# Tutorial MD00: Machine Learning in Materials Sciences — From Basic Concepts to Active Learning


**Arun Mannodi Kanakkithodi**

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Monday, Apr 10, 2023, 8.00 am – 5:00 pm

PURDUE UNIVERSITY | School of Materials Engineering

# Tutorial Outline

**8.00 am – 9.30 am, Arun Mannodi Kanakkithodi:**
Introduction to ML for materials science. Demonstration of training ML models using a DFT dataset of halide perovskite alloys.

**9.30 am – 10.00 am: Break**

**10.00 am – 10.30 am, Austin McDannald:**
Gaussian Process Regression: Detailed description using examples.

**10.30 am – 11.30 am, Austin McDannald:**
Discussion of active learning, Bayesian optimization, autonomous experiments.

**11.30 am – 12.00 pm: General Discussion**

**12.00 pm – 1.30 pm: Lunch Break**

**1.30 pm – 2.30 pm, Saaketh Desai:**
Overview of neural networks for prediction, convolutional neural networks for images.

**2.30 pm – 3.00 pm: General Discussion**

**3.00 pm – 5.00 pm (and beyond):**
Battery Informatics and ML Hackathon.

# Tutorial Instructors

- Arun Mannodi Kanakkithodi: Assistant Professor, Materials Engineering, Purdue University. Computational materials scientist using high-throughput DFT and ML for materials design.
- Austin McDannald: Materials Research Engineer, National Institute of Standards and Technology
- Saaketh Desai: Postdoctoral Researcher, Sandia National Laboratory
- Shijing Sun: Research Scientist, Energy and Materials, Toyota Research Institute

# MRS Bulletin Article in Press

## A Framework for Materials Informatics Education through Workshops

Arun Mannodi-Kanakkithodi[1], Austin McDannald[2], Shijing Sun[3], Saaketh Desai[4], Keith Brown[5] and A. Gilad Kusne[2]

**Abstract**

The burgeoning field of materials informatics necessitates a focus on educating the next generation of materials scientists in the concepts of data science, artificial intelligence (AI), and machine learning (ML). In addition to incorporating these topics in undergraduate and graduate curricula, regular hands-on workshops present the most effective medium to initiate researchers to informatics and have them start applying the best AI/ML tools to their own research. With the help of the Materials Research Society (MRS), members of the MRS AI staging committee, and a dedicated team of instructors, we successfully conducted workshops covering the essential concepts of AI/ML as applied to materials data, at both the spring and fall meetings in 2022, with plans to make this a regular feature in future meetings. In this article, we discuss the importance of materials informatics education via the lens of these workshops, including details such as learning and implementing specific algorithms, the crucial nuts and bolts of ML, and using competitions to increase interest and participation.

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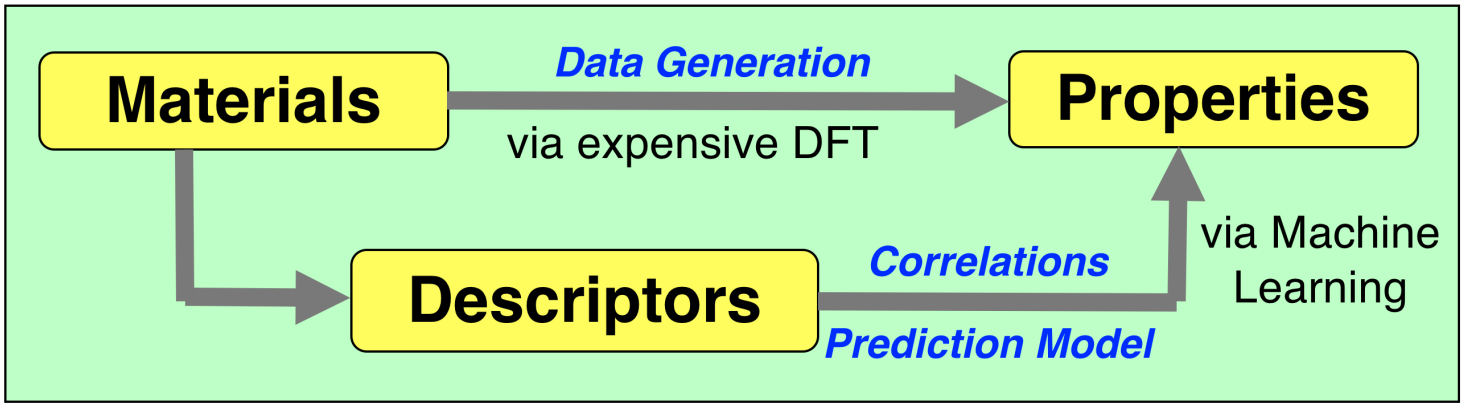
# PART 1:

