GUIDE FOR MVT ON MANIFOLDS PYTHON CODE

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The purpose of this document is to guide a new or returning researcher through the progress made implementing Python methods to refine the non-contact set in solutions to the obstacle problem with Green's function defined on a cylinder. I'll show you around each of the various functions, detail how they work, and suggest some exercises to try. The code is accessible in the "MVT on Manifolds 2.py" and inspiration is taken from the following paper, among others:

A shape optimization approach for simulating contact of elastic membranes with rigid obstacles, Sharma and Rangarajan

Let's begin at the top of the .py document.

IMPORTATIONS

Python documents come with a limited number of built-in functions, but to do most scientific computing you'll need to import packages of methods. <code>numpy</code> is a critically important package to any numerical calculations and, thankfully, its methods appear to mimic those of MATLAB. For most scientific researchers using Python, <code>matplotlib.pyplot</code> is the go-to package for visualizing data. It has an immense library of possibilities and just might surprise you with its versatility. <code>scipy</code> is another hugely popular package with more specialized functions, which we will use for finite element analysis and function optimization. Finally, <code>sympy</code> is a package to help make geometry more intuitive.

Importing a package "as" another name allows you to reference that package by the abbreviation of your choice. np and plt are standard abbreviations for their respective packages.

PARAMETERS

In the PARAMETERS section, you'll find definitions of global variables which act as important parameters throughout the document. Whenever you'd like to change something about the shape optimization, all of your parameters can be found in one place. These variables are "visible" inside all the functions we will create in the document, so they can be referenced anywhere. If you introduce more parameters, consider defining them in this space. Let's see what these variables mean:

- L the length of the cylinder (don't change this)
- R the radius of the cylinder
- r variable in the differential equation for the solution to the obstacle problem in the non-contact set. I.e., controls the "force" pushing up on the elastic membrane.
- C the circumference of of the cylinder
- z0, t0 the (z,θ) coordinates of the singularity in Green's function defined on the cylinder
- resolution the number of grid points (along each axis) at which to compute values
 of Green's function, the signed distance function, and solutions to the differential
 equations. Total number of points is approximately

```
resolution[0]*resolution[1].
```

• R_guess - we will initially guess that the shape of the noncontact region is a circle. Its radius is manipulable with this parameter.

The other parameters have not yet been implemented, as they are involved with the process of refining the shape of the noncontact set, which is left to you! Detailed explanations of these parameters can be found in Sharma and Rangarajan.

<u>Interact</u>

- Compile the code. If you're using Spyder 5, like I do, That's the green play button.
- In your console, type any of the parameter names and Return. Are they reading their correct values?
- Change a parameter value by deleting the old value from the document and typing a new value. Recompile, then make sure that the value has actually changed.
- Ask Python the question "C == 2*pi*R". Does it return what you expected?

CONVENIENCE

I needed to write π a lot, so I made it two characters instead of five.

ASSEMBLY

The assembly() function should execute the main steps of the shape optimization algorithm in the correct sequence. It's not even close to finished! Some of the methods are currently just trivial (they return what is inputted) and for the finished product you will likely need a while loop over the methods that should be iterated until satisfactory shape resolution is achieved. I think the general framework is correct for the first iteration, at least.

<u>Interact</u>

• In your console, try calling assembly() and observe the figures currently being produced. Vary the parameter r and try to discern what changes in these figures (one figure will remain unchanged).

FORMULAS

In this section, you'll find two important formulas which define Green's function and a paraboloid on a cylinder. The former is Dr. LeCrone's masterpiece and the latter will define the initial signed distance function ϕ , designed to be negative in the noncontact region and positive in the contact region. Both functions contain necessary and optional parameters. The necessary parameters z, t are the coordinates at which you'd like to know the value of the function. z0, t0 are, again, the location of the singularity in Green's function. By default, they are the values from the PARAMETERS section, but can be changed locally as well for testing purposes.

Interact

- Ask for the value of Green's function at some various locations on the cylinder. You may want to use L and C. Make sure to try asking for the value at the singularity, too.
- Do the same thing for the paraboloid function.
- In the G_cyl function, what is the purpose of the variable k? Try exploring the np.arange function by typing np.arange (-10,10). Now, do you see np.sum in the return statement? Try to make sense of what's going on here.
- Try to compute 5^3 , $\cosh(\pi)$, and $\frac{C}{2\pi}$ in the console.

COMPLEX FUNCTIONS

These functions do the heavy lifting in this project. When I say "COMPLEX", I mean they took me a while to figure out how to code properly and they do rather intricate tasks. No imaginary numbers in this project, yet! Let's go through them one-by-one.

initializeMesh (plot=False)

The first of the complex functions creates a Delaunay triangulation object tri from the scipy.spatial class, spanning a cylinder with length and radius set previously in PARAMETERS. Essentially, the function creates lists of evenly spaced numbers in z and θ (lines 96-103), uses them to create grids of points (lines 104-105), then combines the grid and "triangulates" the surface of the cylinder into acute triangular elements (lines 107-111).

Triangulation objects have many important attributes. You should become very comfortable with the documentation at the following link, which details parameters you can pass into the Delaunay function and the attributes to the output object:

https://docs.scipy.org/doc/scipy/reference/generated/scipy.spatial.Delaunay.html

Notice that I declare tri a global variable in the first line of this function. This means that during any particular execution of the code, tri is accessible from all other places in the code once initializeMesh(). For instance, if in a single execution I call initializeMesh(), then call findBoundary(), tri can be referenced, used, and manipulated inside findBoundary(). I will continue this organizational technique throughout the functions that I wrote, just for the sake of clarity.

The optional plot parameter allows you to visualize the triangulated mesh on the "unraveled" cylinder.

tri is returned for convenience with manual manipulation, even though returning it is sort of redundant after declaring it a global variable.

Interact

• In the console, create and store a triangulation object using initializeMesh(). (Hint: see line 55 in assembly).

- Print out some of the attributes of your triangulation object. If you called it tri, like I did, do this by typing tri.points, tri.simplices, tri.vertex_neighbor_vertices, etc. The attributes that I listed were the most
 - important ones to me, thus far. If you want to learn about the others, absolutely go for it!
 - Further understand the dimensions of the attributed arrays by asking for their shape. I use numpy's shape function endlessly:
 - https://numpy.org/doc/stable/reference/generated/numpy.shape.html
- Compare the number of points in the triangulation with the expected number, given your resolution parameter. Any differences come from the fact that the mesh is not rectangular, but triangular. I'm sure there's a better way to code it, but at least I got close!
- Test out the optional plot parameter by asking for initializeMesh (True) or initializeMesh (plot=True). Change the resolution and try again!
- Create your own custom triangulation object by following the structure of the Example within the Delaunay documentation page. Create your list of points, triangulate them, and plot them.
- In a new Python document, create two functions first() and second(). In first(), declare an integer variable a = 143. Then, in second(), try to print out that variable with print(a). Call both functions in sequence in the same execution. Now, declare a a global variable by changing the line to global a = 143. Try executing both functions in sequence again.

findBoundary(phis, tri, plot=False)

```
| def | findBoundary(phis, tri, plot=False):
| global D | global dD | global iDs | global iDs | global iDs | global iDs | global iOs | global iCs |
```

This function figures out which nodes in the triangulation can be considered part of the non-contact set/domain D, the boundary ∂D , and the contact set C. Lists of all points in each of these subdomains are found in global variables D, dD, and C. Indices that locate these points within the entire list of points tri.points are found in global variables iDs, idDs, and iCs.

findBoundary takes as required inputs phis and tri, the latter of which should be our friend the Delaunay triangulation object. phis is the list of values of the signed distance function φ at each node of the triangulation, in the correct order. In other words, phis [n] should equal

φ(tri.points[n]). The function should be general enough to accept phis and tri after every iteration of updating, as phis will be changed in updatePhi and tri will be changed in conformMesh.

Essentially, the function uses np.where to locate the indices at which phis has values greater or less than zero. Then, to define a boundary, it loops through each node in D, retrieves its immediate neighboring nodes using the $vertex_neighbor_vertices$ attribute, and isolates the neighboring nodes which are *not* a part of D (or equivalently a part of D). It's possible for the loop to identify the same boundary point more than once, so line 143 takes care of duplicates.

The optional plot parameter again cleanly visualizes the each determined region of the cylinder.

Interact

- Copy lines 55-57 from assembly and execute them in the console, either one by one or all together. Make one minor change: go ahead and set plot=True.
- Observe the output visual. The red dots are located at nodes in C, green dots in D, and black dots in ∂D . If you're using Spyder, make sure to uncheck "Fit plots to window" or just Undock the figures so that you can zoom in and out.
- Take a look at each of the new variables (D, dD, idDs, etc.) to make sense of them.
- Experiment with numpy's where function a bit. Create an array x = np.arange(-10,10) and ask np.where(x < 0). Now ask for np.where(x < 0, x, "Positive"). Reshape the array with x = x.reshape(5,4). Ask the same questions. Useful, huh?</p>

```
conformMesh(phis, tri)
```

The first complex function that you'll have to construct is one which adjusts the locations of the boundary nodes in the triangulation so that they approximate the true boundary a little better, but algorithmically preserves the "quality" of the other elements as best as possible. The inputs are just a suggestion/prediction; you might need to change them.

```
FEM(tri, D, dD, iDs, idDs, plot=True)
```

```
| def | FER(tri, D, dD, iDs, idDs, plot=True):
| def |
```

FEM stands for Finite Element Method, so this function provides the artillery to solve complicated differential equations in meshed regions using linear algebra. FEM takes as input the triangulation \mathtt{tri} , the non-contact set D, the boundary dD, and the locators \mathtt{iDs} and \mathtt{idDs} . It uses this information to find the solution to the obstacle problem U and the solution to the harmonic equation V.

