Introduction to Scientific Computing I

Amir Farbin

What is Data Science?

- From *Wikipedia*: Data science is an interdisciplinary field that uses scientific methods, processes, algorithms and systems to extract knowledge and insights from data in various forms…

- There are concepts that unify statistics, data analysis, machine learning, …

- Take techniques from mathematics, statistics, information science, and computer science

- Apply it to a domain:

  - science: biology, physics, psychology, …

  - business analytics, …

Data Science @ UTA

- College of Science is in the process of getting approval for undergraduate BA and BS degrees in Data Science.

- Tentative New Courses:

    - DATA 1301: Introduction to Data Science
    - DATA 1401/2: Introduction to Scientific Computing 1 and 2
    - DATA 34xx: Data Mining, Management, and Curation
    - DATA 34xx: Statistical Modeling
    - DATA 34xx: Simulation
    - DATA 34xx: Machine Learning
    - DATA 43xx: Data Problems
    - DATA 43xx: Data Capstone Project 1 and 2

Logistics

- ***Lectures***: Monday/Wednesday
    - No official Textbook. Unique class. Not following an existing paradigm.
        - Lecture and labs are essential.
        - Welcome to use any python book as a reference.
        - We will learn to use online docs as resource.
        - ***Quizzes*** (10%): Short and Easy. “Pop”: Randomly scheduled. Meant mostly as attendance tool.
            - Drop 2 lowest grades (including being sick, unless previously made arrangements).
- **Lab** (40%) Friday
    - Hands-on: I’ll walk through something.
    - **Lab**: (10%) has to be accomplished in during the session (maybe end of day).
    - **Homework** (30%): Remainder is general is “Homework”. Due by following lab session.
- 3 **Exams** (30%): During lab session. Similar to Homework. Drop 1 lowest grade. No makeups.
- **Final** (20%): Comprehensive… similar to homework.

Logistics (2)

- Homework Policy
    - You can work with others, but do not copy/paste code from another student.
    - Submitted via git (Version Control System).
- Help
    - ***Clinic***: We are hiring a TA. Intend to have three, 3-hour sessions a week (TBA), where you can ask for help.
        - ***Office Hours*****:** Open door policy. Generally at UTA MWF after (class) 12 pm. Best to let me know after class or e-mail.
- ***Laptop*** (with a physical keyboard).
    - Need to have a laptop for this class
        - Doesn’t matter what OS you run… all you need is a browser.
    - If you don’t have a laptop, you can rent one. Details by Wednesday.
- We will use TACC (Texas Advanced Computing Center) for all of the coursework.
- First lab (this Friday), will be to get setup.

Topics

- Computer System Basics:
    - CPU, GPU (co-processor), RAM, Hard Drive/SSD, OS, cache, memory hierarchy
    - Base-n numbers, ASCII vs binary, high-level vs machine code,
    - Networking(TCP/IP), HTTP, FTP, terminal, SSH,
    - Shell, filesystem, IO (Disk vs RAM), text editor, IDE
- Math (limited and in context)
    - Probability Theory: Distributions, Bayes Theorem, …
    - Linear Algebra
    - Numerical Methods
- Programming Concepts
    - Compiler vs interpreter, history of programming languages, code structures (arrays, etc)
    - Programming constructs: If, loop, functions, ...
    - Functional programming
    - Object-oriented programming
- Data
    - Structures: Array, Linked List, Stack, Queue, Binary Tree, Binary Search Tree, Heap, Hashing, Graph, Matrix, Advanced Data Structures, ...
    - Storage formats: CSV, H5, …
    - Data Manipulation and Mining
    - Tools: Pandas
- Data Science Concepts
    - Matrix / Tensor operations
    - Histograms
    - Classification
    - Regression
    - Tools: numpy, scikit-learn,
- Algorithmic thinking
    - Time and space complexity (“Big O” notation and analysis of algorithms)
    - Sort
    - Graph algorithms

Style

- Really a Python Programming Class taught from a Data Science perspective.
- Introduce and then reinforce data science concepts through successively more advanced implementations each introducing new programming techniques and culminating in use of advanced libraries.
- For example,
  - Learn about distributions and histogram
  - Example: Construct histograms
    - by hand
    - procedurally
    - write histogramming functions
    - write histogramming object oriented classes
    - use standard libraries that provide histogramming

What do *I* do ?

Was the Universe an Accident?

