Machine Learning for Materials Scientists: An Introductory Guide Towards Best Practices

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This Editorial is intended for materials scientists interested in performing machine learning-centered research. We cover broad guidelines and best practices regarding the obtaining and treatment of data, feature engineering, model training, validation, evaluation and comparison, popular repositories for materials data and benchmarking datasets, model and architecture sharing, and finally publication. In addition, we include interactive Jupyter notebooks with example Python code to demonstrate some of the concepts, workflows, and best practices discussed.

Overall, the data-driven methods and machine learning workflows and considerations are presented in a simple way, allowing interested readers to more intelligently guide their machine learning research using the suggested references, best practices, and their own materials domain expertise.

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Machine Learning for Materials Scientists:

An introductory guide towards best practices

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Abstract

This Editorial is intended for materials scientists interested in performing machine learning-centered research. We cover broad guidelines and best practices regarding the obtaining and treatment of data, feature engineering, model training, validation, evaluation and comparison, popular repositories for materials data and benchmarking

datasets, model and architecture sharing, and finally publication. In addition, we include interactive Jupyter notebooks with example Python code to demonstrate some of the concepts, workflows, and best practices discussed. Overall, the data-driven methods and machine learning workflows and considerations are presented in a simple way, allowing interested readers to more intelligently guide their machine learning research using the suggested references, best practices, and their own materials domain expertise.

Keywords

Machine learning, neural networks, materials science, materials informatics, data science, common pitfalls, best practices, example code, Python, interactive notebooks, Jupyter

Introduction

Materials scientists are constantly striving to advance their ability to understand, predict and improve materials properties. Due to the high cost of traditional trial-and-error methods in materials research (often in the form of repeated rounds of material synthesis and characterization), material scientists have increasingly relied on simulation and modeling methods to understand and predict materials properties *a priori*. Materials informatics (MI) is a resulting branch of materials science that utilizes high-throughput computation to analyze large databases of materials properties to gain unique insights. More recently, data-driven methods such as machine learning (ML) have been adopted in MI to study the wealth of existing experimental and computational data in materials science, leading to a paradigm shift in the way materials science research is conducted.

However, there exist many challenges and “gotchas” when implementing ML techniques in materials science. Furthermore, many experimental materials scientists lack the know-how to get started in data-driven research, and there is a lack of recommended best practices for implementing such methods in materials science. As such, this Editorial is designed to

assist those materials science scholars who wish to perform data-driven materials research. We demonstrate a typical ML project step-by-step (Figure 1 on page 24), starting with loading and processing data, splitting data, feature engineering, fitting different ML models, evaluating model performance, comparing performance across models, and visualizing the results. We also cover sharing and publication of the model and architecture, with the goal of unifying research reporting and facilitating collaboration this emerging field. Throughout this process, we highlight some of the challenges and common mistakes encountered during a typical ML study in materials science, as well as approaches to overcome or address them. Highlighting the best practices will improve the research and manuscript quality, and ensure reproducible results.

To demonstrate some of the best practices discussed throughout this Editorial, we have created several interactive Jupyter notebooks with relevant Python code structured in a tutorial format (Table 1). The sections in this Editorial that include accompanying notebooks are marked with an asterisk*. The notebooks walk the readers through a basic ML study in materials science: the prediction of heat capacity for solid inorganic compounds. We demonstrate this by implementing several classical machine learning as well as neural network models from the well-known Python packages `scikit-learn` and `PyTorch`, respectively. The Jupyter notebooks can be accessed at the online GitHub repository: <https://github.com/anthony-wang/BestPractices>. Setup, usage, further instructions and pertinent information can also be found there. Please note, an intermediate knowledge of the Python programming language and general programming principles is required.

Table 1: List of accompanying Jupyter notebooks and the topics demonstrated.

#	Notebook contents
1	Loading data; examining, processing, cleaning up of data
2	Splitting data into train/validation/test datasets
3	Featurizing data; modeling with classical models, evaluating models, effect of different train/validation/test splits
4	Modeling with neural networks, evaluating models, exporting models, avoiding overfitting
5	Visualizing results

Meaningful machine learning

Machine learning is a powerful tool, but not every materials science problem is a nail. It is important to delineate when to use ML, and when it may be more appropriate to use other methods. Consider what value ML can add to your project and whether there are more suitable approaches. Machine learning is most useful when human learning is impossible, such as where the data and interactions within the data are too complex and intractable for human understanding and conceptualization. Contrarily, machine learning often fails to find meaningful relationships and representations from small amounts of data, when a human mind would otherwise likely succeed.

When developing ML tools and workflows, consider how (and with what ease) they can be used not only by yourself, but by others in the research community. If another researcher wants to use your method, will they be able to do so, and will it be worth it for them? For example, if you include data from *ab initio* calculations such as density functional theory (DFT), or crystal structure as one of the input features of your ML model, would it not be simpler for other researchers to use DFT or other simulation methods themselves, instead of using your ML model?

Another limitation to consider when using ML as a tool is the model interpretability vs. predictive power trade-off. If you are looking for physical or chemical insights into your materials, you are unlikely to find them when using powerful and complex models such as neural networks: these models—while they can exhibit high model performance—are usually too complex to be easily understood. These are so-called “black-box” models because outside of their inputs and outputs, it is nearly impossible for a human to grasp the inner model workings and its decision making processes. In contrast, simpler models might be easier to understand, but tend to lack the predictive power of the more complex models.

In general, a good ML project should do one or more of the following: screen or down-select candidate materials from a pool of known compounds for a given application or property,¹⁻³ acquire and process data to gain new insights,^{4,5} conceptualize new modeling ap-

proaches,^{6–10} or explore ML in materials-specific applications.^{1,11–13} Consider these points when you judge the applicability of ML for your project.

Machine learning in materials science

Machine learning has been applied in the study of many inorganic material properties, such as mechanical, electronic, thermodynamic, and transport properties. It has also been used in many different material application areas, such as photovoltaic materials, materials for energy storage, catalysts/photocatalysts, thermoelectric materials, high-temperature superconductors, and high entropy and metallic glass alloys. We highlight some current examples in the literature of inorganic material properties and their application areas in Table 2. Here, we are not attempting to summarize the methods or results of these studies; instead, we advise the interested reader to refer to the cited works as well as other well-written reviews available in the literature.^{3,14–24}

Table 2: Examples of using machine learning in the study of inorganic materials.

Material properties	Refs.
Mechanical properties	1,6,9,25–30
Formation energy	7,9,29,31–34
Band gap	6,9,29,35–39
Density of states	40,41
Crystal structure / stability	32,42–52
Debye temperature / heat capacity	6,53,54
Thermal expansion coefficient	6,53
Thermal conductivity	6,53,55–57
Seebeck coefficient	56,58
Material classes	Refs.
Photovoltaic materials	34,59,60
Energy storage	61–65
Catalysts / photocatalysts	2,66–71
Thermoelectric materials	4,13,56,72,73
High-temperature superconductors	74,74–80
High entropy alloys	81,82
Metallic glass alloys / glass-forming ability	34,83,84

Working with materials data

Data source

Some of the more commonly-used repositories for materials property data are shown below in Table 3.

Table 3: Comparison of materials data repositories with predominantly property information.

Name	Structure information	Mechanical properties	Thermal properties	Electronic properties	API*	Data license	Refs.
Materials Project	Y	Y	Y	Y	Y	CC BY 4.0	85
Open Quantum Materials Database	Y	N	Y	Y	Y	CC BY 4.0	86
AFLOW for Materials Discovery	Y	Y	Y	Y	Y	†	87
NOvel MAterials Discovery (NOMAD)	Y	Y	Y	Y	Y	CC BY 4.0	88
Open Materials Database	Y	N	Y	Y	Y	CC BY 4.0	89
Citrine Informatics	Y	Y	Y	Y	Y	CC BY	90
Materials Platform for Data Science (MPDS)	Y	Y	Y	Y	Y	CC BY 4.0	91
AiiDA / Materials Cloud	Y	Y	Y	Y	Y	Varies	92,93
NREL MatDB	Y	N	Y	Y	N	Own license	94
NIST TRC Alloy Data	N	N	Y	N	On request	Free	95
NIST TRC ThermoData	N	N	Y	N		NIST SRD	96
NIST JARVIS-DFT /-ML Database	Y	Y	Y	Y	Y	Public domain	97,98
MatWeb	N	Y	Y	N	N	Paid	99
Total Materia	N	Y	Y	N	N	Paid	100
Ansys Granta (Material-Universe repository)	N	Y	Y	N	N	Paid	101
MATDAT	N	Y	Y	N	N	Paid	102

*: An “application programming interface” is a set of defined functions, procedures, methods or classes which enable a structured way of exchanging data between programs. In the framework of a materials data repository, an API facilitates, *e.g.*, the uploading, examining, downloading of data, and other forms of interactions between the user and the repository.

†: not specified.

Other repositories that host predominantly crystal structure information are shown below in Table 4. While these repositories do not necessarily host material property information, the structure information contained within these repositories are also valuable.

Table 4: Comparison of materials data repositories with predominantly structure information.

Name	# records	API	Data license	Refs.
Cambridge Structural Database (CSD)	1,055,780	Y	Paid	103
Inorganic Crystal Structure Database (ICSD)	216,302	N	Paid	104
Pearson’s Crystal Data (PCD)	335,000	N	Paid	105
International Centre for Diffraction Data (ICDD)	1,004,568	N	Paid	106
Crystallography Open Database (COD)	455,714	Y	Open-access	107
Pauling File	357,612	Y	Paid	108
CrystMet database	160,000	N	Paid	109

Note: values for number of records were updated as of the submission date (May 2020).

There is an ever-increasing number of materials informatics-related resources and repositories; as such, only the more commonly used repositories are mentioned above. Keep in mind that each dataset is different, and may contain domain-specific information and features that are restricted to certain research fields or applications. There may also be differences in the methodologies with which the data are experimentally or computationally derived, curated, and recorded in these databases. As a result of this, the values for material properties might not be directly comparable across the different repositories. Be mindful of this when you are comparing property data across the repositories, especially if you plan on aggregating or merging data from different sources.

Dataset size & composition*

When collecting your dataset for your ML study, be mindful of your dataset size. Ensure that your dataset size is large enough and includes most examples of the combinations of material compositions in the material space you want to study. It is also important to consider data balance or bias in your datasets. Does your data form clusters based on

chemical formula, test condition, structure type, or other criteria? Are some clusters greatly over- or under-represented? Many statistical models used in ML are frequentist in nature, and will be influenced by dataset imbalance or bias. Visualization techniques such as t-distributed stochastic neighbor embedding (t-SNE¹¹⁰), uniform manifold approximation and projection (UMAP¹¹¹), or even simple elemental prevalence mapping¹¹² may be useful in investigating dataset imbalance and bias.

Lastly, if your dataset is too large (a rare luxury in the materials science field), you may find yourself having to wait a long time to train and validate your models during the prototyping phase of your project. In this case, you can sub-sample your dataset into a small-scale “toy dataset”, and use that to test and adjust your models. Once you have tuned your models to your satisfaction on the toy dataset, you can then carry on and apply them to the full dataset. When sampling the original dataset to create the toy dataset, be aware that you do not introduce any dataset biases through your sampling. Also keep in mind that not all performance-related problems can be fixed by sub-sampling your data. If your model can only train successfully on the toy dataset, and cannot train on the full dataset (*e.g.*, due to memory or time constraints), you may wish to focus on improving its performance first.

Data version control

Be sure to save an archival copy of your raw dataset as obtained, and be sure that you can retrieve it at any time. If you make any changes to your dataset, clearly record the steps of the changes and ensure that you are able to reproduce them on the dataset in the future if needed. To simplify version control, consider using a version control system (such as Git,¹¹³ Mercurial¹¹⁴ or Subversion¹¹⁵) for your datasets.

Cleanup and processing*

Once you have curated your dataset, examine and explore the data on a high level to see if there are any obvious flaws or issues. These may—and often do—include missing or unre-

alistic values (*e.g.*, NaN's, or negative values/positive values where you don't expect them), outliers or infinite values, badly-formatted or corrupt values (*e.g.*, wrong text encoding, numbers stored in non-numeric format), non-matching data formats or data schema caused by changes in the repository, and other irregularities. If you find any irregularities, deal with them in an appropriate way, and be careful not to introduce any bias or irregularities of your own. Make sure you document any data cleanup and processing steps you performed; this is an important step in ensuring reproducibility that is often overlooked in ML studies. In addition, during your model prototyping stage, you may find some additional problematic data samples which adversarially affect your model performance. In this case, consider performing another round of data cleanup before finalizing your model.

Train-validation-test split*

Split your data once into three datasets: train, validation, and test. The split should be performed in a reproducible way (*e.g.*, by assigning a random seed and shuffling the dataset); alternatively, you can save the split datasets as files for reuse. Make sure that no same (or similar) data appear in the test dataset, if they are already present in the train or validation dataset. For example, if you have several measurements of a chemical compound that are performed at different measurement conditions in the train dataset (*e.g.*, temperature or pressure), during the testing phase, your model would likely perform well if it is asked to predict the property of the same compound at a different condition. This, however, gives you an inflated estimate of how well the model will generalize in cases where it hasn't seen a particular chemical compound before. For a truly rigorous evaluation of your model's generalization performance, you should take care to avoid this data leakage when you split your data.

During the training stage, models may only be shown the training data as part of the learning process. Validation data may be used to assess and tune different model hyperparameters, and may be compared with the predictions of different model/hyperparameter

combinations to evaluate a model's performance. In contrast, test data may only be used in order to evaluate a model's performance as a final step, after the model has been finalized. Models *must not* be trained *nor* tuned on the test dataset. Use the same train, validation, and test datasets for all modeling and model comparison/benchmarking steps.

The training dataset can be further partitioned to be used for cross-validation (CV). CV is a method that is often employed to estimate the true ability of a model to predict on new unseen data, and to catch model-specific problems such as overfitting or selection bias.¹¹⁶ One typical method is k -fold cross-validation. In k -fold CV, the training dataset is first randomly partitioned into K subsets (remember to note down your partitioning details). Then, for each k of the data subsets $k = 1, 2, \dots, K$, the model is trained on the combined data of the other $K - 1$ subsets, and then evaluated using the k^{th} subset. The resulting K prediction errors are then typically averaged to give a more accurate estimate of the model's true predictive performance compared to evaluating the model performance on one single train/validation/test split. Typical choices for K in the literature are 5 or 10. In the case of a small input dataset size, k -fold CV or other methods of cross-validation can also be used as a data re-sampling technique for models that are more robust against overfitting on the validation set (*e.g.*, linear regression).

