

Does the *TSP* intersect the *NNG*?

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SYNOPSIS

Does the Euclidean TSP for a finite set of points P share an edge with P 's nearest neighbor graph?

¹ Or its k -NNG? Or the Delaunay Graph? Or indeed any poly-time computable graph spanning the input points? We investigate this question experimentally by checking the validity of this conjecture for various instances in TSPLIB, for which the optimal solutions have been provided and for other synthetic data-sets (e.g. uniformly and non-uniformly generated points) for which we can compute optimal or near-optimal tours using Concorde.

DESCRIPTION

The question posed in the title came about while working on the Horsefly problem, a generalization of the famously *NP*-hard Travelling Salesman Problem ². One line of attack was to get at some kind of structure theorem by identifying a candidate set of good edges from which a near-optimal solution to the horsefly problem could be constructed. But first off, would this approach work for the special case of the TSP? Answering " $TSP \cap NNG \stackrel{?}{=} \emptyset$ " seemed like a good place to start. However, all attempts at constructing examples where the intersection is *empty* failed. And so did a literature search! The closest matching reference we found was [HS14] which *eliminates* edges that cannot be part of a Euclidean TSP tour on a given instance of points, based on checking a few simple, local geometric inequalities. ³ There was also a very much related discussion thread on David Eppstein's [webpage](#). A small counter-example is given near the bottom of that link.

But the thread says nothing about whether the DT *must* intersect the TSP at least a certain fraction of times, or indeed even once. ⁴

See also this [blogpost](#) on the topic, which talks about using the Delaunay Triangulations for generating heuristically good (no bounds are given) TSP tours. Another approach using Del Tris is taken in [this technical report](#)

Knowledge of some family of easily computed edges that are necessarily part of a TSP solution could potentially be used to speed up some of the existing solutions to TSP using combinatorial optimization methods; see, e.g., Concorde [App+09] and other papers of Bill Cook.

5

¹In this article, we will assume the NNG to be undirected i.e. after constructing the nearest neighbor graph for a point-set we will throw away the edge directions.

²In this report by "*TSP*", we mean *TSP*-cycle and not *TSP*-path, although the question is still interesting for the path case. One reason for focusing only on the path case, is that the Concorde library (to the author's knowledge) computes only optimal cycle solutions and **not** optimal path solutions!

³The author believes this will be a useful reference for future work

⁴Perhaps, we can follow up with Dillencourt or Eppstein if they have notes on this?

⁵The landmark PTAS'es for the TSP, such as those of Mitchell [Mit99] and Arora[Aro96], are too complicated to be put

To spur our intuition, we investigate the conjecture experimentally in this short report ⁶ using TSPLIB and Concorde in tandem. TSPLIB [Rei91] is an online collection of medium to large scale instances of the Metric, the Euclidean and a few other variants of the TSP Concorde can compute the optimal solutions in nearly all the instances; the certificate of optimality — as always! — coming from the comparison of the computed tour-length against a lower bounds (also computed by Concorde).

For starters, we investigate the following questions ⁷: for each symmetric 2-D Euclidean TSP instance from TSPLIB for which we have an optimal solution, does

- ❖ $TSP \cap (k\text{-})NNG \stackrel{?}{=} \emptyset$, for $k = 1, 2, \dots$
- ❖ $TSP \cap \text{Delaunay Graph} \stackrel{?}{=} \emptyset$
- ❖ For question 1 what fraction (a fourth?, a fifth?) of the n edges of a TSP-tour share its edges with the k -NNG does the TSP intersect for various values of k ?
- ❖ Are there any structural patterns observed in the intersections? Specifically, does *at least* one edge from the intersection with the 1-NNG have one of its *vertices* on the convex hull? ⁸ More generally, is this true for every layer of the onion, and not just the outer layer (i.e, the convex hull)?

See also the Appendix II for a running wishlist of questions that come out during discussions.

As an aid in constructing possible counter-examples, a GUI interface is provided to mouse-in points and then run various tests on the points inputted.

If you don't have Python 3.7+ on your machine, download the free [Anaconda](#) distro of Python; it comes with most of the batteries included. See Appendix I for instructions on how to install and run the code.

into code (yes, even Python!). On the other hand, the Concorde library [App+09] or Helsgaun's methods [Hel00] use a whole kitchen-sink of practical techniques such as k -local swaps, branch-and-bound, branch-and-cut to generate near-optimal (if not optimal) tours very fast. But it would be interesting to investigate the behavior of the various graphs with respect to the techniques used in the PTAS'es of Mitchell and Arora. Maybe we can augment them with the probabilistic method (the pigeon-hole principle on steroids!) or something from Ramsey Theory to prove the existence of an intersection??

⁶This report has been written as a literate program [Knu84; Ram08] to weave together the code, documentations, explanations and generated data into the same document. Brickbats and bouquets on the author's preliminary stab at Literate Programming are most welcome.

⁷Experimental answers to other questions will be barnacled onto the report as it grows

⁸This indeed seemed to be the case in all the author's failed attempts at a counter-example, and so a proof/disproof of this conjecture would be helpful

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1 OVERALL STRUCTURE OF TSPNNG.PY

The `tspnng.py` file at a high level divided into the following chunks, each of which is expanded upon in the coming sections. The `main.py` file used to run the `main()` function from the command-line is more of a scratchpad for testing the functions in this file, and later pointing the main to the appropriate test harnesses inside the `tspnng.py` file. Hence `main.py` will be developed independently of this document for convenience because it will be subject to continuous changes. .

4a $\langle \textit{tspnng.py} \text{ 4a} \rangle \equiv$

$\langle \textit{Headers} \text{ 4b} \rangle$
 $\langle \textit{Data Generation} \text{ 5} \rangle$
 $\langle \textit{Generic utility classes and functions} \text{ 10a} \rangle$
 $\langle \textit{Functions for plotting and interacting} \text{ 11} \rangle$
 $\langle \textit{Functions for generating various graphs} \text{ 18} \rangle$
 $\langle \textit{Functions dealing with intersecting two geometric graphs} \text{ 28b} \rangle$
 $\langle \textit{Testing hypotheses} \text{ 29c} \rangle$

4b $\langle \textit{Headers} \text{ 4b} \rangle \equiv$ (4a) 13b▷

```
import matplotlib.pyplot as plt
import matplotlib as mpl
from matplotlib import rc
rc('font',**{'family':'serif','serif':['Palatino']})
rc('text', usetex=True)

import scipy as sp
import numpy as np
import random
import networkx as nx

from sklearn.cluster import KMeans
import argparse, os, sys, time
from colorama import init, Fore, Style, Back
init() # this line does nothing on Linux/Mac,
      # but is important for Windows to display
      # colored text. See https://pypi.org/project/colorama/
import yaml
```

2 DATA GENERATION

$$\begin{aligned}
 5 \quad \langle \textit{Data Generation } 5 \rangle &\equiv & (4a) \\
 \langle \textit{TSPLIB data } 7 \rangle & \\
 \langle \textit{Synthetic data } 9 \rangle &
 \end{aligned}$$

TSPLIB data-sets

Figure 1 is a screenshot of the entire opening page of [Rei91] that should more than suffice as an intro to this popular set of benchmarks for various TSP-like problems.⁹

TSPLIB is a library of sample instances for the TSP (and related problems) from various sources and of various types. Instances of the following problem classes are available.

