Evolutionary Computation

2023/24

Master Artificial Intelligence

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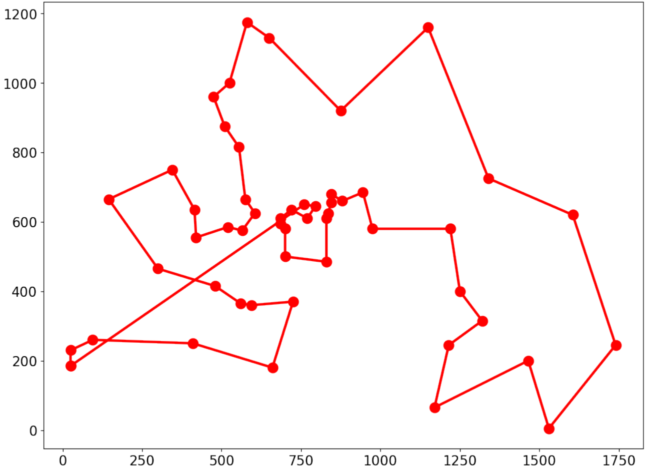
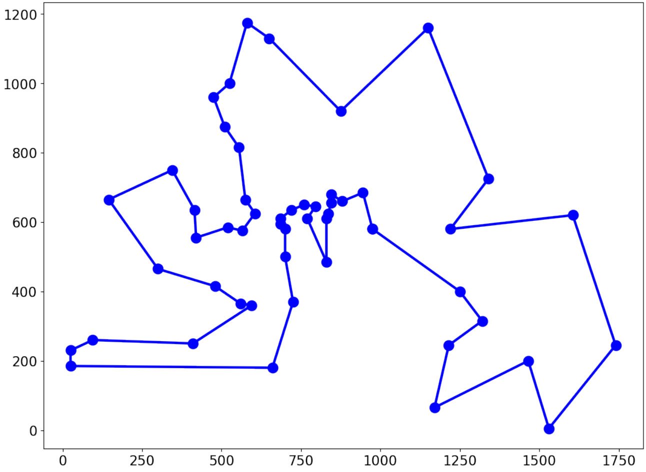
23/24

traveling salesperson problem: first impressions



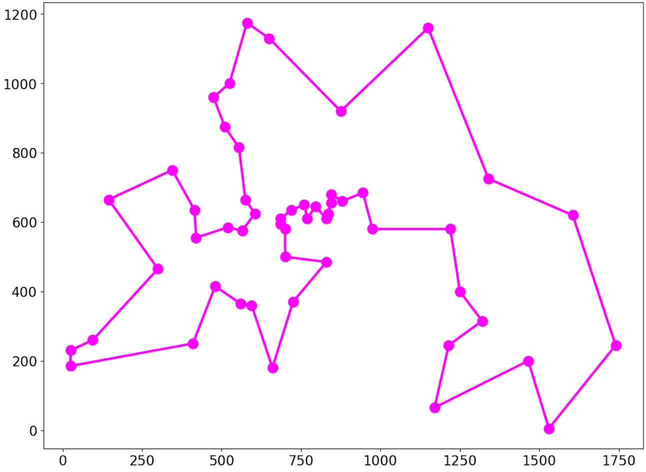
a closest-neighbor tour: 8.49% relative error

traveling salesperson problem: first impressions



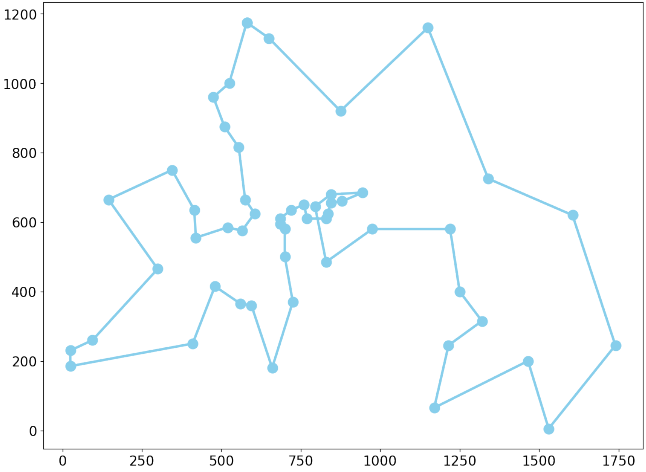
a pair-center tour: 7.28% relative error

traveling salesperson problem: first impressions



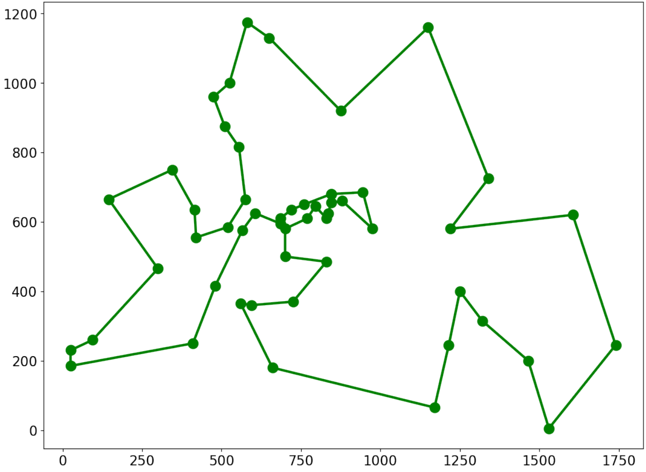
the best tour (known for this example): 0% relative error

traveling salesperson problem: first impressions



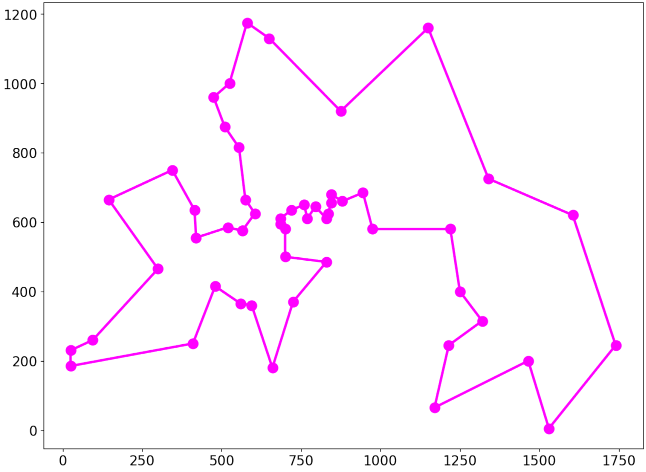
a quick tour (with Monte Carlo): 2.32% relative error

traveling salesperson problem: first impressions



a genetic algorithm tour: 8.37% relative error

traveling salesperson problem: first impressions



the best tour (known for this example): 0% relative error

lower bounds on tour length of TSP

- simple bound: sum of minimal distances to neighbors
- Held-Karp bound
  (typically comes close to 1% on random instances and below 2% on TSPLIB, arguments for the bound are quite complicated)

upper bounds on tour length of TSP

- tour around minimal spanning tree yields $\leq 2 \cdot L_{opt}$
  runtime $\mathcal{O}(n^2)$
- Christofides algorithm yields $\leq 1.5 \cdot L_{opt}$
  runtime $\mathcal{O}(n^2 \log n)$

known solving algorithms for TSP

- brute force exhaustive search $\mathcal{O}(n!)$
  (quite easy to implement)
- Bellman-Held-Karp dynamic programming for Euclidean TSP
  $\mathcal{O}(n^2 2^n)$ time and $\mathcal{O}(n2^n)$ space
  (not covered here, please refer to advanced algorithms in computer science)
- state-of-the-art solver Concorde.
- state-of-the-art approximative solver LKH.

known approximation heuristics for TSP

start with some small tour generated by a simple heuristic, then:

- use 2-opt moves (modifing tour by changing two edges, for instance, to eliminate crossings in Euclidean TSP);
- or use 3-opt moves (modifing tour by changing three edges);
- or use Lin-Kernighan heuristic algorithm
  (variable mixture of 2-opt and 3-opt moves),
  currently the best known heuristic strategy.

TSP on a grid

let's take a look at a regular $m \times n$ grid (e.g. checker board)

- an optimal tour on a regular grid is easy to build
- optimal length:
  - $L_{opt} = n \cdot m$ if n or m even
  - $L_{opt} = n \cdot m - 1 + \sqrt{2}$ if $n \cdot m$ odd
- there are many! optimal tours

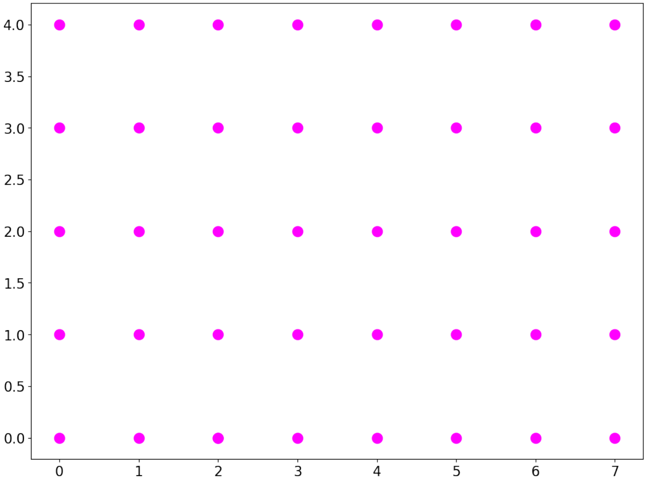
More on traveling salesperson problem

- The version of the TSP problem as shown until now is a special case of a more general problem definition:
- Let $G = (V, E)$ be a graph. V are the nodes (or locations), E are the edges (or connections) with some weight (e.g., distance, time, cost).
- Goal: find a minimal tour through all nodes.
- Particularly we talked about the Euclidean TSP, where the nodes are points in the Euclidean plane and the distance among all pairs, hence complete graph, is just the Euclidean distance.
- One step to be more general is, just require the triangular condition to be met (then, possibly, the pair-center approach cannot be used as we have no distances for the centers), this is called the metric TSP (mTSP).
- Moreover, the distances might be asymmetric, i.e., going in one direction is different from going in the other (ATSP).
- or we have additional conditions: open loop, arrival time windows, asymmetric distances, interrupted tours, etc.

More recent results on the eTSP

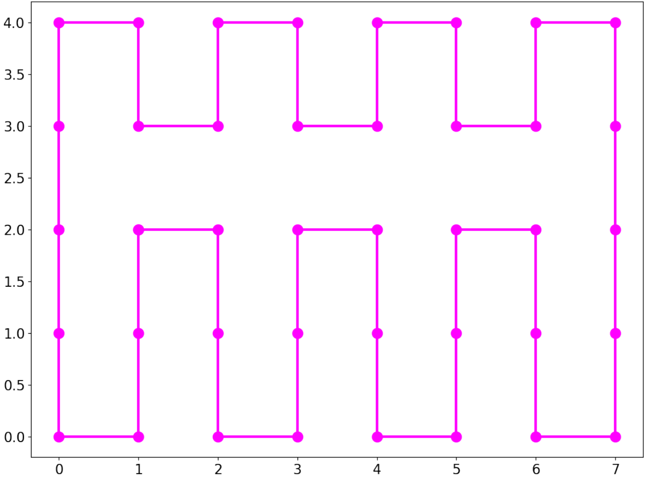
- In the 90's it was shown that eTSP can be solved in $\mathcal{O}(2^{O(\sqrt{n}\log n)})$.
- In the 10's this was improved to $\mathcal{O}(2^{\sqrt{n}})$, and with certain arguments that further improvement may be very unlikely.
- One recent result of complexity theory is that eTSP has a polynomial time approximation scheme (PTAS) of $\mathcal{O}_{\varepsilon,d}(n\log n)$ (with fixed error ε and fixed dimension d), however, an implementation is not available (to my knowledge).
- This has been improved to $\mathcal{O}_{\varepsilon,d}(n)$ with high probability (2013).

