AI FOR MATTERS

Molecules and Materials

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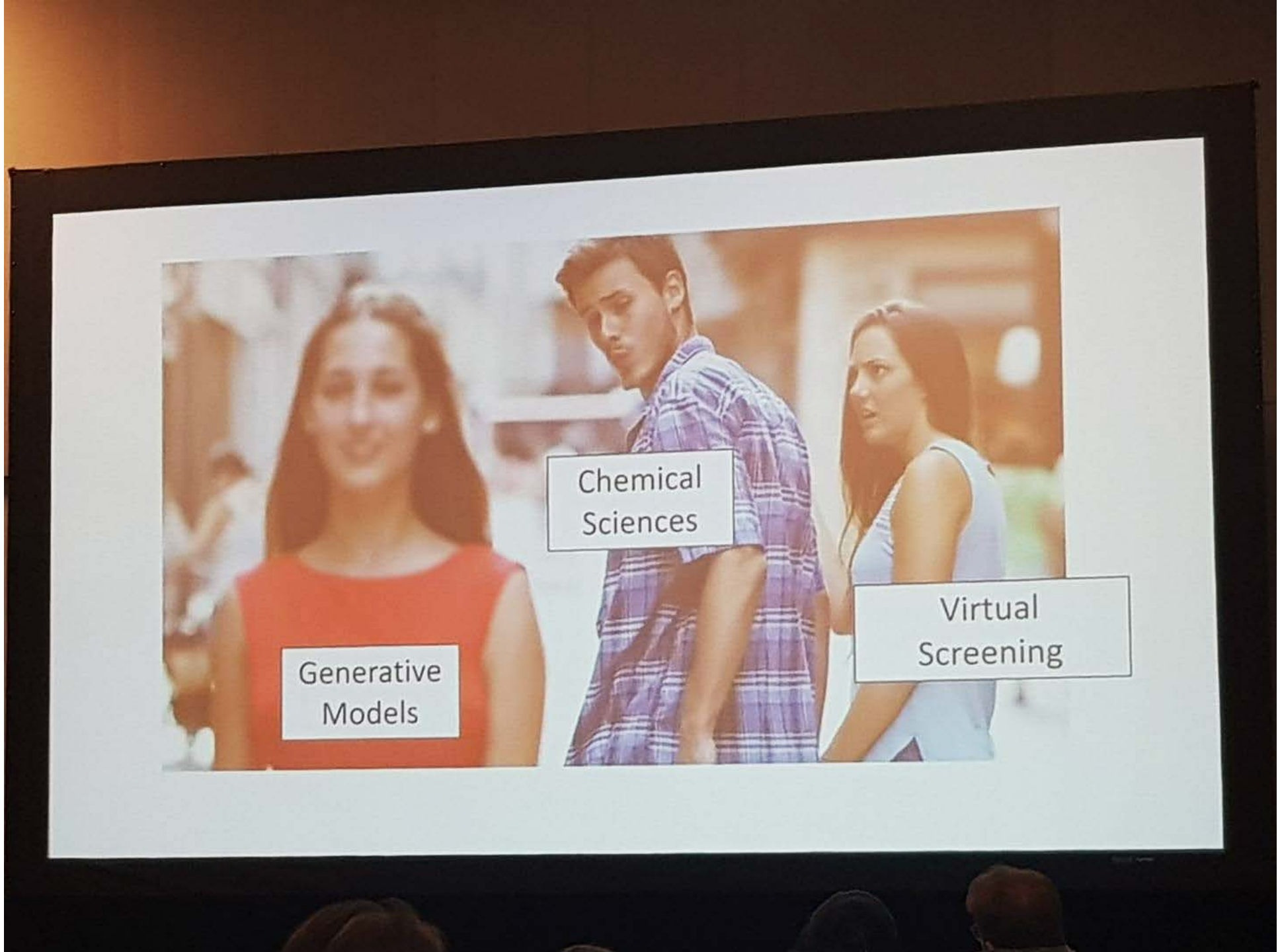
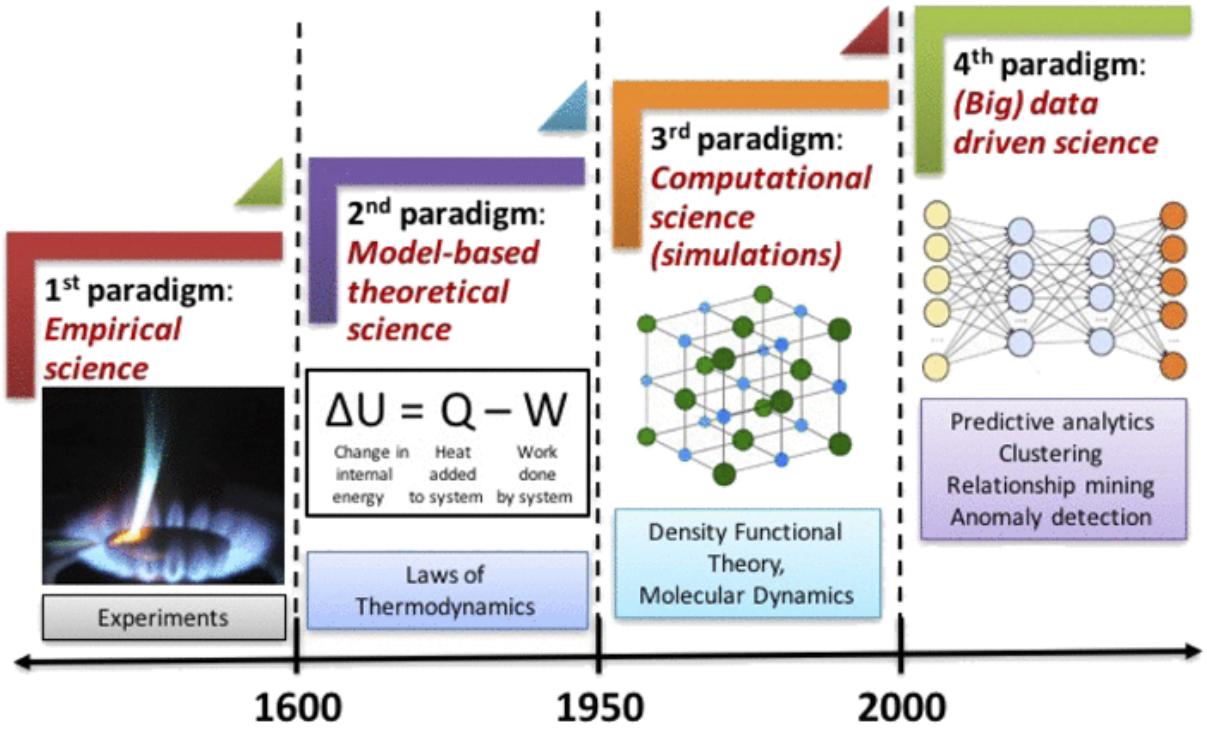
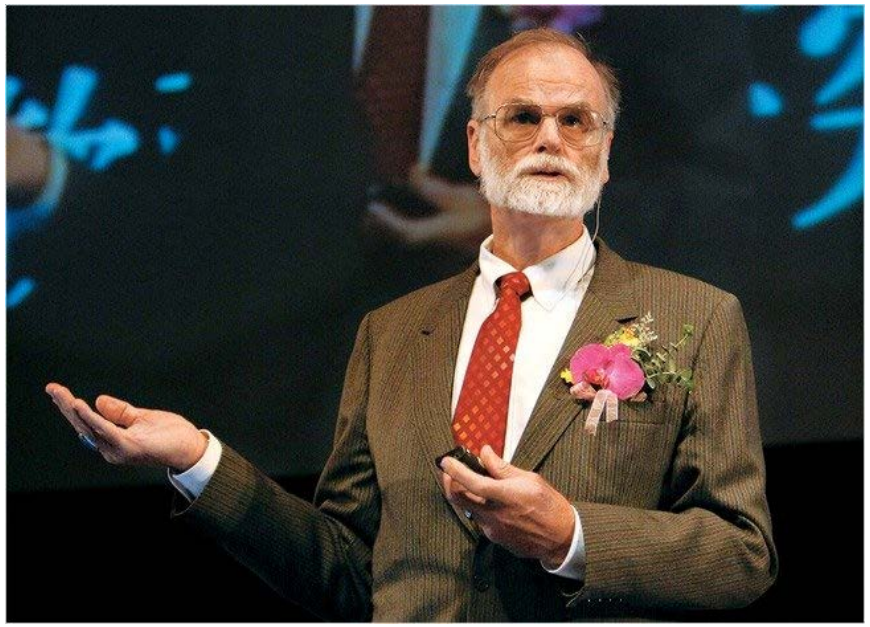
Hanoi, Jan 2019

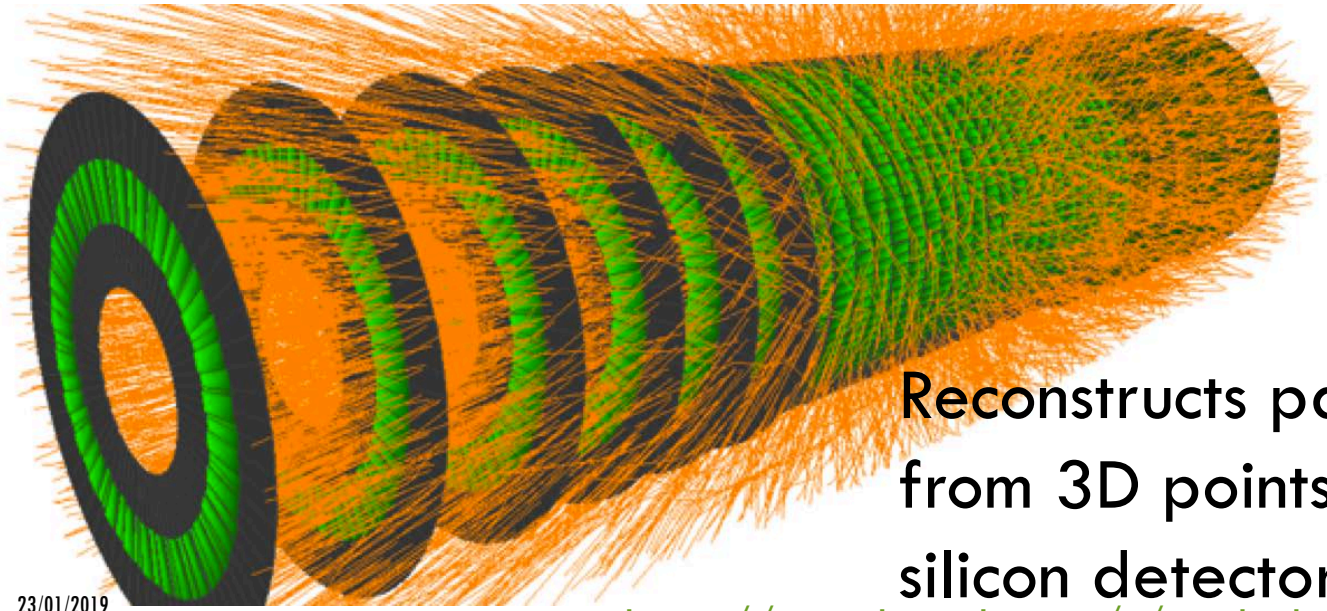

Chemical Sciences
Generative Models
Virtual Screening



Agrawal, A., & Choudhary, A. (2016). Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science. *Apl Materials*, *4*(5), 053208.



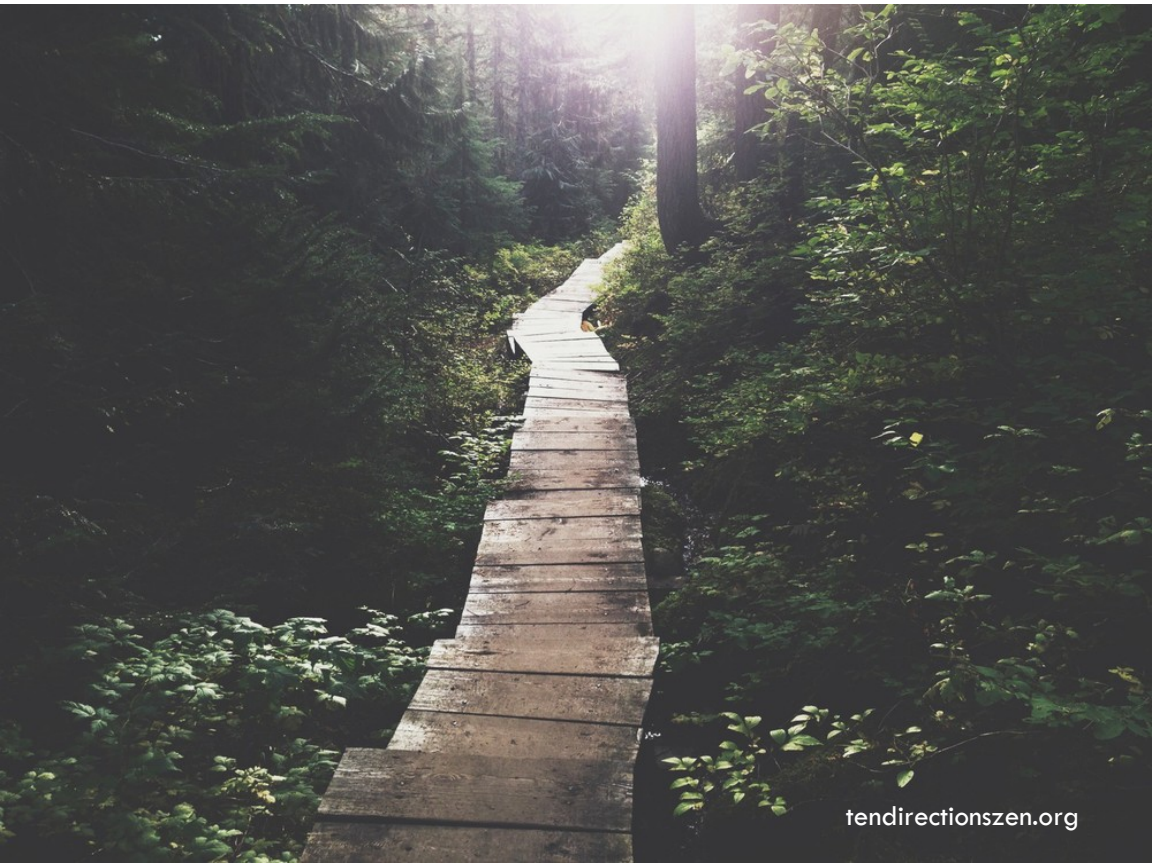
Jim Gray, Turing Award 1998 (1944-2007)
Honoured as father of ***The 4th Paradigm***



Reconstructs particle tracks from 3D points left in the silicon detectors.

https://www.kaggle.com/c/trackml-particle-identification

AI Research: dream

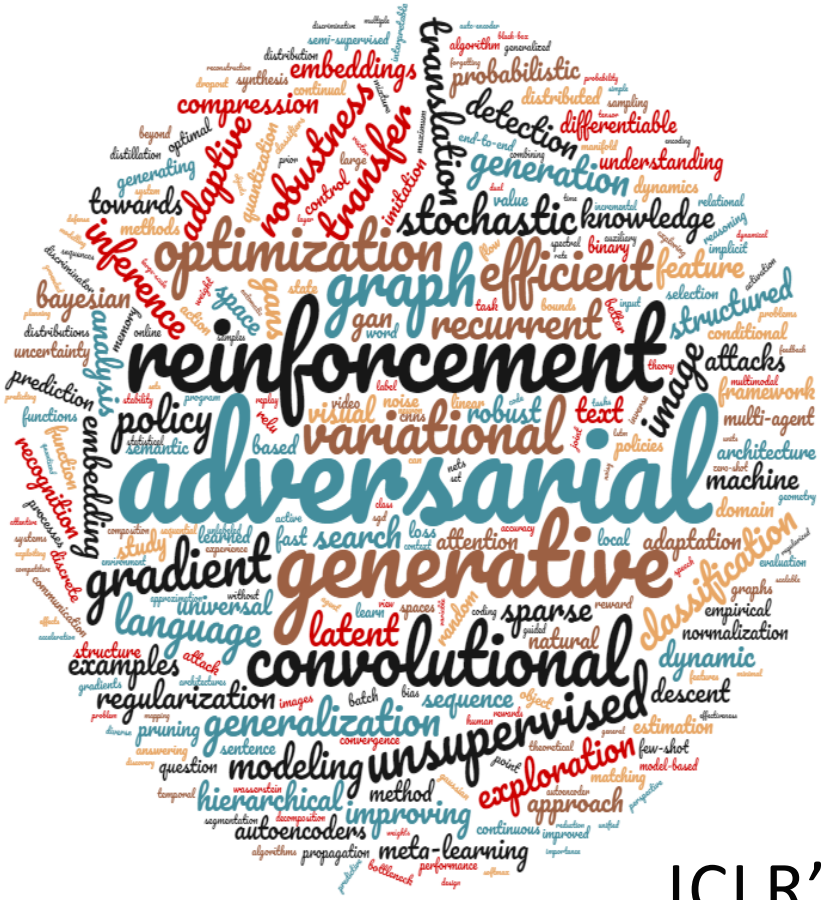


Among the most challenging scientific questions of our time are the corresponding analytic and synthetic problems:

- How does the brain function?
- Can we design a machine which will simulate a brain?

-- *Automata Studies*, 1956.

AI Research: reality



ICLR'19

What makes AI?

Perceiving

Learning

Reasoning

Planning

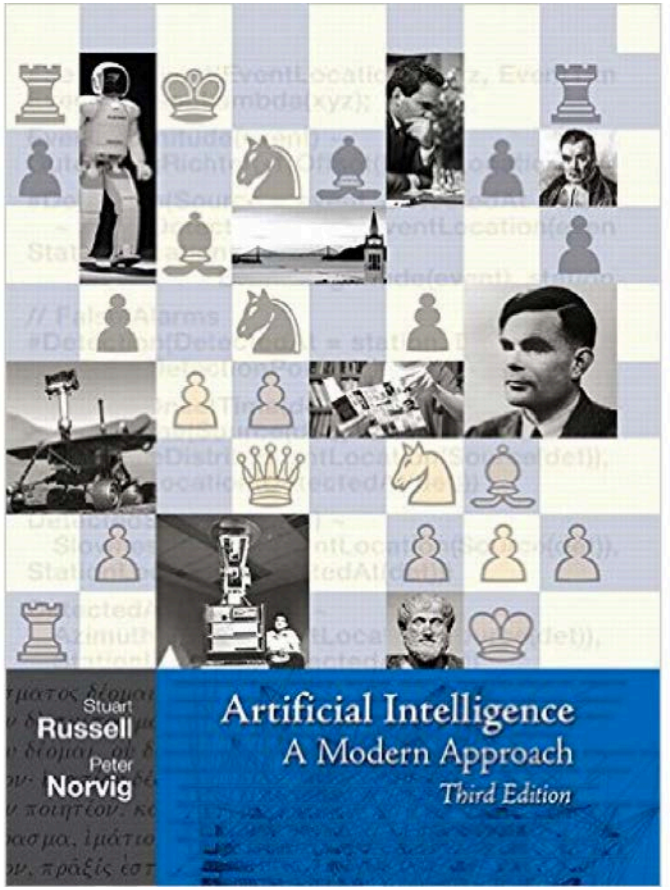
Acting

Robotics

Communicating

Consciousness

Automated discovery



Modern AI is mostly data-driven, as opposed to classic AI, which is mostly expert-driven.

What you can’t design, learn!
(aka variational method)

Filling the slot

- In-domain (intrapolation), e.g., an alloy with a given set of characteristics
- Out-domain (extrapolation), e.g., weather/stock forecasting
- Classsification, recognition, identification
- Action, e.g., driving
- Mapping space, e.g., translation
- Replacing expensive simulations

Estimating semantics, e.g., concept/relation embedding

Assisting experiment designs

Finding unknown, causal relation, e.g., disease-gene

Predicting experiment results, e.g., alloys → phase diagrams → material characteristics

Machine learning settings

Supervised learning

(mostly machin

A → B

Anywhere in between: semi-supervised learning, reinforcement learning, lifelong learning, meta-learning, few-shot learning, knowledge-based ML

Unsupervised learning

han)

$$\mathbf{v} \sim P_{model}(\mathbf{v})$$

$$(\mathbf{v}) \approx P_{data}(\mathbf{v})$$

Will be quickly solved for "easy problems (Andrew Ng)

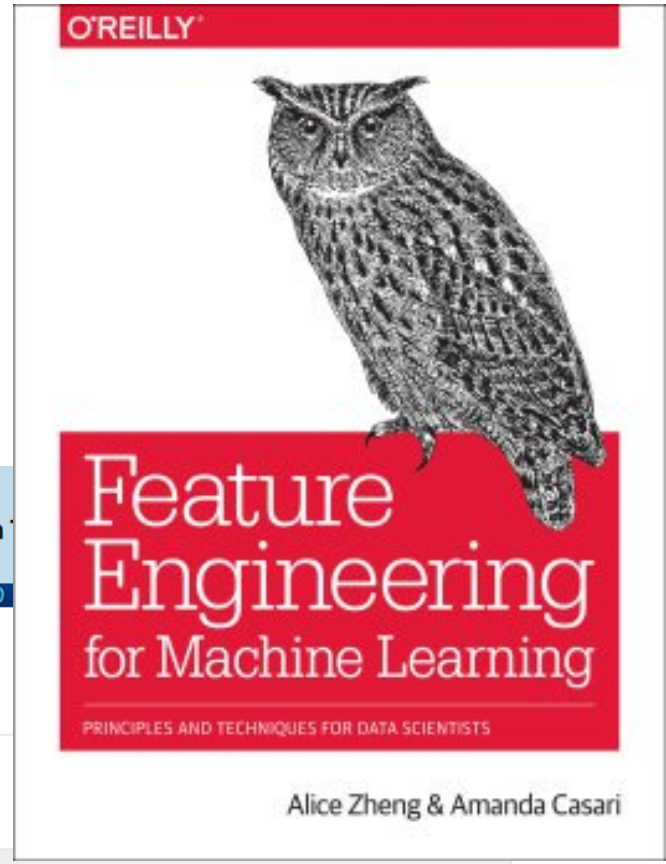
Idea: Over-represent and select

$3M Prize, 3 years

170K patients, 4 years worth of data

Predict length-of-stay next year

Not deep learning yet (early 2013), but strong ensemble needed → suggesting dropout/batch-norm



HERITAGE PROVIDER NETWORK HEALTH PRIZE

Truyen

Dashboard

Leaderboard - Heritage Health Prize

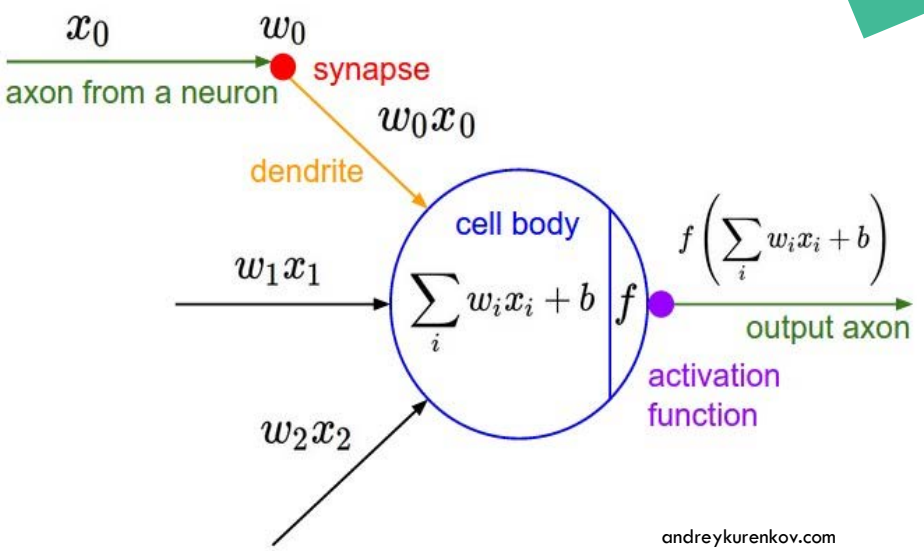
This competition has completed. This leaderboard reflects the final standings.

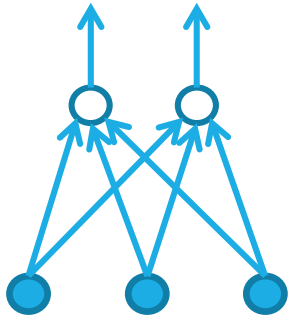
#	Δ1w	Team Name * in the money	Score	Entries	Last Submission UTC (Best – Last Submission)
1	-	POWERDOT *	0.461197	671	Thu, 04 Apr 2013 05:12:00 (-12.3d)
2	↑60	EXL Analytics	0.462247	555	Thu, 04 Apr 2013 00:06:09 (-3.4d)
3	↑15	J.A. Guerrero	0.462417	173	Thu, 04 Apr 2013 06:03:09
47	↓4	Midnight Run	0.467358	60	Fri, 15 Feb 2013 02:18:14 (-194.5d)
48	↓4	PookyPANTS	0.467387	6	Fri, 03 Feb 2012 21:30:44
49	↑31	Vietlabs	0.467543	8	Thu, 28 Mar 2013 22:36:51
50	↓5	jsf	0.467545	18	Wed, 03 Apr 2013 17:31:42 (-118d)

This is me!

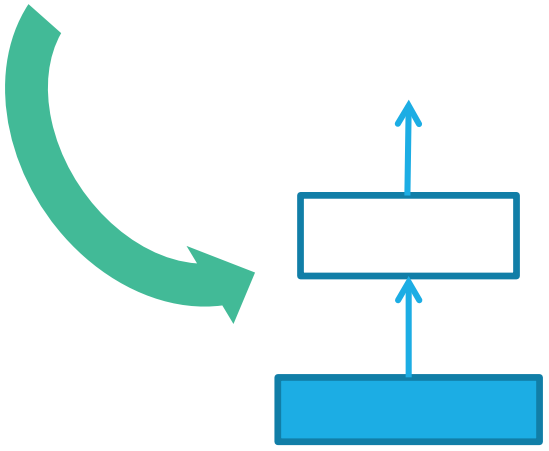
Idea: Filter stacking

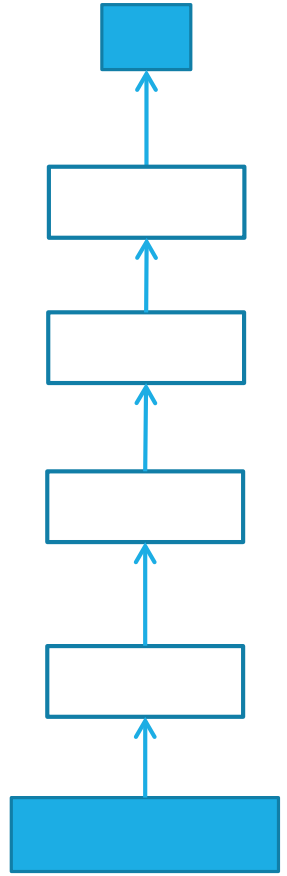
Integrate-and-fire neuron





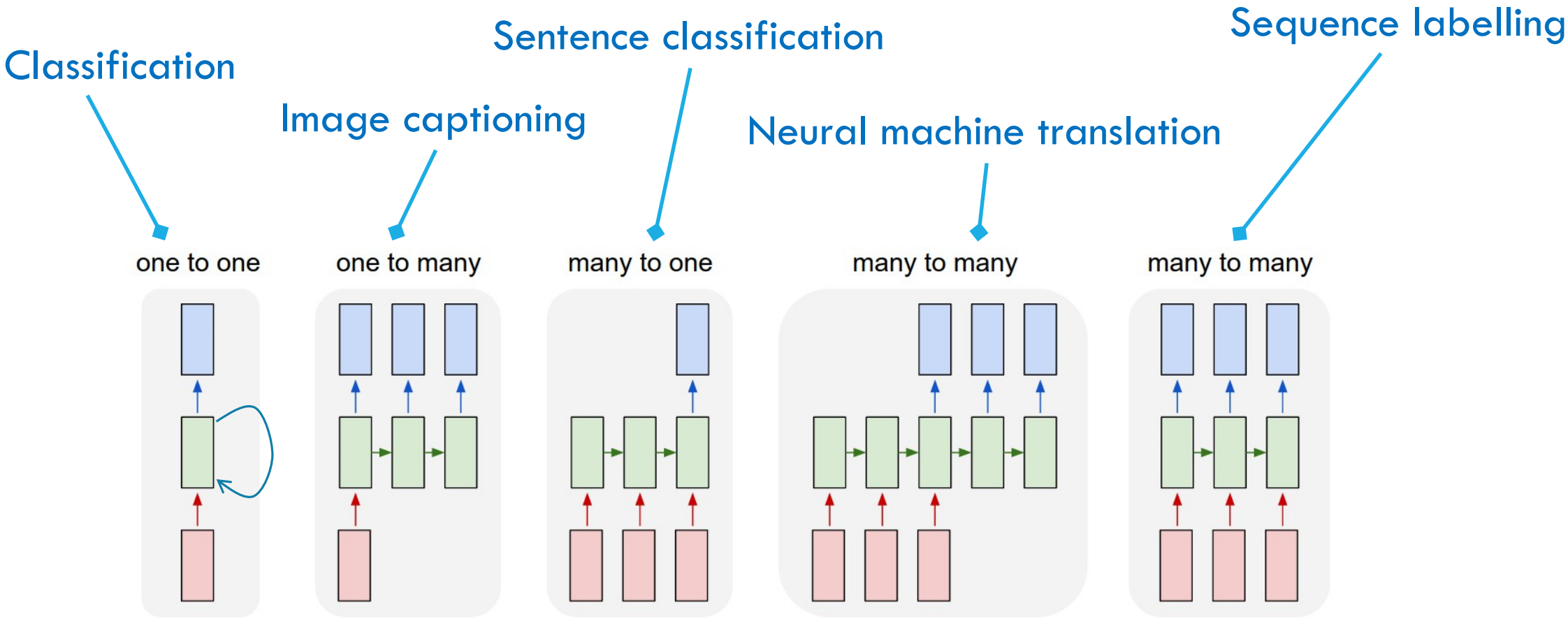
Feature detector





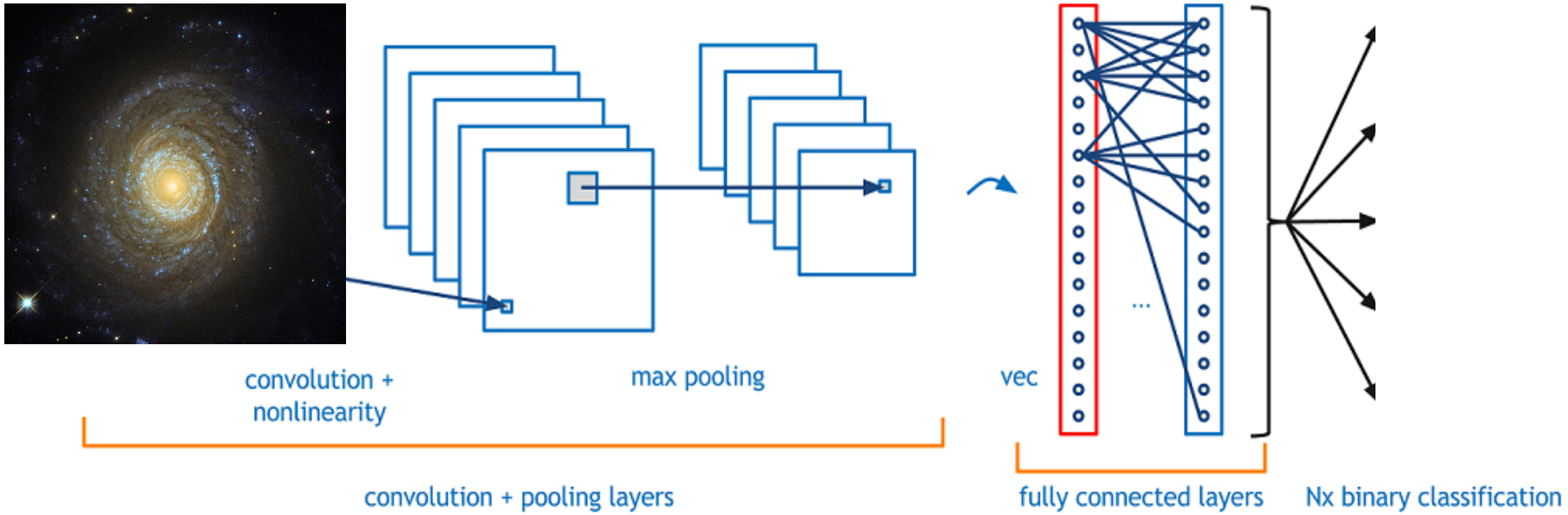
Block representation

Idea: Repeated refinement



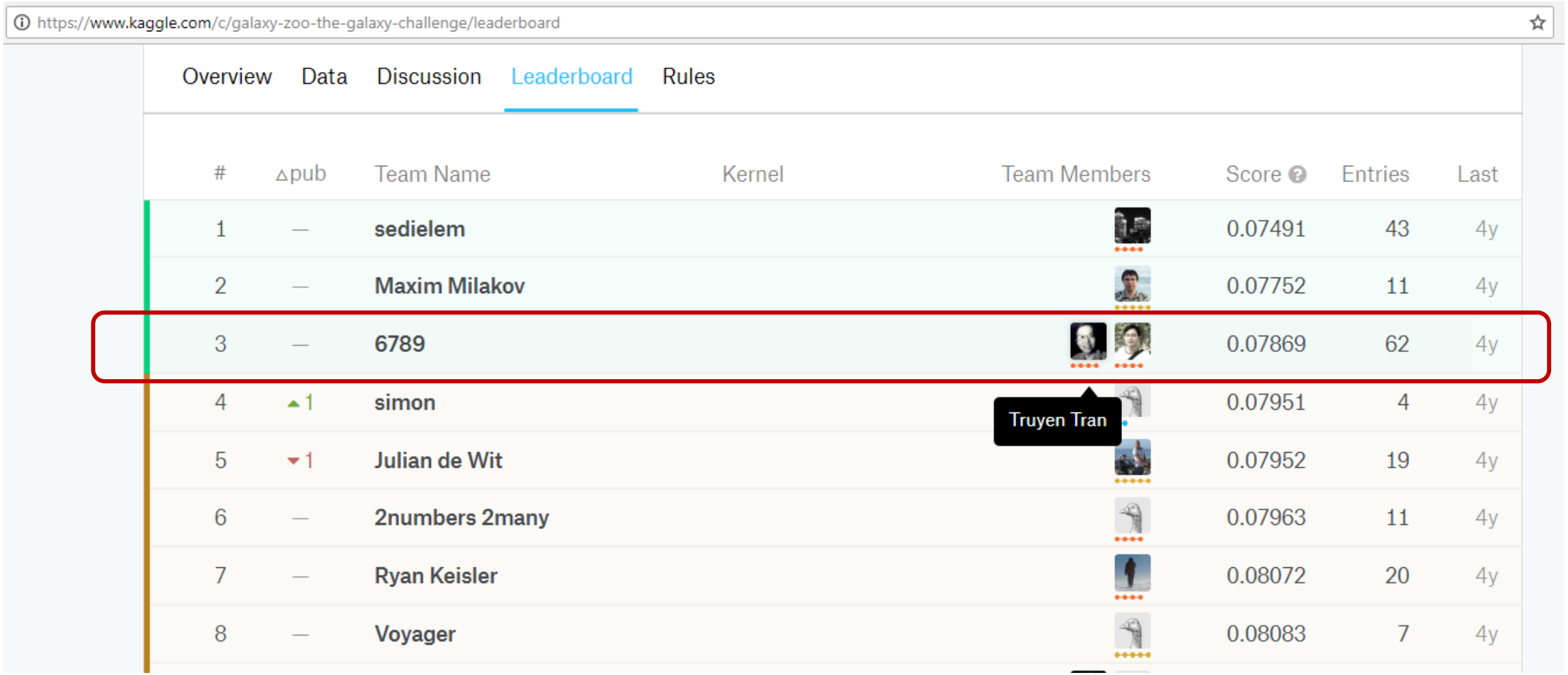
Source: http://karpathy.github.io/assets/rnn/diags.jpeg

Idea: Convolution & composition

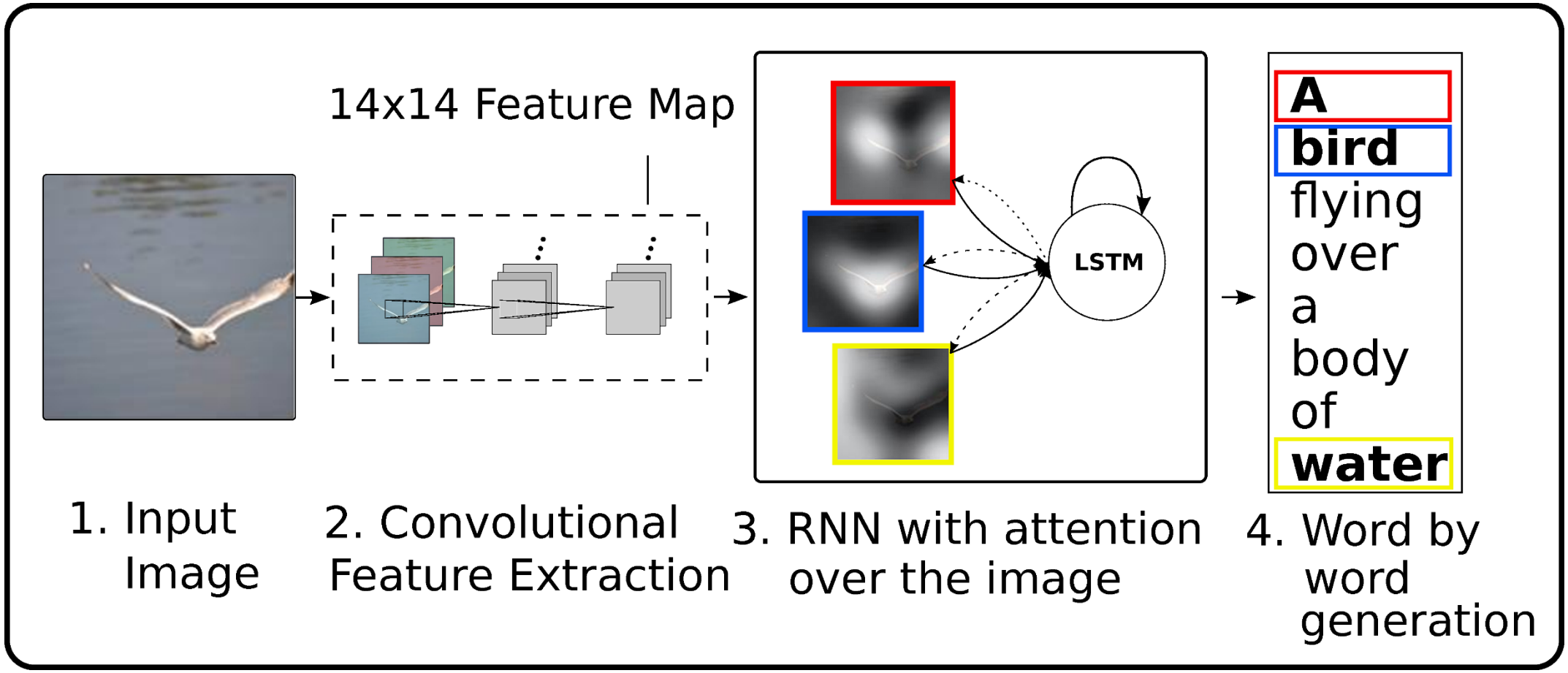


adeshpande3.github.io

Galaxy Zoo challenge: Categorization of galaxy images

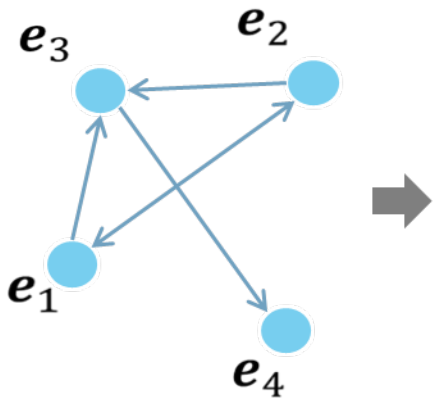


Idea: Attention

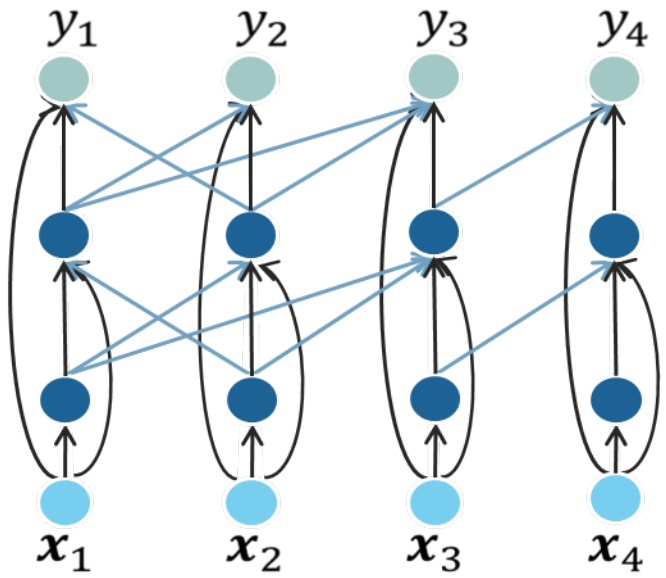


Show, Attend and Tell: Neural Image Caption Generation with Visual Attention, K. Xu , J. Ba, R. Kiros, K. Cho, A. Courville, R. Salakhutdinov, R. Zemel, Y. Bengio

Idea: Message passing

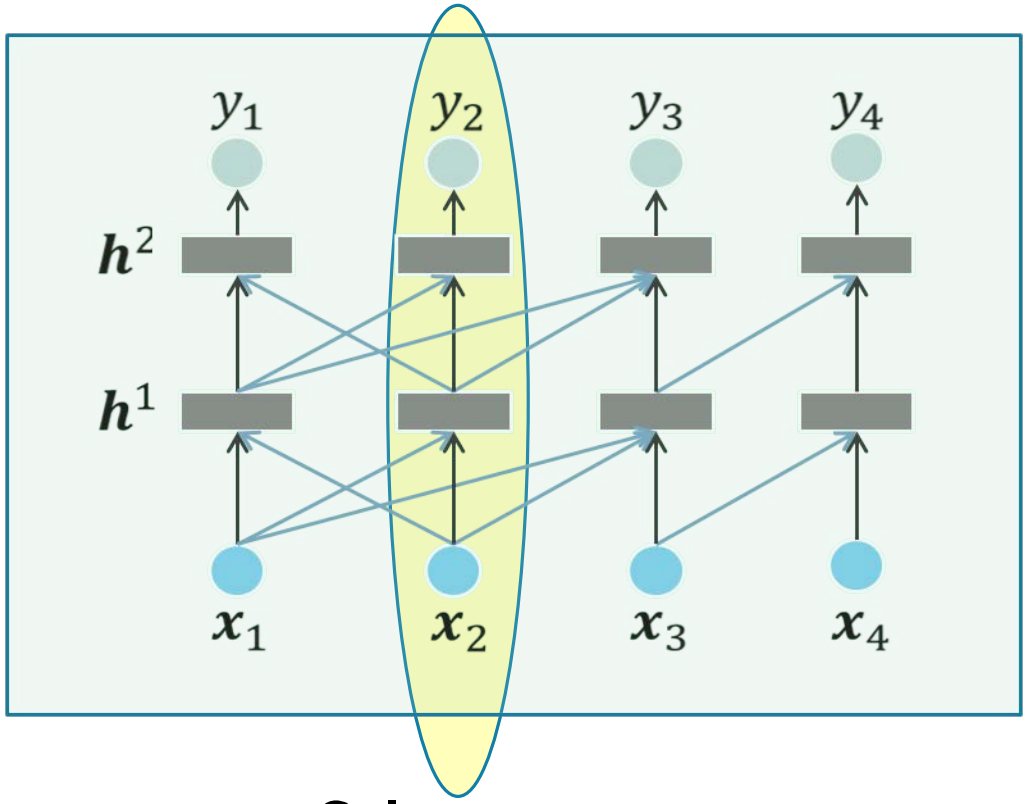


Relation graph



Stacked learning

Thin column



Column nets

#REF: Pham, Trang, et al. "Column Networks for Collective Classification." *AAAI*. 2017.

Generative models

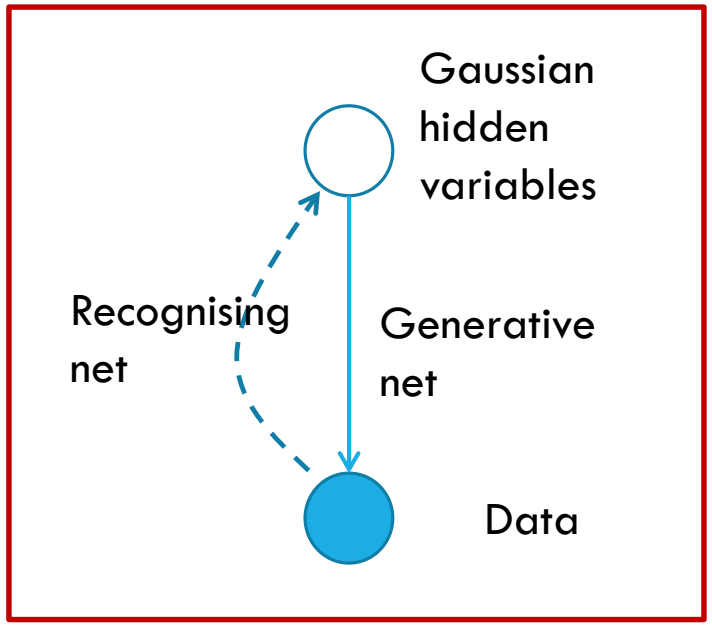
Many applications:

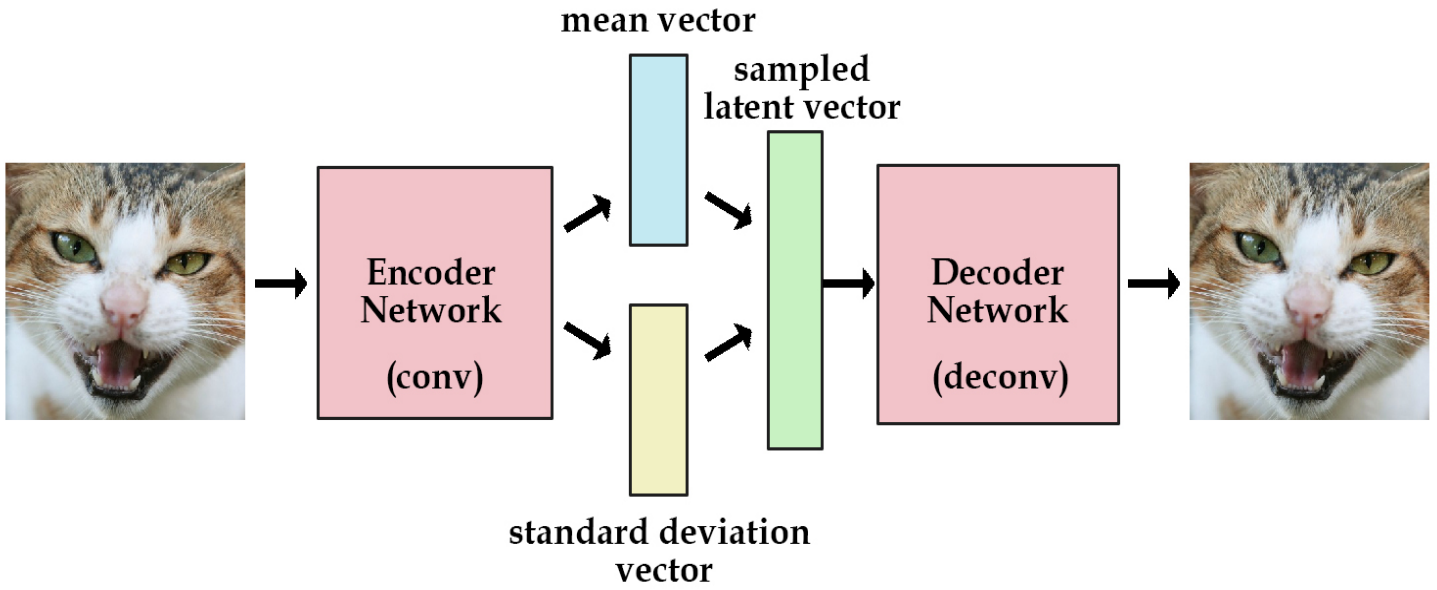
- Text to speech
- **Simulate data that are hard to obtain/share in real life (e.g., healthcare)**
- Generate meaningful sentences conditioned on some input (foreign language, image, video)
- Semi-supervised learning
- Planning

$$\mathbf{v} \sim P_{model}(\mathbf{v})$$
$$P_{model}(\mathbf{v}) \approx P_{data}(\mathbf{v})$$

Variational Autoencoder
(Kingma & Welling, 2014)

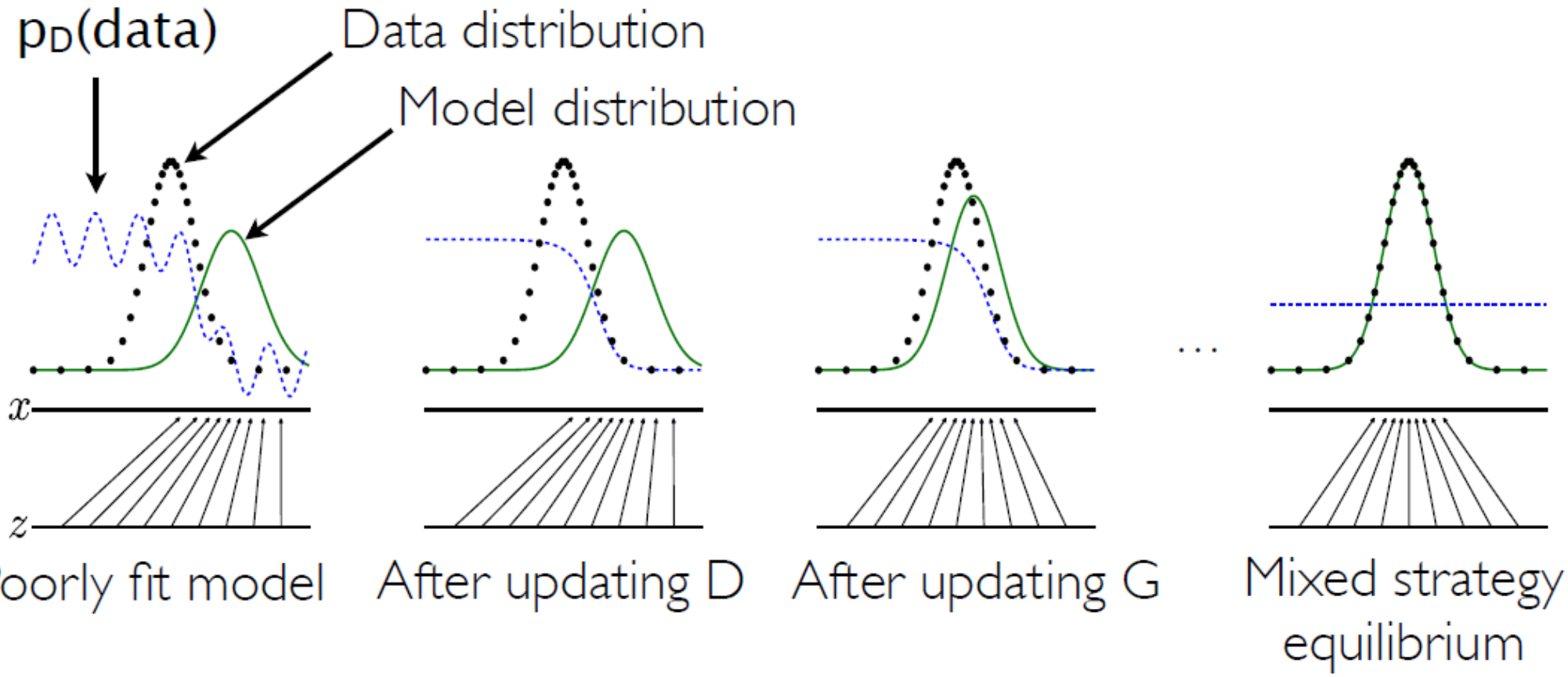
Two separate processes: generative (hidden → visible) versus recognition (visible → hidden)



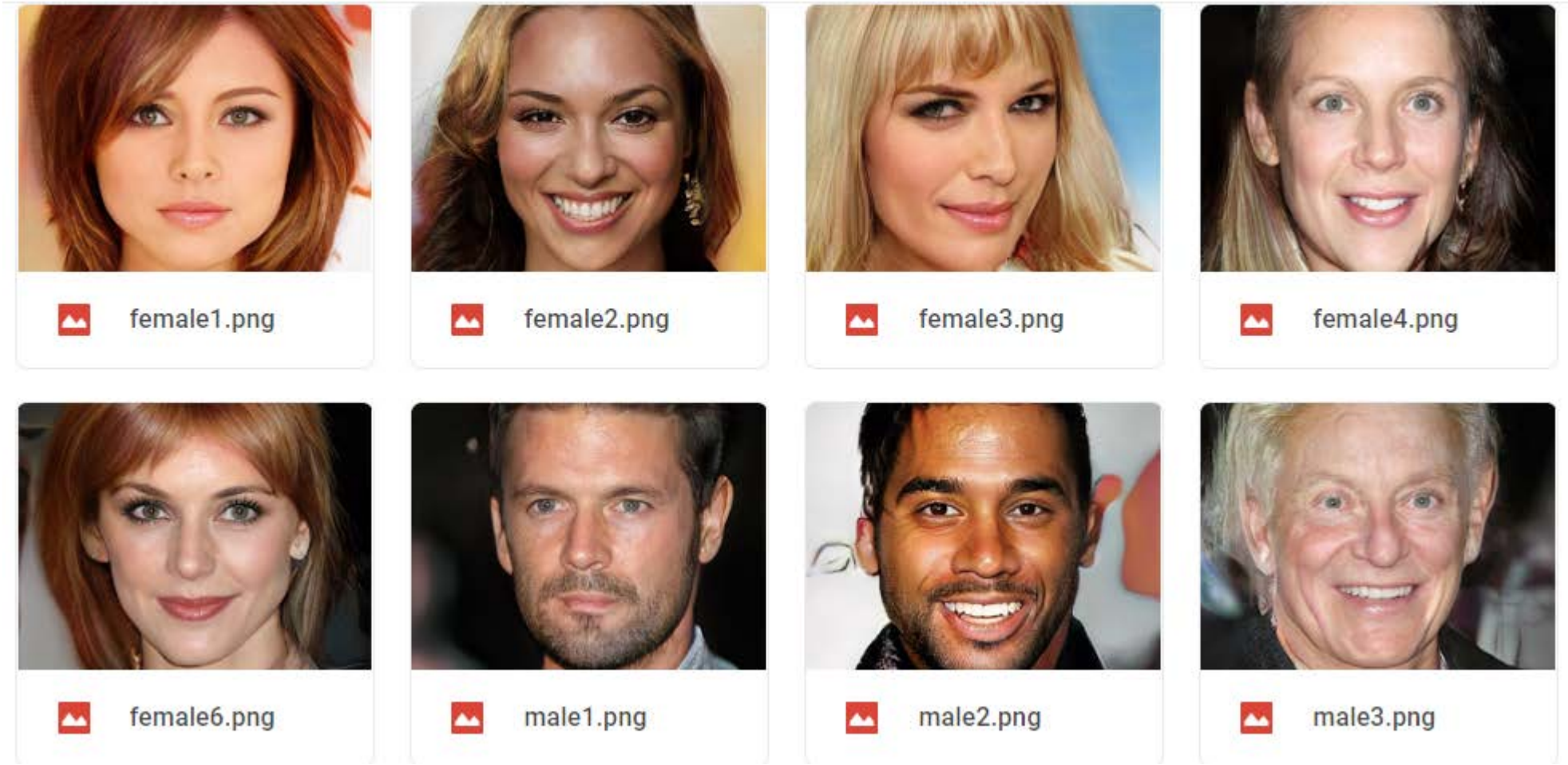


http://kvfrans.com/variational-autoencoders-explained/

Generative adversarial networks
(Adapted from Goodfellow's, NIPS 2014)



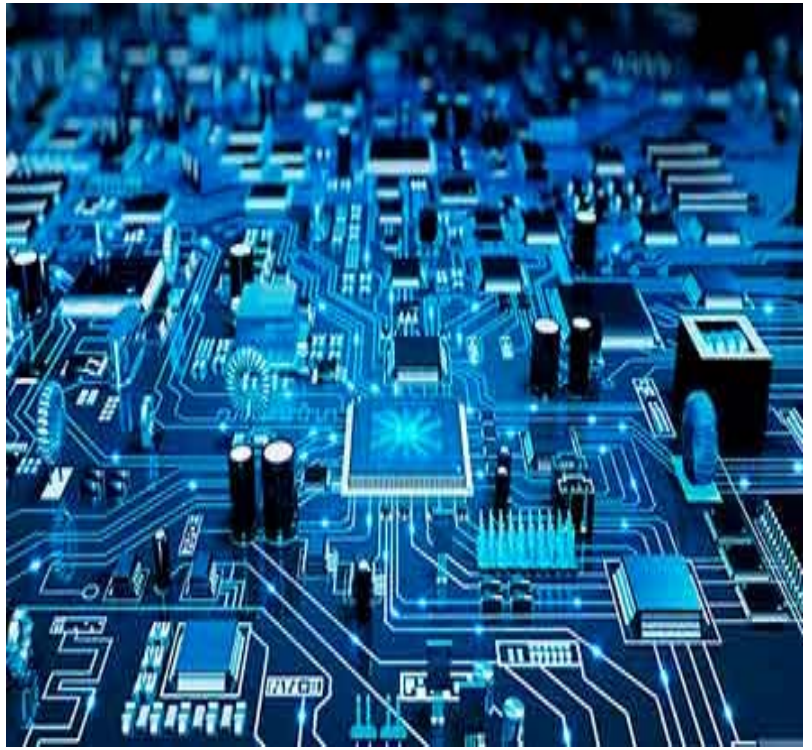
Progressive GAN: Generated images



Karras, T., Aila, T., Laine, S., & Lehtinen, J. (2017). Progressive growing of gans for improved quality, stability, and variation. *arXiv preprint arXiv:1710.10196*.

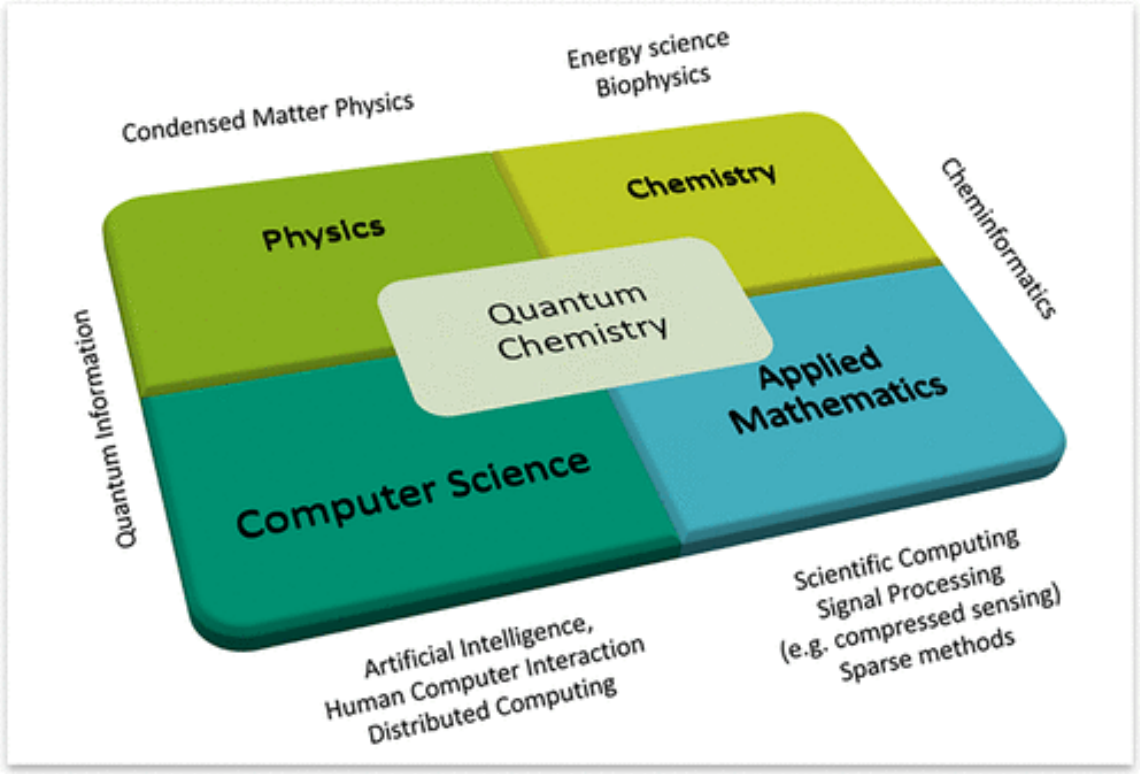
Deep learning vs electronics

- Neuron as feature detector → SENSOR, FILTER
- Multiplicative gates → AND gate, Transistor, Resistor
- Attention mechanism → SWITCH gate
- Memory + forgetting → Capacitor + leakage
- Skip-connection → Short circuit
- Computational graph → Circuit
- Compositionality → Modular design



AI for molecules

- Represent atom/molecular space
- Predict molecular properties
- Estimate chem-chem interaction
- Predict chemical reaction
- Fast search for new molecules
- Plan chemical synthesis



https://pubs.acs.org/doi/full/10.1021/acscentsci.7b00550

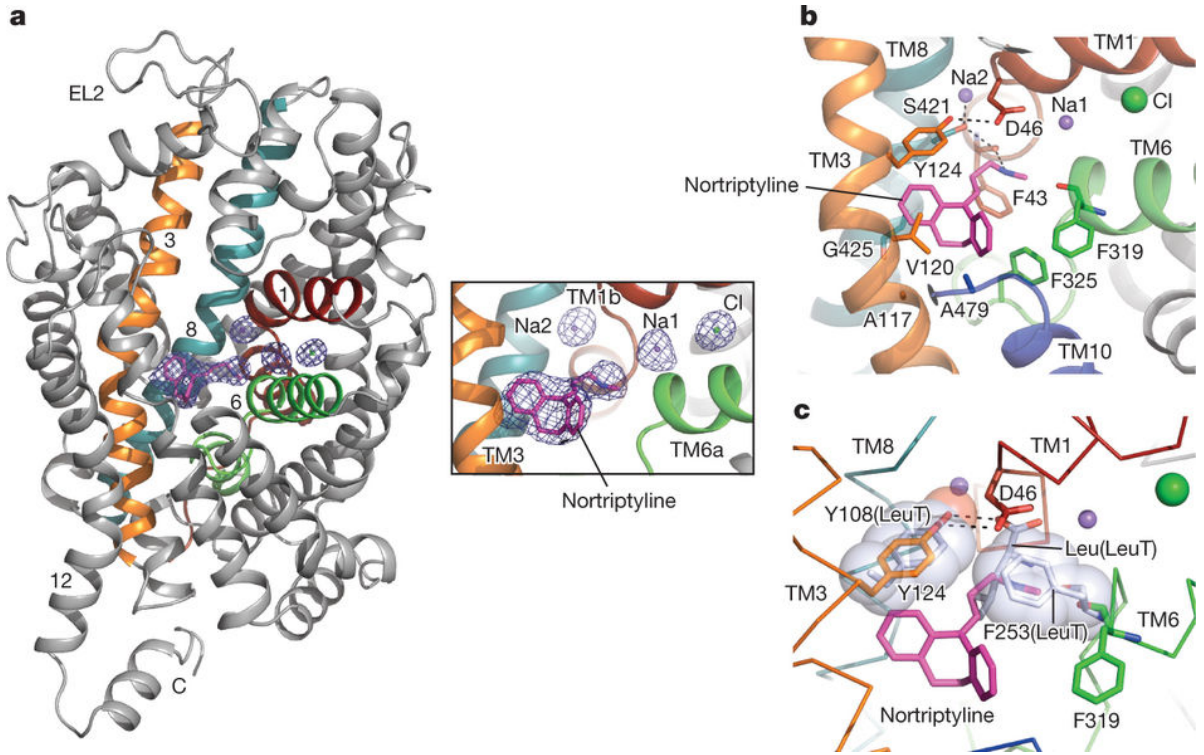
Molecular properties prediction

Traditional techniques:

- Graph kernels (ML)
- Molecular fingerprints (Chemistry)

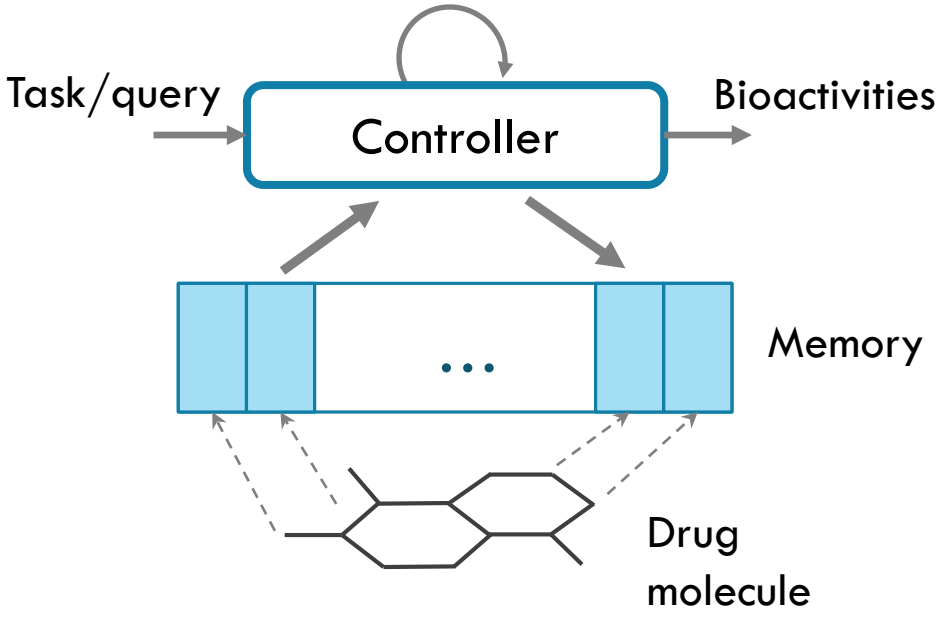
Modern techniques

- Molecule as graph: atoms as nodes, chemical bonds as edges

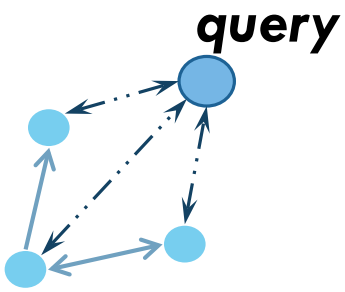


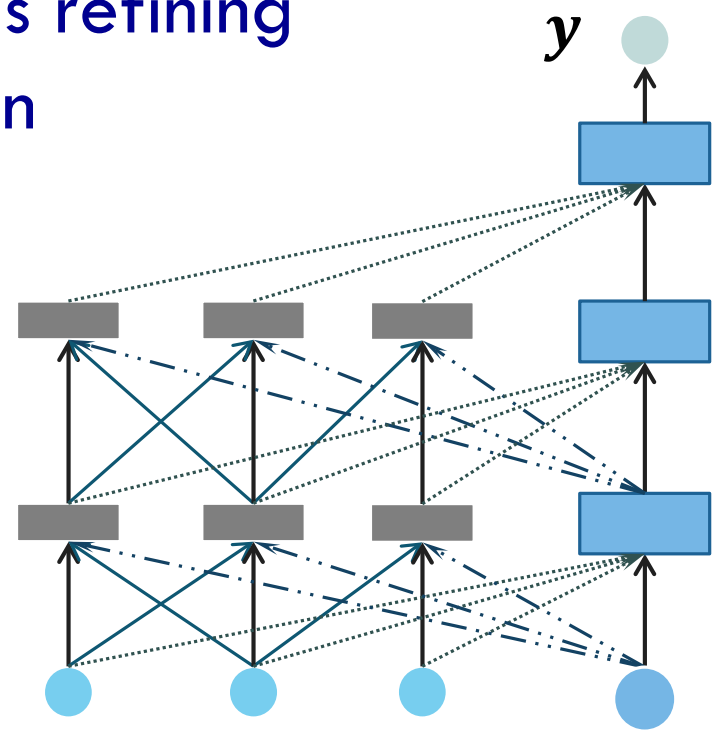
#REF: Penmatsa, Aravind, Kevin H. Wang, and Eric Gouaux. "X-ray structure of dopamine transporter elucidates antidepressant mechanism." *Nature* 503.7474 (2013): 85-90.

Graph memory networks (GMN)



Message passing as refining atom representation





#Ref: Pham, Trang, Truyen Tran, and Svetha Venkatesh. "Graph Memory Networks for Molecular Activity Prediction." *ICPR'18*.

GMN on molecular bioactivities

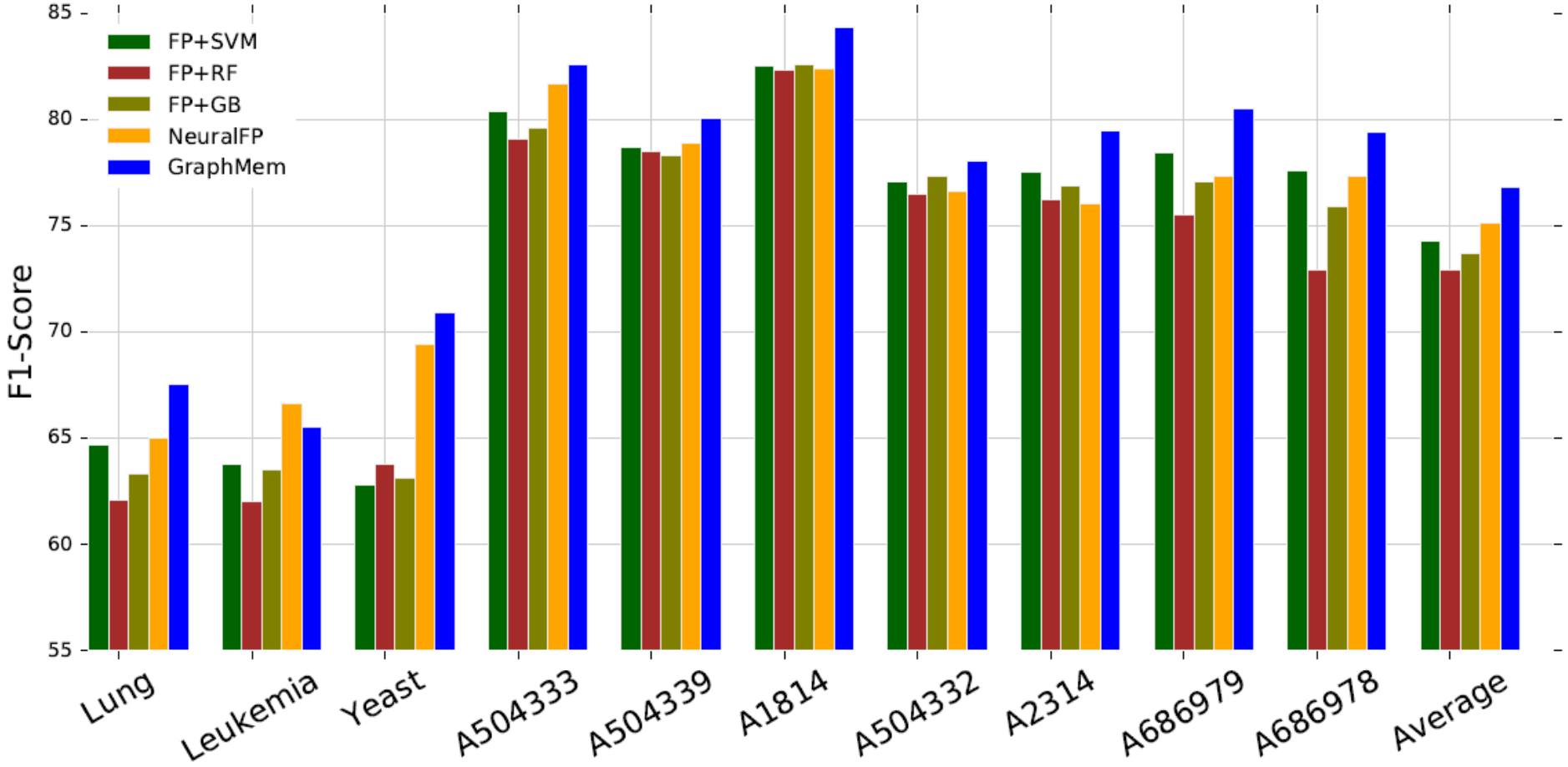
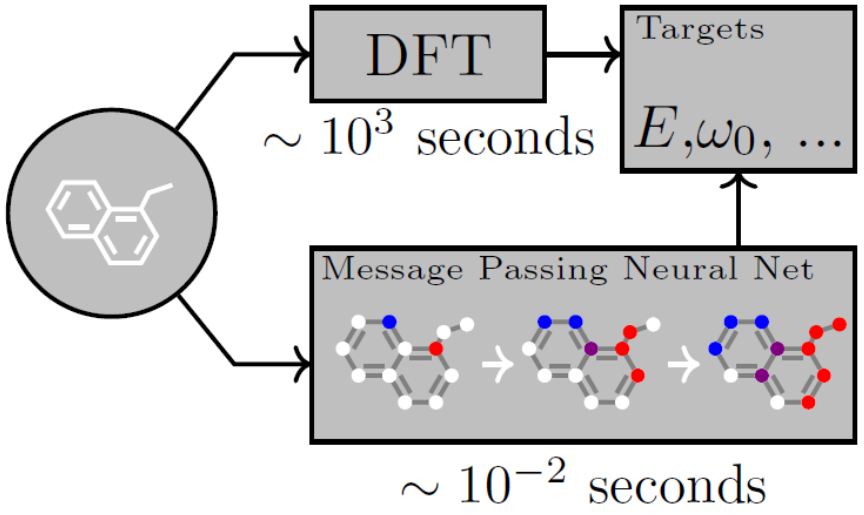


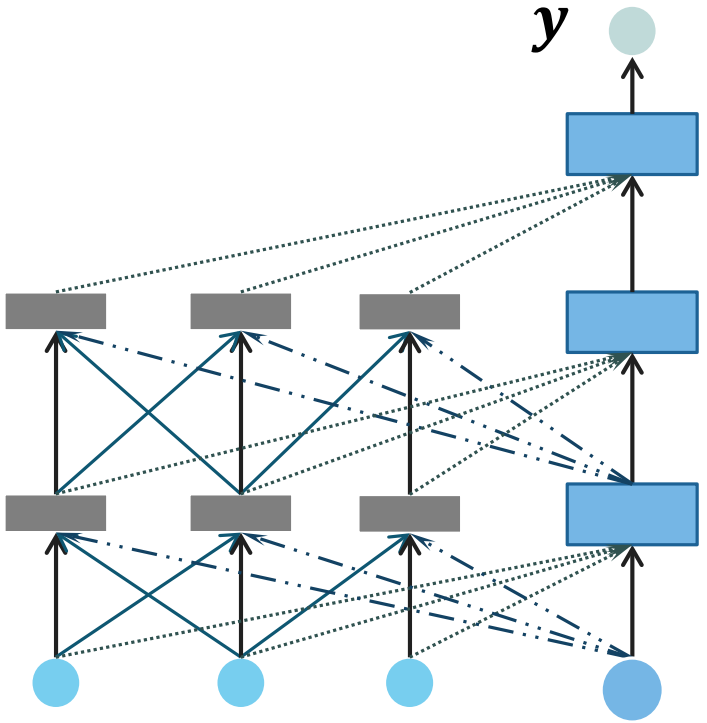
Figure 2: F1-score (%) for NCI datasets. FP = Fingerprint; RF = Random Forests; GBM = Gradient Boosting Machine. Best view in color.

Approximating DFT

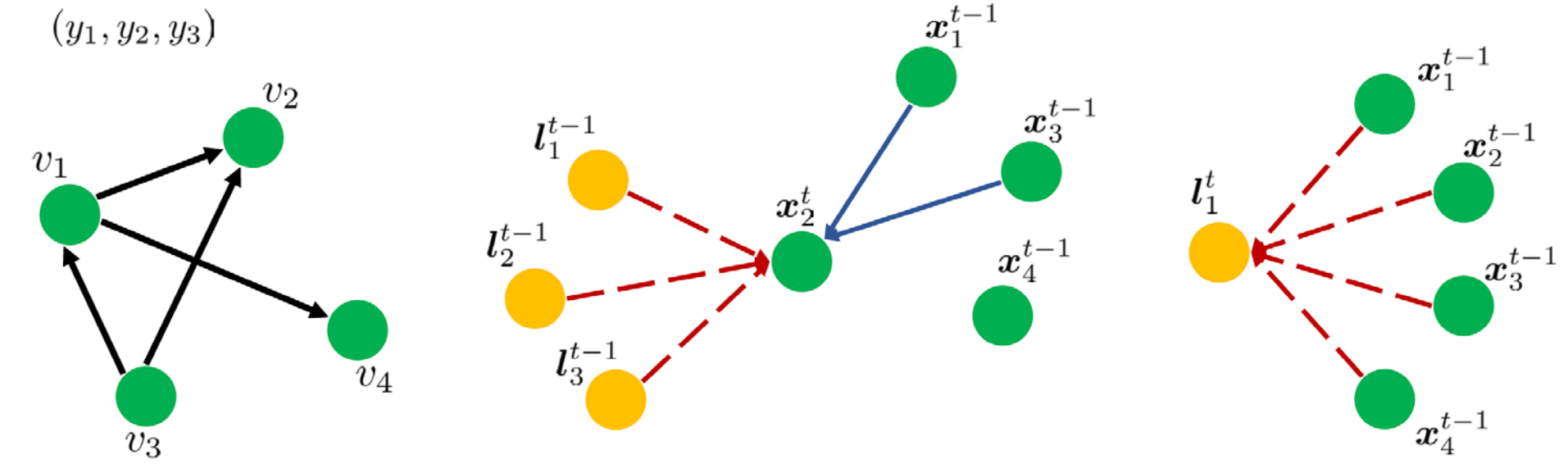
DFT = Density Functional Theory

Gilmer, Justin, et al. "Neural message passing for quantum chemistry." *arXiv preprint arXiv:1704.01212* (2017).





Predict multiple properties



(a) A input graph with 4 nodes and 3 labels

(b) Input node update

(c) Label node update

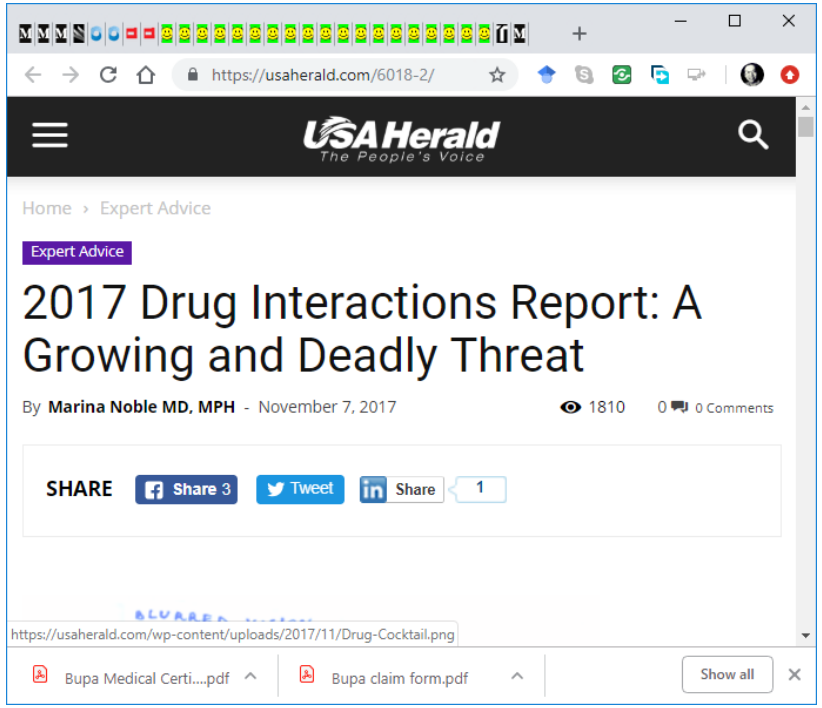
#REF: Do, Kien, et al. "Attentional Multilabel Learning over Graphs-A message passing approach." *Machine Learning, 2019*.

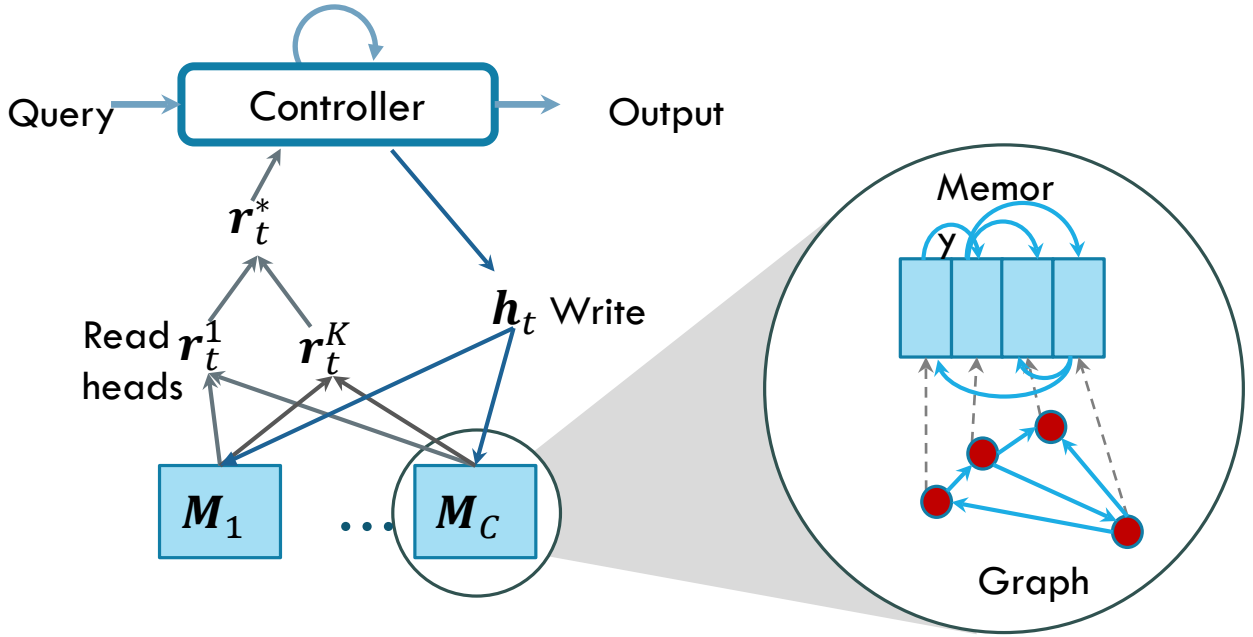
Dataset	Metrics	Fingerprint		SMILES	Molecular Graph		
		SVM	HWN	GRU	WL+SVM	CLN	GAML
9cancers	m-AUC	81.94	85.95	83.29	86.06	88.35	**88.78**
	M-AUC	81.37	85.85	82.74	85.74	88.23	**88.50**
	m-F1	50.63	57.44	55.97	54.55	59.48	**62.03***
	M-F1	50.71	57.29	55.99	54.54	59.50	**62.14***
50proteins	m-AUC	79.85	77.46	79.11	81.62	82.08	**82.82**
	M-AUC	74.77	73.78	75.25	77.60	78.36	**79.35***
	m-F1	17.21	16.37	16.08	17.04	18.37	**20.47***
	M-F1	18.40	15.87	14.96	18.66	17.72	**19.83***

Table 4: The performance in the multi-label classification with graph-structured input (m-X: micro average of X; M-X: macro average). SVM and HWN work on fingerprint representation; GRU works on string representation of molecule known as SMILES; WL+BR and CLN work directly on graph representation. Bold indicates better values. (*) $p < 0.05$.

