

DEEP LEARNING AND THE TRANSFORMATION OF SCIENTIFIC EXPLORATION

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THE RISE OF AI-ENRICHED SCIENTIFIC EXPLORATION

SCIENTIFIC PARADIGMS

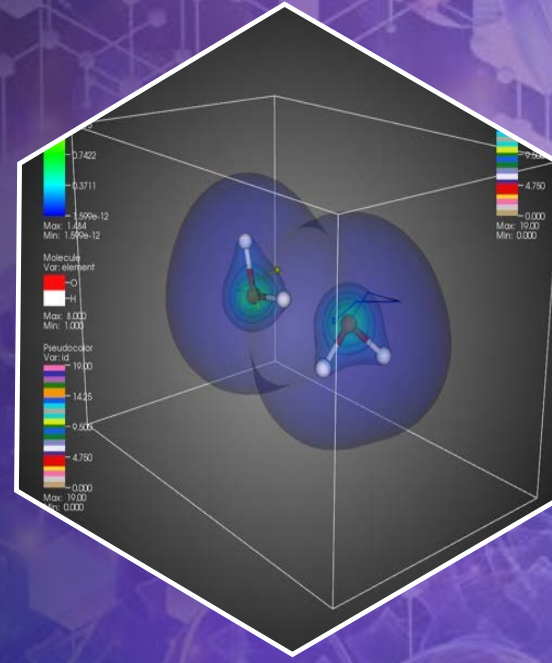
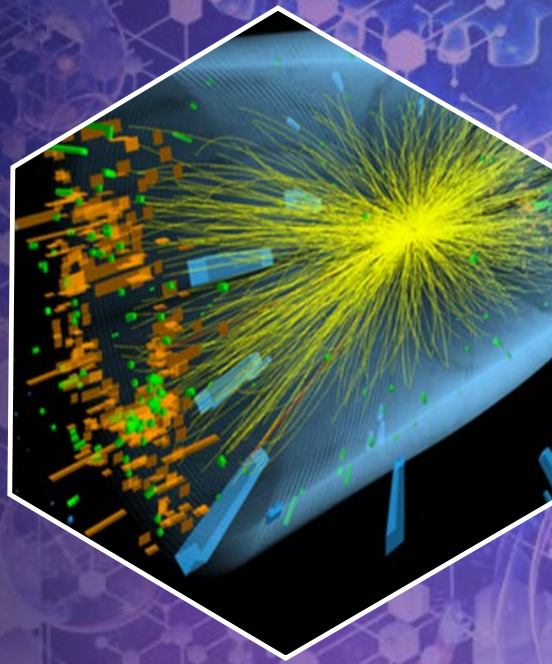
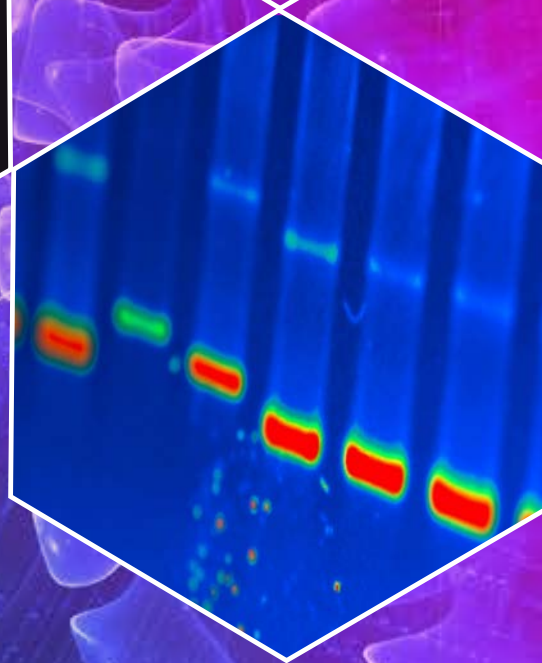
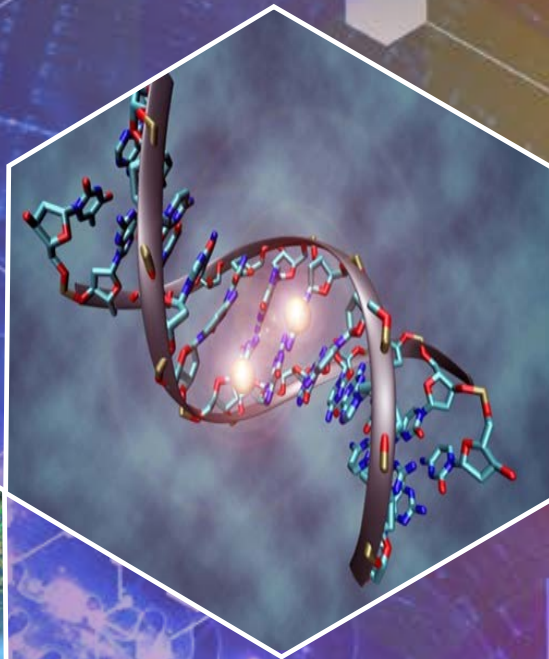
EMPIRICAL