traveling salesperson problem: first impressions



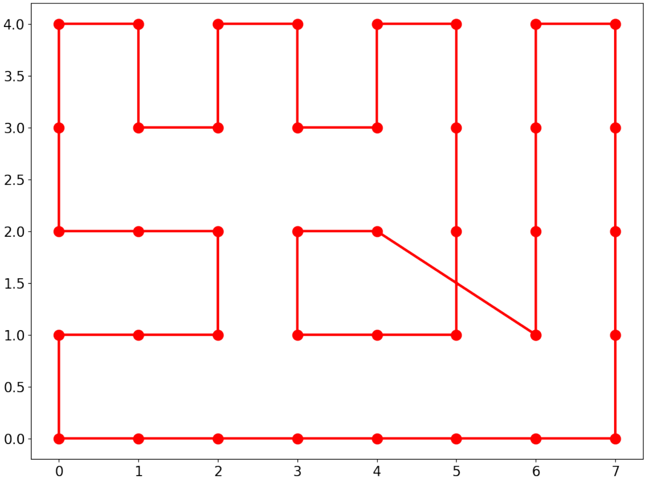
the cities distributed geographically

traveling salesperson problem: first impressions



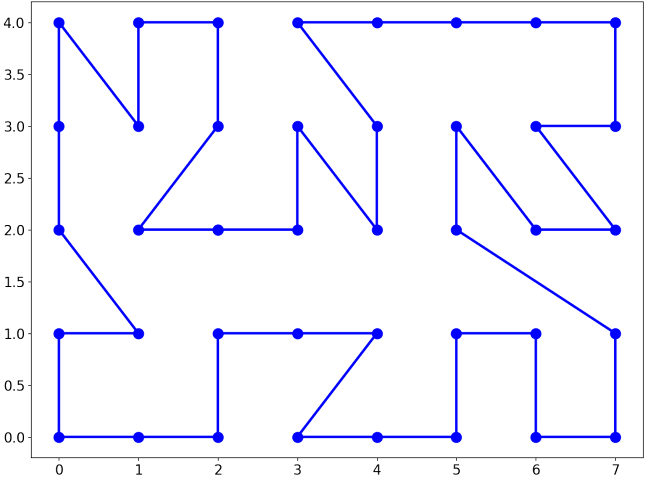
a best tour (trivial for this example): 0% relative error

traveling salesperson problem: first impressions



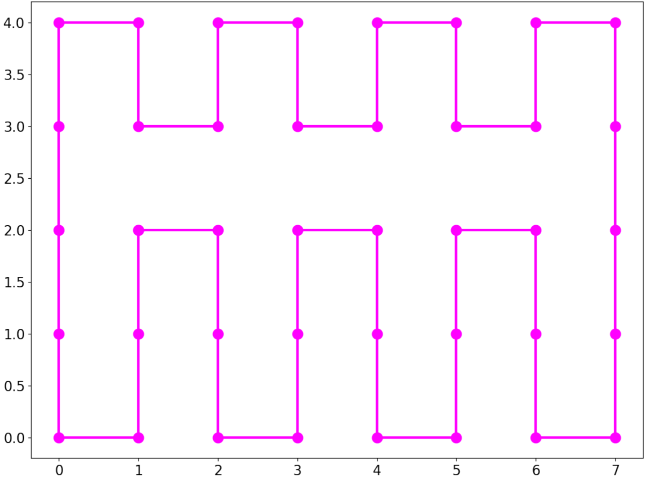
a closest-neighbor tour (with Monte Carlo): 3.09% relative error

traveling salesperson problem: first impressions



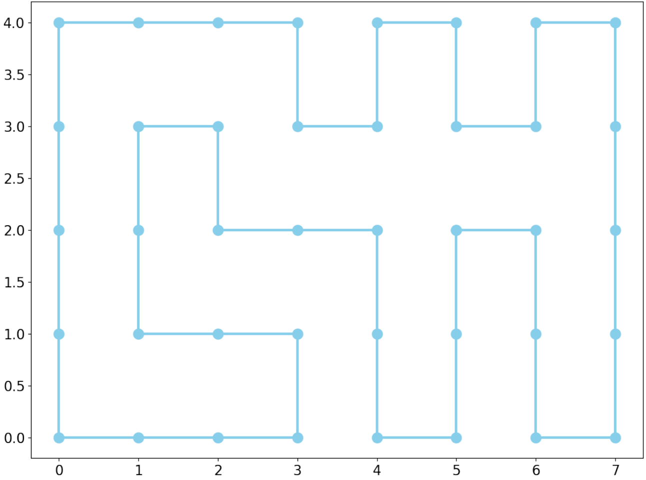
a pair-center tour: 14.46% relative error

traveling salesperson problem: first impressions



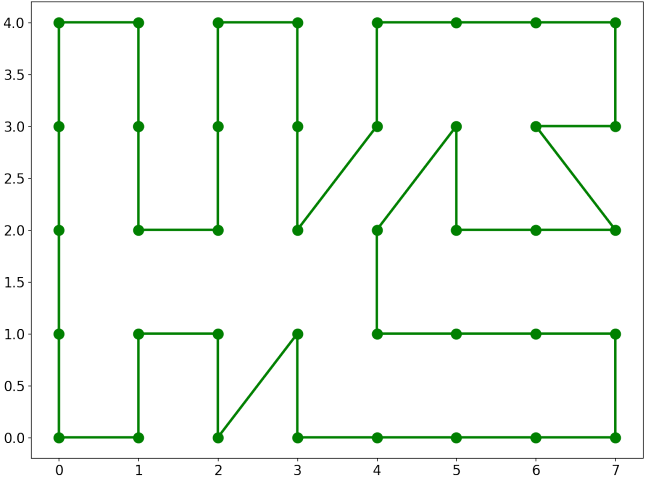
a best tour (trivial for this example): 0% relative error

traveling salesperson problem: first impressions



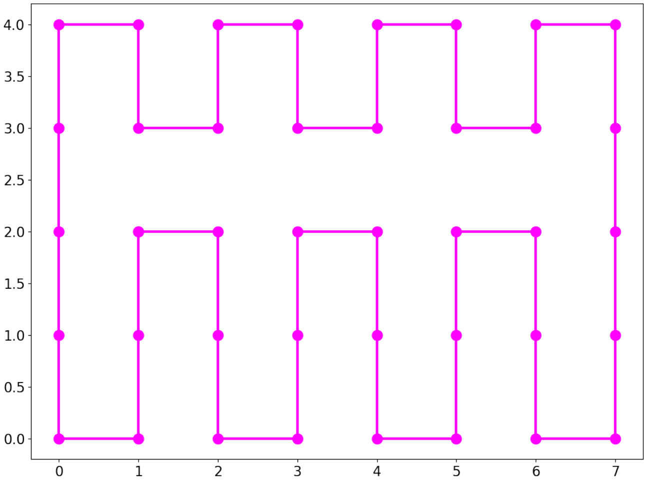
a quick tour (with Monte Carlo): 0.00% relative error

traveling salesperson problem: first impressions



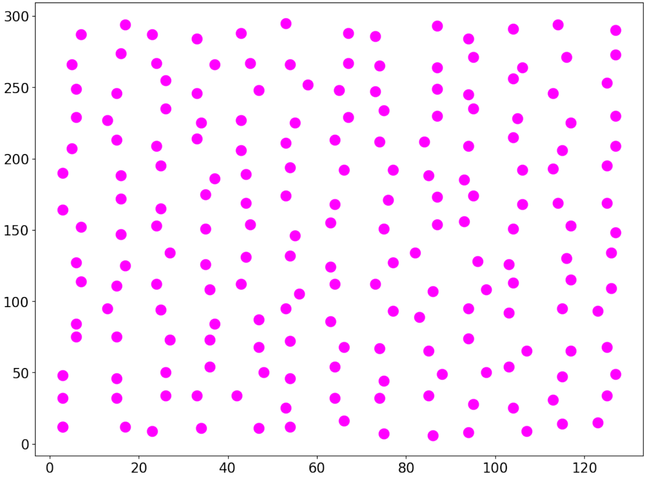
a genetic algorithm tour: 4.14% relative error

traveling salesperson problem: first impressions



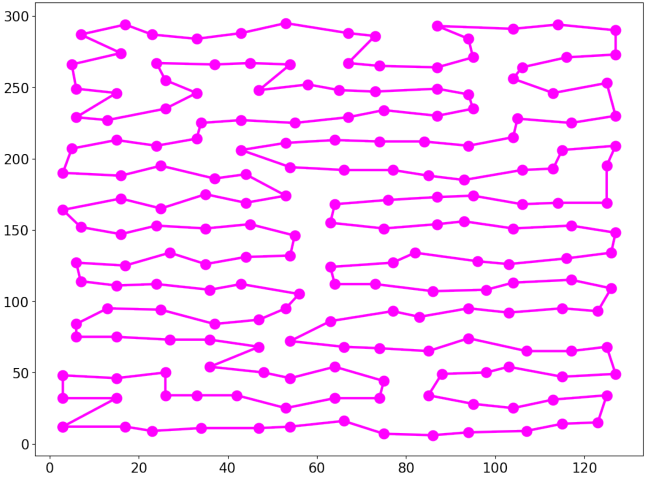
a best tour (trivial for this example): 0% relative error

traveling salesperson problem: first impressions



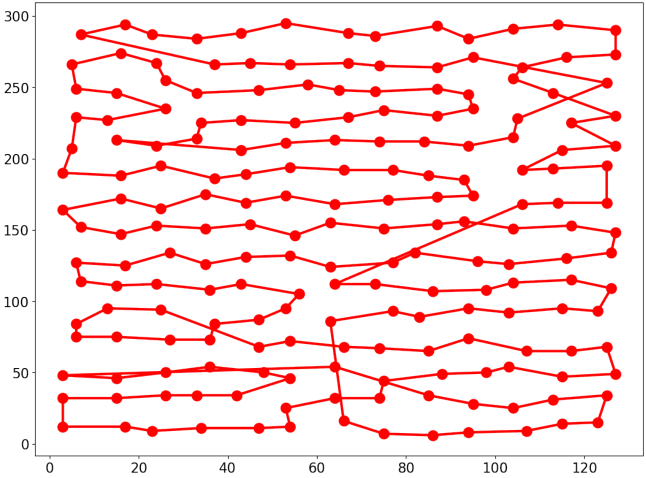
the locations distributed in the plane

traveling salesperson problem: first impressions



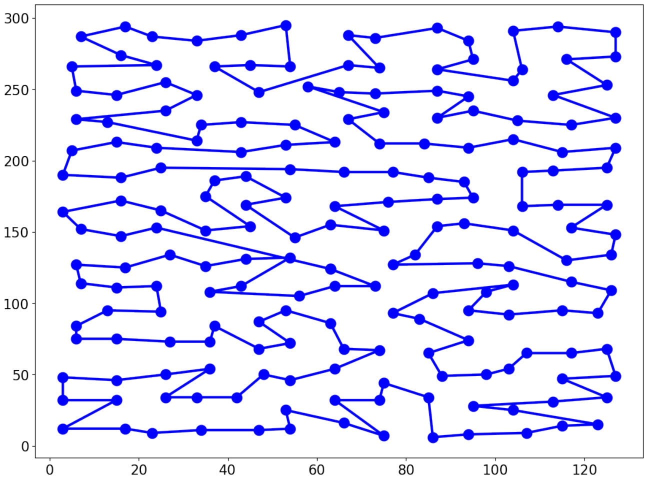
the best tour (known for this example): 0% relative error

traveling salesperson problem: first impressions



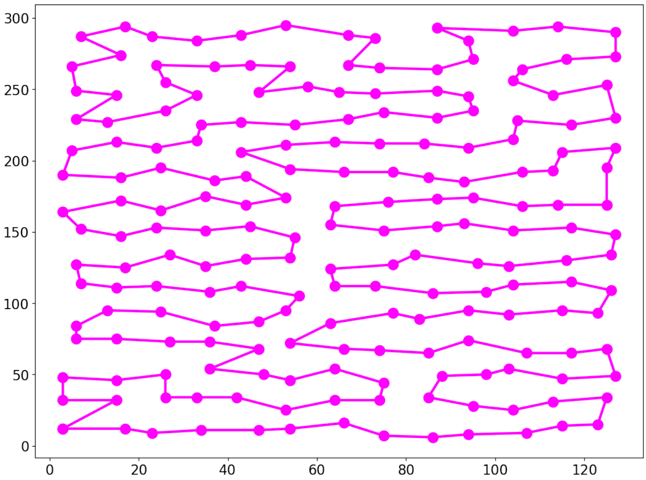
a closest-neighbor tour (with Monte Carlo): 10.23% relative error

traveling salesperson problem: first impressions



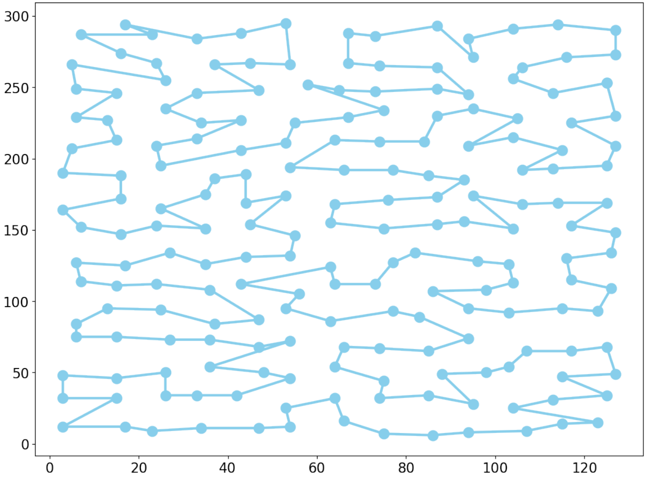
a pair-center tour: 13.93% relative error