Symmetric traveling salesman problem (TSP)
 Given a set of n nodes and distances for each pair of nodes, find a roundtrip of minimal total length visiting each node exactly once. The distance from node i to node j is the same as from node j to node i .

Hamiltonian cycle problem (HCP)
 Given a graph, test if the graph contains a Hamiltonian cycle or not.

Asymmetric traveling salesman problem (ATSP)
 Given a set of n nodes and distances for each pair of nodes, find a roundtrip of minimal total length visiting each node exactly once. In this case, the distance from node i to node j and the distance from node j to node i may be different.

Sequential ordering problem (SOP)
 This problem is an asymmetric traveling salesman problem with additional constraints. Given a set of n nodes and distances for each pair of nodes, find a Hamiltonian path from node 1 to node n of minimal length which takes given precedence constraints into account. Each precedence constraint requires that some node i has to be visited before some other node j .

Capacitated vehicle routing problem (CVRP)
 We are given $n - 1$ nodes, one depot and distances from the nodes to the depot, as well as between nodes. All nodes have demands which can be satisfied by the depot. For delivery to the nodes, trucks with identical capacities are available. The problem is to find tours for the trucks of minimal total length that satisfy the node demands without violating truck capacity constraint. The number of trucks is not specified. Each tour visits a subset of the nodes and starts and terminates at the depot. (Remark: In some data files a collection of alternate depots is given. A CVRP is then given by selecting one of these depots.)

Except, for the Hamiltonian cycle problems, all problems are defined on a complete graph and, at present, all distances are integer numbers. There is a possibility to require that certain edges appear in the solution of a problem.

Figure 1: Screenshot of the opening page of [Rei91]

In this document we will be interested in that subset of instances corresponding to the Symmetric TSP with the standard Euclidean Metric. Pages 9 through 11 of [Rei91] contain 4-column tables with all Symmetric TSP instances. We will be focusing precisely on those instances which have their 3rd column marked “EUC_2D”.

The entire symmetric TSP data-set has been downloaded into the

`./sym-tsp-tsplib/instances/sym-tsp-tsplib/instances/tsplib_symmetric_tsp_instances/`

directory. After writing a small Python script¹⁰ the subset of EUC_2D instances were converted into the convenient YAML format and copied into the

`./sym-tsp-tsplib/instances/sym-tsp-tsplib/instances/euclidean_instances_yaml/`

directory. *Unless otherwise noted, we will restrict our attention to this directory when talking about TSPLIB data.*

To see what the point-sets look like peep into the folder `tsplib_euc2d_pictures_of_instances` contained in the top level directory of the code. Note that the numbers affixed to each instance name indicate the number of points in that instance. See Figure 2 for some examples.

This chunk implements two functions: the first one returns the full path names of each of the Euclidean

⁹Prof. Sandor Fekete has a much larger collection of interesting TSP data-sets, I believe?

¹⁰`tsplib_to_yaml.py` in that same directory

instances in an list and the second one reads in a TSPLIB instance (identified by its file-name e.g. 'berlin52.yml') in the `euclidean_instances_yaml` directory and returns a list of 2D points for that instance.

7 $\langle TSPLIB \text{ data } 7 \rangle \equiv$ (5)

```
def get_names_of_all_euclidean2D_instances(dirpath=\
    "./sym-tsp-tsplib/instances/euclidean_instances_yaml/" ):

    inst_names = []
    for name in os.listdir(dirpath):
        full_path = os.path.join(dirpath, name)
        if os.path.isfile(full_path):
            inst_names.append(name)
    return inst_names

def tsplib_instance_points(instance_file_name,\
    dirpath="./sym-tsp-tsplib/instances/euclidean_instances_yaml/"):

    print(Fore.GREEN+"Reading " + instance_file_name, Style.RESET_ALL)
    with open(dirpath+instance_file_name) as file:
        data = yaml.load(file, Loader=yaml.FullLoader)
        points = np.asarray(data['points'])

    return points
```

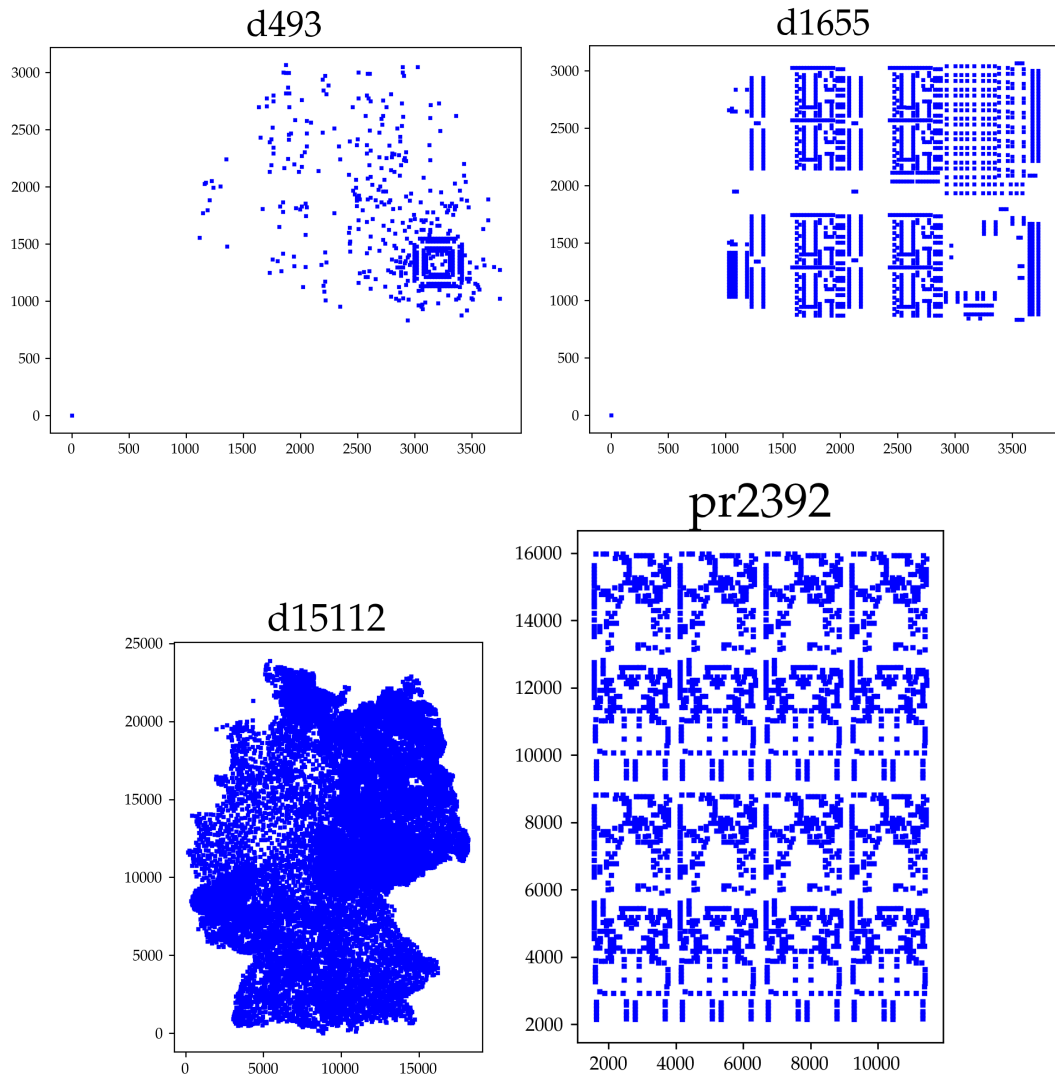


Figure 2: Instances of four TSPLIB data sets for the Symmetric TSP with 2D Euclidean Metric