# Introduction to ML in Materials Science

# Machine Learning in Materials Science




**a** Example dataset

| Material | Property Value |
|---|---|
| Material 1 | $P_1$ |
| Material 2 | $P_2$ |
| ⋮ | ⋮ |
| Material *N* | $P_N$ |

**b** The learning problem

| Material | Property Value |
|---|---|
| Material *X* | ? |

**c** Fingerprinting, learning and prediction

| Material | Fingerprint | Property Value |
|---|---|---|
| Material 1 | $F_{11}, F_{12}, \ldots F_{1M}$ | $P_1$ |
| Material 2 | $F_{21}, F_{22}, \ldots F_{2M}$ | $P_2$ |
| ⋮ | ⋮ | ⋮ |
| Material *N* | $F_{N1}, F_{N2}, \ldots F_{NM}$ | $P_N$ |

Fingerprinting

Learning

$f(F_{i1}, F_{i2}, \ldots, F_{iN}) = P_i$

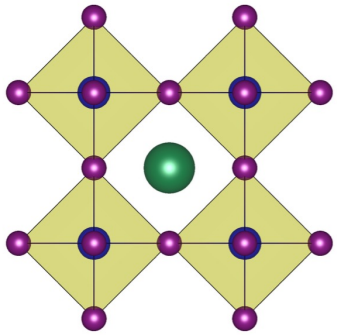
Prediction Model

# Key Ingredient of ML: Feature Vectors / Materials Descriptors / Fingerprints

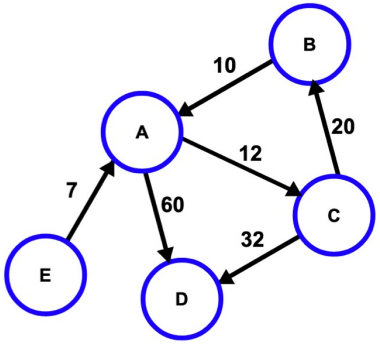
- Numerical representation of materials, input to ML.
- Definition depends on: a) application, b) domain expertise, and c) accuracy desired.
- Requirements: a) intuitive and inexpensive to calculate, b) generalizable to every material in the chemical space, and c) invariant to translation / rotation / permutation of like elements.

# Examples of Fingerprints

3D geometry:
Atom i = (Z,x,y,z)



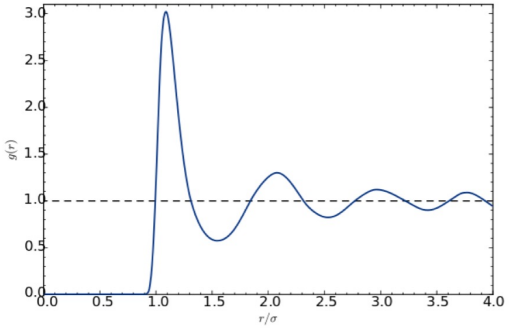
Weighted graph:
atoms & bonds




Coulomb Matrix

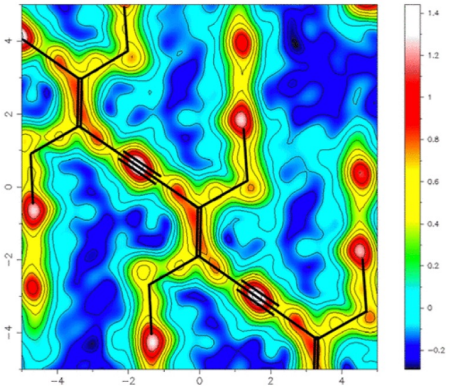
$$M_{IJ} = \begin{cases} 0.5Z_I^{\,2.4} & \text{for } I = J \\ \dfrac{Z_I Z_J}{\left|\boldsymbol{R}_I - \boldsymbol{R}_J\right|} & \text{for } I \neq J \end{cases}$$

