

coordinate-transformation

June 18, 2024

1 Validation of the coordinate transformation function defined in the pymatcal module

1.1 import the modules

```
[ ]: import sys
      sys.path.insert(0, '..')
      import pymatcal
      import numpy as np
      import matplotlib.pyplot as plt
      import matplotlib as mpl
```

1.2 Generate random coordinates

```
[ ]: angle_rad = np.pi/6.0
      input_np = np.array([[5, 5, 0]])

      # randomly generated points
      rng = np.random.default_rng()
      npx = 4
      ydata = rng.integers(low=0, high=180, size=npx)
      xdata = rng.integers(low=0, high=180, size=npx)
```

1.2.1 Shape the coordinates to the desired data shape

```
[ ]: data1 = np.vstack([xdata, ydata, np.zeros(npx)]).T
```

1.3 Perform the transformations

1.3.1 Rotational transformation around x,y = (90,90)

```
[ ]: mr, mt = pymatcal.get_mtransform(angle_rad, 90, 90)
      data2 = pymatcal.coord_transform(
          mr, mt, data1-np.array((90, 90, 0)))
```

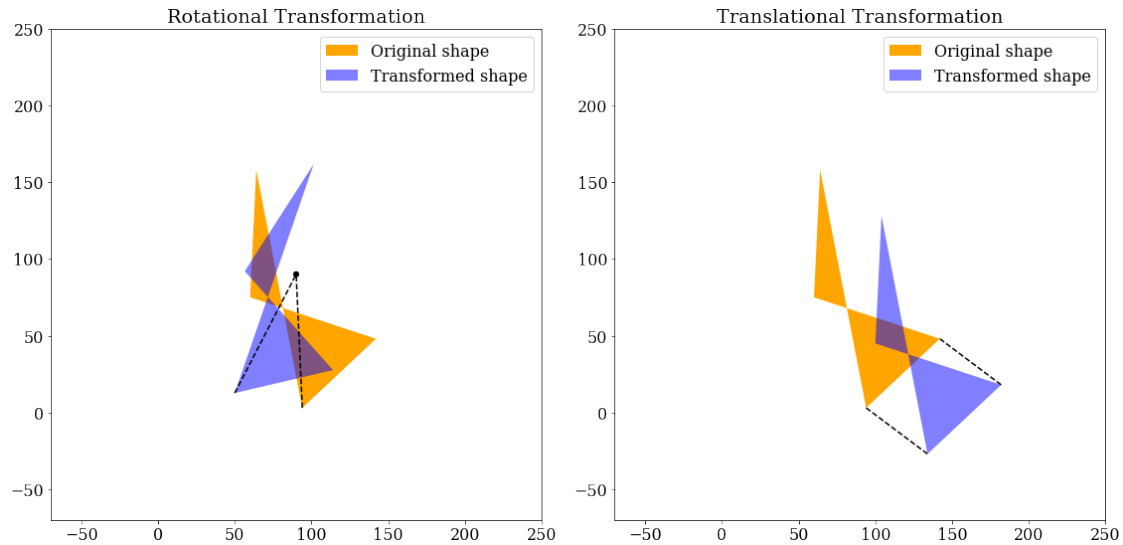
1.3.2 Pure translational transformation by $dx, dy = (40, -30)$

```
[ ]: mr, mt = pymatcal.get_mtransform(0, 40, -30)
data3 = pymatcal.coord_transform(
    mr, mt, data1)
```

1.4 Plot the result

```
[ ]: plt.rcParams["font.family"] = "serif"
mpl.rcParams.update({'font.size': 16})
fig, axs = plt.subplots(1,2,figsize=(16, 10))
for ax in axs:
    ax.set_xlim(-70, 250)
    ax.set_ylim(-70, 250)
    ax.set_aspect('equal')
axs[0].add_patch(mpl.patches.Polygon(data1[:, 0:2], fc='orange',label='Original_
    ↪shape'))
axs[0].add_patch(mpl.patches.Polygon(data2[:, 0:2], alpha=0.5,
    ↪fc='blue',label='Transformed shape'))
axs[0].plot([data1[0, 0], 90],
            [data1[0, 1], 90], c='k',ls='--')
axs[0].plot([data2[0, 0], 90],
            [data2[0, 1], 90], c='k',ls='--')
axs[0].add_patch(mpl.patches.Circle((90, 90), 2, fc='k'))
axs[0].legend()
axs[0].set_title("Rotational Transformation")

axs[1].add_patch(mpl.patches.Polygon(data1[:, 0:2], fc='orange',label='Original_
    ↪shape'))
axs[1].add_patch(mpl.patches.Polygon(data3[:, 0:2], alpha=0.5,
    ↪fc='blue',label='Transformed shape'))
for idx in [0,3]:
    axs[1].plot([data1[idx, 0], data3[idx,0]],
                [data1[idx, 1], data3[idx, 1]], c='k',ls='--')
# axs[1].add_patch(mpl.patches.Circle((90, 90), 2, fc='k'))
axs[1].legend()
axs[1].set_title("Translational Transformation")
fig.tight_layout()
fig.savefig("coordinate-transformation-module.png")
# plt.show()
```



1.4.1 Length is kept the same after the transformation:

```
[ ]: print(np.linalg.norm(data1[0]-data1[2]),np.linalg.norm(data2[0]-data2[2]))
```

```
128.01562404644207 128.01562404644207
128.01562404644207 128.01562404644207
```

1.4.2 All the data points are shifted exactly the way we want

```
[ ]: for dxy in data1-data3:
      print(dxy)
```

```
[-40.  30.   0.]
[-40.  30.   0.]
[-40.  30.   0.]
[-40.  30.   0.]
```

```
[ ]:
```