Synthetic data-sets

Alongside TSPLIB we will also be using synthetic data-sets i.e. uniform and non-uniform point-sets generated inside the unit-square $[0, 1] \times [0, 1]$. Note that each point is represented as a numpy array of size 2.

This chunk generates uniform and non-uniform point sets in $[0, 1] \times [0, 1]$. To generate non-uniform point-sets we basically take a small set of uniformly distributed random points in the square, place a small square centered around each such random point and then generate the appropriate number of points uniformly inside each of those squares.¹¹ The size of the square is proportional to the distance of the sampled point from the boundary of the unit square. Thus you will often see tight clusters near the boundary as you increase the number of input points (`'numpts'`). This was done to make sure all points get generated in the unit square. This would make it convenient for the purposes of plotting. Other non-uniform point-generation schemes will later be considered depending on which direction our investigation proceeds.

9 *⟨Synthetic data 9⟩*≡ (5)

```
def uniform_points(numpts):
    return sp.rand(numpts, 2).tolist()

def non_uniform_points(numpts):

    cluster_size = int(np.sqrt(numpts))
    numcenters   = cluster_size
    centers       = sp.rand(numcenters, 2).tolist()
    scale, points = 4.0, []

    for c in centers:
        cx, cy = c[0], c[1]
        sq_size = min(cx, 1-cx, cy, 1-cy)

        loc_pts_x = np.random.uniform(low = cx-sq_size/scale,
                                       high = cx+sq_size/scale,
                                       size = (cluster_size,))
        loc_pts_y = np.random.uniform(low = cy-sq_size/scale,
                                       high = cy+sq_size/scale,
                                       size = (cluster_size,))

        points.extend(zip(loc_pts_x, loc_pts_y))

    num_remaining_pts = numpts - cluster_size * numcenters
    remaining_pts = sp.rand(num_remaining_pts, 2).tolist()
    points.extend(remaining_pts)
```

¹¹A somewhat similar method was used in Jon Bentley's experimental TSP paper

```
return points
```

3 DATA STORAGE

YAML[BKEI09] is a convenient serialization and data-interchange format that we will be using for serializing output data of different experiments onto disk. Python has particularly good libraries for dealing with YAML. Basically, YAML records data in a format similar to a Python dictionary. Infact the `yaml` module provides a function that transparently encodes any (appropriate) Python dictionary into a YAML file. In the function below, the `data` argument is a dictionary, and `dir_name` and `file_name` are strings.

```
10a  <Generic utility classes and functions 10a>≡ (4a) 10b>
      def write_to_yaml_file(data, dir_name, file_name):
          with open(dir_name + '/' + file_name, 'w') as outfile:
              yaml.dump( data, outfile, default_flow_style = False)
```

4 SETTING UP TSPNNGINPUT CLASS

The following class is used to keep track of the points inserted thus far, along with any other auxiliary information. It basically functions as a convenience wrapper class around the main input data (basically a bunch of points in \mathbb{R}^2) and a wrapper function around various graph generators such as TSP, Delaunary, k -NNG etc.

```
10b  <Generic utility classes and functions 10a>+≡ (4a) <10a>
      class TSPNNGInput:
          def __init__(self, points=[]):
              self.points = points

          def clearAllStates (self):
              self.points = []

          def generate_geometric_graph(self,graph_code):
              pass
```

5 SETTING UP THE INTERACTIVE CANVAS

The following set of code blocks create an interactive matplotlib canvas onto which the user can insert points, and then run the appropriate algorithm to visualize the intersection of the TSP and various graphs.

We first set up the run handler function (each “run” corresponds to a run of the code on a particular data-set generated synthetically) by connecting the keyboard and mouse handlers to the canvas.

```

11  ⟨Functions for plotting and interacting 11⟩≡ (4a) 12▷
    def run_handler():
        fig, ax = plt.subplots()
        run = TSPNNGInput()

        ax.set_xlim([xlim[0], xlim[1]])
        ax.set_ylim([ylim[0], ylim[1]])
        ax.set_aspect(1.0)
        ax.set_xticks([])
        ax.set_yticks([])

        mouseClicked = wrapperEnterRunPointsHandler(fig,ax, run)
        fig.canvas.mpl_connect('button_press_event' , mouseClicked )

        keyPress      = wrapperkeyPressHandler(fig,ax, run)
        fig.canvas.mpl_connect('key_press_event', keyPress      )
        plt.show()

```

There are two principal callback functions `wrapperEnterRunPointsHandler` and `wrapperkeypressHandler` used in the code above. These encode the interaction between the mouse and keyboard to the matplotlib canvas.

First we define the call back function for mouse-clicks. Double-clicking the left mouse button (denoted as “button 1” in the matplotlib world) inserts a small circle patch representing a point. Note that each mouse click clears the canvas and freshly draws the input point-set from scratch. This helps with modifying an existing input to check how solution changes.

```

12  <Functions for plotting and interacting 11>+≡ (4a) <11 13a>
    xlim, ylim = [0,1], [0,1]
    def wrapperEnterRunPointsHandler(fig, ax, run):
        def _enterPointsHandler(event):
            if event.name      == 'button_press_event'      and \
               (event.button   == 1)                        and \
               event.dblclick == True                       and \
               event.xdata    != None                       and \
               event.ydata    != None:
                newPoint = np.asarray([event.xdata, event.ydata])
                run.points.append( newPoint )
                print("You inserted ", newPoint)

                patchSize = (xlim[1]-xlim[0])/130.0

                ax.clear()

                for pt in run.points:
                    ax.add_patch( mpl.patches.Circle( pt, radius = patchSize,
                                                       facecolor='blue', edgecolor='black' ))

                ax.set_title('Points Inserted: ' + str(len(run.points)), \
                             fontdict={'fontsize':25})
                applyAxCorrection(ax)
                fig.canvas.draw()

        return _enterPointsHandler

```

Now a call-back function for keyboard. Pressing ‘i’ or ‘I’ on the keyboard further prompts the user to insert a 2 or 3 letter code to indicate which graph should span the points.

```

13a  <Functions for plotting and interacting 11>+≡ (4a) <12 17b>
    def wrapperkeyPressHandler(fig,ax, run):
        def _keyPressHandler(event):
            if event.key in ['n', 'N', 'u', 'U']:
                <Enter type of point set to generate 16a>
            elif event.key in ['t' or 'T']:
                <Compute TSP and find common edges with various spanning graphs 14>
            elif event.key in ['i', 'I']:
                <Compute spanning graph 15>
            elif event.key in ['x', 'X']:
                <Clear all line segments from the canvas 16b>
            elif event.key in ['c', 'C']:
                <Clear all states and the canvas 17a>
        return _keyPressHandler

```

We now elaborate on the chunks in `wrapperkeypresshandler`, and implement the boring technicalities. You can skip ahead to the next sections, at this point, if you wish.