Radial Distribution Function

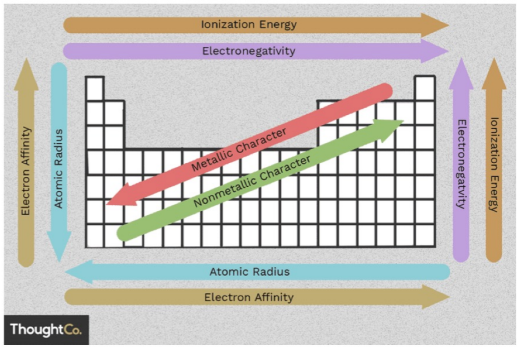



$A_i(\eta) = \exp(-r_{ij}^2/\eta^2)*f(r_{ij})$

Electron Density Distribution

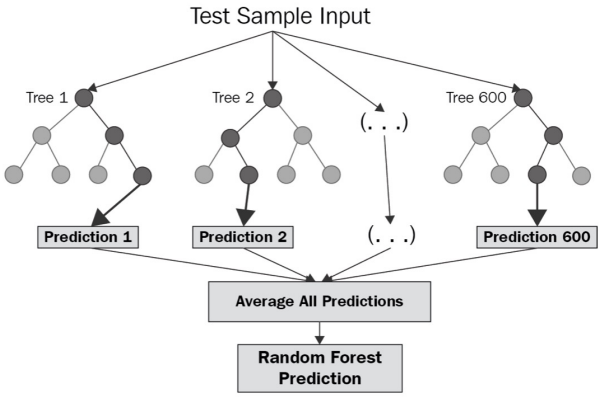


Tabulated elemental properties

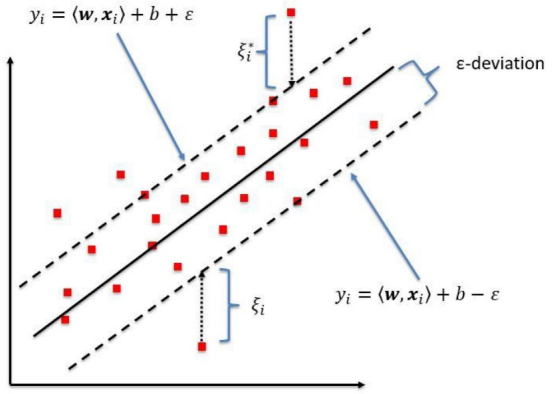


# Examples of ML Techniques

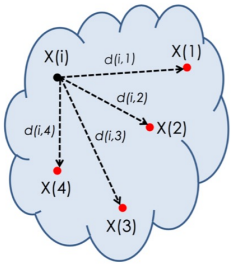
## Random Forest Regression




## Support Vector Regression




## Kernel Ridge Regression




$X(i) = \{x_1, x_2, x_3 \dots x_m\}$

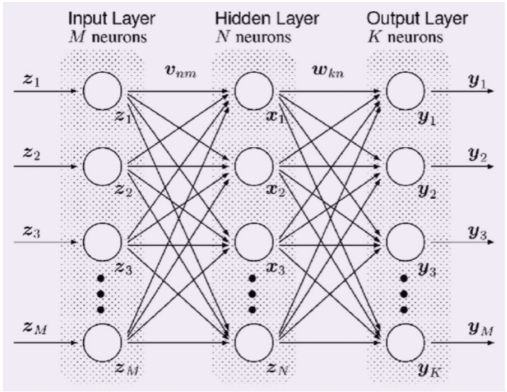
Measure of Similarity: Euclidean Distance

$$d(i,j) = \sqrt{(x_{i1} - x_{j1})^2 + \dots + (x_{im} - x_{jm})^2}$$

Property = Weighted sum of Gaussians

$$f(i) = \sum_{k=1}^{N} a_k \cdot \exp\left(-\frac{1}{2\sigma^2} \cdot [d(i, i_k)]^2\right)$$