Artificial Intelligence may find the answer in data from the Large Hadron Collider

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UNIVERSITY OF TEXAS ARLINGTON

ATLAS EXPERIMENT

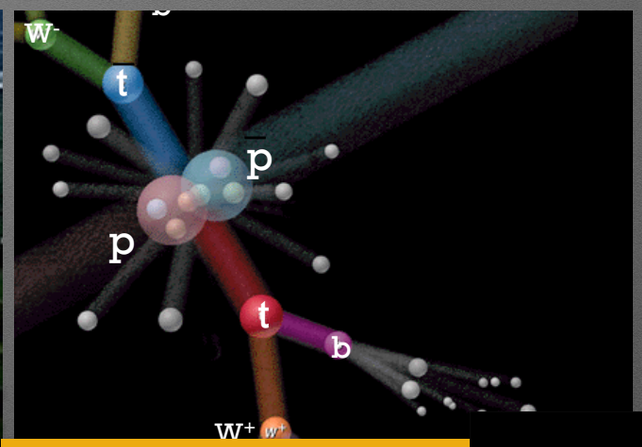
DUNE DEEP UNDERGROUND NEUTRINO EXPERIMENT

What is HEP ?

Large Hadron Collider (LHC)

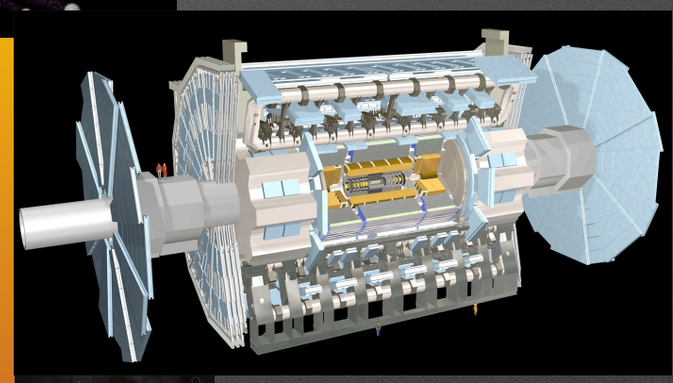
Largest Machine Ever Built

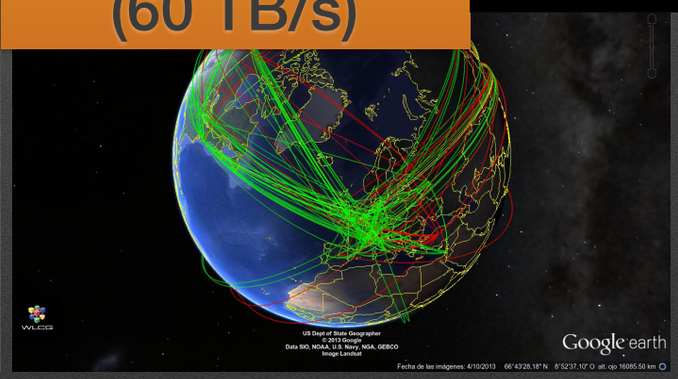
10^{11} Protons Collide 40 Million Times per Second



Create New Particles
Only 1 in 10^{11} are "interesting"

Record with 5 Story 100M Channel "Camera" (60 TB/s)





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Higgs Discovery - Nobel Prize Physics 2013

Physics Letters B 716 (2012) 1–29

Contents lists available at SciVerse ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC ☆

ATLAS Collaboration *

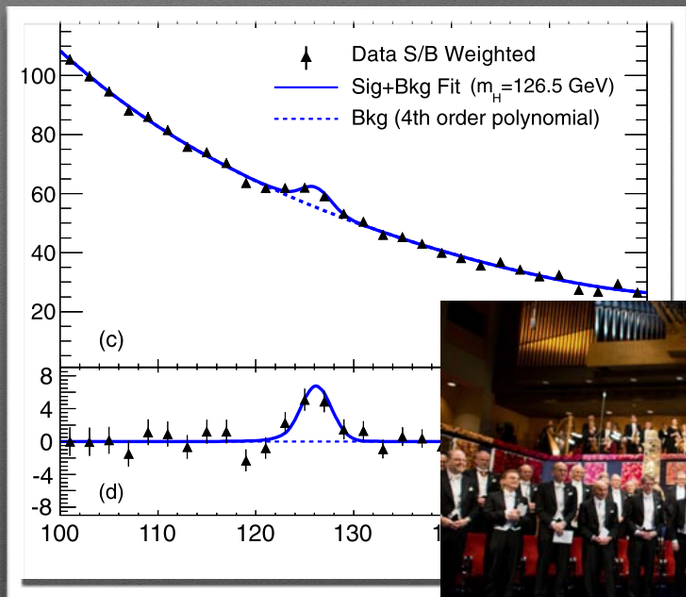
This paper is dedicated to the memory of our ATLAS colleagues who did not live to see the full impact and significance of their contributions to the experiment.