Modeling

Choosing appropriate models & features*

The dataset size will almost always determine your available choices of ML models. For smaller dataset sizes, classical and statistical ML approaches (*e.g.*, regression, support vector machines, k -nearest neighbors, and decision trees) are more suitable. In contrast, neural networks require larger amounts of data, and only start becoming feasible/useful when you have training data points on the order of thousands or more. Typically, ML models such as regression, decision tree/random forest, k -nearest neighbors, and support vector machines

are used on smaller datasets. These algorithms can be further improved by applying bagging, boosting or stacking approaches. There are many existing Python libraries for implementing the above, with perhaps the most well-known being `scikit-learn`.¹¹⁷ For larger datasets, neural networks and deep learning methods are more commonly used. In the scholarly community, the Python libraries `PyTorch`¹¹⁸ and `TensorFlow`¹¹⁹ are often used to implement these architectures.

Feature engineering is important for smaller dataset sizes, and can contribute to a large model performance increase if the features are well-engineered.^{1,54,120} A common way to transform chemical compositions into usable input features for ML studies is through the use of composition-based feature vectors (“CBFVs”). There are numerous forms of the CBFV available, such as `Jarvis`,¹²¹ `Magpie`,³⁴ `mat2vec`,⁴ and `Oliynyk`.¹³ These CBFVs contain values that are either experimentally-derived, calculated through high-throughput computation, or extracted from materials science literature using ML techniques. Instead of featurizing your data using CBFVs, you can also try a simple onehot-encoding of the elements. These CBFV featurization schemes as well as the relevant functions and code for featurizing chemical compositions are included in the online GitHub repository associated with this work.

For sufficiently large datasets and for more “capable” learning architectures like very deep, fully-connected networks^{7,122} or novel attention-based architectures such as `CrabNet`,⁶ feature engineering and the integration of domain knowledge (such as through the use of CBFVs) in the input data becomes irrelevant and does not contribute to a better model performance compared to a simple onehot-encoding.¹¹ Therefore, due to the effort required to curate and evaluate domain knowledge-informed features specific to your research, you may find it more beneficial to seek out additional sources of data, already-established featurization schemes, or use learning methods that don’t require domain-derived features⁶ instead.

Data scaling & normalization*

In most cases, it may be beneficial to scale your input data (X). For a regression task, it may also be helpful to scale the targets (y) as well. Scaling can be done in many ways. Often, the input data is scaled to have zero-mean and unit variance. This allows for more stable gradients and faster model convergence, since the resulting feature dimensions are similar in scale.^{123–126}

This is done by using the transformation:

$$X' = (X - \bar{X})/\sigma_X \tag{1}$$

where $\bar{X}$ denotes the mean and σ_X the standard deviation of X . In some cases, applying the logarithm function to your values before scaling them according to Equation 1 may further improve your model performance.

Keep in mind that the scaling operations must be conducted using solely the statistics from the training dataset (*i.e.*, the train/validation/test datasets are scaled using only the mean and standard deviation values computed from the training data), and that the validation and test data statistics must not be used. Remember also to undo the scaling operation(s) on the target values (if these were scaled) after loss computation, but before performance evaluation. Similar to scaling, normalization of X is recommended for regression tasks. Here it is also important to use only the training data statistics when normalizing input data.

Scaling and normalization are not commutable: their ordering matters. You should scale, then normalize. When undoing this operation, the inverse is required: unnormalize and then unscale.

Keep it simple

Sometimes, especially in the case of small dataset sizes, simpler models can perform better than more complex models on the held-out test data. Some simpler models that you can try are linear (or ridge / lasso) regression, random forest, or k -nearest neighbors.

Furthermore, consider the model complexity–explainability trade-off. Typically, more complex models achieve higher model performance, but have the caveat that they are generally not easily interpretable by humans. In contrast, simpler models are typically assumed to be more easily understood by humans, and lead to better opportunities for model introspection. This is an important consideration in materials science, since synthesis and characterization are costly and time-consuming and the costs must be justified.

Hyperparameter optimization

Depending on your choice of ML model, there may be model hyperparameters that can be tuned. Examples of hyperparameters are the number of neighbors (k) in k -nearest neighbors, the number and depth of trees in a random forest, the kernel type and coefficient in support vector machines, the maximum number of features to consider in gradient boosting, and loss criterion, learning rate and optimizer type in neural networks. These hyperparameters are properties of the models themselves, and can significantly affect your model’s performance, speed (in training and inference), and complexity.

The hyperparameters are not learned by the model during the training step; rather, they are selected by you when you create the model. The recommended way to optimize your model hyperparameters is by training numerous models (each with a different set of hyperparameters) using the same training set, and then evaluating the models’ performance using the same validation set. By doing this, you will be able to identify the set of hyperparameters that generally lead to good-performing models. This is commonly referred to as a “grid search”. Imagine that your model has two continuous-variable hyperparameters, h_1 and h_2 , and that there is a range of values for each of these parameters that you wish to

investigate, $[h_{1,min}, h_{1,max}]$ and $[h_{2,min}, h_{2,max}]$, respectively. You can then define a grid that spans between $(h_{1,min}, h_{2,min})$ and $(h_{1,max}, h_{2,max})$. At each point on this grid, you train a model corresponding to that set of hyperparameters using the training set, and then evaluate its performance on the validation set. After repeating this for every point on the grid, you obtain a mapping that you can then use to determine the best set of hyperparameters for your specific model and data.

Once again, we stress the importance of reserving a held-out test dataset during dataset splitting. By training and optimizing your model on the training and validation datasets, you have effectively tuned—and possibly biased—your model to perform exceptionally well on these data samples. Therefore, the performance metrics of your model on these datasets are no longer good indicators of your model’s true generalization ability. In contrast, evaluating your model’s performance on the held-out test dataset (which your model has never seen before) will give you a much more realistic estimate.

Model evaluation and comparison

Typically, studies in materials science will compare the performance of several ML model and hyperparameter combinations on a given task. Trained models are typically compared by evaluating their performance on the held-out test dataset using computed test metrics such as accuracy, logarithmic loss, precision, recall, F1-score, ROC (receiver operating characteristic curve), and AUC (area under curve) for classification tasks, and r^2 (Pearson correlation coefficient), mean absolute error, and (root) mean squared error for regression tasks. Also consider using cross-validation (as discussed earlier) to give a more accurate estimate of your model’s true performance.

Show your model*

If you are reporting a new model architecture or algorithm, you must include all pertinent information necessary to reproduce, evaluate, and apply your models. This entails providing

the complete source code for your implementation, the hyperparameters used, the random seeds applied (if any), and the pre-trained weights of the models themselves. In addition, clear descriptions and schematics of your new system should be provided, as well as instructions to reproduce your model and work. Ideally, you can show your model and results in an interactive manner, such as through the use of Jupyter notebooks.

Fitting and testing

Avoid overfitting*

In an ML problem, the model is asked to perform two contradicting tasks: (1) minimize its prediction error on the training dataset, and (2) maximize its ability to generalize on unseen data. Depending on how the model, loss criterion, and evaluation methods are set up, the model may end up memorizing the training dataset (an unwanted outcome) rather than learning an adequate representation of the data (the intended outcome). This is called “overfitting”, and usually leads to decreased generalization performance of the model. Overfitting can occur on all kinds of models, although it typically occurs more often on complex models such as random forests, support vector machines and neural networks.

During model training, observe the training metrics such as your loss output and r^2 score on the training and validation set. For example, when training a neural network, you can use a learning curve to track validation error over each epoch during the training process. As the model trains, the validation and training error will ideally decrease. Your training error will approach zero, but this is not the metric we care about! Rather, you should closely observe the validation error. When your validation error increase again while your training error continues to decrease, you are likely memorizing your training data and thus overfitting your data.

Overfitting can have an adverse effect on your model’s ability to generalize (that is, returning a reasonable output prediction for new and unseen data) thus performing poorer

on the test dataset. If you notice that your model overfits your data very easily, consider reducing the complexity of your model, or using regularization.

Beware of random initialization*

Many ML models require an initial guess as a starting point for their internal parameters. In many model implementations (*e.g.*, in `scikit-learn`'s linear regression, random forest, support vector machines, boosting implementations), these initial internal model parameters are provided by your system's random number generator. The same applies for neural network-based models, in the initialization of the weights and biases of the networks and some optimizer parameters. Depending on how sensitive your model is to initialization, different initial states of the models can lead to significant differences in your model performance.

It is therefore important that you ensure reproducible results across different model runs and different models (both for your internal testing and for publication). To accomplish this, you can choose a seed to use for the random number generator. Don't forget to mention this seed in your publication and code. Note that alternative ways of model initialization exist, such as using different estimators for initial parameter guesses as well as different initialization schemes for neural network weights and biases; here, you should note down your changes if you use an alternative implementation.

Avoid p -hacking

Train your models on the training dataset only, and use the validation dataset for tuning your model hyperparameters. *Do not* evaluate your model on the held-out test dataset until you have finished tuning your model, and it is ready for publication. Looking at the test dataset multiple times to pick ideal model hyperparameters is a form of p -hacking and is considered cheating!¹²⁷

Benchmarking and Testing

Reproducibly test various methods*

For comparison / ablation studies against other ML models and/or architectures, make sure you use the same train/validation/test datasets (refer to above for best practices on dataset splitting and management). For the most informative and fair comparison between different published models, consider running the models yourself. If you perform any additional model-specific data manipulation steps, make sure to document them and make them reproducible for your readers.

During the model tuning process, train your models on the train dataset and evaluate their performance on the validation set. After you have finalized your model architecture and hyperparameters, train the models once more on the combined train & validation datasets, and evaluate their performance on the test dataset.

Existing benchmarks

There are some tools and software packages online, which can be used as baselines to judge the performance of your models.^{128–130} Some of these tools can perform automatic feature engineering and testing of several different ML models. We suggest that you download these tools and compare the performance of your models against them. If your model does not perform better, or does not offer any advantages over these existing tools, consider other venues of improvement.

Making publication-ready, reproducible work

Source code & documentation*

Publishing in peer-reviewed journals relies on the foundational principle that the methodology be sufficiently described in order to ensure reproducibility. Therefore, for your ML-based

study, full source code for your models and architecture (if any) must be provided, including implementation details of data processing, data cleanup, data splitting, model training, and model evaluation. If you can, you should also publish your source code under a permissive or an open-source license so that others may (re-)use, improve, collaborate on, and contribute further to your work.¹³¹

Your published source code must be complete—that is, somebody should be able to take your source code verbatim, execute it, and obtain the same results that you did. Required libraries and other software dependencies (if any) must be listed, preferably with the pertinent version numbers. Ideally, these dependencies will be listed in an “environment file” that others can use to directly create a working software environment on their local system. If you use any code or packages developed by others, make sure to adhere to their licenses. Also consider hosting your code in an online, version-controlled repository such as GitHub, GitLab, Bitbucket, DLHub¹³² or similar.

Make sure the source code is well-documented and follows well-established code standards. Instead of writing additional comments to explain your code, considering writing code in a way such that it is self-explanatory without the need for additional comments. This entails using clear variable names, closely following formatting guidelines (such as PEP 8), and writing “explicit” code. Add a “README” file as well that provides your readers with instructions for the installation, setup, usage of your code, and for the reproduction of your published results. To ensure large-scale deployability and consistency on any infrastructure, consider also publishing your project as a containerized application, using tools such as Docker.¹³³

All data should be provided*

All results and datasets reported in the manuscript should be provided with the manuscript; alternatively, code for the users to obtain the data themselves must be given, ideally with clear instructions of the process. Additionally, all raw data—if their licenses allow it—

should be provided with the manuscript as well. In the case where the data cannot be provided, due to licensing, legal, intellectual property protection, or other insurmountable hurdles, an explanation should be given. You are nevertheless encouraged to find alternative solutions for providing data within reason. Examples may be to provide a partial dataset, an anonymized dataset, trained model weights, or instructions for users on how to obtain the dataset themselves. Consult with the owner of the data before considering these approaches, and as always, make sure you adhere to the data license.

Trained models & weights*

Ideally, you should provide a record of all model hyperparameters tested, as well as the best hyperparameters reported. For neural network implementations, the trained weights from the models should also be provided. In this case, be sure to provide the necessary code to recreate the neural network architecture and to load the saved weights for use. Ideally, you should also offer a friendly way to make predictions on user-supplied input data using these saved weights.

Visualizations*

All visualizations shown in the manuscript should be reproducible by a user who accesses your code. Ensure that you have included the required data (and ideally the code) used to generate the visualizations, or have given the users a way to obtain the required data themselves. If there are additional figures, such as in the supplementary information (SI), ensure that they are understandable by themselves and do not require additional explanation. If they do require explanation, provide this in the SI along with the figures.

Some of the typical visualizations that have shown themselves to be generally useful—and are thus commonly shown—in MI studies are: predicted property value vs. actual property value plots (Figure 2), residual error plots and histograms of residual errors (Figure 3), loss curves throughout the training process of a neural network (Figure 4), and element

prevalence visualizations (Figures 5 and 6). The figures are shown together at the end of this manuscript, on page 24.

Benchmark datasets

While there are currently several materials property datasets online which could potentially be used as benchmark datasets for benchmarking model performance in MI, there exist few published train/validation/test splits of these datasets which can be used by researchers to conduct a fair benchmark. Here, we note that examples of such datasets are commonly found in the fields of computer vision (*e.g.*, CIFAR, Google Open Images dataset, CelebFaces, ImageNet) as well as in natural language processing (*e.g.*, Glue, decaNLP, WMT 2014 EN-DE).

Furthermore, the data heterogeneity—in terms of the classes of materials, the reported material properties, or the diversity in the types of compounds and constituent elements—of the available materials datasets are typically quite limited and vary between dataset to dataset. Additionally, the methods to access some of the data stored in the online data repositories are sometimes restricted, and therefore hinder potential MI studies. This is due in part to the fact that certain datasets are proprietary or licensed under terms that do not allow their sharing (whether online or offline).

