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1 Global Feature Reconstruction Error (GFRE) and Distortion (GFRD)

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Example for the usage of the `skcosmo.metrics.global_reconstruction_error` as global feature reconstruction error (GFRE) and `skcosmo.metrics.global_reconstruction_distortion` global feature reconstruction distortion (GFRD)

```
[1]: import numpy as np
import matplotlib.pyplot as plt

from skcosmo.datasets import load_degenerate_CH4_manifold
from skcosmo.metrics import (
    global_reconstruction_error,
    global_reconstruction_distortion,
)

# load features
degenerate_manifold = load_degenerate_CH4_manifold()
soap_features = degenerate_manifold.data.SOAP_power_spectrum
bispectrum_features = degenerate_manifold.data.SOAP_bispectrum

-----
NotADirectoryError                                Traceback (most recent call last)
<ipython-input-1-b71508f861f4> in <module>
     9
    10 # load features
----> 11 degenerate_manifold = load_degenerate_CH4_manifold()
    12 soap_features = degenerate_manifold.data.SOAP_power_spectrum
    13 bispectrum_features = degenerate_manifold.data.SOAP_bispectrum

~/checkouts/readthedocs.org/user_builds/scikit-cosmo/envs/latest/lib/python3.7/site-
packages/skcosmo-0.1.0-py3.7.egg/skcosmo/datasets/_base.py in
load_degenerate_CH4_manifold()
    22     module_path = dirname(__file__)
    23     target_filename = join(module_path, "data", "degenerate_CH4_manifold.npz")
----> 24     raw_data = np.load(target_filename)
    25     data = Bunch(
    26         SOAP_power_spectrum=raw_data["SOAP_power_spectrum"],

~/checkouts/readthedocs.org/user_builds/scikit-cosmo/envs/latest/lib/python3.7/site-
packages/numpy/lib/npzio.py in load(file, mmap_mode, allow_pickle, fix_imports,
encoding)
    415         own_fid = False
    416     else:
--> 417         fid = stack.enter_context(open(os_fspath(file), "rb"))
    418         own_fid = True
    419

NotADirectoryError: [Errno 20] Not a directory:
```

```
'/home/docs/checkouts/readthedocs.org/user_builds/scikit-  
cosmo/envs/latest/lib/python3.7/site-packages/skcosmo-0.1.0-  
py3.7.egg/skcosmo/datasets/data/degenerate_CH4_manifold.npz'
```

```
[2]: gfre_matrix = np.zeros((2, 2))  
print("Computing GFRE...")  
gfre_matrix[0, 0] = global_reconstruction_error(soap_features, soap_features)  
gfre_matrix[0, 1] = global_reconstruction_error(soap_features, bispectrum_features)  
gfre_matrix[1, 0] = global_reconstruction_error(bispectrum_features, soap_features)  
gfre_matrix[1, 1] = global_reconstruction_error(  
    bispectrum_features, bispectrum_features  
)  
print("Computing GFRE finished.")
```

Computing GFRE...

```
-----  
NameError                                Traceback (most recent call last)  
<ipython-input-1-f1b8517c7cba> in <module>  
    1 gfre_matrix = np.zeros((2, 2))  
    2 print("Computing GFRE...")  
----> 3 gfre_matrix[0, 0] = global_reconstruction_error(soap_features, soap_features)  
    4 gfre_matrix[0, 1] = global_reconstruction_error(soap_features,  
bispectrum_features)  
    5 gfre_matrix[1, 0] = global_reconstruction_error(bispectrum_features,  
soap_features)
```

NameError: name 'soap_features' is not defined

```
[3]: gfrd_matrix = np.zeros((2, 2))  
print("Computing GFRD...")  
gfrd_matrix[0, 0] = global_reconstruction_distortion(soap_features, soap_features)  
gfrd_matrix[0, 1] = global_reconstruction_distortion(soap_features,  
bispectrum_features)  
gfrd_matrix[1, 0] = global_reconstruction_distortion(bispectrum_features,  
soap_features)  
gfrd_matrix[1, 1] = global_reconstruction_distortion(  
    bispectrum_features, bispectrum_features  
)  
print("Computing GFRD finished.")
```

