The CESM community is perpetually developing.
Community members want more tools to be able to enhance CESM capabilities and usability.
- Processing CESM timing data for machine learning.
High level goal is to predict performance.
What is Machine Learning

- Machine learning centers on the usage of a subset of algorithms.
- These algorithms seek to become more efficient or effective at a given task.
- The algorithms are trained by providing data to learn from.
Processor Comparison Dataset Motivation

- Simpler scenario to test the workflow.
  - Measure how effectively the machine learning methods can classifying different systems.
- Performing a classification of the hardware to later extend to more complex scenarios.

Classification Area

Classification Area
• Goal: For classification, could the models distinguish between the 3.5GHz Intel i5 vs. 2.5GHz Intel i7 runs.
• Data preprocessed with One Hot Encoding and Standard Scaling [1] [2].
• Models evaluated: SVM, Decision Trees, Random Forests, Multi-layer Perceptron, KNN.
• Principal Component Analysis, Select K Best methods.
Using different hardware, but same run parameters.
Same containerized CESM compset used: Aqua Planet.
4 cores used for each model run.
Running at 5, 10, 15 model days for 6 runs each on both 3.5GHz Intel i5 Vs. 2.5GHz.
• The print statements in the component barriers have been commented out.
• The standing idea is that component barriers on will influence performance.
  – Exploring the performance of the machine learning methods to see if a significant difference can be found.
• Provides a more complex scenario for the machine learning methods.
• Provide some insight as to whether the component barriers are significantly affecting CESM runs.
• Goal: Classifying whether the input data was from a barriers on data point or barriers off data point.
• Similar overall process, with Recursive Feature Elimination (RFE) added for alternative feature selection.
• All ran on Cheyenne.
• All other parameters similar to 3.5GHz Intel i5 Vs. 2.5GHz Intel i7 experiment.
Dimensionality Reduction and Feature Selection Methods

- **PCA**
  - Using linear algebra operations to combine features into new features
- **Select K Best**
  - Using a metric to select k amount of features from the total features
  - Mutual Information Classifier
- **RFE**
  - Builds a model and uses said model’s metrics to select k features
  - Decision tree
Overview of Results for 3.5GHz Intel i5 Vs. 2.5GHz Intel i7 Dataset

- 3.5GHz Intel i5 Vs. 2.5GHz Intel i7 accuracy results:
  - Highest mean accuracy is 99.2% from Decision Trees with Select K Best (example shown in plot below).
  - Lowest mean accuracy is 83.4% from Decision Trees with PCA.

Note: Experiment1_QPC4 refers to 2.3GHz Intel i7 and Experiment1_DT_QPC4 refers to 3.5GHz Intel i5.
Overview of Results Cheyenne Component Barriers on vs Component Barriers Off

- Cheyenne component barriers on vs component barriers off
  - Highest mean accuracy is 66.1% from SVMs with PCA (example plot shown below).
  - Lowest mean accuracy is 30.1% from random forests with Select K Best.

Note: Experiment1_CH4c_QPC4 refers to component barriers off and Experiment1_CH4c_QPC4_barriers refers component barriers on.
Future Work

- Increasing data available.
- Adding further machine learning models.
- Implementing widgets for an interactive notebook.
- Exploring more complex scenarios:
  - Exploring compsets and resolutions

Example plot examining B1850 vs F2000 compsets at two different resolutions for each compset.


I would like to thank my excellent mentors Sheri Mickelson, Brian Dobbins, and John Dennis for their guidance and expertise.

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Special Thanks to the NSF.
Questions

Project GitHub Repository QR Code:
https://github.com/NCAR/SIParCS-2021-Johnson

LinkedIn: https://www.linkedin.com/in/thomas-j-3804a7a6/
GitHub: https://github.com/Herok4Build
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Thomas Johnson III’s:
Cross Validation Methods

- Utilizing Leave One Out Cross Validation, abbreviated LOOCV.
  - The preferred cross validation strategy for tiny datasets [3] [4].
- 10-Fold Stratified Cross Validation, abbreviated SCV [4].

### Diagram of 10-Fold Cross Validation

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<th>Test</th>
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Number of Features for Data

- Cheyenne component barriers on vs. component barriers off using 86 features.
- 3.5GHz Intel i5 Vs. 2.5GHz Intel i7 dataset using 86 features.
### 3.5GHz Intel i5 Vs. 2.5GHz Intel i7 Runs of Aqua World Results

<table>
<thead>
<tr>
<th>Model Group</th>
<th>Mean of LOOCV for PCA</th>
<th>Mean of 10-Fold SCV for PCA</th>
<th>Mean of LOOCV for Select K Best</th>
<th>Mean of 10-Fold SCV for Select K Best</th>
</tr>
</thead>
<tbody>
<tr>
<td>SVMs</td>
<td>89.4%</td>
<td>91.7%</td>
<td>97.6%</td>
<td>97.8%</td>
</tr>
<tr>
<td>Decision Trees</td>
<td>83.4%</td>
<td>83.5%</td>
<td>99.2%</td>
<td>98.8%</td>
</tr>
<tr>
<td>Random Forests</td>
<td>85.8%</td>
<td>86.6%</td>
<td>98%</td>
<td>97.9%</td>
</tr>
<tr>
<td>Multi-layer Perceptron Neural Network</td>
<td>87.1%</td>
<td>89.2%</td>
<td>94.4%</td>
<td>94.5%</td>
</tr>
<tr>
<td>KNN</td>
<td>86.7%</td>
<td>87.7%</td>
<td>95.1%</td>
<td>95%</td>
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</tbody>
</table>
### Component Barriers On Versus Component Barriers Off Results

<table>
<thead>
<tr>
<th>Model Group</th>
<th>Mean of LOOCV for PCA</th>
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<th>Mean of 10-Fold SCV for Select K Best</th>
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</thead>
<tbody>
<tr>
<td>SVMs</td>
<td>66.1%</td>
<td>66.6%</td>
<td>36.2%</td>
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<tr>
<td>Decision Trees</td>
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<td>57.6%</td>
<td>32.2%</td>
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<tr>
<td>Random Forests</td>
<td>62.6%</td>
<td>62.7%</td>
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<tr>
<td>Multi-layer Perceptron Neural Network</td>
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<tr>
<td>KNN</td>
<td>57.1%</td>
<td>62.6%</td>
<td>49.3%</td>
<td>54.5%</td>
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</table>
## Component Barriers On Versus Component Barriers Off Results

<table>
<thead>
<tr>
<th>Model Group</th>
<th>Mean of LOOCV for Recursive Feature Elimination</th>
<th>Mean of 10-Fold SCV for Recursive Feature Elimination</th>
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</thead>
<tbody>
<tr>
<td>SVMs</td>
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<tr>
<td>Decision Trees</td>
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<tr>
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<td>62%</td>
</tr>
<tr>
<td>KNN</td>
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