First we compute the TSP and then print a table mentioning how many of its edges are common to other standard graphs. See <https://pypi.org/project/prettytable/> for more information on the `prettytable` module used to output data to terminal.

```

13b  <Headers 4b>+≡ (4a) <4b>
    from prettytable import PrettyTable

```

14 \langle Compute TSP and find common edges with various spanning graphs 14 $\rangle \equiv$ (13a)

```

tsp_graph = get_concorde_tsp_graph(run.points)
graph_fns = [(get_delaunay_tri_graph, 'Delaunay Triangulation'), \
              (get_mst_graph, 'Minimum Spanning Tree'), \
              (get_onion_graph, 'Onion') ]

tbl = PrettyTable()
tbl.field_names = ["Spanning Graph (G)", "G", "G \cap T", "T", "(G \cap T)/T"]

num_tsp_edges = len(tsp_graph.edges)
for ctr, (fn_body, fn_name) in zip(range(1,1+len(graph_fns)), graph_fns):
    geometric_graph = fn_body(run.points)
    num_graph_edges = len(geometric_graph.edges)
    common_edges = list_common_edges(tsp_graph, geometric_graph)
    num_common_edges_with_tsp = len(common_edges)

    tbl.add_row([fn_name, \
                 num_graph_edges, \
                 num_common_edges_with_tsp, \
                 num_tsp_edges, \
                 "{perc:3.2f}".format(perc=1e2*num_common_edges_with_tsp/num_tsp_edges)+ ' %' ])
print(tbl)
render_graph(tsp_graph,fig,ax)
fig.canvas.draw()

```

In a kind of “dual” demo, we now compute and render the various geometric graphs, and then mention how many edges each graph has in common with the TSP. Thus we can explore the intersection of the TSP with a graph from the point-of-view of both the TSP and the graph.

The user should type the code enclosed in the brackets (e.g. ‘dt’ for delaunay triangulation) to generate the indicated graph that spans the points.

```

15  <Compute spanning graph 15>≡ (13a)
    algo_str = input(Fore.YELLOW + "Enter code for the graph you need to span the points:\n" + Sty
                        "(knng)   k-Nearest Neighbor Graph           \n"           +\
                        "(mst)    Minimum Spanning Tree           \n"           +\
                        "(onion)  Onion                           \n"           +\
                        "(dt)     Delaunay Triangulation           \n"           +\
                        "(conc)   TSP computed by the Concorde TSP library \n" +
                        "(pytsp)  TSP computed by the pure Python TSP library \n")
    algo_str = algo_str.lstrip()

    if algo_str == 'knng':
        k_str = input('==> What value of k do you want? ')
        k      = int(k_str)
        geometric_graph = get_knng_graph(run.points,k)

    elif algo_str == 'mst':
        geometric_graph = get_mst_graph(run.points)

    elif algo_str == 'onion':
        geometric_graph = get_onion_graph(run.points)

    elif algo_str == 'dt':
        geometric_graph = get_delaunay_tri_graph(run.points)

    elif algo_str == 'conc':
        geometric_graph = get_concorde_tsp_graph(run.points)

    elif algo_str == 'pytsp':
        geometric_graph = get_py_tsp_graph(run.points)

    else:
        print(Fore.YELLOW, "I did not recognize that option.", Style.RESET_ALL)
        geometric_graph = None

    common_edges = list_common_edges(get_concorde_tsp_graph(run.points), geometric_graph)
    print("-----")
    print("Number of edges in " + algo_str + " graph (TOTAL)           :", len(geom

```

```
print("Number of edges in " + algo_str + " graph which are also in Concorde TSP      :", len(comm
print("-----", Style.RESET_ALL)
```

```
ax.set_title("Graph Type: " + geometric_graph.graph['type'] + '\n Number of nodes: ' + str(len
render_graph(geometric_graph,fig,ax)
fig.canvas.draw()
```

If you want to enter a uniformly or non-uniformly distributed point-set in the unit-square press ‘u’ or ‘n’ respectively after being prompted.

16a *⟨Enter type of point set to generate 16a⟩≡* (13a)

```
numpts = int(input("\nHow many points should I generate?: "))
run.clearAllStates()
ax.cla()
applyAxCorrection(ax)

ax.set_xticks([])
ax.set_yticks([])
fig.texts = []

if event.key in ['n', 'N']:
    run.points = non_uniform_points(numpts)
else :
    run.points = uniform_points(numpts)

patchSize  = (xlim[1]-xlim[0])/140.0

for site in run.points:
    ax.add_patch(mpl.patches.Circle(site, radius = patchSize, \
                                   facecolor='blue',edgecolor='black' ))

ax.set_title('Points generated: ' + str(len(run.points)), fontdict={'fontsize':25})
fig.canvas.draw()
```

Sometimes, you just want to clear the edges of the network from the graph, so that a new graph can be rendered in its place on the points. For that, you need to press ‘x’ or ‘X’.

16b *⟨Clear all line segments from the canvas 16b⟩≡* (13a)

```
print(Fore.GREEN, 'Removing network edges from canvas' ,Style.RESET_ALL)
ax.lines=[]
applyAxCorrection(ax)
fig.canvas.draw()
```


If you want to wipe the canvas and the point-cloud data (and everything else ...) clean, then press ‘c’.

17a *<Clear all states and the canvas 17a>≡* (13a)

```
run.clearAllStates()
ax.cla()
```

```
applyAxCorrection(ax)
ax.set_xticks([])
ax.set_yticks([])
```

```
fig.texts = []
fig.canvas.draw()
```

Often the `ax` object has to be reset and cleaned of the various segment and circle patches, or even resetting the aspect ratio of the `ax` object to be 1.0. These “cleanup” functions that were called in some of the code blocks above are implemented next.