Another challenge is that the online material property repositories do not offer a “checkpointed” repository state; therefore, the repository and its data may change at any point in time, and there is no easy way to revert or refer back to the state of the repository at an earlier time. Therefore, current ML researchers typically download materials datasets from the repositories and archive them locally to run their benchmarks internally. However, there are recent emerging works from researchers that aim to address this issue of missing benchmark datasets for MI and ML studies in materials science.¹³⁴

Summary

While various machine learning methods, including classical methods and more advanced techniques such as deep learning and neural network-based architectures, have successfully been used for the prediction of materials properties, unique challenges still exist for their application in the domain of materials informatics. There are common pitfalls in the gathering, analysis and reporting of materials science-related data and machine learning results, and in the facilitation of reproduction studies. This Editorial highlights a large number of these issues which are found in submitted manuscripts and published works in the field of materials informatics. Proper observation to the recommendations given above will certainly ensure higher publication standards and more reproducible science in this exciting emerging field.

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Supporting Information Available

The following files are available with this publication:

- Online `GitHub` repository with the interactive Jupyter notebook files, Python source code and example data: <https://github.com/anthony-wang/BestPractices>
- Supplementary Information, containing read-only versions of the Jupyter notebook files

Figures

Figure 1: Schematic of a machine learning study in materials science.

Figure 2: Example predicted vs. actual material property plots, plotted (left) without and (right) with marginal histogram. In addition, lines corresponding to ideal predictions (where the predicted value exactly matches the actual values) and a linear regression fit (for estimating the correlation between the predicted and actual values) are shown.

Figure 3: Example residual error plots, plotted (left) against the actual value and (right) as a histogram with a kernel density estimation (kde). A lower error indicates a more accurate model prediction.

Figure 4: Example loss curve plot of a neural network, showing model performance (loss) evaluated on the train and validation datasets at each epoch throughout the training process. A lower loss indicates a better-performing model.

Figure 5: Example visualization of element prevalence in a dataset, shown as a histogram.

Figure 6: Example visualization of element prevalence in a dataset, shown as a heatmap on a periodic table.

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BestPractices_submitted.pdf (2.22 MiB)

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Supplementary Information for the paper “Machine
Learning for Materials Scientists:
An introductory guide towards best practices”

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Overview of Notebooks

These notebooks are included to illustrate a hypothetical Machine Learning project created following best practices.

The goal of this ML project is to predict the heat capacity of inorganic materials given the chemical composition and condition (the measurement temperature). We will use both classical ML models as well as neural networks.

To do this, we must:

1. Clean and process our dataset, removing obviously erroneous or empty values.
2. Partition our data into train, validation, and test splits.
3. Featurize our data, turning the chemical formulae into CBFVs.
4. Train models on our data and assess the predictive power of the models.
5. Compare the performance of the models fairly and reproducibly.
6. Visualize the prediction results of the models.
7. Share our models and enable others to reproduce your work and aid collaboration.

If you require more information about how to use Jupyter notebooks, you can consult:

- The main README file inside this repository: <https://github.com/anthony-wang/BestPractices/blob/master/README.md> (<https://github.com/anthony-wang/BestPractices/blob/master/README.md>)
- The official Jupyter Notebook documentation: <https://jupyter-notebook.readthedocs.io/en/stable/notebook.html> (<https://jupyter-notebook.readthedocs.io/en/stable/notebook.html>)

To read the main publication for which these notebooks are made, please see:

link coming

Please also consider citing the work if you choose to adopt or adapt the methods and concepts shown in these notebooks or in the publication:

citation coming

Check that libraries are installed

This notebook checks to see if you have the correct version of Python as well as all necessary libraries installed.

Check the [main README file \(https://github.com/anthony-wang/BestPractices/blob/master/README.md\)](https://github.com/anthony-wang/BestPractices/blob/master/README.md) for instructions if anything is missing.

```

In [1]: from __future__ import print_function
        from distutils.version import LooseVersion as Version
        import sys

        try:
            import curses
            curses.setupterm()
            assert curses.tigetnum("colors") > 2
            OK = "\x1b[1;%dm[ OK ]\x1b[0m" % (30 + curses.COLOR_GREEN)
            FAIL = "\x1b[1;%dm[FAIL]\x1b[0m" % (30 + curses.COLOR_RED)
        except:
            OK = '[ OK ]'
            FAIL = '[FAIL]'

        try:
            import importlib
        except ImportError:
            print(FAIL, "Python version 3.4 is required,"
                  " but %s is installed." % sys.version)

        def import_version(pkg, min_ver):
            mod = None
            try:
                mod = importlib.import_module(pkg)
                if pkg in {'PIL'}:
                    ver = mod.VERSION
                else:
                    ver = mod.__version__
                if Version(ver) < min_ver:
                    print(FAIL, "%s version %s or higher required, but %s installed."
                          % (lib, min_ver, ver))
                else:
                    print(OK, '%s version %s' % (pkg, ver))
            except ImportError as imp_err_msg:
                print(FAIL, 'Error in importing %s: %s' % (pkg, imp_err_msg))
            except AttributeError as att_err_msg:
                print(FAIL, 'Error in reading attribute of %s: %s' % (pkg, att_err_msg))
        ))
        return mod

        # first check the python version
        print('Using python in', sys.prefix)
        print(sys.version)
        pyversion = Version(sys.version)
        if pyversion >= "3":
            if pyversion < "3.7":
                print(FAIL, "Python version > 3.7 is required,"
                      " but %s is installed.\n" % sys.version)
            elif pyversion < "3":
                print(FAIL, "Python version > 3.7 is required,"
                      " but %s is installed.\n" % sys.version)
            else:
                print(FAIL, "Unknown Python version: %s\n" % sys.version)

        requirements = {'numpy': '1.18.0',
                        'pandas': '1.0.0',

```

```
'pandas_profiling': '2.4.0',  
'matplotlib': '3.2.0',  
'seaborn': '0.10.0',  
'sklearn': '0.22.0',  
'scipy': '1.4.0',  
'tqdm': '4.43.0',  
'jupyter_client': '6.0.0',  
'ipywidgets': '7.5.0',  
'torch': '1.3.0',}
```

now check the dependencies

```
for lib, required_version in list(requirements.items()):  
    import_version(lib, required_version)
```

Using python in C:\Users\Anthony\Anaconda3\envs\bestpractices

3.7.6 | packaged by conda-forge | (default, Mar 5 2020, 14:47:50) [MSC v.191

6 64 bit (AMD64)]

```
[ OK ] numpy version 1.18.1  
[ OK ] pandas version 1.0.2  
[ OK ] pandas_profiling version 2.4.0  
[ OK ] matplotlib version 3.2.0  
[ OK ] seaborn version 0.10.0  
[ OK ] sklearn version 0.22.2.post1  
[ OK ] scipy version 1.4.1  
[ OK ] tqdm version 4.43.0  
[ OK ] jupyter_client version 6.1.2  
[ OK ] ipywidgets version 7.5.1  
[ OK ] torch version 1.3.1
```


Data loading, cleanup and processing

The first step to a ML project is to obtain the dataset you will be working with. There are many repositories for materials science-specific data (whether online or offline)---consult the accompanying paper for a list of the more commonly used ones.

Once you have identified the repository and dataset you will use for your project, you will have to download it to your local machine, or establish a way to reliably access the dataset. Consult the documentation of the repository for how to do this.

For this tutorial, we have collected heat capacity (C_p) data from the [NIST-JANAF Thermochemical Tables](https://doi.org/10.18434/T42S31) (<https://doi.org/10.18434/T42S31>).

```
In [1]: import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
%config InlineBackend.figure_format='retina'

from pandas_profiling import ProfileReport
```

Load data

Using Pandas, we read in the dataset into a DataFrame.

We also print the shape of the DataFrame, which indicates the number of rows and columns in this dataset.

```
In [2]: PATH = os.getcwd()
data_path = os.path.join(PATH, '../data/cp_data_demo.csv')

df = pd.read_csv(data_path)
print(f'Original DataFrame shape: {df.shape}')

Original DataFrame shape: (4583, 3)
```

This means that our input dataset has 4583 data samples, each with 3 variables.

Examine the data

We examine some rows and look at the data's basic statistics.

We see that the dataset contains information about the formula, measurement condition (in this case, temperature in K), and the target property, heat capacity (in J/(mol * K)).

```
In [3]: df.head(10)
```

Out[3]:

	FORMULA	CONDITION: Temperature (K)	PROPERTY: Heat Capacity (J/mol K)
0	B2O3	1400.0	134.306
1	B2O3	1300.0	131.294
2	B2O3	1200.0	128.072
3	B2O3	1100.0	124.516
4	B2O3	1000.0	120.625
5	B2O3	900.0	116.190
6	B2O3	800.0	111.169
7	B2O3	723.0	106.692
8	B2O3	700.0	105.228
9	B2O3	600.0	98.115

First thing you should notice: we have many observations of the same compound (B2O3) but measured at different measurement conditions, resulting in a different property value.

We can get some simple summary statistics of the DataFrame by calling the `.describe()` method on the database.

```
In [4]: df.describe()
```

Out[4]:

	CONDITION: Temperature (K)	PROPERTY: Heat Capacity (J/mol K)
count	4579.000000	4576.000000
mean	1170.920341	107.483627
std	741.254366	67.019055
min	-2000.000000	-102.215000
25%	600.000000	61.312500
50%	1000.000000	89.497000
75%	1600.000000	135.645000
max	4700.000000	494.967000

Using the `pandas-profiling` library, we can generate a more in-depth report of our starting dataset. Note that generating this profile report might take upwards of 20 seconds.

```
In [5]: profile = ProfileReport(df.copy(), title='Pandas Profiling Report of Cp dataset',
                                html={'style':{'full_width':True}})
        profile.to_widgets()
```

Report generated with [pandas-profiling \(https://github.com/pandas-profiling/pandas-profiling\)](https://github.com/pandas-profiling/pandas-profiling).

Notice a few things from the profile report:

- We have some missing cells in the dataset ("Overview" tab)
- We have some unrealistic Temperature and Heat Capacity values in the dataset ("Variables" tab)
- We have some missing Temperature, Formula and Heat Capacity values in the dataset ("Variables" tab)

Also notice that on the "Overview" tab, there is the following warning: `FORMULA` has a high cardinality: 245 distinct values.

Cardinality is the number of distinct values in a column of a table, relative to the number of rows in the table. In our dataset, we have a total of 4583 data observations, but only 245 distinct formulae. We will have to keep this in mind later, when we process and split the dataset.

Rename the column names for brevity

```
In [6]: df.columns
```

```
Out[6]: Index(['FORMULA', 'CONDITION: Temperature (K)',
               'PROPERTY: Heat Capacity (J/mol K)'],
              dtype='object')
```

```
In [7]: rename_dict = {'FORMULA': 'formula',
                      'CONDITION: Temperature (K)': 'T',
                      'PROPERTY: Heat Capacity (J/mol K)': 'Cp'}
df = df.rename(columns=rename_dict)
df.columns
```

```
Out[7]: Index(['formula', 'T', 'Cp'], dtype='object')
```

Check for and remove NaN values

Here we can use the built-in Pandas methods to check for NaN values in the dataset, which are missing values. We then remove the dataset rows which contain NaN values.

```
In [8]: # Check for NaNs in the respective dataset columns, and get the indices
df2 = df.copy()
bool_nans_formula = df2['formula'].isnull()
bool_nans_T = df2['T'].isnull()
bool_nans_Cp = df2['Cp'].isnull()

# Drop the rows of the DataFrame which contain NaNs
df2 = df2.drop(df2.loc[bool_nans_formula].index, axis=0)
df2 = df2.drop(df2.loc[bool_nans_T].index, axis=0)
df2 = df2.drop(df2.loc[bool_nans_Cp].index, axis=0)

print(f'DataFrame shape before dropping NaNs: {df.shape}')
print(f'DataFrame shape after dropping NaNs: {df2.shape}')
```

```
DataFrame shape before dropping NaNs: (4583, 3)
```

```
DataFrame shape after dropping NaNs: (4570, 3)
```

Pandas also includes the convenient built-in method `.dropna()` to check for and remove NaNs in-place:

```
In [9]: df3 = df.copy()
df3 = df3.dropna(axis=0, how='any')

print(f'DataFrame shape before dropping NaNs: {df.shape}')
print(f'DataFrame shape after dropping NaNs: {df3.shape}')

df = df3.copy()
```

```
DataFrame shape before dropping NaNs: (4583, 3)
```

```
DataFrame shape after dropping NaNs: (4570, 3)
```

Check for and remove unrealistic values

In some cases, you might also get data values that simply don't make sense. For our case, this could be negative values in the temperature or heat capacity values.

```
In [10]: bool_invalid_T = df['T'] < 0
          bool_invalid_Cp = df['Cp'] < 0

          df = df.drop(df.loc[bool_invalid_T].index, axis=0)
          df = df.drop(df.loc[bool_invalid_Cp].index, axis=0)

          print(f'Cleaned DataFrame shape: {df.shape}')
```

Cleaned DataFrame shape: (4564, 3)

Save cleaned data to csv

Finally, after cleaning and processing the data, you can save it to disk in a cleaned state for you to use later.

Pandas allows us to save our data as a comma separated value .csv file.

```
In [11]: out_path = os.path.join(PATH, '../data/cp_data_cleaned.csv')
          df.to_csv(out_path, index=False)
```

Note, your data can be saved in other file formats (such as hdf5) or in databases (such as SQL), but we will not go into the details of these formats.

Typically, the amount of data you can gather for your ML project isn't large enough to warrant these approaches.

Splitting data into the train/validation/test dataset

It is important to split your full dataset into train/validation/test datasets, and reliably use the same datasets for your modeling tasks later.

Using different train/validation/test splits can dramatically affect your model performance (as seen here by the variance in r^2 scores for 30 models which have been trained on 30 different dataset splits) [1]:

[1]: C. Clement, S. K. Kauwe, T. D. Sparks, Benchmark AFLOW Data Sets for Machine Learning, figshare 2020, DOI: [10.6084/m9.figshare.11954742](https://doi.org/10.6084/m9.figshare.11954742) (<https://dx.doi.org/10.6084/m9.figshare.11954742>).

```
In [1]: import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
%config InlineBackend.figure_format='retina'

from sklearn.model_selection import train_test_split

# Set a random seed to ensure reproducibility across runs
RNG_SEED = 42
np.random.seed(seed=RNG_SEED)
```

Load the pre-processed dataset

We will start with the processed dataset that we saved from the last notebook.

```
In [2]: PATH = os.getcwd()
data_path = os.path.join(PATH, '../data/cp_data_cleaned.csv')

df = pd.read_csv(data_path)
print(f'Full DataFrame shape: {df.shape}')
```

Full DataFrame shape: (4564, 3)

```
In [3]: df.head(10)
```

Out[3]:

	formula	T	Cp
0	B2O3	1400.0	134.306
1	B2O3	1300.0	131.294
2	B2O3	1200.0	128.072
3	B2O3	1100.0	124.516
4	B2O3	1000.0	120.625
5	B2O3	900.0	116.190
6	B2O3	800.0	111.169
7	B2O3	723.0	106.692
8	B2O3	700.0	105.228
9	B2O3	600.0	98.115

Separate the DataFrame into your input variables (X) and target variables (y)

The X will be used as the input data, and y will be used as the prediction targets for your ML model.