traveling salesperson problem: first impressions



the best tour (known for this example): 0% relative error

traveling salesperson problem: first impressions



a quick tour (with Monte Carlo): 9.66% relative error

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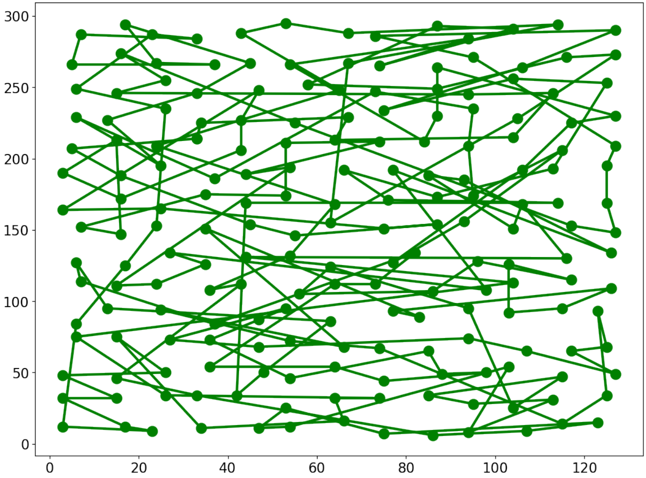
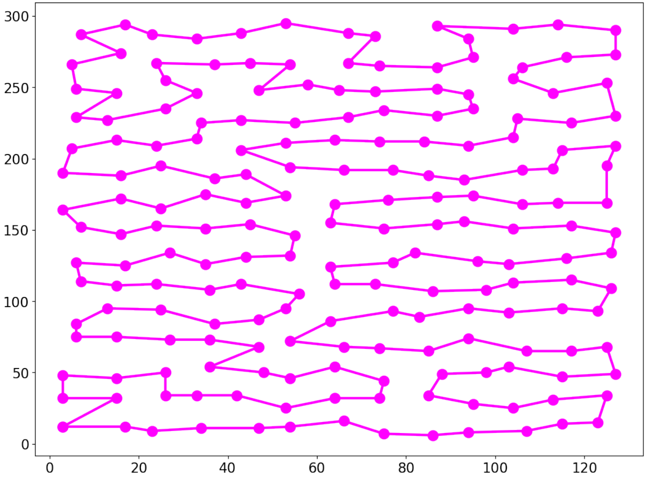


a genetic algorithm (GA) tour: 205.65% relative error

traveling salesperson problem: first impressions



the best tour (known for this example): 0% relative error

errors for the above heuristics

problem	heuristic	relative error
berlin52	closest neighbor tour	8.49
	quick tour	2.32
	pair-center tour	7.28
	genetic algorithm tour	8.37
	pair-center tour improved	0.00
	Lin-Kernighan tour	0.00
rat195	closest neighbor tour	10.23
	quick tour	9.66
	pair-center tour	13.93
	genetic algorithm tour	205.65
	pair-center tour improved	1.16
	Lin-Kernighan tour	0.00
block40	closest neighbor tour	3.09
	quick tour	0.00
	pair-center tour	14.46
	genetic algorithm tour	4.14
	improved pair-center tour	0.00
	Lin-Kernighan tour	0.00

Your goal: make GA-tour consistently better than pair-center tour or quick tour.

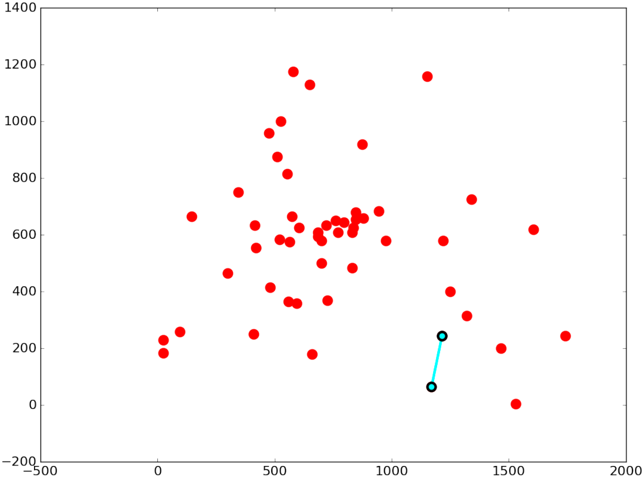
How does the closest-neighbor algorithms work?

The classical closest-neighbor algorithm is a greedy algorithm with a small random component:

- select a random city
- while there are still unconnected cities
  - connect to the closest unconnected neighbor
  - use a random tie break
- connect the first with the last city

- runtime is $\mathcal{O}(n^2)$,
- can be run in Monte Carlo fashion keeping the shortest tour
- worst tour may have a length up to $0.5 \cdot \log n \cdot L_{opt}$

animation of the closest-neighbor algorithm



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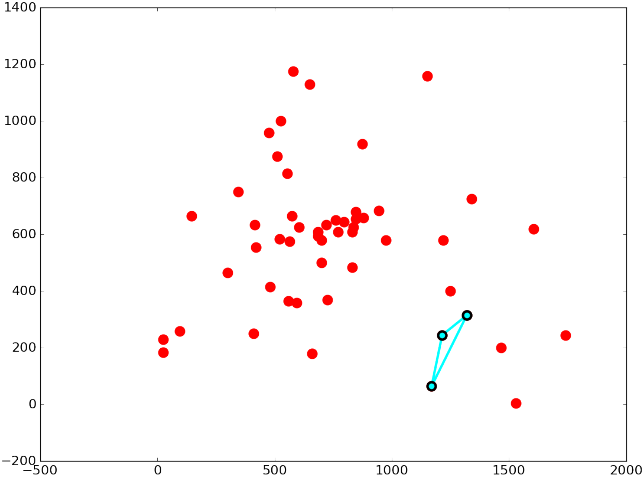

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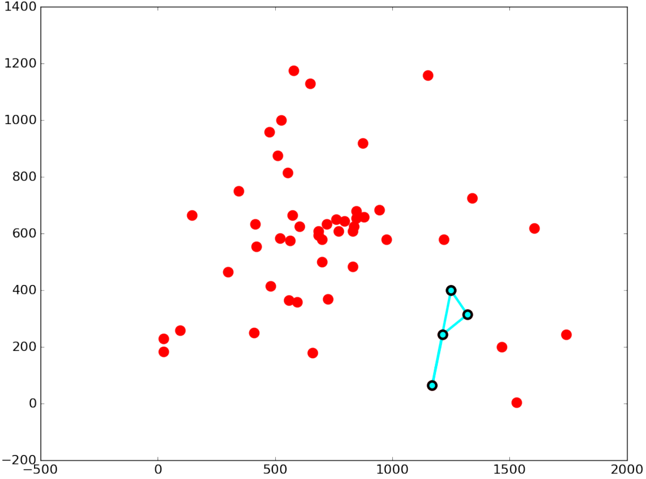

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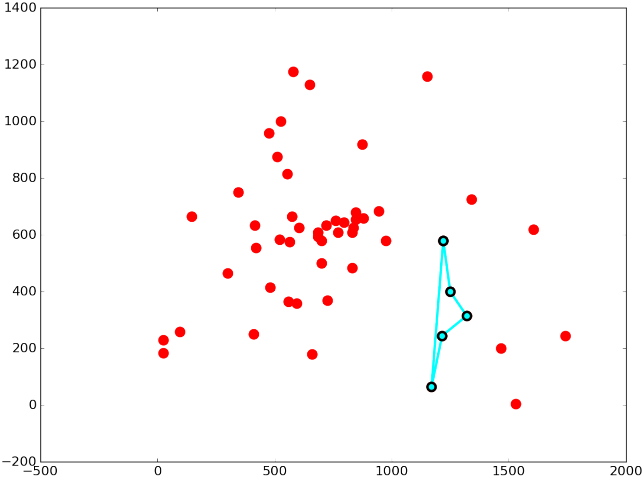

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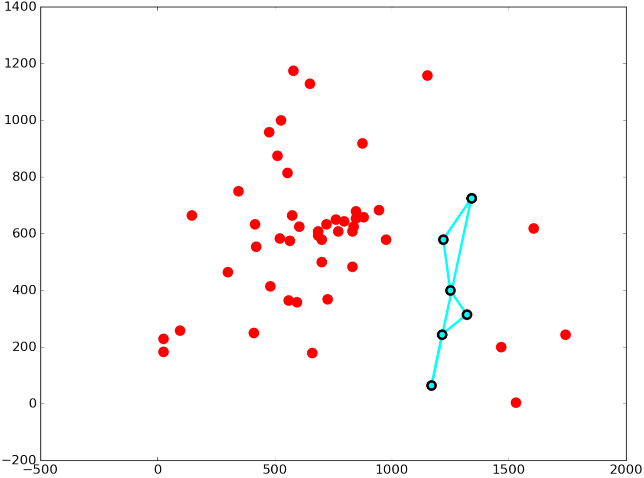

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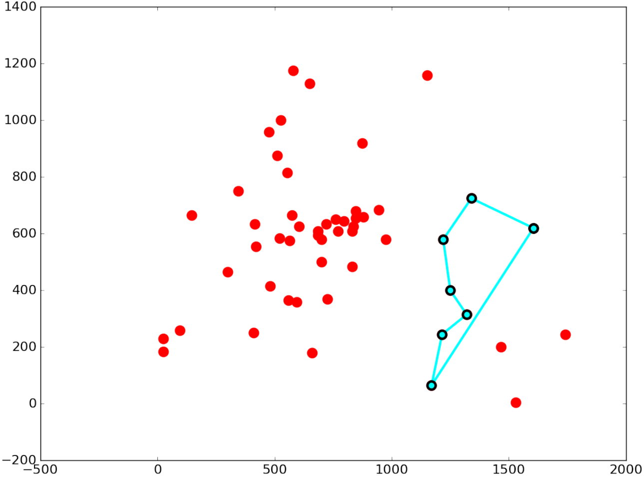

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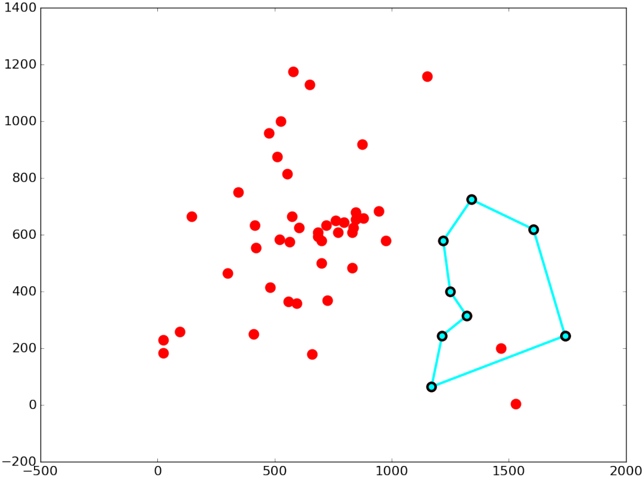

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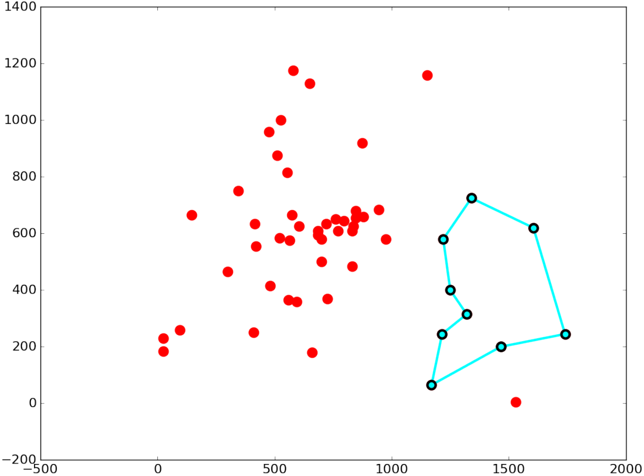

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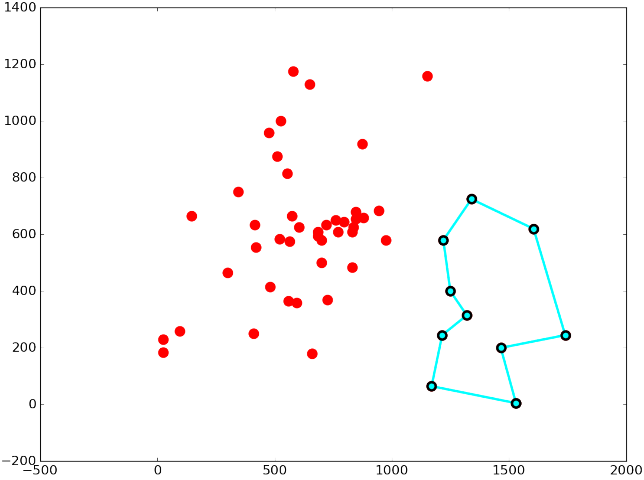

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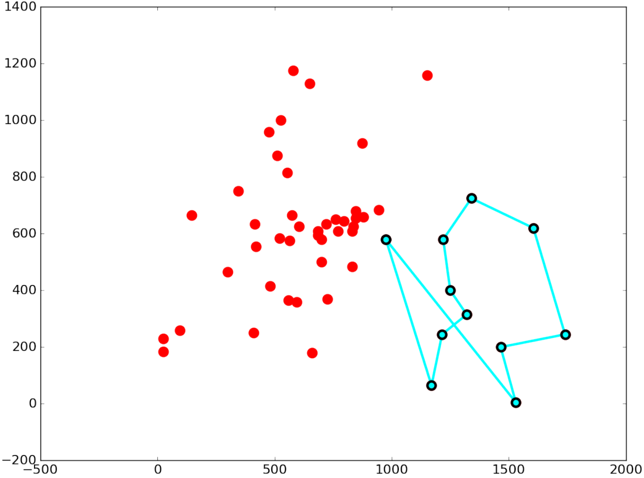

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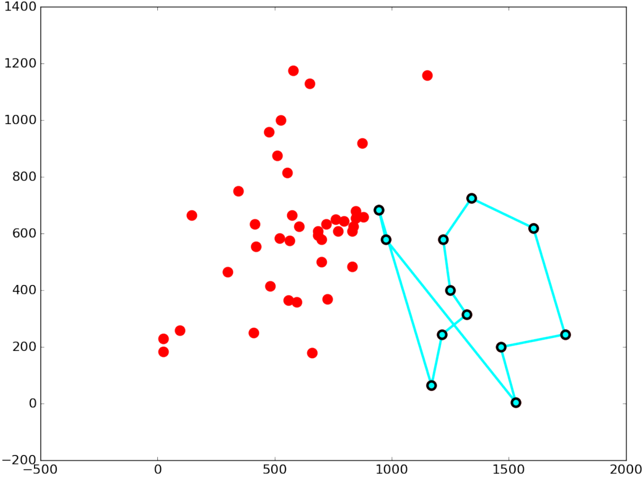

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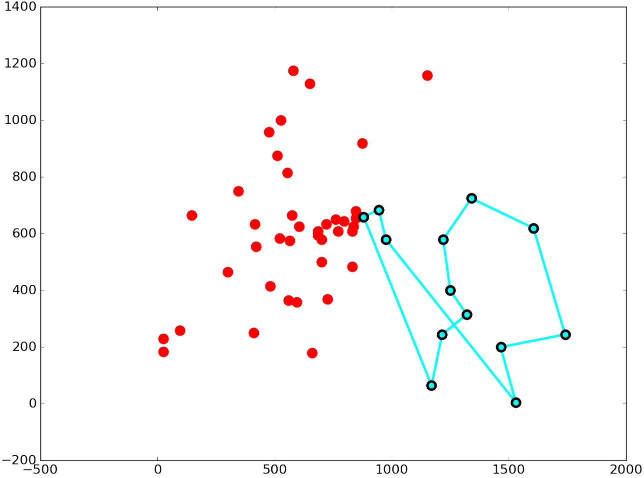

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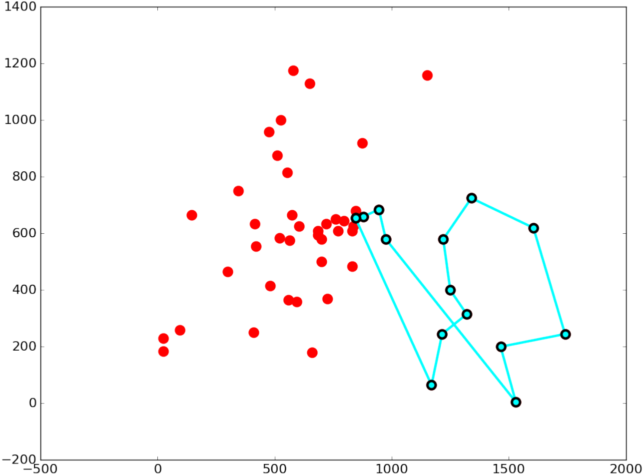

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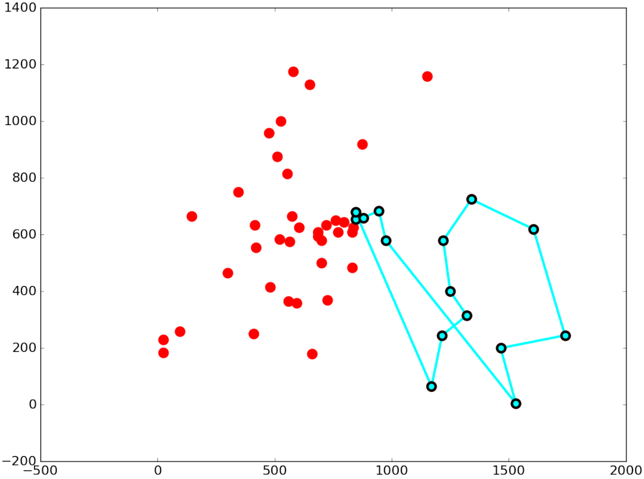

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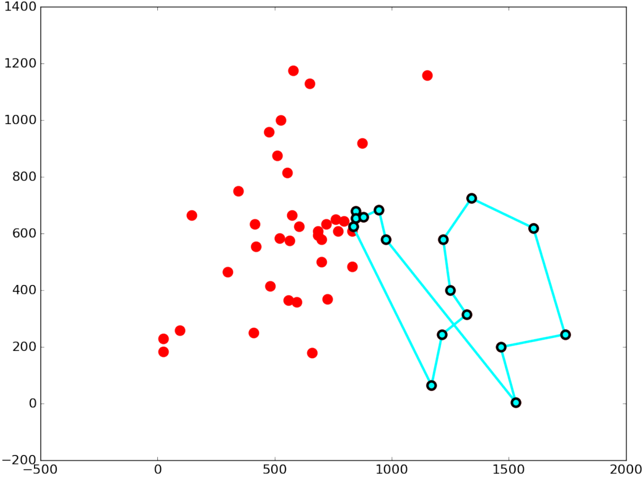

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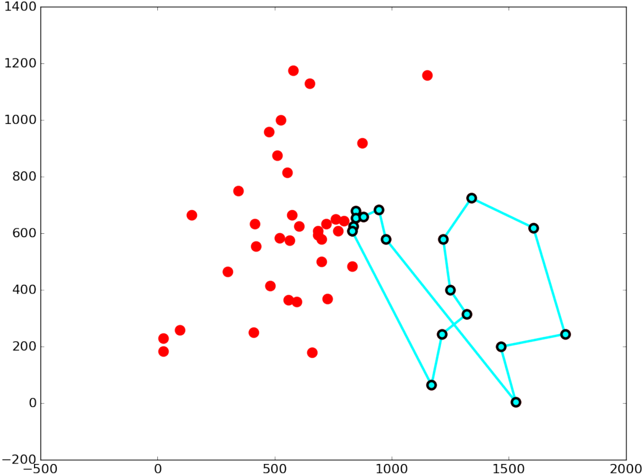

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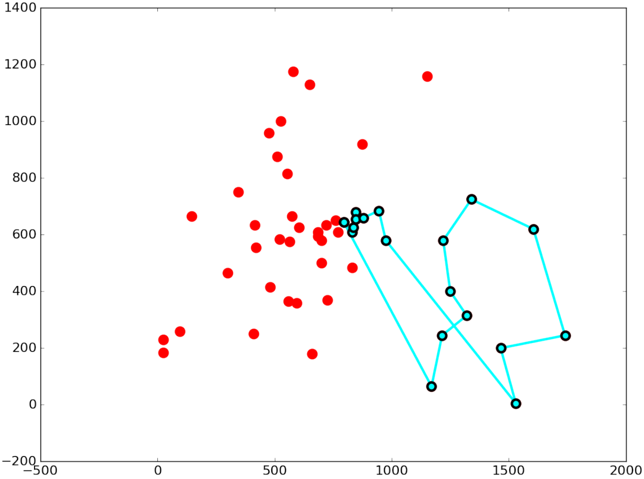

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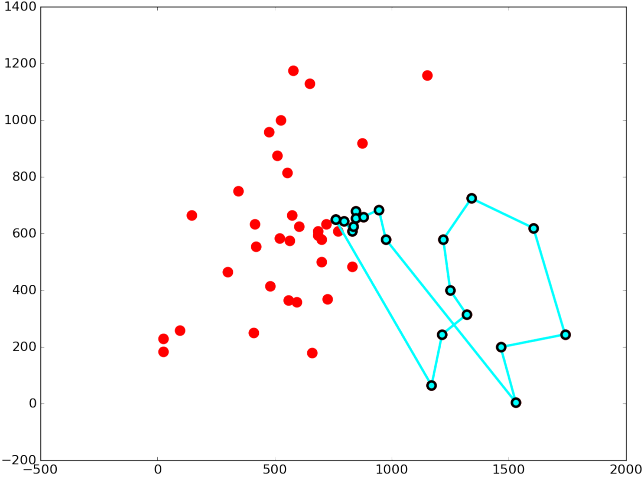

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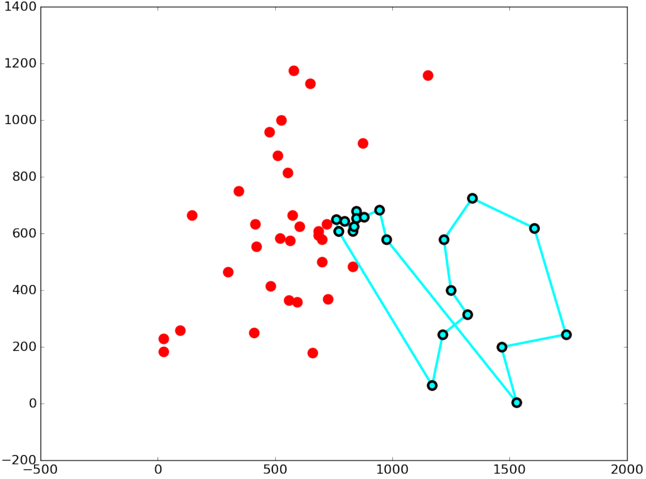

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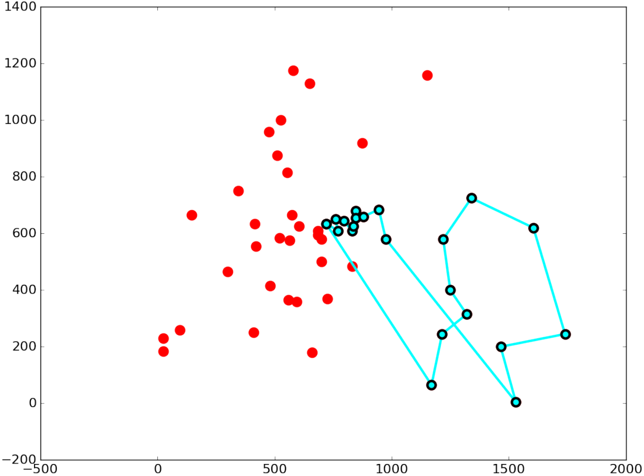

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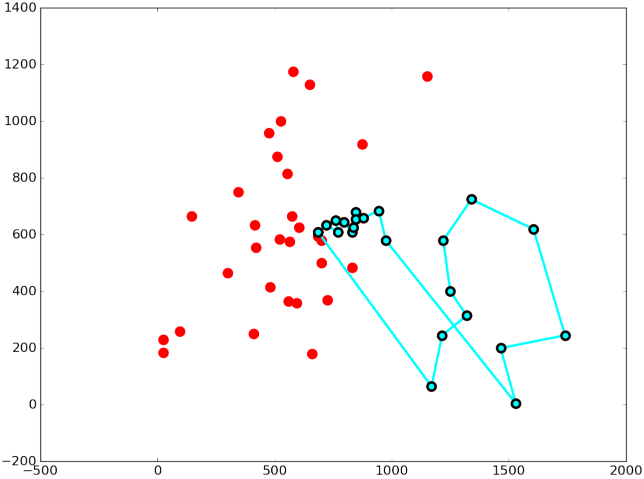

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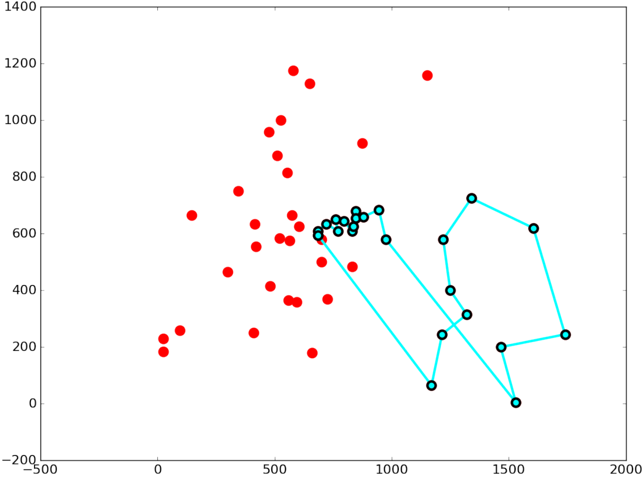