17b *<Functions for plotting and interacting 11>+≡* (4a) <13a 27a>

```
def applyAxCorrection(ax):
    ax.set_xlim([xlim[0], xlim[1]])
    ax.set_ylim([ylim[0], ylim[1]])
    ax.set_aspect(1.0)
```

```
def clearPatches(ax):
    for index , patch in zip(range(len(ax.patches)), ax.patches):
        if isinstance(patch, mpl.patches.Polygon) == True:
            patch.remove()
    ax.lines[:] = []
    applyAxCorrection(ax)
```

```
def clearAxPolygonPatches(ax):

    for index , patch in zip(range(len(ax.patches)), ax.patches):
        if isinstance(patch, mpl.patches.Polygon) == True:
            patch.remove()
    ax.lines[:] = []
    applyAxCorrection(ax)
```

6 GENERATING VARIOUS GEOMETRIC GRAPHS

For manipulating abstract graphs we use the NetworkX [HSSC08]¹². This section deals with generating the various geometric graphs using packages like Scipy and Sklearn and then converting them into a NetworkX graph with the necessary edge and node attributes. Note that all the nodes in the abstract constructed below have the same numbering across all graphs have the same numbering across all graphs: namely, the order in which the points occur in the `points` array argument.

k -NNG

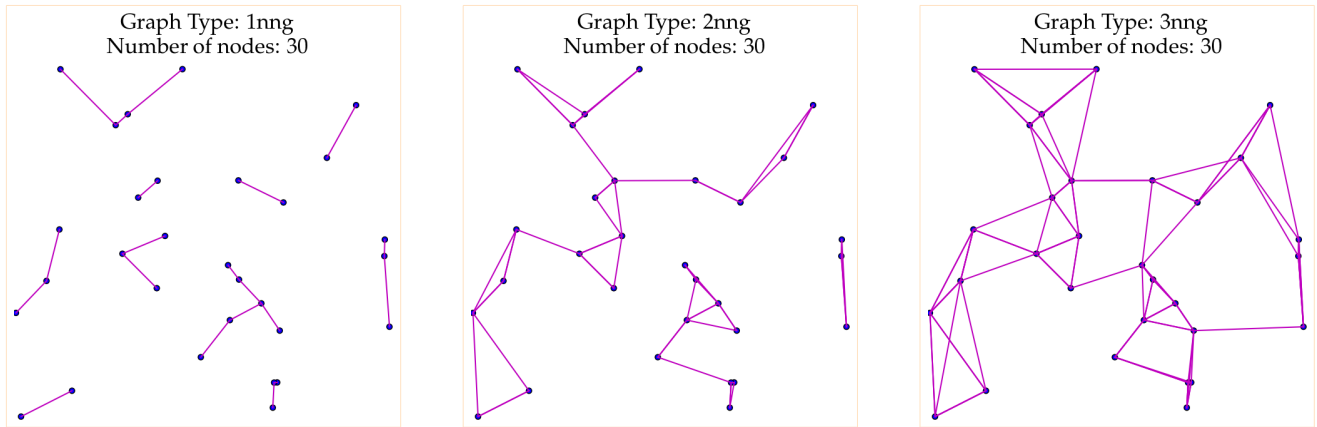


Figure 3: Generating the k -NNG graphs with Scikit-Learn for various value of k on the same set of 30 randomly generated points. Note that we are considering these graphs as undirected.

We use the nearest neighbor routine from the Scikit-learn [Ped+11] library. The documentation for the various nearest neighbor methods implemented therein can be found at <https://bit.ly/3nTQkqV>. Note that for the nearest-neighbor function of sklearn the k -nearest-neighbors of a point includes the point itself. Thus we use $(k + 1)$ in the argument to the `NearestNeighbors` function below, and take the last k elements in the list returned — the neighbors of a point are reported by that function in increasing order of distance from that point.

18 *<Functions for generating various graphs 18>≡* (4a) 20>

```
def get_knng_graph(points,k):
    from sklearn.neighbors import NearestNeighbors
    points      = np.array(points)
    coords      = [{"coords":pt} for pt in points]
    knng_graph = nx.Graph()
    knng_graph.add_nodes_from(zip(range(len(points)), coords))
    nbrs = NearestNeighbors(n_neighbors=(k+1), algorithm='ball_tree').fit(points)
    distances, indices = nbrs.kneighbors(points)
    edge_list = []

    for nbidxs in indices:
```

¹²already available inside the Anaconda Python distribution by default

```
nfix = nbidxs[0]
edge_list.extend([(nfix,nvar) for nvar in nbidxs[1:]])

knng_graph.add_edges_from( edge_list )
knng_graph.graph['type']    = str(k)+'nng'
knng_graph.graph['weight'] = None # TODO, also edge weights for each edge!!!
return knng_graph
```

Delaunay Triangulation

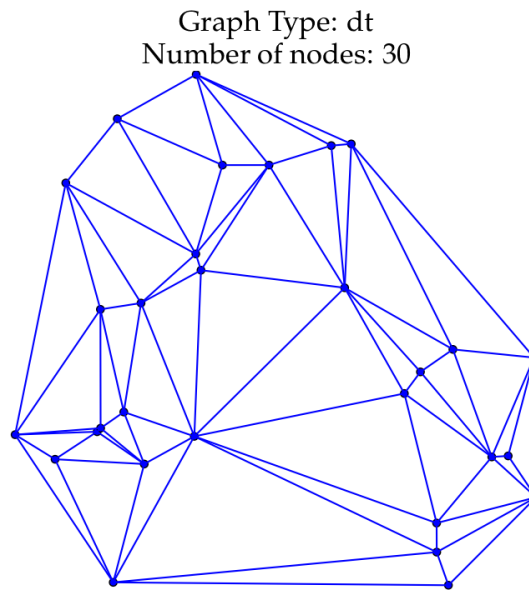


Figure 4: Example of a Delaunay Triangulation computed by SciPy on 30 randomly generated points

We use the [blackbox routine](#) for computing this graph implemented in Scipy [\[Vir+20\]](#).

20 \langle Functions for generating various graphs 18 $\rangle + \equiv$ (4a) \triangleleft 18 21 \triangleright

```
def get_delaunay_tri_graph(points):
    from scipy.spatial import Delaunay
    points      = np.array(points)
    coords      = [{"coods":pt} for pt in points]
    tri         = Delaunay(points)
    deltri_graph = nx.Graph()

    deltri_graph.add_nodes_from(zip(range(len(points)), coords))

    edge_list = []
    for (i,j,k) in tri.simplices:
        edge_list.extend([(i,j),(j,k),(k,i)])
    deltri_graph.add_edges_from( edge_list )

    total_weight_of_edges = 0.0
    for edge in deltri_graph.edges:
        n1, n2 = edge
        pt1 = deltri_graph.nodes[n1]['coods']
        pt2 = deltri_graph.nodes[n2]['coods']
        edge_wt = np.linalg.norm(pt1-pt2)

        deltri_graph.edges[n1,n2]['weight'] = edge_wt
    total_weight_of_edges = total_weight_of_edges + edge_wt
```

```

deltri_graph.graph['weight'] = total_weight_of_edges
deltri_graph.graph['type']   = 'dt'

return deltri_graph

```

Minimum Spanning Tree

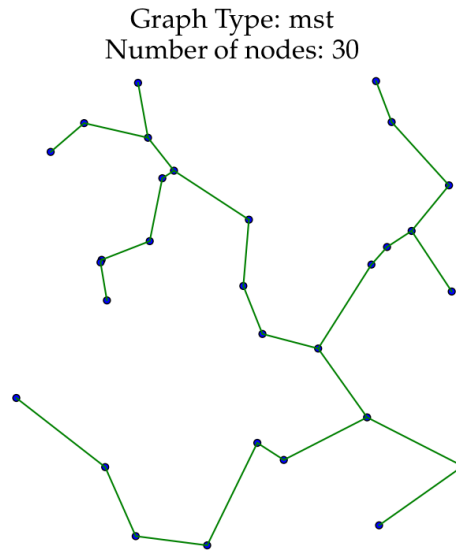


Figure 5: Example of a Minimum Spanning Tree computed by NetworkX on 30 randomly generated points

From elementary CG, we know that the MST of a set of points in the plane is a subset of the delaunay triangulation. Thus to compute the MST, it suffices to compute the MST of the corresponding delaunay triangulation. See [this page](#) for a documentation of the code in NetworkX used to compute the MST on an abstract weighted undirected graph. Note that along with the Kruskal method (used below), both Prim's and Boruvka's algorithms have also been implemented in that library.