## Neural Networks



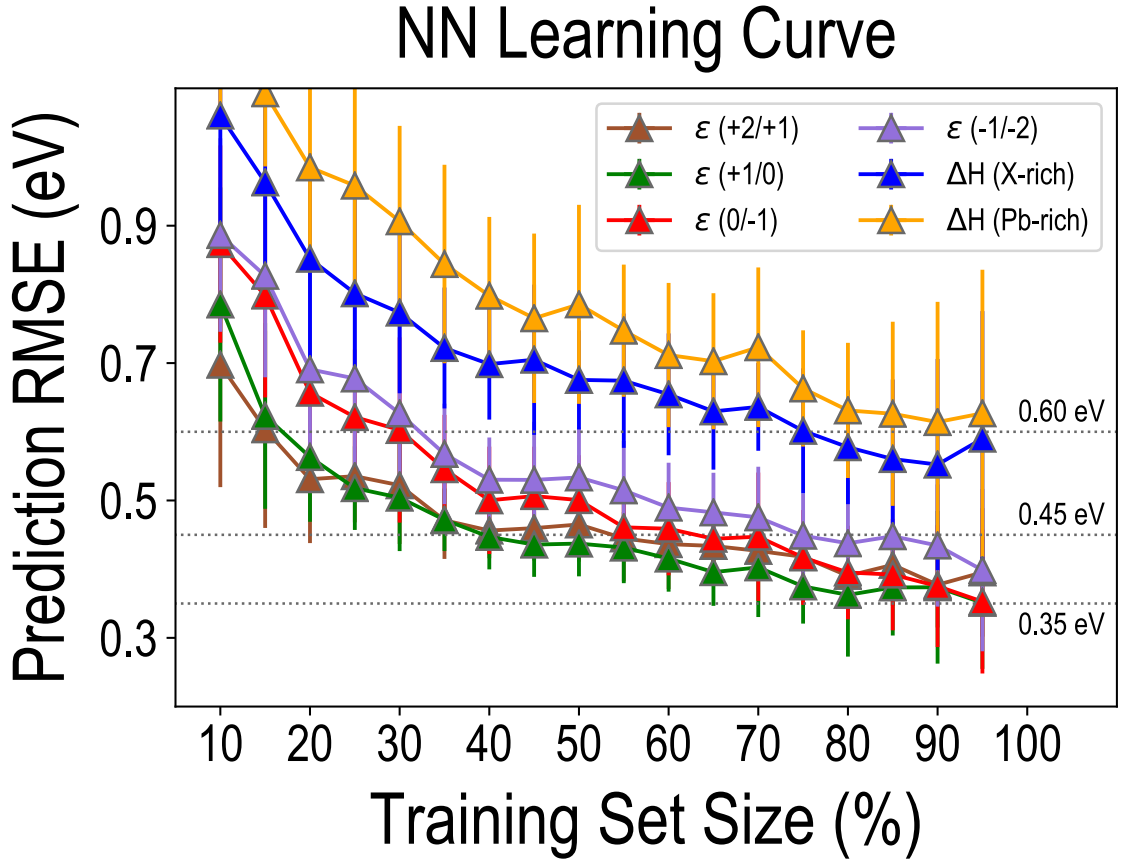
# Types of Machine Learning

- Supervised learning: From labeled training data, find the unknown function connecting known inputs to unknown outputs, based on extrapolation of patterns.
- Unsupervised learning: Find patterns in unlabeled data, leading to clustering of samples.
- Semi-supervised learning: Representations learned from a mix of unlabeled and labeled data.
- Reinforcement learning: Finding optimal or sufficiently good actions for a situation to maximize a reward.

# Nuts and Bolts of ML

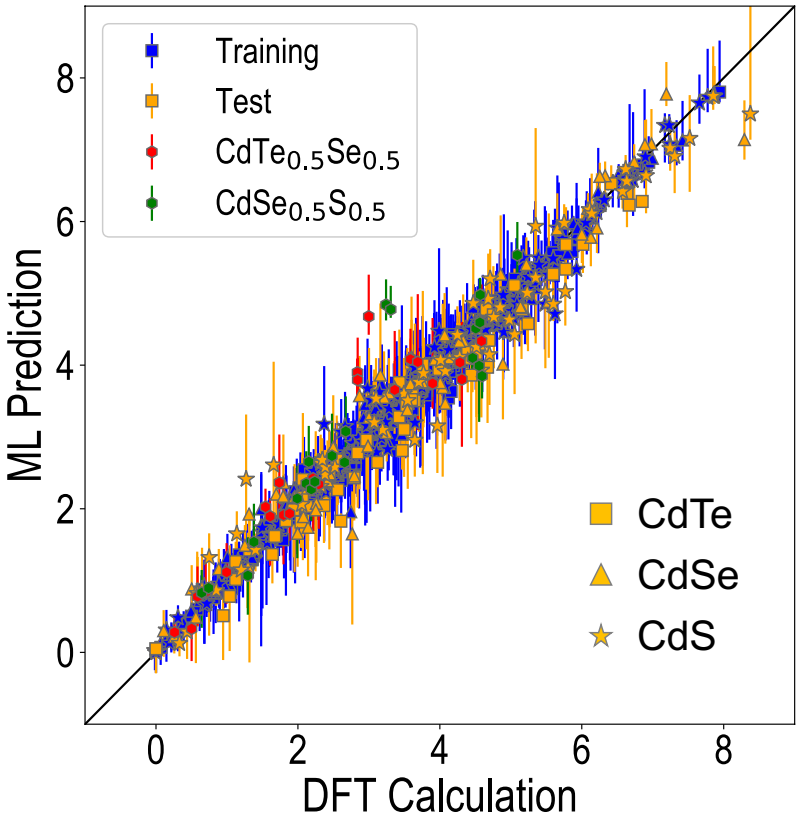
- Data: Divide into training, validation, and test sets.
- Descriptors: enumerate for all data points, perform dimensionality reduction and feature scaling.
- Cross-validation: n-fold, leave-one-out.
- Hyperparameter optimization: grid-search, Bayesian.
- Best model: optimized w.r.t. training data and descriptor size, CV, and HPO; choose error definition.
- Quality and quantity of data and descriptors: prevent underfitting. CV, HPO, regularization: prevent overfitting.

