NCAP-COALESCE
CarbOnaceous AerosoL Emissions, Source apportionment & ClimatE impacts
Understanding scientific complexities related to carbonaceous aerosols focussing on issues underlying their origin and fate, and their role as drivers of regional climate change over India.

Research BRIEFS

pyGNMF: A Python library for implementation of generalised non-negative matrix factorisation method

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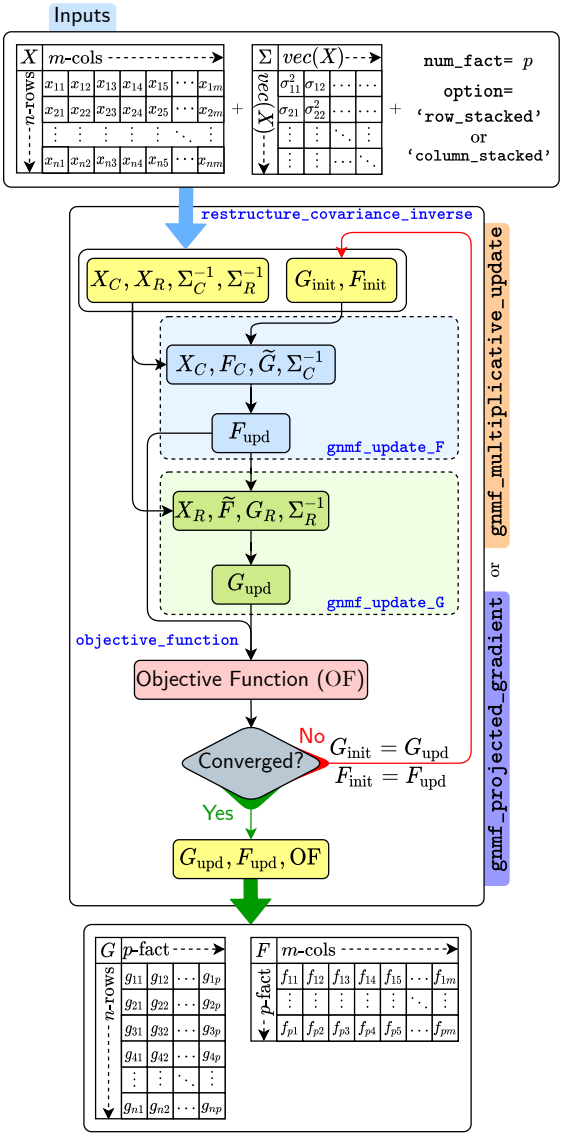

Key highlights:

- Python implementation of Generalised Non-Negative Matrix Factorisation (GNMF) method.
- Optimised code and easy to use functions for quick GNMF application.
- pyGNMF implementation of GNMF method can be used for variety of application subject to availability of the covariance matrix.

Summary of your Research:

This study introduces pyGNMF, a Python library for the implementation of a the recently proposed generalised non-negative matrix factorisation (GNMF) method. GNMF factorises a non-negative matrix into a product of two non-negative matrices by incorporating error-covariance information between different elements of the dataset. In literature, several non-negative matrix factorisation (NNMF) methods such as NMF, glsNMF and LS-NMF are available; however, they assume different forms of the error-covariance matrix. In particular, NMF assumes identity error-covariance matrix, LS-NMF assumes diagonal error-covariance matrix, and glsNMF assumes errors to be correlated in only one direction (rows or columns).

In contrast, GNMF can incorporate the full error-covariance information and depending on the error-covariance structure, GNMF subsumes these methods as special cases. The parent article introduces two approaches to solve the problem by using projected gradient-based and multiplicative updates and is demonstrated on an air pollution source apportionment problem. Both these approaches have been incorporated into the pyGNMF library. The mathematical nature of GNMF method makes it domain-agnostic, enabling users from different domains to deploy GNMF for their non-negative matrix factorisation applications.

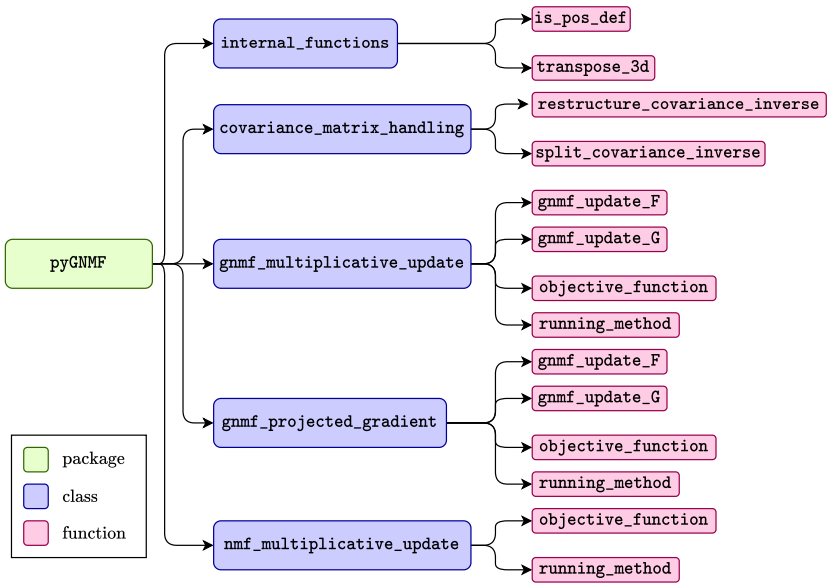

Figure: pyGNMF Package Structure.

Code 4: Code for using test example for `gnmf_projected_gradient` method.

```
from scipy import io
import pyGNMF.gnmf_projected_gradient as gproj

example_data = io.loadmat("illustrative_example.mat")
X_matrix = example_data['x_matrix']
covariance = example_data['covariance']
num_fact = 3

GMat, FMat, OFunc = gproj.running_method(
   X_matrix,            ## Matrix to be factorised
   covariance,          ## Covariance matrix
   G_init='random',     ## Random initialisation
   F_init='random',     ## Random initialisation
   beta=0.1,            ## Parameter -- Step-length
   sigma=0.0001,        ## Parameter -- Step-length
   alpha_init_G=1,      ## Initial value of alpha_G
   alpha_init_F=1,      ## Initial value of alpha_F
   option='row_stacked', ## Cov. corresponds to row-stacked elements of X matrix.
   num_fact=3,          ## Number of factors
   num_init=5,          ## Number of initialisations
   max_iter=500000,     ## Maximum number of iterations
   tolerance=1e-8       ## Tolerance value for convergence
)
```

Take away/conclusion :

pyGNMF package makes implementation of GNMF method easy for any application under consideration. The code snippet shows the sample code for running GNMF method with an illustrated example which is part of the code. It also shows different options available to fine-tune the method.

Research Article citation

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