NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Artificial Intelligence for Materials Science Workshop: Hands-On Session

Peter Bajcsy, Austin McDannald, Brain DeCost, Daniel Wines, Kamal Choudhary

AIMS: July 18, 2024

https://jarvis.nist.gov

https://github.com/usnistgov/aims2024_workshop/

Joint Automated Repository for Various Integrated Simulations

7/18/2024

Outline

1. Foundational Concepts of AI-Based Modeling: Peter Bajcsy
   - NN-Calculator
2. Leveraging DFT, GNNs and GPTs for Accurate Predictions: Daniel Wines, Brian DeCost, Kamal Choudhary
   - JARVIS-DFT
   - ALIGNN and ALIGNN-FF
   - AtomGPT
3. Gaussian Processes and Active Learning: Austin McDannald

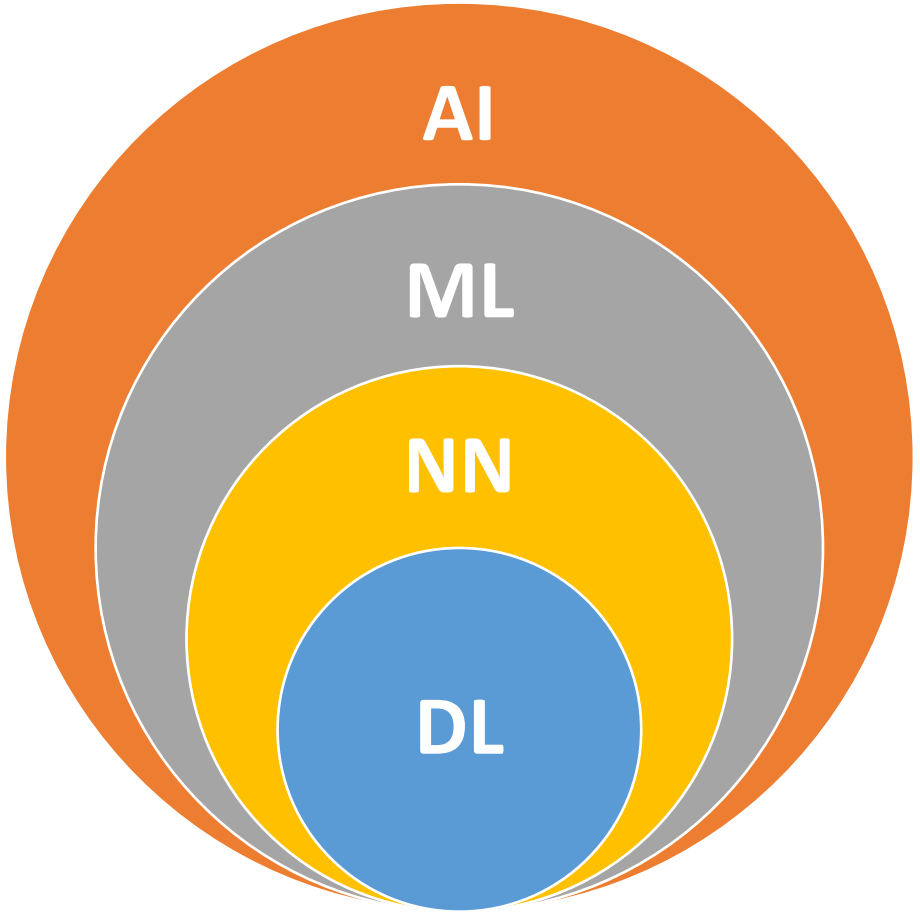
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Neural Network Calculator for Learning About Artificial Intelligence-Based Modeling

Peter Bajcsy, Ph.D.
Information Technology Laboratory
National Institute of Standards and Technology

2024 Artificial Intelligence for Materials Science (AIMS) Workshop, July 17-18, 2024

Terminology



- AI: Artificial intelligence is the overarching system.
- ML: Machine learning is a subset of AI.
- NN: Neural networks are the backbone of deep learning algorithms.
- DL: Neural network of more than three layers, including the inputs and the output.

URL

1. Why are we interested in Neural Networks?

Neural Networks Can Sort and Label Your Pictures

CATS

DOGS

Neural Network Can Assist/Replace a Human

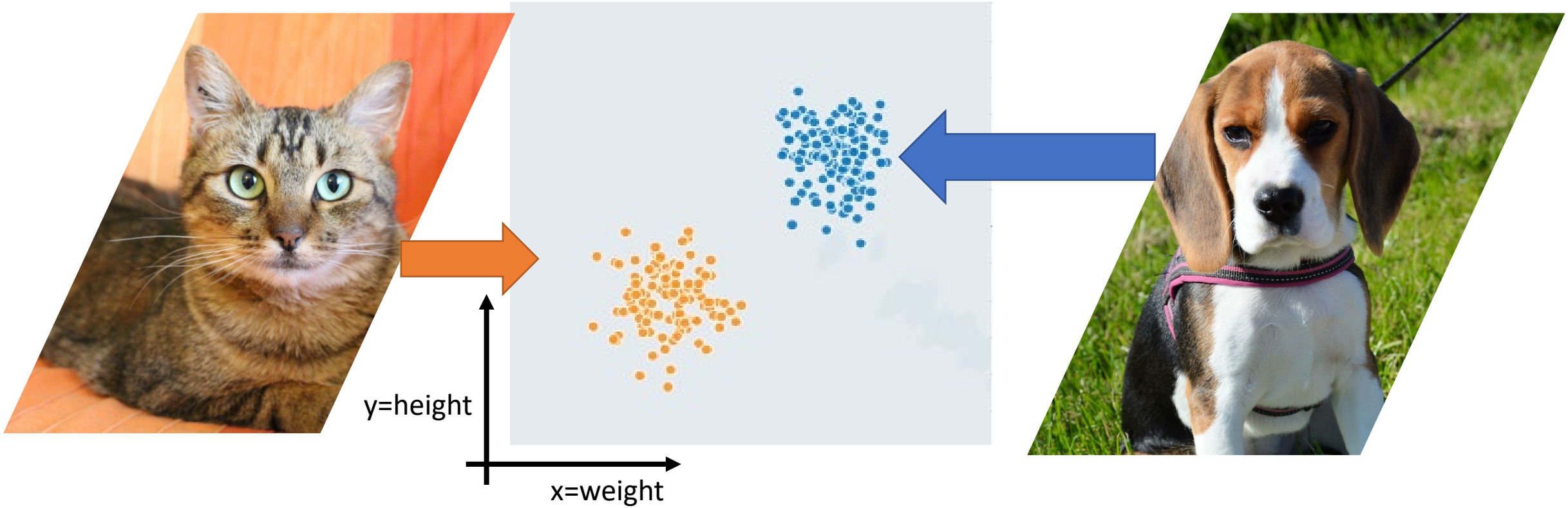
1. Why are Scientists interested in Neural Networks?

Relevance of AI to Metrology:

- Neural Networks can classify pictures into classes →
  - Tasks: classification, object detection, segmentation, tracking, recognition
- Neural Networks can assist humans →
  - Learn from training data: labeled and partially unlabeled.
  - Learn from past models: a priori knowledge and simulations.
- Neural Networks can outperform humans →
  - Task metrics: overall accuracy (NN do not get tired) beyond visual detection limits and speed.
- Neural Networks can save us a lot of time →
  - Automation of tasks: processing TB of images, detecting outliers, and leading to discovery.

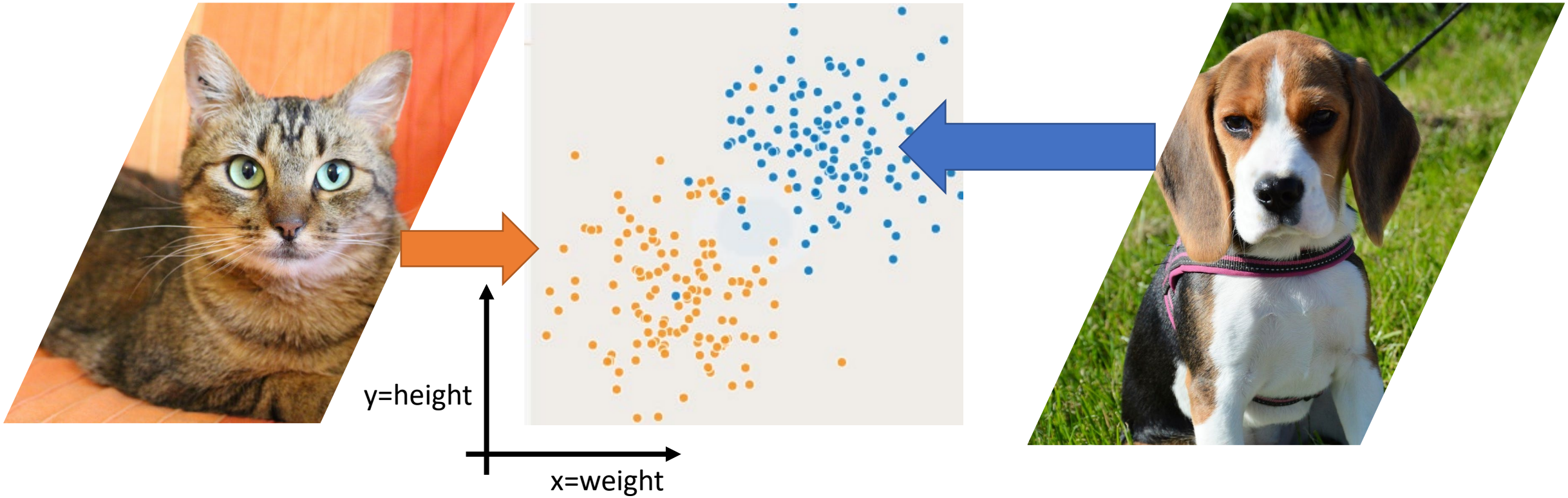
2. How to describe two-class inputs and create a complex boundary separating two classes?

Cats & Dogs Described by 2D Points (x, y): Ideal Data



Height & weight = properties of dogs and cats

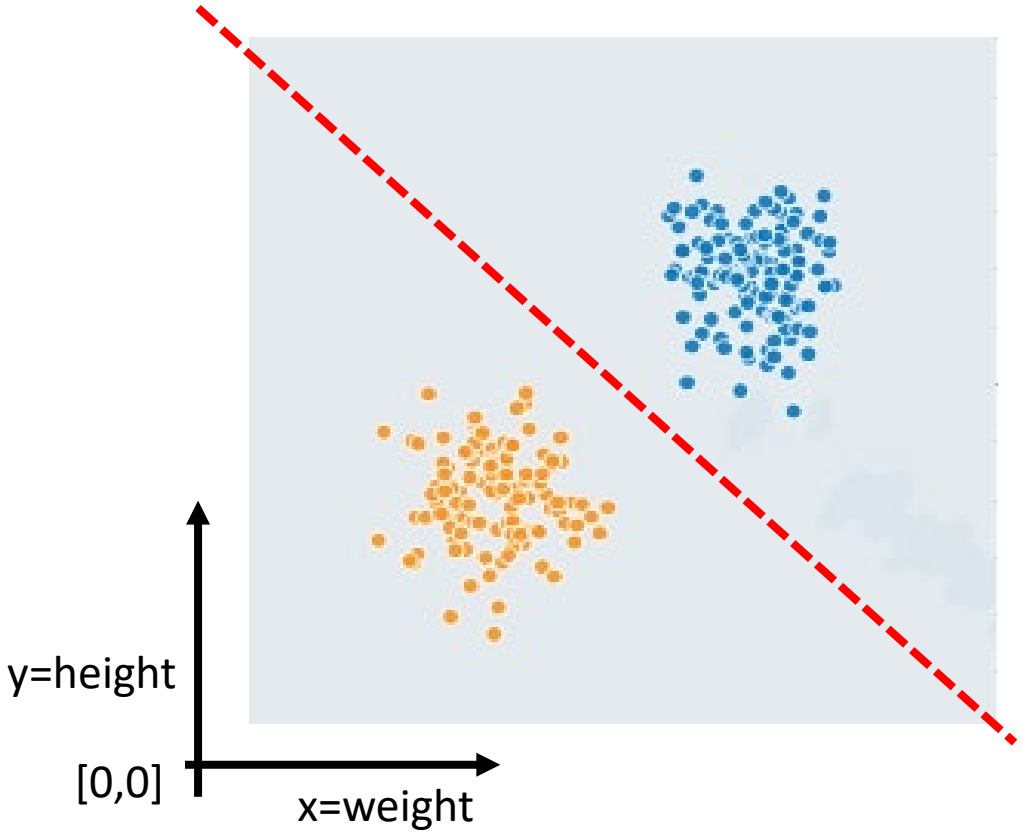
Cats & Dogs Described by 2D Points (x, y): Real Data



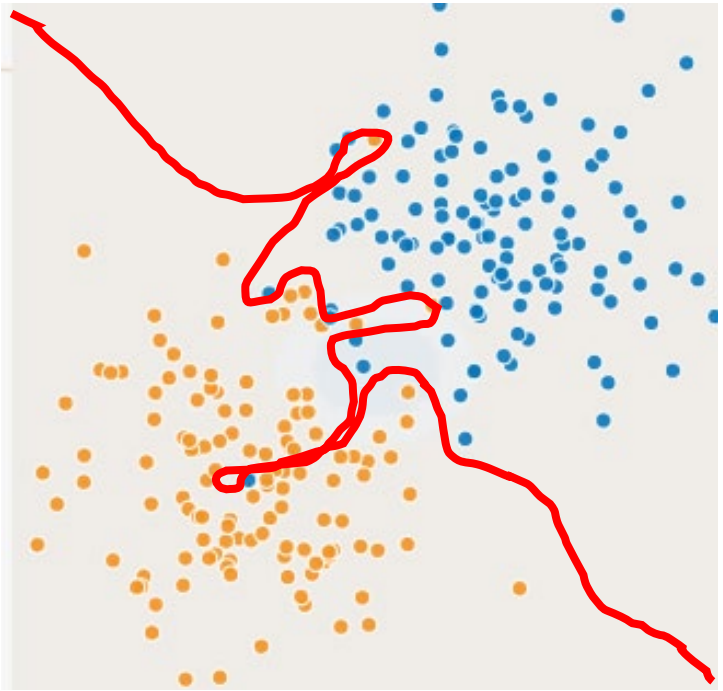
Separation of properties → accuracy of “Dogs versus Cats” classification

Types of Boundaries

Linear boundary

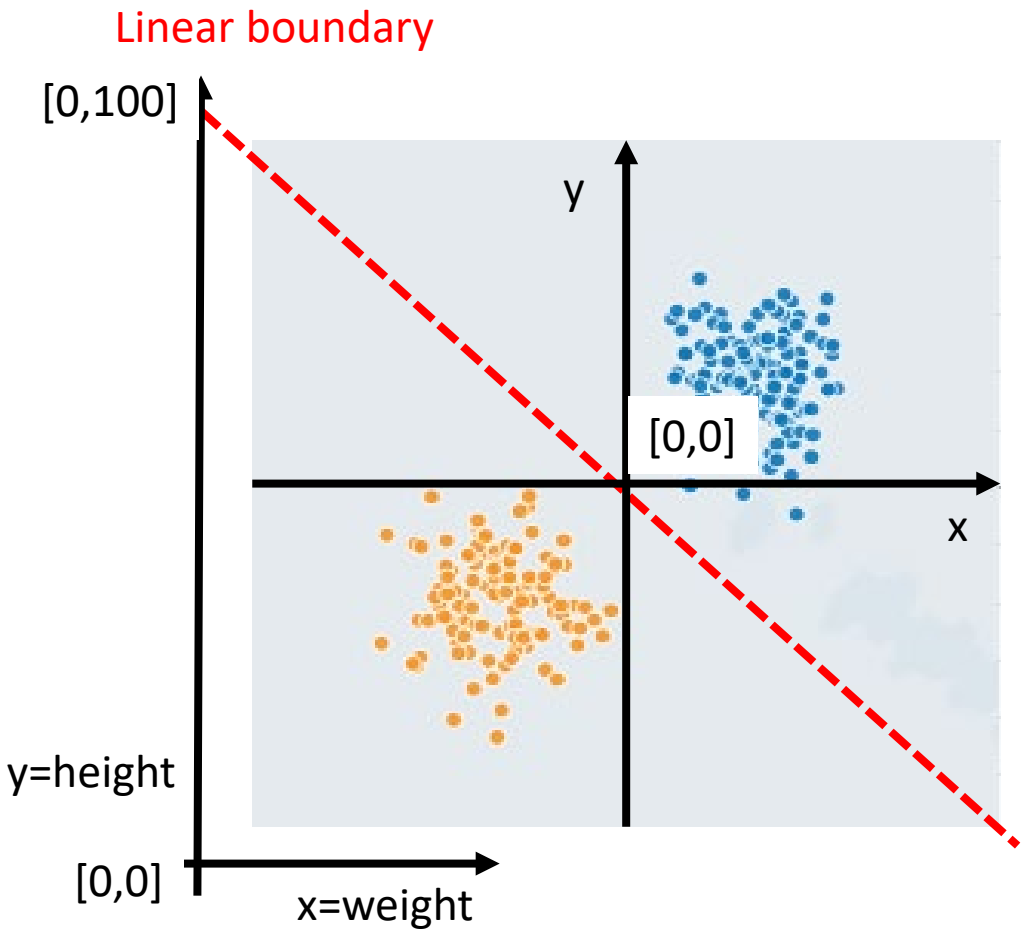


Non-linear boundary



How to describe and derive these boundaries automatically?

Linear Boundaries



$$Boundary: x + y = 100$$

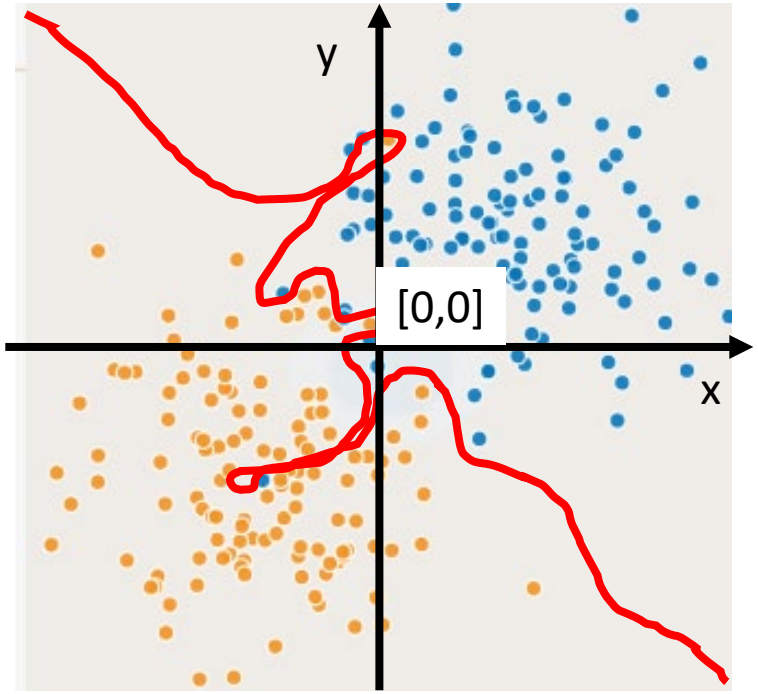
$$Boundary: x + y = 0$$

$$Math\ model: if\ x + y < 0\ then\ orange\ else\ blue$$

How to describe and derive these boundaries automatically?

Nonlinear Boundaries

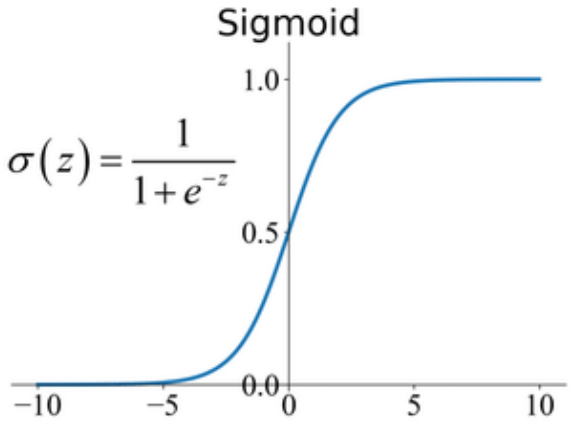
Non-linear boundary



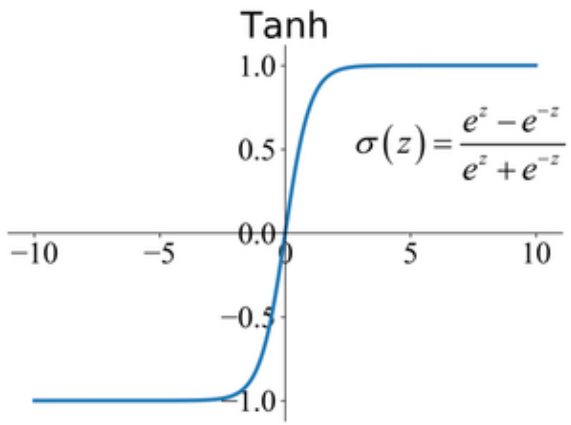
How to describe a nonlinear boundary using x and y?

How to derive the boundary description automatically?