FEM starts by concatenating the lists of boundary nodes and non-contact nodes into D_{-} , which is supposed to resemble "the closure of D" (lines 173-174). The remainder of the function is focused on populating the *shape matrices* Ku, Kv and *force matrices* Fu, Fv with the correct values.

This code was mostly created by Dr. LeCrone in MATLAB and adapted to Python by me, so he is by far the most knowledgeable about the details here. Notice, though, the overarching nested loop structure. The function loops through every index \pm corresponding to points in D_. If \pm corresponds with a boundary point, it populates the corresponding elements of the matrices a certain way (lines 184-188). However, if \pm corresponds to a non-contact point, the corresponding elements of the matrices are populated a different way (lines 190-213). Eventually, the matrices are used to solve two matrix equations, as is traditionally done in Finite Element Method, yielding solutions to two different differential equations related to the obstacle problem.

Use the optional plot input to visualize both solutions.

The second function you'll need to create has to take as input the solutions to the differential equations and make algorithmic adjustments to the signed distance function ϕ to refine the approximation of the boundary of the non-contact set (hence the title "shape optimization" from Sharma-Rangarajan). The last four functions should be compatible in an iterative, looping format, general enough to accept and handle each updated phis and tri.

<u>Interact</u>

Call assembly() again and ponder the sequence in which the functions are currently executed. With Dr. LeCrone, discuss the modifications to the overall structure of the assembly necessary to complete an iterative, looping optimization process (instead of a single initialization). The loop will probably be a while loop, executing until a certain condition or level of tolerance is satisfied.

HELPER FUNCTIONS

Helper functions are quicker algorithms that will be useful in coding the complex functions. They make a task easier by reducing a common problem into a few short inputs.

```
get_Gs(locs) and get_phis(locs)
```

These functions take as input a list of locations on the cylinder and outputs the values of Green's function or paraboloid at those locations using list comprehension (fast!).

unique(a)

Takes a 1 (2)-dimensional array a and outputs an array of equal dimension with duplicate elements (rows) removed. There's a numpy routine for this (numpy.unique), but I found it difficult to figure out, so I drafted up my own. Feel free to use my method or the one made by experts at your leisure!

vnvFinder(tri, k)

Delaunay triangulation objects have a useful attribute called <code>vertex_neighbor_vertices</code> which is simple in theory but difficult to code. The method allows you to input a particular node index and get the indices of all neighboring nodes. Luckily, <code>scipy</code> has taken care of most of the hard work for us, but they left some gymnastics for the user. Luckily for <code>you</code>, I've taken care of the rest of those gymnastics so that you can use the feature quickly.

Input the triangulation object tri and the index k of the node in question. Outputted are the indices of the neighboring vertices.

<u>Interact</u>

• Create and store a triangulation object tri using initializeMesh(). Use vnvFinder() to find the indices of the neighbor vertices to vertex number 1000. Print tri.points[1000] and tri.points[vnvFinder(tri, 1000)].

shoelaceArea(vertices) and
sumSideSquare(vertices)

```
def shoelaceArea(vertices):
    z,t = np.transpose(vertices)
292
293    return 1/2*(np.dot(z,np.roll(t,-1)) - np.dot(np.roll(z,-1),t))
294
295
296
297    def sumSideSquare(vertices):
298
299    return sum(np.sum((vertices - np.roll(vertices,1,axis=0))**2, axis=1))
```

Blazing fast algorithms to find the *signed area* and *sum of squared side lengths* of a simple polygon given the coordinate locations of its vertices. Input vertices as a 2-dimensional array and get the quantities you want. It's that simple. I used these when coding the next few helper methods, so these are helpers to helpers.

getQ(vertices)

Gets the "quality factor" Q of a triangle, a sort of measure of the area-to-perimeter ratio of the triangle. A high quality triangle is close to equilateral while a low quality triangle is very scalene/obtuse. This method is necessary in conjunction with the next few in updating the triangulation in an algorithmically clean way.