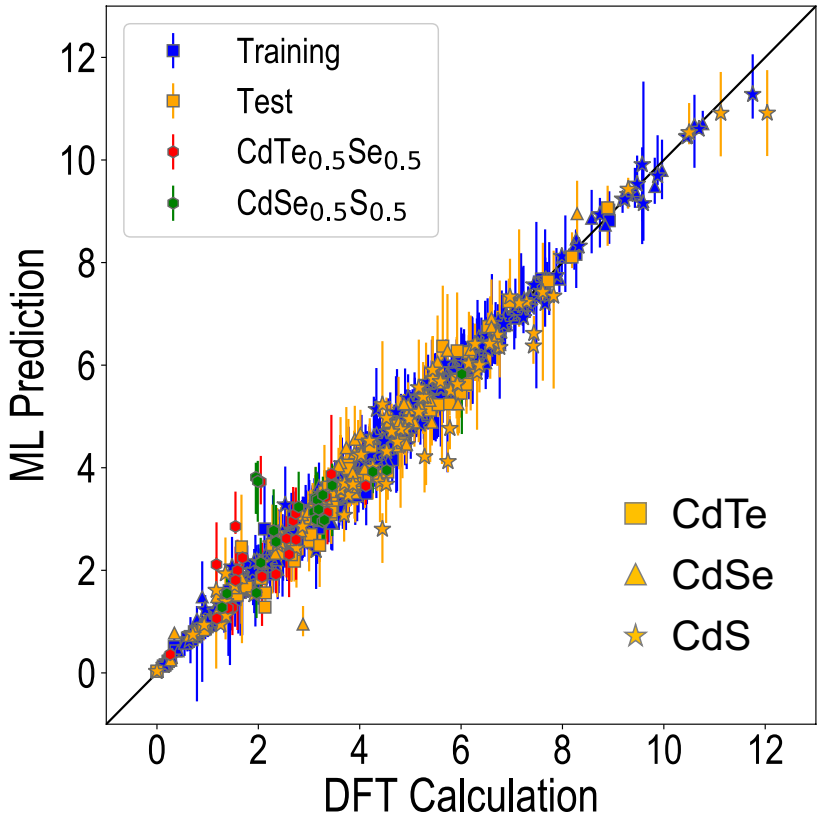
# Training Data Size: Learning Curves




Iteratively change training set size (and descriptor dimensions) until test error saturates → learning curve.

