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Strategies to scale computationally: bigger data

For some applications the amount of examples, features (or both) and/or the speed at which they need to be processed are challenging for traditional approaches. In these cases scikit-learn has a number of options you can consider to make your system scale.

Scaling with instances using out-of-core learning

Out-of-core (or "external memory") learning is a technique used to learn from data that cannot fit in a computer's main memory (RAM).

Here is a sketch of a system designed to achieve this goal:

1. a way to stream instances
2. a way to extract features from instances
3. an incremental algorithm

Streaming instances

Basically, 1. may be a reader that yields instances from files on a hard drive, a database, from a network stream etc. However, details on how to achieve this are beyond the scope of this documentation.

Extracting features

2. could be any relevant way to extract features among the different :ref:`feature extraction <feature_extraction>` methods supported by scikit-learn. However, when working with data that needs vectorization and where the set of features or values is not known in advance one should take explicit care. A good example is text classification where unknown terms are likely to be found during training. It is possible to use a stateful vectorizer if making multiple passes over the data is reasonable from an application point of view. Otherwise, one can turn up the difficulty by using a stateless feature extractor. Currently the preferred way to do this is to use the so-called :ref:`hashing trick<feature_hashing>` as implemented by :class:`sklearn.feature_extraction.FeatureHasher` for datasets with categorical variables represented as list of Python dicts or :class:`sklearn.feature_extraction.text.HashingVectorizer` for text documents.

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Incremental learning

Finally, for 3. we have a number of options inside scikit-learn. Although not all algorithms can learn incrementally (i.e. without seeing all the instances at once), all estimators implementing the `partial_fit` API are candidates. Actually, the ability to learn incrementally from a mini-batch of instances (sometimes called "online learning") is key to out-of-core learning as it guarantees that at any given time there will be only a small amount of instances in the main memory. Choosing a good size for the mini-batch that balances relevancy and memory footprint could involve some tuning [1].

Here is a list of incremental estimators for different tasks:

- Classification

  - :class:`sklearn.naive_bayes.MultinomialNB`

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  - :class:`sklearn.naive_bayes.BernoulliNB`

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  - :class:`sklearn.linear_model.Perceptron`

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  - :class:`sklearn.linear_model.SGDClassifier`

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  - :class:`sklearn.linear_model.PassiveAggressiveClassifier`

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  - :class:`sklearn.neural_network.MLPClassifier`

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- Regression

  - :class:`sklearn.linear_model.SGDRegressor`

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  - :class:`sklearn.linear_model.PassiveAggressiveRegressor`

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- :class:`sklearn.neural_network.MLPRegressor`

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- Clustering

  - :class:`sklearn.cluster.MiniBatchKMeans`

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  - :class:`sklearn.cluster.Birch`

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- Decomposition / feature Extraction

  - :class:`sklearn.decomposition.MiniBatchDictionaryLearning`

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  - :class:`sklearn.decomposition.IncrementalPCA`

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  - :class:`sklearn.decomposition.LatentDirichletAllocation`

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- Preprocessing

  - :class:`sklearn.preprocessing.StandardScaler`

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  - :class:`sklearn.preprocessing.MinMaxScaler`

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For classification, a somewhat important thing to note is that although a stateless feature extraction routine may be able to cope with new/unseen attributes, the incremental learner itself may be unable to cope with new/unseen targets classes. In this case you have to pass all the possible classes to the first `partial_fit` call using the `classes=` parameter.

Another aspect to consider when choosing a proper algorithm is that not all of them put the same importance on each example over time. Namely, the `Perceptron` is still sensitive to badly labeled examples even after many examples whereas the `SGD*` and `PassiveAggressive*` families are more robust to this kind of artifacts. Conversely, the latter also tend to give less importance to remarkably different, yet properly labeled examples when they come late in the stream as their learning rate decreases over time.

Examples

Finally, we have a full-fledged example of :ref:`sphx_glr_auto_examples_applications_plot_out_of_core_classification.py`. It is aimed at providing a starting point for people wanting to build out-of-core learning systems and demonstrates most of the notions discussed above.

Furthermore, it also shows the evolution of the performance of different algorithms with the number of processed examples.

Now looking at the computation time of the different parts, we see that the vectorization is much more expensive than learning itself. From the different algorithms, `MultinomialNB` is the most expensive, but its overhead can be mitigated by increasing the size of the mini-batches (exercise: change `minibatch_size` to 100 and 10000 in the program and compare).

Notes

[1] Depending on the algorithm the mini-batch size can influence results or not. SGD*, PassiveAggressive*, and discrete NaiveBayes are truly online and are not affected by batch size. Conversely, MiniBatchKMeans convergence rate is affected by the batch size. Also, its memory footprint can vary dramatically with batch size.