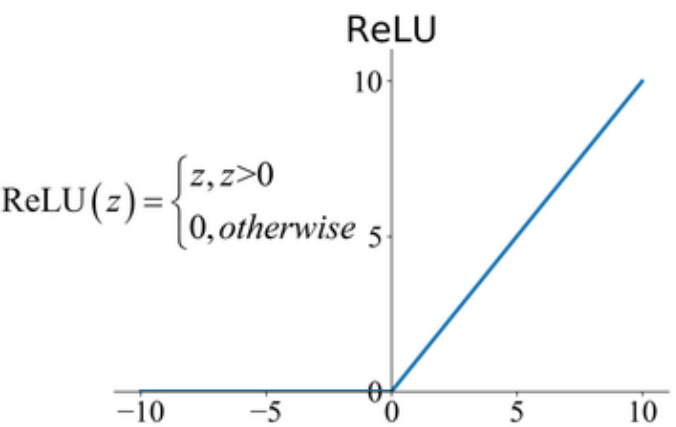
Describe nonlinear boundary using x and y



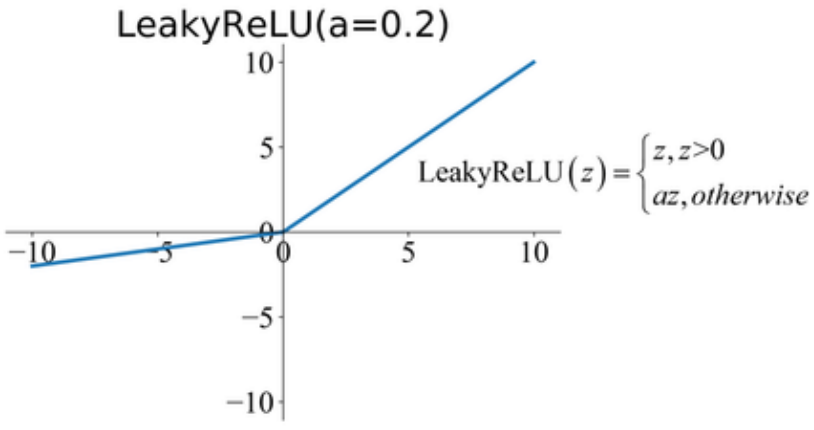
(a)



(b)



(c)



(d)

Nonlinear operators: (a) Sigmoid, (b) Tanh, (c) ReLU, and (d) LReLU.

$Linear\ Boundary$:
$x + y = 0$

$Nonlinear\ Boundary$:
$Tanh(x + y) = 0$

Nonlinear operators on features

$Nonlinear\ Boundary$:
$(x^2 + y^2) = 100$

Nonlinear features

$Nonlinear\ Boundary$:
$\mathrm{Tanh}(x^2 + y^2) = 100$

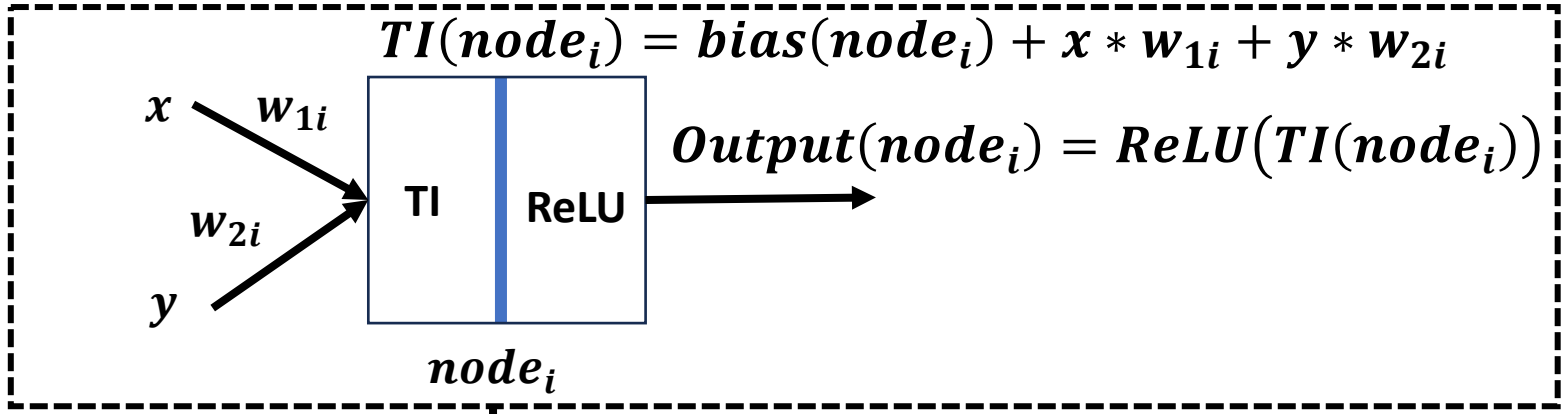
Nonlinear operators & nonlinear features

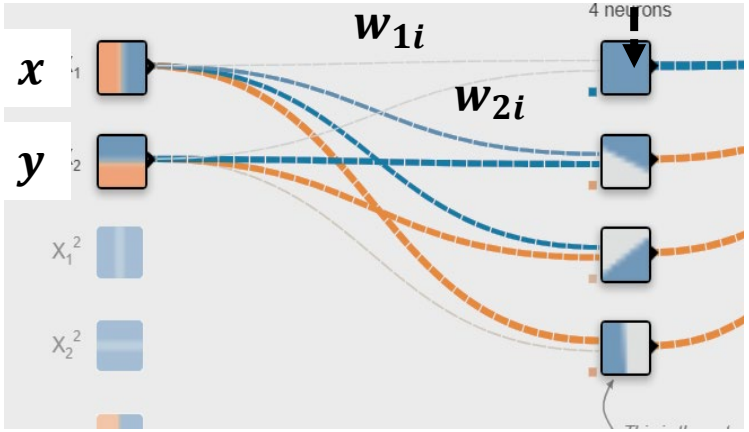
Prepare NN model for non-linear boundary

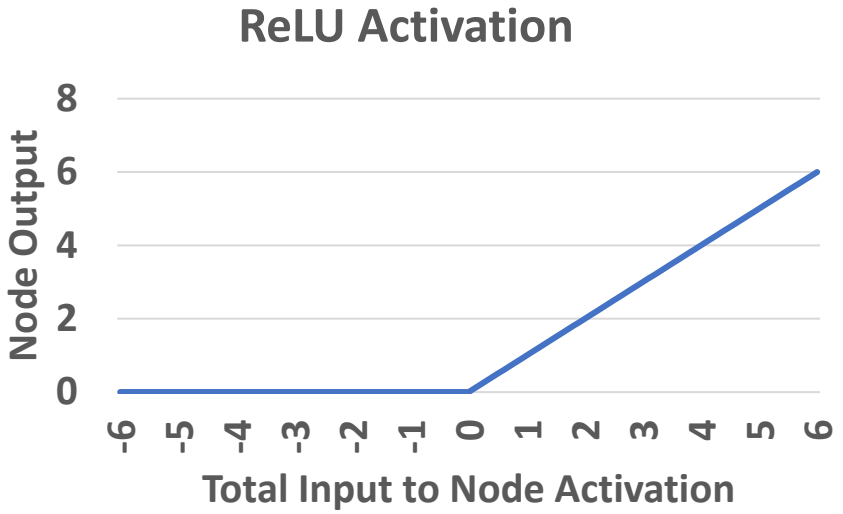
Mathematical Model

$$TI(node_i) = bias(node_i) + x * w_{1i} + y * w_{2i}$$

$$Output(node_i) = ReLU\big(TI(node_i)\big)$$



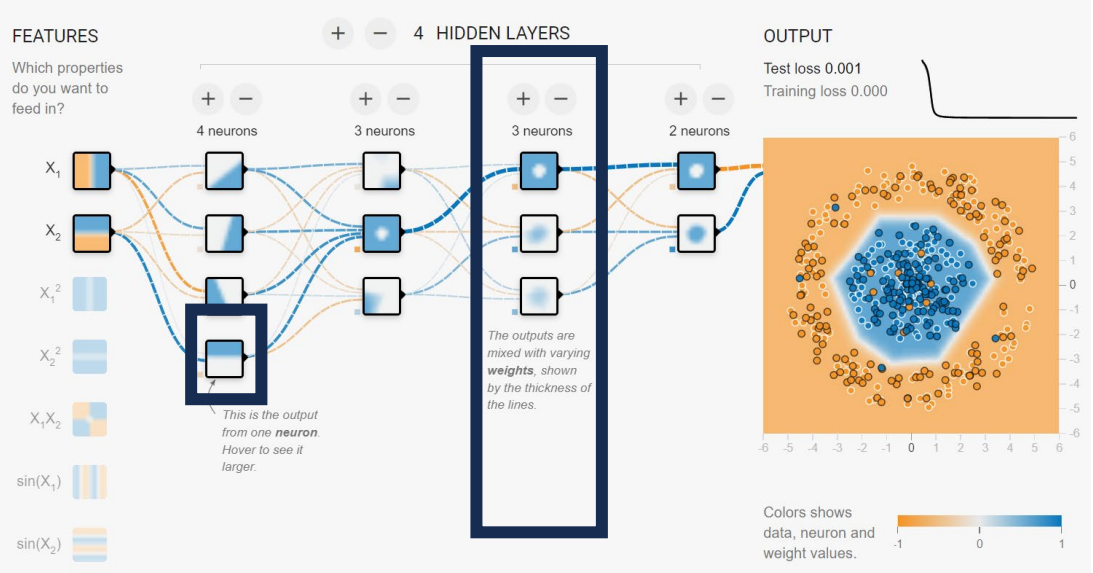




Derive boundary description automatically

1. Step - Configure Neural Network architecture (layers, nodes, connectivity)
2. Step – Prepare (input, output) pairs (images and labels)
3. Step – Initialize all weights in NN with random numbers
4. Step – Train weights so that the multiplications, additions, and nonlinear operators convert input to output (images of cats/dogs to labels of cats/dogs)
5. Step – Evaluate the accuracy of trained NN on test (input, output) pairs

Input:
(x, y) coordinates



Output:
Label of (x, y) coordinates = {Orange, Blue)

2. How Are Scientists Creating Complex Boundary?

Relevance of AI to Metrology:

- Describe boundaries mathematically
  - → Boundaries are unknown in discoveries!
- Linear boundaries can be described directly with x and y
  - → Linear regression is rarely accurate for complex biomedical phenomena!
- Nonlinear boundaries must be described with nonlinear transformations (nonlinear features and operators/activations)
  - → ReLU is the most frequently used in practice. The choice might depend on the convergence of the model training.
- Nonlinear boundary description can be derived automatically by training Neural Networks (NN) with training data.
  - → NN are graphs of connected linear and non-linear computational units. The graph nodes and edges have coefficients that are applied to each input to produce a prediction output.

3. How do you learn primitive neural network concepts interactively?

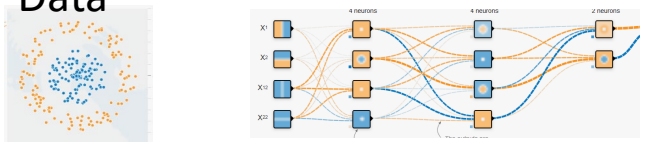
- https://pages.nist.gov/nn-calculator/
- Four simple exercises
  1. Simple to complex NN architecture
  2. Linear to non-linear features
  3. Linear to non-linear activation functions
  4. Well-separated to inseparable (interleaved) classes

Learning about NNs Using a Web-Based "NN Calculator"

Memory Operations: MC, MR, M+, M-, MS, AVG

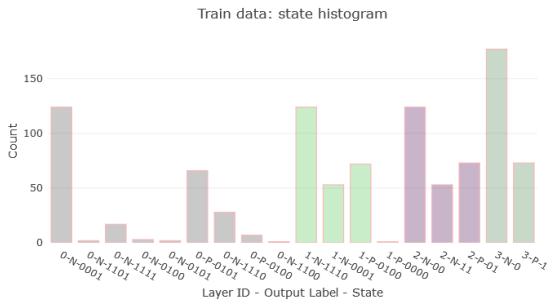
Data

NN



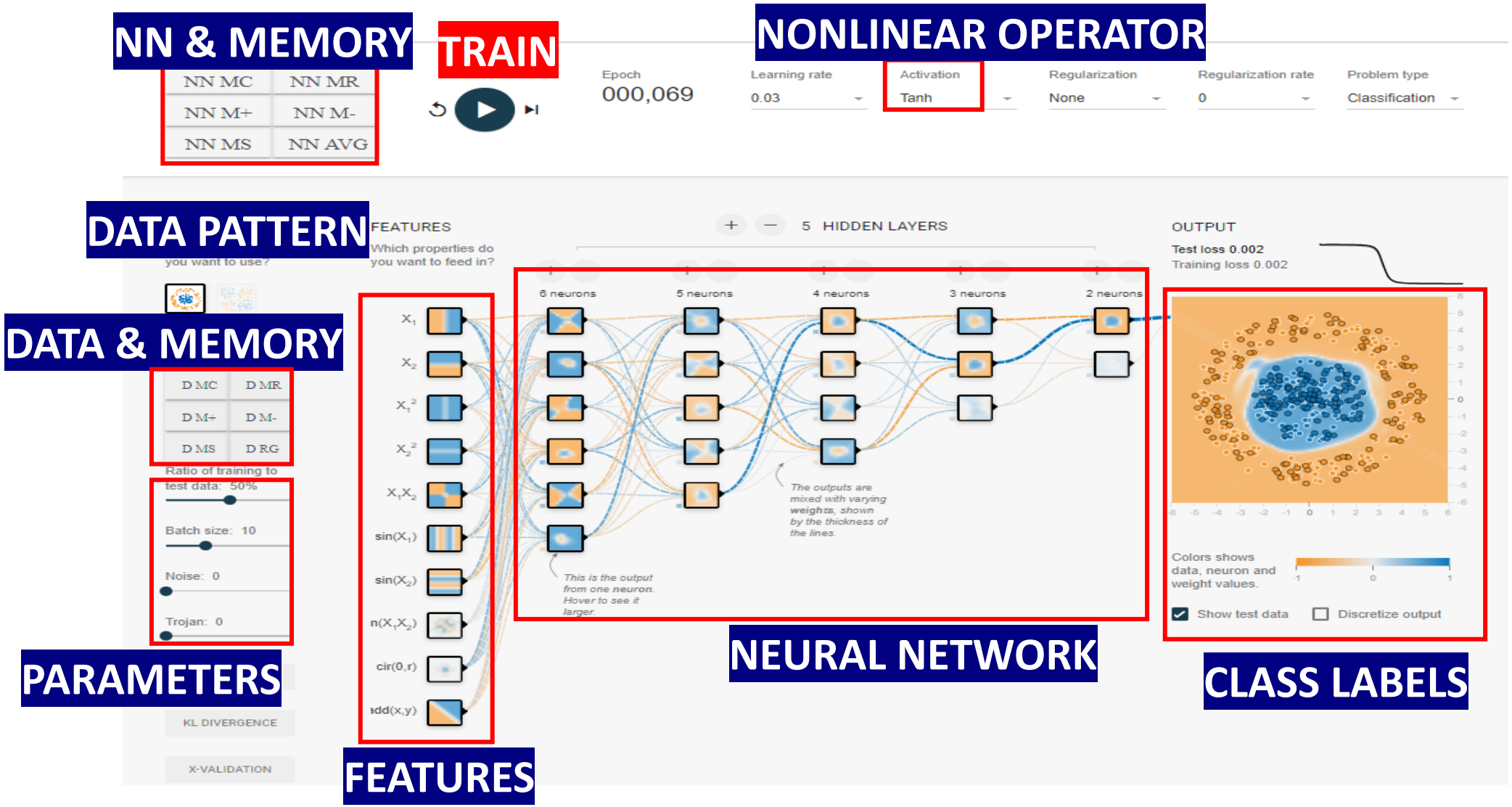
Operands: 2D data and NN

Display: NN, Data, Results



NN Operators: design, parametrize, train, infer, inefficiency, sensitivity

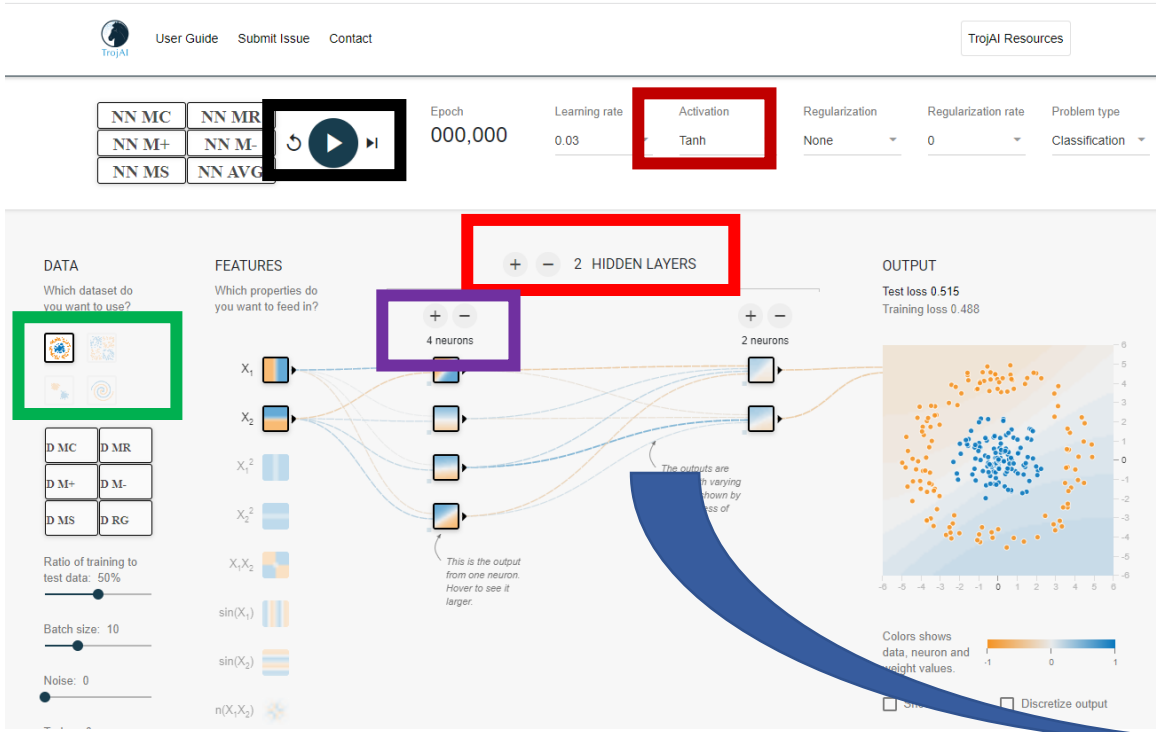
NN Calculator Layout

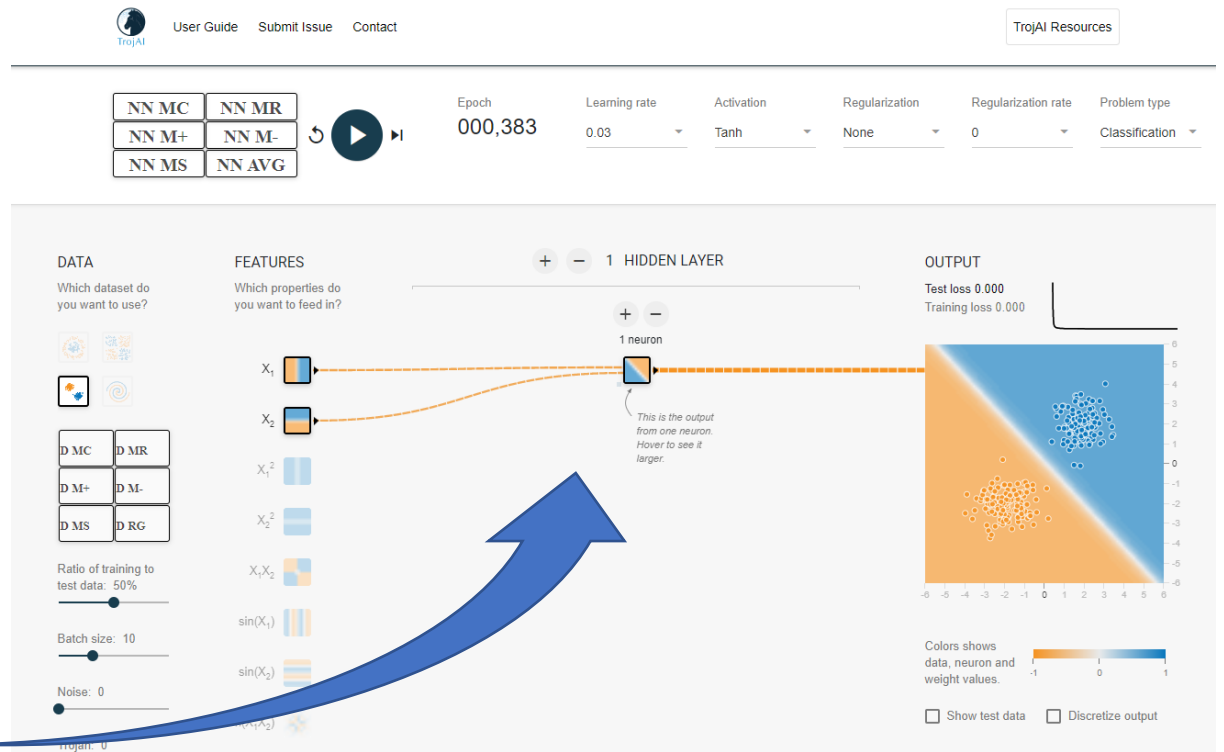


NN calculator: https://pages.nist.gov/nn-calculator/

EX #1: Modify the NN to a single node

1. Remove layers
2. Remove nodes
3. Select data pattern with cluster pattern
4. Select Linear activation function
5. Train

