously Powerful**
Cloud Dataprep is built on top of powerful Google Cloud Dataflow service. Cloud Dataprep is auto-scalable and can easily handle processing massive data sets.

**Supports Common Data Sources of Any Size**
Process diverse datasets - structured and unstructured. Transform data stored in CSV, JSON, or relational Table formats. Prepare datasets of any size, megabytes to terabytes, with equal ease.


Untitled Flow > package_log_3 – 2
Grid
Columns
Full Dataset - 785.29kB
5 Columns
20,000 Rows
3 Data Types
Preview
column2
column3
column4
column5
0 - 1
13 Categories
0
AZ
CA
AK
NM
WA
KS
OK
MN
1
SUGGESTIONS
Delete rows where sourcerownumber() == 4
Affects all columns, 1 row
column5
Overview
Patterns
SUMMARY
TOP VALUES
MISMA
None
OUTLIE
None
57
56
55
54
53
Run Job
7 Columns
Columns: All
Transformed - 3 Columns
Source
to be dropped
column6
column1
column7
1.42B - 1.45B
0 - 499
10,000 Categories
1,000 Categories
152 - 9M
1424860400
1430020400
1438298400
1438380400
1436414400
1438167400
1438271020
1437008760
1438623160
1438557900
1430173580
37
495
395
72
320
266
195
351
429
96
164
1LOCWA4000790
1LOCKS5000950
1LOCOK6000228
1LOCOK7000310
1LOCMN8000344
1LOCMN900097
1LOC
4000790
5000950
6000228
7000310
8000344
900097
Switch to editor
Cancel
Add to Recipe
ransformation
Column
required
Between two positions
starting from 5
ending at 7


Untitled Flow > package_log_3
Grid Columns Full Dataset - 785.29kB 5 Columns 21,000 Rows 3 Data Types
Untitled Flow > package_log_3
Run Job
Grid Columns Full Dataset - 785.29kB 5 Columns 21,000 Rows 3 Data Types
column5
Overview Patterns
SUMMARY
Valid 20,000 95.2%
Unique 500 2.4%
Outliers 0 0.0%
Mismatched 0 0.0%
Missing 1,000 4.8%
STATISTICS
Minimum 0.00
Lower Quartile 124.00
Median 249.00
Upper Quartile 373.00
Maximum 499.00
Average 249.05
Standard Deviation 144.17
TOP VALUES
369 57
111 56
37 56
386 55
11 54
149 54
273 54
280 54
368 54
379 54
452 54
172 53
237 53
300 53
MISMATCHED VALUES
None
OUTLIERS
None
VALUE HISTOGRAM
SUGGESTIONS
Cancel
Modify
Add to Recipe
Keep rows where ismismatched(column3, ['State'])
column3
401 ERROR
401 ERROR
401 ERROR
Affects all columns, 1000 rows
Delete rows where ismismatched(column3, ['State'])
column3
401 ERROR
401 ERROR
401 ERROR
Affects all columns, 1000 rows
Create a new column from ismismatched(column3, ['State'])
column3 column1
AZ false
CA false
AK false
Affects 1 column, all rows
Creates 1 column
Set column3 to IFMISMATCHED(column3, ['State
column3
AZ
CA
AK
Affects 1 column, all rows
Changes 1 column

# Machine Learning

# Two flavors of machine learning

API

Vision

Translation

Speech BETA

Natural Language

## Pre-Trained Models

Storage

BigQuery

Datalab

TF

Tensor Flow

Pipelines

Model Management

## Build Your Own Model

# Google Cloud Machine Learning Services

cloud.google.com/translate/

Enter a word or phrase: Hello world
Translate from: English
Translate to: Albanian
TRANSLATE

cloud.google.com/natural-language/

Try the API

Google, headquartered in Mountain View, unveiled the new Android phone at the Consumer Electronic Show. Sundar Pichai said in his keynote that users love their new Android phones.

ANALYZE

Enter text in English, Spanish or Japanese

cloud.google.com/vision/

Try the API

Drag image file here or
Browse from your computer

cloud.google.com/speech/

Convert your voice to text right now

Click on the microphone icon to start recording

English (United States)

# Cloud ML Engine

- **PaaS** for Tensorflow
- **Scale** your training up to 100 workers
- Automatic **monitoring** and **logging**
- Easy  transition from training to **prediction**
- Built in model **version management**
- **No lock-in.** Option to download your trained models for on-premise or mobile deployment

# CloudML is part of a bigger picture

## Capture
Pub/Sub

## Store
Cloud Storage

BigQuery

Cloud SQL

Datastore

BigTable

## Process
Dataflow
Dataproc

## Analyze
BigQuery

Dataflow

Datalab

## Insight
Cloud ML Engine

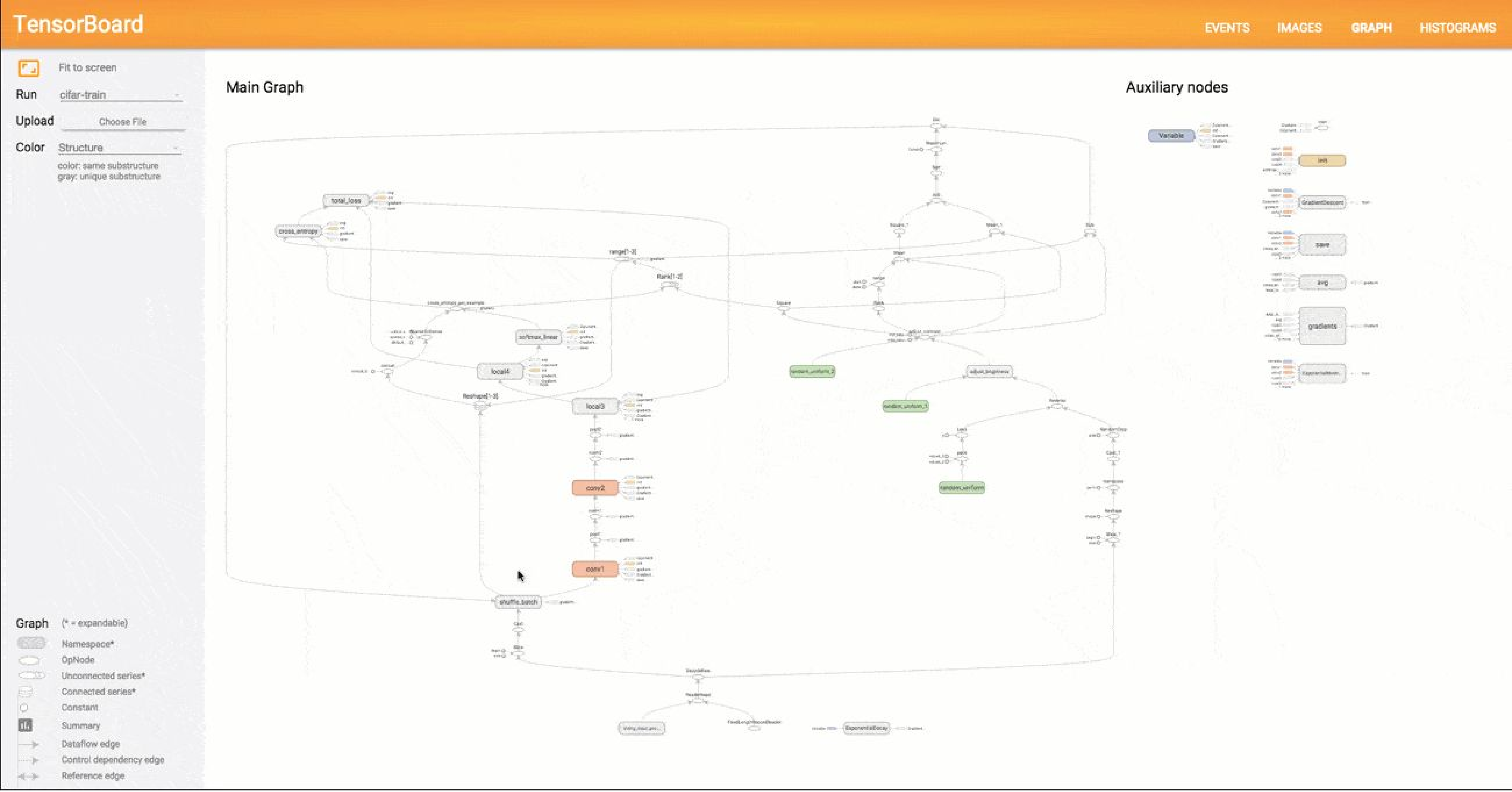
# TensorFlow

- World's most popular ML framework
- Developer friendly yet performance optimized
- **Powers over 100 Google services**
- Managed infrastructure with Cloud ML
- Tutorials at https://www.tensorflow.org

# Linear Regression VS Neural Network

```python
import tensorflow as tf

#Define input feature columns
sq_footage = tf.contrib.layers.real_valued_column("sq_footage")
feature_columns = [sq_footage]

#Define input function
def input_fn(feature_data,label_data=None):
  return {"sq_footage":feature_data}, label_data

#Instantiate Linear Regression Model
estimator = tf.contrib.learn.LinearRegressor(
  feature_columns=feature_columns,
  optimizer=tf.train.FtrlOptimizer(learning_rate=100))

#Train
estimator.fit(
  input_fn=lambda:input_fn(tf.constant([1000,2000]),
                           tf.constant([100000,200000])),
  steps=100)

#Predict
estimator.predict(input_fn=lambda: input_fn(tf.constant([3000])))
```

```python
import tensorflow as tf

#Define input feature columns
sq_footage = tf.contrib.layers.real_valued_column("sq_footage")
feature_columns = [sq_footage]

#Define input function
def input_fn(feature_data,label_data=None):
  return {"sq_footage":feature_data}, label_data

#Instantiate Neural Network Model
estimator = tf.contrib.learn.DNNRegressor(
  feature_columns=feature_columns, hidden_units=[10,10])


#Train
estimator.fit(
  input_fn=lambda:input_fn(tf.constant([1000,2000]),
                           tf.constant([100000,200000])),
  steps=100)

#Predict
estimator.predict(input_fn=lambda: input_fn(tf.constant([3000])))
```


TensorBoard
EVENTS
IMAGES
GRAPH
HISTOGRAMS
Fit to screen
Run
cifar-train
Upload
Choose File
Color
Structure
color: same substructure
gray: unique substructure
Main Graph
Auxiliary nodes
total_loss
cross_entropy
softmax_linear
local4
local3
conv2
conv1
shuffle_batch
adjust_brightness
Variable
init
GradientDescent
save
avg
gradients
Graph
(* = expandable)
Namespace*
OpNode
Unconnected series*
Connected series*
Constant
Summary
Dataflow edge
Control dependency edge
Reference edge

Google Cloud Datalab Cop

Notebook ▾ Add Code

# Copy Number se

The goal of this notebook is to in

This table contains all available T
Genome Wide SNP6 array, as of
recent archives (eg`broad.mit.`
types was downloaded from the
Each of these segmentation files
During ETL the sample identifer
the SDRF file in the associated m

In order to work with BigQuery,
the name(s) of the table(s) you a

```
import gcp.bigquery a
cn_BQtable = bq.Table
```

From now on, we will refer to thi
table name each time.

Let's start by taking a look at the

```
%bigquery schema --ta
```

| name | type |
|---|---|
| ParticipantBarcode | STRII |
| SampleBarcode | STRII |
| SampleTypeLetterCode | STRII |
| AliquotBarcode | STRII |
| Study | STRII |
| Platform | STRII |
| Chromosome | STRII |
| Start | INTE( |
| End | INTE( |
| Num_Probes | INTE( |
| Segment_Mean | FLOA |

Unlike most other molecular dat
microRNAs, this data is produce
sizes and positions of these segn

Google Cloud Datalab Copy Number segmen

Notebook ▾ Add Co

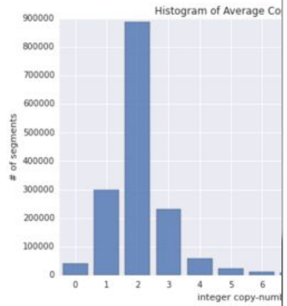
Now we'll use matplotlib to create some simple visual

```
import numpy as np
import matplotlib.pyplot as plt
```

For the segment means, let's invert the log-transform

```
%%sql --module getCNhist

SELECT
  lin_bin,
  COUNT(*) AS n
FROM (
  SELECT
    Segment_Mean,
    (2.*POW(2,Segment_Mean)) AS lin_
    INTEGER(((2.*POW(2,Segment_Mean)
  FROM
    $t
  WHERE
    ( (End-Start+1)>1000 AND SampleT
GROUP BY
  lin_bin
HAVING
  ( n > 2000 )
ORDER BY
  lin_bin ASC
```

```
CNhist = bq.Query(getCNhist,t=cn_BQt
bar_width=0.80
plt.bar(CNhist['lin_bin']+0.1,CNhist
plt.xticks(CNhist['lin_bin']+0.5,CNh
plt.title('Histogram of Average Copy
plt.ylabel('# of segments');
plt.xlabel('integer copy-number');
```




The histogram illustrates that the vast majority of the
either side representing deletions (left) and amplificat

Google Cloud Datalab Copy Number segmen

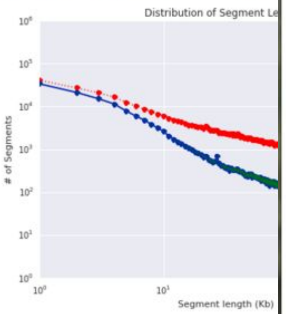
Notebook ▾ Add Co

```
  bin
ORDER BY
  bin ASC
```

```
%%sql --module getSLhist_1k_amp

SELECT
  bin,
  COUNT(*) AS n
FROM (
  SELECT
    (END-Start+1) AS segLength,
    INTEGER((END-Start+1)/1000) AS b
  FROM
    $t
  WHERE
    (END-Start+1)<1000000 AND Sample
GROUP BY
  bin
ORDER BY
  bin ASC
```

```
SLhistDel = bq.Query(getSLhist_1k_de
SLhistAmp = bq.Query(getSLhist_1k_am
```

```
plt.plot(SLhist_1k['bin'],SLhist_1k[
plt.plot(SLhistDel['bin'],SLhistDel[
plt.plot(SLhistAmp['bin'],SLhistDel[
plt.xscale('log');
plt.yscale('log');
plt.xlabel('Segment length (Kb)');
plt.ylabel('# of Segments');
plt.title('Distribution of Segment L
```




The amplification and deletion distributions are nearly
from this graph that a majority of the segments less th
lengths >100Kb are copy-number neutral.

Google Cloud Datalab Copy Number segments (autosaved)

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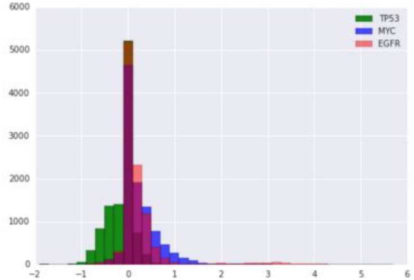
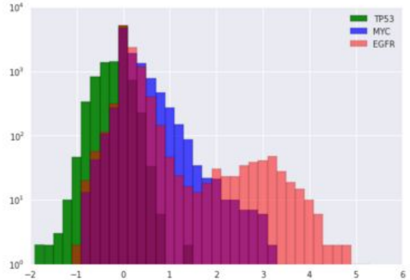
And now we'll take a look at histograms of the average copy-number for these three genes. TP53 (in green) shows a significant number of partial deletions (CN<0), while MYC (in blue) shows some partial amplifications -- more frequently than EGFR, while EGFR (pale red) shows a few extreme amplifications (log2(CN/2) > 2). The final figure shows the same histograms on a semi-log plot to bring up the rarer events.

```
binWidth = 0.2
binVals = np.arange(-2+(binWidth/2.), 6-(binWidth/2.), binWidth)
plt.hist(tp53CN['avgCN'],bins=binVals,normed=False,color='green',alpha=0.9,label='TP53');
plt.hist(mycCN ['avgCN'],bins=binVals,normed=False,color='blue',alpha=0.7,label='MYC');
plt.hist(egfrCN['avgCN'],bins=binVals,normed=False,color='red',alpha=0.5,label='EGFR');
plt.legend(loc='upper right');
```




```
plt.hist(tp53CN['avgCN'],bins=binVals,normed=False,color='green',alpha=0.9,label='TP53');
plt.hist(mycCN ['avgCN'],bins=binVals,normed=False,color='blue',alpha=0.7,label='MYC');
plt.hist(egfrCN['avgCN'],bins=binVals,normed=False,color='red',alpha=0.5,label='EGFR');
plt.yscale('log');
plt.legend(loc='upper right');
```



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- National Institutes of Health
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| 1 TB<br>Queries per month | Basic Cluster<br>Sized 5 nodes or fewer | 5 GB-Months<br>Regional storage | 28<br>Instance hours per day<br>5 GB<br>Cloud Storage |

Google Cloud Public Datasets Program

**Mission:**
Facilitate the onboarding of datasets into Google Cloud products

# Thank you

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