ARTICLE INFO

Article history:
Received 31 July 2012
Received in revised form 8 August 2012
Accepted 11 August 2012
Available online 14 August 2012
Editor: W.-D. Schlatter

ABSTRACT

A search for the Standard Model Higgs boson in proton–proton collisions with the ATLAS detector at the LHC is presented. The datasets used correspond to integrated luminosities of approximately 4.8 fb^{-1} collected at $\sqrt{s} = 7$ TeV in 2011 and 5.8 fb^{-1} at $\sqrt{s} = 8$ TeV in 2012. Individual searches in the channels $H \to ZZ^{(*)} \to 4\ell$, $H \to \gamma\gamma$ and $H \to WW^{(*)} \to e\nu\mu\nu$ in the 8 TeV data are combined with previously published results of searches for $H \to ZZ^{(*)}$, $WW^{(*)}$, $b\bar{b}$ and $\tau^+\tau^-$ in the 7 TeV data and results from improved analyses of the $H \to ZZ^{(*)} \to 4\ell$ and $H \to \gamma\gamma$ channels in the 7 TeV data. Clear evidence for the production of a neutral boson with a measured mass of 126.0 ± 0.4 (stat) ± 0.4 (sys) GeV is presented. This observation, which has a significance of 5.9 standard deviations, corresponding to a background fluctuation probability of 1.7×10^{-9}, is compatible with the production and decay of the Standard Model Higgs boson.