21 *<Functions for generating various graphs 18>+≡* (4a) <20 22>

```

def get_mst_graph(points):

    points = np.array(points)
    deltri_graph = get_delaunay_tri_graph(points)
    mst_graph = nx.algorithms.tree.mst.minimum_spanning_tree(deltri_graph, \
                                                             algorithm='kruskal')

    mst_graph.graph['type']   = 'mst'
    return mst_graph

```

The Onion

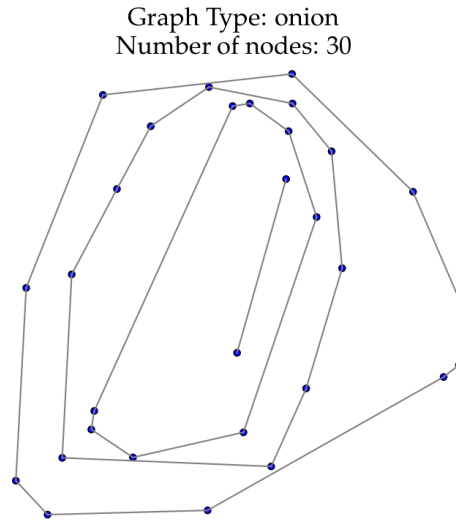


Figure 6: Example of the Onion graph computed with QHull (through SciPy) on 30 randomly generated points

Here we compute successive convex-hull of the point-set: compute the convex hull of the points, delete the hull points, compute the convex hull of this smaller point-set, repeating this process till we run out of points.

The resulting sequence of convex layers form a graph called the onion.

22 *⟨Functions for generating various graphs 18⟩*+≡ (4a) <21 25a>

```
def get_onion_graph(points):
    from scipy.spatial import ConvexHull
    points      = np.asarray(points)
    points_tmp  = points.copy()
    numpts     = len(points)
    onion_graph = nx.Graph()
    numpts_proc = -1

    ⟨ Definition of circular_edge_zip 23c⟩
    while len(points_tmp) >= 3:
        ⟨Generate convex hull of points remaining in points_tmp 23a⟩
        ⟨Update onion_graph 23b⟩
        ⟨Remove points reported in the convex hull from points_tmp 23d⟩

    if len(points_tmp) == 2:
        ⟨Join two remaining points by an edge in onion_graph 24a⟩
    elif len(points_tmp) == 1:
        ⟨Add the remaining points as a node in onion_graph 24b⟩
```

```

onion_graph.graph['type'] = 'onion'
return onion_graph

```

Note that the convex hull is computed by Scipy using the Qhull library as mentioned in the [docs](#).

23a \langle Generate convex hull of points remaining in points_tmp 23a $\rangle \equiv$ (22)

```

hull          = ConvexHull(points_tmp)
pts_on_hull   = [points_tmp[i] for i in hull.vertices]
coords        = [{"coods":pt} for pt in pts_on_hull]

```

23b \langle Update onion_graph 23b $\rangle \equiv$ (22)

```

new_node_idx = range(numpts_proc+1, numpts_proc+len(hull.vertices)+1)
onion_graph.add_nodes_from(zip(new_node_idx, coords))
onion_graph.add_edges_from(circular_edge_zip(new_node_idx))

```

Given a set of node ids of a graph provided as a list of integers, the following function, returns a cycle of edges with successive nodes joined in the order provided. e.g. $[1, 2, 3] \rightarrow [(1, 2), (2, 3), (3, 1)]$. Convenient to have this defined separately.

23c \langle Definition of circular_edge_zip 23c $\rangle \equiv$ (22)

```

def circular_edge_zip(xs):
    xs = list(xs) # in the event that xs is of the zip or range type
    if len(xs) in [0,1] :
        zi1 = []
    elif len(xs) == 2 :
        zi1 = [(xs[0],xs[1])]
    else:
        zi1 = list(zip(xs,xs[1:]+xs[:1]))
    return zi1

```

23d \langle Remove points reported in the convex hull from points_tmp 23d $\rangle \equiv$ (22)

```

numpts_proc = numpts_proc + len(hull.vertices)
rem_pts_idx = list(set(range(len(points_tmp))-set(hull.vertices))
points_tmp  = [ points_tmp[idx] for idx in rem_pts_idx ]
coords      = [{"coods":pt} for pt in points]

```

There are two edge cases: when only two points and one point remain. These cases, cannot be handled by Qhull (It reports an error at the terminal, saying it needs at least three points must be provided as input). Hence the separate treatment in the following two chunks.

When two nodes, remain, we just join them by an edge.

24a $\langle \text{Join two remaining points by an edge in onion_graph 24a} \rangle \equiv$ (22)

```

p, l = numpts_proc+1, numpts_proc+2
onion_graph.add_node(p)
onion_graph.add_node(l)
onion_graph.nodes[p]['coods'] = points_tmp[0]
onion_graph.nodes[l]['coods'] = points_tmp[1]
onion_graph.add_edge(p,l)

```

No edges to add here, just the node.

24b $\langle \text{Add the remaining points as a node in onion_graph 24b} \rangle \equiv$ (22)

```

l = numpts_proc+1
onion_graph.add_node(l)
onion_graph.nodes[l]['cood'] = points_tmp[0]

```

Traveling Saleman Tour (Cycle)

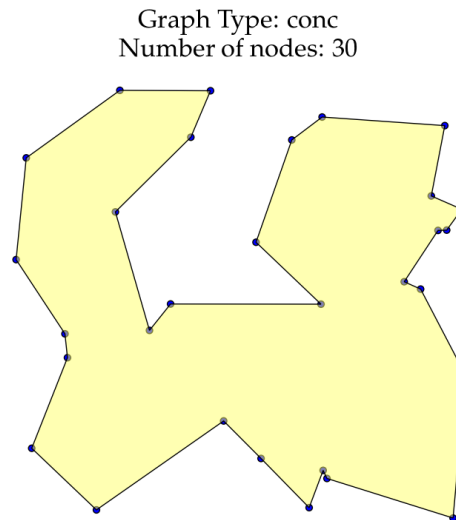


Figure 7: Example of an optimal TSP tour computed with Concorde on 30 randomly generated points

We use two separate independent routines that each compute the TSP. One is the `tsp` module available at <https://pypi.org/project/tsp/> the other being, Concorde, through its Python interface (whose github page can be accessed at <https://github.com/jvkersch/pyconcorde>). Anedoctally speaking the first solver works relatively quickly on point-sets upto size 30. Because of its simplicity, we used it in the intial stages of writing this report. It is clearly not competitive with Concorde (which can solve a 300 size instances in a couple of seconds), but it serves as a useful backup routine, in the event that a machine faces problems with the installation of PyConcorde.