Computing GFRD...

```
-----  
NameError                                Traceback (most recent call last)  
<ipython-input-1-524fc5cb8cd1> in <module>  
    1 gfrd_matrix = np.zeros((2, 2))  
    2 print("Computing GFRD...")  
----> 3 gfrd_matrix[0, 0] = global_reconstruction_distortion(soap_features,  
soap_features)  
    4 gfrd_matrix[0, 1] = global_reconstruction_distortion(soap_features,  
bispectrum_features)  
    5 gfrd_matrix[1, 0] = global_reconstruction_distortion(bispectrum_features,  
soap_features)
```

NameError: name 'soap_features' is not defined

It can be seen that the reconstruction of the 4-body features using 3-body features has a nonnegligible error showing that 4-body features adds additional information in a linear regression sense for this dataset. Furthermore, it can be seen that 3-body features can be reconstructed using 4-body with a negligible error but high distortion.

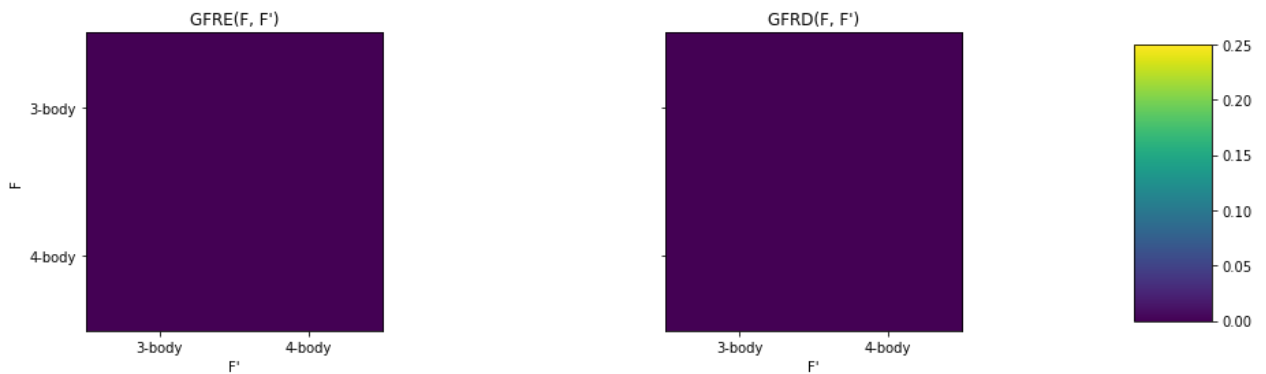
```
[4]: fig, axes = plt.subplots(1, 2, figsize=(16, 4))  
    pcm1 = axes[0].imshow(gfre_matrix, vmin=0, vmax=0.25)
```

```

pcm2 = axes[1].imshow(gfrd_matrix, vmin=0, vmax=0.25)
axes[0].set_ylabel("F")
axes[0].set_xlabel("F'")
axes[1].set_xlabel("F'")
axes[0].set_title("GFRE(F, F')")
axes[1].set_title("GFRD(F, F')")
axes[0].set_xticks([0, 1])
axes[0].set_xticklabels(["3-body", "4-body"])
axes[1].set_xticks([0, 1])
axes[1].set_xticklabels(["3-body", "4-body"])
axes[0].set_yticks([0, 1])
axes[0].set_yticklabels(["3-body", "4-body"])
axes[1].set_yticks([0, 1])
axes[1].set_yticklabels(["", ""])

fig.subplots_adjust(right=0.8)
cbar_ax = fig.add_axes([0.85, 0.15, 0.05, 0.7])
fig.colorbar(pcm2, cax=cbar_ax)
plt.show()

```



[]: