kernelmethods for pattern analysis and machine learning in python

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Abstract

Kernel methods have proven to be powerful techniques for pattern analysis and machine learning (ML) in a variety of domains. However, many of their original or advanced implementations remain in Matlab. With the incredible rise and adoption of Python in the ML and data science world, there is a clear need for a well-defined library that enables not only the use of popular kernels, but also allows easy definition of customized kernels to fine-tune them for diverse applications. The kernelmethods library fills that important void in the python ML ecosystem in a domain-agnostic fashion, allowing the sample data type to be anything from numerical, categorical, graphs or a combination of them. In addition, this library provides a number of well-defined classes to make various kernel-based operations efficient (for large scale datasets), modular (for ease of domain adaptation), and inter-operable (across different ecosystems). The library is available at https://github.com/raamana/kernelmethods

Keywords: kernel methods, data structure, support vector machines, pattern analysis, multiple kernel learning, python, machine learning

1. Introduction

Kernel methods (KM) demonstrated their potential in pattern analysis and machine learning (ML) in a diverse array of domains such as image processing, text analysis, bioinformatics and medicine (Shawe-Taylor et al., 2004). Much of their power and popularity boils down to the kernel trick and the modularity of the kernel learning algorithms. The kernel functions enable the study of non-linear relations in the high-dimensional data by efficiently embedding them in an inner-product feature-space. Kernel-learning algorithms operate exclusively on the the pairwise inner products (so called gram- or kernel-matrix) without needing to know the original representation. This modularity led to efficient and robust algorithms such as the support vector machines (SVM) that performed well in diverse ML applications (Burges, 1998; Vapnik, 2000).

With rapid growth and adoption of open source software, ML libraries have become available in most languages, including but not limited to Java, Python, C++, and Matlab (MLOSS, 2007). Although these languages have varying levels of support for kernel methods, basic functionality of standard kernel functions and SVMs is generally available in many popular ML libraries (online repo, 2007). However, to fully leverage the power of kernel methods, researchers need to be able to develop, use and fine-tune custom kernel
functions and algorithms for their unique application, dataset or domain. But unfortunately many existing libraries are neither easily modifiable nor extensible, and allow limited functionality typically restricted to using predefined kernel functions and algorithms. There have been attempts to address this e.g. JKernelMachines and KELP in Java (Picard et al., 2013; Filice et al., 2017), and kernlab in R (Karatzoglou et al., 2004). But no such library exists in Python, despite its incredible adoption and accelerated growth in ML, data science and research software development in general (Raamana, 2018). Popular libraries like scikit-learn (Pedregosa et al., 2011) provide only basic kernel functions, and implementing new kernels or methods is neither easy nor well-defined. This challenge is even more apparent when attempting to implement advanced methods such as multiple kernel learning (MKL) (Gönen and Alpaydın, 2011; Raamana et al., 2015) and hyper-kernels (Ong et al., 2005). Moreover, common and necessary kernel operations such as normalization, centering and alignment etc are simply missing, in addition to the lack of thorough kernel-oriented validation of such implementations.

kernelmethods aims to fill this important gap in the python ecosystem, to provide a scikit-learn-like library focused on kernel methods, with the following goals: 1) an intuitive API, 2) deep extensibility allowing for easy customization and optimization for diverse needs, and 3) high modularity allowing different data types (from numbers to categorical to graphs to trees) as well as mixed data types (e.g. in medical, epidemiological and biostatistics applications). kernelmethods is a pure python library released under the Apache 2.0 license, implements the best practices in research software engineering, along with continuous integration and a test suite with over 95% coverage. By filling an important gap, we believe this library would strengthen the python ML ecosystem and advance the state of the art in kernel methods. The source code is available at https://github.com/raamana/kernelmethods and the corresponding auto-generated documentation is available at https://raamana.github.io/kernelmethods.

2. Design of the kernelmethods library

kernelmethods offers the following features 1) popular kernel functions, 2) KernelMatrix class, 3) container classes to manage large collections of kernel matrices, 4) kernel operations and utilities module, and 5) drop-in Estimator classes for ease of use in the python ML ecosystem. It is designed to ease the development of advanced functionality such as customized, composite or hyper kernels.

2.1 The KernelMatrix class

The KernelMatrix is a self-contained class for the Gram matrix induced by a kernel function on a given sample $X$. This class defines the central data structure for all kernel methods, as it acts a key bridge between input data space and the learning algorithms (Shawe-Taylor et al., 2004). The library

- computes only the elements needed, saving computation and storage
- supports both callable and attribute access, allowing easy access to partial or random portions of KernelMatrix.
• allows parallel computation of different parts of \texttt{KernelMatrix} to speed up processing of large scale datasets (when $N > 50K$)

• allows user-defined attributes, which is ideal for easy identification among a large collection of KMs from generating, filtering and ranking applications for MKL

• implements necessary kernel operations such as centering and normalization, which are different from those manipulating regular matrices and

• exposes several convenience attributes (norms, diagonal and centered versions) and classes for ease of extensibility e.g. \texttt{ConstantKernelMatrix}, \texttt{KernelMatrixPrecomputed}.