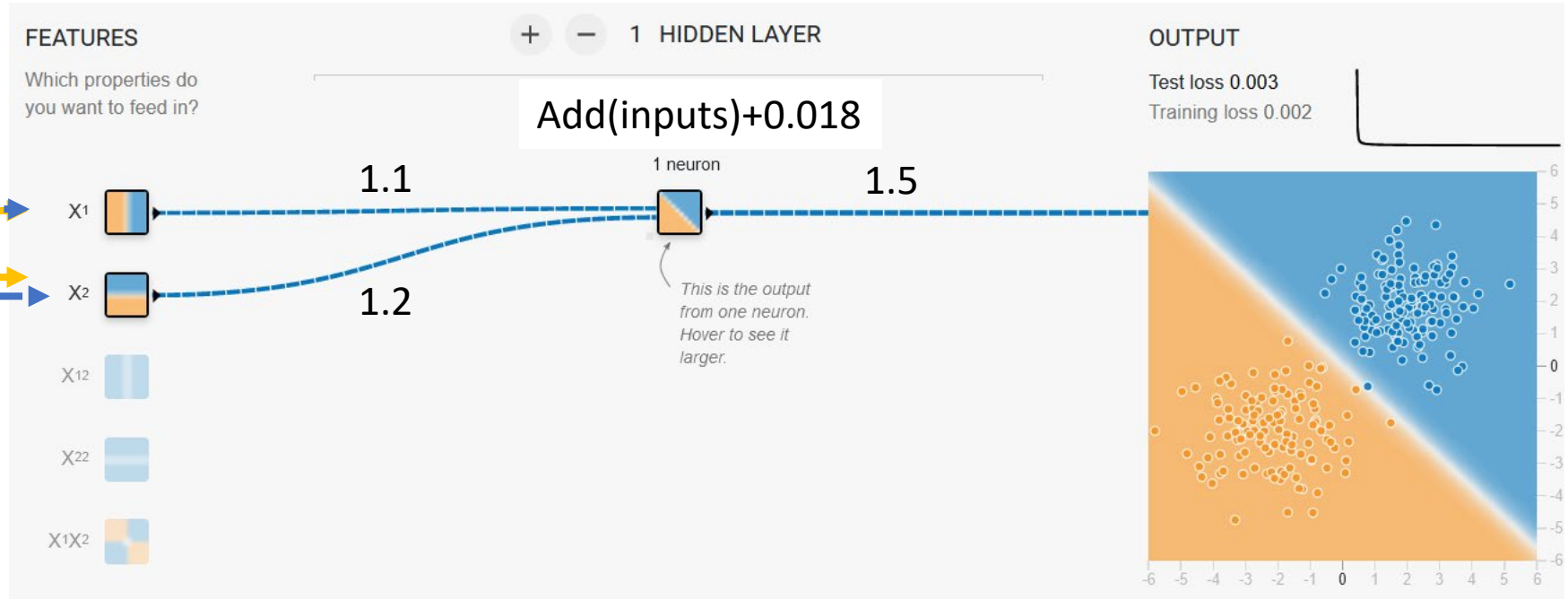


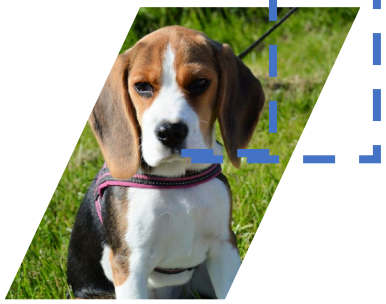


Single node NN with Linear activation function

$Math\ model\colon\ if\ x + y\ < 0$
$then\ orange(N)\ else\ blue\ (P)$

Linear Activation



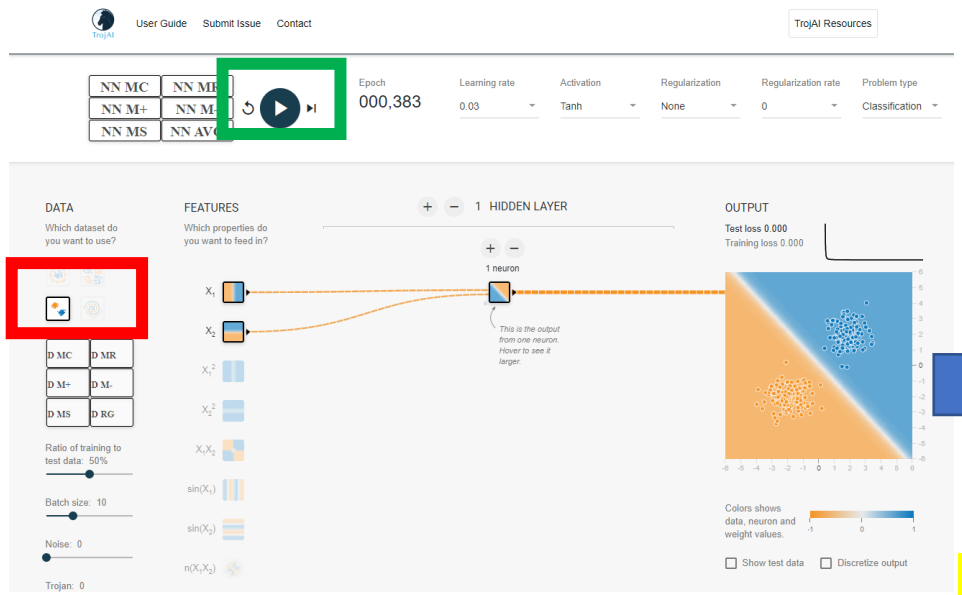


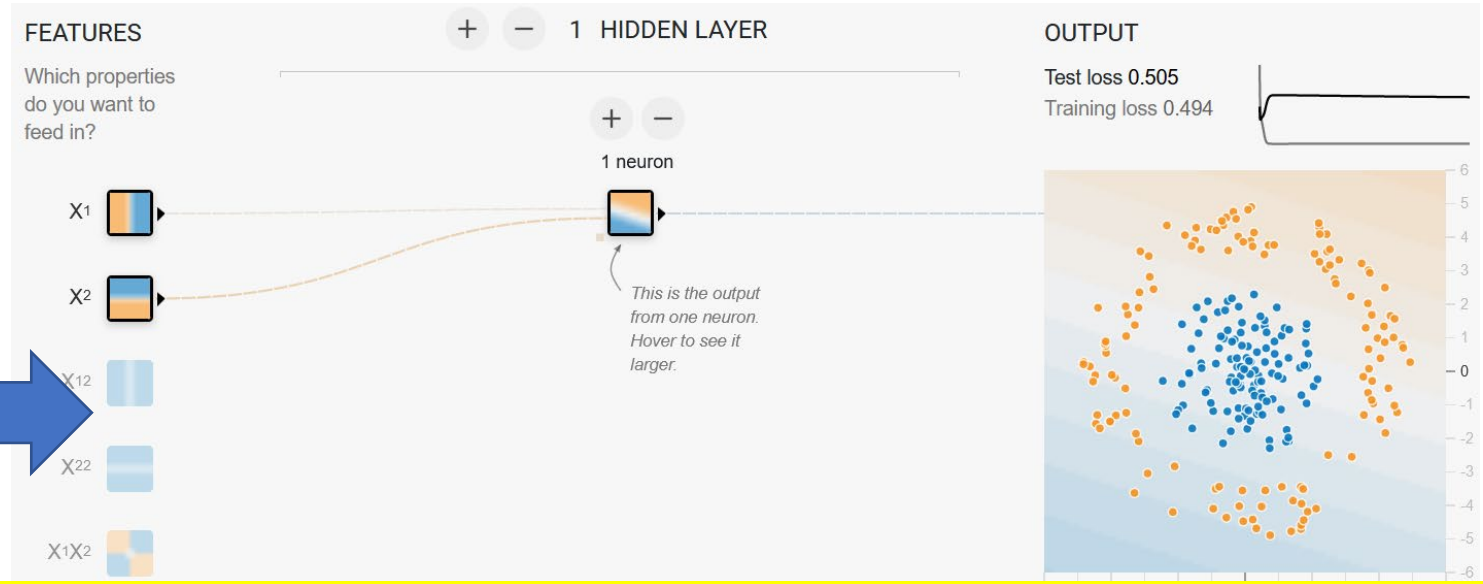
$NN\ model\colon\ if\ 1.5 * \big((1.1 * x + 1.2 * y) + 0.018\big) < 0$
$then\ orange\ (N)\ else\ blue\ (P)$

If 1.65 * x + 1.8 * y + 0.027 < 0 then orange (N) else blue P)

Complexity of Data Patterns

- Switch data patterns
- Train



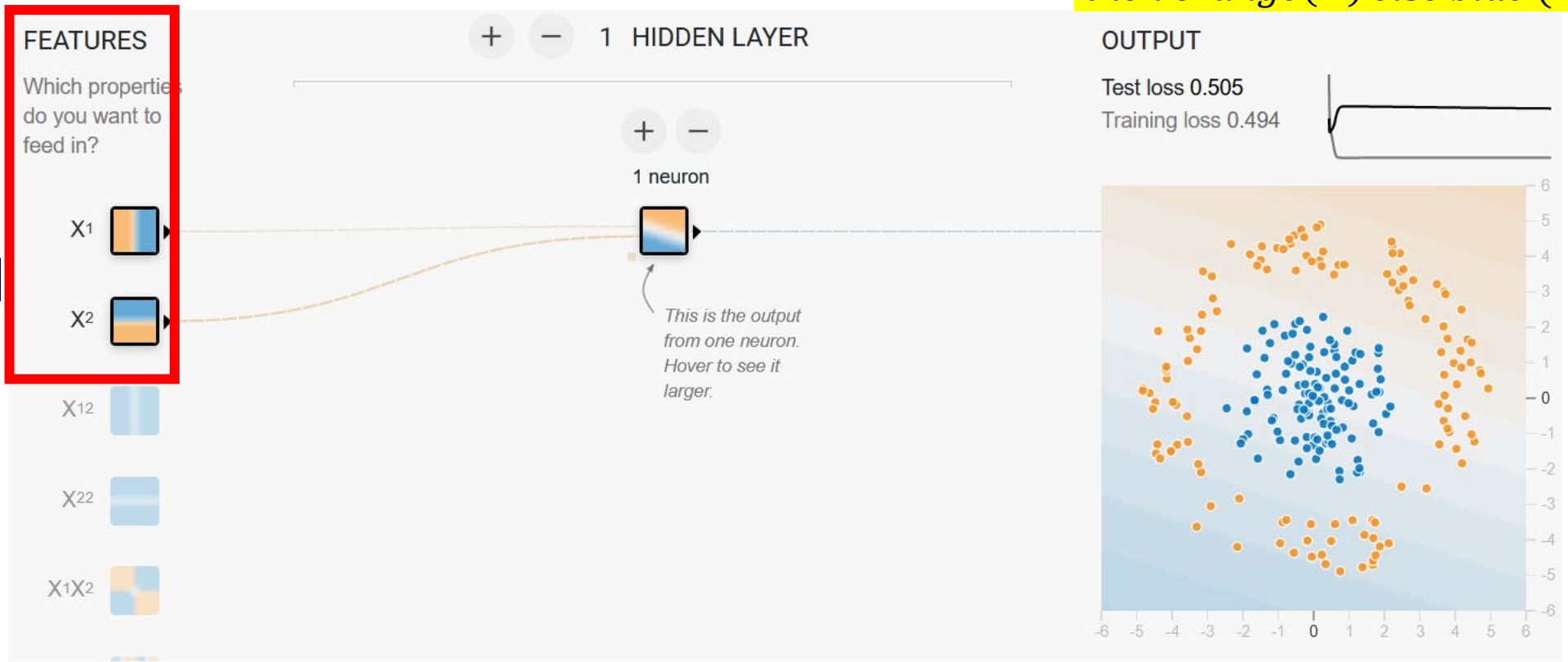


NN model: FAILED
– could not come up with an accurate labeling formula based on x & y

Why did the model fail?

Linear Activation

$Math: if\ x^2 + y^2 > r^2$
$then\ orange(N)\ else\ blue\ (P)$



$NN\ model: FAILED$
$-\ could\ not\ come\ up\ with\ an\ accurate\ labeling\ formula\ based\ on\ x\ \&\ y$

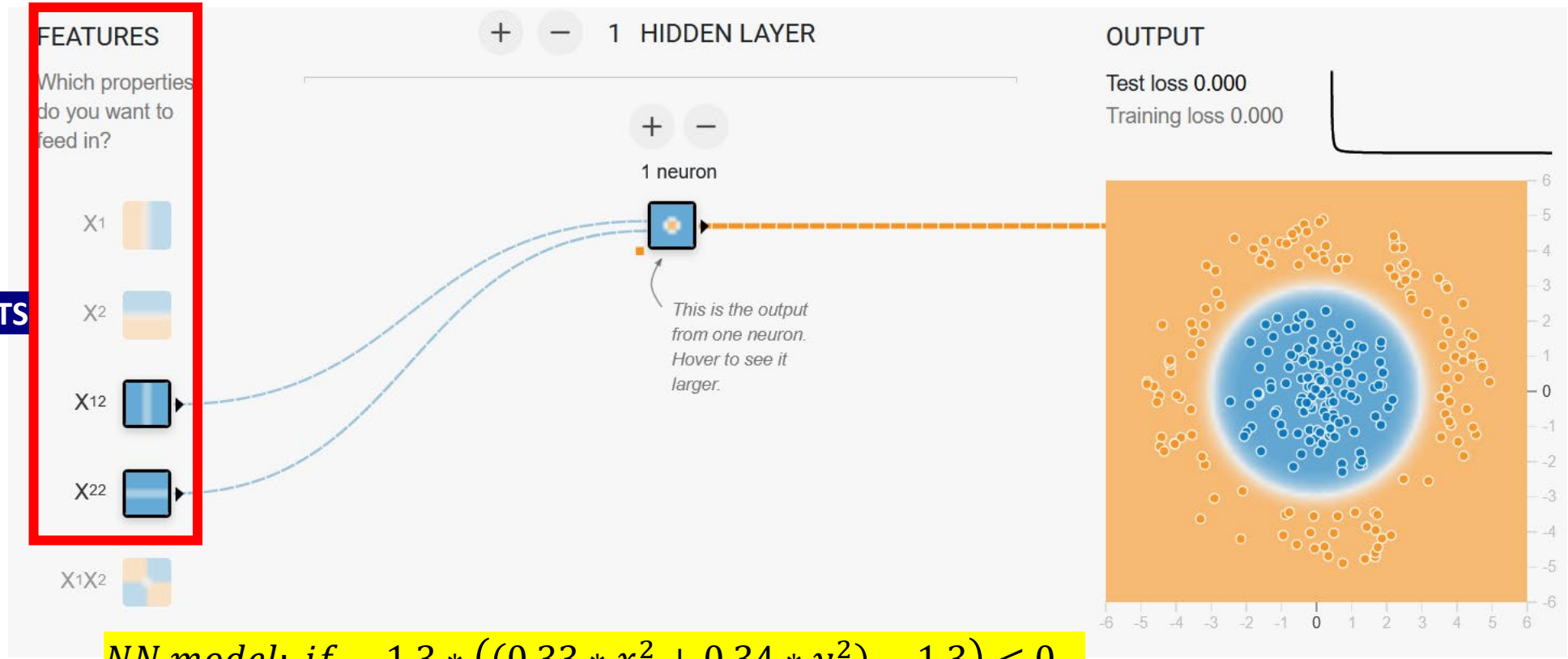
Solution 1:
- Create non-linear features

Solution 2:
- Add 3 more nodes
- Switch to Tanh activation function

EX #2: Non-Linear Features (x^2 and y^2)

$Math: if\ x^2 + y^2 > r^2$
$then\ orange(N)\ else\ blue\ (P)$

Linear Activation



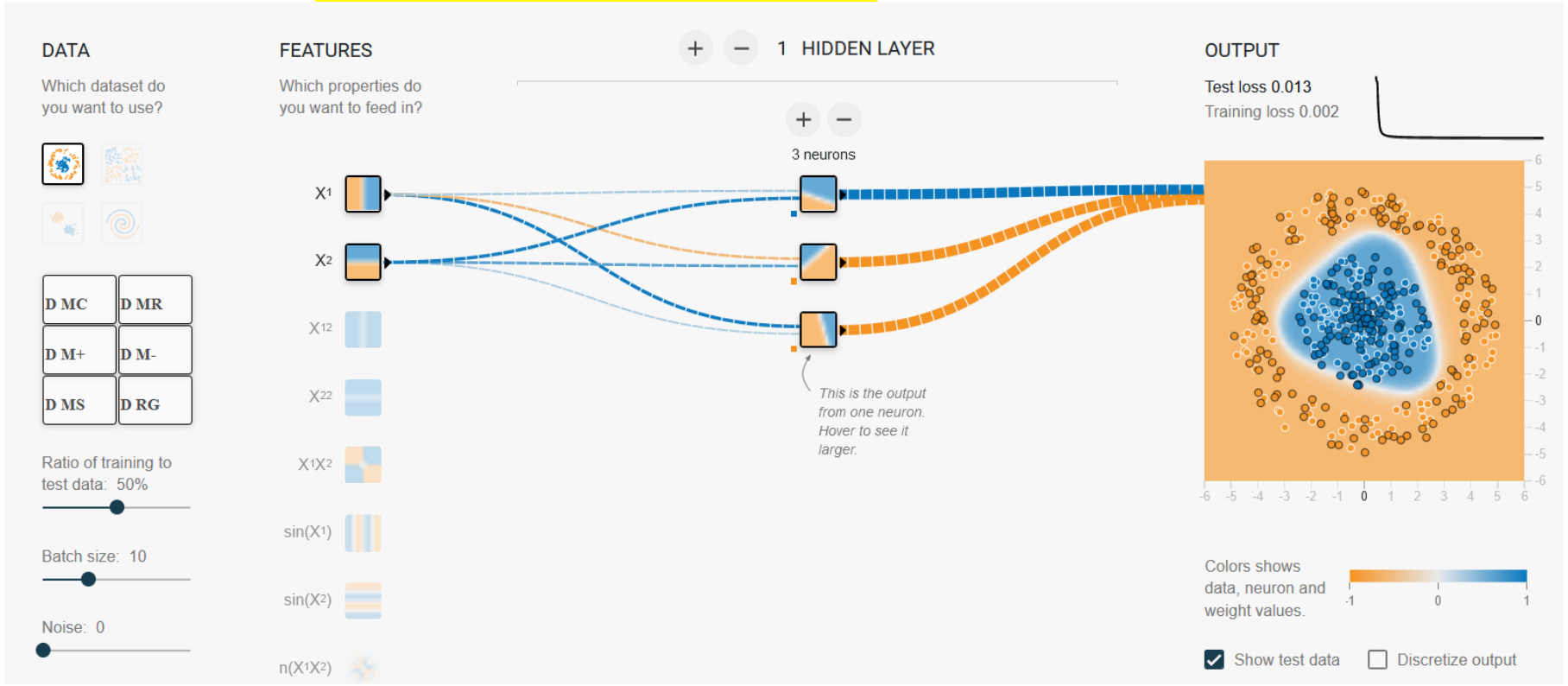
$NN\ model: if\ -1.3 * \left((0.33 * x^2 + 0.34 * y^2) - 1.3\right) < 0$
$then\ orange(N)\ else\ blue\ (P)$

If - 0.429 * x^2 - 0.442 * y^2 + 1.69 < 0 then orange (N) else blue (P) → radius ~ Sqrt(1.69/0.433) = 1.97

EX #3: Non-Linear Tanh Activation

$Math: if\ x^2 + y^2 > r^2$
$then\ orange(N)\ else\ blue\ (P)$

Tanh Activation

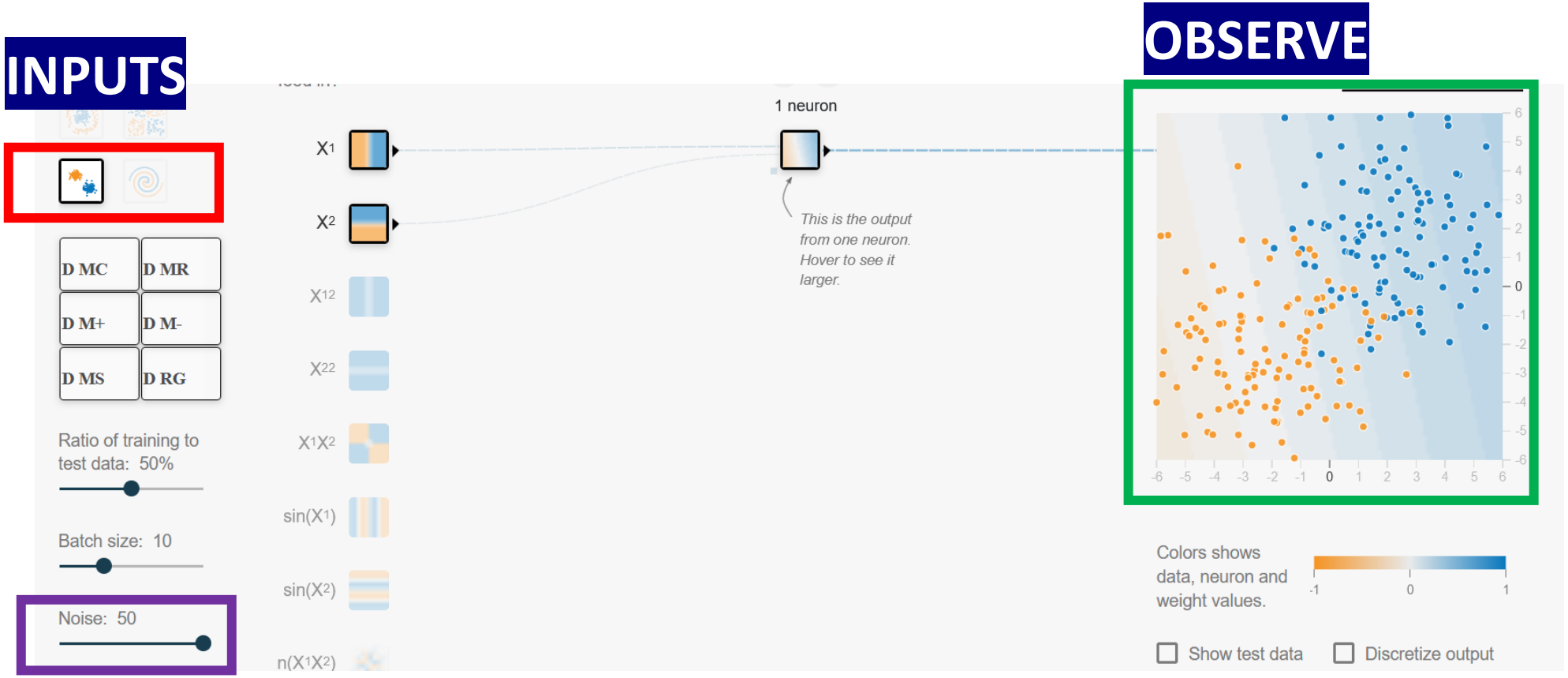


Test loss 0.013
Training loss 0.002

$NN\ model: if$ 4 * tanh(1.7 + 0.32 * x + 0.94 * y) – 4 * tanh(-1.9 - 0.59 *x + 0.66 * y) – 4 * tanh(-2.0 + 0.96 * x + 0.27 * y) < 0
$then\ orange\ (N)\ else\ blue\ (P)$

EX #4: Test well-separated and interleaved patterns

- Select a dataset with cluster pattern
- Use the “Noise” slider bar



Thank You

- URL: https://pages.nist.gov/nn-calculator/
- Questions: peter.bajcsy@nist.gov

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Leveraging Density Functional Theory (DFT), Graph Neural Networks (GNN) & Generative Pre-trained Transformers (GPTs) for Accurate Predictions: JARVIS-DFT, ALIGNN, AtomGPT

Daniel Wines, Brian DeCost and Kamal Choudhary

https://jarvis.nist.gov

Joint Automated Repository for Various Integrated Simulations

7/18/2024

JARVIS-DFT

NIST MATERIAL MEASUREMENT LABORATORY

jarvis.nist.gov/jarvisdft/

NIST

JARVIS Publications Colab Downloads Tutorials Events Log In / Sign Up Help

Density Functional Theory (DFT)

Click on periodic table elements (e.g., Ni-Al-) or enter a chemical formula (e.g., Al2O3) or enter a JARVIS-ID (e.g., JVASP-1002) and click Search.

Mo-S- Search Refresh

https://jarvis.nist.gov/jarvisdft/

how 100 entries Search:

id	formula	Spg	SpgNum	crys	func	E_form	OPT_gap	MBJ_gap	hse_gap	Kv	Gv	poisson	spillage	slme	mag	type
JVASP-664	MoS2	P-6m2	187	hexagonal	OptB88vdW	-0.88454	1.658	-	-	-	-	-	0.003	-	0.0	2D
JVASP-730	MoS2	R-3m	166	trigonal	OptB88vdW	-0.60967	0.000	-	-	-	-	-	0.976	-	-0.0	2D
JVASP-100856	MoS3	P2_1/m	11	monoclinic	OptB88vdW	-0.34773	0.443	-	-	-	-	-	-	-	0.0	3D
JVASP-111117	MoS2	P-3m1	164	trigonal	OptB88vdW	-0.69305	0.000	0.0	-	-	-	-	-	-	0.0	3D
JVASP-127507	MoS	Pm-3m	221	cubic	OptB88vdW	-0.18293	0.000	-	-	-	-	-	-	-	0.0	3D
JVASP-132473	MoS3I	P1	1	triclinic	OptB88vdW	0.06061	0.651	-	-	-	-	-	-	-	3.993	3D
JVASP-144515	Mo3S4	P-1	2	triclinic	OptB88vdW	-0.73826	0.000	-	-	-	-	-	-	-	0.0	3D
JVASP-228	MoS2	R-3m	166	trigonal	OptB88vdW	-0.69909	0.000	0.0	-	51.32	45.47	0.19	0.852	-	0.0	3D
JVASP-28379	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.95754	0.958	1.364	-	71.48	44.27	0.26	-	33.92	-	3D
JVASP-28413	MoS2	P-3m1	164	trigonal	OptB88vdW	-0.92268	1.207	1.471	-	-	-	-	-	32.7	0.0	3D
JVASP-28733	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.96160	0.921	-	-	70.62	47.69	0.23	0.013	-	0.0	3D
JVASP-34138	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.96135	0.920	1.356	-	-	-	-	-	33.93	0.0	3D

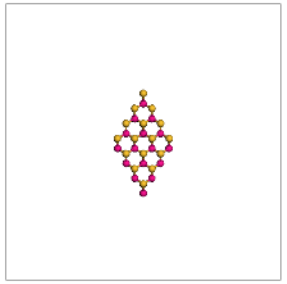
JARVIS API JARVIS-DFT JARVIS-ML JARVIS-FF JARVIS-Tools Documentation Publications Report bug/Contact

Structure XRD DOS Bands Spillage Optics(GGA) Elastic Thermoelectric Convergence

ID: JVASP-664	Functional: OptB88vdW	Primitive cell	Primitive cell	Conventional cell	Conventional cell
Chemical formula: MoS2	Formation energy/atom (eV): -0.88454	a 3.19 Å	α: 90.0 °	a 3.19 Å	α: 90.0 °
Space-group:P-6m2 (187)	Relaxed energy/atom (eV):-5.21029	b 3.19 Å	β: 90.0 °	b 3.19 Å	β: 90.0 °
Crystal system:hexagonal	Point group:-6m2	c 34.88 Å	γ: 120.0 °	c 34.88 Å	γ: 120.0 °
Data source:JARVIS-DFT-VASP	Material type:SingleLayer	Density (gcm⁻³):0.866	Volume (Å³):306.988	nAtoms_prim:3	nAtoms_conv:3
SCF direct bandgap (eV):1.683	SCF indirect bandgap (eV):1.658	Magnetic moment (μB):0.0	Exfoliation energy (meV/atom):	Packing fraction:0.069	Number of species:2
Band direct gap (eV):1.71	Band indirect gap (eV):1.71	TBmBJ direct gap (eV):	TBmBJ indirect gap (eV):	HSE06 direct gap (eV):2.49	HSE06 indirect gap (eV):2.36
Voigt bulk mod. (GPa):	Voigt shear mod. (GPa):	Poisson ratio:	Anisotropy ratio:	Solar SLME (%):	Solar SQ (%):
Max. IR mode (cm⁻¹):	Max. Raman mode (cm⁻¹):	Min. IR mode (cm⁻¹):	Min. FD phonon (cm⁻¹):-0.0	Cut-off (eV):650	K-point length (Å):25

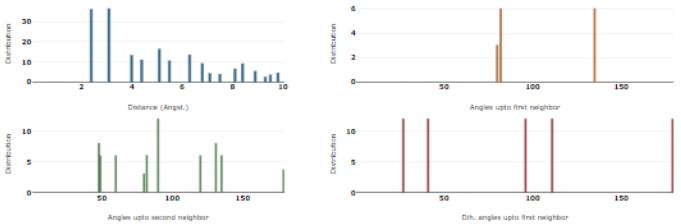
Show POSCAR Show POSCAR-conv Show XYZ format Show CIF format

Visualizing Atomic structure



Atomic Structure Analysis

The following shows the radial, angle and dihedral distribution function plots.



JARVIS-DFT

NIST MATERIAL MEASUREMENT LABORATORY

Features	JARVIS-DFT
#Materials (Struct., E_f, E_g)	80000
DFT functional/methods	vdW-DFT-OptB88, TBmBJ, DFT+SOC
K-point/cut-off	Converged for each material
SCF convergence criteria	Energy & Forces
Elastic tensors & point phonos	17402
Piezoelectric, IR spect.	4801
Dielectric tensors (w/o ion)	4801 (15860)
Electric field gradients	11865
SuperCon Tc	2200 (1058 ambient condition)

Features	JARVIS-DFT
2D monolayers	1011
Raman spectra	400
Seebeck, Power Factors	23210
Solar SLME	8614
Spin-orbit Coupling Spillage	11383
WannierTB	1771
STM images	1432
Surfaces	300
Defects	400
Interfaces	1.4 trillion (IU), 600 (ASJ)

Hands-on: JARVIS-DFT Analysis

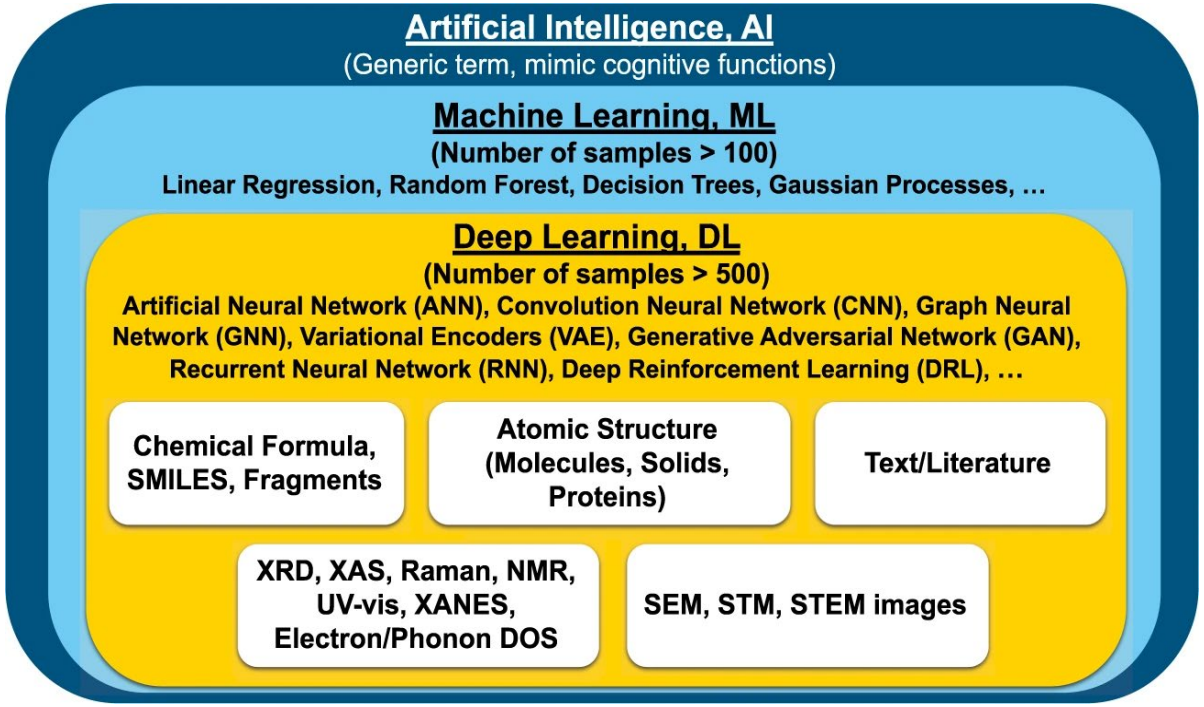
NIST MATERIAL MEASUREMENT LABORATORY

Part-2

2.1 https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/JARVIS_QuantumEspressoColab_Basic_Example.ipynb
2.2 https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/Analyzing_data_in_the_JARVIS_DFT_dataset.ipynb
2.3 https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/Basic_ML.ipynb
2.4 https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/alignn_jarvis_leaderboard.ipynb
2.5 https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/Train_ALIGNNFF_Mlearn.ipynb
2.6 https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/atomgpt_example.ipynb
2.7 (optional) https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/AtomVisionImageClassification.ipynb

Deep learning for materials

NIST MATERIAL MEASUREMENT LABORATORY



npj | computational materials

Explore content · About the journal · Publish with us

nature > npj computational materials > review articles > article

Review Article | Open Access | Published: 05 April 2022

Recent advances and applications of deep learning methods in materials science

Kamal Choudhary, Brian DeCost, Chi Chen, Anubhav Jain, Francesca Tavazza, Ryan Cohn, Cheol Woo Park, Alok Choudhary, Ankit Agrawal, Simon J. L. Billinge, Elizabeth Holm, Shyue Ping Ong & Chris Wolverton

npj Computational Materials **8**, Article number: 59 (2022) | Cite this article

REVIEW ARTICLE | OCTOBER 18 2023

Recent progress in the JARVIS infrastructure for next-generation data-driven materials design

Daniel Wines ; Ramya Gurunathan ; Kevin F. Garrity ; Brian DeCost ; Adam J. Biacchi ; Francesca Tavazza ; Kamal Choudhary

Check for updates

+ Author & Article Information

Appl. Phys. Rev. 10, 041302 (2023)

https://doi.org/10.1063/5.0159299 **Article history**

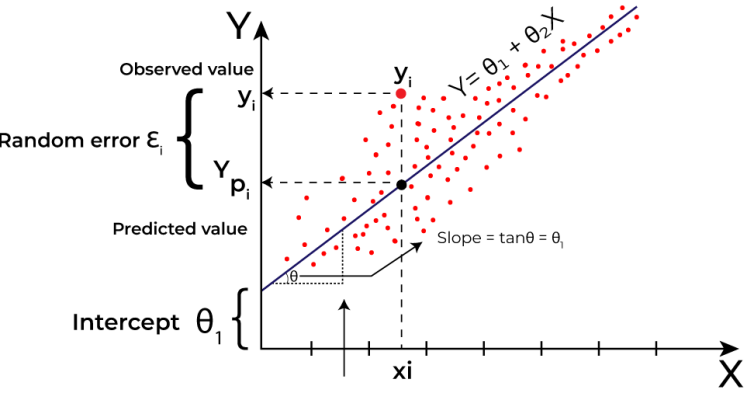
Tour of Machine Learning Models

- **Dimensionality reduction**: feature extraction technique that aims to reduce the number of input features
  - PCA, t-SNE, UMAP
- **Instance methods**: Compares instances in data with a similarity measure to identify best matches
  - K-Nearest Neighbor, Self-Organizing Maps (SOM)
- **Regression**: Establish relationship between independent variable X and dependent variable Y by iteratively optimizing errors made in predictions, most of these can be used for classification as well
  - Logistic Regression, Neural networks, Decision trees
- **Clustering Models**: describes the class of problem, different from classification, works with unlabeled data
  - Hierarchical Clustering, k-Means
- **Regularization models**: penalizes models based on their complexity
  - Ridge regression, LASSO, Elatic Net
- **Bayesian algorithms**: apply Bayes' Theorem for problems
  - Naïve Bayes, Bayesian Network
- **Ensemble algorithms**: models composed of multiple weaker models that are independently trained and whose predictions are combined in some way to make the overall predictions better
  - Random Forest, Gradient Boosted Regression Trees, AdaBoost
- **Neural Network Algorithms**: inspired by the structure and/or function of biological neural networks
  - Multilayer Perceptrons, convolution NN, Graph NN, transformers, Auto-encoders, diffusion models

https://machinelearningmastery.com/a-tour-of-machine-learning-algorithms/ ,
https://www.geeksforgeeks.org/machine-learning-algorithms/

ML Models

Linear Regression



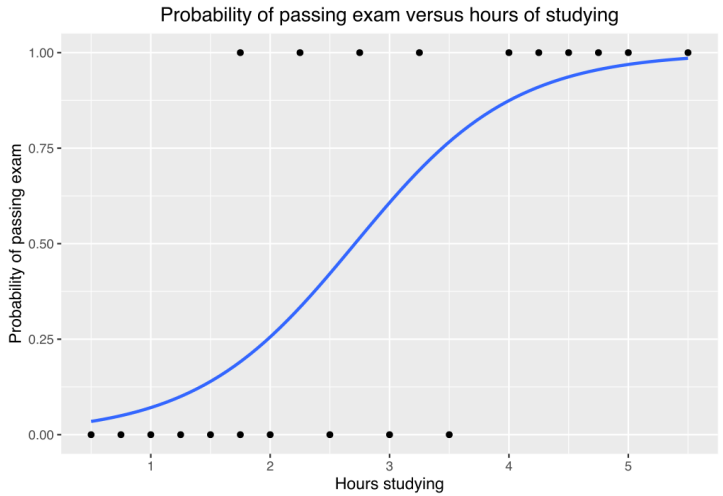
$$y = \beta_0 + \beta_1 x$$

- y is the dependent variable.
- x is the independent variable.
- β0 is the y-intercept of the line.
- β1 is the slope of the line.
- To estimate $\beta 0$ and $\beta 1$, we minimize the sum of the squared residuals:

$$\text{RSS} = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p$$

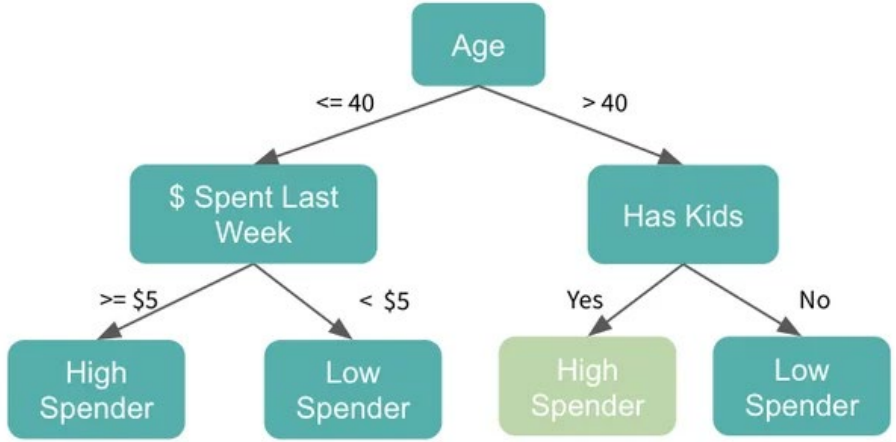
Logistic Regression



- Log-odds of an event as a linear combination of one or more independent variables
- Used for predicting a binary or categorical dependent variable.

$$p(x) = \frac{1}{1 + e^{-(x-\mu)/s}}$$

Tree based methods



Tree-based models use a series of if-then rules to generate predictions from one or more decision trees: RandomForest, GBM

Gini Impurity:

$$Gini = 1 - \sum_{i=1}^{n} p_i^2$$

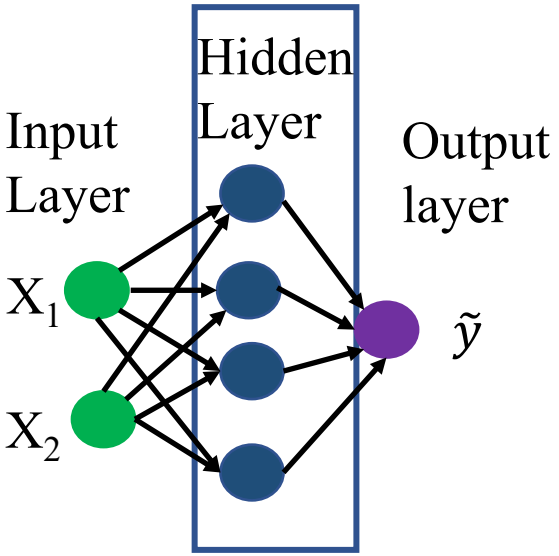
Where p_i is the proportion of samples belonging to class i in the node.

$$Entropy = -\sum_{i=1}^{n} p_i \log_2(p_i)$$

Deep learning for materials

NIST MATERIAL MEASUREMENT LABORATORY

Standard NN



1) Forward propagation

$z^{[l]} = W^{[l]} a^{[l-1]} + b^{[l]}$

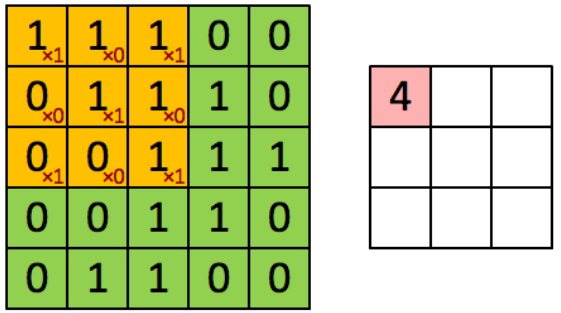
$a^{[1]} = \sigma(z^{[l]}); \quad a^{[0]} = X$

2) $Cost, J(W, b) = f(y - \tilde{y})$

3) Gradient descent (∇J):
minimize cost with W,b

4) Backpropagation:
chain rule to get, $\frac{\partial J}{\partial W}$

ConvolutionNN



1	0	1
0	1	0
1	0	1

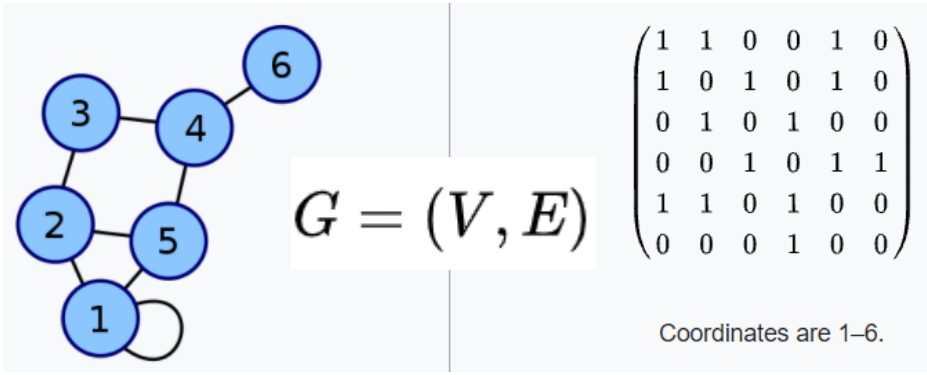
1) Convolution:
element-wise multiplication & sum

2) Pool: Max, Average, Sum

3) Fully Connected: Standard NN

Shared weights (Learnable filters), regularized version of NNs

GraphConvNN



Types: un/weighted, un/directed, line, Hetero/Homogenous, Multigraph

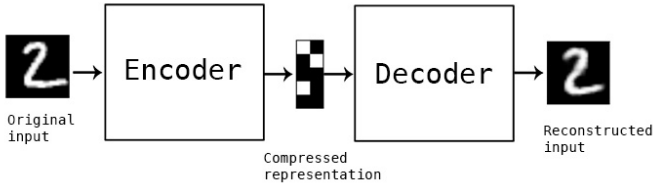
1) Adjacency matrix, N x N (N: #nodes),
2) D: degree of node
3) Update node representation using message passing, GPU efficient
4) Update equation is local, neighborhood of a node only, independent of graph size

$$h_i^{\ell+1} = f(h_i^{\ell}, \{h_j^{\ell}\}_{j \in \mathcal{N}_i})$$

Deep learning for materials

NIST MATERIAL MEASUREMENT LABORATORY

AutoEncoders



Used for Dimensionality reduction or feature learning:

1) Encoding functions: *x* to a latent dimension *z*

$$\mathbf{z} = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$$

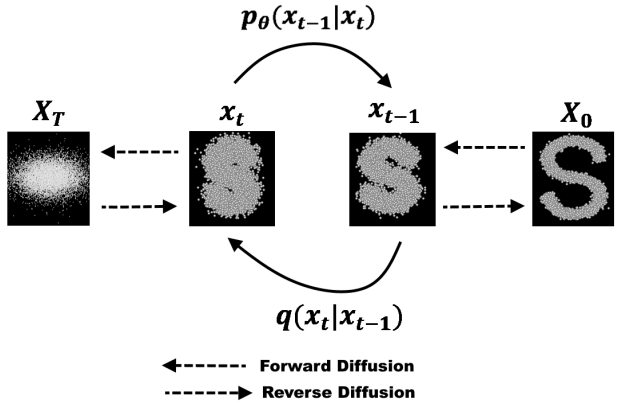
2) Decoding functions: *z* to x

$$\mathbf{x}' = \sigma'(\mathbf{W}'\mathbf{z} + \mathbf{b}')$$

3) Loss function

$$\mathcal{L}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|^2$$
$$\|\mathbf{x} - \sigma'(\mathbf{W}'(\sigma(\mathbf{W}\mathbf{x} + \mathbf{b})) + \mathbf{b}')\|^2$$

Diffusion Models



Reverse diffusion process, starting from random noise

1)Forward diffusion: gradually adds noise over time steps

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \prod_{t=1}^{T} \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

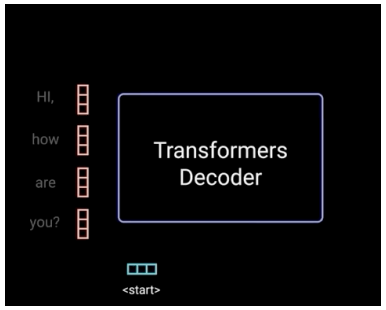
2) Reverse Diffusion Process:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

3) Training Objective and sampling:

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}}[\, \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\|^2 \,]$$

Transformers



1) Self-attention: calculates the relevance between each pair of input tokens.