# Example: ML Regression

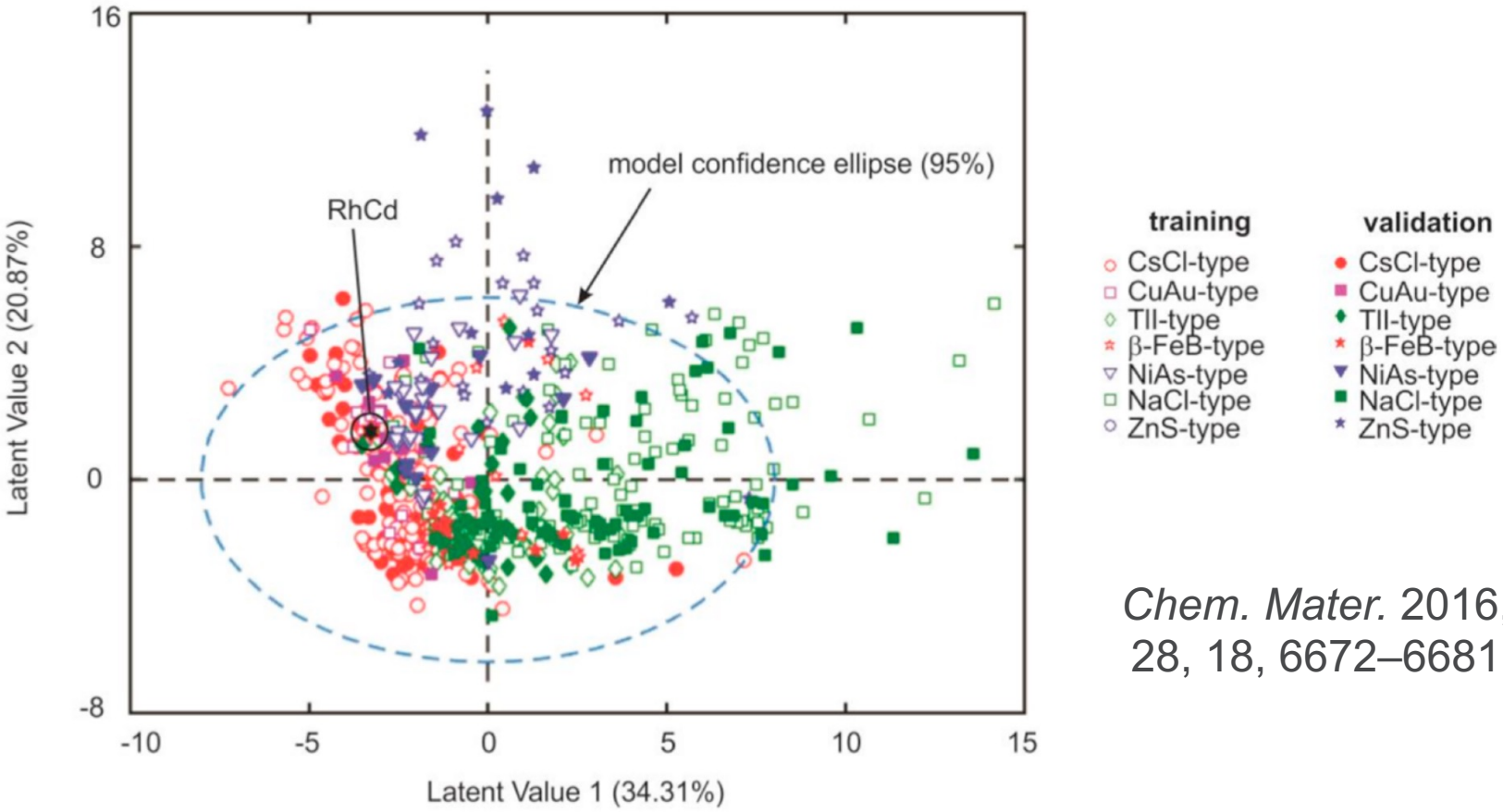



Predicting defect formation energy in semiconductors.

*npj Comput Mater.* **6,** 39 (2020)

# Example: ML Classification




*Chem. Mater.* 2016, 28, 18, 6672–6681

Classifying AB compounds into different structure types.

# Linear Regression

- Linear regression model prediction form:
  $y = \boldsymbol{\theta}_0 + \boldsymbol{\theta}_1 x_1 + \boldsymbol{\theta}_2 x_2 + \ldots + \boldsymbol{\theta}_m x_m$; or, $y = h_{\boldsymbol{\theta}}(x) = \boldsymbol{\theta}^T.\mathbf{x}$

- MSE cost function for a linear regression model:

$$\mathrm{MSE}(\mathbf{X}, h_\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(\theta^T \cdot \mathbf{x}^{(i)} - y^{(i)}\right)^2$$

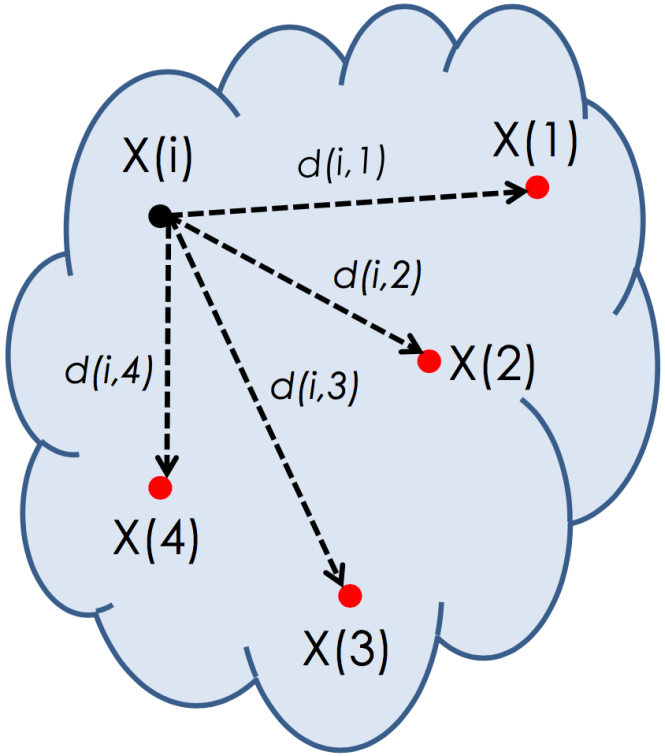
- Direct estimation of $\boldsymbol{\theta}$ using the formula below (indirect method uses GD):

$$\hat{\theta} = \left(\mathbf{X}^T \cdot \mathbf{X}\right)^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

- Easy extension to Polynomial regression.

# Kernel Ridge Regression

*Chemical Space*




$X(i) = \{x_1, x_2, x_3 \ldots x_m\}$

## KERNEL RIDGE REGRESSION (KRR)

Measure of Similarity: Euclidean Distance

$$d(i,j) = \sqrt{(x_{i1} - x_{j1})^2 + \ldots + (x_{im} - x_{jm})^2}$$

Property = Weighted sum of Gaussians

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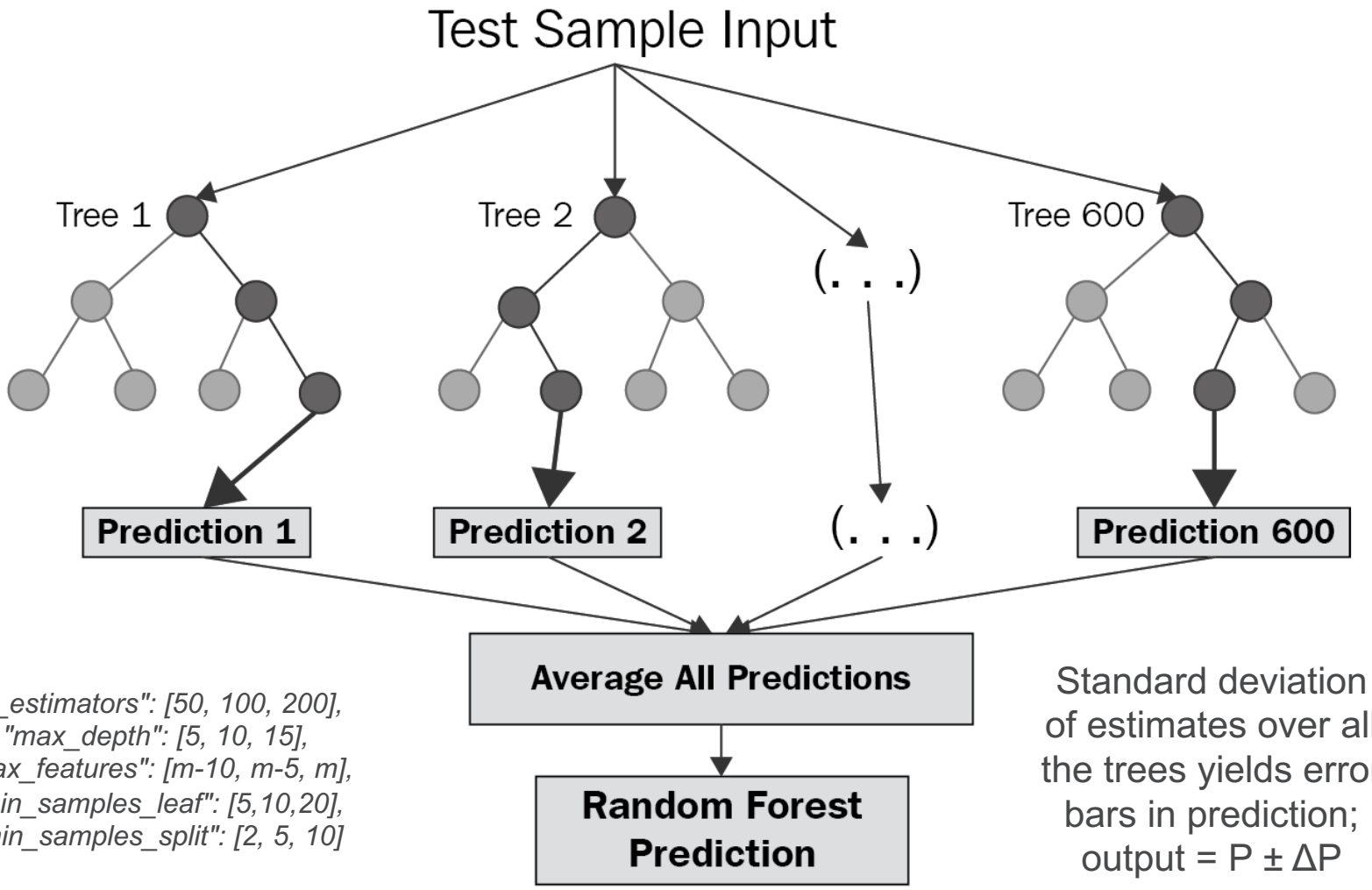
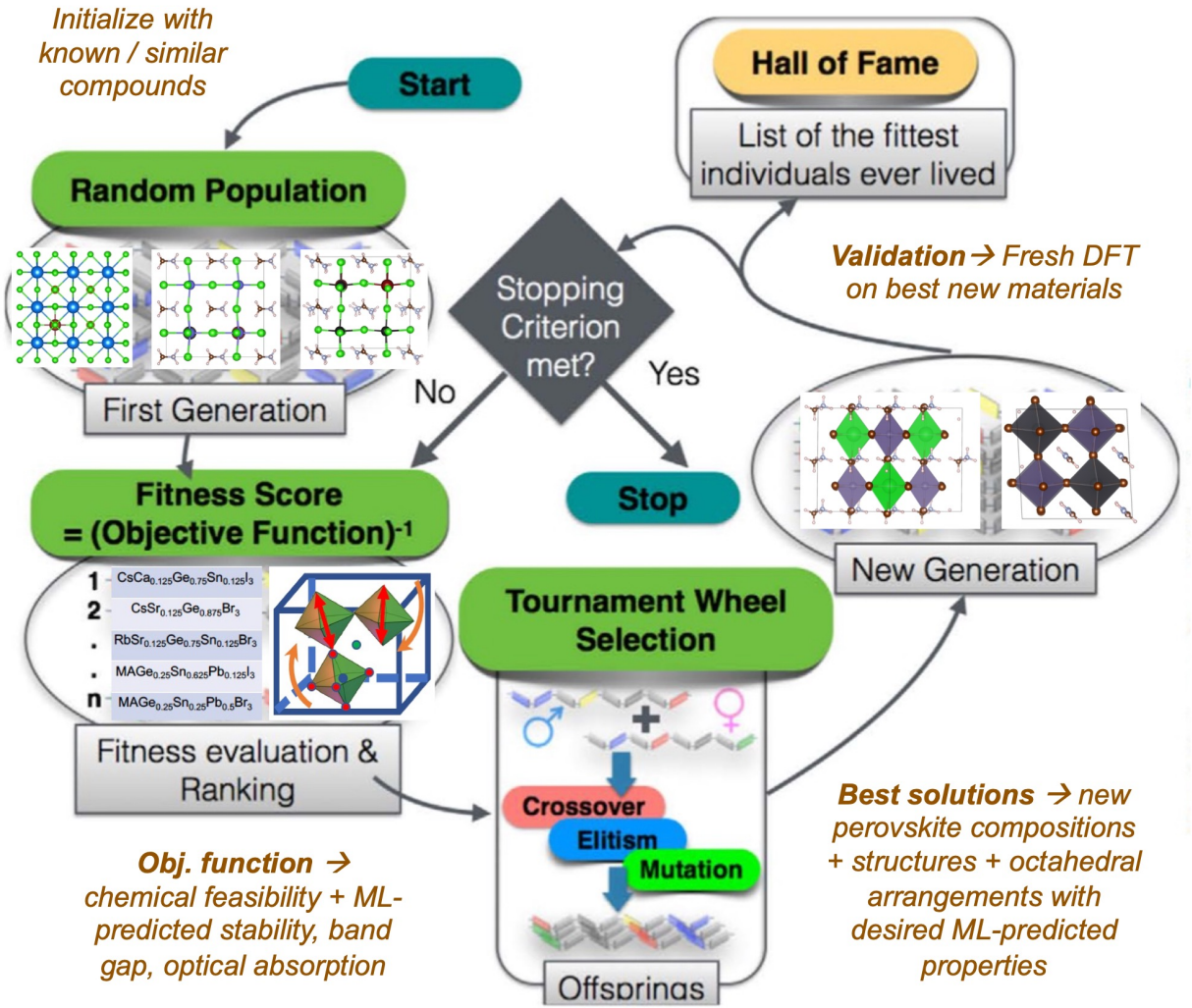