THEORETICAL

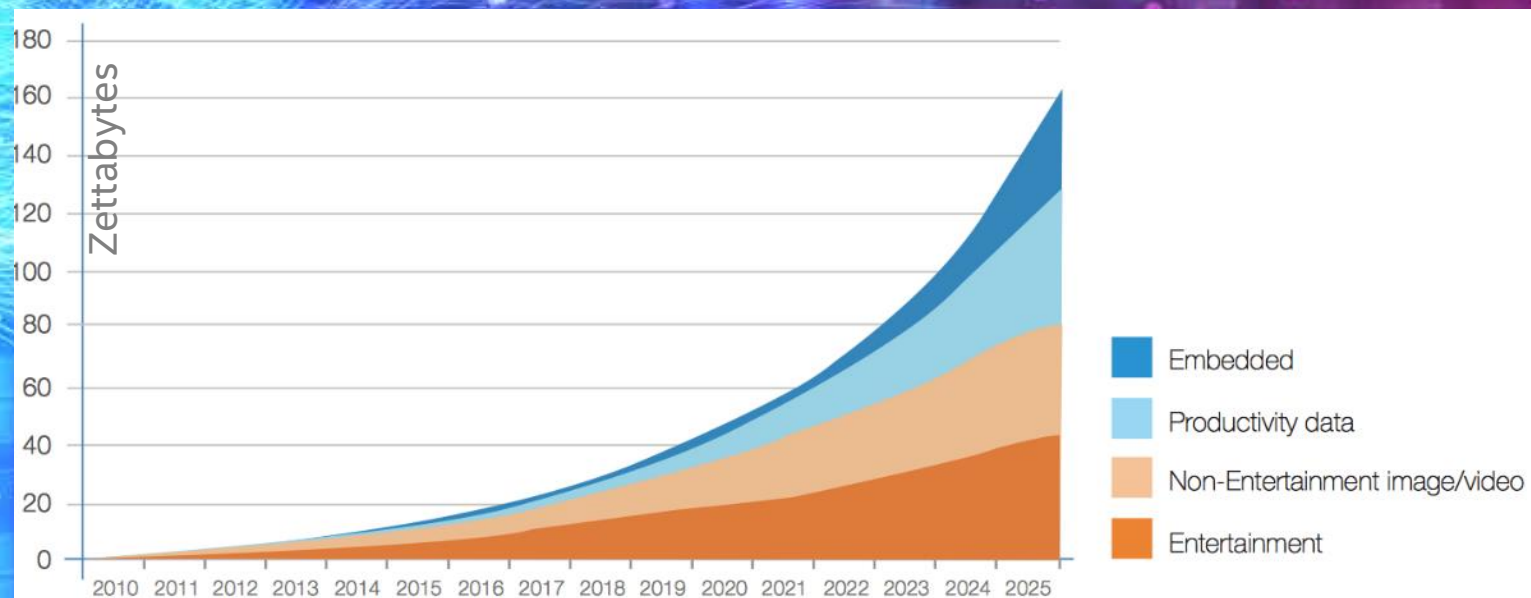
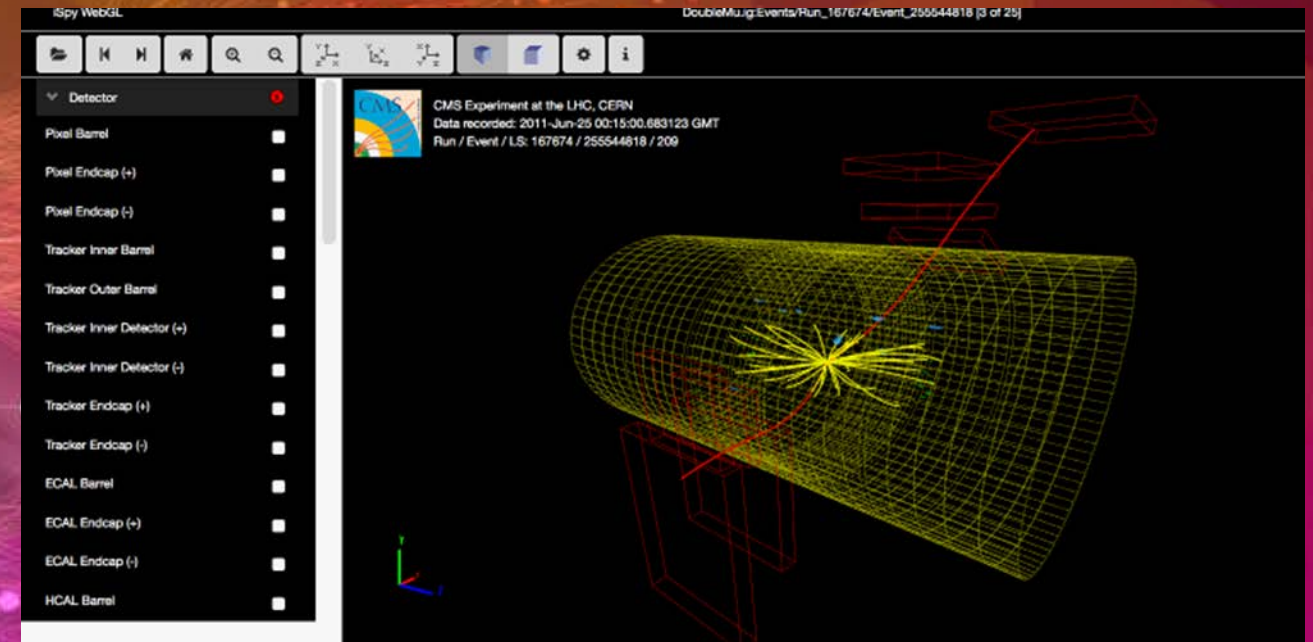
COMPUTATIONAL

DATA EXPLORATION (PROGRAMMED)

PHENOMENON EXPLORATION (ML)



THE CAMBRIAN EXPLOSION OF DATA



Source: IDC's Data Age study, sponsored by Seagate, April 2017

DAILY BY 2020

AVERAGE INTERNET USER 1.5 GB

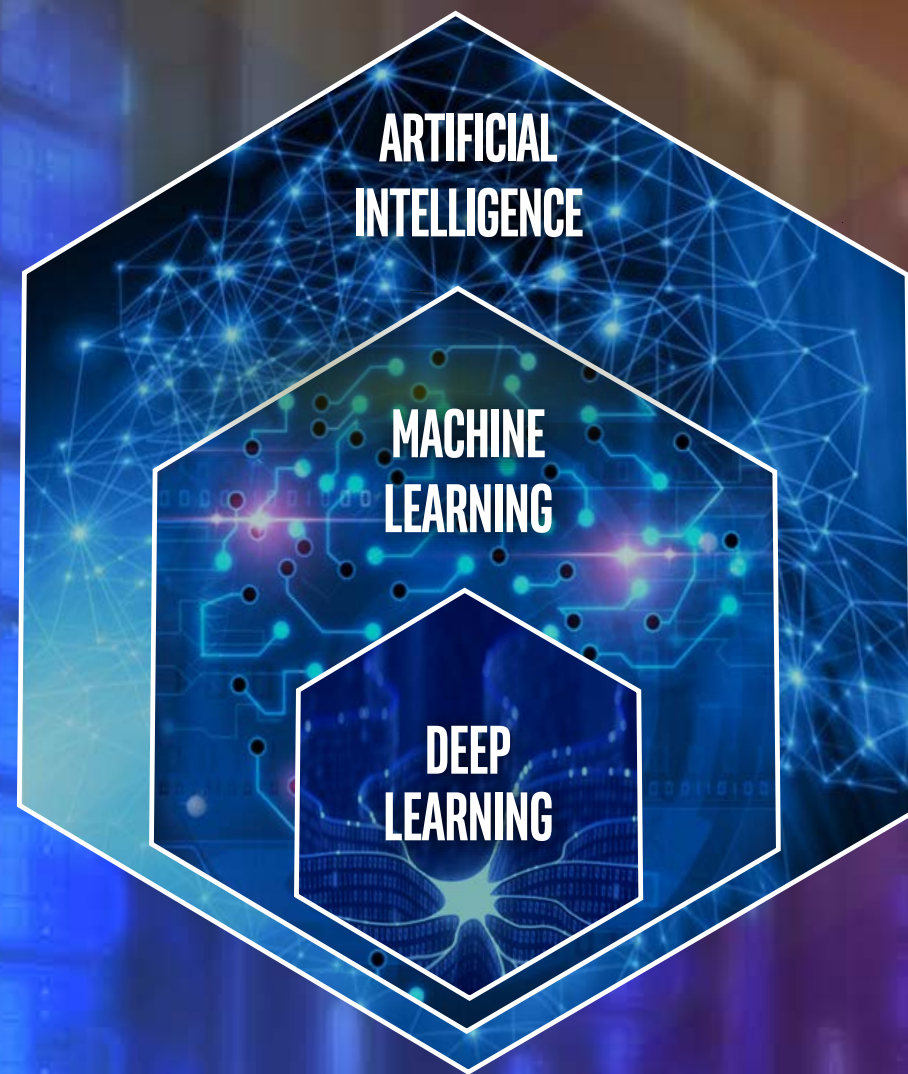
AUTONOMOUS VEHICLE 4 TB

CONNECTED AIRPLANE 5 TB

SMART FACTORY 1 PB

CLOUD VIDEO PROVIDER 750 PB

ZETTA DATA × EXA COMPUTING × MACHINE LEARNING



DEEP LEARNING IN HPC AND SCIENCE

SPEECH

ADAS

VISION

ALPHA GO

TYPES OF ANALYTICS/ML (PARTIAL LIST)