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

2) Multi-head attention: focus on different parts of the input sequence simultaneously

3) $$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W^O$$

$$\text{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

4) Positional Encoding: instead of RNN, use PE to convey the order of elements in the sequence

$$\text{PE}_{(pos,2i)} = \sin\left(\frac{pos}{10000^{2i/d_{\text{model}}}}\right)$$
$$\text{PE}_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{2i/d_{\text{model}}}}\right)$$

ALIGNN

NIST MATERIAL MEASUREMENT LABORATORY

Atomistic Line Graph Neural Network

github.com/usnistgov/alignn

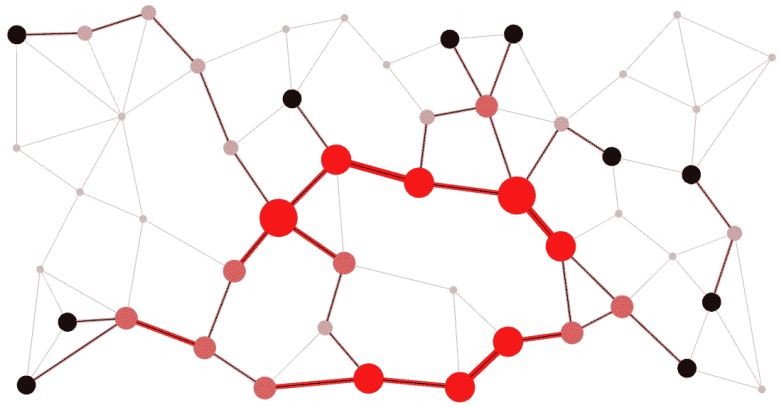
usnistgov / alignn

Type / to

Code | Issues 23 | Pull requests 5 | Discussions | Actions | Proje

alignn Public

Edit Pins



npj | computational materials

Explore content | About the journal | Publish with us

nature > npj computational materials > articles > article

Article | Open Access | Published: 15 November 2021

Atomistic Line Graph Neural Network for improved materials property predictions

Kamal Choudhary & Brian DeCost

npj Computational Materials **7**, Article number: 185 (2021) | Cite this article

Digital Discovery

ROYAL SOCIETY OF CHEMISTRY

PAPER

View Article Online
View Journal

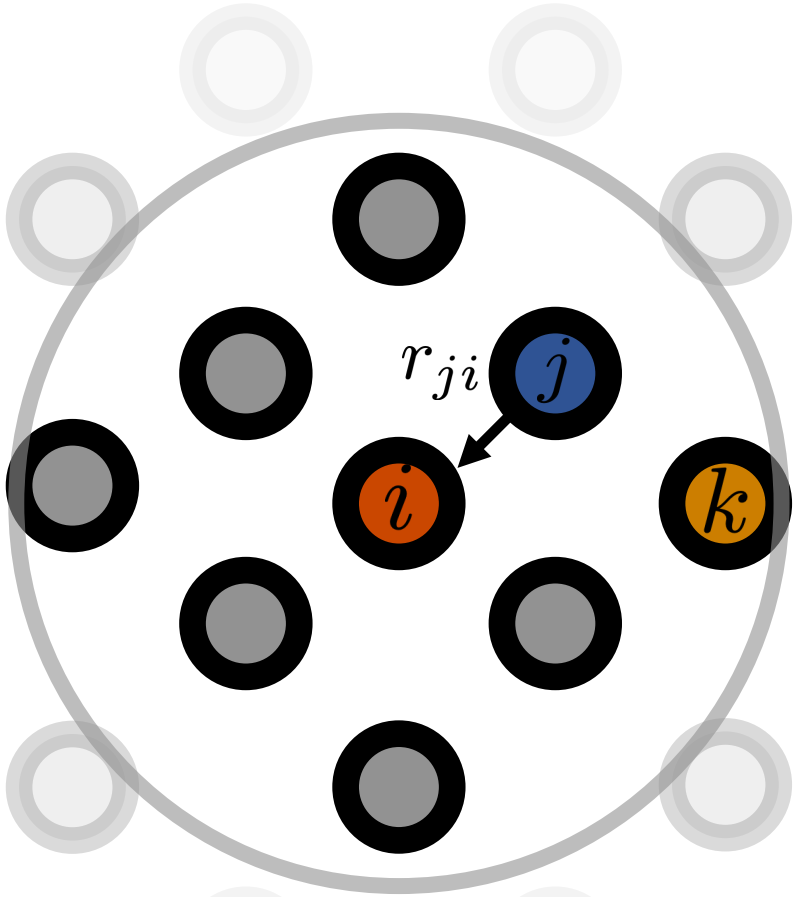
Check for updates

Cite this: DOI: 10.1039/d2dd00096b

Unified graph neural network force-field for the periodic table: solid state applications

Kamal Choudhary, *[ab] Brian DeCost, [c] Lily Major, [de] Keith Butler, [e] Jeyan Thiyagalingam [e] and Francesca Tavazza [c]

Interatomic potentials



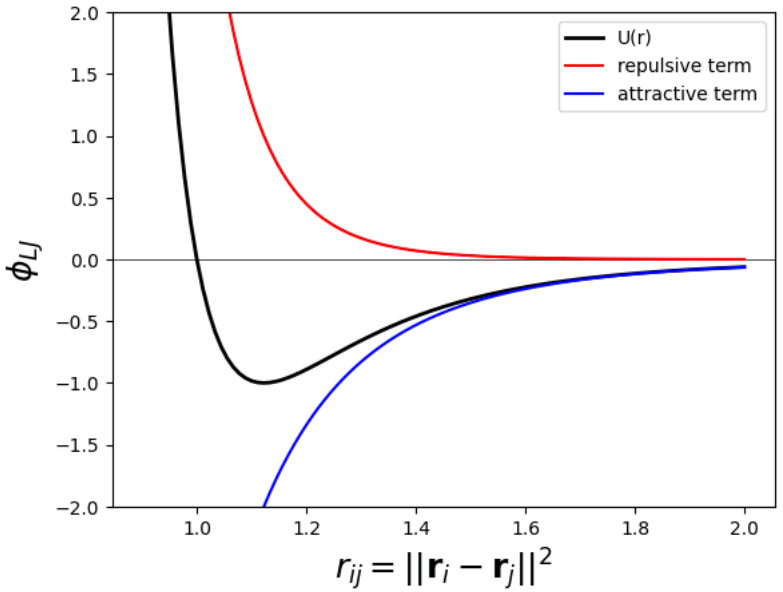
Expand the potential U({r}) in terms of n-body interactions

$$U(\{\mathbf{r}\}) = \sum_i \phi_1(\mathbf{r}_i) + \sum_i \sum_j \phi_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_i \sum_j \sum_k \phi_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots$$

Lennard Jones potential: repulsive and attractive terms

$$U(\{\mathbf{r}\}) = \sum_i \sum_j \phi_{LJ}(r_{ij})$$

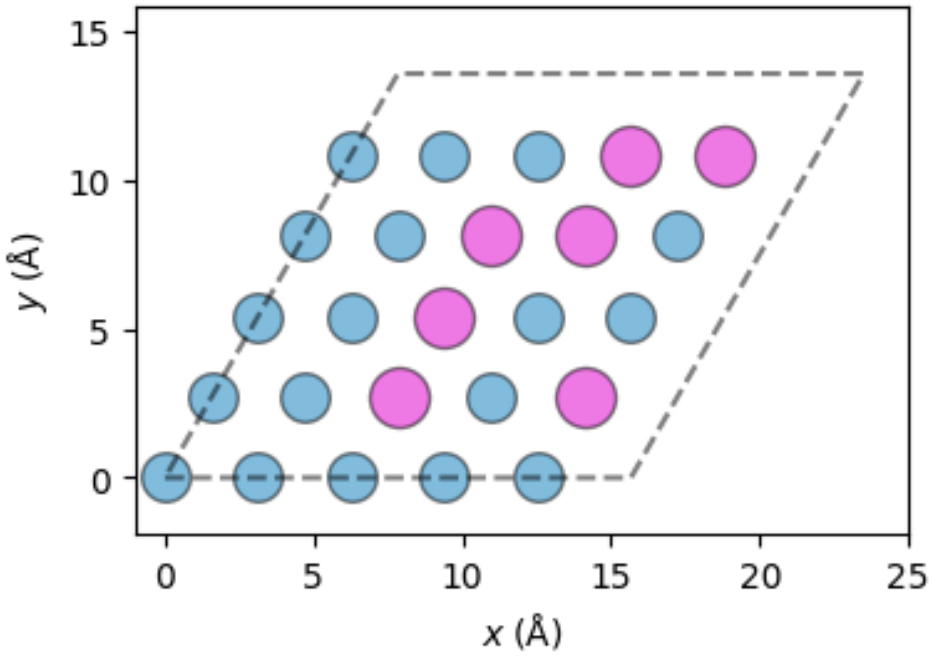
$$\phi_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

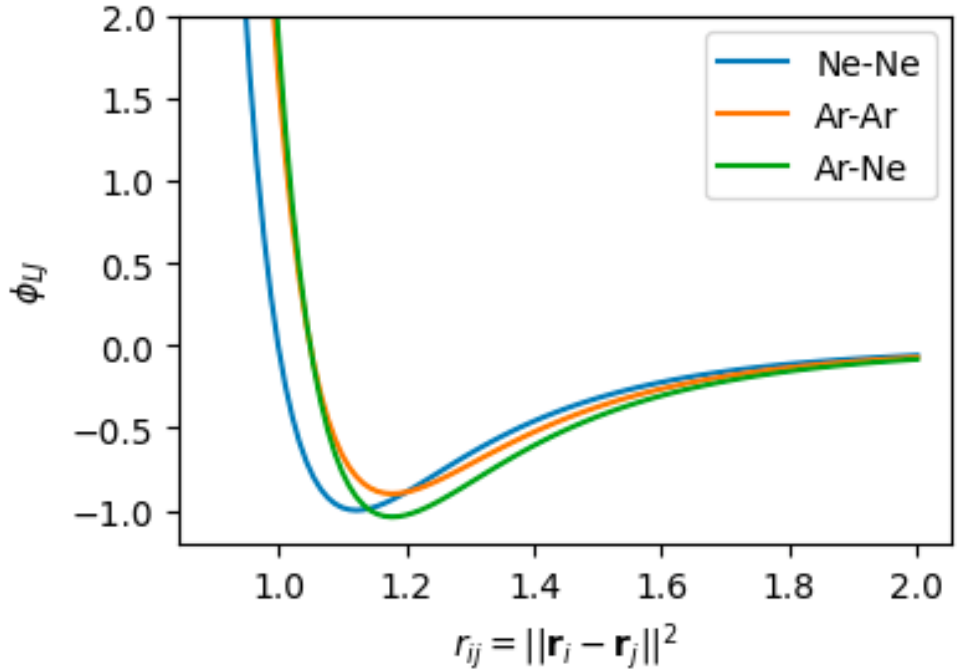


Multicomponent systems

For example, Ne-Ar system

Add separately-parameterized pair potentials for each combination of species





1. Model size scales unfavorably with species considered, especially with more complex potential forms
2. Low model capacity limits ability to capture complex environment-dependent bonding

From pair potentials to (simple) GNN potentials

1. replace pairwise polynomials φ_2 with a simple neural network
2. use multiple rounds of pairwise interaction!

that's the entire core idea.

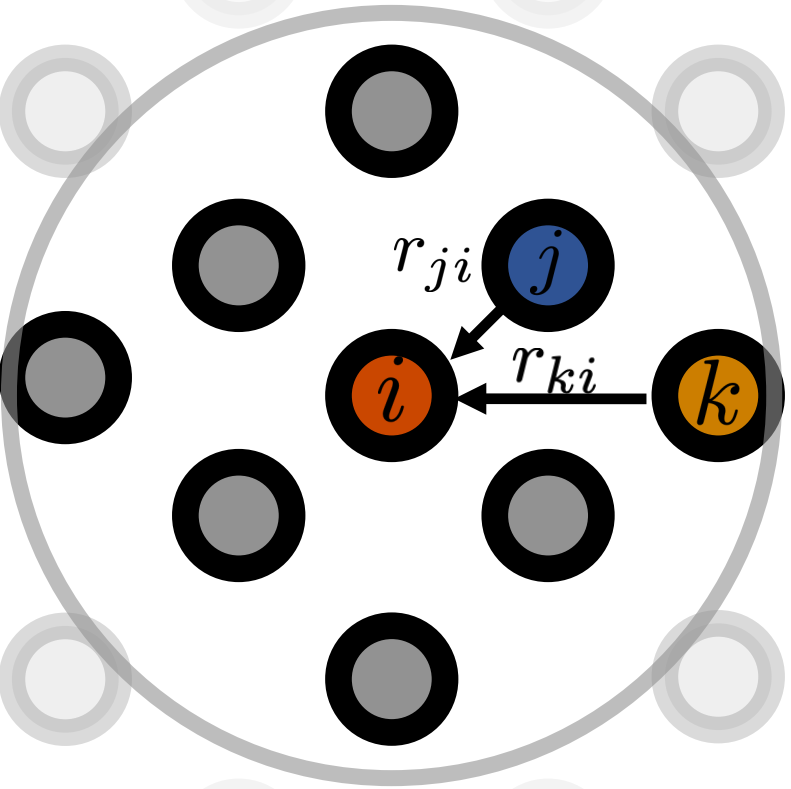
Basic CGCNN interaction: $$\mathbf{x}_i^{l+1} = \sum_j \phi_{ffn}\left([\mathbf{x}_i^l; \mathbf{x}_j^l; b(\mathbf{r}_j - \mathbf{r}_i)]\right)$$

$\mathbf{x}^\ell$	Atom representation
$b(\mathbf{r}_j - \mathbf{r}_i)$	Radial basis
ϕ_{ffn}	Feedforward network
$[a; b]$	Vector concatenation

Variants:
- Atom input featurization
- Spatial basis functions
- Specific neural network architecture
- Incorporation of higher-order functions (angles, dihedrals, …)

Unpacking pair interactions in GNNs

$$W\left([\mathbf{x}_i; \mathbf{x}_j; b(\mathbf{r}_j - \mathbf{r}_i)]\right) = W_d\mathbf{x}_i + W_s\mathbf{x}_j + W_r b(\mathbf{r}_j - \mathbf{r}_i)$$



Expand bond lengths with some basis functions (e.g. Gaussian RBF)

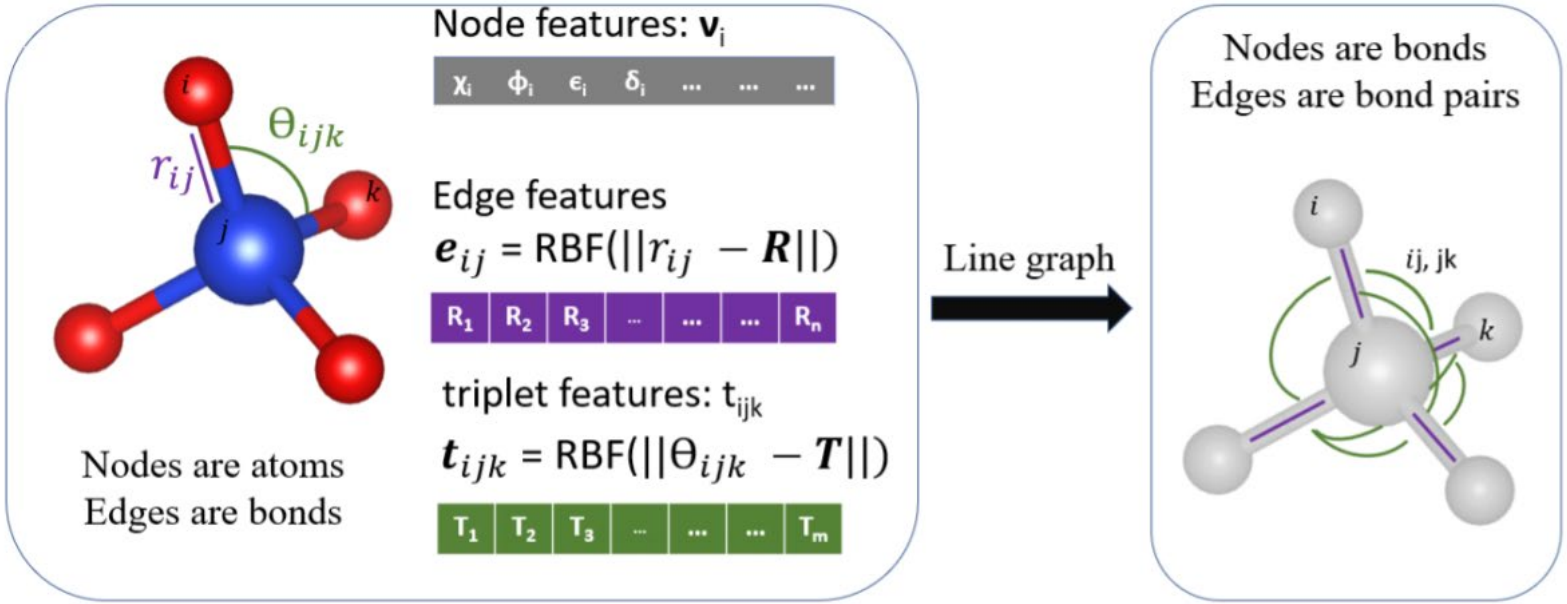
Construct smooth radial functions

Add conditional bias for pair species

$$\beta_{ji} = \exp\left(-\left(r_{ji} - \mathbf{c}\right)/\ell\right)$$

Atomistic Graph & Line Graph

Explicitly represent pairwise and triplet (bond angle) interactions using line graph
Possible to extend for n-body, *e.g.* line graph of line graph