*"n_estimators": [50, 100, 200],*
*"max_depth": [5, 10, 15],*
*"max_features": [m-10, m-5, m],*
*"min_samples_leaf": [5,10,20],*
*"min_samples_split": [2, 5, 10]*

Standard deviation of estimates over all the trees yields error bars in prediction; output = P ± ΔP

# Genetic Algorithm



# PART 1 SUMMARY

- Definition and basic principles of materials informatics.
- Key steps in ML: materials data, materials descriptors, techniques for regression and classification.
- Linear regression, RFR, KRR, GA.
- NEXT: A detailed supervised learning case study → predicting (DFT computed) properties of a chemical space of halide perovskite alloys.

# MRS Bulletin Article in Press

## A Framework for Materials Informatics Education through Workshops

Arun Mannodi-Kanakkithodi[1], Austin McDannald[2], Shijing Sun[3], Saaketh Desai[4], Keith Brown[5] and A. Gilad Kusne[2]

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# PART 2, CASE STUDY: Data-Driven Design of Halide Perovskite Alloys

https://github.com/mannodiarun/mrs_spring_tutorial/blob/perovs_dft_ml/DFT-ML-GA.ipynb

Or directly open
https://colab.research.google.com/github/mannodiarun/mrs_spring_tutorial/blob/perovs_dft_ml/DFT-ML-GA.ipynb

https://tinyurl.com/257ruuue

# PART 3:
# Gaussian Process Regression & Active Learning

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

GPR notebook: https://tinyurl.com/3db88ka5

AL notebook: https://tinyurl.com/2zu9n7aj

# PART 4:
# Neural Network Regression and Classification

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

Regression notebook: https://tinyurl.com/yf3sx74c

Classification notebook: https://tinyurl.com/5n7kecyr