2.2 Defining Kernel Functions

Creating new kernel functions is trivial, which boils down to inheriting from the \texttt{BaseKernelFunction}, implementing the \texttt{__call__} method, and giving it a human readable \texttt{__str__}. This implementation design, focusing on nothing more than two vectors $x$ and $y$, makes it easy for non-expert users and developers alike to define new and interesting kernels for their unique applications. For example, implementing the entire \texttt{Chi2Kernel} is as simple as:

```python
class Chi2Kernel(BaseKernelFunction):
    def __init__(self, gamma=1.0):
        super().__init__(name='chi2')
        self.gamma = gamma

    def __call__(self, x, y):
        """Actual implementation of kernel func""
        # not shown are a lot of checks and validation
        return np.exp(-self.gamma * np.nansum(np.power(x - y, 2) / (x + y)))

    def __str__(self):
        """human readable repr""
        return "{}(gamma={})".format(self.name, self.gamma)
```

This frees the users from the burden of having to worry about verifying its implementation is PSD, as all kernel functions are validated to satisfy the Mercer’s condition (Shawe-Taylor et al., 2004), which make them interoperable with rest of the kernel machinery. Such abstraction of the implementation and application of the kernel function is exactly how this library becomes domain-agnostic, deferring the handling of the data type down to the data structures holding the features, such as \texttt{pyradigm} (Raamana et al., 2017), and the particular domain-relevant kernel in question.

2.3 Utilities

Besides being able to apply basic kernels on a given sample, this library provides necessary kernel operations, such as normalization, centering, product, alignment evaluation, linear combination and ranking (by various performance metrics) of kernel matrices. While kernel functions are commonly applied on a single sample, this class is designed to allow two
samples to be attached with potentially differing number of \textit{samplets}\textsuperscript{1}. This is not possible in scikit-learn where kernel implementations are hard-coded for specific definitions.

### 2.4 Container classes

The library also provides \texttt{KernelSet} and \texttt{KernelBucket} container classes for easy management of a large collection of kernels. Dealing with a diverse configuration of kernels is necessary for automatic kernel selection and optimization in applications such as Multiple Kernel Learning (MKL), hyper kernel and the like (Gönen and Alpaydın, 2011).

### 2.5 Domain agnostic

Besides the numerical kernels, we designed this library to make it easy to develop categorical, string and graph kernels, owing to its great modularity i.e. feature data-type and iteration of the sample are encapsulated into that particular kernel function and the generic \texttt{KernelMatrix} class, and they do not interact with the rest of the library. For example, implementing a categorical kernel function is as simple as:

\begin{verbatim}
class MatchCountKernel(BaseKernelFunction):
    def __init__(self, return_perc=True): # Constructor
        self.return_perc = return_perc
        super().__init__('MatchPerc' if self.return_perc else 'MatchCount')

    def __call__(self, vec_c, vec_d):
        """vec_c, vec_d : array of equal-sized categorical variables""
        match_count = np.sum(vec_c==vec_d)
        if self.return_perc:
            return match_count / len(vec_d)
        else:
            return match_count
\end{verbatim}

### 2.6 Interoperability

Moreover, drop-in \texttt{Estimator} classes are provided for seamless usage in the scikit-learn ecosystem. For example, SVM with any arbitrary user-defined kernel (on any data type) can be achieved easily with only a few lines of code:

\begin{verbatim}
from kernelmethods import KernelMachine # valid sklearn estimator
from userlib import custom_metric # user-defined kernel function
km = KernelMachine(custom_metric) # learning algorithm is another option
km.fit(X=sample_data, y=targets) # can be dropped in as estimator anywhere
predicted_y = km.predict(sample_data)
\end{verbatim}

\footnote{1. We define the term \textit{samplet} here to be a single data point in a given sample i.e. one row in the feature matrix $X$ of size $n \times p$.}
3. Validation

The `kernelmethods` library is tested thoroughly under continuous integration with over 95% test coverage. In addition, we run few experiments here to not only demonstrate its utility but also to serve as an additional validation at the level of the library. Following (Picard et al., 2013), we evaluate this library, as well as scikit-learn, on 4 datasets from the UCI repo using the same algorithms and parameters (repeated holdout cross-validation, 80% training, 20 repetitions). The accuracy estimates for 4 libraries for the default SMO option (gaussian kernel with $\sigma = 0.1$) are shown in Table 1. This demonstrates the `kernelmethods` is performing just as well as the other libraries as expected. The minor differences across libraries are due to differences in implementation of the formulae and parameter interpretation.

Table 1: Accuracy estimates of SVM from `kernelmethods`, Weka and JKernelMachines on UCI data sets, which perform similarly, as expected.

| Dataset (N x p)    | Weka     | JKernelMachines | scikit-learn | `kernelmethods` |
|-------------------|----------|----------------|--------------|-----------------|
| ionosphere (351x34)| 0.861 ± 0.041 | 0.915 ± 0.025  | 0.9465 ± 0.027 | 0.9451 ± 0.0263 |
| heart (270x13)    | 0.840 ± 0.038 | 0.831 ± 0.043  | 0.8167 ± 0.050 | 0.8037 ± 0.0348 |
| breast-cancer (638x10) | 0.973 ± 0.013 | 0.942 ± 0.018  | 0.9745 ± 0.011 | 0.9704 ± 0.0149 |
| german (1000x24)  | 0.754 ± 0.023 | 0.689 ± 0.029  | 0.7583 ± 0.026 | 0.7282 ± 0.0274 |

With further tuning (dataset-specific kernel function and parameters), the performance can be improved. As such an exercise would be domain-specific, broader discussion (of dataset properties, performance optimization and trade-offs) is beyond the scope of this software paper.

3.1 Future work

We plan to extend the `kernelmethods` library in many important directions: 1) providing base classes for MKL and HyperKernel (as well as their popular variations) to enable the user focus on higher-level domain-specific optimizations, 2) support for missing data and covariates (when estimating similarity), and 3) supporting broader domains such as graphs, trees and sequences, which have exciting applications in most biomedical research domains.

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