CLASSIFICATION

REGRESSION

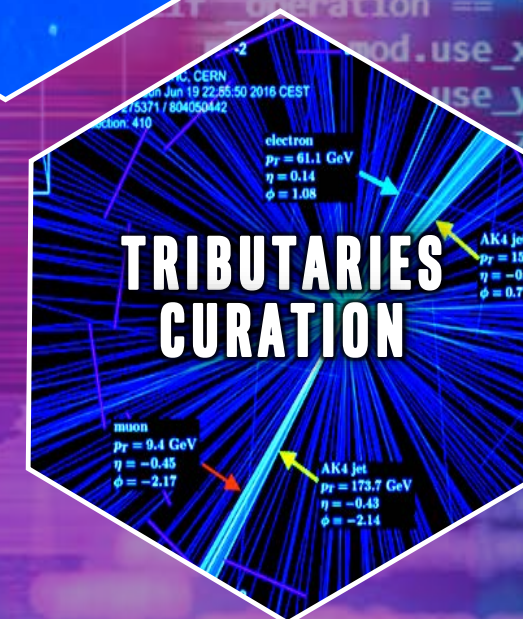
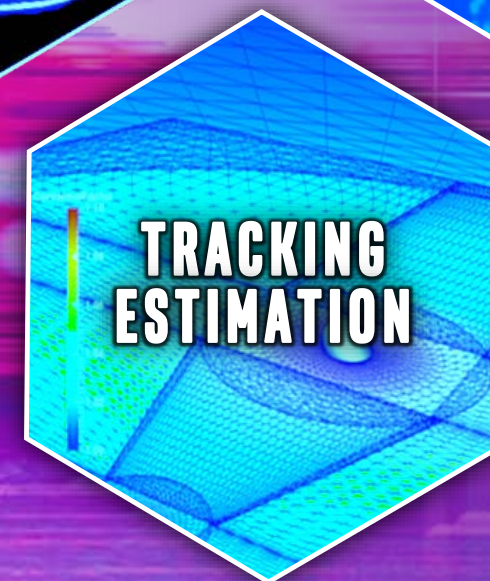
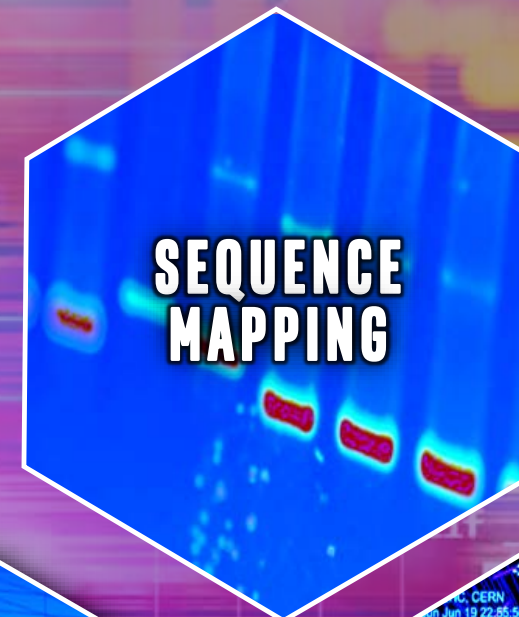
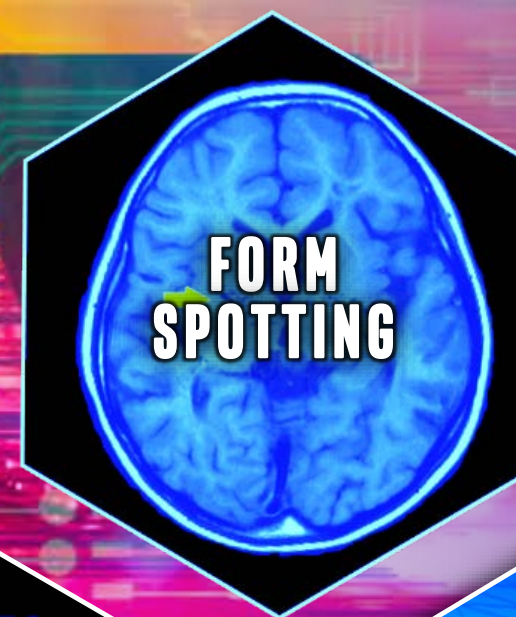
CLUSTERING

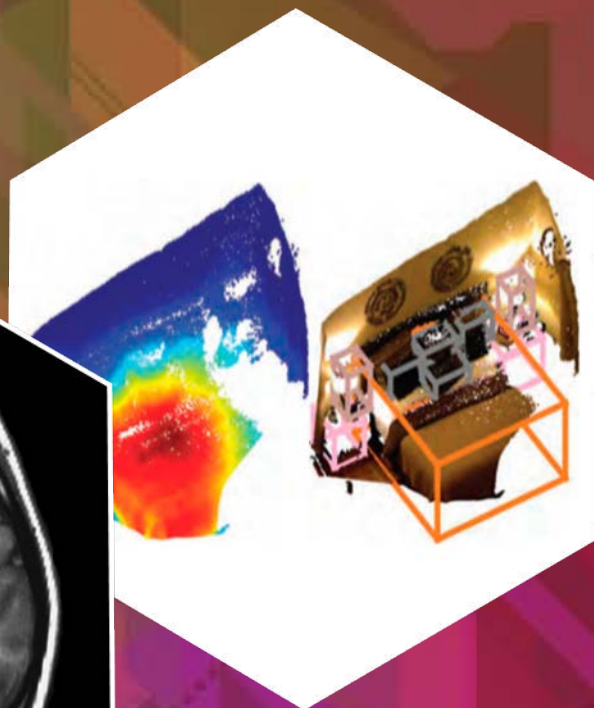
FEATURE LEARNING

ANOMALY DETECTION

MACHINE LEARNING

CLASSES OF APPLICATION SCHEMES





- ▶ Finding a 'kind of pattern' in multi-dimensional elaborate data
- ▶ Lots of examples available
- ▶ Weak signal in a sea of noise
- ▶ No mathematical/statistical model

Applicable DL techniques:

Pattern classification
Feature learning
Anomaly detection

Supervised learning:

Data tagging

FORM SPOTTING

FINDING A BLADE OF GRASS IN A HAYSTACK

FORM SPOTTING NEUROSCIENCE



<http://brainiak.org>

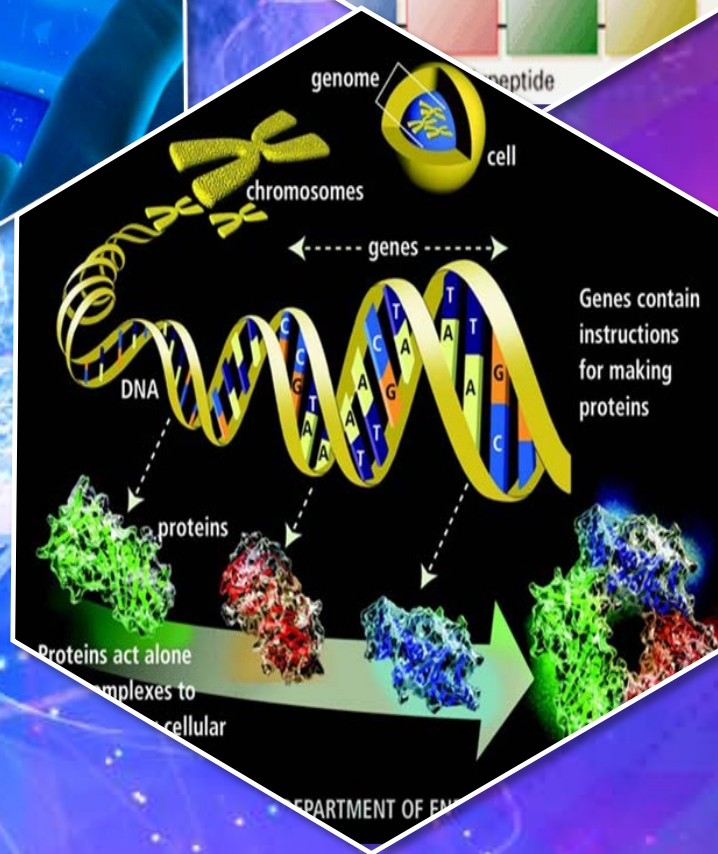
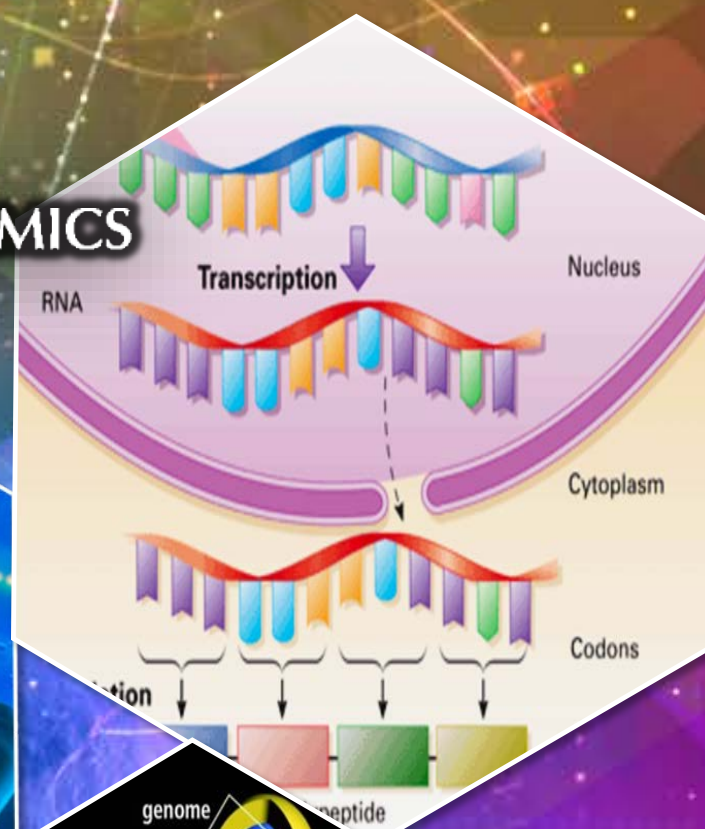
Princeton Neuroscience Institute mapped the human mind in real time for improved diagnosis and treatment of brain disorders and mental illness.

Typical single scan (~1 million voxels) evaluated in seconds vs hours.

BrainIAK - Developing the next generation in fMRI brain imaging.



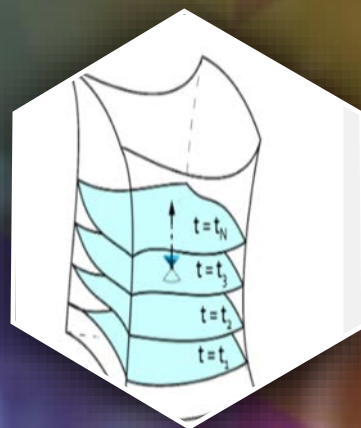
SYNTHETIC GENOMICS



FORM SPOTTING GENOMICS

- ▶ 10^4 x speed up boost: annotate 1 million genes in <1hr vs. weeks with traditional tools
- ▶ Assign function to millions of uncharacterized proteins
- ▶ Semantic Search: discover proteins with related function even without sequence similarity
- ▶ Early stages of protein design: predict in seconds impact of every possible AA change

Joint effort of SGI and Intel



TRACKING ESTIMATION

- ▶ Well defined functions/model; compute intensive
- ▶ Major reduction (e.g., 10^4 x) required to enable real-time or rapid iterations

Applicable DL techniques:

Regression

Supervised learning:

Full model training the DL Shadowing Estimator

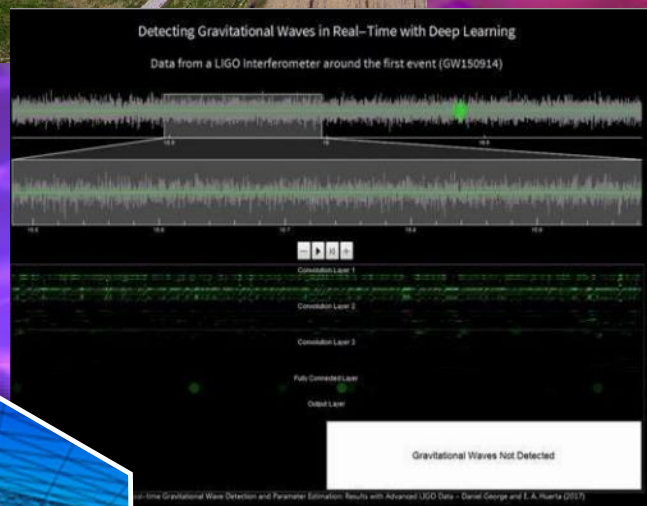
$$\lim_{\Delta t \rightarrow 0^+} \int_{\Omega} D(t_1, x) \frac{\varphi(t_1 - \Delta t, x) - \varphi(t_1, x)}{(-\Delta t)} dx$$

$$\lim_{\Delta t \rightarrow 0^+} \int_0^T \int_{\Omega} D(t_1, x) \frac{\partial \varphi}{\partial t_1}(t_1, x) dx dt_1$$

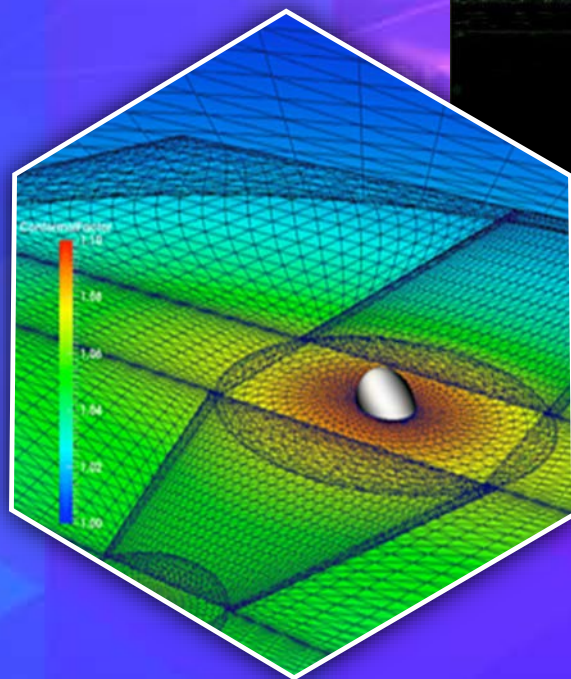
**DL
TRACKER**

TRACKING ESTIMATION

DETECTION OF GRAVITATIONAL WAVES (LIGO)



- ▶ Laser Interferometer Gravitational-Wave Observatory (LIGO) labs
- ▶ Detection of gravitational waves from binary black hole mergers
- ▶ Process array of sensors for directing a high-focus radio telescope
- ▶ Real-time multimessenger detection (DNN)
>10⁴ speedup: multiple days to 'real-time'
(George, D. , Huerta, E. A.: *Deep Neural Networks to Enable Real-time Multimessenger Astrophysics*)

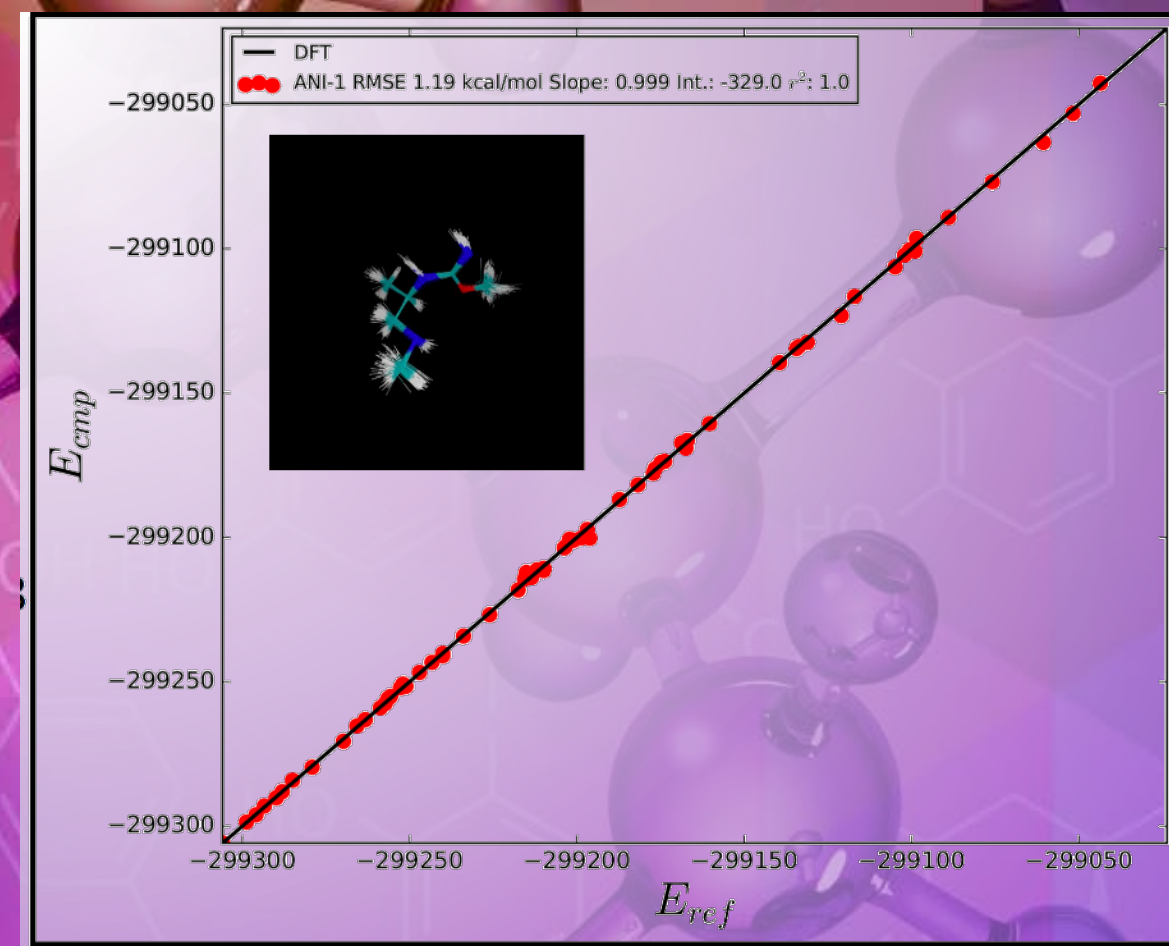
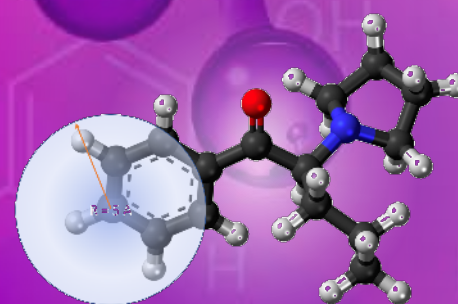


<https://www.ligo.caltech.edu>

TRACKING ESTIMATION

APPROXIMATING THE BEHAVIOR OF MOLECULES

- ▶ Predicting behavior of organic molecules
- ▶ Compute intensive Kohn-Sham Density-Functional Theory (DFT) equations
- ▶ Database of 20 million conformations
- ▶ Chemically accurate DL
- ▶ 10^5 speedup; $\sim 6 \times 10^{-4}$ power reduction



Source: Mastering Computational Chemistry with Deep Learning, Isayev, O, University of North Carolina Chapel Hill

SEQUENCE MAPPING

- ▶ Creating output sequence based on context based, multi-dimensional, continuous input sequence

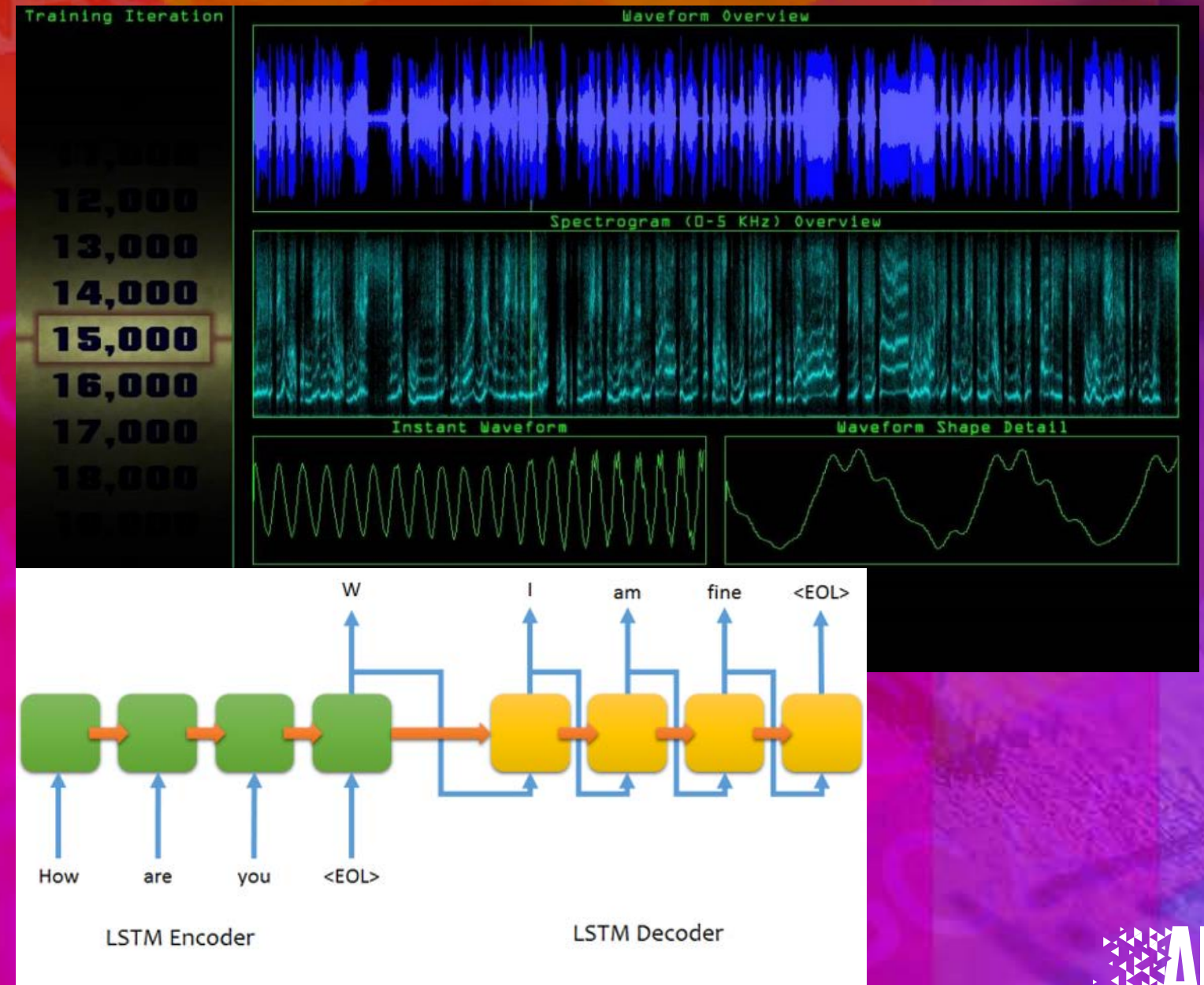
Applicable DL techniques:

Neural Machine Translation (NMT)

Sequence-to-sequence transformation

Supervised learning:

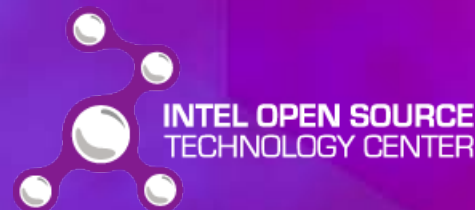
Sequence examples tagging



SEQUENCE MAPPING

CONTEXTUAL SPEECH GENERATION

- ▶ Stephen Hawking device – effective translation of cheek movements to cursor and mouse controls
- ▶ Machine Learning, multi-context
- ▶ Customized language models
- ▶ High accuracy at predicting syllables and words
- ▶ ACAT (Assistive Contextually Aware Toolkit) by Intel Labs
- ▶ Added Speech Synthesis

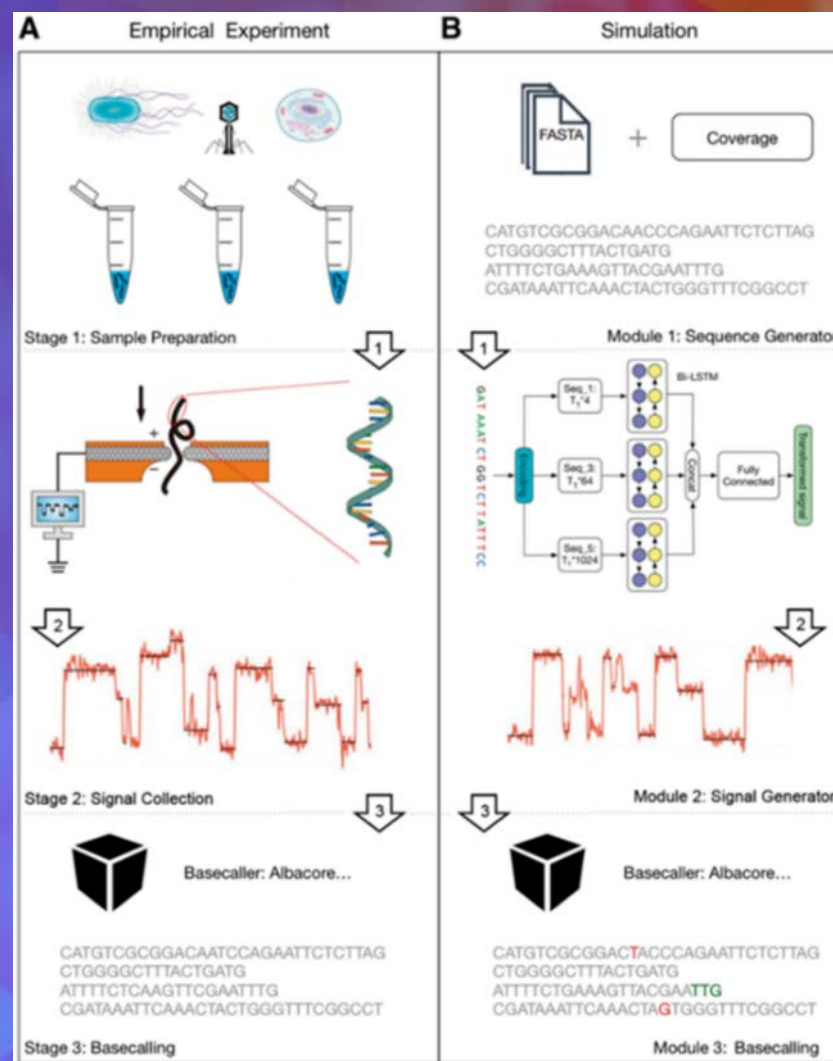


<https://01.org/acat>

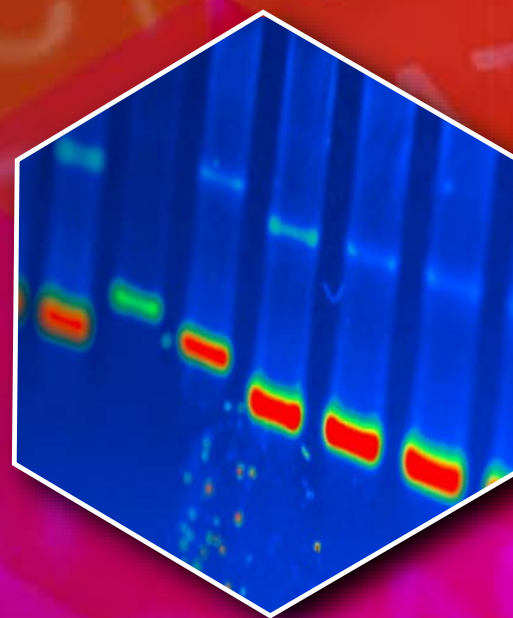


SEQUENCE MAPPING

GENOMICS - NANOPORE SEQUENCING



Yu Li et al.: DeepSimulator: a deep simulator for Nanopore sequencing.



Oxford
NANOPORE
Technologies®

جامعة الملك عبدالله
للعلوم والتقنية

King Abdullah University of
Science and Technology



- ▶ DNA/RNA high TPT sequencing by Oxford Nanopore Tech
- ▶ From noisy electrical waveforms, predicting sequence of ATCGs
- ▶ DeepSimulator mimics entire pipeline, similar to experimental
- ▶ Addressing repetitive regions

SPACE EXPLORATION

- ▶ Solution space too large for scientist trial-and-error
- ▶ Lack of model to guide exploration

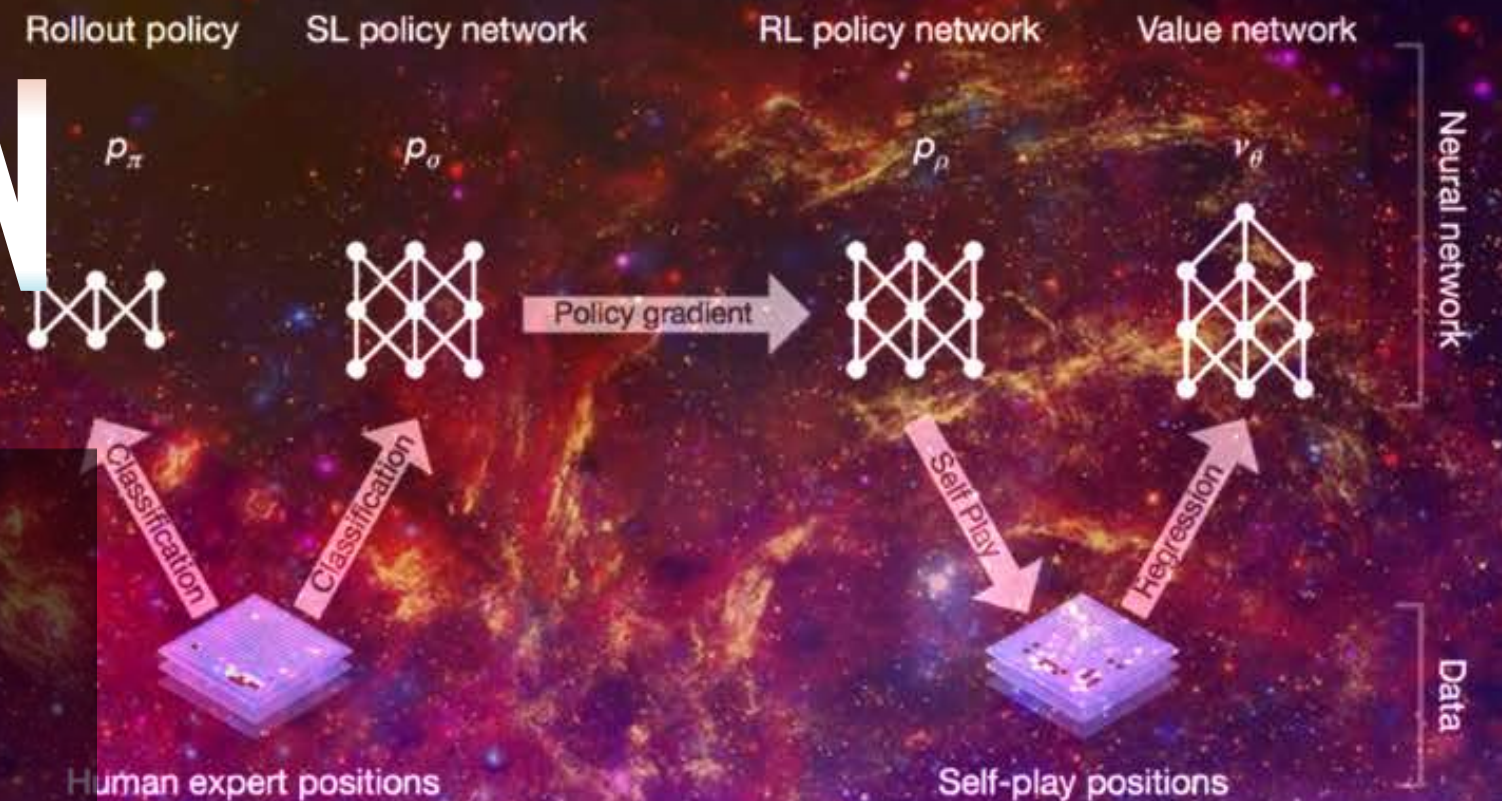
Applicable DL techniques:

Reinforcement Learning (RL)

Meta Learning (learning how to best learn)

+ previous methods to evaluate branches

Unsupervised learning



Source: <https://medium.com/@karpathy/alphago-in-context-c47718cb95a5>

Policy network

Value network

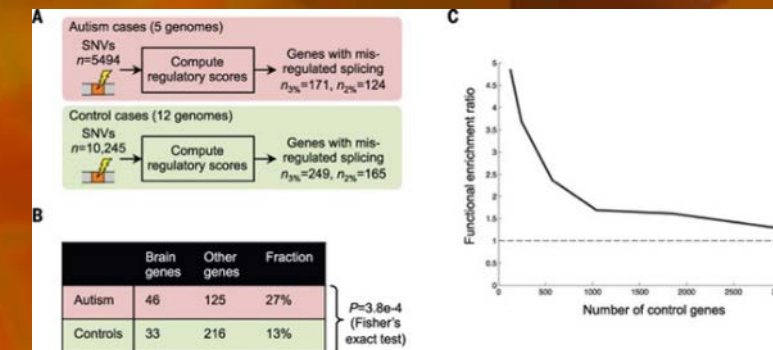
$p_{\sigma/p}(a|s)$

$v_\theta(s')$

s

s'

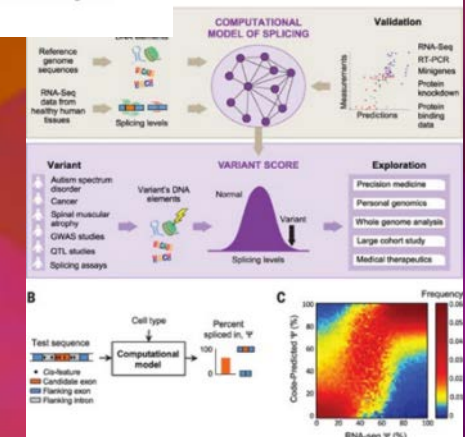
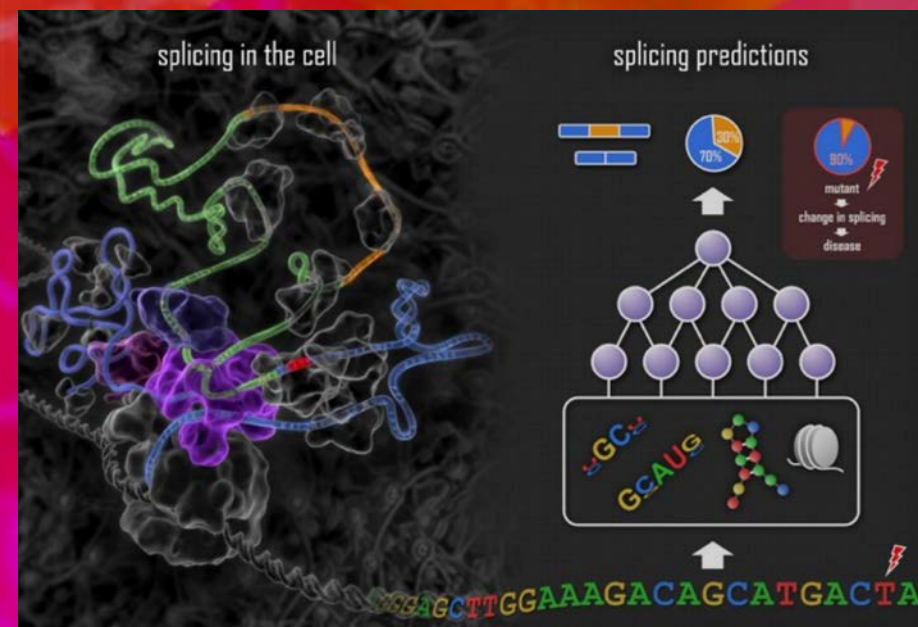
SPACE EXPLORATION REVEALING THE GENETIC ORIGINS OF DISEASE



Hui Y. Xiong et al. Science
2015;347:1254806

- ▶ Ranking of genetic mutations based on how living cells 'read' DNA
- ▶ DL learns genetic instructions for proper splicing, protein production
- ▶ Evaluate mutations and likelihood of causing disease
- ▶ Facilitate discovery of unexpected genetic determinants of autism, cancer, spinal muscular atrophy
- ▶ Challenge – which mutations to try?

(H. Y. Xiong. et al.: *The human splicing code reveals new insights into genetic determinants of disease*, Science 347)



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- ▶ Finding preferred path in complex space : *Neural Arch Search with Reinforcement Learning*
(by Zoph, B. and Le, Q. V.)
- ▶ “Use ML for ML Itself”

TRIBUTARIES CURATION

- ▶ Massive number of data sources
- ▶ Data curation: intelligent filtering at the source
- ▶ Combined learning of filtering functions & data analysis

Applicable DL techniques:

Ensemble Learning: central plus
Distributed processing
Multiple ML techniques

Unsupervised Learning

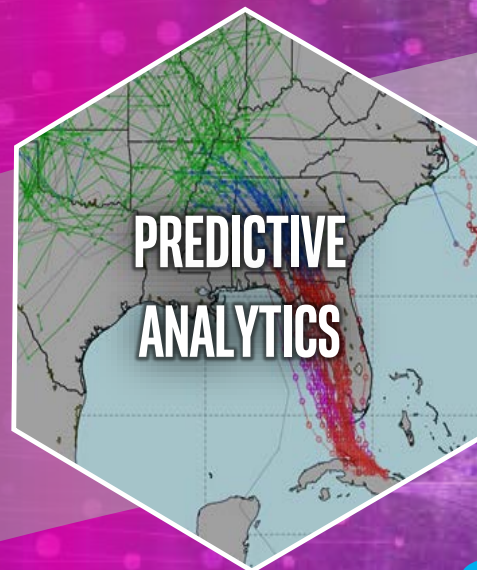
FROM PAST/PRESENT TO THE FUTURE FROM PREDICTIONS TO TAKING ACTION



PAST



PRESENT

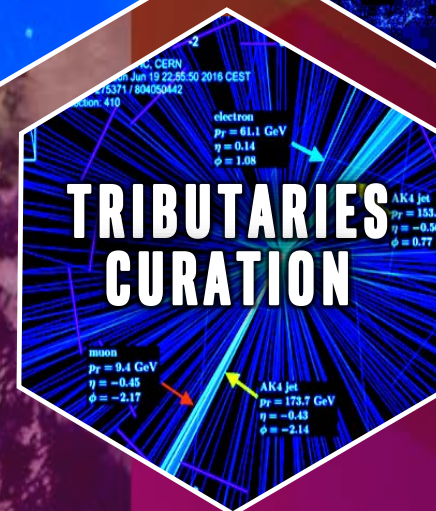
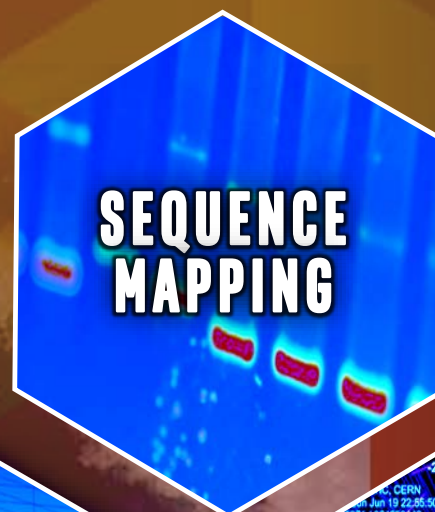
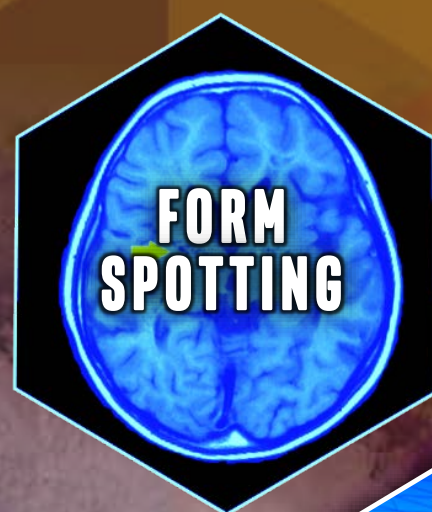


FUTURE

ANALYTICS CURVE

OUTLOOK: CHALLENGES AND OPPORTUNITIES

- ▶ Address lack of theory and explainability
- ▶ Understand limits of supervised & unsupervised learning
- ▶ Update skillset of senior scientists
- ▶ Fully utilize ML targeted 'solver' capabilities – “ 10^4 factor”
- ▶ Evolve from a dataset to tapping flowing phenomenon
- ▶ Harness ML as a creative co-explorer



SUMMARY CALL TO ACTION

ANALYTICS CURVE



EMBRACE AI AS A TOOL OF CHOICE AND A 'CREATIVE PARTNER'