- Graph level prediction, e.g. energy
- Node level predictions, e.g. charges
- Node level derivatives, e.g. forces
- Edge level predictions, e.g. LJ params

nisaba.nist.gov Tesla V100

Performance on the JARVIS-DFT Dataset

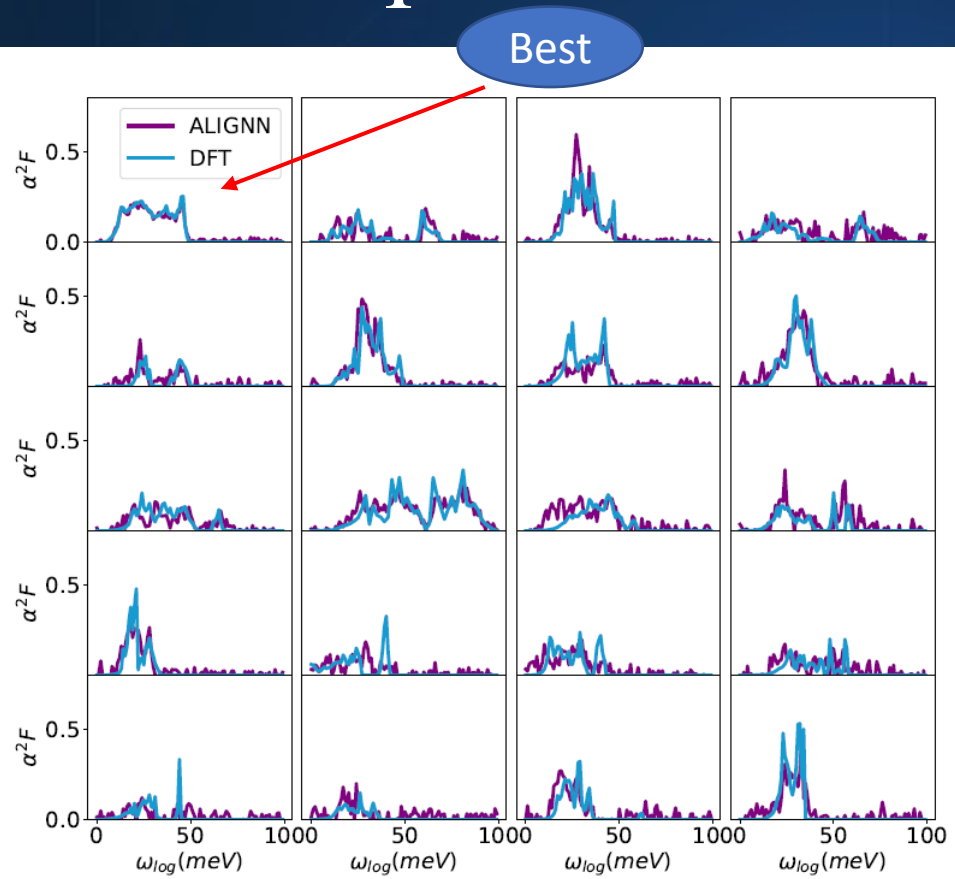
NIST MATERIAL MEASUREMENT LABORATORY

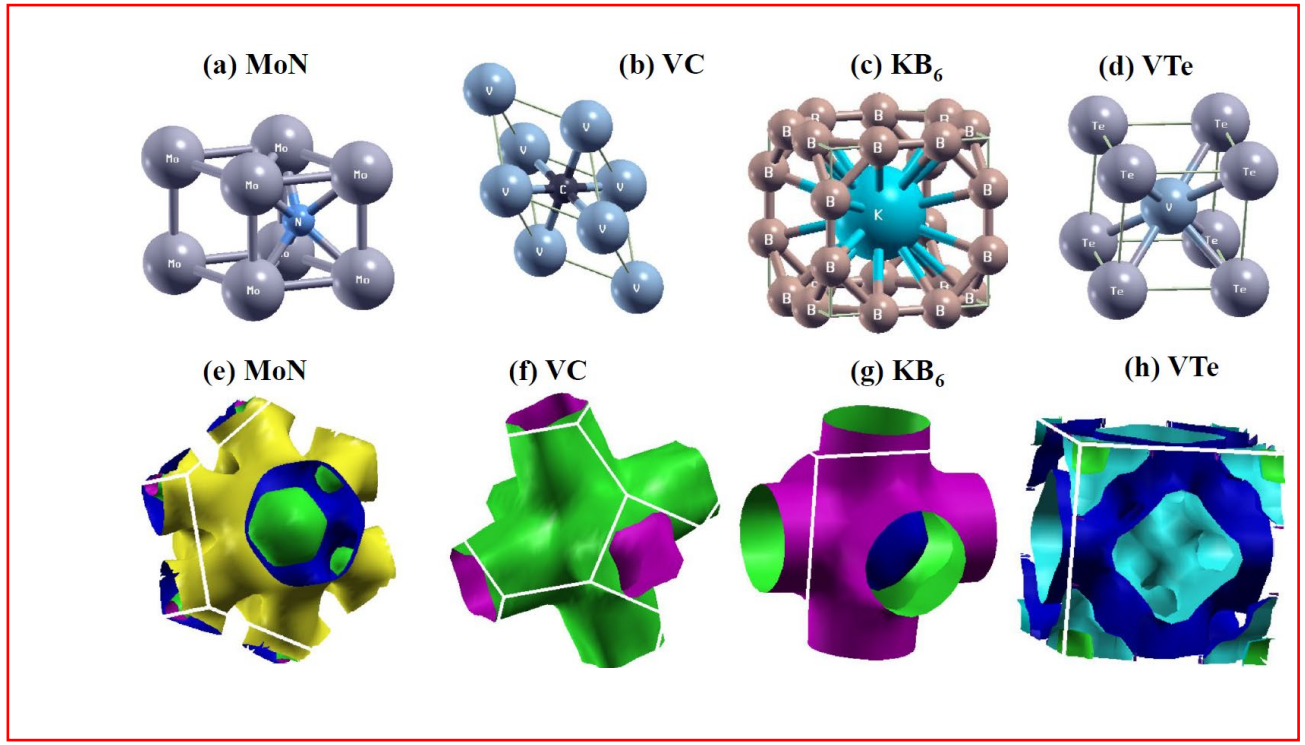
Property	Units	MAD	CFID	CGCNN	ALIGNN	MAD: MAE
Formation energy	eV(atom)$^{-1}$	0.86	0.14	0.063	0.033	26.06
Bandgap (OPT)	eV	0.99	0.30	0.20	0.14	7.07
Total energy	eV(atom)$^{-1}$	1.78	0.24	0.078	0.037	48.11
Ehull	eV	1.14	0.22	0.17	0.076	15.00
Bandgap (MBJ)	eV	1.79	0.53	0.41	0.31	5.77
Kv	GPa	52.80	14.12	14.47	10.40	5.08
Gv	GPa	27.16	11.98	11.75	9.48	2.86
Mag. mom	μB	1.27	0.45	0.37	0.26	4.88
SLME (%)	No unit	10.93	6.22	5.66	4.52	2.42
Spillage	No unit	0.52	0.39	0.40	0.35	1.49
Kpoint-length	Å	17.88	9.68	10.60	9.51	1.88
Plane-wave cutoff	eV	260.4	139.4	151.0	133.8	1.95
ϵ_x (OPT)	No unit	57.40	24.83	27.17	20.40	2.81
ϵ_y (OPT)	No unit	57.54	25.03	26.62	19.99	2.88
ϵ_z (OPT)	No unit	56.03	24.77	25.69	19.57	2.86

Trained on ~55k materials

- Total energy, Formation energy , Ehull
- Bandgap (OPT), Bandgap (MBJ)
- Kv, Gv
- Mag. mom
- ϵx (OPT/MBJ), ϵy (OPT), ϵz (OPT), ϵ (DFPT:elec+ionic)
- Max. piezo. stress coeff (eij)
- Solar-SLME (%)
- Topological-Spillage
- 2D-Exfo. energy
- Kpoint-length
- Plane-wave cutoff
- Max. Electric field gradient
- avg. m_e, avg. m_h
- n-Seebeck, n-PF, p-Seebeck, p-PF

BCS Superconductors





npj | computational materials

Explore content · About the journal · Publish with us

nature › npj computational materials › articles › article

Article | Open access | Published: 22 November 2022

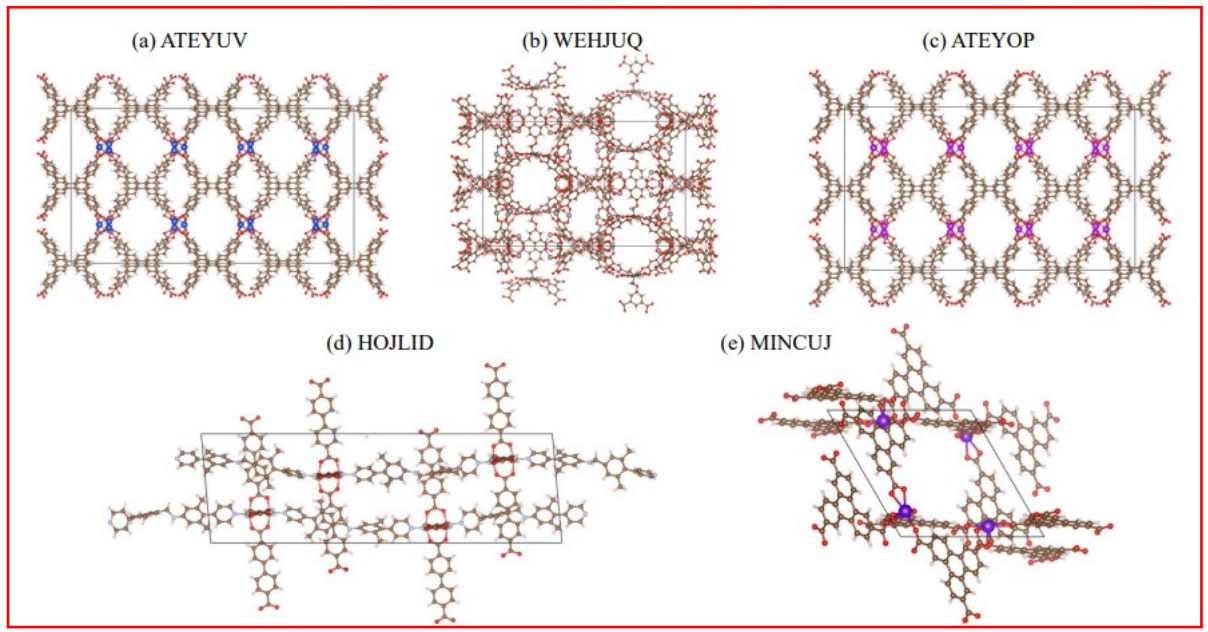
Designing high-T_C superconductors with BCS-inspired screening, density functional theory, and deep-learning

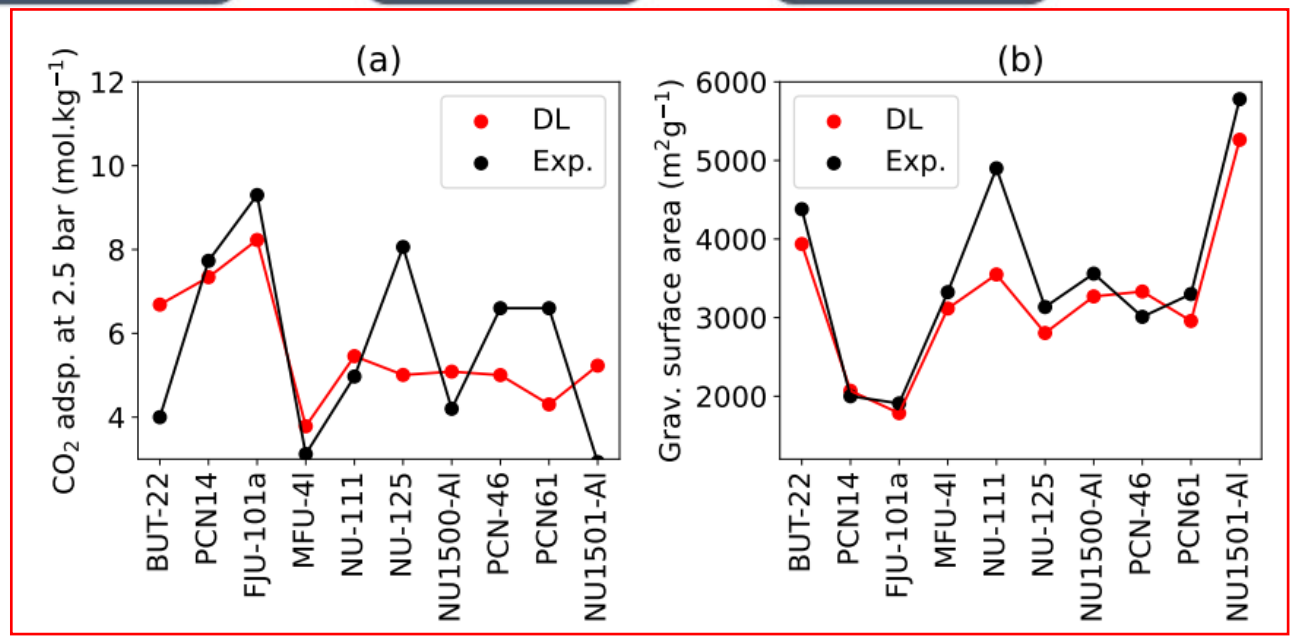
Kamal Choudhary & Kevin Garrity

- Prediction on 10 % test data
- 8293 out of 431778 materials in COD as superconductors
- First predicting Eliashberg function, then Tc → 6 % improvement
- ALIGNN for both scalar and spectral learning

CO_2 capture & MOFs

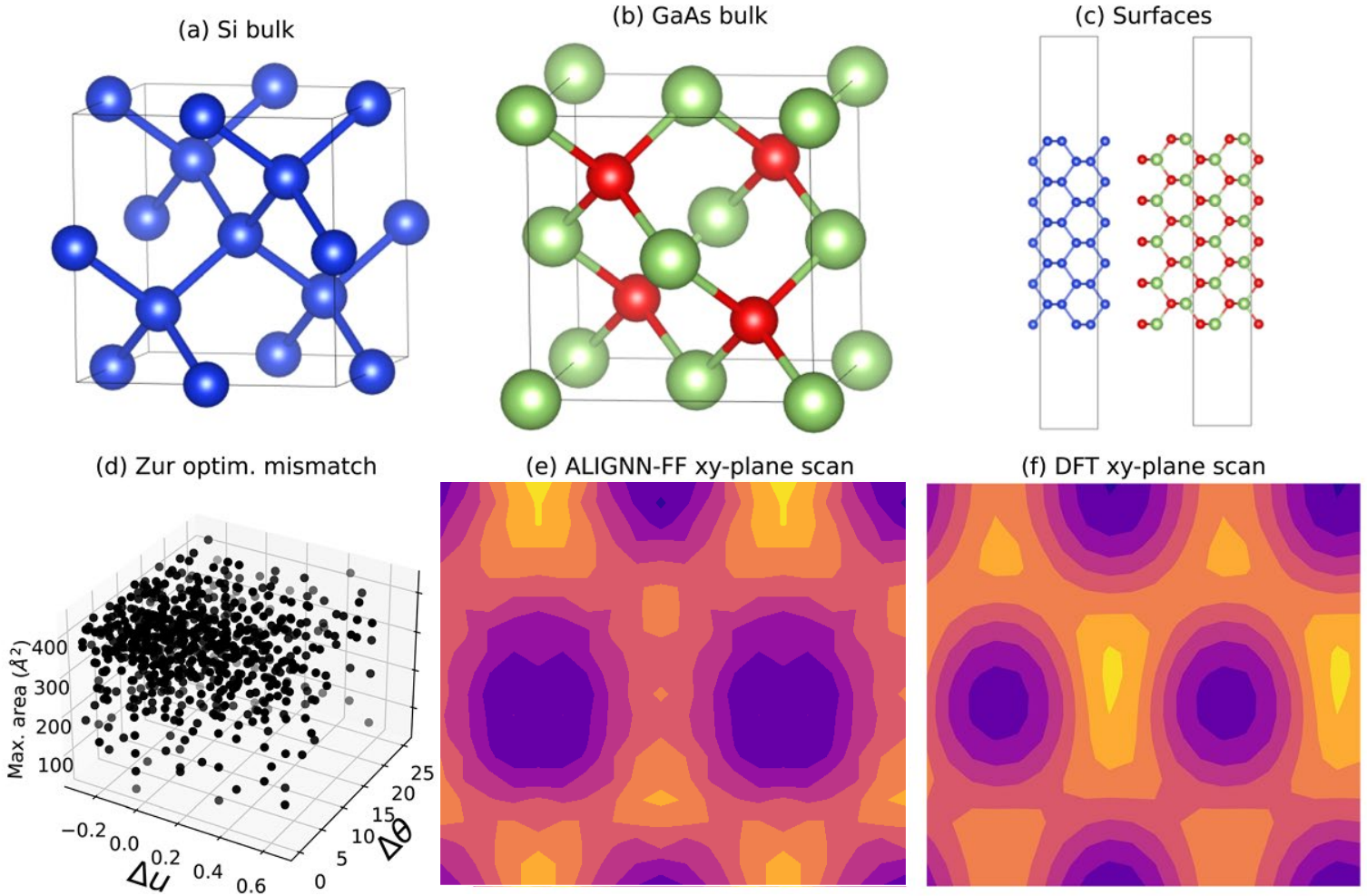
DL model for predicting CO_2 adsorption in MOFs (using hMOF GCMC data)



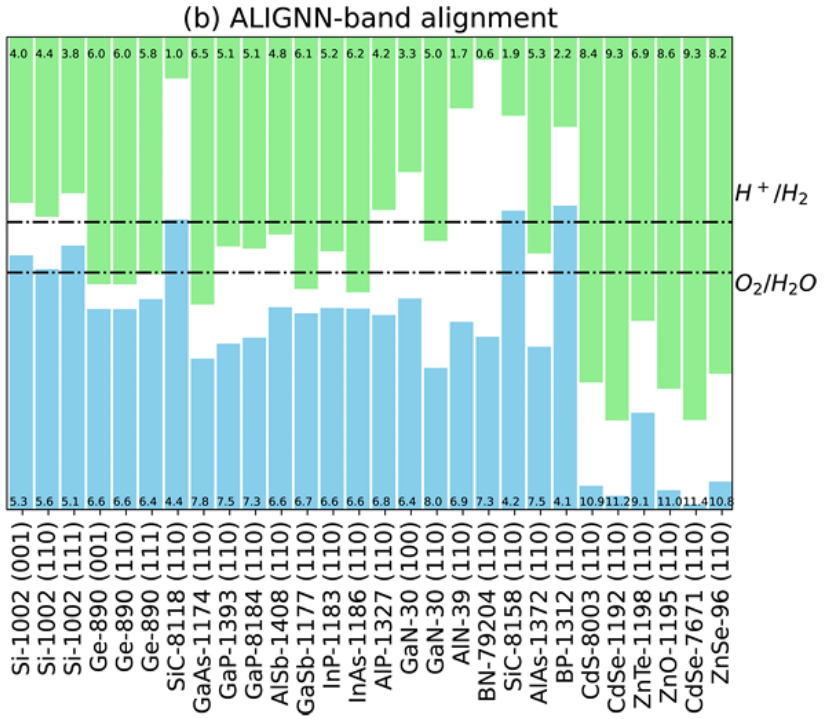


Choudhary et al., Computational Materials Science 210, 111388 (2022)

InterMat: Interface Materials Design (Semicons)



- ALIGNN+DFT for accelerated interface design
- Benchmarked band-offset predictions
- General workflow for materials design



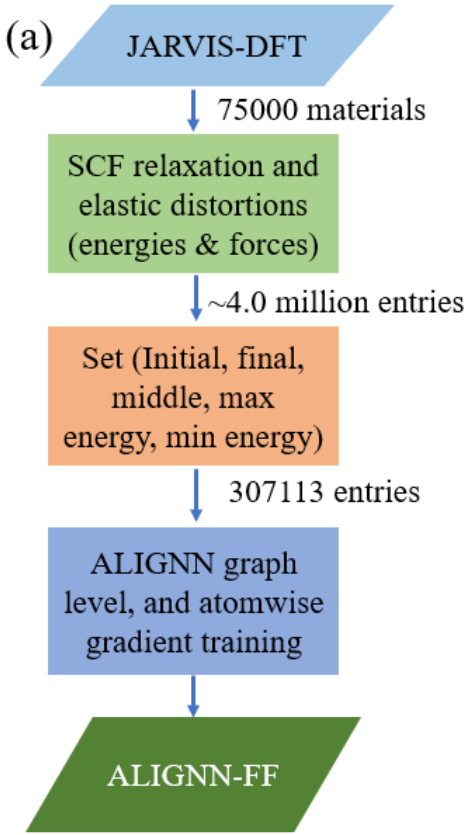
DOI: 10.1039/D4DD00031E (Paper) *Digital Discovery*, 2024, Advance Article

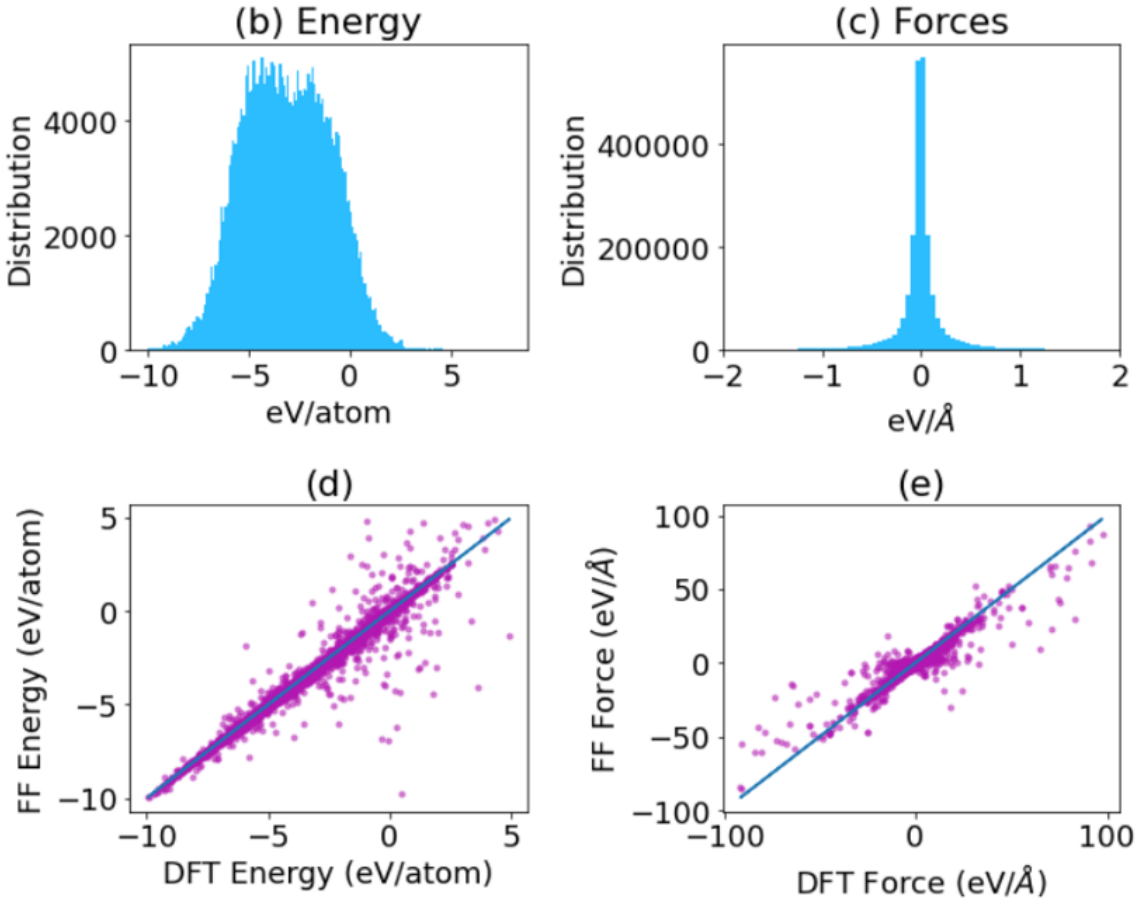
InterMat: accelerating band offset prediction in semiconductor interfaces with DFT and deep learning†