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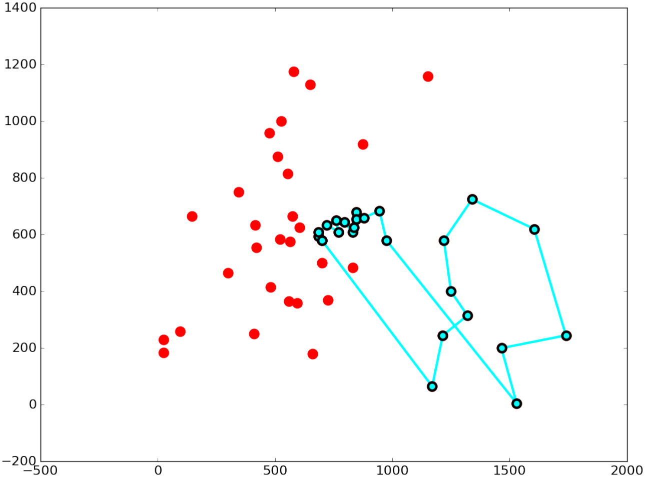

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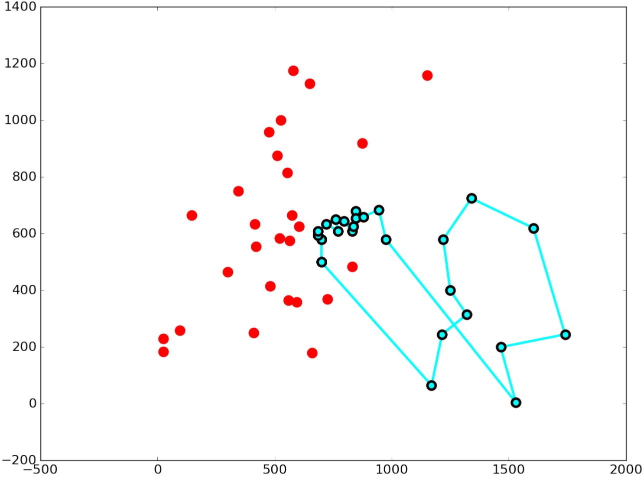

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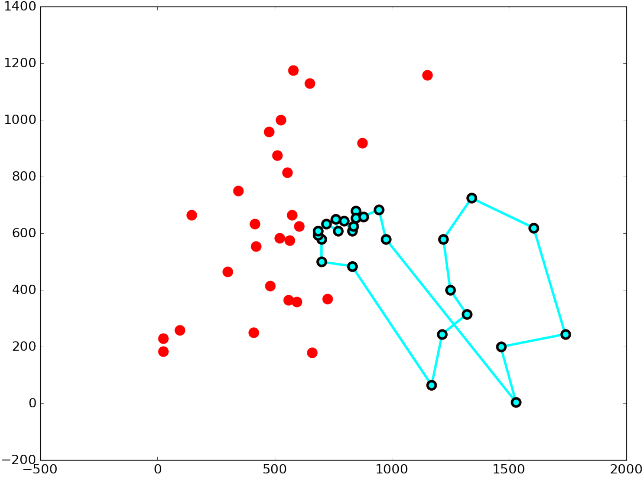

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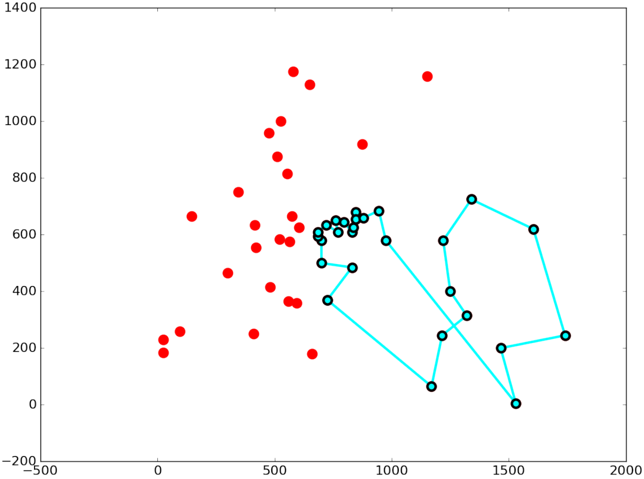

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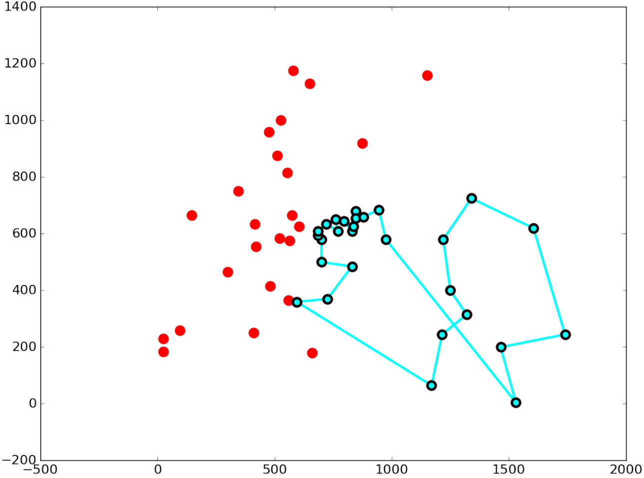

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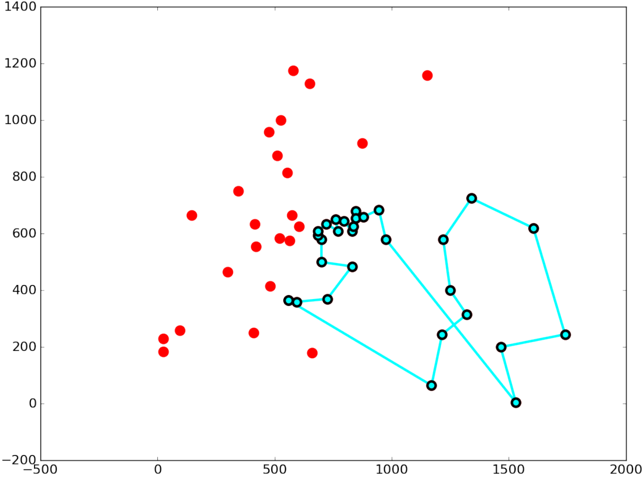

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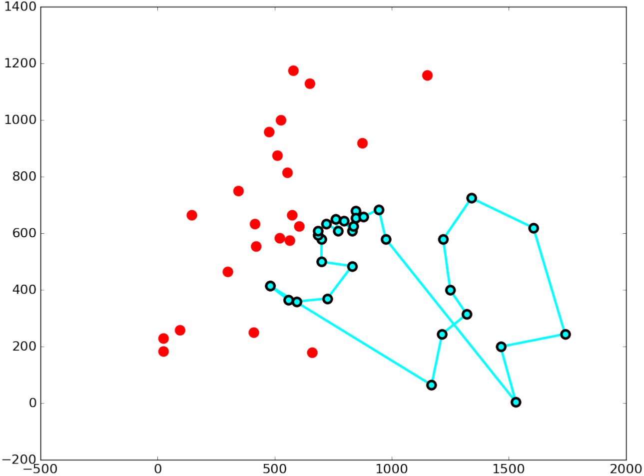

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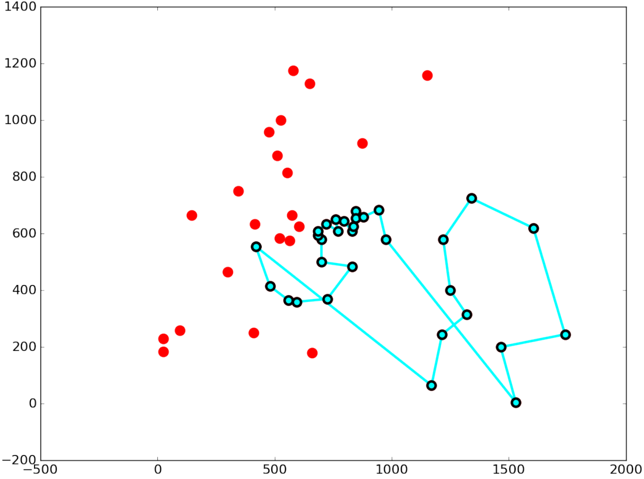

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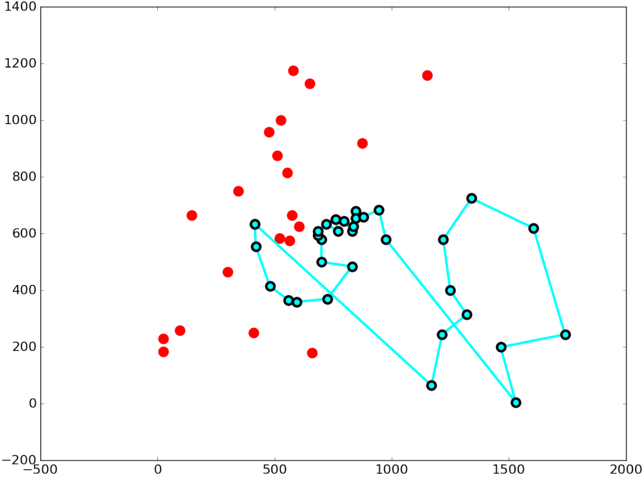

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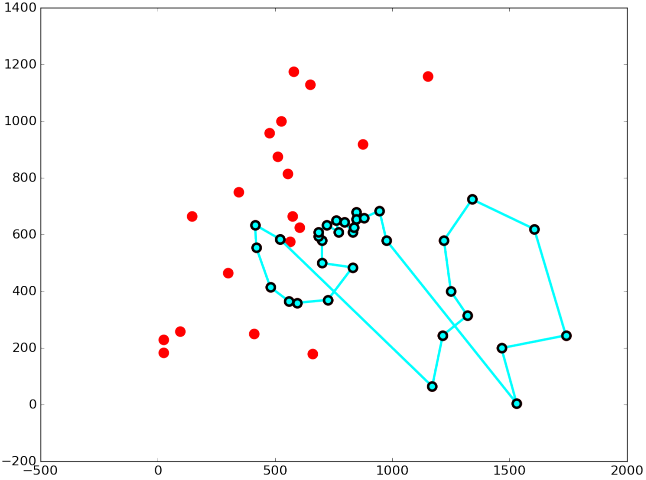

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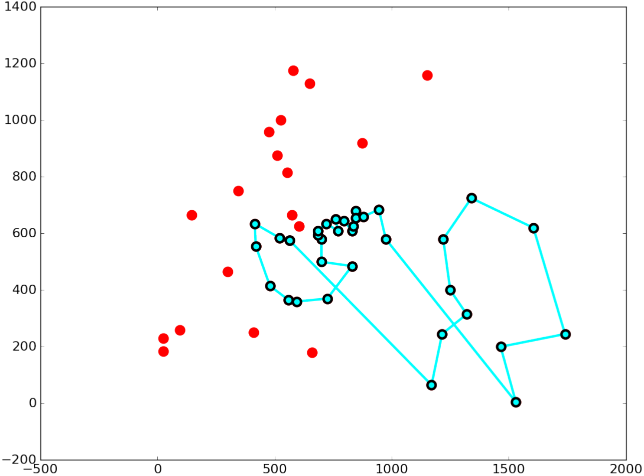

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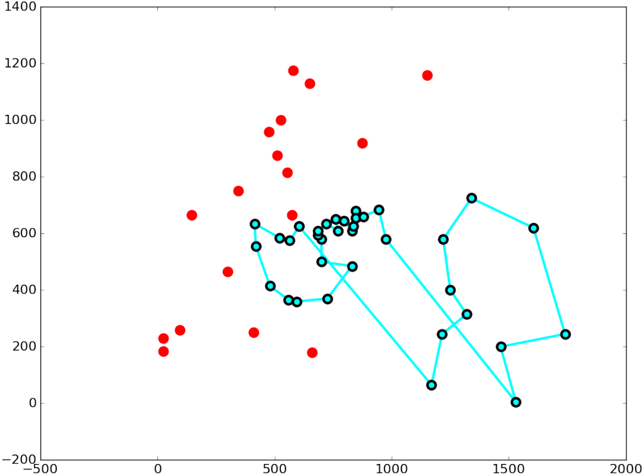