If your target variables are discrete (such as `metal / non-metal` or types of crystal structures), then you will be performing a classification task. In our case, since our target variables are continuous values (heat capacity), we are performing a regression task.

```
In [4]: X = df[['formula', 'T']]
        y = df['Cp']

        print(f'Shape of X: {X.shape}')
        print(f'Shape of y: {y.shape}')
```

Shape of X: (4564, 2)

Shape of y: (4564,)

Splitting data (and a word of caution)

Normally, we could simply split the data with a simple `sklearn` function

The scikit-learn `train_test_split` function randomly splits a dataset into train and test datasets. Typically, you can use `train_test_split` to first split your data into "train" and "test" datasets, and then use the function again to split your "train" data into "train" and "validation" dataset splits.

As a rule of thumb, you can roughly aim for the following dataset proportions when splitting your data:

	train split	validation split	test split
proportion of original dataset	50% to 70%	20% to 30%	10% to 20%

If you have copious amounts of data, it may suffice to train your models on just 50% of the data; that way, you have a larger amount of data samples to validate and to test with. If you however have a smaller dataset and thus very few training samples for your models, you may wish to increase your proportion of training data during dataset splitting.

```
In [5]: X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, random_state=RNG_SEED)

        print(X_train.shape)
        print(X_test.shape)
```

(3651, 2)

(913, 2)

But wait, what's wrong here?

We have to make sure that our dataset splits contain mutually exclusive formulae (e.g., all the data samples associated with "Al₂O₃" is *either* in the train, validation, or test dataset, but *not in multiple*)!

```
In [6]: num_rows = len(X_train)
print(f'There are in total {num_rows} rows in the X_train DataFrame.')

num_unique_formulae = len(X_train['formula'].unique())
print(f'But there are only {num_unique_formulae} unique formulae!\n')

print('Unique formulae and their number of occurrences in the X_train DataFrame:')
print(X_train['formula'].value_counts(), '\n')
print('Unique formulae and their number of occurrences in the X_test DataFrame:')
print(X_test['formula'].value_counts())
```

There are in total 3651 rows in the X_train DataFrame.
But there are only 244 unique formulae!

Unique formulae and their number of occurrences in the X_train DataFrame:

W1	40
N1Ti1	38
N1Zr1	33
B1Ti1	33
O2Zr1	30
..	
I4Si1	4
N2O4	3
K1	2
Hg1O1	1
I4Ti1	1

Name: formula, Length: 244, dtype: int64

Unique formulae and their number of occurrences in the X_test DataFrame:

Ca1S1	10
N0.465V1	10
Be2O4Si1	10
O3W1	9
W1	9
..	
H2Mg1	1
O2Pb1	1
Fe1H3O3	1
Hf1	1
I1K1	1

Name: formula, Length: 229, dtype: int64

There are in total 3651 rows in the X_train DataFrame. But there are only 244 unique formulae! In fact, you will see that the same formulae are often present in the X_train and X_test DataFrames!

That's not good, because now we have instances of the same chemical compound appearing in *both* the training and test data. Which means the model can cheat and in essence just memorize the training data, and during testing, look up the nearby values present in the training data!

So how do we mitigate this?

Be aware of leaking data between datasets

We have to first group the data by chemical formula, then split the data according to the chemical formulae. That way, all data points associated with each formula are either in the training dataset or in the test dataset, *but not in both at the same time*.

Splitting data, cautiously (manually)

First we get a list of all of the unique formulae in the dataset.

```
In [7]: unique_formulae = X['formula'].unique()
print(f'{len(unique_formulae)} unique formulae:\n{unique_formulae}')
```

244 unique formulae:

```
['B2O3' 'Be1I2' 'Be1F3Li1' 'Al1Cl4K1' 'Al2Be1O4' 'B2H4O4' 'B2Mg1' 'Be1F2'
'B1H4Na1' 'Br2Ca1' 'Al1N1' 'Al1Cl6Na3' 'Ba1H2O2' 'Al1Br3' 'Br3Zr1'
'Br2Ti1' 'B1Ti1' 'Be2O4Si1' 'Br2Pb1' 'Al1' 'Br2Hg2' 'B1H3O3' 'Br3Ti1'
'C1Cu1N1' 'B1' 'Al1F6Na3' 'Ca1H2O2' 'B2Be3O6' 'Al1Cl4Na1' 'Al1Cl6K3'
'C0.98Nb1' 'Br2Hg1' 'Al1Cl1O1' 'Cl1H4N1O4' 'Be1F4Li2' 'C1Mg1O3' 'Br1H4N1'
'Ca1I2' 'Al1F6Li3' 'Br4Mo1' 'Ba1' 'Br4Ti1' 'Ba1Br2' 'Be1O4S1' 'Ba1F2'
'Ba1I2' 'Cl2Fe1' 'C1K1N1' 'Be1H2O2' 'Cs1' 'Al1H4Li1' 'C1Be2' 'Cr1'
'Cs2O4S1' 'Cl1Cu1' 'Cu1F2' 'Al2O3' 'B1N1' 'Co1O4S1' 'Cu1O1' 'Br1Na1'
'Cr2O3' 'Cs1F1' 'Cr2N1' 'Cl1Li1' 'Fe0.877S1' 'Cl1Na1' 'F2Hg1' 'Fe1H2O2'
'Cs1H1O1' 'Br3Mo1' 'Br2Sr1' 'Cl2Hg2' 'Fe1O1' 'Co1' 'Cl1Cs1' 'Cu1H2O2'
'Al1Li1O2' 'Co1F2' 'Br2Fe1' 'Fe1I2' 'Ga1' 'Cl1Li1O4' 'Cl2Cu1' 'Fe0.947O1'
'Be1Cl2' 'Cl1K1' 'F1Na1' 'H3O4P1' 'Fe3O4' 'H1Na1O1' 'Fe2O12S3' 'H1Na1'
'Cl1Na1O4' 'B1F4K1' 'Cu1O4S1' 'H1Li1' 'F2H1K1' 'B1H4Li1' 'Hg1O1' 'Be3N2'
'Fe1' 'I2Mo1' 'Cu1F1' 'Cr1N1' 'Fe1H3O3' 'I1Li1' 'Al1I3' 'Fe1S1'
'Al2Cl9K3' 'I2Pb1' 'I4Zr1' 'Hg1I2' 'H4I1N1' 'Hf1' 'F2Hg2' 'I2Sr1'
'C1K2O3' 'C1N1Na1' 'H2O4W1' 'Ca1S1' 'K2O4S1' 'I2Mg1' 'Mg1O3Si1' 'Li3N1'
'I2Zr1' 'H2Mg1' 'I2Ti1' 'H1K1' 'Mg1O4W1' 'I4Ti1' 'H1K1O1' 'I2' 'Mn1'
'F1K1' 'Li2O3Si1' 'K2O1' 'Mg1O4S1' 'Al1Na1O2' 'Mo1O2.889' 'Mo1O2.750'
'N0.465V1' 'Mg2O4Ti1' 'K1O2' 'Mo1O3' 'C1Na2O3' 'K2S1' 'Mo1S2' 'Li2O3Ti1'
'I4Mo1' 'Ba1S1' 'Na2O3Si1' 'I3Mo1' 'Mg1S1' 'Cu2O5S1' 'K2O2' 'Mg1O3Ti1'
'Na2S2' 'I3Ti1' 'Li2O2' 'I3Zr1' 'Al2Mg1O4' 'N1Ti1' 'N1V1' 'Na1O2' 'Ni1S1'
'Na2O1' 'I4Si1' 'B1Li1O2' 'O1Ti1' 'H1Li1O1' 'Nb1O1' 'F2Mg1' 'Nb1' 'O3Ti2'
'Ca1' 'Nb1O2' 'O3Pb1Si1' 'O4Pb3' 'O3W1' 'O7Ti4' 'K1' 'O4V2' 'O2.90W1'
'Ca1Cl2' 'Pb1' 'Na2O5Si2' 'O5Ti3' 'O5V2' 'Mg3N2' 'Mg2O4Si1' 'Mo1O2.875'
'Br1K1' 'Br2Mo1' 'Cl1H4N1' 'Cu1' 'F1Li1' 'Fe1S2' 'H2O2Sr1' 'I1K1' 'I1Na1'
'K2O3Si1' 'Li2O4S1' 'Li2O5Si2' 'Mg1' 'Mg2Si1' 'Mo2S3' 'N1Zr1' 'N2O4'
'N4Si3' 'N5P3' 'Na2O2' 'Na2S1' 'Nb2O5' 'Ni1' 'Ni1S2' 'Ni3S2' 'Ni3S4'
'O10P4' 'O1Pb1' 'O1Sr1' 'O1V1' 'O2.72W1' 'O2.96W1' 'O2Pb1' 'O2Si1'
'O2Ti1' 'O2Zr1' 'O3V2' 'O4Pb2Si1' 'O4S1Zn1' 'O4Si1Zr1' 'P1' 'P4S3'
'Pb1S1' 'Rb1' 'S1' 'S1Sr1' 'Sr1' 'Ti1' 'V1' 'W1' 'Zn1' 'Zr1']
```

```

In [8]: # Set a random seed to ensure reproducibility across runs
np.random.seed(seed=RNG_SEED)

# Store a list of all unique formulae
all_formulae = unique_formulae.copy()

# Define the proportional size of the dataset split
val_size = 0.20
test_size = 0.10
train_size = 1 - val_size - test_size

# Calculate the number of samples in each dataset split
num_val_samples = int(round(val_size * len(unique_formulae)))
num_test_samples = int(round(test_size * len(unique_formulae)))
num_train_samples = int(round((1 - val_size - test_size) * len(unique_formulae)))

# Randomly choose the formulae for the validation dataset, and remove those from the unique formulae list
val_formulae = np.random.choice(all_formulae, size=num_val_samples, replace=False)
all_formulae = [f for f in all_formulae if f not in val_formulae]

# Randomly choose the formulae for the test dataset, and remove those from the unique formulae list
test_formulae = np.random.choice(all_formulae, size=num_test_samples, replace=False)
all_formulae = [f for f in all_formulae if f not in test_formulae]

# The remaining formulae will be used for the training dataset
train_formulae = all_formulae.copy()

print('Number of training formulae:', len(train_formulae))
print('Number of validation formulae:', len(val_formulae))
print('Number of testing formulae:', len(test_formulae))

```

```

Number of training formulae: 171
Number of validation formulae: 49
Number of testing formulae: 24

```

```
In [9]: # Split the original dataset into the train/validation/test datasets using the
        formulae lists above
df_train = df[df['formula'].isin(train_formulae)]
df_val = df[df['formula'].isin(val_formulae)]
df_test = df[df['formula'].isin(test_formulae)]

print(f'train dataset shape: {df_train.shape}')
print(f'validation dataset shape: {df_val.shape}')
print(f'test dataset shape: {df_test.shape}\n')

print(df_train.head(), '\n')
print(df_val.head(), '\n')
print(df_test.head(), '\n')
```

```
train dataset shape: (3214, 3)
validation dataset shape: (980, 3)
test dataset shape: (370, 3)
```

	formula	T	Cp
0	B2O3	1400.0	134.306
1	B2O3	1300.0	131.294
2	B2O3	1200.0	128.072
3	B2O3	1100.0	124.516
4	B2O3	1000.0	120.625

	formula	T	Cp
82	B2Mg1	1900.0	92.242
83	B2Mg1	1800.0	90.249
84	B2Mg1	1700.0	88.162
85	B2Mg1	1600.0	85.981
86	B2Mg1	1500.0	83.643

	formula	T	Cp
192	Ba1H2O2	900.00	134.892
193	Ba1H2O2	800.00	130.834
194	Ba1H2O2	700.00	126.775
195	Ba1H2O2	681.15	126.022
196	Ba1H2O2	600.00	122.717

To be sure that we really only have mutually exclusive formulae within each of the datasets (e.g., all the data samples associated with "Al₂O₃" is *either* in the train, validation, or test dataset, but *not in multiple*), we can do the following to check:

```
In [10]: train_formulae = set(df_train['formula'].unique())
val_formulae = set(df_val['formula'].unique())
test_formulae = set(df_test['formula'].unique())

common_formulae1 = train_formulae.intersection(test_formulae)
common_formulae2 = train_formulae.intersection(val_formulae)
common_formulae3 = test_formulae.intersection(val_formulae)

print(f'# of common formulae in intersection 1: {len(common_formulae1)}; common formulae: {common_formulae1}')
print(f'# of common formulae in intersection 2: {len(common_formulae2)}; common formulae: {common_formulae2}')
print(f'# of common formulae in intersection 3: {len(common_formulae3)}; common formulae: {common_formulae3}')
```

```
# of common formulae in intersection 1: 0; common formulae: set()
# of common formulae in intersection 2: 0; common formulae: set()
# of common formulae in intersection 3: 0; common formulae: set()
```

Save split datasets to csv

Finally, after splitting the dataset into train/validation/test dataset splits, you can save them to disk for you to use later.

By saving these dataset splits into files, you can then later reproducibly use these same exact splits during your subsequent model training and comparison steps. Use the same datasets for all your models---that way, you can ensure a fair comparison.

Also, when you publish your results, you can include these dataset splits, so that others can use the exact datasets in their own studies.

```
In [11]: # saving these splits into csv files
PATH = os.getcwd()

train_path = os.path.join(PATH, '../data/cp_train.csv')
val_path = os.path.join(PATH, '../data/cp_val.csv')
test_path = os.path.join(PATH, '../data/cp_test.csv')

df_train.to_csv(train_path, index=False)
df_val.to_csv(val_path, index=False)
df_test.to_csv(test_path, index=False)
```

Remember, keep the test dataset locked away and forget about it until you have finalized your model! **Never look at the test dataset!!**

Data Featurization

Here, we will show some simple examples of featurizing materials composition data using so-called "composition-based feature vectors", or CBFVs. This method represents a single chemical formula as one vector based on its constituent atoms' chemical properties (refer to the paper for more information and references).

Note that the steps shown in this notebook are intended to demonstrate the best practices associated with featurizing materials data, using *one* way of featurizing materials composition data as an example. Depending on your input data and your particular modeling needs, the data featurization method and procedure you use may be different than the example shown here.

```
In [1]: import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
%config InlineBackend.figure_format='retina'

from collections import OrderedDict

# Set a random seed to ensure reproducibility across runs
RNG_SEED = 42
np.random.seed(RNG_SEED)
```

Loading data

We will start with the dataset splits that we saved from the last notebook.

```
In [2]: PATH = os.getcwd()
train_path = os.path.join(PATH, '../data/cp_train.csv')
val_path = os.path.join(PATH, '../data/cp_val.csv')
test_path = os.path.join(PATH, '../data/cp_test.csv')

df_train = pd.read_csv(train_path)
df_val = pd.read_csv(val_path)
df_test = pd.read_csv(test_path)

print(f'df_train DataFrame shape: {df_train.shape}')
print(f'df_val DataFrame shape: {df_val.shape}')
print(f'df_test DataFrame shape: {df_test.shape}')

df_train DataFrame shape: (3214, 3)
df_val DataFrame shape: (980, 3)
df_test DataFrame shape: (370, 3)
```

Sub-sampling your data (optional)

If your dataset is too large, you can subsample it to be a smaller size. This is useful for prototyping and for making quick sanity tests of new models / parameters.

Just be aware that you do not introduce any bias into your data through the sampling.

```
In [3]: # Sub-sample the data. Set the random_state to make the sampling reproducible
        # every time.
df_train_sampled = df_train.sample(n=2000, random_state=RNG_SEED)
df_val_sampled = df_val.sample(n=200, random_state=RNG_SEED)
df_test_sampled = df_test.sample(n=200, random_state=RNG_SEED)

print(f'df_train_sampled DataFrame shape: {df_train_sampled.shape}')
print(f'df_val_sampled DataFrame shape: {df_val_sampled.shape}')
print(f'df_test_sampled DataFrame shape: {df_test_sampled.shape}')

df_train_sampled DataFrame shape: (2000, 3)
df_val_sampled DataFrame shape: (200, 3)
df_test_sampled DataFrame shape: (200, 3)
```

Generate features using the CBFV package

To featurize the chemical compositions from a chemical formula (e.g. "Al2O3") into a composition-based feature vector (CBFV), we use the open-source [CBFV package \(https://github.com/kaaiian/CBFV\)](https://github.com/kaaiian/CBFV).

We have downloaded and saved a local copy of the package into this repository for your convenience. For the most updated version, refer to the GitHub repository linked above.

```
In [4]: # Import the package and the generate_features function
        from CBFV.cbfv.composition import generate_features
```

The `generate_features` function from the CBFV package expects an input DataFrame containing at least the columns `['formula', 'target']`. You may also have extra feature columns (e.g., `temperature` or `pressure`, other measurement conditions, etc.).

In our dataset, `Cp` represents the target variable, and `T` is the measurement condition. Since the `generate_features` function expects the target variable column to be named `target`, we have to rename the `Cp` column.


```
In [5]: print('DataFrame column names before renaming:')
print(df_train.columns)
print(df_val.columns)
print(df_test.columns)

rename_dict = {'Cp': 'target'}
df_train = df_train.rename(columns=rename_dict)
df_val = df_val.rename(columns=rename_dict)
df_test = df_test.rename(columns=rename_dict)

df_train_sampled = df_train_sampled.rename(columns=rename_dict)
df_val_sampled = df_val_sampled.rename(columns=rename_dict)
df_test_sampled = df_test_sampled.rename(columns=rename_dict)

print('\nDataFrame column names after renaming:')
print(df_train.columns)
print(df_val.columns)
print(df_test.columns)
```

```
DataFrame column names before renaming:
Index(['formula', 'T', 'Cp'], dtype='object')
Index(['formula', 'T', 'Cp'], dtype='object')
Index(['formula', 'T', 'Cp'], dtype='object')
```

```
DataFrame column names after renaming:
Index(['formula', 'T', 'target'], dtype='object')
Index(['formula', 'T', 'target'], dtype='object')
Index(['formula', 'T', 'target'], dtype='object')
```

Now we can use the `generate_features` function to generate the CBFVs from the input data.

Note that we have specified several keyword arguments in our call to `generate_features` :

- `elem_prop='oliynyk'`
- `drop_duplicates=False`
- `extend_features=True`
- `sum_feat=True`

A short explanation for the choice of keyword arguments is below:

- The `elem_prop` parameter specifies which CBFV featurization scheme to use (there are several). For this tutorial, we have chosen to use the `oliynyk` CBFV featurization scheme.
- The `drop_duplicates` parameter specifies whether to drop duplicate formulae during featurization. In our case, we want to preserve duplicate formulae in our data (`True`), since we have multiple heat capacity measurements (performed at different temperatures) for the same compound.
- The `extend_features` parameter specifies whether to include extended features (features that are not part of [`'formula'`, `'target'`]) in the featurized data. In our case, this is our measurement temperature, and we want to include this information (`True`), since this is pertinent information for the heat capacity prediction.
- The `sum_feat` parameter specifies whether to calculate the sum features when generating the CBFVs for the chemical formulae. We do in our case (`True`).

For more information about the `generate_features` function and the CBFV featurization scheme, refer to the GitHub repository and the accompanying paper to this notebook.


```
In [8]: X_train_unscaled.shape
```

```
Out[8]: (2000, 177)
```

Note the `sum` features in the CBFV, which we have included by using `sum_feat=True` in the call to `generate_features`.

Also note the temperature column `T` at the end of this featurized data.

What we have done above is featurize the input data. In the featurized data, each row contains a unique CBFV that describes a given chemical composition.

Data scaling & normalization

For numerical input data, scaling and normalization of the features often improves the model performance. Scaling can partially correct the discrepancy between the orders of magnitudes of the features (e.g., some numerical features being much larger or smaller than others). This typically improves the model learning performance, and in turn, improves the model performance.

We will scale then normalize our input data using scikit-learn's built-in `StandardScaler` class and `normalize` function.

Note, in addition to `StandardScaler`, other scalers such as `RobustScaler` and `MinMaxScaler` are also available in scikit-learn. Consult the documentation for the details and when to use them.

```
In [9]: from sklearn.preprocessing import StandardScaler
        from sklearn.preprocessing import normalize
```

Scaling the data

First, we instantiate the scaler object.

In a `StandardScaler` object:

- During the `fit` process, the statistics of the input data (mean and standard deviation) are computed.
- Then, during the `transform` process, the mean and standard deviation values calculated above are used to scale the data to having zero-mean and unit variance.

Therefore, for the first time usage of the scaler, we call the `.fit_transform()` method to fit the scaler to the input data, and then to transform the same data. For subsequent uses, since we have already computed the statistics, we only call the `.transform()` method to scale data.

Note: you should *only* `.fit()` the scaler using the training dataset statistics, and then use these same statistics from the training dataset to `.transform()` the other datasets (validation and train).

```
In [10]: scaler = StandardScaler()

X_train = scaler.fit_transform(X_train_unscaled)
X_val = scaler.transform(X_val_unscaled)
X_test = scaler.transform(X_test_unscaled)
```

Normalizing the scaled data

We repeat a similar process for normalizing the data. Here, there is no need to first fit the normalizer, since the normalizer scales the rows of the input data to unit norm independently of other rows.

The normalizer is different to a Scaler in that the normalizer acts row-wise, whereas a Scaler acts column-wise on the input data.

```
In [11]: X_train = normalize(X_train)
X_val = normalize(X_val)
X_test = normalize(X_test)
```

Modeling using "classical" machine learning models

Here we implement some classical ML models from `sklearn` :

- Ridge regression
- Support vector machine
- Linear support vector machine
- Random forest
- Extra trees
- Adaptive boosting
- Gradient boosting
- k-nearest neighbors
- Dummy (if you can't beat this, something is wrong.)

Note: the Dummy model types from `sklearn` act as a good sanity check for your ML studies. If your models do not perform significantly better than the equivalent Dummy models, then you should know that something has gone wrong in your model implementation.

```
In [12]: from time import time

from sklearn.dummy import DummyRegressor

from sklearn.linear_model import Ridge

from sklearn.ensemble import AdaBoostRegressor
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import ExtraTreesRegressor
from sklearn.ensemble import RandomForestRegressor

from sklearn.neighbors import KNeighborsRegressor

from sklearn.svm import SVR
from sklearn.svm import LinearSVR

from sklearn.metrics import r2_score
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error
```

In addition, we define some helper functions.

```

In [13]: def instantiate_model(model_name):
    model = model_name()
    return model

def fit_model(model, X_train, y_train):
    ti = time()
    model = instantiate_model(model)
    model.fit(X_train, y_train)
    fit_time = time() - ti
    return model, fit_time

def evaluate_model(model, X, y_act):
    y_pred = model.predict(X)
    r2 = r2_score(y_act, y_pred)
    mae = mean_absolute_error(y_act, y_pred)
    rmse_val = mean_squared_error(y_act, y_pred, squared=False)
    return r2, mae, rmse_val

def fit_evaluate_model(model, model_name, X_train, y_train, X_val, y_act_val):
    model, fit_time = fit_model(model, X_train, y_train)
    r2_train, mae_train, rmse_train = evaluate_model(model, X_train, y_train)
    r2_val, mae_val, rmse_val = evaluate_model(model, X_val, y_act_val)
    result_dict = {
        'model_name': model_name,
        'model_name_pretty': type(model).__name__,
        'model_params': model.get_params(),
        'fit_time': fit_time,
        'r2_train': r2_train,
        'mae_train': mae_train,
        'rmse_train': rmse_train,
        'r2_val': r2_val,
        'mae_val': mae_val,
        'rmse_val': rmse_val}
    return model, result_dict

def append_result_df(df, result_dict):
    df_result_appended = df.append(result_dict, ignore_index=True)
    return df_result_appended

def append_model_dict(dic, model_name, model):
    dic[model_name] = model
    return dic

```

Build an empty DataFrame to store model results:

[illegible]

Out[14]:

```
In [15]: # Build a dictionary of model names
         classic_model_names = OrderedDict({
             'dumr': DummyRegressor,
             'rr': Ridge,
             'abr': AdaBoostRegressor,
             'gbr': GradientBoostingRegressor,
             'rfr': RandomForestRegressor,
             'etr': ExtraTreesRegressor,
             'svr': SVR,
             'lsvr': LinearSVR,
             'knr': KNeighborsRegressor,
         })
```


Instantiate and fit the models

Now, we can fit the ML models.

We will loop through each of the models listed above. For each of the models, we will:

- instantiate the model (with default parameters)
- fit the model using the training data
- use the fitted model to generate predictions from the validation data
- evaluate the performance of the model using the predictions
- store the results in a DataFrame for analysis

Note: this may take several minutes, depending on your hardware/software environment, dataset size and featurization scheme (CBFV).

```
In [16]: # Instantiate a dictionary to store the model objects
         classic_models = OrderedDict()

         # Keep track of elapsed time
         ti = time()

         # Loop through each model type, fit and predict, and evaluate and store result
         s
         for model_name, model in classic_model_names.items():
             print(f'Now fitting and evaluating model {model_name}: {model.__name__}')
             model, result_dict = fit_evaluate_model(model, model_name, X_train, y_train, X_val, y_val)
             df_classics = append_result_df(df_classics, result_dict)
             classic_models = append_model_dict(classic_models, model_name, model)

         dt = time() - ti
         print(f'Finished fitting {len(classic_models)} models, total time: {dt:0.2f} s')
```

```
Now fitting and evaluating model dumr: DummyRegressor
Now fitting and evaluating model rr: Ridge
Now fitting and evaluating model abr: AdaBoostRegressor
Now fitting and evaluating model gbr: GradientBoostingRegressor
Now fitting and evaluating model rfr: RandomForestRegressor
Now fitting and evaluating model etr: ExtraTreesRegressor
Now fitting and evaluating model svr: SVR
Now fitting and evaluating model lsvr: LinearSVR
Now fitting and evaluating model knr: KNeighborsRegressor
Finished fitting 9 models, total time: 21.38 s
```

Now, we can look at the results.

You will notice, that some of the models (such as RandomForestRegressor, ExtraTreesRegressor and GradientBoostingRegressor) have completely memorized the training data, as evidenced by the very high `r2_train` scores of ~1.0.

```
In [17]: # Sort in order of increasing validation r2 score
df_classics = df_classics.sort_values('r2_val', ignore_index=True)
df_classics
```

Out[17]:

	model_name	model_name_pretty	model_params	fit_time	r2_train	mae_train	rmse_
0	dumr	DummyRegressor	{'constant': None, 'quantile': None, 'strategy': ...}	0.000000	0.000000	47.451805	60.60
1	lsvr	LinearSVR	{'C': 1.0, 'dual': True, 'epsilon': 0.0, 'fit_...	0.008975	0.763989	16.961421	29.44
2	svr	SVR	{'C': 1.0, 'cache_size': 200, 'coef0': 0.0, 'd...	0.653226	0.763306	16.726278	29.48
3	knr	KNeighborsRegressor	{'algorithm': 'auto', 'leaf_size': 30, 'metric...	0.046875	0.981784	3.902671	8.17
4	abr	AdaBoostRegressor	{'base_estimator': None, 'learning_rate': 1.0, ...}	1.740368	0.922253	14.174608	16.89
5	rr	Ridge	{'alpha': 1.0, 'copy_X': True, 'fit_intercept'...	0.027902	0.875762	14.425002	21.36
6	rfr	RandomForestRegressor	{'bootstrap': True, 'ccp_alpha': 0.0, 'criteri...	8.986937	0.998316	1.216542	2.48
7	etr	ExtraTreesRegressor	{'bootstrap': False, 'ccp_alpha': 0.0, 'criter...	4.108041	0.999995	0.010897	0.11
8	gbr	GradientBoostingRegressor	{'alpha': 0.9, 'ccp_alpha': 0.0, 'criterion': ...}	4.803637	0.985051	5.360182	7.40

You can now also access the full details of the models by inspecting the `classic_models` dictionary that we populated.