#REF: Do, Kien, et al. "Attentional Multilabel Learning over Graphs-A message passing approach." *Machine Learning 2019*.

Chemical-chemical interaction via *Relational Dynamic Memory Networks*





#REF: Pham, Trang, Truyen Tran, and Svetha Venkatesh. "Relational dynamic memory networks." *arXiv preprint arXiv:1808.04247*(2018).

Results on STITCH database

	CCI900		CCI800	
	AUC	F1-score	AUC	F1-score
Random Forests	94.3	86.4	98.2	94.1
Highway Networks	94.7	88.4	98.5	94.7
DeepCCI [31]	96.5	92.2	99.1	97.3
RDMN	96.6	92.6	99.1	97.4
RDMN+multiAtt	97.3	93.4	99.1	97.8
RDMN+FP	97.8	93.3	99.4	98.0
RDMN+multiAtt+FP	98.0	94.1	99.5	98.1
RDMN+SMILES	98.1	94.3	99.7	97.8
RDMN+multiAtt+SMILES	**98.1**	**94.6**	**99.8**	**98.3**

Table 3 The performance on the CCI datasets reported in AUC and F1-score. *FP* stands for fingerprint and *multiAtt* stands for multiple attentions.

Chemical reaction product prediction as reinforcement learning

Input: Molecules

Output: Molecules

Model: Graph morphism

Method: Graph transformation policy network (GTPN)

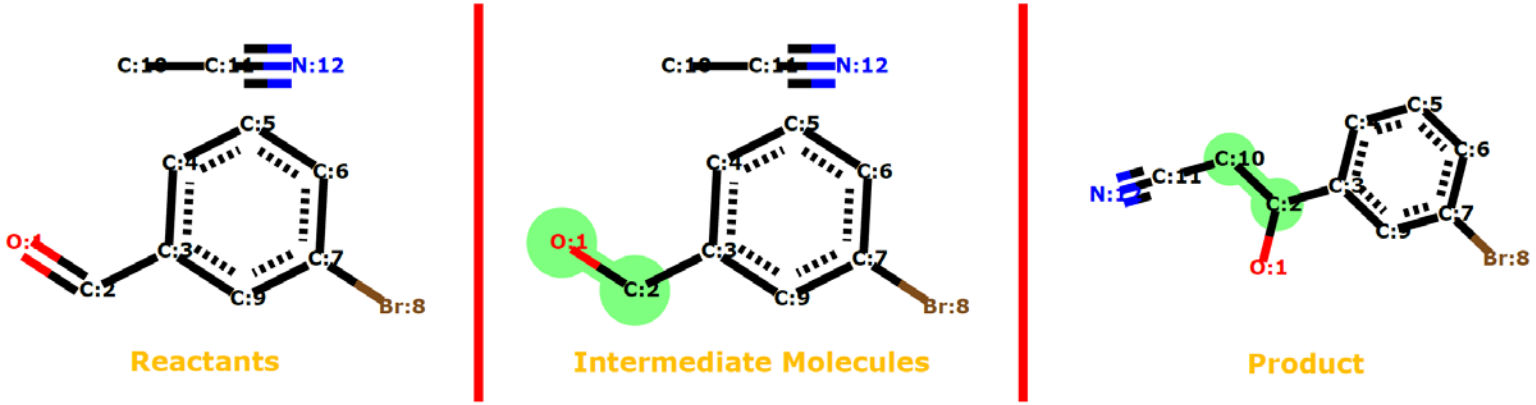


Figure 1: A sample reaction represented as a set of graph transformations from reactants (leftmost) to products (rightmost). Atoms are labeled with their type (Carbon, Oxygen,...) and their index (1, 2,...) in the molecular graph. The atom pairs that change connectivity and their new bonds (if existed) are highlighted in green. There are two bond changes in this case: 1) The double bond between O:1 and C:2 becomes single. 2) A new single bond between C:2 and C:10 is added.

Do, Kien, Truyen Tran, and Svetha Venkatesh. "Graph Transformation Policy Network for Chemical Reaction Prediction." *arXiv preprint arXiv:1812.09441* (2018).

GTPN results

Model	*USPTO-15k*			*USPTO*		
	P@1	*P@3*	*P@5*	*P@1*	*P@3*	*P@5*
WLDN (Jin et al., 2017)	*76.7*	*85.6*	***86.8***	*79.6*	***87.7***	***89.2***
Seq2Seq (Schwaller et al., 2018)	-	-	-	80.3⋆	86.2⋆	87.5⋆
GTPN	72.31	-	-	71.26	-	-
GTPN♢	74.56	82.62	84.23	73.25	80.56	83.53
GTPN♢♣	74.56	83.19	84.97	73.25	84.31	85.76
GTPN♢♠	**82.39**	85.60	86.68	**83.20**	84.97	85.90
GTPN♢♠♣	**82.39**	**85.73**	**86.78**	**83.20**	86.03	86.48

Table 3: Results for reaction prediction. *P@k* is precision at k. State-of-the-art results from (Jin et al., 2017) are written in italic. Results from (Schwaller et al., 2018) are marked with ⋆ and they are computed on a slightly different version of USPTO that contains only single-product reactions. Best results are highlighted in bold. ♢: With beam search (beam width = 20), ♠: Invalid product removal, ♣: Duplicated product removal.

Molecular generation: Case of drug

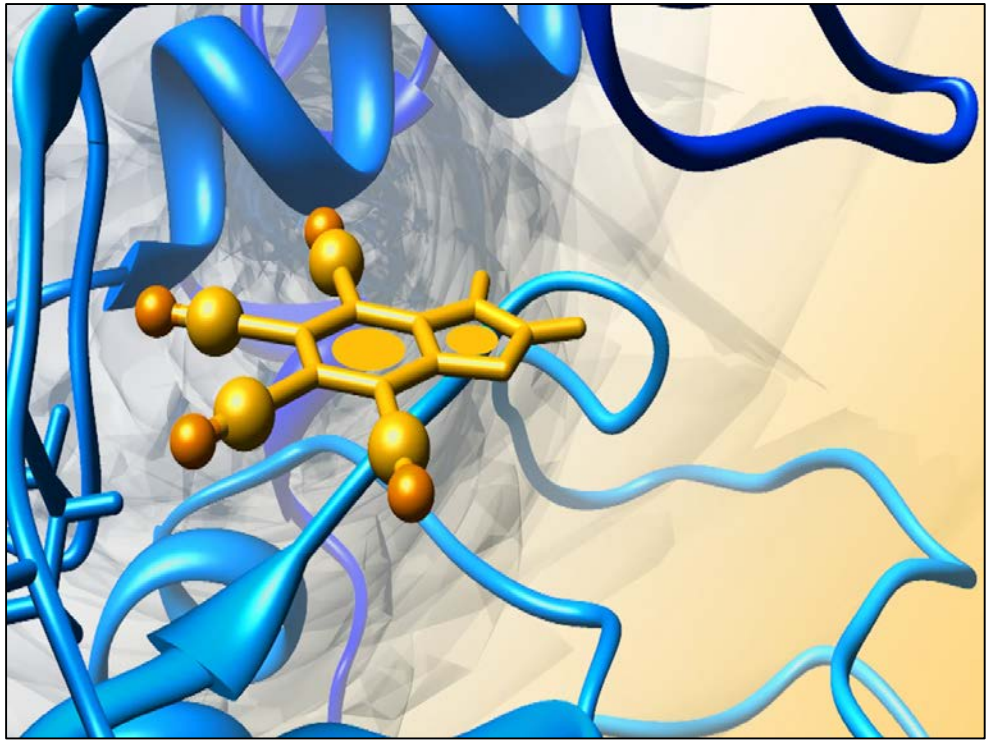
The space of drugs is estimated to be 1e+23 to 1e+60

- Only 1e+8 substances synthesized thus far.

It is impossible to model this space fully.

The current technologies are not mature for graph generations.

But approximate techniques do exist.



Source: pharmafactz.com

Combinatorial chemistry

Generate variations on a template

Returns a list of molecules from this template that

- Bind to the pocket with good pharmacodynamics?
- Have good pharmacokinetics?
- Are synthetically accessible?

#REF: Talk by Chloé-Agathe Azencott titled “Machine learning for therapeutic research”, 12/10/2017

AI approach to molecule design

Representing molecules using fingerprints

Representing graph as string, and use sequence VAEs or GANs.

Graph VAE & GAN

- Model nodes & interactions
- Model cliques

Sequences

- Iterative methods

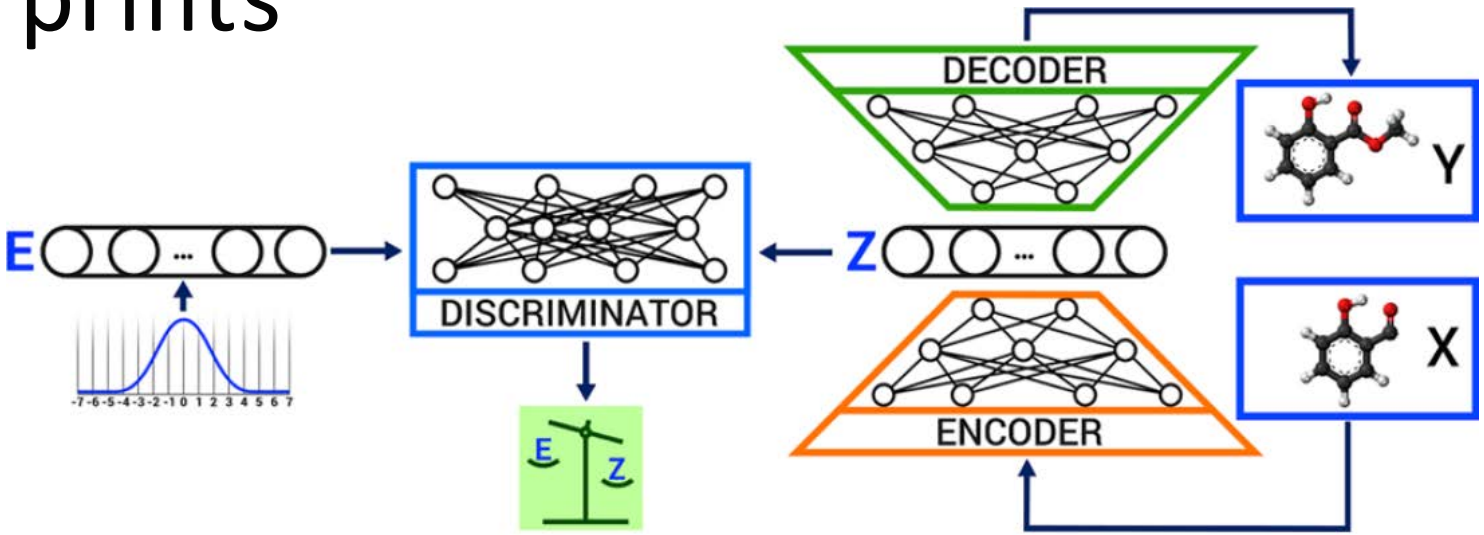
Reinforcement learning

- Discrete objectives

Any combination of these + memory.

Kadurin, Artur, et al. "The cornucopia of meaningful leads: Applying deep adversarial autoencoders for new molecule development in oncology." *Oncotarget* 8.7 (2017): 10883.

Molecule → fingerprints



Input of the encoder : the fingerprint of a molecule

The decoder outputs the predicted fingerprint .

The generative model generates a vector E, which is then discriminated from the latent vector of the real molecule by the discriminator.

Molecule → string

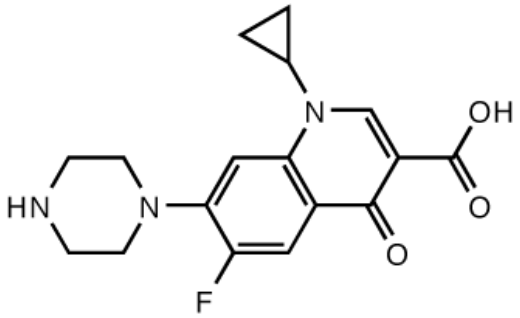
Using SMILES representation of molecule, to convert a molecular graph into a string

- SMILES = Simplified Molecular-Input Line-Entry System

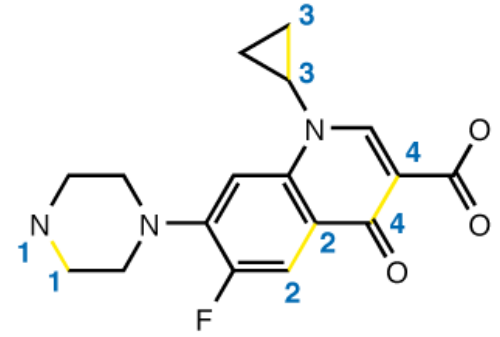
Then using sequence-to-sequence + VAE/GAN to model the continuous space that encodes/decodes SMILES strings

- Allow easy optimization on the continuous space

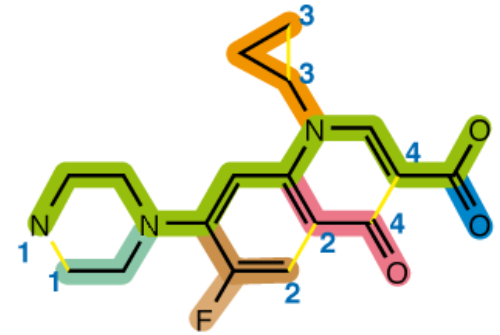
A



B



C



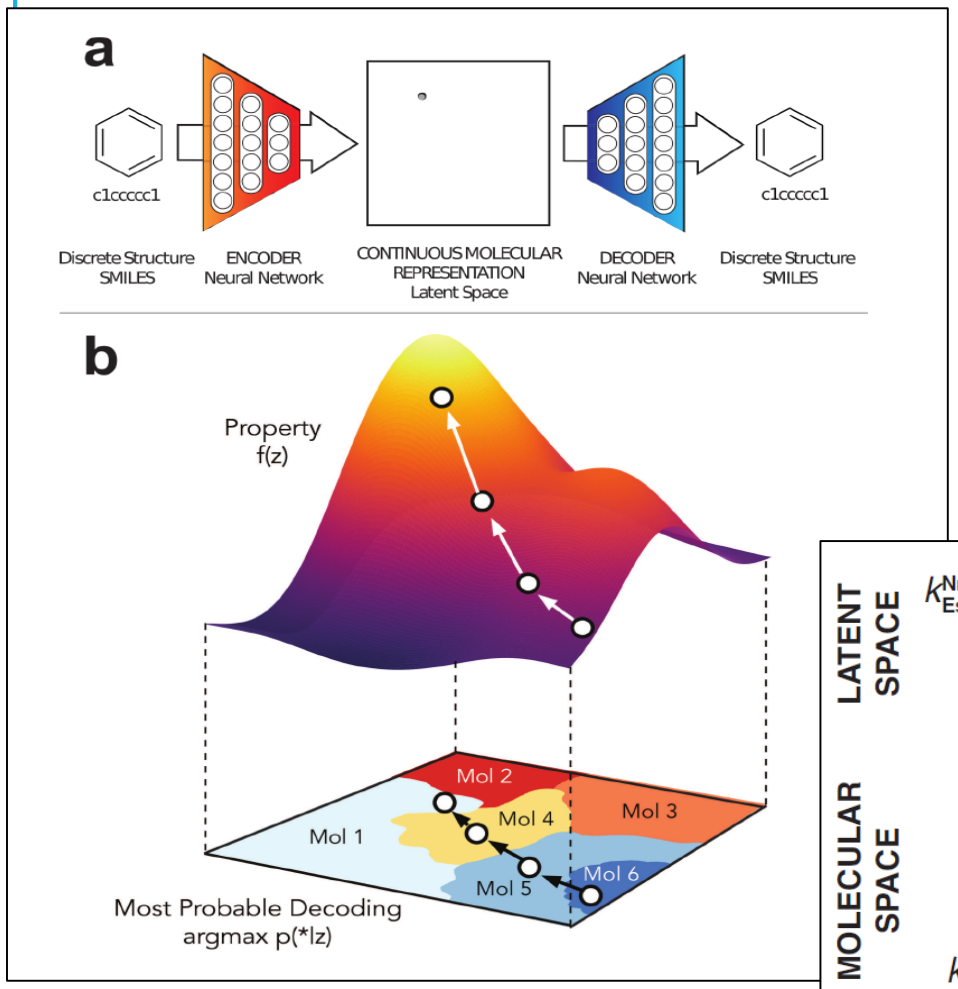
D

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

Source: wikipedia.org

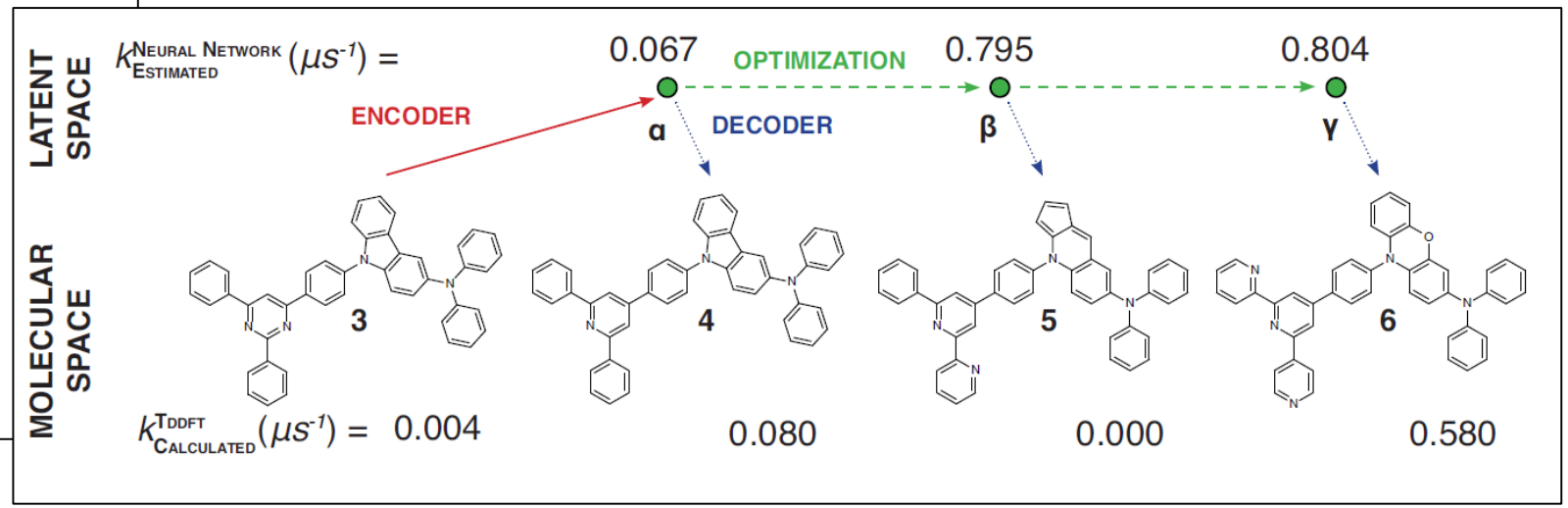
#REF: Gómez-Bombarelli, Rafael, et al. "Automatic chemical design using a data-driven continuous representation of molecules." *arXiv preprint arXiv:1610.02415* (2016).

VAE for molecular space modelling



Uses VAE for sequence-to-sequence.

Gómez-Bombarelli, Rafael, et al. "Automatic chemical design using a data-driven continuous representation of molecules." *ACS Central Science* (2016).



Drawbacks of string representation

String → graphs is not unique!

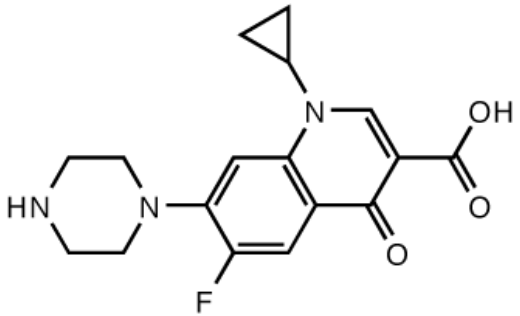
Lots of string are invalid

Precise 3D information is lost

Short range in graph may become long range in string

A better way is to encode/decode graph directly.

A



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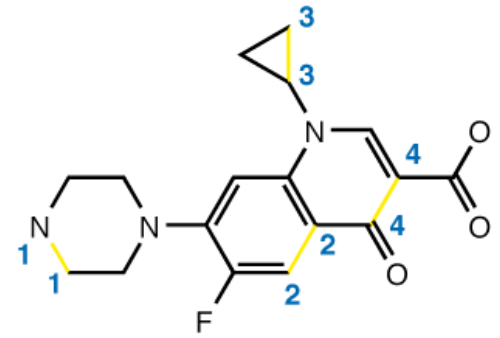
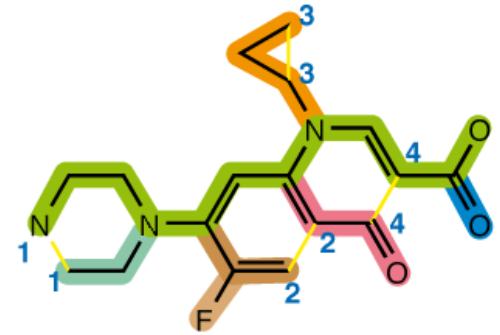


C



D

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

Source: wikipedia.org

#REF: Gómez-Bombarelli, Rafael, et al. "Automatic chemical design using a data-driven continuous representation of molecules." *arXiv preprint arXiv:1610.02415* (2016).

Better approach: Generating molecular graphs directly

No regular, fixed-size structures

Graphs are ***permutation invariant***:

- #permutations are exponential function of #nodes
- The probability of a generated graph G need to be marginalized over all possible permutations

Multiple objectives:

- **Diversity** of generated graphs
- **Smoothness** of latent space
- Agreement with or optimization of multiple design objectives

GraphVAE

Handles irregular structures

- Predict the whole adjacency matrix, node types and edge types

Deals with variable size graph

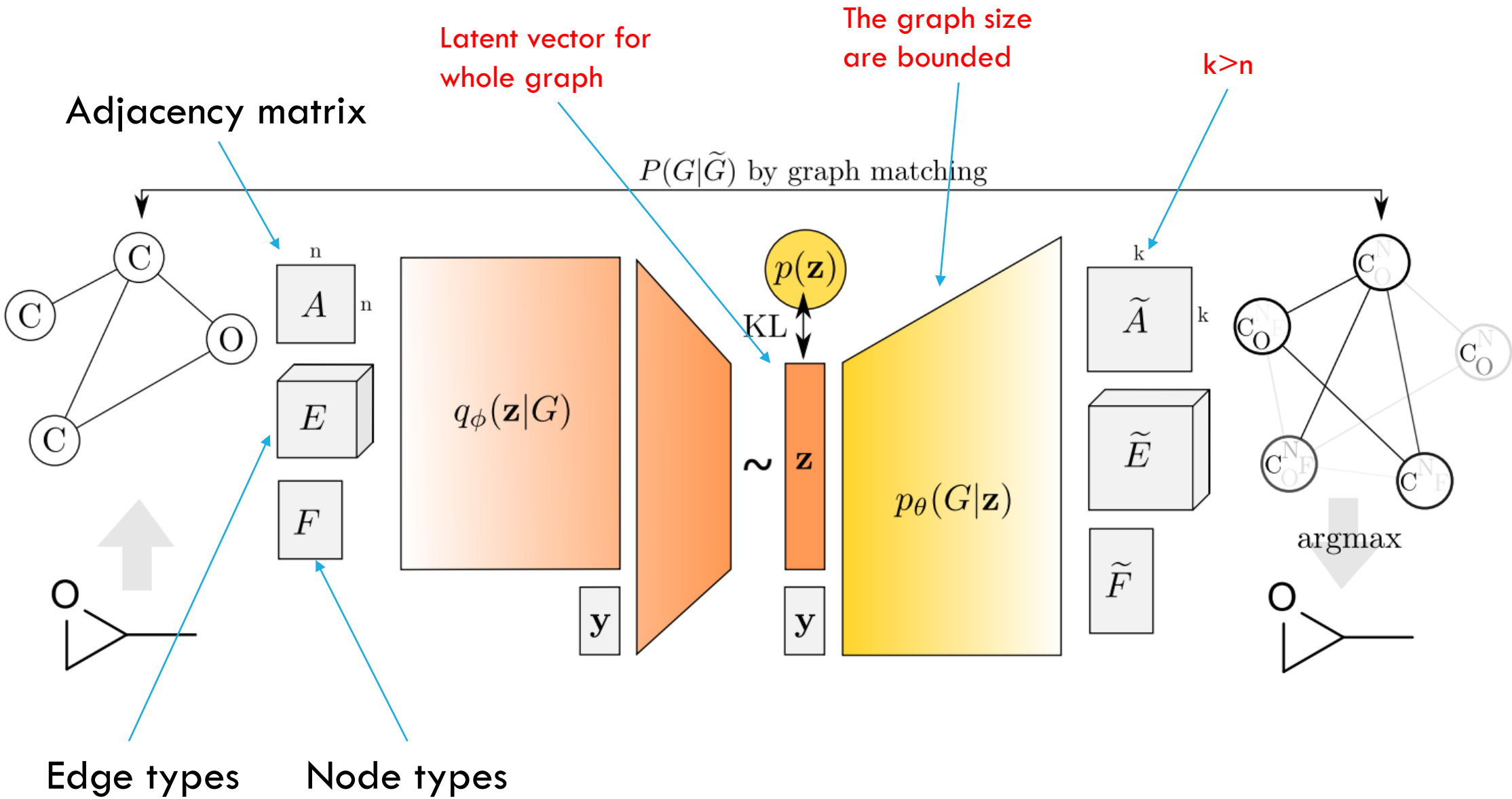
- Bounded by the size of the largest graph in training data.

Handles permutation invariance

- Matching every pair of nodes in 2 graphs

Partially promotes diversity

#REF: Simonovsky, M., & Komodakis, N. (2018). GraphVAE: Towards Generation of Small Graphs Using Variational Autoencoders. *arXiv preprint arXiv:1802.03480*.



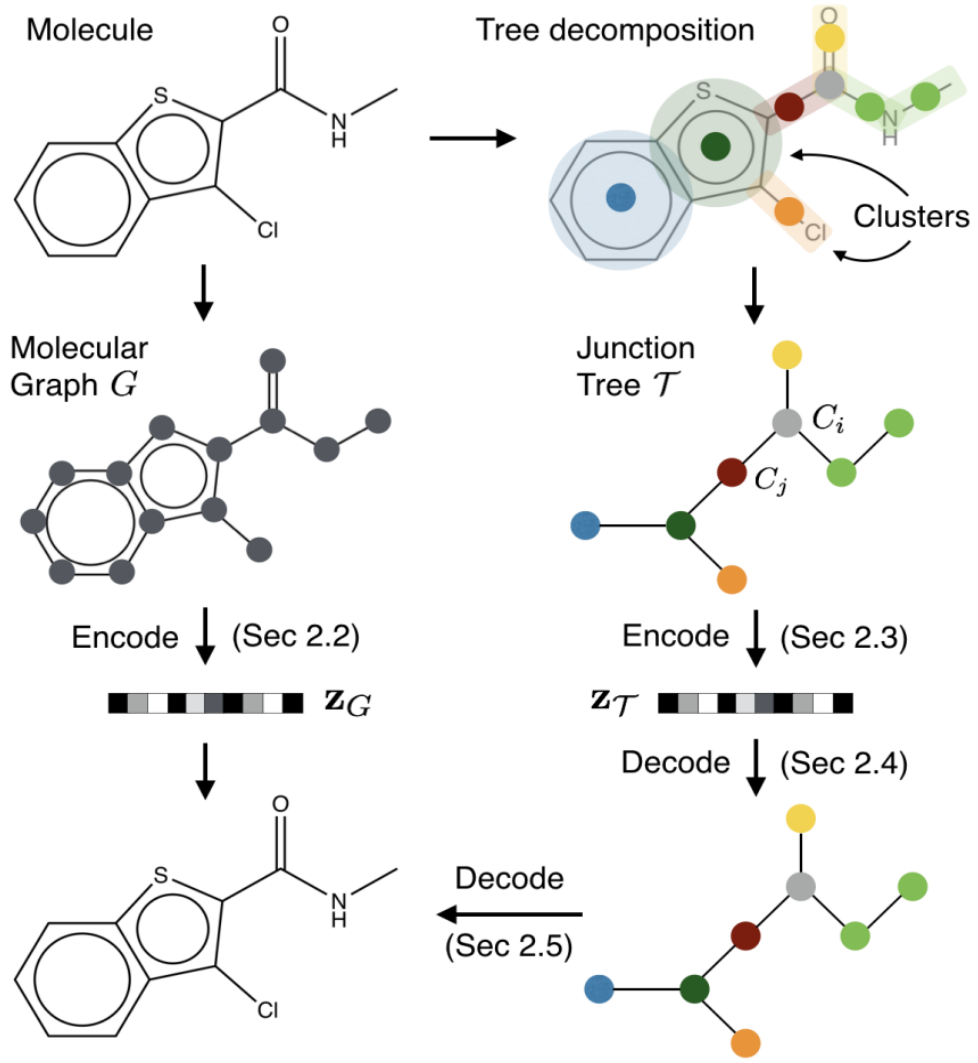
#REF: Simonovsky, M., & Komodakis, N. (2018). GraphVAE: Towards Generation of Small Graphs Using Variational Autoencoders. *arXiv preprint arXiv:1802.03480*.

Junction tree VAE

Junction tree is a way to build a “thick-tree” out of a graph

Cluster vocab:

- rings
- bonds
- atoms



Jin, W., Barzilay, R., & Jaakkola, T. (2018). Junction Tree Variational Autoencoder for Molecular Graph Generation. *ICML'18*.

Algorithm 2 Tree decomposition of molecule $G = (V, E)$

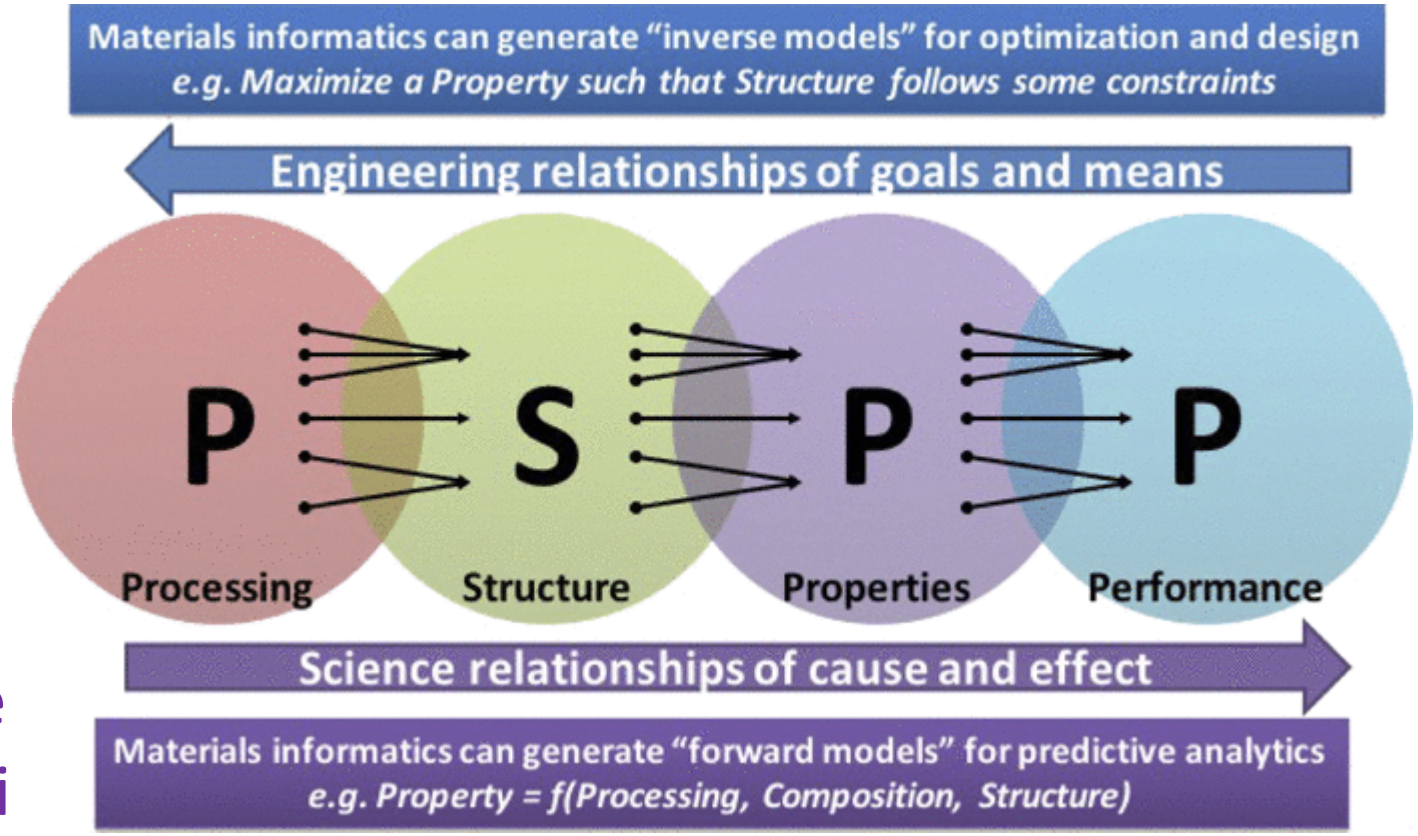
$V_1 \leftarrow$ the set of bonds $(u, v) \in E$ that do not belong to any rings.
$V_2 \leftarrow$ the set of simple rings of G.
for r_1, r_2 **in** V_2 **do**
  Merge rings r_1, r_2 into one ring if they share more than two atoms (bridged rings).
end for
$V_0 \leftarrow$ atoms being the intersection of three or more clusters in $V_1 \cup V_2$.
$\mathcal{V} \leftarrow V_0 \cup V_1 \cup V_2$
$\mathcal{E} \leftarrow \{(i, j, c) \in \mathcal{V} \times \mathcal{V} \times \mathbb{R} \mid |i \cap j| > 0\}$. Set $c = \infty$ if $i \in V_0$ or $j \in V_0$, and $c = 1$ otherwise.
Return The maximum spanning tree over cluster graph $(\mathcal{V}, \mathcal{E})$.

Method	Reconstruction	Validity
CVAE	44.6%	0.7%
GVAE	53.7%	7.2%
SD-VAE[2]	76.2%	43.5%
GraphVAE	-	13.5%
JT-VAE	**76.7%**	**100.0%**

Jin, W., Barzilay, R., & Jaakkola, T. (2018). Junction Tree Variational Autoencoder for Molecular Graph Generation. *ICML'18*.

AI for materials

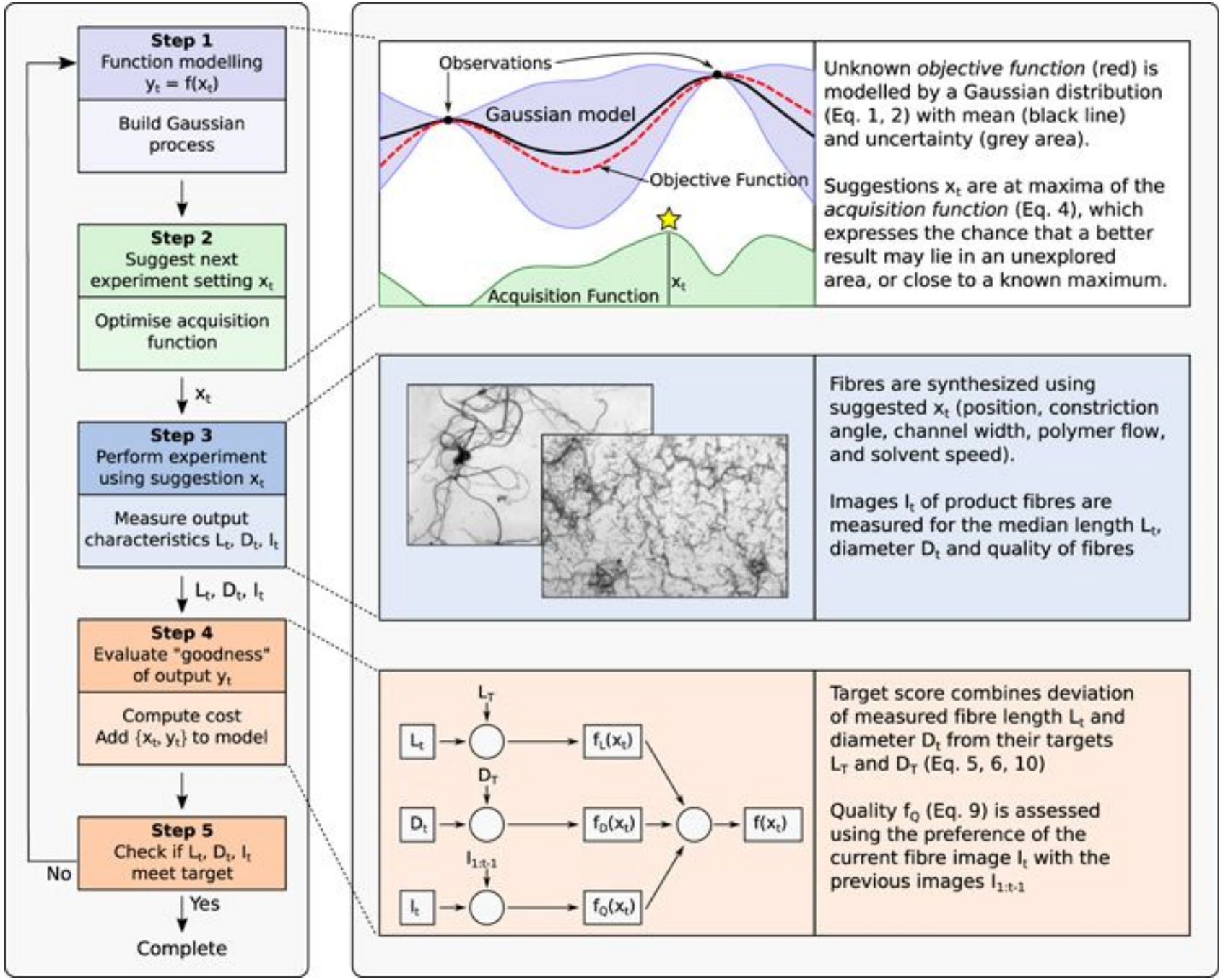
- Characterise the space of materials
- Represent crystals
- Map alloy composition → phase diagram
- Inverse design: Map phase diagram → alloy compositi
- Generate alloys
- Optimize processing parameters



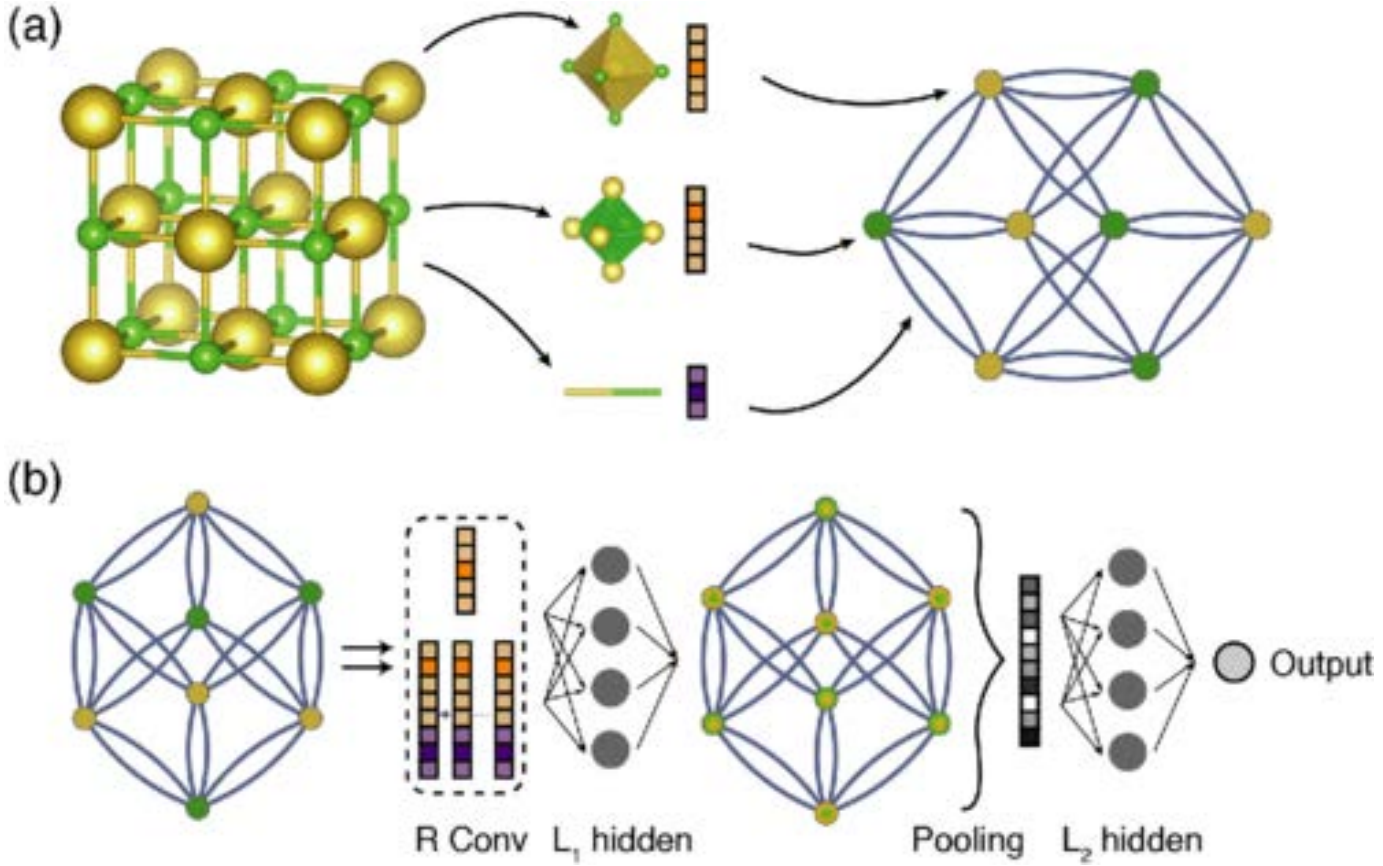
Agrawal, A., & Choudhary, A. (2016). Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science. *Apl Materials*, *4*(5), 053208.

Bayesian optimization for short polymer fiber

Li, Cheng, David Rubín de Celis Leal, Santu Rana, Sunil Gupta, Alessandra Sutti, Stewart Greenhill, Teo Slezak, Murray Height, and Svetha Venkatesh. "Rapid Bayesian optimisation for synthesis of short polymer fiber materials." *Scientific reports* 7, no. 1 (2017): 5683.



Crystal as a graph neural net



Xie, Tian, and Jeffrey C. Grossman. "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties." *Physical review letters* 120.14 (2018): 145301.

Computing materials similarity

Strong features are highly but nonlinearly predictive of properties (e.g., formation energy)

The relationship between features & properties can be locally linear

Materials that share the same feature-property relationship may be functionally similar

electronic reprint

IUCrJ

ISSN: 2052-2525
www.iucrj.org

Committee machine that votes for similarity between materials

Duong-Nguyen Nguyen, Tien-Lam Pham, Viet-Cuong Nguyen, Tuan-Dung Ho, Truyen Tran, Keisuke Takahashi and Hieu-Chi Dam

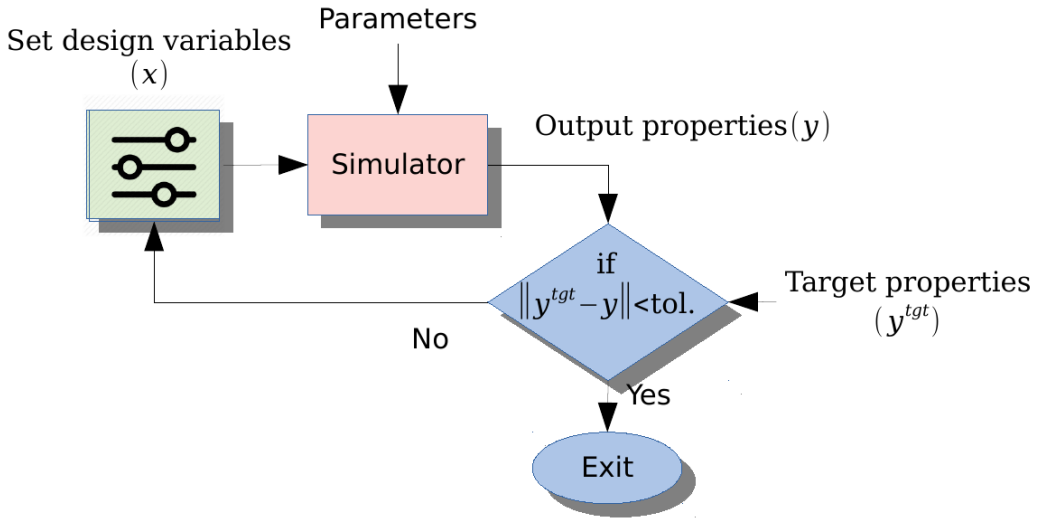
IUCrJ (2018). 5, 830–840

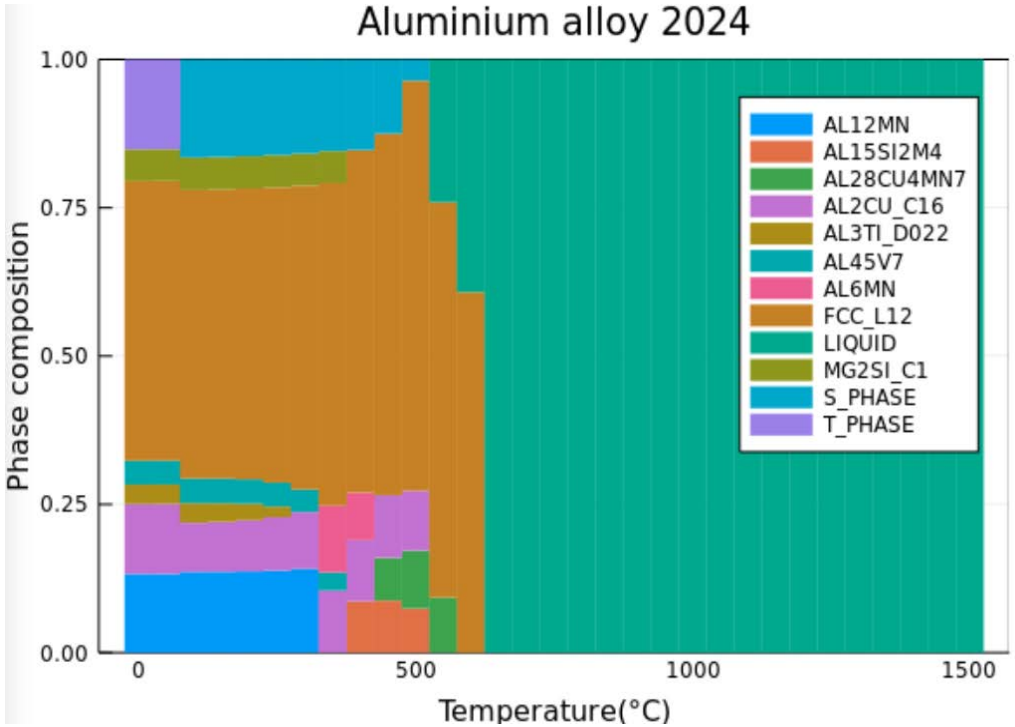
IUCr Journals
CRYSTALLOGRAPHY JOURNALS ONLINE

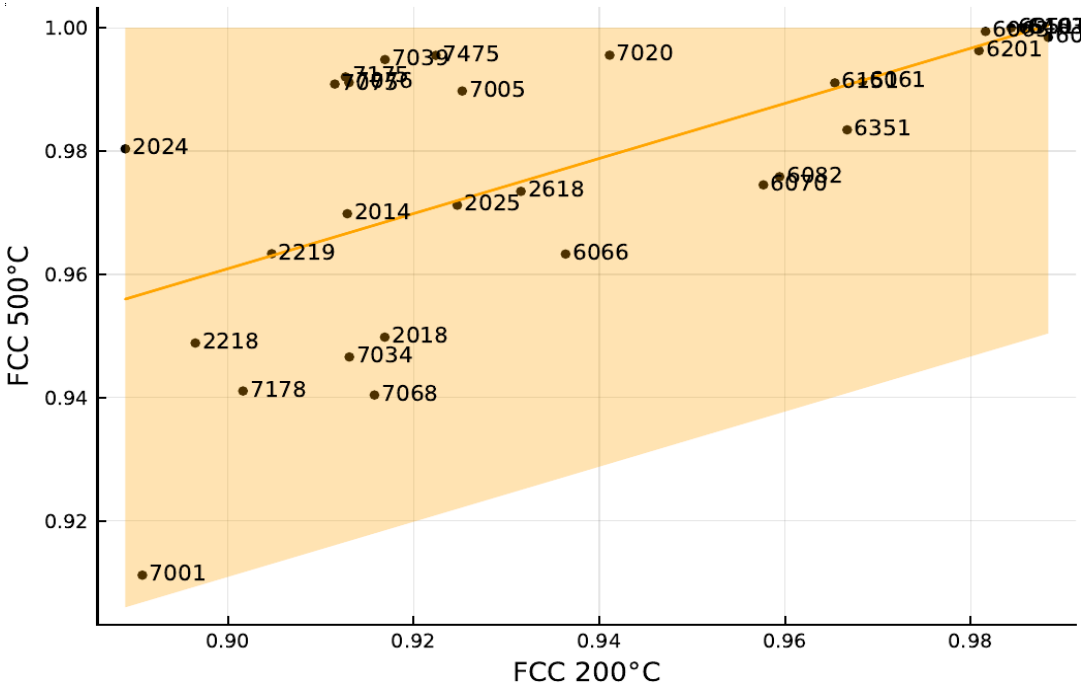
#REF: Nguyen, P., Tran, T., Gupta, S., Rana, S., & Venkatesh, S. Incomplete Conditional Density Estimation for Fast Materials Discovery. *SDM'19*

Alloy space exploration

- Scientific innovations are expensive
- One search per specific target
- Availability of growing data

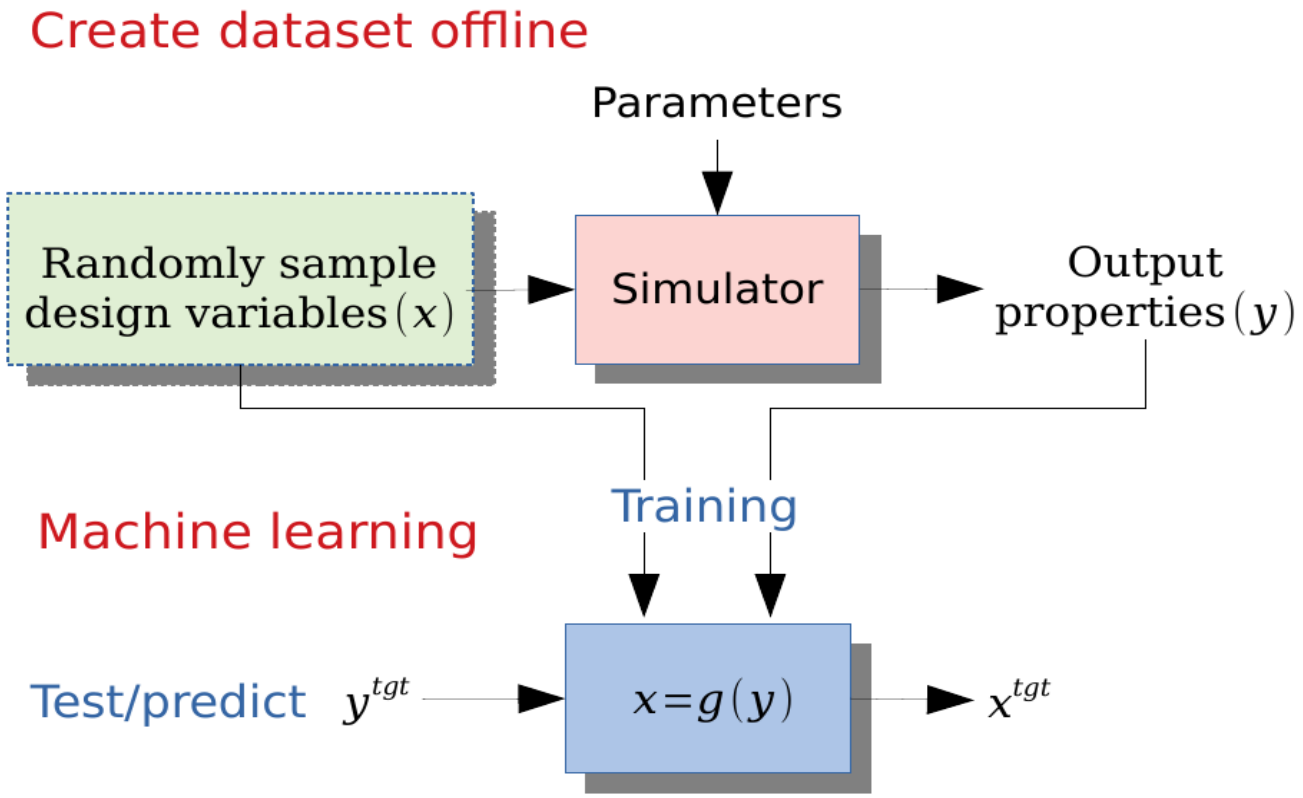






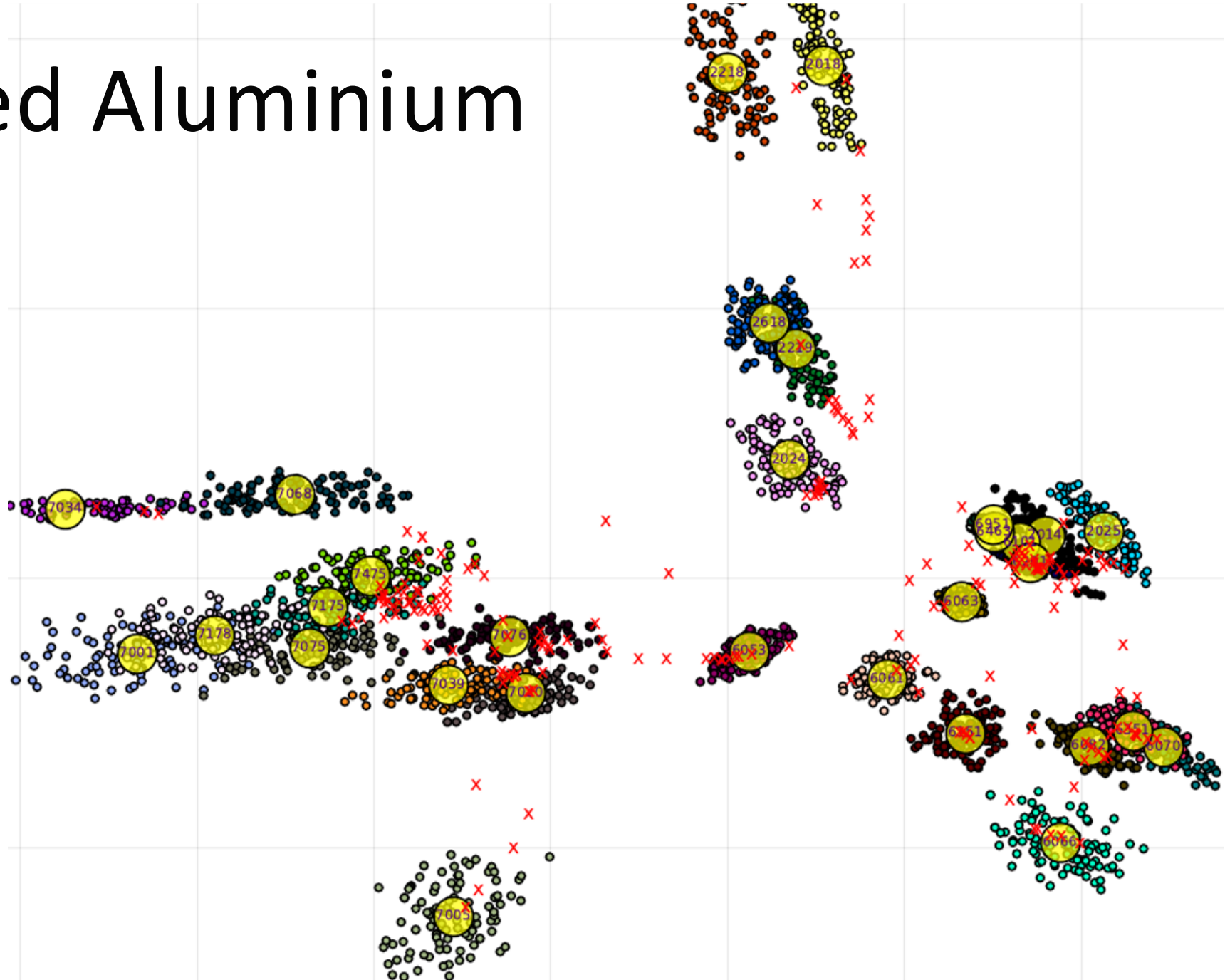
Inverse design

- Leverage the existing data and query the simulators in an offline mode
- Avoid the global optimization by learning the inverse design function $f^{-1}(y)$
- Predict design variables in a single step



$$\boldsymbol{x}^{\text{target}} = g\left(\boldsymbol{y}^{\text{target}}\right)$$

Generated Aluminium alloys



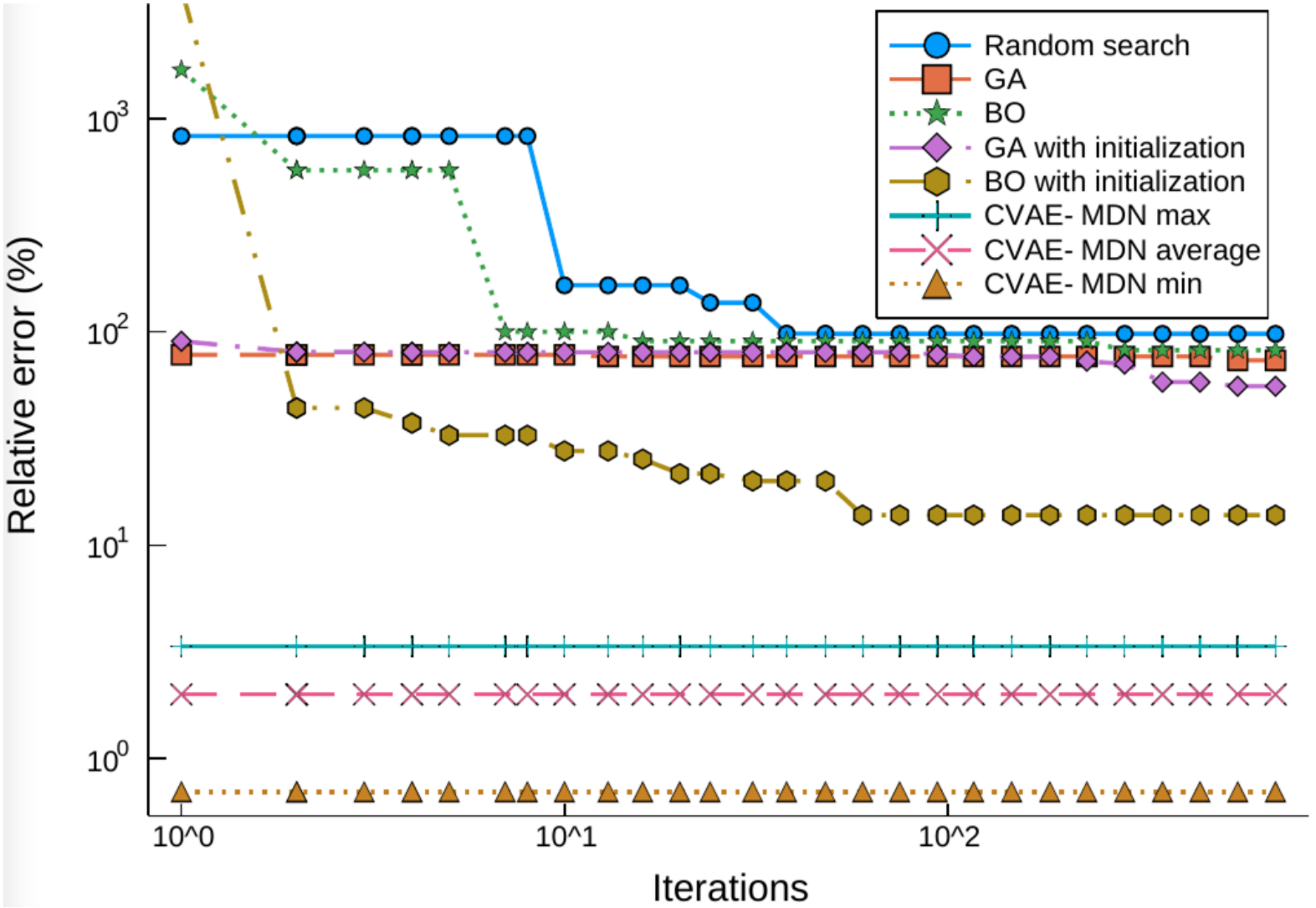
Full phase specification

	Known-alloy dataset		BO-search dataset	
Method	**Relative (%)**	**Absolute (%)**	**Relative (%)**	**Absolute (%)**
RF	3.21 ± 0.02	0.00 ± 0.00	6.37 ± 2.13	0.01 ± 0.00
MLP	1.10 ± 0.03	0.00 ± 0.00	3.41 ± 1.48	0.01 ± 0.01
MDN	0.52 ± 0.00	0.00 ± 0.00	2.95 ± 1.32	0.00 ± 0.01

50% phase missing

	Known-alloy dataset		BO-search dataset	
Method	**Relative (%)**	**Absolute (%)**	**Relative (%)**	**Absolute (%)**
RF	4.38 ± 0.01	0.00 ± 0.00	8.49 ± 1.34	0.01 ± 0.01
MLP	3.43 ± 0.07	0.00 ± 0.00	11.91 ± 2.54	0.03 ± 0.02
MDN	2.28 ± 0.22	0.00 ± 0.00	7.83 ± 1.11	0.01 ± 0.01
CVAE-MLP	2.50 ± 0.24 (a)	0.00 ± 0.00	7.42 ± 2.03 (e)	0.01 ± 0.01 (i)
CVAE-MDN	2.08 ± 0.12 (b)	0.00 ± 0.00	4.23 ± 0.67 (f)	0.00 ± 0.00 (j)
CGAN-MLP	3.18 ± 0.18 (c)	0.00 ± 0.00	8.39 ± 2.33 (g)	0.00 ± 0.00 (k)
CGAN-MDN	2.30 ± 0.18 (d)	0.00 ± 0.00	7.38 ± 0.70 (h)	0.00 ± 0.00 (l)

Search time comparisons



Recent context

NIPS Workshop on Molecular and Materials Sciences (2017, 2018)

The International Workshop on Machine Learning for Materials Science 2018

2018 Workshop on Machine Learning in Materials Science (April 2018)

AI-driven Acceleration Platform for Materials (Jan 2018, CIFAR Report)

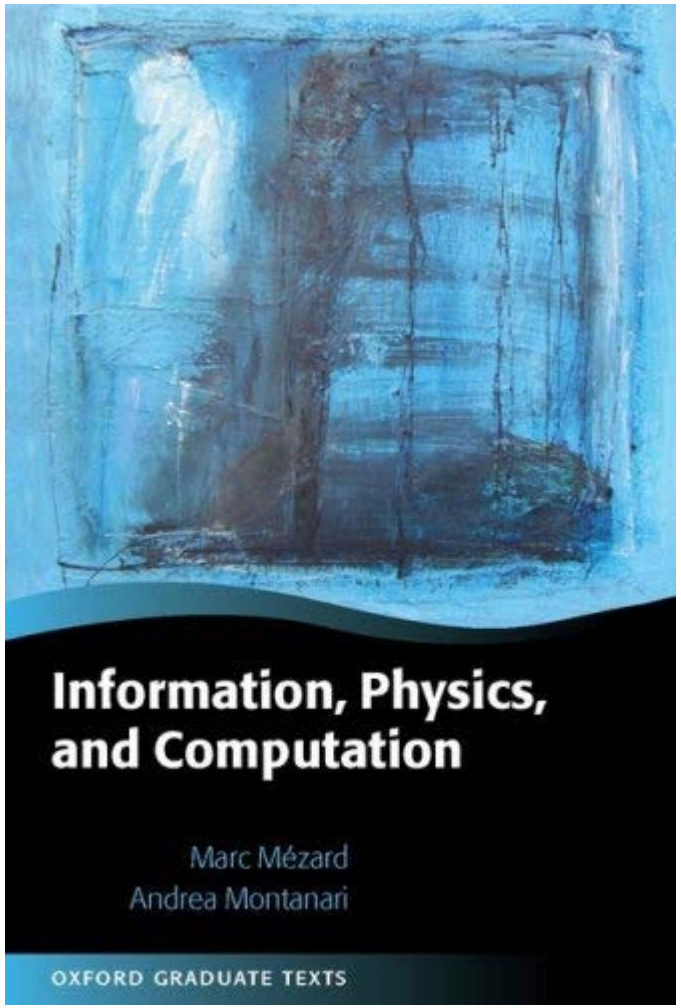
Workshop on Deep Learning for Physical Sciences (Dec 2017)

Machine learning for materials research: Bootcamp & workshop (June 2017)

International Workshop on Machine Learning for Materials Science (March 2017, Finland)

Understanding Many-Particle Systems with Machine Learning (Sept-Dec 2016)

Remarks


Information, Physics,
and Computation
Marc Mézard
Andrea Montanari
OXFORD GRADUATE TEXTS

Machine learning a physics theory?

Expressiveness

- Can represent the complexity of the world
- Can compute anything computable

Learnability

- Have mechanism to learn from the training signals

Generalizability

- Work on unseen data

AI as physics

Intelligence as self-organizing phenomena: reducing ignorance/entropy

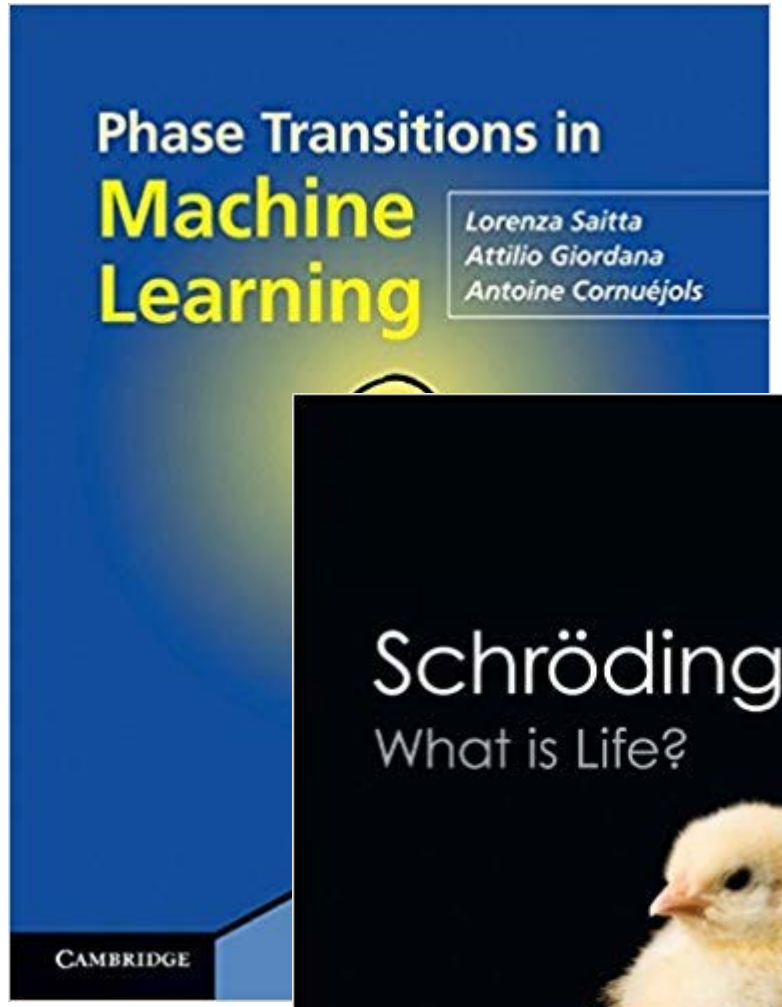
Neural networks as a statistical mechanical system

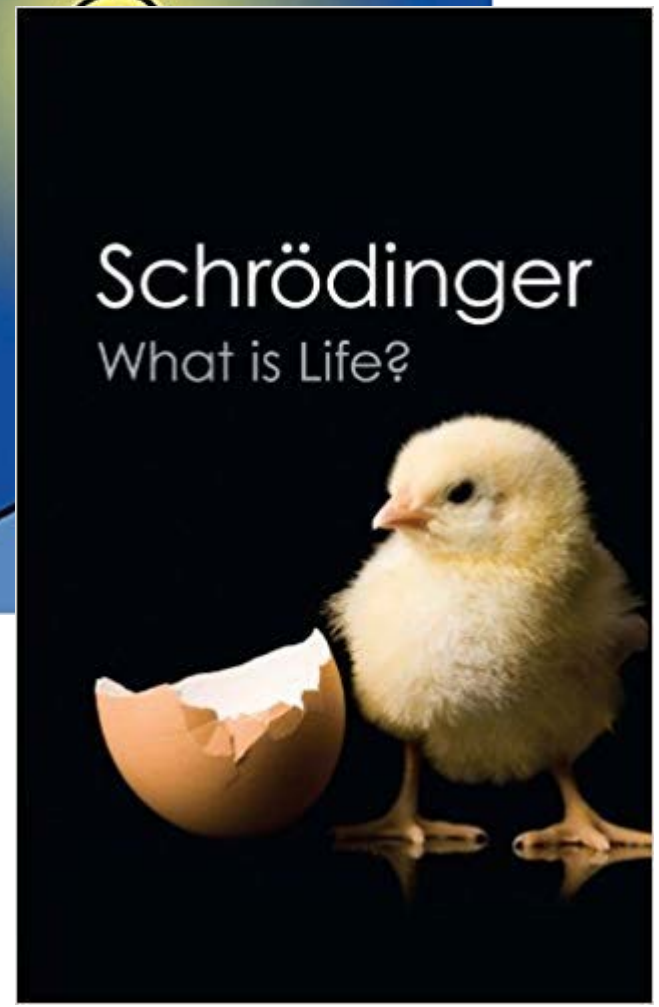
Learning as variational optimization

Inference in probabilistic graphical models as Bethe free-energy minimization

Phase transition may occur in AI systems

Ultimate AI must solve the **consciousness problem**, which may require quantum physics (or a new physics)





Life has low entropy

Physics of Restricted Boltzmann machines

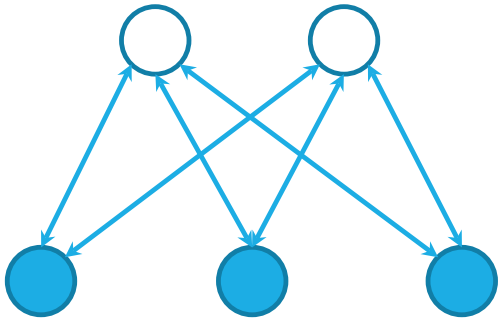
Boltzmann machines as a generalization of Ising model

Restricted Boltzmann machine as a simplified version, but with hidden variables to denote underlying unobserved processes

Stack of RBMs is akin to renormalization trick in physics

$$p(\mathbf{v}, \mathbf{h}; \psi) \propto \exp\left[-E(\mathbf{v}, \mathbf{h}; \psi)\right]$$

energy



Restricted Boltzmann Machine (~1994, 2001)

RBM for n-body problem

Carleo, Giuseppe, and Matthias Troyer. "Solving the quantum many-body problem with artificial neural networks." *Science*355.6325 (2017): 602-606.

Torlai, Giacomo, et al. "Many-body quantum state tomography with neural networks." *arXiv preprint arXiv:1703.05334* (2017).

Nomura, Yusuke, et al. "Restricted Boltzmann machine learning for solving strongly correlated quantum systems." *Physical Review B* 96.20 (2017): 205152.

Gao, Xun, and Lu-Ming Duan. "Efficient representation of quantum many-body states with deep neural networks." *Nature communications* 8.1 (2017): 662.

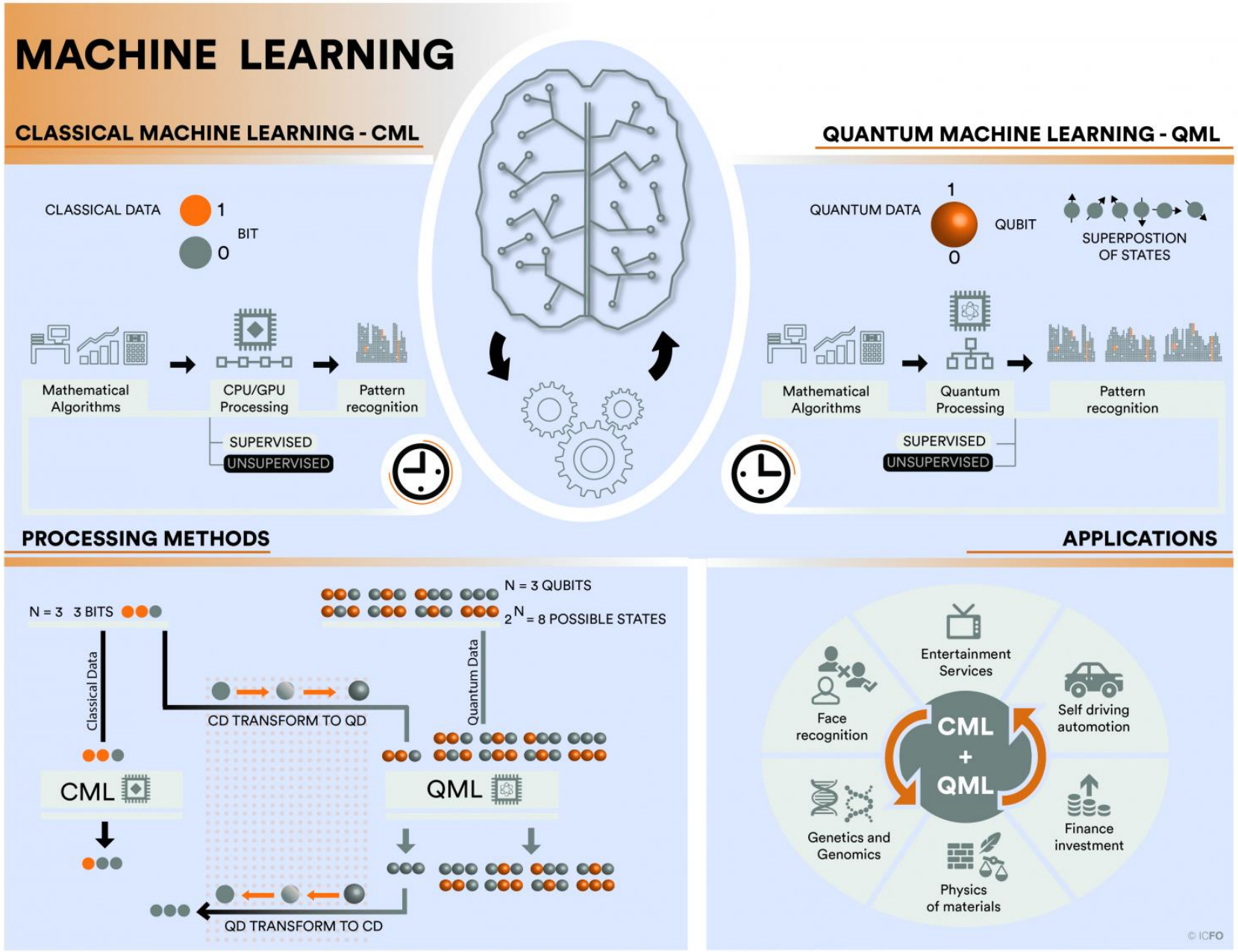
Chen, Jing, et al. "On the equivalence of restricted Boltzmann machines and tensor network states." *arXiv preprint arXiv:1701.04831* (2017).

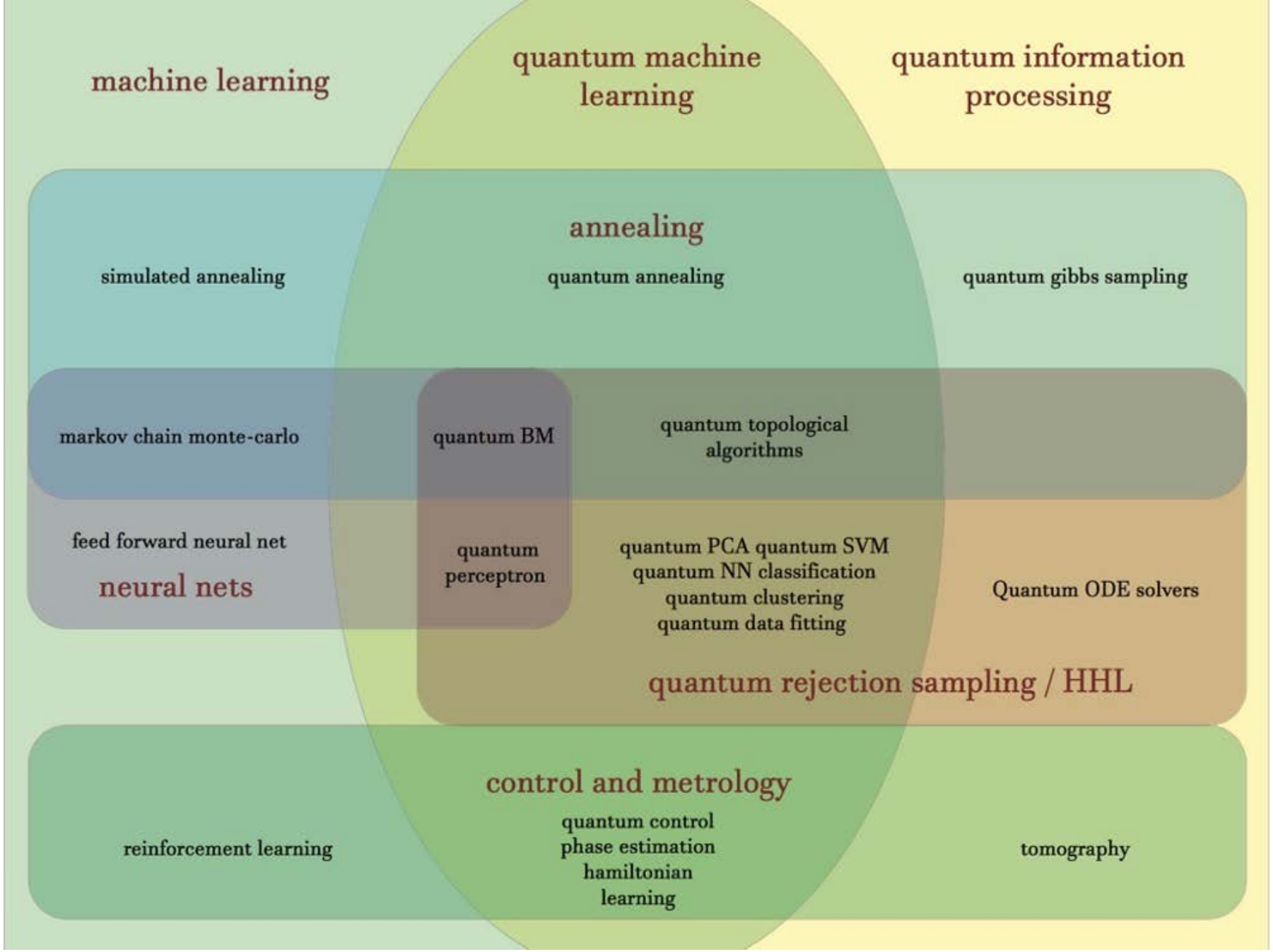
Rao, Wen-Jia, et al. "Identifying product order with restricted Boltzmann machines." *Physical Review B* 97.9 (2018): 094207.

Quantum machine learning

Quantum Machine Learning, Jacob Biamonte, Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe and Seth Lloyd, *Nature* 549, 195–202 14 September 2017

Read more at:
https://phys.org/news/2017-09-quantum-machines.html#jCp





https://medium.com/@_NicT_/quantum-machine-learning-c5ab31f6b4d

Prediction versus understanding

We can predict well without understanding (e.g., planet/star motion Newton).

Guessing the God's many complex behaviours versus knowing his few universal laws.

Some open challenges

Can AI/ML discover a new phase of matter ?

Would AI/ML discover new algorithms for us ?

Would it be possible for us to make progress on fermion sign problem?

Non-stochastic, or better ways for optimizing, renormalizing, and evolving Neural Networks.

Information pattern aware structure learning of neural networks

#REF: Liu, Jin-Guo, Shuo-Hui Li, and Lei Wang. "Lecture Note on Deep Learning and Quantum Many-Body Computation." (2018).