Interact

• Create any set of three vertices v defining a triangle (as a 3 x 2 matrix). Call shoelaceArea(v), sumSideSquare(v), and getQ(v). Do this with a few triangles and get a sense for the functions.

worstQ(iVertex, tri, direction, lamb,
returnall=False)

Pretty dang cool little method that may be my most treasured piece of code that I created in this document. Input the index of any node <code>iVertex</code>, the triangulation <code>tri</code>, then the <code>direction</code> ('z' or 't') and distance <code>lamb</code> that you'd like to perturb the vertex. The method temporarily changes the location of some node in the triangulation and calculates the quality factor of each element containing that node, i.e. each element in the *1-ring*. The lowest quality factor calculated among those elements is returned. I know it sounds niche, but it turns out to be useful for adjusting the triangulation in smart ways.

What the heck am I doing in this method? It's a little complicated and unenlightening to explain, but I've left my original personal comments in the code document for future reference. Hopefully the next function makes the idea a little clearer.

optimizeQ(iVertex, tri, direction, guess=0)

```
def optimizeQ(iVertex, tri, direction, guess=0):
    func = lambda lamb : -1*worstQ(iVertex, tri, direction, lamb)
    return fmin(func, guess)
```

Now, I'm using worstQ to my advantage with fmin, a scipy function used to find a local minimum of a continuous function. As required by fmin, I create a quick function using worstQ, fixing iVertex, tri, and direction, but allowing lamb to fluctuate. I multiply in -1 so that my fmin is really an "fmax" (does not exist, don't try to find it in scipy). fmin then uses an optimization algorithm to determine the local extremum of the function I pass in, which should be somewhere around the optional parameter guess.

Think about what this is doing for a second: we're perturbing the location of a node in the triangulation to figure out the location at which the *worst quality triangle in the 1-ring is at a maximum*. It is in this configuration that the elements are closest to equilateral, in total.

This will be useful in <code>conformMesh()</code>. You'll be moving vertices around to best fit an estimation of the non-contact boundary, then "controlling the damage" to the local equilateral-ness of elements, requiring slight changes to elements in the entire mesh.

QPlot1d(iVertex, tri, direction, lambs, includeAll=True, includeMin=True)

```
def QPlot1d(iVertex, tri, direction, lambs, includeall=True, includemin=True):
346
347
    Qs = []
    for lamb in lambs:
        Q = worstQ(iVertex, tri, direction, lamb, returnall=True)
350
    Qs = np.array([Q]) if len(Qs)==0 else np.vstack((Qs, Q))
351
    if includeall: [plt.plot(lambs, Qs[:,1]) for 1 in range(len(Qs[0]))]
352
    if includemin: plt.plot(lambs, np.min(Qs, axis=1), 'k', linewidth=4)
plt.xlabel(r"Perturbation $\lambda\seta\")
plt.ylabel(r"Quality $Qs\")
355
    plt.grid()
357
    return
```

I wanted to visualize this complicated idea, and if you do too, you've come to the right place.

Side note: this is a helper function which doesn't provide elegance to another part of the code, but instead actually helps the user understand what's going on! Feel free to include your own methods of this sort during your coding journey.

Same inputs as worstQ, except that you supply a bunch of values lambs at which you'd like to measure the worst quality. In a more human way, you're visually doing what optimizeQ is doing. QPlotld can plot the quality of each triangle in the 1-ring at each perturbation value (with optional parameter includeall) and can bold the worst quality at each lamb (with parameter includemin).

<u>Interact</u>

 Get a triangulation tri from initializeMesh(). Call QPlotld, centralizing node number 1000, perturbing along the 't' axis, with 50 lamb values between -0.08 and 0.08.
 Try to make sense of what you see by adjusting some of these parameters. It's really cool stuff!

projectToZeroLine(points, i)

Quick function that does a series of geometric calculations using Python's sympy package.

Input points, a 3 x 3 array which defines coordinate locations of vertices of a triangle in 3-dimensional $(z,\theta,\varphi(z,\theta))$ space. One or two points have $\varphi>0$ while the other(s) have $\varphi<0$. That means the z,θ plane intersects the triangle formed by points, and the intersection is a line segment. Finally, input index i and find the closest point projection onto that line segment.

This method should, again, be useful when you code conformMesh. I've done my best to give a headstart into the development of that method with this helper and optimizeQ.

Disclaimer: it's actually not possible to perform a closest point projection onto a line segment with sympy, and I'm not sure you can find a publicly available package with that functionality. What I've done is a closest point projection onto the *line* formed by intersection the whole plane formed by points and the z, θ plane.

Interact

(Advanced) Resolve the disclaimer: modify this method to actually project onto the line segment produced by intersecting the triangle formed by points and the z, θ plane. Do this by first projecting onto the line (as I've already done), then checking to see if your projection is contained within the segment encompassed by the triangle (this will take work). If so, leave the projection be. If not, move the projection to the closer endpoint of the segment.