Kamal Choudhary * and Kevin F. Garrity

DOI: 10.1039/D4DD00031E Digital Discovery, 202

Unified GNN Force-field





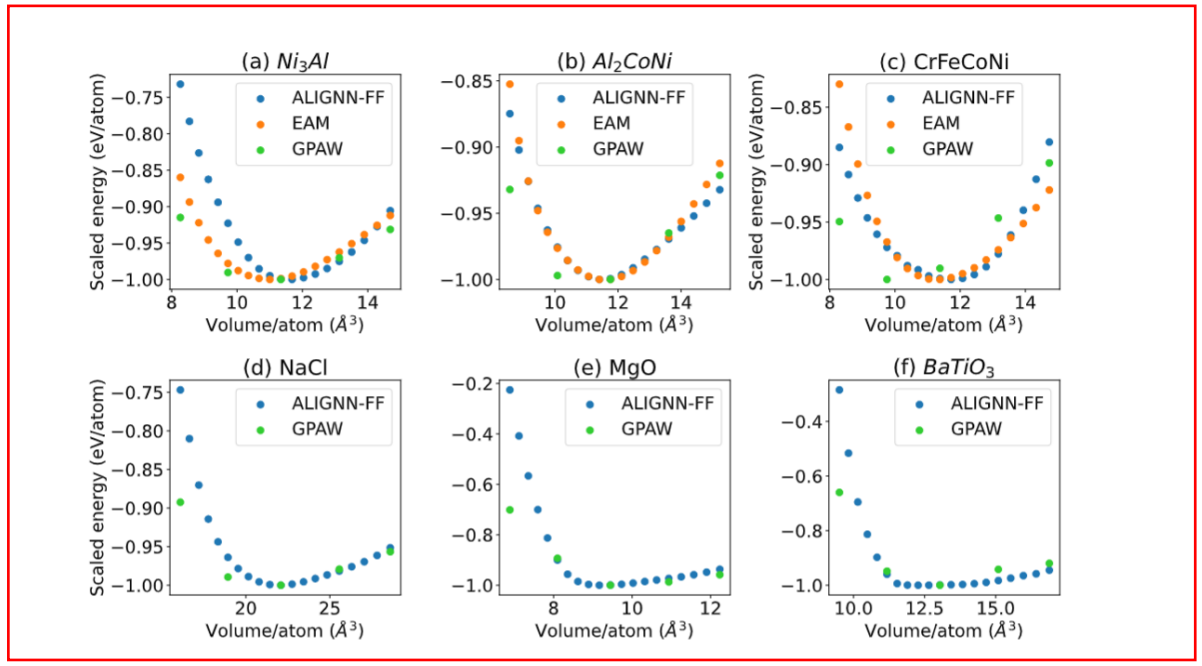
Weight	MAE-Energies (eV/atom)	MAE-Forces (eV/Å)
0.1	0.034	0.092
0.5	0.044	0.089
1.0	0.051	0.088
5.0	0.082	0.054
10.0	0.086	0.047

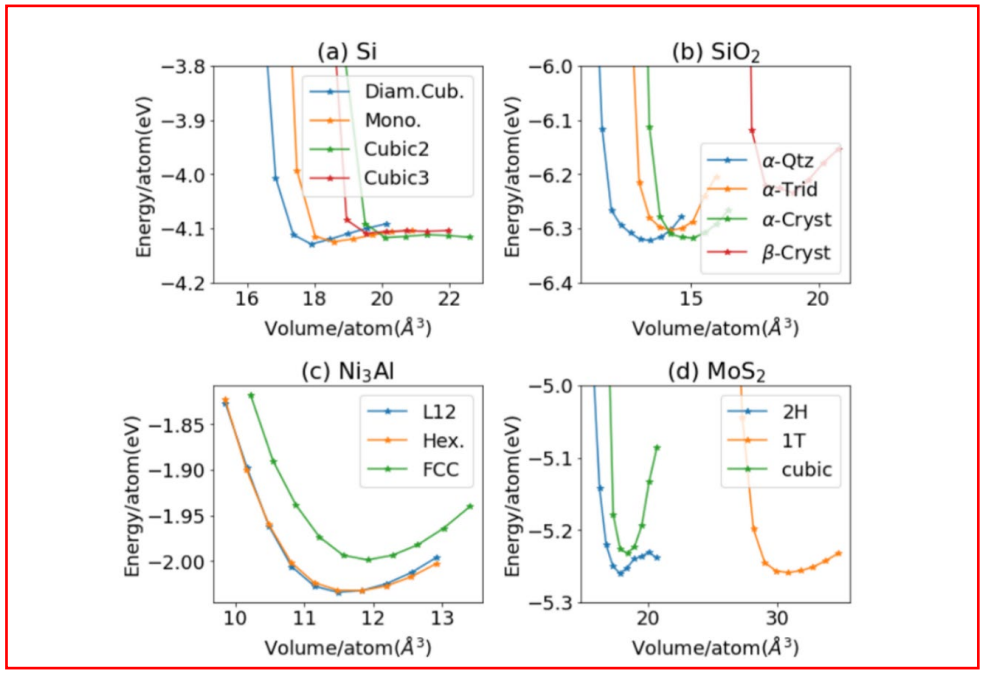
Simulate any combination of 89 elements from the periodic table

$$m_i \frac{\mathrm{d}^2 r_i(t)}{\mathrm{d}t^2} = \sum_j F_{ij}(t) = -\sum_j \nabla_i U\left(r_{ij}(t)\right)$$

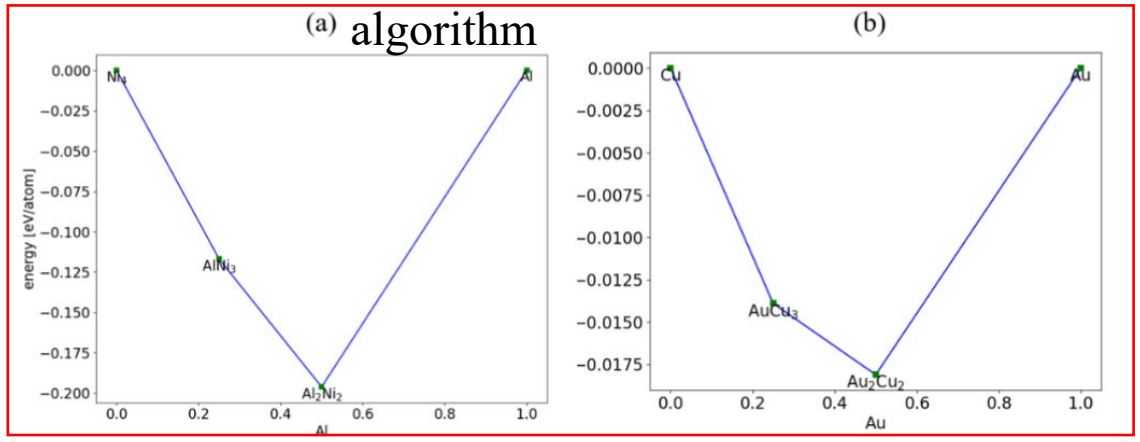
Unified GNN Force-field

EV-curves





Genetic algorithm



Digital Discovery

ROYAL SOCIETY OF CHEMISTRY

PAPER

View Article Online
View Journal

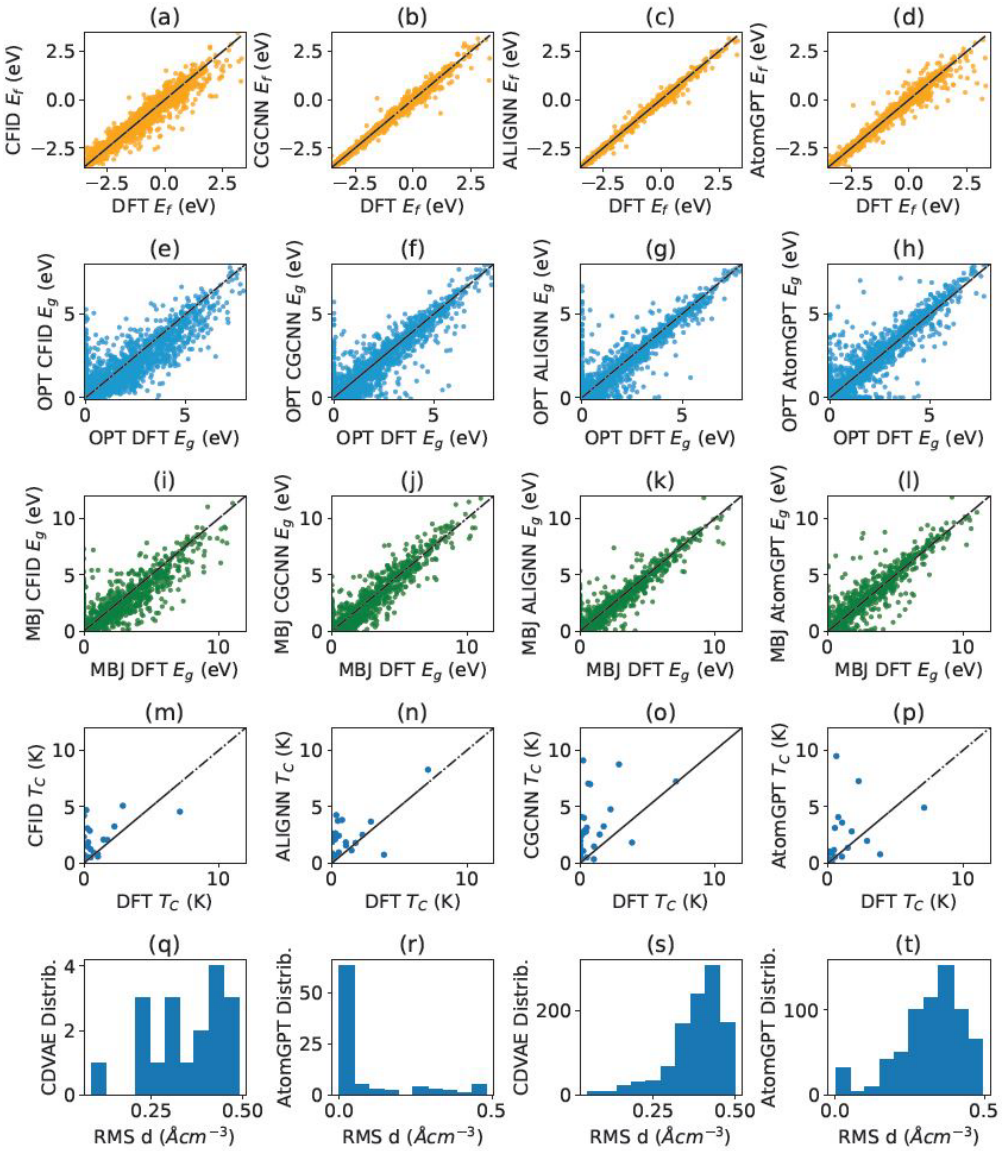
Check for updates

Cite this: DOI: 10.1039/d2dd00096b

Unified graph neural network force-field for the periodic table: solid state applications

Kamal Choudhary, *ab Brian DeCost, c Lily Major, de Keith Butler, e Jeyan Thiyagalingam e and Francesca Tavazza c

AtomGPT



Forward models				
Prop/MAE	CFID	CGCNN	ALIGNN	AtomGPT
E_{form} (eV/atom)	0.142	0.063	**0.033**	0.072
OPT E_g (eV)	0.299	0.199	0.142	**0.139**
MBJ E_g (eV)	0.531	0.407	**0.310**	0.319
T_C (K)	1.99	2.60	2.03	**1.54**

Inverse models		
Database/RMSE	CDVAE	AtomGPT
SuperConDB	0.24	**0.08**
Carbon24	0.36	**0.32**

AtomGPT: Atomistic Generative Pretrained Transformer for Forward and Inverse Materials Design

Kamal Choudhary*

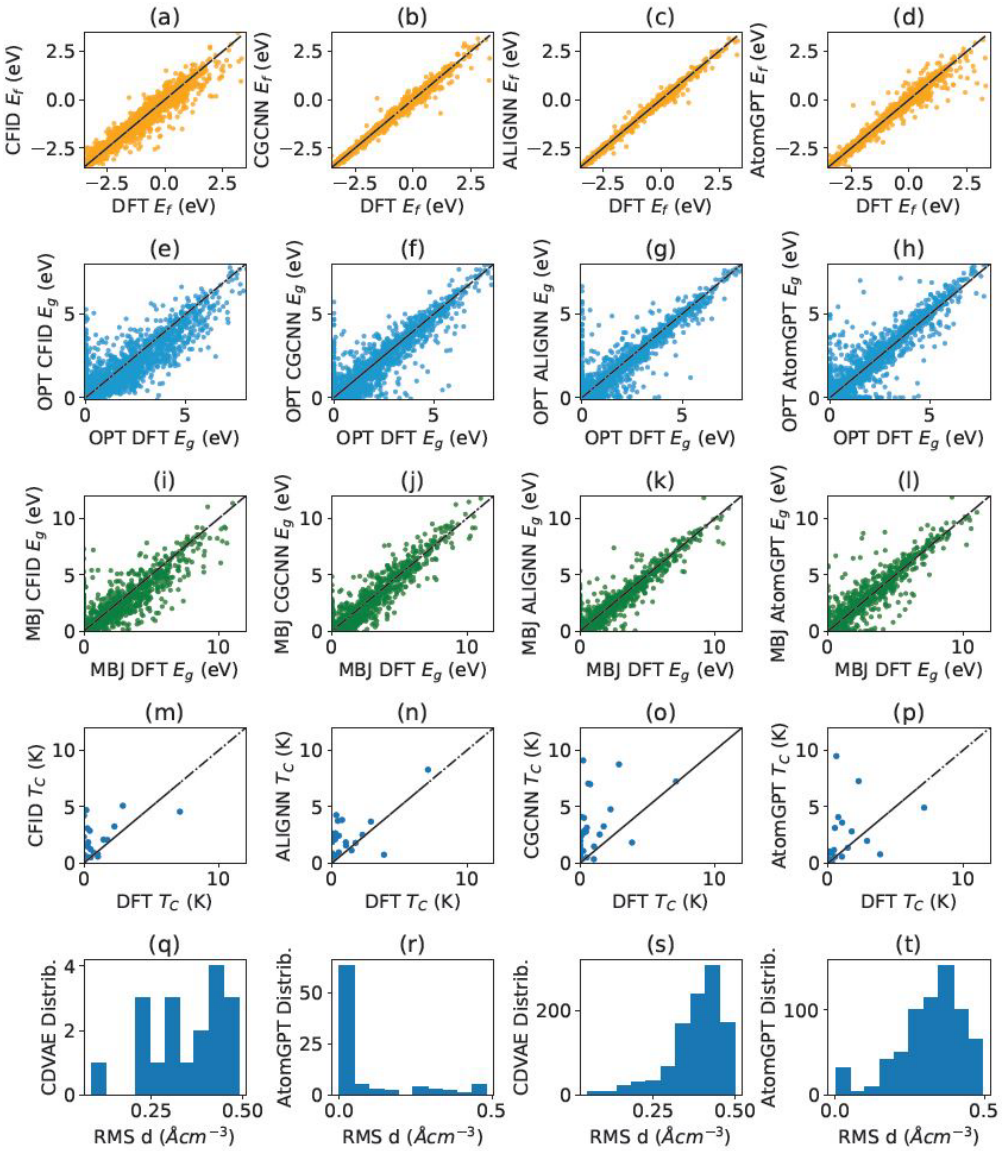
Cite this: *J. Phys. Chem. Lett.* 2024, 15, XXX, 6909−6917

Publication Date: June 27, 2024

https://doi.org/10.1021/acs.jpclett.4c01126

Generated structures relaxed with ALIGNN-FF before DFT-superconductivity workflow

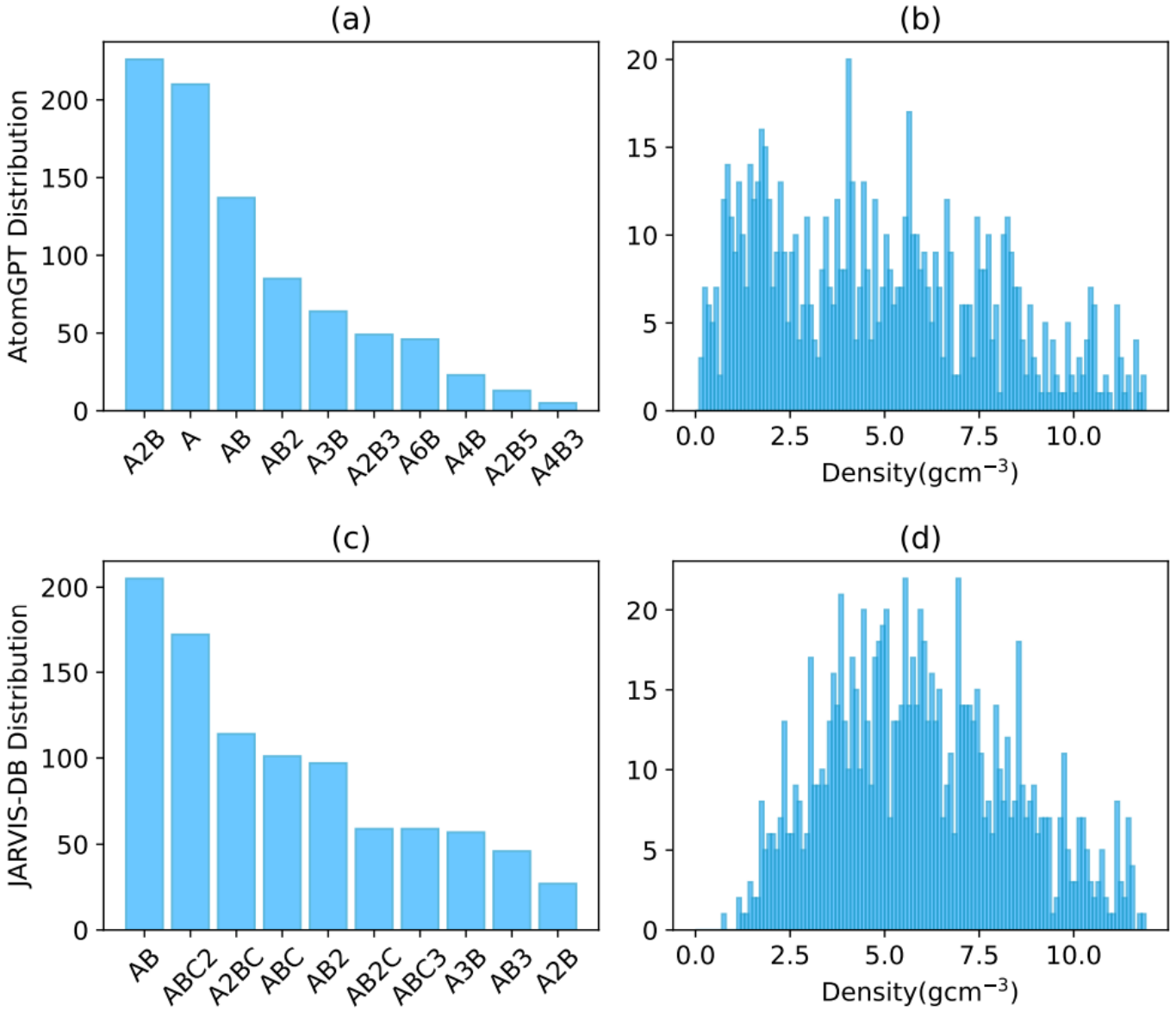
AtomGPT



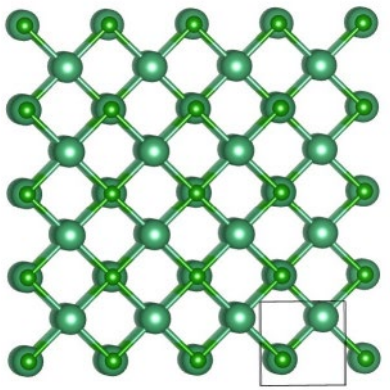
Forward models				
Prop/MAE	CFID	CGCNN	ALIGNN	AtomGPT
E_{form} (eV/atom)	0.142	0.063	**0.033**	0.072
OPT E_g (eV)	0.299	0.199	0.142	**0.139**
MBJ E_g (eV)	0.531	0.407	**0.310**	0.319
T_C (K)	1.99	2.60	2.03	**1.54**

Inverse models			
	Database/RMSE	CDVAE	AtomGPT
	SuperConDB	0.24	**0.08**
	Carbon24	0.36	**0.32**

AtomGPT



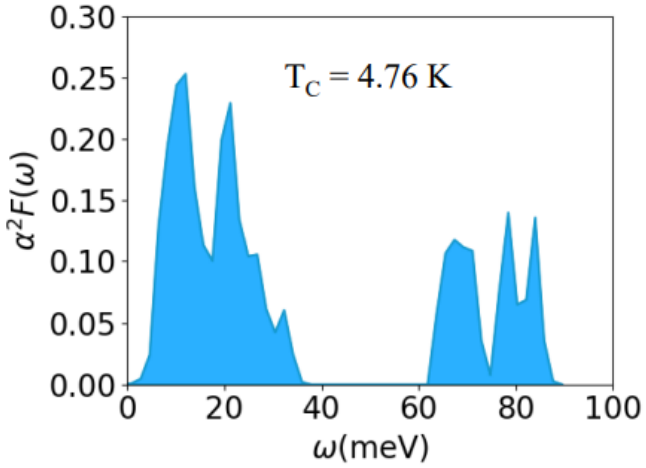
a) Nb_2B structure



$$T_c = \frac{\omega_{log}}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]$$

$$\omega_{log} = \exp\left[\frac{\int d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln \omega}{\int d\omega \frac{\alpha^2 F(\omega)}{\omega}}\right]$$

b) Eliashberg function



AtomGPT Demo

atomgpt_example.ipynb

File Edit View Insert Runtime Tools Help

Code + Text | Copy to Drive

AtomGPT example: https://pubs.acs.org/doi/10.1021/acs.jpclett.4c01126

Author: kamal.choudhary@nist.gov

```
[ ] !pip install -q condacolab
    import condacolab
    condacolab.install()
```

```
Downloading https://github.com/conda-forge/miniforge/releases/download/23.11.0-0/Mambaforge-23.11.0-0-Linux-x86_64.sh
Installing...
Adjusting configuration...
Patching environment...
Done in 0:00:13
Restarting kernel...
```

Installation

```
[ ] %%time
    import os
    os.chdir('/content')
```

https://colab.research.google.com/github/knc6/jarvis-tools-notebooks/blob/master/jarvis-tools-notebooks/atomgpt_example.ipynb

AIMS 2024

Gaussian Processes and Active Learning

Austin McDannald

Austin.McDannald@NIST.gov

National Institute of Standards and Technology
U.S. Department of Commerce

MATERIAL MEASUREMENT LABORATORY

Annual Machine Learning for Materials Research Boot Camp and Workshop

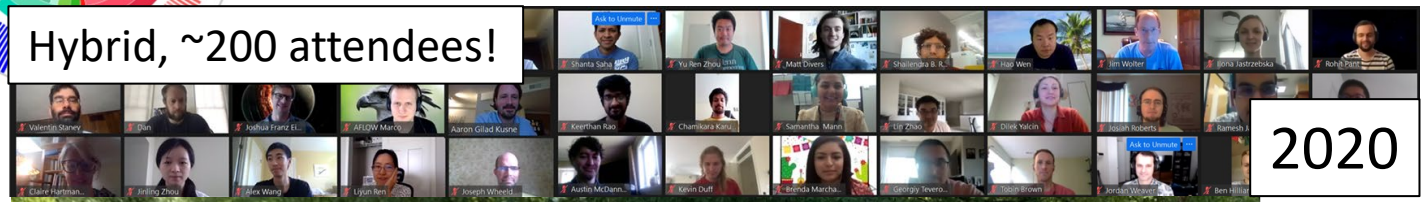
Date: July 22-25 2024

Location: Online

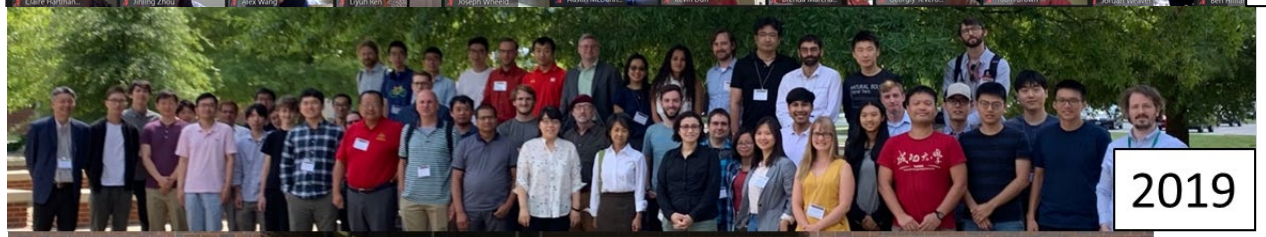
NIST National Institute of Standards and Technology U.S. Department of Commerce

University of Maryland 18 56

Hybrid, ~200 attendees!