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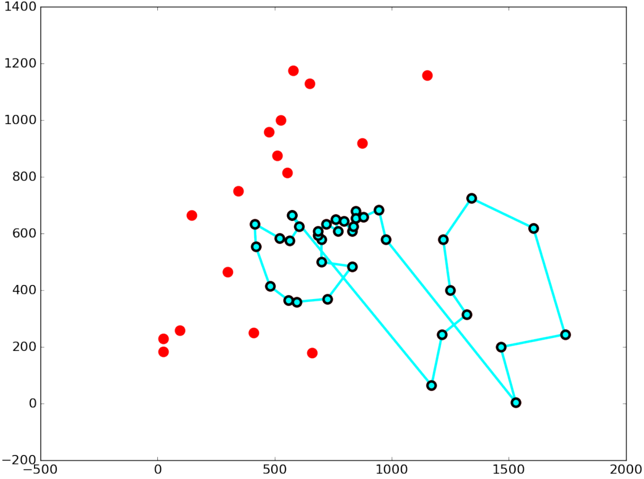
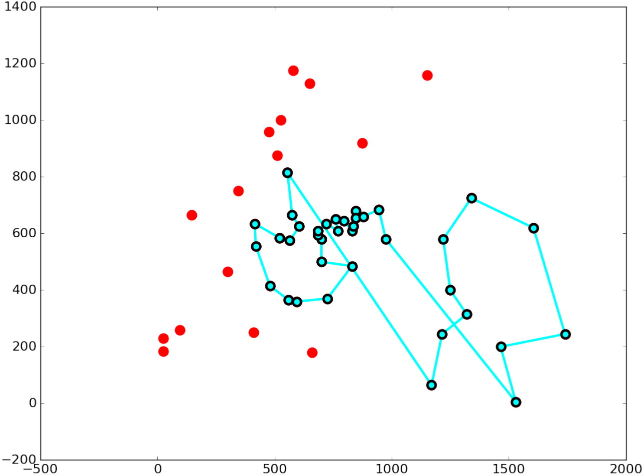


animation of the closest-neighbor algorithm



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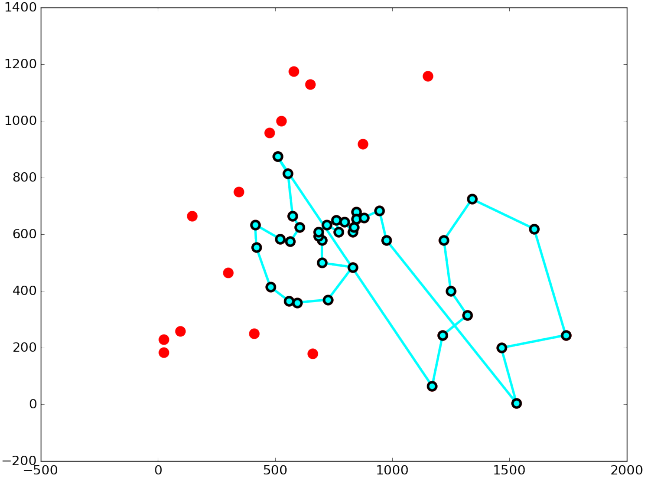

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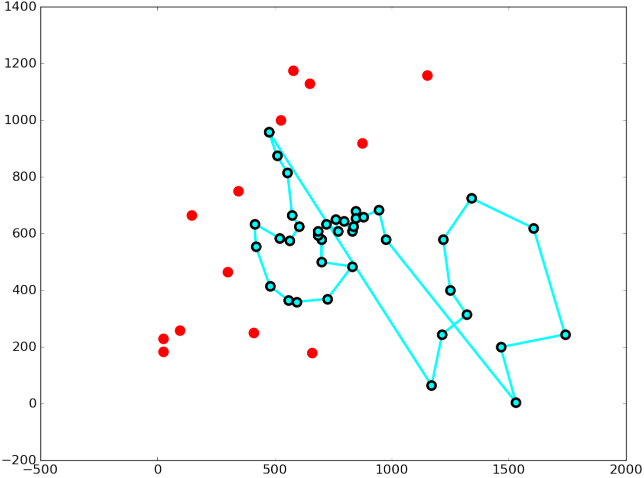

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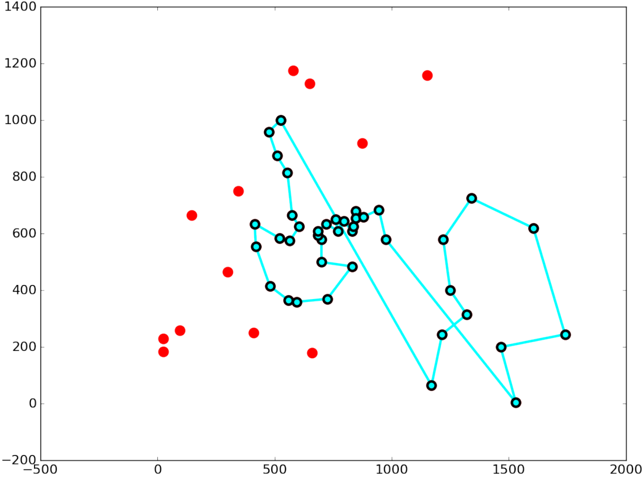

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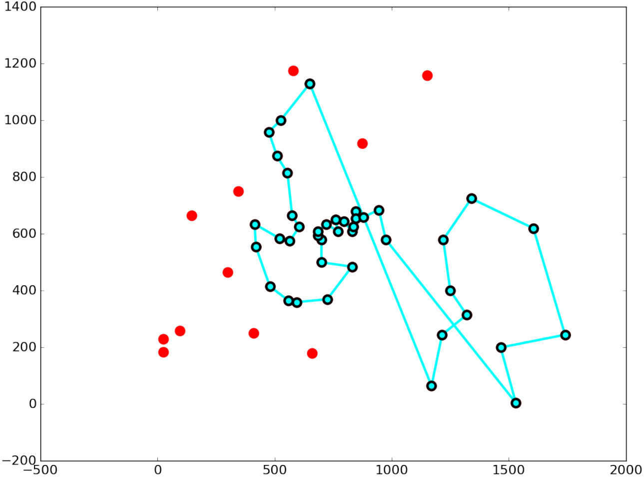

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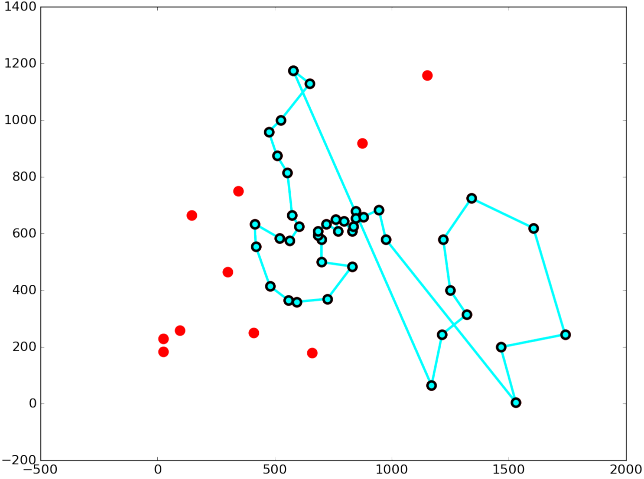

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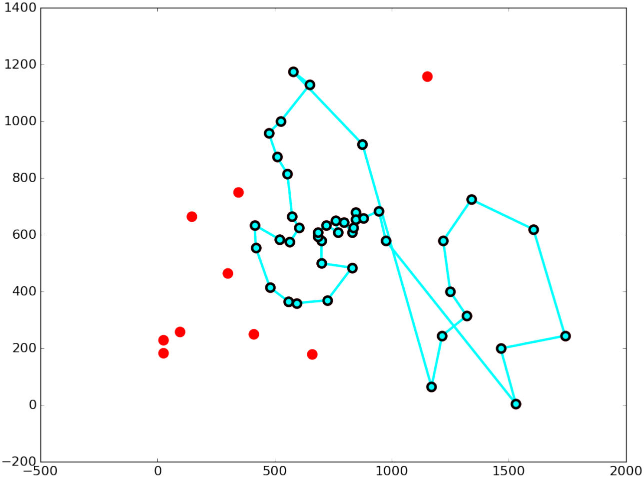

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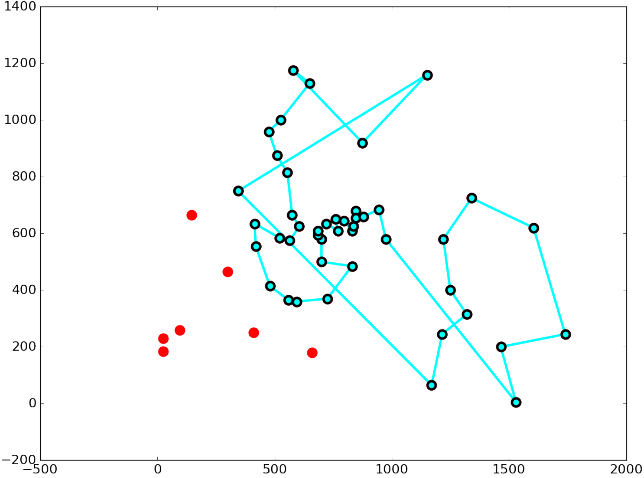

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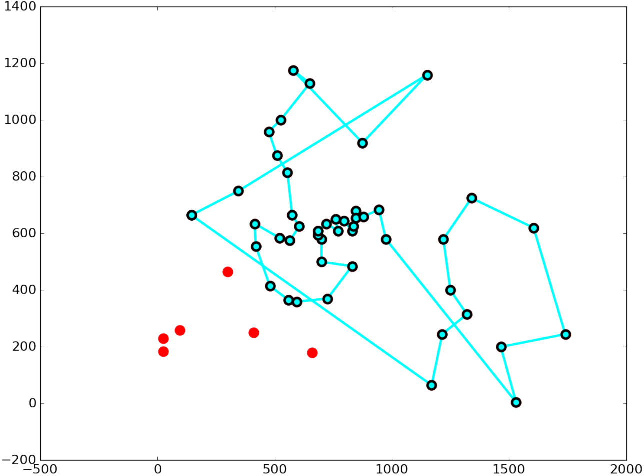

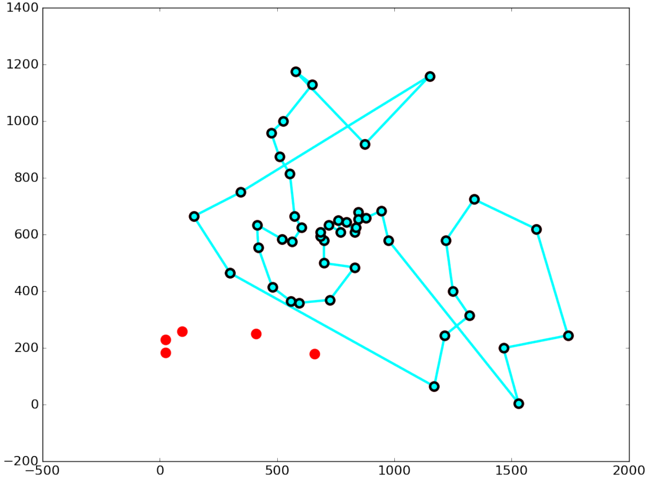
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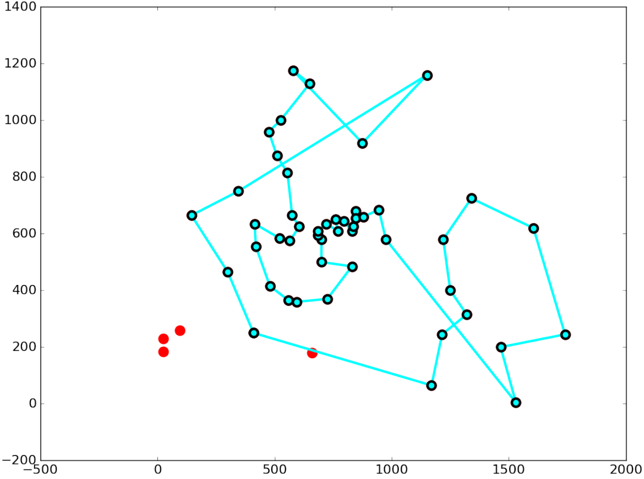

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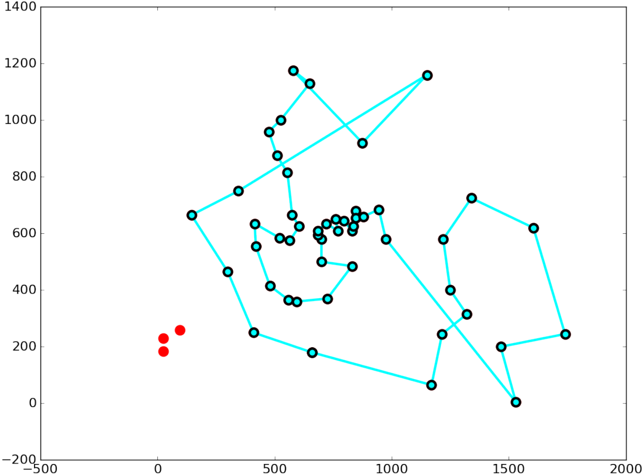