In [18]: classic_models

```

Out[18]: OrderedDict([('dumr',
                        DummyRegressor(constant=None, quantile=None, strategy='mean')),
                        ('rr',
                         Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=Non
e,
                                normalize=False, random_state=None, solver='auto', tol=0.
001)),
                        ('abr',
                         AdaBoostRegressor(base_estimator=None, learning_rate=1.0, loss
='linear',
                                           n_estimators=50, random_state=None)),
                        ('gbr',
                         GradientBoostingRegressor(alpha=0.9, ccp_alpha=0.0, criterion
='friedman_mse',
                                                    init=None, learning_rate=0.1, loss='l
s', max_depth=3,
                                                    max_features=None, max_leaf_nodes=Non
e,
                                                    min_impurity_decrease=0.0, min_impuri
ty_split=None,
                                                    min_samples_leaf=1, min_samples_split
=2,
                                                    min_weight_fraction_leaf=0.0, n_estim
ators=100,
                                                    n_iter_no_change=None, presort='depre
cated',
                                                    random_state=None, subsample=1.0, tol
=0.0001,
                                                    validation_fraction=0.1, verbose=0, w
arm_start=False)),
                        ('rfr',
                         RandomForestRegressor(bootstrap=True, ccp_alpha=0.0, criterion
='mse',
                                              max_depth=None, max_features='auto', max_
leaf_nodes=None,
                                              max_samples=None, min_impurity_decrease=
0.0,
                                              min_impurity_split=None, min_samples_leaf
=1,
                                              min_samples_split=2, min_weight_fraction_
leaf=0.0,
                                              n_estimators=100, n_jobs=None, oob_score=
False,
                                              random_state=None, verbose=0, warm_start=
False)),
                        ('etr',
                         ExtraTreesRegressor(bootstrap=False, ccp_alpha=0.0, criterion
='mse',
                                              max_depth=None, max_features='auto', max_le
af_nodes=None,
                                              max_samples=None, min_impurity_decrease=0.
0,
                                              min_impurity_split=None, min_samples_leaf=
1,
                                              min_samples_split=2, min_weight_fraction_le
af=0.0,
                                              n_estimators=100, n_jobs=None, oob_score=Fa

```

```

lse,
                                random_state=None, verbose=0, warm_start=Fa
lse)),
                                ('svr',
                                SVR(C=1.0, cache_size=200, coef0=0.0, degree=3, epsilon=0.1, ga
mma='scale',
                                kernel='rbf', max_iter=-1, shrinking=True, tol=0.001, verbo
se=False)),
                                ('lsvr',
                                LinearSVR(C=1.0, dual=True, epsilon=0.0, fit_intercept=True,
                                intercept_scaling=1.0, loss='epsilon_insensitive', ma
x_iter=1000,
                                random_state=None, tol=0.0001, verbose=0)),
                                ('knnr',
                                KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='min
kowski',
                                metric_params=None, n_jobs=None, n_neighbor
s=5, p=2,
                                weights='uniform'))))]]

```

Evaluating model performance on validation dataset

Now comes the time to evaluate the trained models on the validation set.

Remember, we use the same validation set to evaluate all models. This ensures a fair comparison.

In addition, we plot the predicted vs. actual plots using the predictions made by each trained model on the same validation set.

```

In [19]: def plot_pred_act(act, pred, model, reg_line=True, label=''):
            xy_max = np.max([np.max(act), np.max(pred)])

            plot = plt.figure(figsize=(6,6))
            plt.plot(act, pred, 'o', ms=9, mec='k', mfc='silver', alpha=0.4)
            plt.plot([0, xy_max], [0, xy_max], 'k--', label='ideal')
            if reg_line:
                polyfit = np.polyfit(act, pred, deg=1)
                reg_ys = np.poly1d(polyfit)(np.unique(act))
                plt.plot(np.unique(act), reg_ys, alpha=0.8, label='linear fit')
            plt.axis('scaled')
            plt.xlabel(f'Actual {label}')
            plt.ylabel(f'Predicted {label}')
            plt.title(f'{type(model).__name__}, r2: {r2_score(act, pred):0.4f}')
            plt.legend(loc='upper left')

            return plot

```

```
In [20]: for row in range(df_classics.shape[0]):
          model_name = df_classics.iloc[row]['model_name']

          model = classic_models[model_name]
          y_act_val = y_val
          y_pred_val = model.predict(X_val)

          plot = plot_pred_act(y_act_val, y_pred_val, model, reg_line=True, label=
'$\mathrm{C}_p$ (J / mol K)')
```

AdaBoostRegressor, r2: 0.8528

Ridge, r2: 0.8551

Re-training the best-performing model on combined train + validation dataset

After you have finalized your model, you can re-train your model (using the same hyperparameters) again on the combined train + validation datasets, and finally, evaluate your model on the held-out test dataset.

By training on the combined train + validation dataset after you have finished tuning your model, you give it more training data, which should lead to an increase in the model performance.

```
In [21]: # Find the best-performing model that we have tested
best_row = df_classics.iloc[-1, :].copy()

# Get the model type and model parameters
model_name = best_row['model_name']
model_params = best_row['model_params']

# Instantiate the model again using the parameters
model = classic_model_names[model_name](**model_params)
print(model)

GradientBoostingRegressor(alpha=0.9, ccp_alpha=0.0, criterion='friedman_mse',
                           init=None, learning_rate=0.1, loss='ls', max_depth=
3,
                           max_features=None, max_leaf_nodes=None,
                           min_impurity_decrease=0.0, min_impurity_split=None,
                           min_samples_leaf=1, min_samples_split=2,
                           min_weight_fraction_leaf=0.0, n_estimators=100,
                           n_iter_no_change=None, presort='deprecated',
                           random_state=None, subsample=1.0, tol=0.0001,
                           validation_fraction=0.1, verbose=0, warm_start=False)
e)
```

```
In [22]: # Concatenate the train and validation datasets together
X_train_new = np.concatenate((X_train, X_val), axis=0)
y_train_new = pd.concat((y_train, y_val), axis=0)

print(X_train_new.shape)

(2200, 177)
```

Finally, we can fit the model on the combined train + validation dataset.

```
In [23]: ti = time()

model.fit(X_train_new, y_train_new)

dt = time() - ti
print(f'Finished fitting best model, total time: {dt:0.2f} s')

Finished fitting best model, total time: 5.44 s
```

Testing the re-trained model on the test dataset

After re-fitting the best model on the train+validation dataset, you can finally test it on the test dataset.

Remember: you should only do this *once*!

```
In [24]: y_act_test = y_test
y_pred_test = model.predict(X_test)

r2, mae, rmse = evaluate_model(model, X_test, y_test)
print(f'r2: {r2:0.4f}')
print(f'mae: {mae:0.4f}')
print(f'rmse: {rmse:0.4f}')

plot = plot_pred_act(y_act_test, y_pred_test, model, reg_line=True, label='$\mathrm{C}_p$ (J / mol K)')

r2: 0.8442
mae: 17.1236
rmse: 31.0274
```

We see that our model achieves decent performance on the held-out test dataset.

Effect of train/validation/test dataset split

Using different train/validation/test splits can dramatically affect your model performance, even for classical ML models.

Here, we provide a little demonstration.


```

In [27]: splits = range(10)
df_splits = pd.DataFrame(columns=['split',
                                  'r2_train',
                                  'mae_train',
                                  'rmse_train',
                                  'r2_val',
                                  'mae_val',
                                  'rmse_val'])

for split in splits:
    print(f'Fitting and evaluating random split {split}')
    X_train = X_train_original.sample(frac=0.7, random_state=split)
    y_train = y_train_original[X_train.index]

    scaler = StandardScaler()
    X_train = normalize(scaler.fit_transform(X_train))
    X_val = normalize(scaler.transform(X_val_unscaled))
    X_test = normalize(scaler.transform(X_test_unscaled))

    model = AdaBoostRegressor()
    model.fit(X_train, y_train)
    y_act_val = y_val
    y_pred_val = model.predict(X_val)

    r2_train, mae_train, rmse_train = evaluate_model(model, X_train, y_train)
    r2_val, mae_val, rmse_val = evaluate_model(model, X_val, y_val)
    result_dict = {
        'split': split,
        'r2_train': r2_train,
        'mae_train': mae_train,
        'rmse_train': rmse_train,
        'r2_val': r2_val,
        'mae_val': mae_val,
        'rmse_val': rmse_val}

    df_splits = append_result_df(df_splits, result_dict)

```

```

Fitting and evaluating random split 0
Fitting and evaluating random split 1
Fitting and evaluating random split 2
Fitting and evaluating random split 3
Fitting and evaluating random split 4
Fitting and evaluating random split 5
Fitting and evaluating random split 6
Fitting and evaluating random split 7
Fitting and evaluating random split 8
Fitting and evaluating random split 9

```

```
In [28]: df_splits['split'] = df_splits['split'].astype(int)
df_splits
```

Out[28]:

	split	r2_train	mae_train	rmse_train	r2_val	mae_val	rmse_val
0	0	0.921647	14.237594	16.979393	0.815858	23.865538	34.461629
1	1	0.927656	13.501629	16.265329	0.808852	22.688912	35.111086
2	2	0.922515	14.448165	17.079006	0.817551	23.744004	34.302802
3	3	0.926511	13.651451	16.537507	0.831742	20.315320	32.941742
4	4	0.924336	13.983030	16.703454	0.822637	22.490512	33.821357
5	5	0.925542	13.714406	16.610536	0.811329	23.408679	34.882859
6	6	0.927083	13.872571	16.567055	0.818648	23.621438	34.199530
7	7	0.921361	14.275176	16.893382	0.823097	23.931573	33.777476
8	8	0.918063	14.508259	17.281824	0.824275	23.186429	33.664755
9	9	0.919256	14.204361	16.984472	0.824302	23.008472	33.662190

We then plot the train and validation r^2 scores for each of the 10 models.

Note the high variability in the $r2_val$ score. In contrast, the variability in the $r2_train$ score is comparatively lower.

```
In [29]: df_splits.plot('split', ['r2_train', 'r2_val'], kind='bar')
plt.title(f'Performance of {type(model).__name__}\nwith {len(splits)} differen
t data splits')
plt.ylim((0.5, 1.0))
plt.ylabel('$r^2$')
plt.xlabel('Split #')
plt.legend(loc='lower right', framealpha=0.9)
plt.show()
```

This effect is even more pronounced when we plot the mean absolute error (MAE).

```
In [30]: df_splits.plot('split', ['mae_train', 'mae_val'], kind='bar')
plt.title(f'Performance of {type(model).__name__}\nwith {len(splits)} different data splits')
plt.ylabel('MAE in  $C_p$  (J / mol K)')
plt.xlabel('Split #')
plt.legend(loc='lower right', framealpha=0.9)
plt.show()
```

Therefore, typically the average value of all the scores are reported, as this gives a much more accurate estimate of how well the model actually performs.

```
In [31]: avg_r2_val = df_splits['r2_val'].mean()
avg_mae_val = df_splits['mae_val'].mean()

print(f'Average validation r2: {avg_r2_val:0.4f}')
print(f'Average validation MAE: {avg_mae_val:0.4f}')
```

```
Average validation r2: 0.8198
Average validation MAE: 23.0261
```

Modeling using neural network / deep learning-based models

In this notebook, we will cover how to implement a simple neural network for the modeling of heat capacity.

We will load, prepare featurize, and scale/normalize the input datasets the same way as we did in the pervious notebook. For more information about the individual steps, you can consult that notebook.

```
In [1]: import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
%config InlineBackend.figure_format='retina'

from collections import OrderedDict

from CBFV.cbfv.composition import generate_features

from sklearn.preprocessing import RobustScaler
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import normalize

from sklearn.metrics import r2_score
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error

import torch
from torch import nn
from torch.utils.data import Dataset, DataLoader

import torch.optim as optim

# Set a random seed to ensure reproducibility across runs
RNG_SEED = 42
np.random.seed(RNG_SEED)
torch.manual_seed(RNG_SEED)
```

```
Out[1]: <torch._C.Generator at 0x24e8007e510>
```

Featurizing and scaling data

Nothing new here---same steps as we've done in the previous notebook.

```
In [2]: PATH = os.getcwd()
train_path = os.path.join(PATH, '../data/cp_train.csv')
val_path = os.path.join(PATH, '../data/cp_val.csv')
test_path = os.path.join(PATH, '../data/cp_test.csv')

df_train = pd.read_csv(train_path)
df_val = pd.read_csv(val_path)
df_test = pd.read_csv(test_path)

print(f'df_train DataFrame shape: {df_train.shape}')
print(f'df_val DataFrame shape: {df_val.shape}')
print(f'df_test DataFrame shape: {df_test.shape}')

df_train DataFrame shape: (3214, 3)
df_val DataFrame shape: (980, 3)
df_test DataFrame shape: (370, 3)
```

Here we do not sub-sample the datasets into smaller datasets like we did in the previous notebook. Typically, the more data you have for neural networks, the better the networks will be able to train, and the better they will perform (as long as they are well-conditioned).

Additionally, the performance of PyTorch is very good for modern computers, especially if you have a modern CUDA-capable graphics processing unit (GPU) such as an Nvidia GPU to accelerate the computations. Our dataset is small enough to fit into almost all modern computers or CUDA-capable GPUs.

```
In [3]: rename_dict = {'Cp': 'target'}
df_train = df_train.rename(columns=rename_dict)
df_val = df_val.rename(columns=rename_dict)
df_test = df_test.rename(columns=rename_dict)

X_train_unscaled, y_train, formulae_train, skipped_train = generate_features(df_train, elem_prop='oliynyk', drop_duplicates=False, extend_features=True, sum_feat=True)
X_val_unscaled, y_val, formulae_val, skipped_val = generate_features(df_val, elem_prop='oliynyk', drop_duplicates=False, extend_features=True, sum_feat=True)
X_test_unscaled, y_test, formulae_test, skipped_test = generate_features(df_test, elem_prop='oliynyk', drop_duplicates=False, extend_features=True, sum_feat=True)
```

```
Processing Input Data: 100% ██████████  
██████| 3214/3214 [00:00<00:00, 28074.71it/s]  
Assigning Features...:   0%|  
| 0/3214 [00:00<?, ?it/s]
```

Featurizing Compositions...

[illegible]

Creating Pandas Objects...

```
Processing Input Data: 100%|██████████|  
██████████| 980/980 [00:00<00:00, 28050.95it/s]  
Assigning Features...: 100%|██████████|  
██████████| 980/980 [00:00<00:00, 23381.48it/s]  
Processing Input Data: 100%|██████████|  
██████████| 370/370 [00:00<00:00, 28536.88it/s]
```

Featurizing Compositions...

Creating Pandas Objects...

```
Assigning Features...: 100%|██████████████████████████████████████  
██████████ | 370/370 [00:00<00:00, 21791.04it/s]
```

Featurizing Compositions...

Creating Pandas Objects...

```
In [4]: X_train_unscaled.head()
```

Out[4]:

	sum_Atomic_Number	sum_Atomic_Weight	sum_Period	sum_group	sum_families	sum_Metal
0	34.0	69.6202	10.0	74.0	33.0	0.0
1	34.0	69.6202	10.0	74.0	33.0	0.0
2	34.0	69.6202	10.0	74.0	33.0	0.0
3	34.0	69.6202	10.0	74.0	33.0	0.0
4	34.0	69.6202	10.0	74.0	33.0	0.0

5 rows × 177 columns

```
In [5]: scaler = StandardScaler()

X_train = scaler.fit_transform(X_train_unscaled)
X_val = scaler.transform(X_val_unscaled)
X_test = scaler.transform(X_test_unscaled)

X_train = normalize(X_train)
X_val = normalize(X_val)
X_test = normalize(X_test)
```

Building a neural network

This is where you get to be the architect, and design your own neural network!

For sake of clarity (and to ensure that this tutorial runs on all the potatoes of this world), we will define a simple dense fully-connected neural network (which we will call `DenseNet`) as an example.

The input layer of `DenseNet` accepts input data in the dimension of each row of the input data, which is equal to the number of features in our CBFV featurization scheme. In our particular example, when featurized using the `oliynyk` featurizer, the input dimension is 177 (it is the second dimension when you view `X_train.shape`).

The output layer dimension of `DenseNet` is 1, because we want to predict one value (heat capacity).

In addition, `DenseNet` can have one or more "hidden layers" that are attached between the input and output layers. These can be any arbitrary dimensions > 1 you want to choose.

Defining the network in PyTorch

```

In [6]: class DenseNet(nn.Module):
        """
        This implements a dynamically-built dense fully-connected neural network
        with Leaky ReLU activation and optional dropout.

        Parameters
        -----
        input_dims: int
            Number of input features (required).
        hidden_dims: list of ints
            Number of hidden features, where each integer represents the number of
            hidden features in each subsequent hidden linear layer (optional,
            default=[64, 32]).
        output_dims: int
            Number of output features (optional, default=1).
        dropout: float
            the dropout value (optional, default=0.0).
        """
        def __init__(self,
                      input_dims,
                      hidden_dims=[64, 32],
                      output_dims=1,
                      dropout=0.0):
            super().__init__()

            self.input_dims = input_dims
            self.hidden_dims = hidden_dims
            self.output_dims = output_dims

            self.dropout = dropout

            # Build a sub-block of linear networks
            def fc_block(in_dim, out_dim, *args, **kwargs):
                return nn.Sequential(
                    nn.Linear(in_dim, out_dim, *args, **kwargs),
                    nn.Dropout(p=self.dropout),
                    nn.LeakyReLU()
                )

            # Build overall network architecture
            self.network = nn.ModuleList([
                nn.Sequential(
                    nn.Linear(input_dims, self.hidden_dims[0]),
                    nn.Dropout(p=self.dropout),
                    nn.LeakyReLU()
                )
            ])

            hidden_layer_sizes = zip(self.hidden_dims[:-1], self.hidden_dims[1:])
            self.network.extend([
                fc_block(in_dim, out_dim) for in_dim, out_dim
                in hidden_layer_sizes
            ])

            self.network.extend([
                nn.Linear(hidden_dims[-1], output_dims)
            ])

```

```

    )

def forward(self, x):
    """
    Forward pass of the DenseNet model.

    Parameters
    -----
    x: torch.Tensor
        A representation of the chemical compounds in the shape
        (n_compounds, n_feats).

    Returns
    -----
    y: torch.Tensor
        The element property prediction with the shape 1.
    """
    for i, subnet in enumerate(self.network):
        x = subnet(x)

    y = x

    return y

```

Specifying the compute device for calculations

Before we run the neural network, we can first check if your machine has a CUDA-capable device. CUDA is a specific set of application instructions (application programming interfaces, APIs) that PyTorch can use to accelerate some of the calculations performed in neural networks.

Generally, a relatively recent GPU from Nvidia will support CUDA capabilities, and can be used to accelerate neural network computations in PyTorch.

In case you do not have a CUDA-capable device, PyTorch will fall back to using the CPU. Depending on the complexity of your model, training and predicting using a CPU can take significantly longer than using a CUDA-capable GPU.

Consult the [PyTorch \(https://pytorch.org/docs/stable/torch.html\)](https://pytorch.org/docs/stable/torch.html) and [CUDA \(https://docs.nvidia.com/cuda/\)](https://docs.nvidia.com/cuda/) documentation for more information.

```
In [7]: CUDA_available = torch.cuda.is_available()
print(f'CUDA is available: {CUDA_available}')

if CUDA_available:
    compute_device = torch.device('cuda')
else:
    compute_device = torch.device('cpu')

print(f'Compute device for PyTorch: {compute_device}')
```

```
CUDA is available: True
Compute device for PyTorch: cuda
```

Defining the data loader and dataset structure

Here we define a dataloader class specific for loading CBFV-type datasets.

We also define the CBFV dataset class that tells PyTorch how our dataset is structured, and how to grab individual data samples from our dataset.


```

In [8]: class CBFVDataLoader():
        """
        Parameters
        -----
        train_data: np.ndarray or pd.DataFrame or pd.Series
            name of csv file containing cif and properties
        val_data: np.ndarray or pd.DataFrame or pd.Series
            name of csv file containing cif and properties
        test_data: np.ndarray or pd.DataFrame or pd.Series
            name of csv file containing cif and properties
        batch_size: float, optional (default=64)
            Step size for the Gaussian filter
        random_state: int, optional (default=42)
            Random seed for sampling the dataset. Only used if validation data is
            not given.
        shuffle: bool, optional (default=True)
            Whether to shuffle the datasets or not
        """
        def __init__(self, train_data, val_data, test_data,
                      batch_size=64, num_workers=1, random_state=42,
                      shuffle=True, pin_memory=True):

            self.train_data = train_data
            self.val_data = val_data
            self.test_data = test_data

            self.batch_size = batch_size
            self.num_workers = num_workers
            self.pin_memory = pin_memory

            self.shuffle = shuffle
            self.random_state = random_state

        def get_data_loaders(self, batch_size=1):
            """
            Input the dataset, get train test split
            """
            train_dataset = CBFVDataset(self.train_data)
            val_dataset = CBFVDataset(self.val_data)
            test_dataset = CBFVDataset(self.test_data)

            train_loader = DataLoader(train_dataset,
                                     batch_size=self.batch_size,
                                     pin_memory=self.pin_memory,
                                     shuffle=self.shuffle)

            val_loader = DataLoader(val_dataset,
                                   batch_size=self.batch_size,
                                   pin_memory=self.pin_memory,
                                   shuffle=self.shuffle)

            test_loader = DataLoader(test_dataset,
                                    batch_size=self.batch_size,
                                    pin_memory=self.pin_memory,
                                    shuffle=False)

```

```

        return train_loader, val_loader, test_loader

class CBFVDataset(Dataset):
    """
    Get X and y from CBFV-based dataset.
    """
    def __init__(self, dataset):
        self.data = dataset

        self.X = np.array(self.data[0])
        self.y = np.array(self.data[1])
        self.shape = [(self.X.shape), (self.y.shape)]

    def __str__(self):
        string = f'CBFVDataset with X.shape {self.X.shape}'
        return string

    def __len__(self):
        return self.X.shape[0]

    def __getitem__(self, idx):
        X = self.X[[idx], :]
        y = self.y[idx]

        X = torch.as_tensor(X)
        y = torch.as_tensor(np.array(y))

        return (X, y)

```

Here we choose a batch size for loading data, and initialize the DataLoader for loading the featurized input data.

We also get the data loaders corresponding to the train, validation, and test datasets.

```

In [9]: train_data = (X_train, y_train)
        val_data = (X_val, y_val)
        test_data = (X_test, y_test)

        # Instantiate the DataLoader
        batch_size = 128
        data_loaders = CBFVDataLoader(train_data, val_data, test_data, batch_size=batch_size)
        train_loader, val_loader, test_loader = data_loaders.get_data_loaders()

```

Instantiating a DenseNet model

Now, we can instantiate... an instance of the DenseNet model.

```
In [10]: # Get input dimension size from the dataset
example_data = train_loader.dataset.data[0]
input_dims = example_data.shape[-1]

# Instantiate the model
model = DenseNet(input_dims, hidden_dims=[16], dropout=0.0)
print(model)

DenseNet(
  (network): ModuleList(
    (0): Sequential(
      (0): Linear(in_features=177, out_features=16, bias=True)
      (1): Dropout(p=0.0, inplace=False)
      (2): LeakyReLU(negative_slope=0.01)
    )
    (1): Linear(in_features=16, out_features=1, bias=True)
  )
)
```

Defining the loss criterion & optimizer

Here, we see the model and its individual layers and components printed nicely.

We then instantiate and initialize the loss criterion and optimizer.

Note, there are many choices of loss criteria and optimizers that are provided by PyTorch, each with their benefits and limitations, and a myriad of parameters. Consult the PyTorch documentation for further details.

```
In [11]: # Initialize the loss criterion
criterion = nn.L1Loss()
print('Loss criterion: ')
print(criterion)

# Initialize the optimizer
optim_lr = 1e-2
optimizer = optim.Adam(model.parameters(), lr=optim_lr)
print('\nOptimizer: ')
print(optimizer)
```

```
Loss criterion:
L1Loss()
```

```
Optimizer:
Adam (
  Parameter Group 0
    amsgrad: False
    betas: (0.9, 0.999)
    eps: 1e-08
    lr: 0.01
    weight_decay: 0
)
```

Moving the model to the compute device

Then, we can move the model and loss criterion computation to the compute device.

If you have a GPU, this will transfer and attach the required resources to the GPU. If you have a CPU, then everything will remain on the CPU.

```
In [12]: # Move the model and criterion to the compute device
         model = model.to(compute_device)
         criterion = criterion.to(compute_device)
```

Defining some additional helper functions

We define some scalar functions and helper functions to evaluate and visualize model results.

```
In [13]: class Scaler():
    def __init__(self, data):
        self.data = torch.as_tensor(data)
        self.mean = torch.mean(self.data)
        self.std = torch.std(self.data)

    def scale(self, data):
        data = torch.as_tensor(data)
        data_scaled = (data - self.mean) / self.std
        return data_scaled

    def unscale(self, data_scaled):
        data_scaled = torch.as_tensor(data_scaled)
        data = data_scaled * self.std + self.mean
        return data

    def state_dict(self):
        return {'mean': self.mean,
                'std': self.std}

    def load_state_dict(self, state_dict):
        self.mean = state_dict['mean']
        self.std = state_dict['std']

class MeanLogNormScaler():
    def __init__(self, data):
        self.data = torch.as_tensor(data)
        self.logdata = torch.log(self.data)
        self.mean = torch.mean(self.logdata)
        self.std = torch.std(self.logdata)

    def scale(self, data):
        data = torch.as_tensor(data)
        data_scaled = (torch.log(data) - self.mean) / self.std
        return data_scaled

    def unscale(self, data_scaled):
        data_scaled = torch.as_tensor(data_scaled) * self.std + self.mean
        data = torch.exp(data_scaled)
        return data

    def state_dict(self):
        return {'mean': self.mean,
                'std': self.std}

    def load_state_dict(self, state_dict):
        self.mean = state_dict['mean']
        self.std = state_dict['std']
```

```

In [14]: def predict(model, data_loader):
    target_list = []
    pred_list = []

    model.eval()
    with torch.no_grad():
        for i, data_output in enumerate(data_loader):
            X, y_act = data_output
            X = X.to(compute_device,
                      dtype=data_type,
                      non_blocking=True)
            y_act = y_act.cpu().flatten().tolist()
            y_pred = model.forward(X).cpu().flatten().tolist()

            # Unscale target values
            y_pred = target_scaler.unscale(y_pred).tolist()

            targets = y_act
            predictions = y_pred
            target_list.extend(targets)
            pred_list.extend(predictions)
    model.train()

    return target_list, pred_list

def evaluate(target, pred):
    r2 = r2_score(target, pred)
    mae = mean_absolute_error(target, pred)
    rmse = mean_squared_error(target, pred, squared=False)
    output = (r2, mae, rmse)
    return output

def print_scores(scores, label=''):
    r2, mae, rmse = scores
    print(f'{label} r2: {r2:0.4f}')
    print(f'{label} mae: {mae:0.4f}')
    print(f'{label} rmse: {rmse:0.4f}')
    return scores

def plot_pred_act(act, pred, model, reg_line=True, label=''):
    xy_max = np.max([np.max(act), np.max(pred)])

    plot = plt.figure(figsize=(6,6))
    plt.plot(act, pred, 'o', ms=9, mec='k', mfc='silver', alpha=0.4)
    plt.plot([0, xy_max], [0, xy_max], 'k--', label='ideal')
    if reg_line:
        polyfit = np.polyfit(act, pred, deg=1)
        reg_ys = np.poly1d(polyfit)(np.unique(act))
        plt.plot(np.unique(act), reg_ys, alpha=0.8, label='linear fit')
    plt.axis('scaled')
    plt.xlabel(f'Actual {label}')
    plt.ylabel(f'Predicted {label}')
    plt.title(f'{type(model).__name__}, r2: {r2_score(act, pred):0.4f}')

```

```
plt.legend(loc='upper left')

return plot
```

We scale the target variables.

```
In [15]: y_train = [data[1].numpy().tolist() for data in train_loader]
y_train = [item for sublist in y_train for item in sublist]

y_train = train_loader.dataset.y

target_scaler = MeanLogNormScaler(y_train)
```

Training the neural network

And finally, we train the neural network.

This is the training procedure for the neural network:

- for each epoch :
 - iterate through the train dataset using `train_loader` :
 - scale the target data
 - transfer input (`X`) and target (`y`) data to compute device
 - reset the optimizer's gradient to zero
 - compute the output of the model (forward pass)
 - calculate the loss of the model (between the predicted and true target values)
 - propagate the loss backwards through the model (backpropagation)
 - update the weights throughout the model
 - if `epoch == print_every` :
 - print the current epoch (to keep track of training progress)
 - if `epoch == plot_every` :
 - evaluate the model on the validation dataset using `val_loader`
 - plot predicted vs. actual value plots
 - print the train and val r^2 , MAE and RMSE scores of the model

Note: training this network may take up to tens of minutes, depending on your hardware configuration and whether or not you have a CUDA-capable device.

```

In [16]: data_type = torch.float
         epochs = 500

         print_every = 20
         plot_every = 50

         for epoch in range(epochs):
             if epoch % print_every == 0 or epoch == epochs - 1:
                 print(f'epoch: {epoch}')
             if epoch % plot_every == 0:
                 target_train, pred_train = predict(model, train_loader)
                 train_scores = evaluate(target_train, pred_train)
                 print_scores(train_scores, label='train')

                 target_val, pred_val = predict(model, val_loader)
                 val_scores = evaluate(target_val, pred_val)
                 print_scores(val_scores, label='val')
                 plot_pred_act(target_val, pred_val, model, label='$\mathrm{C}_\mathrm{p}$ / mol K')
                 plt.show()

             for i, data_output in enumerate(train_loader):
                 X, y = data_output
                 y = target_scaler.scale(y)

                 X = X.to(compute_device,
                           dtype=data_type,
                           non_blocking=True)
                 y = y.to(compute_device,
                           dtype=data_type,
                           non_blocking=True)

                 optimizer.zero_grad()
                 output = model.forward(X).flatten()
                 loss = criterion(output.view(-1), y.view(-1))
                 loss.backward()
                 optimizer.step()

```


epoch: 0
train r2: -0.1487
train mae: 46.4704
train rmse: 64.9909
val r2: -0.0830
val mae: 52.6671
val rmse: 83.5762

epoch: 20
epoch: 40
train r2: 0.9813
train mae: 4.3085
train rmse: 8.2817
val r2: 0.8492
val mae: 16.8082
val rmse: 31.1895

epoch: 60
epoch: 80
epoch: 100
train r2: 0.9833
train mae: 3.9003
train rmse: 7.8337
val r2: 0.8583
val mae: 16.2121
val rmse: 30.2252

epoch: 120
epoch: 140
train r2: 0.9840
train mae: 3.6218
train rmse: 7.6821
val r2: 0.8673
val mae: 15.5079
val rmse: 29.2527

epoch: 160
epoch: 180
epoch: 200
train r2: 0.9866
train mae: 3.1012
train rmse: 7.0212
val r2: 0.8663
val mae: 15.8610
val rmse: 29.3698

epoch: 220
epoch: 240
train r2: 0.9861
train mae: 3.4834
train rmse: 7.1619
val r2: 0.8756
val mae: 15.2939
val rmse: 28.3246

epoch: 260
epoch: 280
epoch: 300
train r2: 0.9872
train mae: 3.0628
train rmse: 6.8711
val r2: 0.8720
val mae: 15.8923
val rmse: 28.7362

epoch: 320
epoch: 340
train r2: 0.9874
train mae: 3.0447
train rmse: 6.8130
val r2: 0.8812
val mae: 15.2294
val rmse: 27.6838

epoch: 360
epoch: 380
epoch: 400
train r2: 0.9872
train mae: 3.2069
train rmse: 6.8730
val r2: 0.8833
val mae: 15.1164
val rmse: 27.4352

epoch: 420
epoch: 440
train r2: 0.9878
train mae: 2.9436
train rmse: 6.7003
val r2: 0.8823
val mae: 15.3402
val rmse: 27.5488

epoch: 460
epoch: 480
epoch: 499

Now, with our trained neural network, we can evaluate the performance of the model (at the end of the training phase) on the validation dataset.

```
In [17]: target_val, pred_val = predict(model, val_loader)
scores = evaluate(target_val, pred_val)

print_scores(scores, label='val')

plot = plot_pred_act(target_val, pred_val, model, label='$\mathrm{C}_p$ $\mathrm{p}$ (J / mol K)')
```

```
val r2: 0.8833
val mae: 15.3854
val rmse: 27.4286
```

Keeping track of training progress -- avoid overfitting

Note, you can keep track of the training progress by saving the train and validation metrics such as r^2 and MAE at every epoch. Then, you can plot so-called "loss curves" that show the loss of the model vs. epoch throughout the training process. This gives you additional insight into your model training process, and helps you diagnose issues such as overfitting, improper model/optimizer/loss parameters, and so on.

Once you start tracking these performance metrics during your training loop, you can also implement more advanced training techniques such as "early stopping". In early stopping, you observe the performance metrics (such as validation r^2 or MAE) over the training epochs, and you stop the training process if you observe that the metrics are not improving any more (meaning your model is fully trained), or if the metrics are increasing again after reaching a minimum (meaning your model is overfitting the training set).

Evaluating model performance on test dataset

And finally evaluate the performance on the test dataset. **Remember:** you should only do this *once*!


```
In [18]: target_test, pred_test = predict(model, test_loader)
scores = evaluate(target_test, pred_test)

print_scores(scores, label='test')

plot = plot_pred_act(target_test, pred_test, model, label=' $\mathrm{C}_p$  (J / mol K)')
```

test r2: 0.8899
test mae: 14.2758
test rmse: 25.8626

Exporting PyTorch models

Now that we've got a (reasonably well-performing) model, we can export the weights and biases from the model to what is referred to as a "checkpoint" file.

The advantages of exporting your model to a checkpoint file are manifold. For example, when you want to re-use the model again later (to make further predictions, or even to continue training), you don't have to train the model from scratch again. For our current `DenseNet` model, this may not seem like a big deal, since it trains within minutes. But once you start moving on to larger and larger models, model training time can reach hours, days---even weeks!

Another advantage is that you can greatly enhance the reproducibility of your work. If you export your models, other researchers can then recreate your model architecture on their system, then load your weights into the model to get exactly the model you trained. This allows them to use your model as-is, and enables them to reproduce your work---an important step if they are to judge the merit of your work.

With that said, we will now use PyTorch's built-in methods to export (1) our `DenseNet` model, and (2) our `target_scaler` (we need to export our `target_scaler` object as well, because we need to use it to unscale the model predictions to get back the true prediction values).

Saving the model + target scaler

```
In [19]: save_dict = {'weights': model.state_dict(),
                    'scaler_state': target_scaler.state_dict()}
print(save_dict)

{'weights': OrderedDict([('network.0.0.weight', tensor([[ 0.7553,  0.9386,
 0.3842, ...,  0.0225,  0.4568,  2.6430],
 [ 0.2389,  0.2387,  0.1926, ..., -0.3318,  0.0269,  3.4188],
 [-1.3899, -1.3630, -0.7993, ...,  1.0238,  0.6904, -3.7036],
 ...,
 [-0.8147, -0.8653, -0.6919, ...,  1.1902,  1.1137, -2.3598],
 [ 0.4363,  0.4713,  0.2978, ..., -1.2085, -0.8724,  1.3804],
 [ 0.2154,  0.4221, -0.0204, ..., -0.4609, -0.0218,  2.9495]],
 device='cuda:0')), ('network.0.0.bias', tensor([-2.3551e-01, -1.4669e-
01,  1.0728e-02,  1.2264e-01, -5.2010e-01,
 -5.2636e-01, -1.8640e-01, -2.3231e-01, -1.4808e-01,  4.8181e-02,
 3.2689e-01, -8.2749e-02, -5.8574e-01, -1.0106e-01,  1.7105e-01,
 -8.1883e-06], device='cuda:0')), ('network.1.weight', tensor([[ 0.227
2,  0.1508, -0.1535,  0.0698, -0.5781, -0.6211,  0.2401,  0.0881,
 0.2408, -0.1805, -0.2659,  0.2306, -0.3568, -0.1981,  0.1904,  0.14
82]],
 device='cuda:0')), ('network.1.bias', tensor([-0.0122], device='cuda:
0')))], 'scaler_state': {'mean': tensor(4.5152, dtype=torch.float64), 'std':
tensor(0.5749, dtype=torch.float64)}}
```

```
In [20]: pth_path = ('model_checkpoint.pth') # .pth is commonly used as the file extension
         torch.save(save_dict, pth_path)
```

Navigate to your notebooks directory. You should now find a file named 'model_checkpoint.pth'. Since the DenseNet model is small, the checkpoint file weighs in relatively lightly at 13KB. Bigger models will have more weights & biases, and will require more storage space for the checkpoint file.

Loading the model + target scaler

Of course, if you provide the facilities to **save** a model, you should also provide facilities to **load** them and to recreate your model back.

Thankfully, PyTorch makes this also easy.

```
In [21]: # First, clear the variables for model and target_scaler.
         # We want to start with a clean slate.
         model = None
         target_scaler = None
         del model
         del target_scaler
```

We start by recreating the DenseNet model and the target_scaler that we originally built. This model will be initialized with random weights & biases, which we will then overload (overwrite) afterwards with the values from the checkpoint file.

Make sure that you create the same model and target_scaler here as the ones you saved the checkpoint file from. Otherwise you will not be able to load the checkpoint file, or it will produce unexpected results.

```
In [22]: # Instantiate the model.
# The model will be randomly initialized, but we will overwrite
# all weights and biases when we load the checkpoint.
model = DenseNet(input_dims, hidden_dims=[16], dropout=0.0)
model = model.to(compute_device)
print(model)

# Instantiate the target_scaler.
# We initialize this target_scaler with a vector of zeros,
# but we will overwrite its internal parameters
# when we load the checkpoint.
target_scaler = MeanLogNormScaler(torch.zeros(42))
```

```
DenseNet(
  (network): ModuleList(
    (0): Sequential(
      (0): Linear(in_features=177, out_features=16, bias=True)
      (1): Dropout(p=0.0, inplace=False)
      (2): LeakyReLU(negative_slope=0.01)
    )
    (1): Linear(in_features=16, out_features=1, bias=True)
  )
)
```

```
In [23]: # Load the checkpoint and map it to the compute device
pth_path = ('model_checkpoint.pth')
checkpoint = torch.load(pth_path, map_location=compute_device)

# Load the state dictionaries back into the model and target_scaler
model.load_state_dict(checkpoint['weights'])
target_scaler.load_state_dict(checkpoint['scaler_state'])
```

Checking the loaded model

```
In [24]: target_test, pred_test = predict(model, test_loader)
scores = evaluate(target_test, pred_test)

print_scores(scores, label='test')

plot = plot_pred_act(target_test, pred_test, model, label=' $\mathrm{C}_p$  (J / mol K)')
```

test r2: 0.8899
test mae: 14.2758
test rmse: 25.8626

Hooray!

Visualizing results

Here, we will show some typical examples of visualizations that are used often to show results in ML studies in materials science.

We will use the open-source `ML_figures` [package \(https://github.com/kaaiian/ML_figures\)](https://github.com/kaaiian/ML_figures) and the example data provided by the package to generate these figures.

```
In [1]: import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
%config InlineBackend.figure_format='retina'

# Import the ML_figures package and the figure-plotting functions
from ML_figures.figures import act_pred
from ML_figures.figures import residual, residual_hist
from ML_figures.figures import loss_curve
from ML_figures.figures import element_prevalence
```

Predicted vs. actual value plots

These plots, you have already seen before in the previous notebooks.

```
In [2]: # Read in example act vs. pred data
df_act_pred = pd.read_csv('ML_figures/example_data/act_pred.csv')
y_act, y_pred = df_act_pred.iloc[:, 1], df_act_pred.iloc[:, 2]

act_pred(y_act, y_pred,
         reg_line=True,
         save_dir='ML_figures/example_figures')

act_pred(y_act, y_pred,
         name='example_no_hist',
         x_hist=False, y_hist=False,
         reg_line=True,
         save_dir='ML_figures/example_figures')
```

Residual error plots

Residual error plots show how far your model's predictions deviate from the actual values. They are using the same data used in the predicted vs. actual plots; however, instead of plotting predicted vs. actual values, residual error plots plot (predicted - actual) vs. actual values.

This lets you visually analyze your model's prediction error on a straight horizontal line.

Alternatively, you can plot the residual errors on a histogram, and optionally with a kernel density estimation (kde).

```
In [3]: residual(y_act, y_pred,  
               save_dir='ML_figures/example_figures')  
  
residual_hist(y_act, y_pred,  
             save_dir='ML_figures/example_figures')
```

Loss curves

Loss curves show the loss of a neural network model vs. epoch throughout the training process. It is typically evaluated using the training and validation dataset at the end of each epoch (or every n epochs, where n is a small number, if evaluating every epoch takes too many resources).

Typically, loss curves plot the model performance (such as r^2 score) or loss (such as MAE) against epoch.

```
In [4]: # Read in loss curve data
df_lc = pd.read_csv('ML_figures/example_data/training_progress.csv')
epoch = df_lc['epoch']
train_err, val_err = df_lc['mae_train'], df_lc['mae_val']

loss_curve(epoch, train_err, val_err,
            save_dir='ML_figures/example_figures')
```

Visualizing elemental prevalence

Depending on your dataset, what you are studying, and how the compounds/constituent elements of the compounds in the dataset are distributed, it may be useful to visualize the elemental prevalence in your dataset.

These figures let you visualize the relative amount of certain elements vs. other elements present in your dataset, and can help you in identifying dataset biases, imbalanced datasets, or other issues.

```
In [5]: # Visualize element prevalence
formula = df_act_pred.iloc[:, 0]

element_prevalence(formula,
                    save_dir='ML_figures/example_figures',
                    log_scale=False)
element_prevalence(formula,
                    save_dir='ML_figures/example_figures',
                    name='example_log',
                    log_scale=True)

plt.rcParams.update({'font.size': 12})
element_prevalence(formula,
                    save_dir='ML_figures/example_figures',
                    ptable_fig=False,
                    log_scale=False)
element_prevalence(formula,
                    save_dir='ML_figures/example_figures',
                    name='example_log',
                    ptable_fig=False,
                    log_scale=True)
```

BestPractices paper - SI.pdf (3.00 MiB)

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