2020



2019

2018

2017

2016

Introduce researchers from industry, national labs, and academia to ML theory and tools for rapid data analysis.

- 4 days of lectures and **hands-on** exercises (e.g. noise reduction, unsupervised and supervised techniques, computer vision, etc.) includes ML for robot science!

- Focus on handling real data, both experimental and computational.

- Open-source, Python-based modules

- Symposium on Friday

https://umd-mse.catalog.instructure.com/courses/mlmr-2024

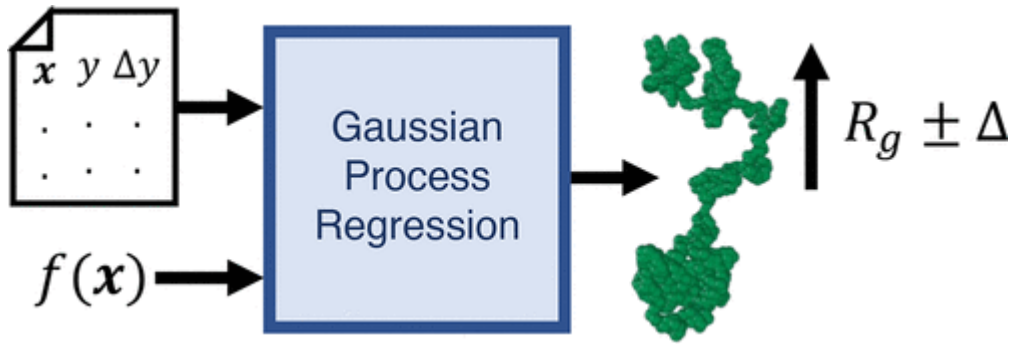
Contact: aaron.kusne@nist.gov

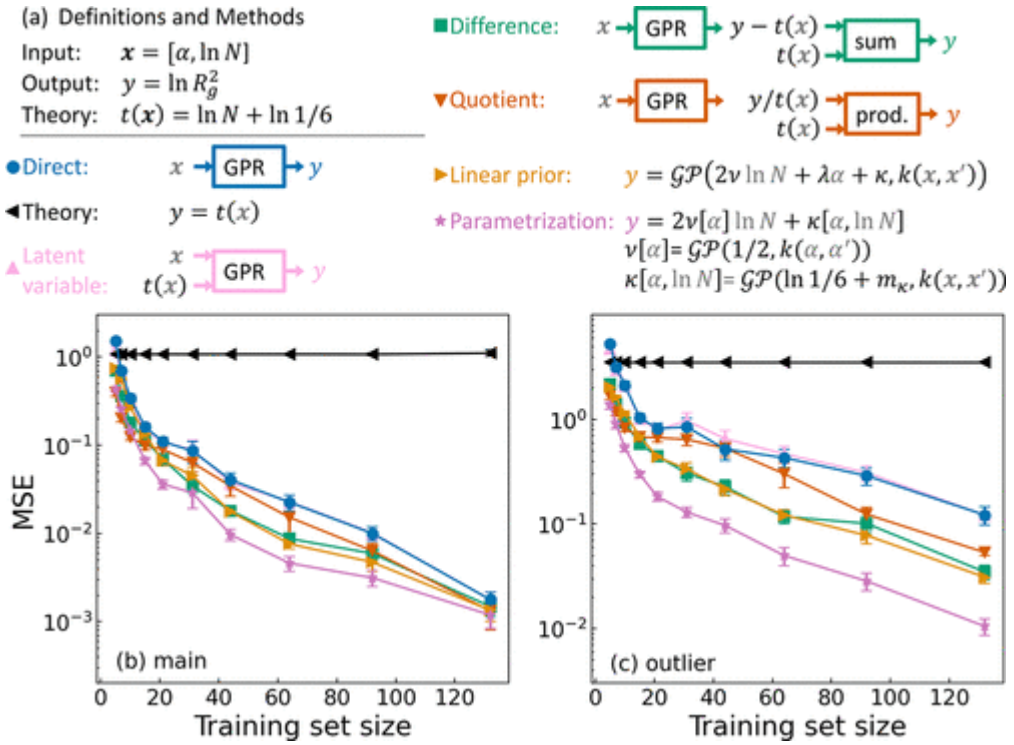
To the Gaussian Process Colab Notebook!

https://tinyurl.com/3db88ka5

https://github.com/mannodiarun/mrs_spring_tutorial/tree/GP_and_AL

Leveraging Theory for Enhanced Machine Learning





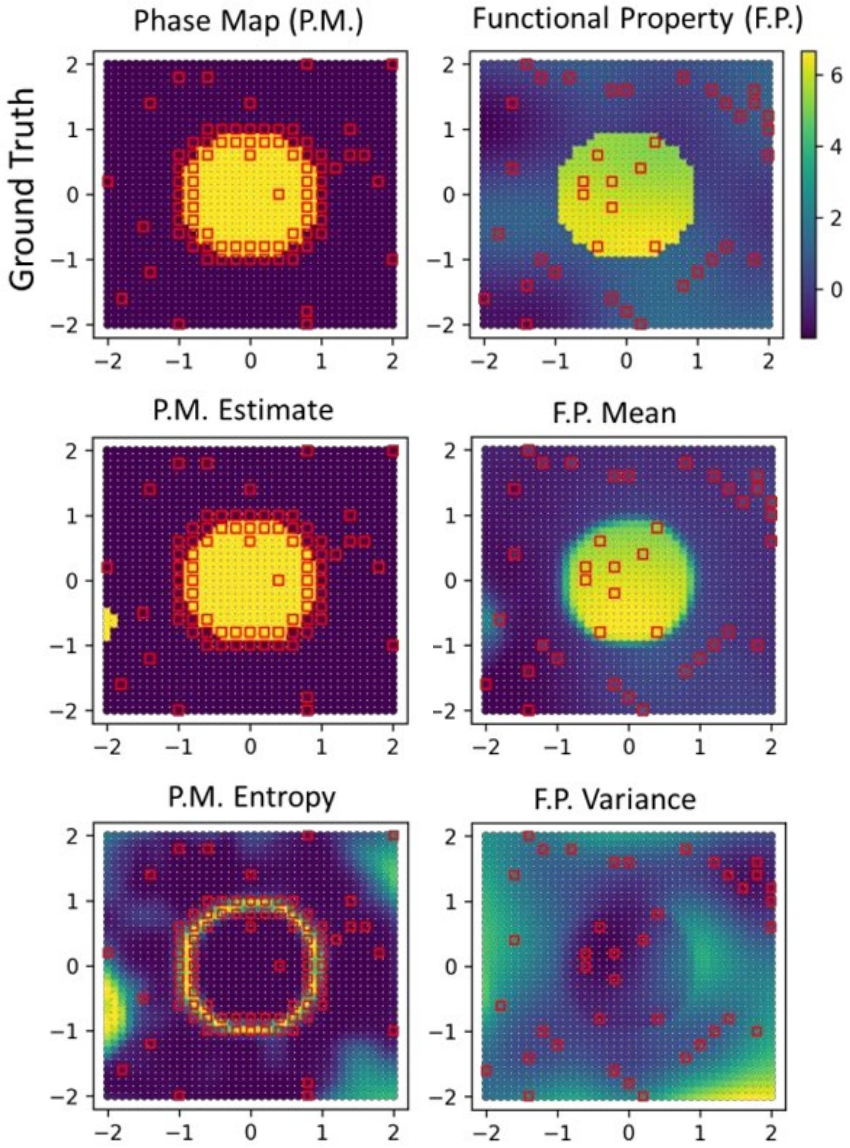
Goal: Predict the Radius of Gyration (R_g) of a single polymer chain given the chain length and solvent quality.

Need computationally expensive molecular dynamics (MD) simulations to calculate R_g.

Used GPR with different methods for encoding theory to interpolate and extrapolate from the MD simulations with propagated uncertainty.

D. J. Audus, A. McDannald, B. DeCost *ACS Macro Lett. 2022, 11, 9, 1117–1122*
https://doi.org/10.1021/acsmacrolett.2c00369

Joint Inference



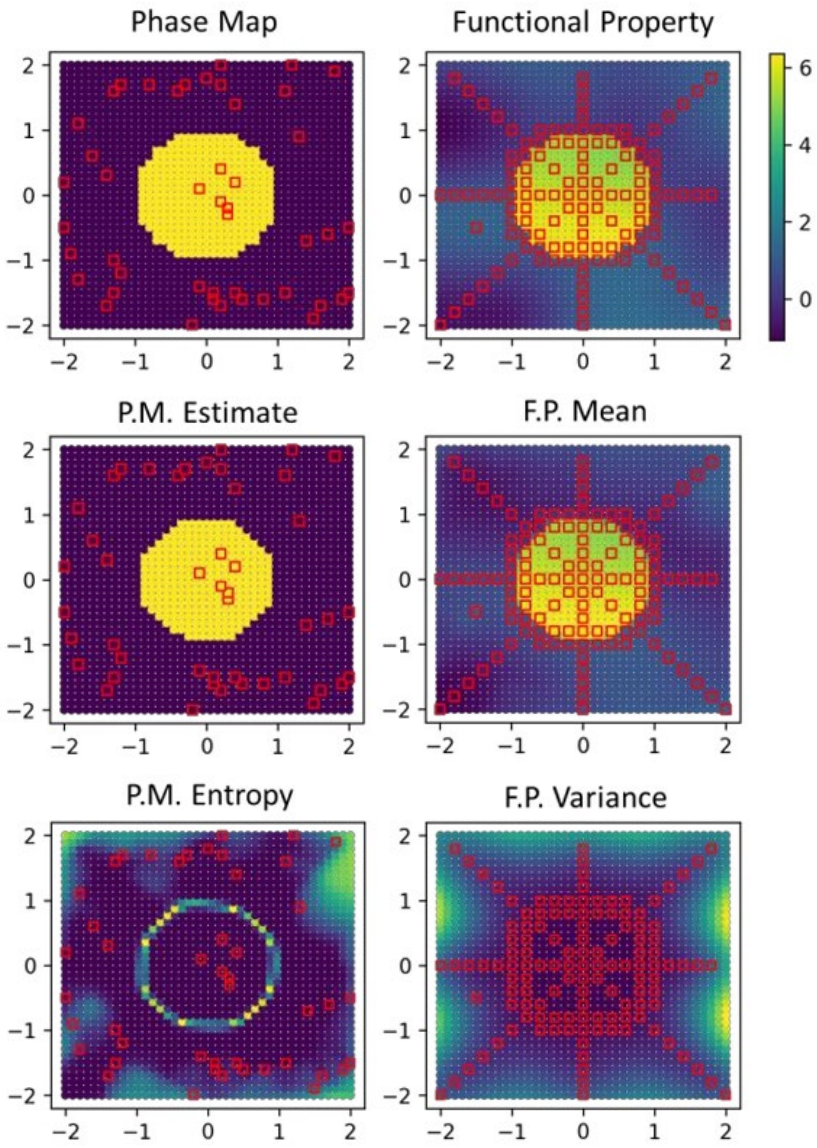
Lots of data of Phase Map
Not much data on Property

Not much data of Phase Map
Lots of data on Property

Phase Map and Functional Property are Co-Regionalized

Joint inference:
data on one informs the other

SAGE:
arXiv:2311.06228



To the Active Learning Colab Notebook!

https://tinyurl.com/2zu9n7aj

https://github.com/mannodiarun/mrs_spring_tutorial/tree/GP_and_AL

Hermes: Scientific AI

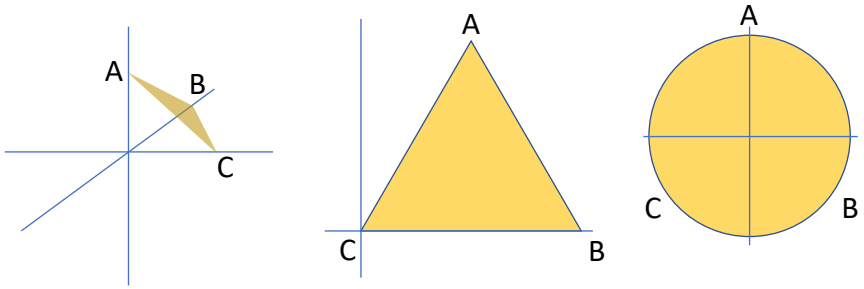
NIST MATERIAL MEASUREMENT LABORATORY

Motivation:

- Off-the-shelf ML algorithms – Don't account for physics
- Hermes – Repository of ML for Mat. Sci
- Convenient Construction of Autonomous Workflows

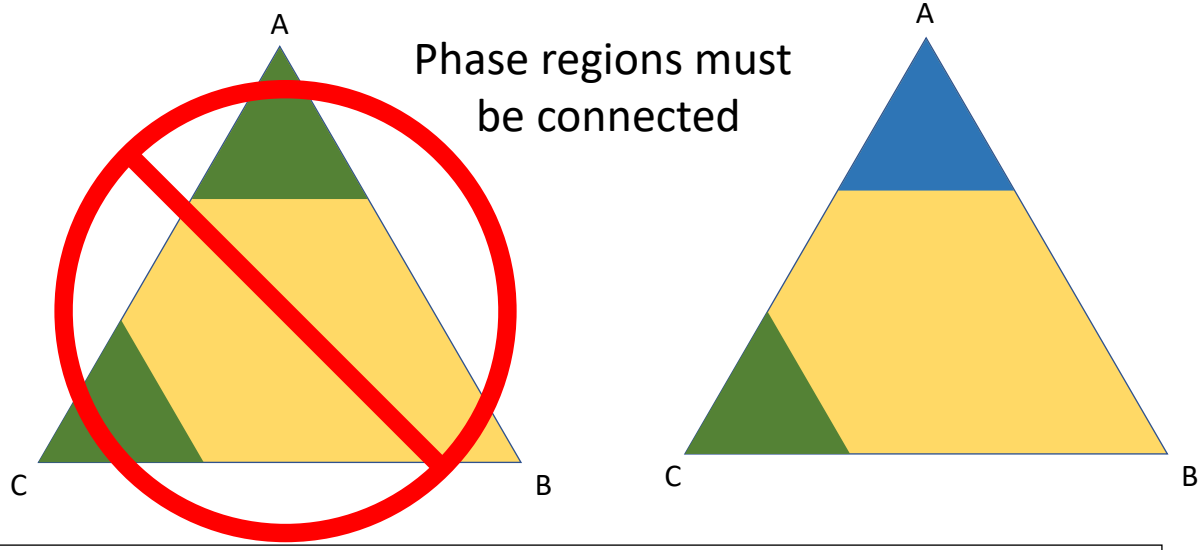
Example:

- XRD Phase Mapping of Combi wafer
  - Domain could be:



- Hermes: easily work & translate between domains

Phase Mapping: Contiguous Constraint



- EBSD Grain Mapping
  - Same Contiguous Constraint

Hermes:
Code repository for autonomous systems.
Fork us on GitHub
https://github.com/usnistgov/hermes/tree/main

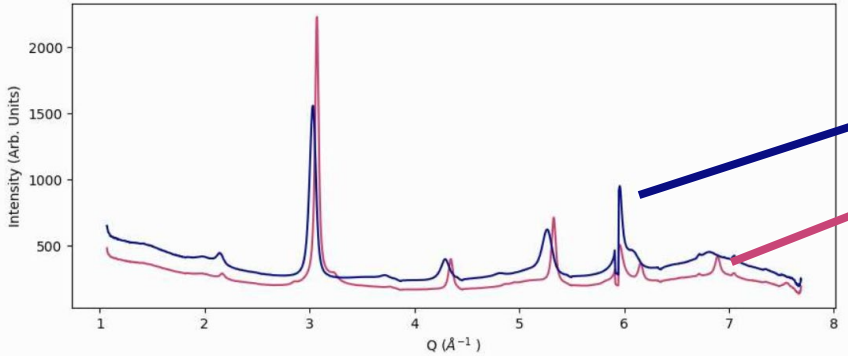
Questions?

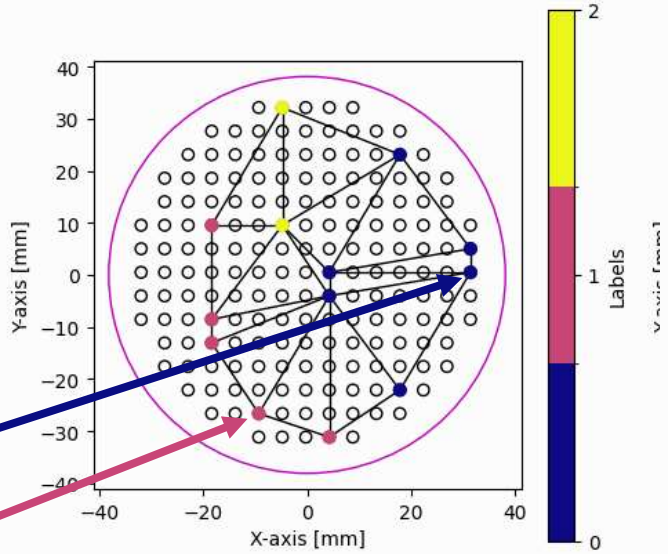
Combi Phase Mapping

Autonomous Phase Mapping with XRD at CHESS

Probabilistically

Take XRD measurements





Graph Cut Partitioning

Predict across the whole domain

With Uncertainty Propagation

Choose Next Measurement

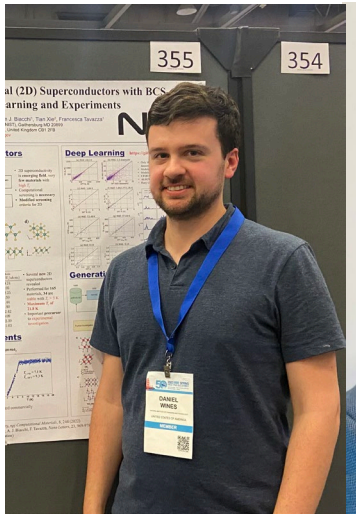
Postdoctoral Opportunities

NRC Postdoc Opportunities:
Many project opportunities for recent PhDs interested in quantum materials, machine learning, computation, and materials design.

- Open to U.S. citizens
- Proposal deadlines:
  Feb. 1st and Aug. 1st

Acknowledgement and Collaboration

NIST
National Institute of Standards and Technology
U.S. Department of Commerce



D. Wines
(NIST, 642)

K. Choudhary
(NIST, 642)

F. Tavazza
(NIST, 643)

B. DeCost
(NIST, 643)

K. F. Garrity
(NIST, 643)

A. McDannald
(NIST, 643)

H. Joress
(NIST, 643)

Los Alamos NATIONAL LABORATORY EST. 1943
Microsoft
West Virginia University
UNIVERSITY OF TORONTO
KIT Karlsruher Institut für Technologie
PURDUE UNIVERSITY
WASHINGTON UNIVERSITY IN ST. LOUIS 1853
UNIVERSITY OF MARYLAND 18 56
UMBC
Argonne NATIONAL LABORATORY
OAK RIDGE National Laboratory
AIR FORCE RESEARCH LABORATORY
VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY
NORTHWESTERN UNIVERSITY 1851
RUTGERS THE STATE UNIVERSITY OF NEW JERSEY 1766
TEXAS A&M UNIVERSITY 1876
UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN
ASU Arizona State University
GEORGE MASON UNIVERSITY
Sandia National Laboratories