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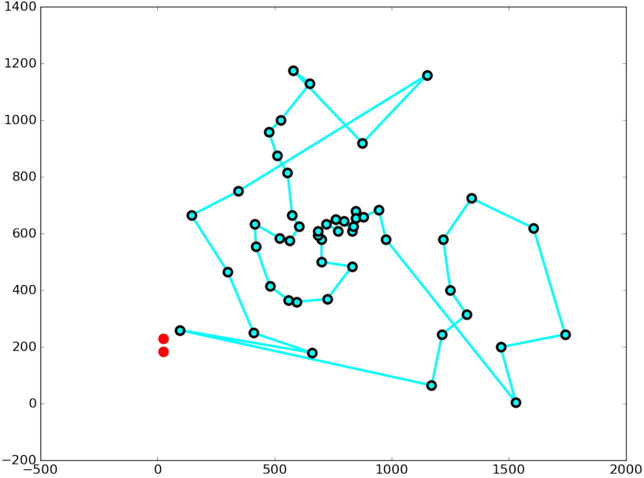

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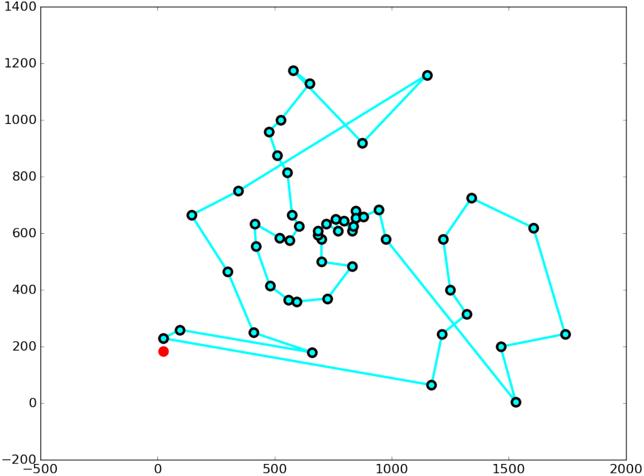

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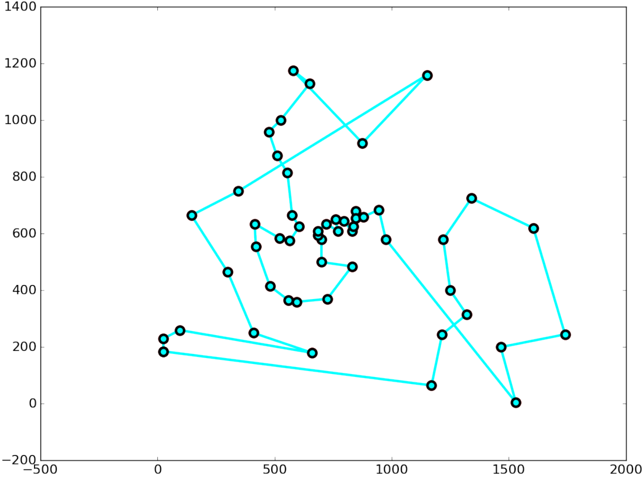


How does the quick tour algorithm work?

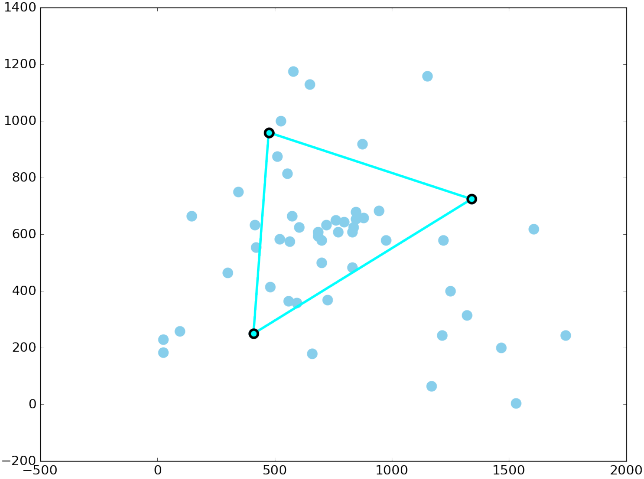
The quick tour algorithm is my own contribution (but found to be known as *insertion/addition approach*) for this course. It is a probabilistic greedy algorithm:

- select three random cities to form an initial triangular tour
- while there are still unconnected cities
  - choose a random (closest) unconnected city
  - expand the current tour by inserting the new city such that the tour increment is minimal

- runtime is in $\mathcal{O}(n^2)$,
- the random version can be run in Monte Carlo fashion keeping the shortest tour
- worst tour may have a length up to $2 \cdot L_{opt}$

There are more similar approaches, e.g., nearest addition or farthest addition.

animation of the quick tour algorithm



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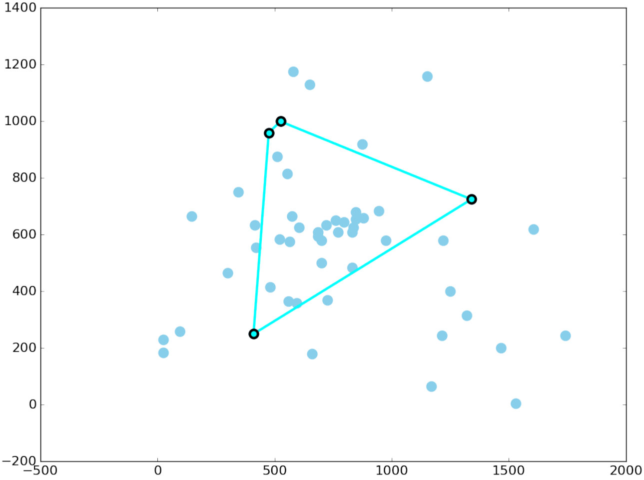

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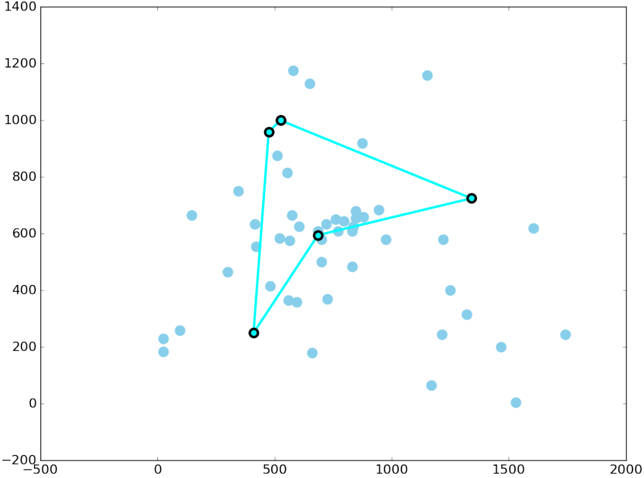

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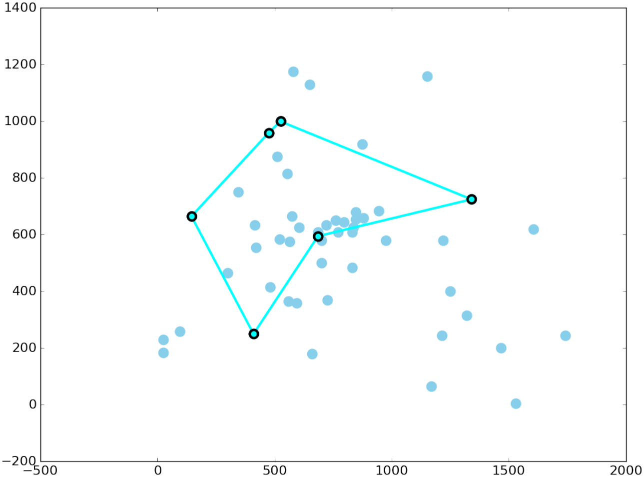

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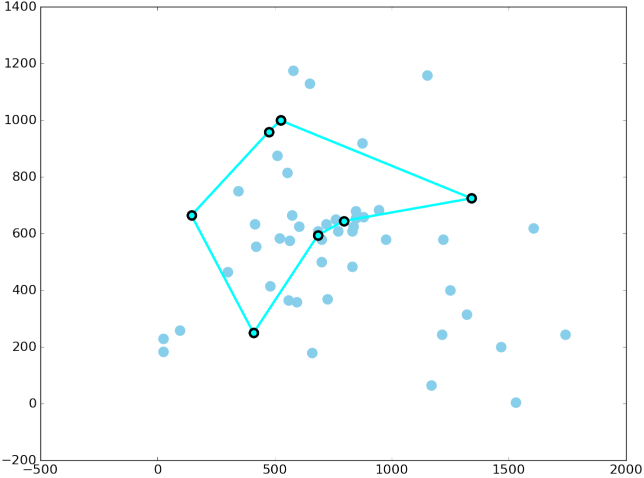

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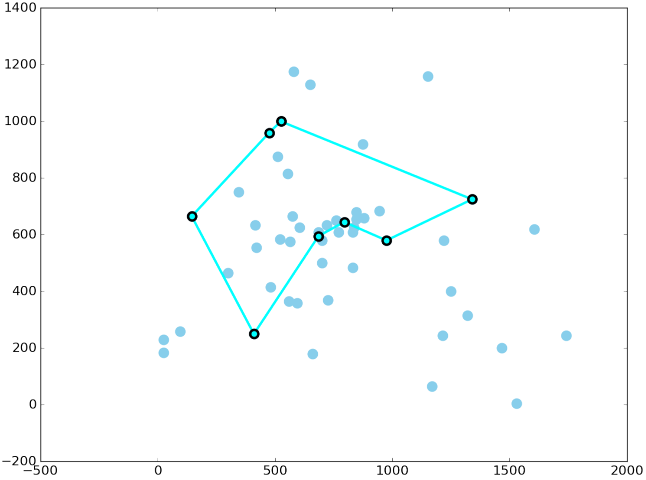

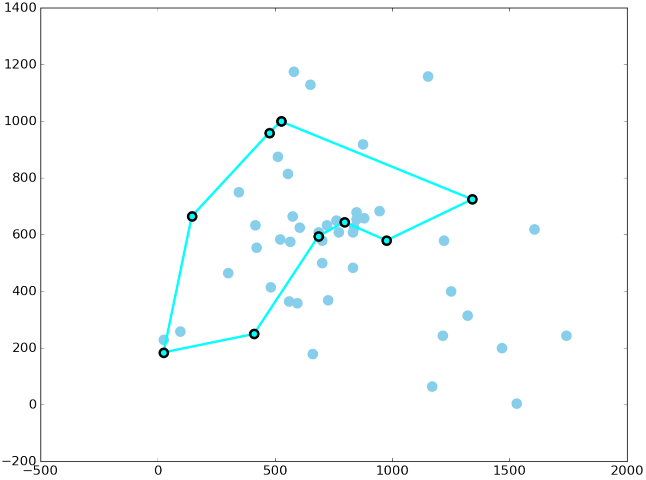
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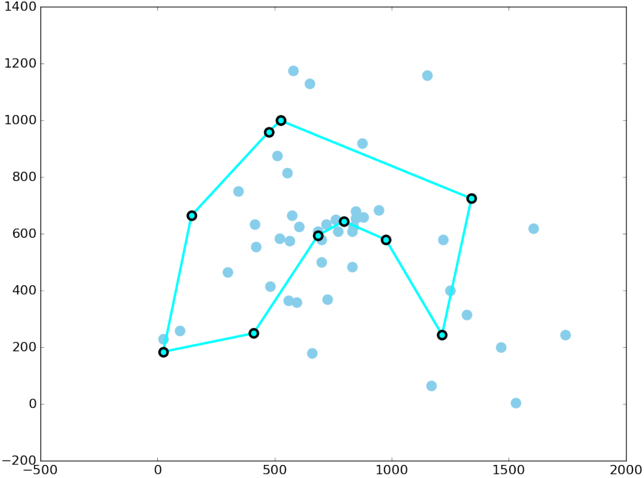

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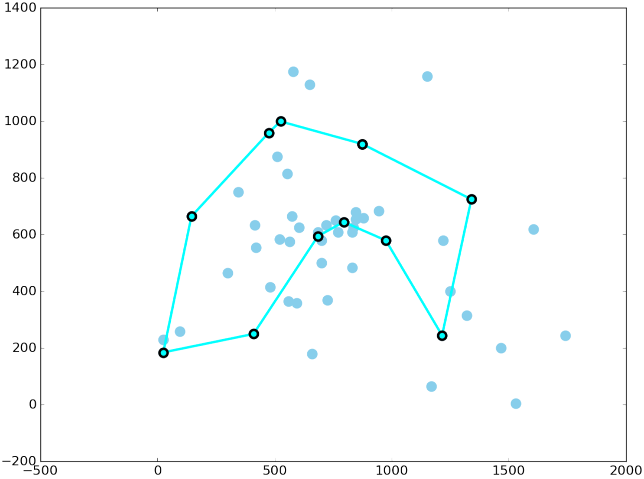