* Using the tsp library

25a *⟨Functions for generating various graphs 18⟩+≡* (4a) ◁22 26▷

```
def get_py_tsp_graph(points):
    import tsp
    points = np.array(points)
    coords = [{"coods":pt} for pt in points]
    ⟨Generate TSP cycle and convert into NetworkX graph 25b⟩
    ⟨Compute weight of each edge and total edge weight 25c⟩
    ⟨Set graph attributes 25d⟩
    return tsp_graph
```

25b *⟨Generate TSP cycle and convert into NetworkX graph 25b⟩≡* (25a)

```
t = tsp.tsp(points)
idxs_along_tsp = t[1]
tsp_graph = nx.Graph()

tsp_graph.add_nodes_from(zip(range(len(points)), coords))
edge_list = list(zip(idxs_along_tsp, idxs_along_tsp[1:])) + \
              [(idxs_along_tsp[-1],idxs_along_tsp[0])]
tsp_graph.add_edges_from( edge_list )
```

25c *⟨Compute weight of each edge and total edge weight 25c⟩≡* (25a)

```
total_weight_of_edges = 0.0
for edge in tsp_graph.edges:

    n1, n2 = edge
    pt1 = tsp_graph.nodes[n1]['coods']
    pt2 = tsp_graph.nodes[n2]['coods']
    edge_wt = np.linalg.norm(pt1-pt2)

    tsp_graph.edges[n1,n2]['weight'] = edge_wt
    total_weight_of_edges = total_weight_of_edges + edge_wt
```

25d *⟨Set graph attributes 25d⟩≡* (25a)

```
tsp_graph.graph['weight'] = total_weight_of_edges
tsp_graph.graph['type'] = 'pytsp'
```

* Using the Pyconcorde library

This library is a thin interface around Concorde. Installing Pyconcorde automatically installs Concorde and other required libraries such as QSOpt. Instructions for installation are given in Appendix I.

Note that for the EUC_2D cases, the Concorde solver works only on points with integer coordinates. Since our synthetic data-sets will be generated inside the unit-square, we scale by the amount `scale_factor` and then rounded to an integer using `int()`. For a sufficiently large value `scaling_factor`, ordering of points reported by Concorde should be the same as if the algorithm was run on the unscaled points.

Note that Concorde crashes when you pass it only three points. Probably something to do with its internals. Of course for the case of one or two points, the package explicitly informs us that we must pass a longer list.

26 *⟨Functions for generating various graphs 18⟩+≡ (4a) <25a*

```
def get_concorde_tsp_graph(points, scaling_factor=1000):
    from concorde.tsp import TSPSolver
    points = np.array(points)
    coords = [{"coods":pt} for pt in points]

    xs = [int(scaling_factor*pt[0]) for pt in points]
    ys = [int(scaling_factor*pt[1]) for pt in points]
    solver = TSPSolver.from_data(xs, ys, norm='EUC_2D', name=None)
    print(Fore.GREEN)
    solution = solver.solve()
    print(Style.RESET_ALL)

    concorde_tsp_graph=nx.Graph()

    idxs_along_tsp = solution.tour
    concorde_tsp_graph.add_nodes_from(zip(range(len(points)), coords))
    edge_list = list(zip(idxs_along_tsp, idxs_along_tsp[1:])) + \
        [(idxs_along_tsp[-1],idxs_along_tsp[0])]
    concorde_tsp_graph.add_edges_from( edge_list )

    concorde_tsp_graph.graph['type']    = 'conc'
    concorde_tsp_graph.graph['found_tour_p'] = solution.found_tour
    concorde_tsp_graph.graph['weight'] = None ### TODO!!
    return concorde_tsp_graph
```

Graph Powers

7 RENDERING THE GRAPHS

For this we just draw each edge of the geometric graph as a straight line segment between the points (each of which happens to be a node of the graph).

For the special case of the TSP, we render it as a polygon patch, because the interior needs to be colored.

```

27a  <Functions for plotting and interacting 11>+≡ (4a) <17b>
def render_graph(G,fig,ax):
    if G is None:
        return
    <Set up edge colors depending on graph type 27b>
    if G.graph['type'] not in ['conc', 'pytsp']:
        <Iterate through graph edges and draw as segments 27c>
    else:
        <Draw tour as polygon patch 28a>

    ax.axis('off') # turn off box surrounding plot
    fig.canvas.draw()

27b  <Set up edge colors depending on graph type 27b>≡ (27a)
    edgecol = None
    if G.graph['type'] == 'mst':
        edgecol = 'g'
    elif G.graph['type'] == 'onion':
        edgecol = 'gray'
    elif G.graph['type'] in ['conc','pytsp']:
        edgecol = 'r'
    elif G.graph['type'] == 'dt':
        edgecol = 'b'
    elif G.graph['type'][-3:] == 'nng':
        edgecol = 'm'

27c  <Iterate through graph edges and draw as segments 27c>≡ (27a)

    for elt in list(G.nodes(data=True)):
        print(elt)

    for (nidx1, nidx2) in G.edges:
        x1, y1 = G.nodes[nidx1]['coods']
        x2, y2 = G.nodes[nidx2]['coods']
        ax.plot([x1,x2],[y1,y2],'-', color=edgecol)

```

Because the *interior* of the tour has to be colored, we render it as a polygon patch, and not just as a bunch of edges. Since I've stored the tour as a generic graph, the `.edges` data member of such a container, does not necessarily report the edges in the order encountered along the TSP.

But this order can trivially be extracted using depth first search.

28a $\langle \textit{Draw tour as polygon patch 28a} \rangle \equiv$ (27a)

```

from networkx.algorithms.traversal.depth_first_search import dfs_edges
node_coods = []
for (nidx1, nidx2) in dfs_edges(G):
    node_coods.append(G.nodes[nidx1]['coods'])
    node_coods.append(G.nodes[nidx2]['coods'])

node_coods = np.asarray(node_coods)
from matplotlib.patches import Polygon
from matplotlib.collections import PatchCollection

polygon = Polygon(node_coods, closed=True, \
                   facecolor=(255/255, 255/255, 102/255,0.5), \
                   edgecolor='k', linewidth=1)
ax.add_patch(polygon)

```

8 FINDING COMMON EDGES BETWEEN TWO GRAPHS

It is possible the same edge may exist in both the graphs but the indices recorded in the nodes may be in a different order. Hence, we explicitly define edges from two different graphs on the same set of nodes as being equal, if they are equal as sorted lists.

