

FRITZ-HABER-INSTITUT
MAX-PLANCK-GESELLSCHAFT

IPAM Workshop

***From Passive to Active:
Generative and Reinforcement
Learning with Physics***

A Review

Coffee Talk

on 4th November 2019

What are you talking about?



The screenshot shows the IPAM website with a navigation menu including PROGRAMS, VIDEOS, NEWS, PEOPLE, YOUR VISIT, ABOUT IPAM, DONATE, and CONTACT US. A search bar for Google Custom Search is also present. The main content area features a blue header with the text 'Long Programs' and a breadcrumb trail: 'Programs > Long Programs > Machine Learning for Physics and the Physics of Learning'. Below this, the program title 'Machine Learning for Physics and the Physics of Learning' is displayed with the dates 'SEPTEMBER 4 - DECEMBER 8, 2019'. A dark navigation bar contains five tabs: OVERVIEW (selected), PARTICIPANT LIST, SEMINAR SERIES, ACTIVITIES, and APPLICATION. The 'Overview' section contains a paragraph about Machine Learning (ML) and a small image of a starry night sky.

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Google Custom Search

Long Programs

[Programs](#) > [Long Programs](#) > Machine Learning for Physics and the Physics of Learning

Machine Learning for Physics and the Physics of Learning

SEPTEMBER 4 - DECEMBER 8, 2019

OVERVIEW PARTICIPANT LIST SEMINAR SERIES ACTIVITIES APPLICATION

Overview

Machine Learning (ML) is quickly providing new powerful tools for physicists and chemists to extract essential information from large amounts of data, either from experiments or simulations. Significant steps forward in every branch of the physical sciences could be made by embracing, developing and applying the methods of machine learning to interrogate high-dimensional complex data in a way that has not been possible before.



What are you talking about?

Workshop I: From Passive to Active: Generative and Reinforcement Learning with Physics

Part of the Long Program [Machine Learning for Physics and the Physics of Learning](#)