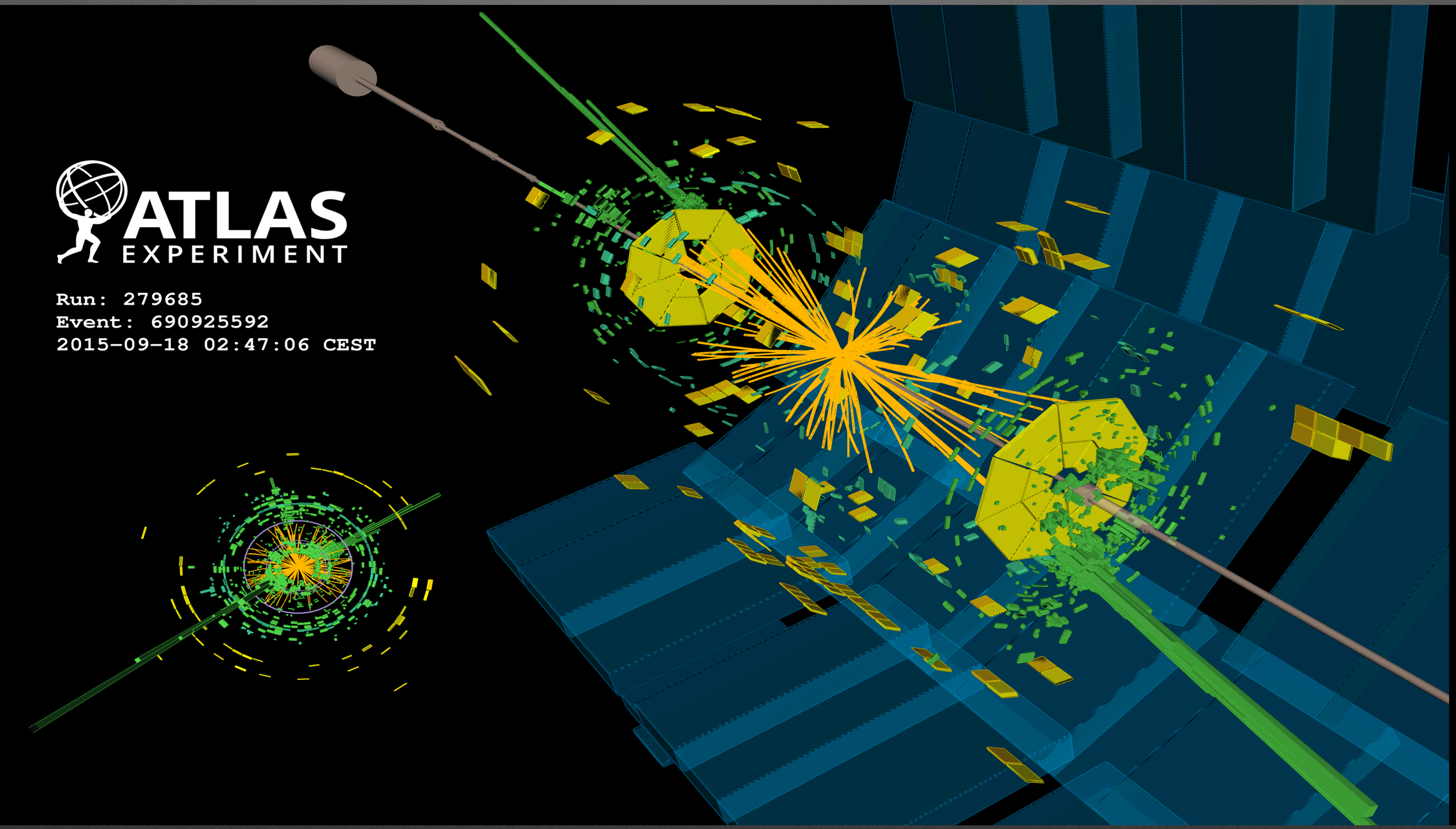
Last Piece of the Standard Model

Best Tested Theory… Ever.

Not Done… Higgs is Light! Possibilities:

- *Fine-tuned Theory*: Accident or Multiverse + Anthropic Principle
- *Mechanism*: Supersymmetry, Extra-Dimensions, Sub-structure
  - Focus of LHC
- *Design?*

Deep Learning in High Energy Physics



- Requires lots of computing
- Upgrade to LHC will give us 100x the data.
  - We won’t have 100x the computing power or storage.
- Use Artificial Intelligence and newest processors…

Animal Brains

- The brain takes in sensory data… ***builds hierarchical models of the world***.
- So effectively, a ***representation*** of the input is assembled in the brain.
  - Eyes see a limited window… but…
  - Location Cells
  - Imagining locations

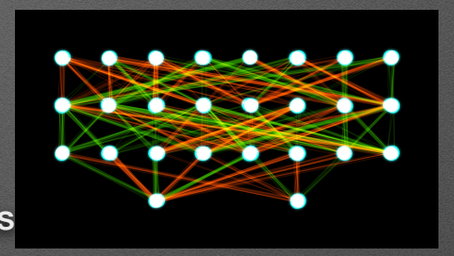
Brief History of AI

Artificial Intelligence

- Goal: Systems that reason and act as well as or better than humans
- Heuristic AI (1990's)
- Machine Learning AI
  - Knowledge learned from data
- Neural Networks ~ Brain inspired computing (1943)
  - Universal Computation Theorem (1989)
  - Multi-layer hidden networks (a.k.a. Deep) (1965)
  - Vanishing Gradient Problem (1991)

Deep Learning Renaissance (> 2007 - now)

- Driven by:
  - New NN Innovation
  - Big Data
  - Graphical Processing Units

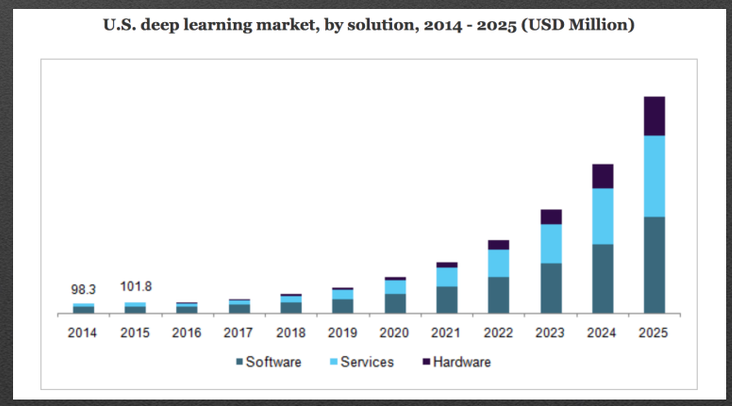


- Amazing Feats

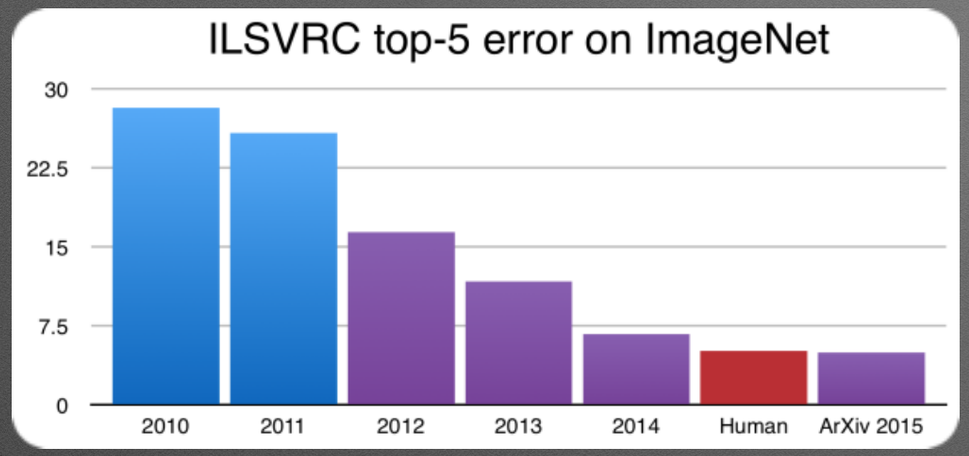
WIRED STAFF SCIENCE 06.26.12 11:15 AM

GOOGLE'S ARTIFICIAL BRAIN LEARNS TO FIND CAT VIDEOS

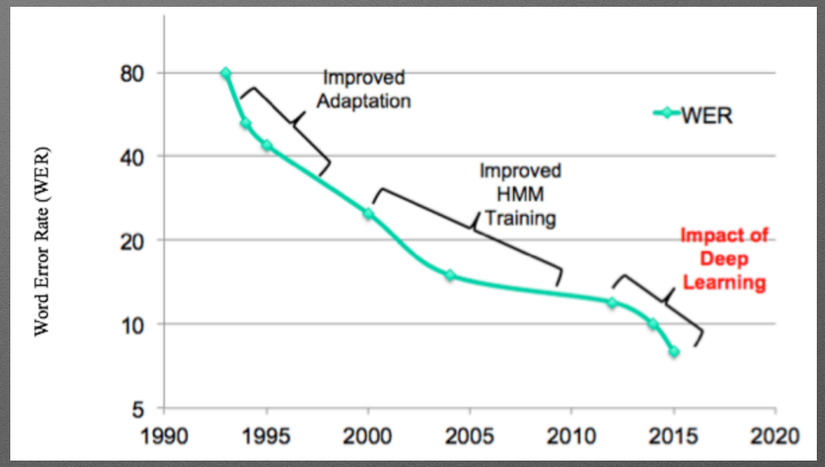
- Market Growth
- Industry Adoption



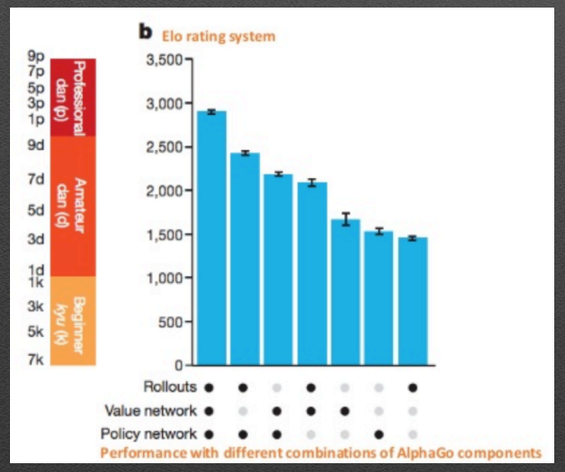
Amazing Feats : Some Examples



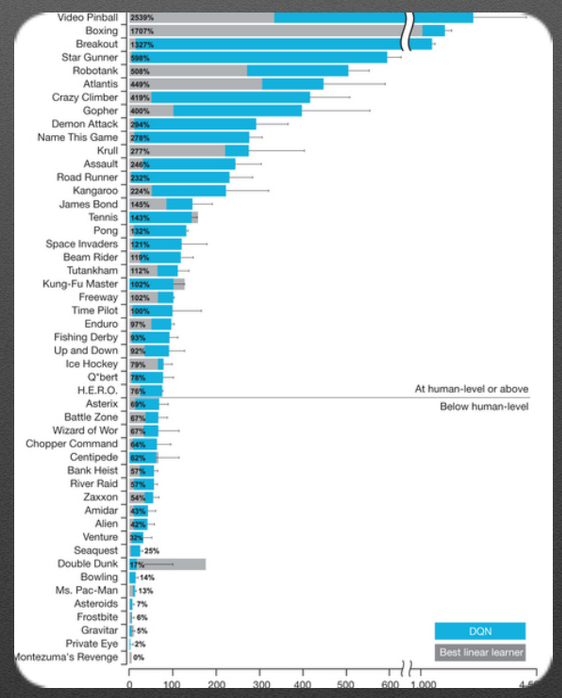
ImageNet Outperforms humans



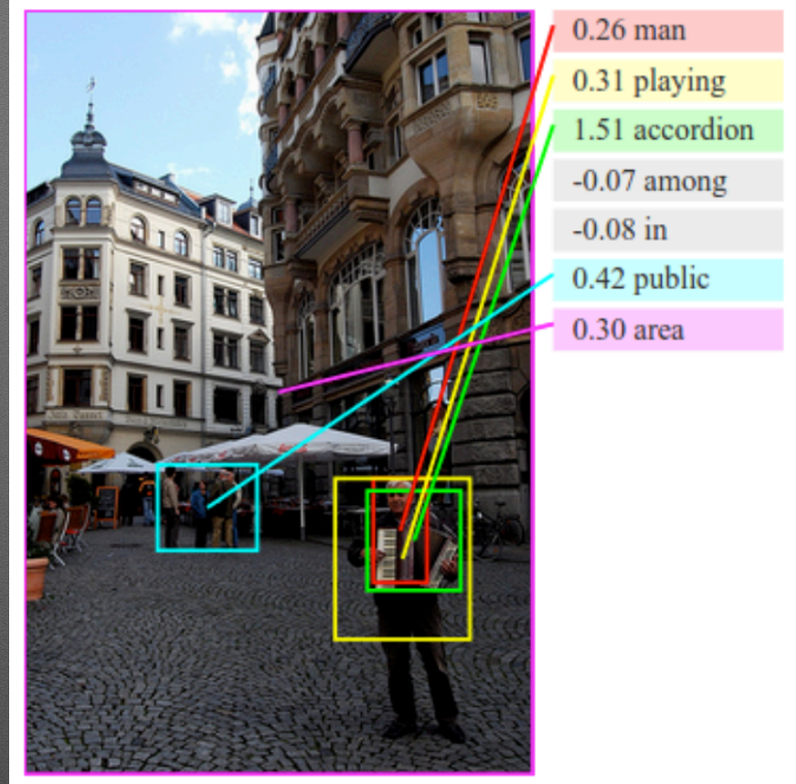
Rapid Advances in Speech Recognition

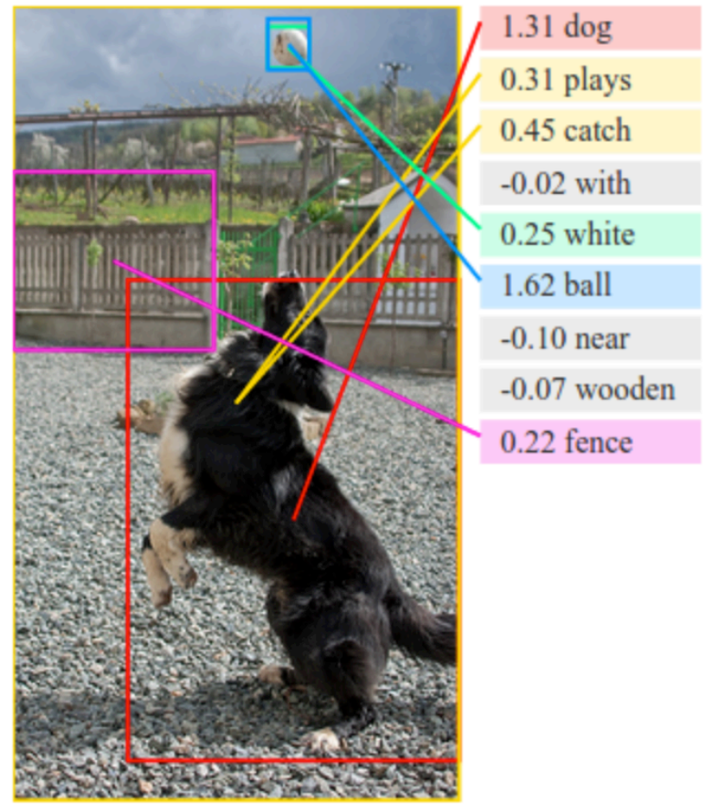


AlphaGo beats Lee Sedol



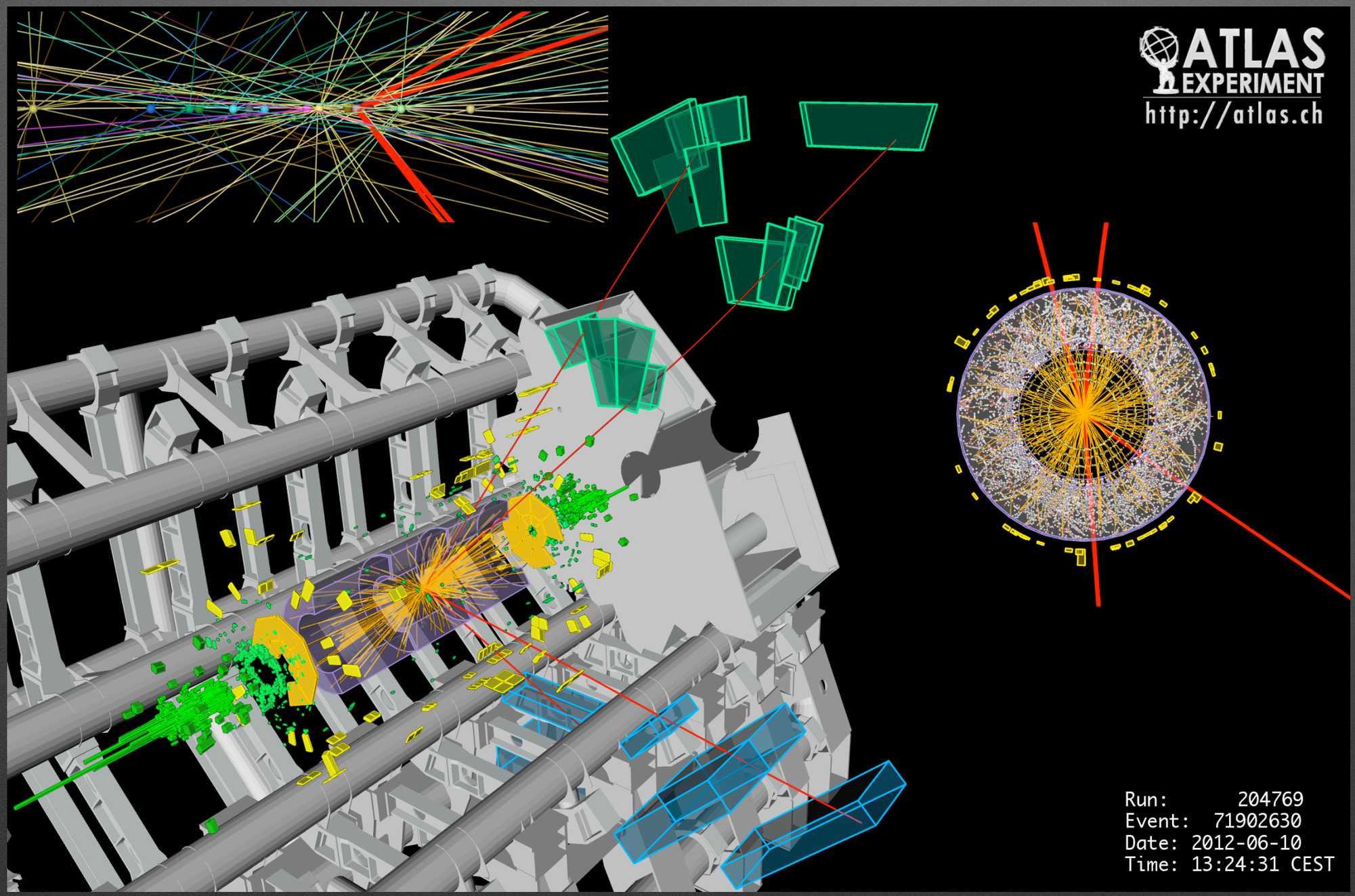
Human Level control in playing Atari games





Deep Learning can be used to tell a story with context through data

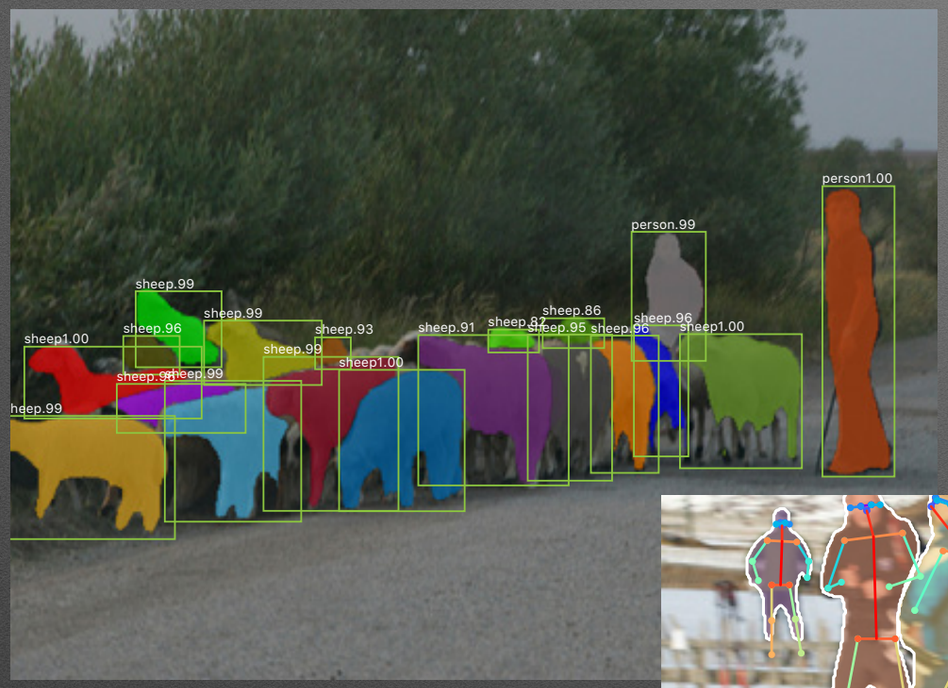
Used in HEP to understand what physics is happening

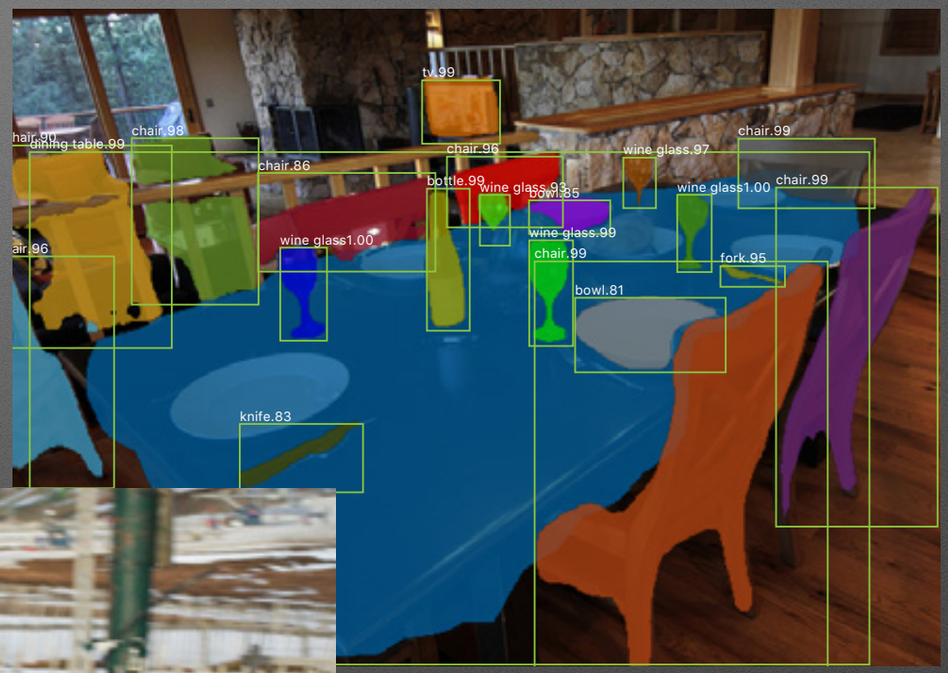


$H \rightarrow ZZ \rightarrow 4\ell$

We can use deep learning object tagging techniques in the data to find the decaying particle

Amazing Feats : Some More Examples





https://arxiv.org/pdf/1703.06870.pdf

Why go Deep?

Better Algorithms

- Better results
- Solution where there is none
- Make sense of complicated data

Easier Development

- Feature Learning, not Feature Engineering
- Save time and cost

Faster Algorithms

- DNNs Faster than traditional Algs
- Neuromorphic processors

Why Physicists ?

High Energy Physicists (HEP) ideally suited

- HEP Systems and Machine Learning and Deep Learning Systems confront similar challenges
- Decades of Experience at the Data Frontier
- Bridge between science and industry
- HEP scientists are also engineers by training

MOVE OVER, CODERS—PHYSICISTS WILL SOON RULE SILICON VALLEY

… it's happening across Silicon Valley. …, ***the things that just about every internet company needs to do are more and more suited to the skill set of a physicist***.

new wave of data science and AI is something that suits physicists right down to their socks.

"There is something very natural about a physicist going into machine learning … more natural than a computer scientist."

Physicists know how to handle data … building these enormously complex systems requires its own breed of abstract thought.