28b $\langle \textit{Functions dealing with intersecting two geometric graphs 28b} \rangle \equiv$ (4a) 29a \triangleright

```

def edge_equal_p(e1,e2):
    e1 = sorted(list(e1))
    e2 = sorted(list(e2))
    return (e1==e2)

```

To find the set of edges common to two graphs on the same set of nodes, we take each edge from one of the graphs and check whether it exists in the other.

29a \langle Functions dealing with intersecting two geometric graphs 28b $\rangle + \equiv$ (4a) \langle 28b 29b \rangle

```
def list_common_edges(g1, g2):
    common_edges = []
    for e1 in g1.edges:
        for e2 in g2.edges:
            if edge_equal_p(e1,e2):
                common_edges.append(e1)
    return common_edges
```

Finally, just a small function that tests if two graphs intersect.

29b \langle Functions dealing with intersecting two geometric graphs 28b $\rangle + \equiv$ (4a) \langle 29a

```
def graphs_intersect_p(g1,g2):
    flag = False
    if list_common_edges(g1,g2):
        flag = True
    return flag
```

9 HYPOTHESIS TESTING!

29c \langle Testing hypotheses 29c $\rangle \equiv$ (4a)

9 REFERENCES

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Appendices

I INSTALLING AND RUNNING THE CODE

The program can be downloaded from Github: <https://github.com/gtelang/tspnng>. Alternatively open a terminal and run the command, `git clone https://github.com/gtelang/tspnng.git`

The only other prerequisites for running the code, are the [Anaconda](#) distribution of Python 3 and a couple of other packages. To check if the Python executable is in your path (and that it is Python 3.7+) run the command `python --version`. If it succeeds, you have installed Anaconda!

The additional packages required can be installed by:

```
pip install colorama prettytable tsp13
git clone https://github.com/jvkersch/pyconcorde
cd pyconcorde
pip install -e .
```

To run the program, cd into the code's top-level folder, then type ¹⁴ any one of:

- ❖ `python src/main.py --interactive`
- ❖ `python src/main.py --batchtest`
- ❖ `python src/main.py --file <points.yaml>`

Interactive Mode

In this mode, one can mouse-in points onto a canvas (with double-clicks), run various network algorithms and render the them onto a GUI canvas.

Once you finish mousing in the points, press 'i'; that will open up a prompt at the terminal, asking which network do you want to compute on those points. Enter the code in the brackets.

If you don't want to mouse-in points, and just want to plaster uniformly distributed random points on the canvas, press u, and then type into the terminal the number of points. Same for non-uniform distributed points: for that press n.

Please note, in `interactive` mode you might see a warning in your terminal:

```
CoreApplication::exec: The event loop is already running
```

Please ignore it! It doesn't affect any of the results. Something in the the internals of Matplotlib that uses Qt triggers that message. `¬\('∩')_/_`.

¹³If you don't have superuser access during installation, add the flag `--user` at the end

¹⁴On Windows replace, the forward slash '/' by '\'

If you have any trouble — or detect a bug! — we can hash things out on Slack, Github or email.

II LAUNDRY-LIST OF QUESTIONS/VARIANTS/CONJECTURES

HAMILTONICITY STRUCTURE

We know that the Delaunay Triangulation of a set of points need not be Hamiltonian. In fact *detecting* Hamiltonicity of a Delaunay Triangulation is famously *NP*-complete [Dil96]

Two useful facts before we proceed:

Folklore

The cube of any connected, unweighted, graph is Hamiltonian. ¹⁵.

Fleischner's theorem [Geo09]

The square of any 2-vertex connected, unweighted, graph is Hamiltonian. ¹⁶

And so the following questions are natural:

- ❖ Based on the experiments results shown in this report, can we claim $TSP \subseteq DT^k$ or $TSP \subseteq MST^k$ in \mathbb{R}^2 for a *small* constant k ? I'd wager $k = 2, 3$ or, at worst, some very slowly growing function of n ¹⁷
- ❖ For $G = MST^3$, how good is the any (or the shortest??) Hamilton cycle through G in approximating the TSP? ¹⁸ Surely, this must be known, right? For the arrangement of n points at the roots of unity suggests that the approximation could be as bad as 3.
- ❖ What is the likelihood of MST^2 of n points $\in \mathbb{R}^2$ in general position being Hamiltonian? Any characterization of such point-sets?
- ❖ Given a set of points in \mathbb{R}^2 , does *ANY* (weakly/strongly) simple polygon and *ANY* triangulation on those points have an edge in common? This is surely not true, right?!

TSP \rightarrow Delaunay

- ❖ Suppose by some magic black box (Concorde! ☺) one has obtained the TSP tour through n points. Can we then compute the Delaunay Triangulation (or MST. Recall $MST \subseteq DT$) of the point-set in $O(n)$ time? It certainly seems so going by the high number of edges in the TSP common to the Delaunay and MST as suggested by the tests in this writeup. Surely the $TSP \rightarrow MST$ question in $O(n)$ time has been studied? Maybe the Okabe book on Voronoi etc. has something on this?

¹⁵It is sufficient to prove this fact for any tree, and then use it on the spanning tree of the given graph

¹⁶This last theorem certainly applies to Delaunay triangulations of general point-sets. By the square of a delaunay triangulation, I mean to say: throw away the edge weights and consider the square of the underlying unweighted graph. Once the new edges are added, consider them weighted with the natural euclidean distance between their endpoints

¹⁷ $\log(n)$ maybe?

¹⁸This is a cute vertex analog of the standard edge-doubling based 2-OPT heuristic, but is detecting such a cycle for a small MST power polytime? I'd bet yes. Probably the FPT experts have something to say on this topic.

This is kind of resonant of Melkman (i.e. simple poly chain \rightarrow convex hull in $O(n)$). Samir Khuller also had work (SODA 1992, iirc) in which he was able to compute a $O(1)$ (1.25, was it?) approximations to low-weight spanning trees of max degree 3 on point-sets in \mathbb{R}^2 , from an MST in linear time. That work was based on a very nice generalization of the triangle inequality¹⁹. Might that be exploitable here? Check his work.

It's, of course, complete baloney to compute triangulations or MSTs in this manner but when did *that* ever stop a computer scientist from being metaphysical?

- ❖ (Bizarre idea!!) Is the Min Weight (MW), or even better, the Min-Angle Maximizing (MAM) Triangulation of the TSP and its external pockets close to being Delaunay in some sense²⁰? Note that both MW and MAM triangulations of simple polygons can be computed by D.P. Should be fun to try this out experimentally. See also Sandor's ALENEX paper from 2015 where he did something about computing "bad" triangulations (iirc he wanted to minimize maximum angle i.e. make triangle skinny or sth), maybe compare against the triangulations obtained from his code, just to see how bad the TSP \rightarrow Delaunay heuristic is compared to the "bad end" of the spectrum?

¹⁹which bounded the perimeter of a triangle in terms of the sums of the distances of a point X to the points of that triangle. It generalizes the Δ inequality, when we set X to any of the vertices of the triangle. I forget the exact coefficients of his inequality which was linear or something

²⁰e.g. how good is the maximum value of the minimum angle in a triangle over all triangles different from OPT