SEPTEMBER 23 - 27, 2019

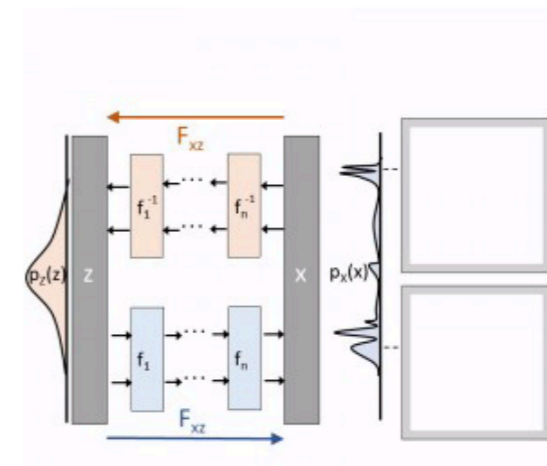
 OVERVIEW

 SPEAKER LIST

 SCHEDULE

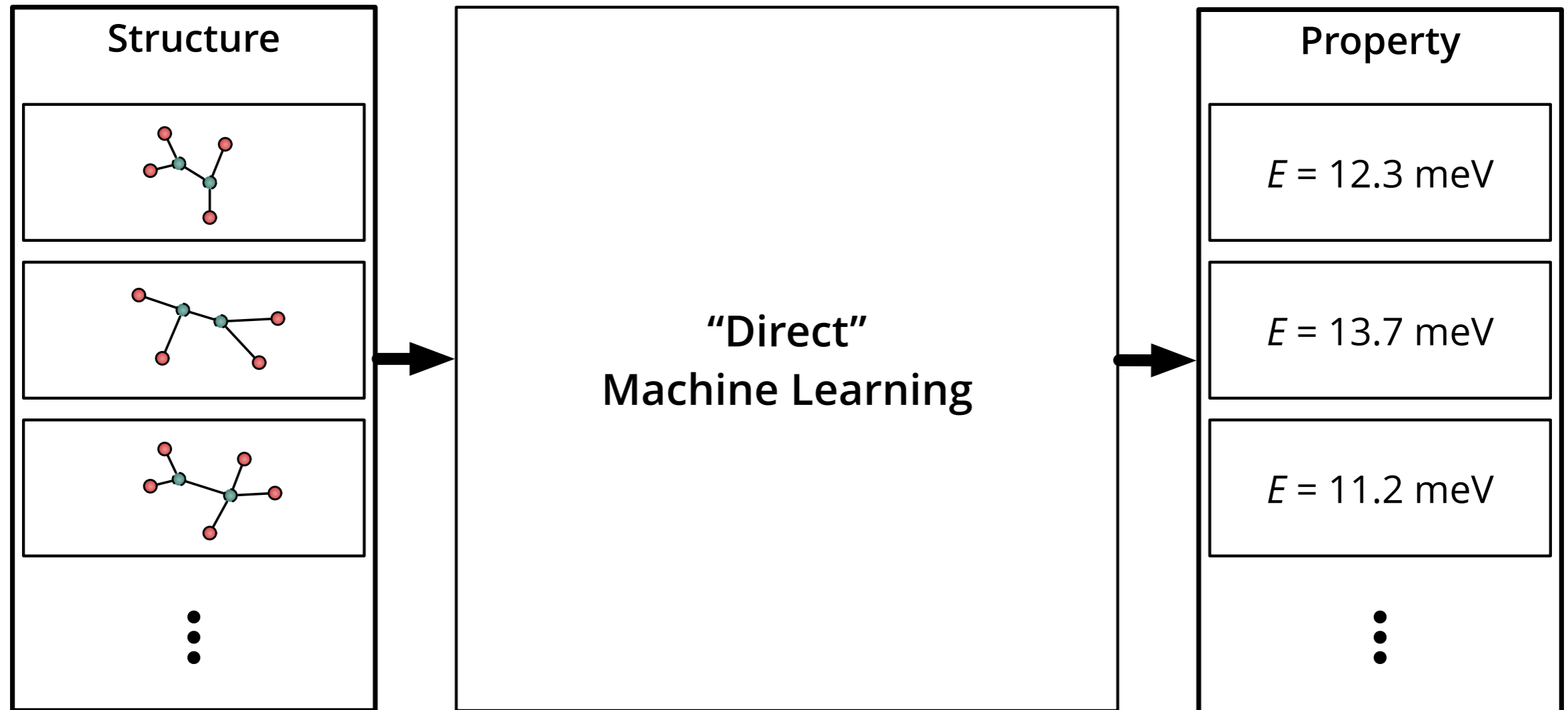
Overview

How can we design a costly experiment in an informationally optimal way? How can we generate complex structures under strong physical constraints? How should we structure the stages of learning or observing in a changing, reactive or adversarial environment? This workshop will address these questions by means of active learning, sequential decision making, experimental design, reinforcement learning, interactive learning or generative learning. In other words, the workshop will examine how to plan experiments in order to use information in a cost-optimal way. It will also include the application of these modalities to training complex models, such as deep architectures, and the transfer of these ideas to the generation of physically-relevant complex structures such as chemical structures, molecular structures, scalar or vector fields in fluid dynamics or electrodynamics, proposal steps for Markov chain Monte Carlo of physical systems etc. In all of these areas, we would like to be able to generate fairly complex structures that have rather strict physical constraints (such as conservation laws, differentiability, smoothness, etc). The constraints make generation of valid structures harder on one hand, but they may also be used to guide the search.

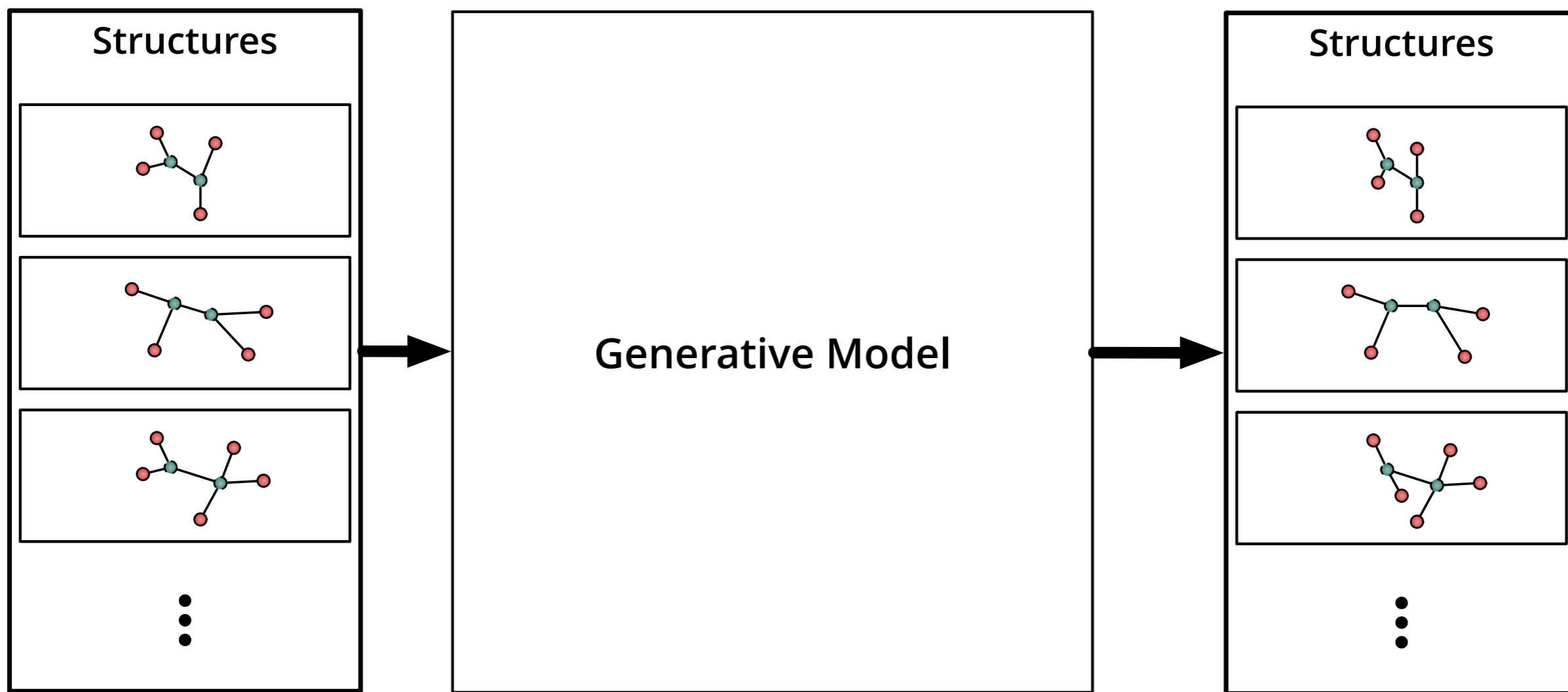


<http://www.ipam.ucla.edu/programs/workshops/workshop-i-from-passive-to-active-generative-and-reinforcement-learning-with-physics/> for talk recordings see the last slide!

Generative Learning



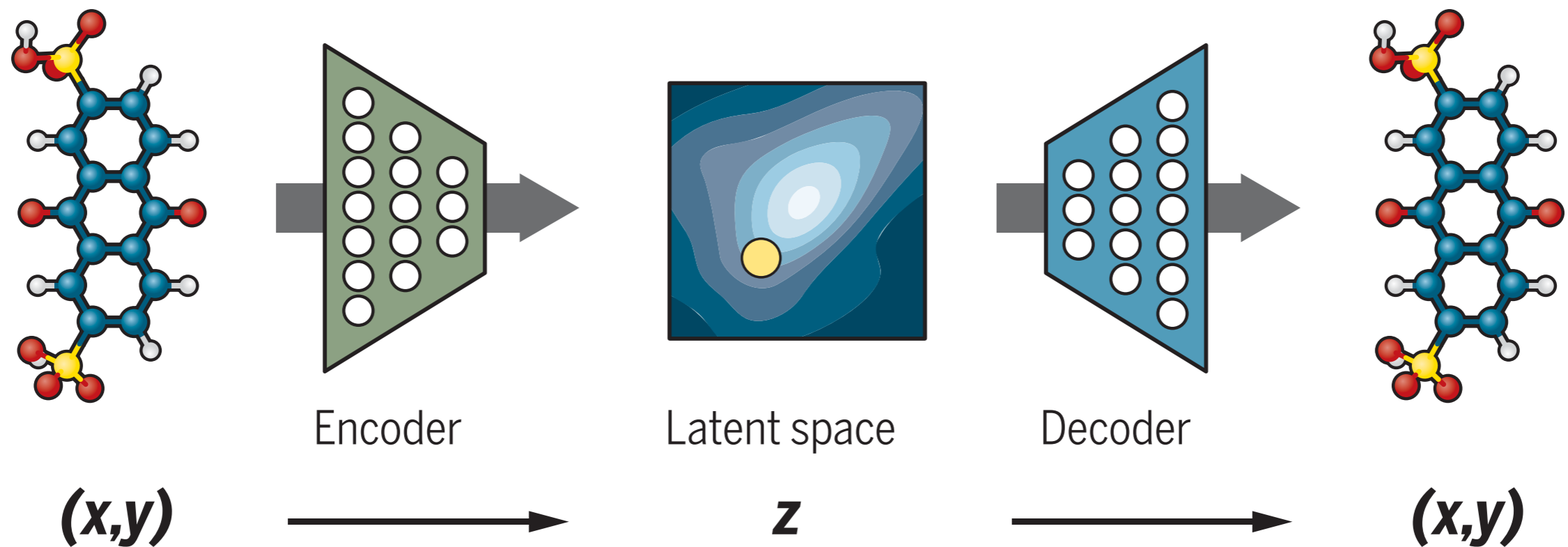
Generative Learning



Generative Learning

- Learn data probability distribution
- Learn representation of data
- Directed generation of structures

VAE: Variational autoencoders

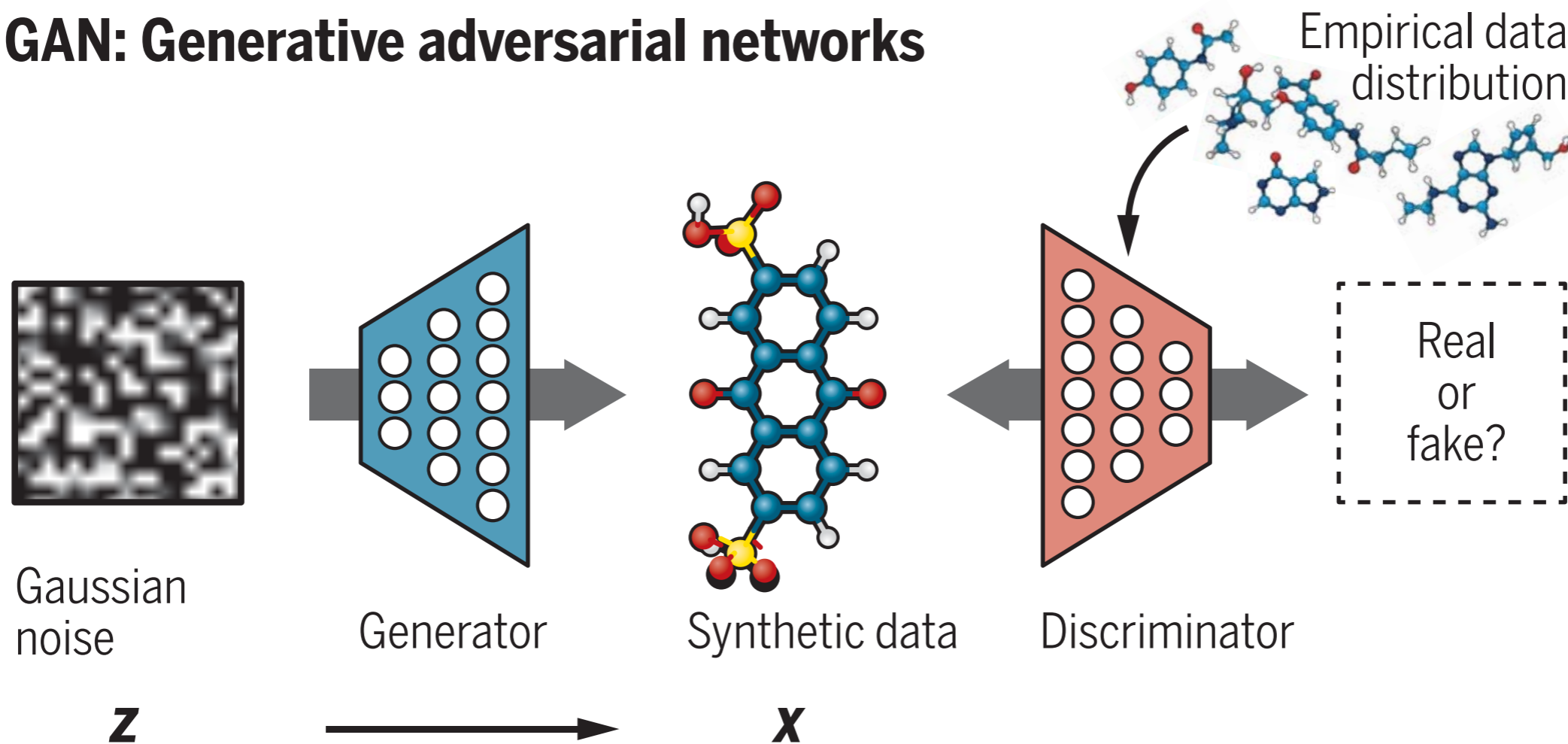


Sanchez-Lengeling *et al.*, Science 361 (2018)

VAE Papers

- Boltzmann Generators: Noé et al.; doi.org/10.1126/science.aaw1147
- Molecule Generation
 - Graph Convolutional Decoder: Bresson and Laurent; arxiv.org/abs/1906.03412
 - Junction Tree VAE: Jin et al.; arxiv.org/abs/1802.04364
- VAE for Solid-State Materials: Noh et al.; doi.org/10.1016/j.matt.2019.08.017
- Normalising Flows: Rezende and Mohamed; arxiv.org/abs/1505.05770

GAN: Generative adversarial networks



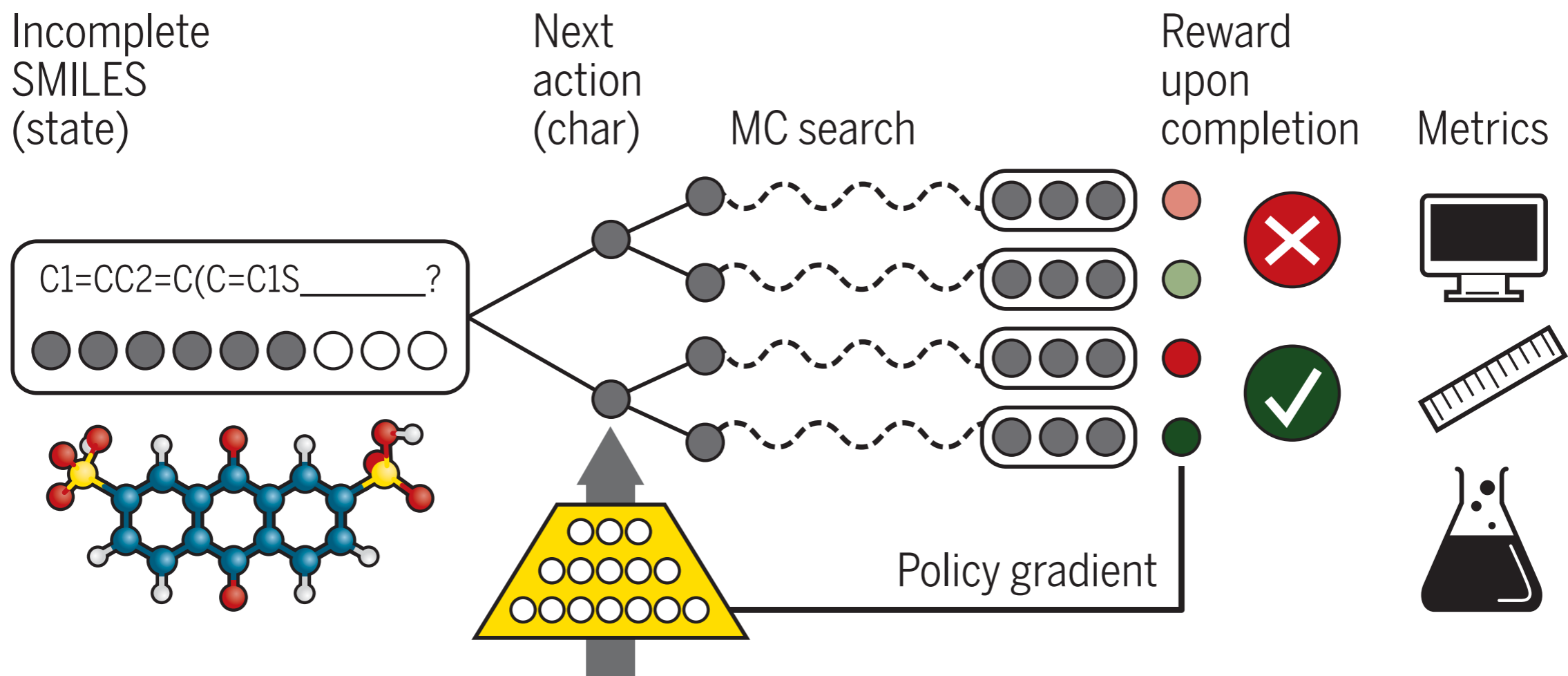
Sanchez-Lengeling *et al.*, Science 361 (2018)

GAN Papers

- MolGAN: De Cao and Kipf; arxiv.org/abs/1805.11973
- Generation of 3D point sets with G-SchNet: Gebauer et al.; arxiv.org/abs/1906.00957
- **BONUS**
SELFIES: Krenn et al. ; arxiv.org/abs/1905.13741
(alternative to SMILES)

RL: Reinforcement learning

Policy gradient with Monte Carlo tree search (MCTS)



Sanchez-Lengeling *et al.*, Science 361 (2018)

RL Papers

- Optimization of Molecules with RL: Zhou et al.; doi.org/10.1038/s41598-019-47148-x
- Graph Convolutional Policy Network: You et al.; arxiv.org/abs/1806.02473

Bonus Papers!

- Tensor Field Networks (NNs with explicit equivariance to rotations and translation): Schmidt et al.; arxiv.org/abs/1802.08219 (stay tuned, might give a seminar in 2020)
- SchnOrb (NN to predict molecular wavefunctions directly): Schütt et al.; arxiv.org/abs/1906.10033
- Quantum Monte Carlo with DNNs:
 - PauliNet: Hermann et al.; arxiv.org/abs/1909.08423 (recommended!)
 - FermiNet: Pfau et al.; arxiv.org/abs/1909.02487 (DeepMind)
- sGDML: Chmiela et al.; doi.org/10.1016/j.cpc.2019.02.007 (non-NN force field with gradients!)

Talk Recordings

- Talks can be found at: <http://www.ipam.ucla.edu/programs/workshops/workshop-i-from-passive-to-active-generative-and-reinforcement-learning-with-physics/?tab=schedule> ; the recordings are very good!
- Some recommended talks:
 - Tess Smidt
 - Patrick Riley
 - Alexandre Tkatchenko
 - Frank Noé
 - Lars Ruthotto (mathematical background on DNNs)