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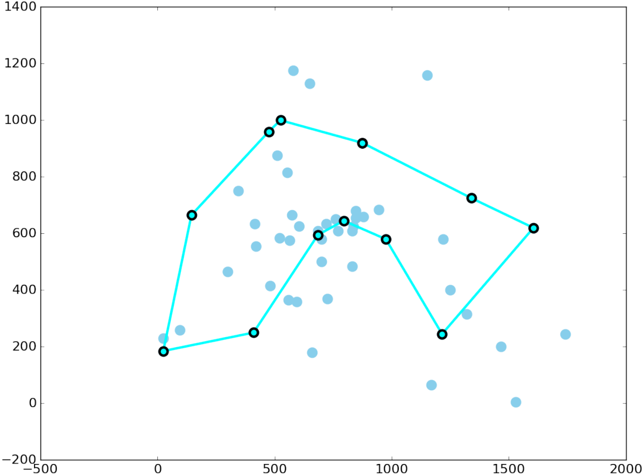

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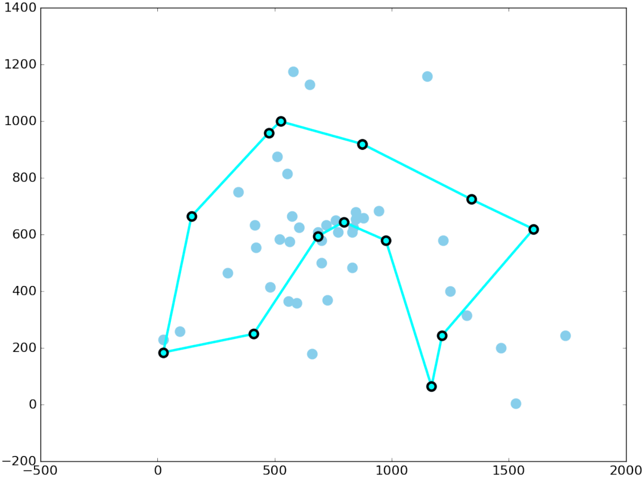

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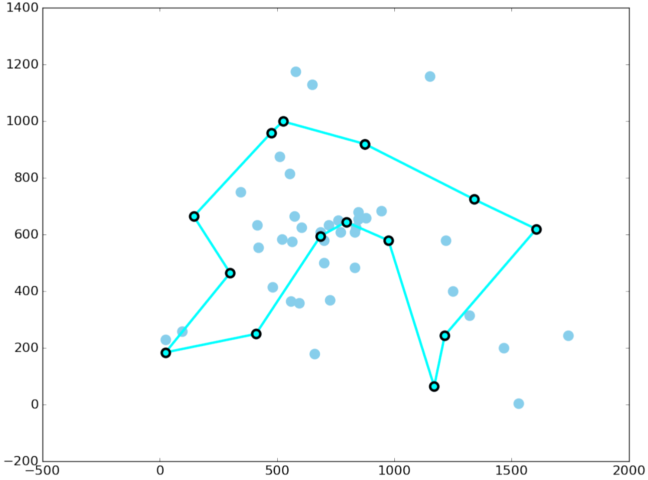

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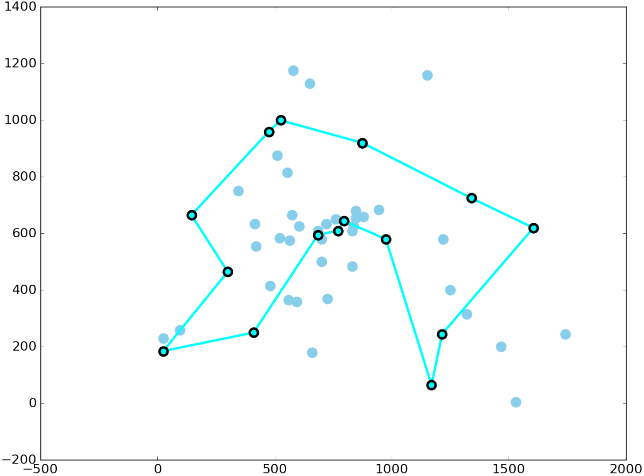

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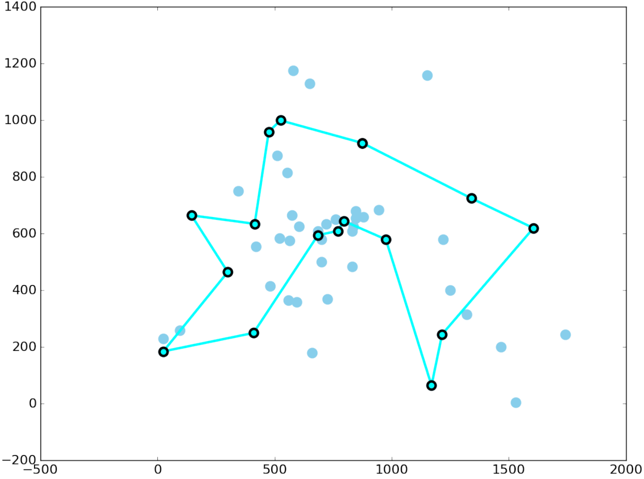

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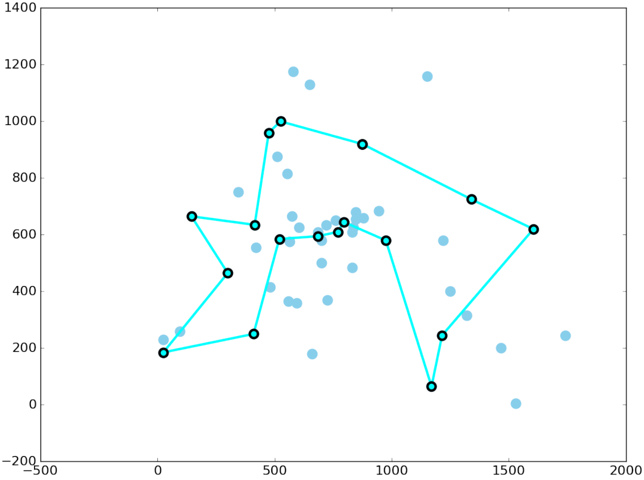

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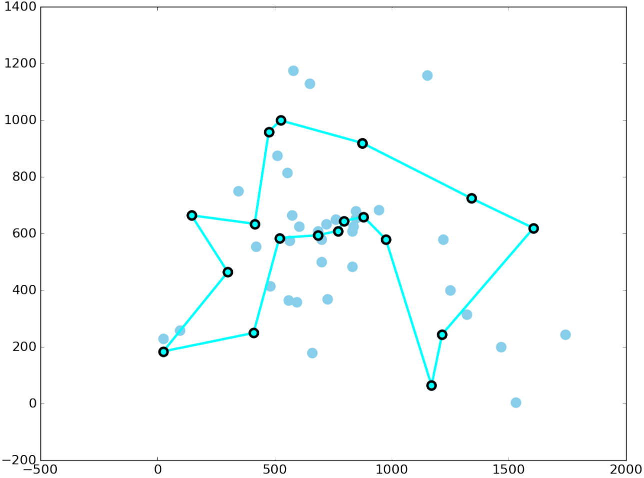

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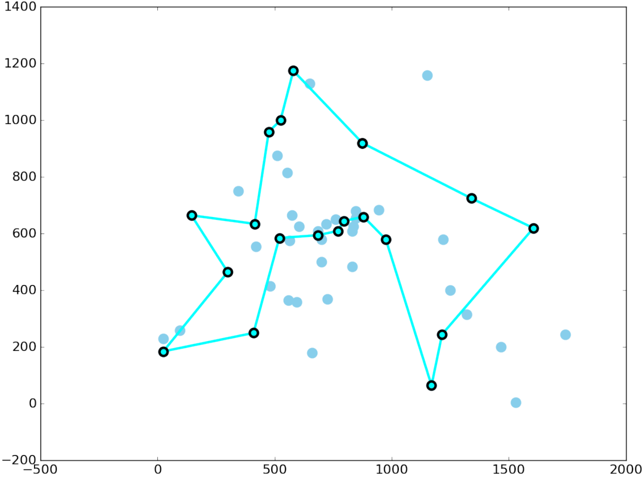

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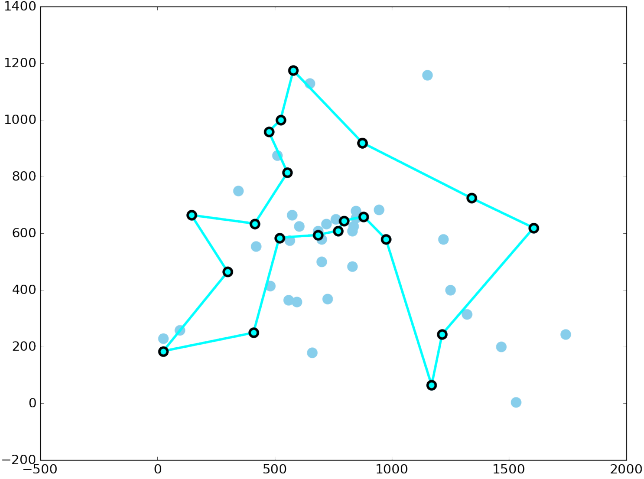

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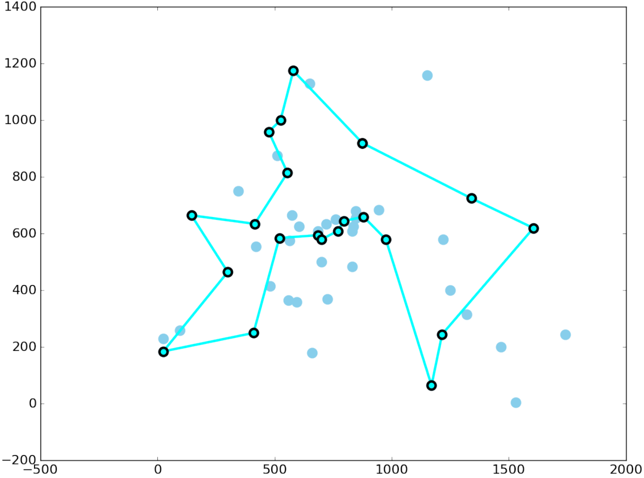

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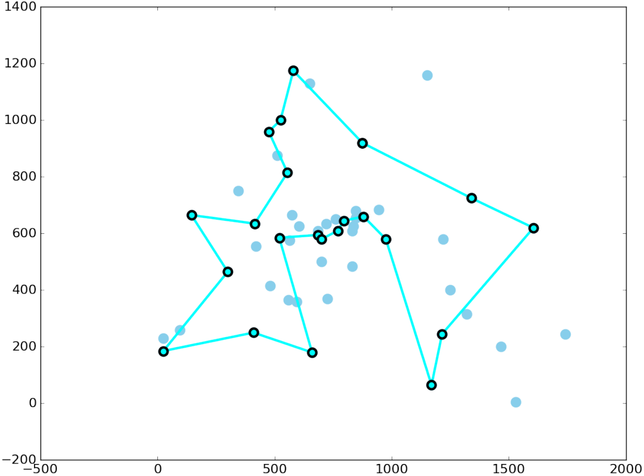

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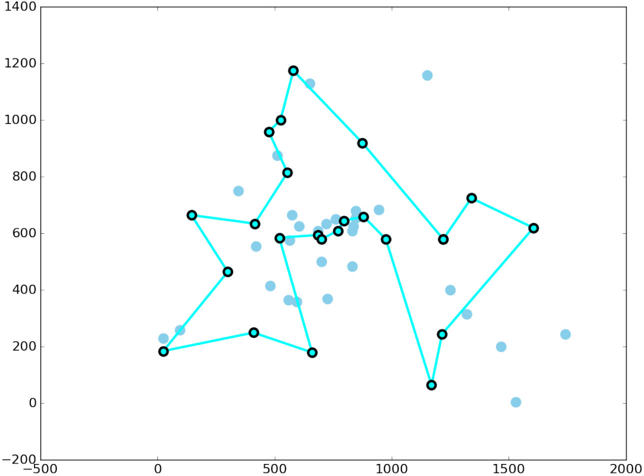

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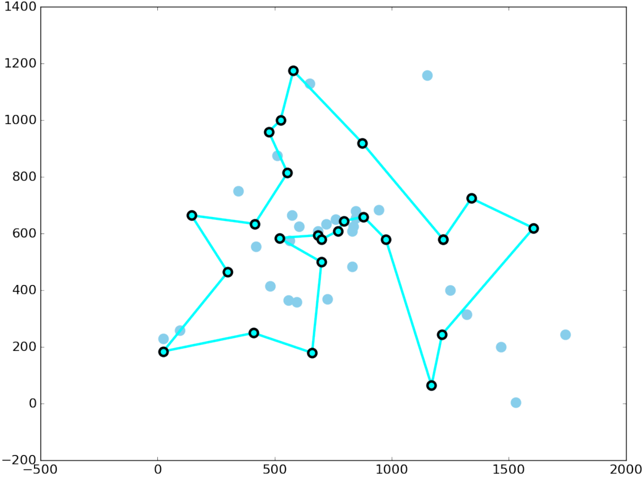

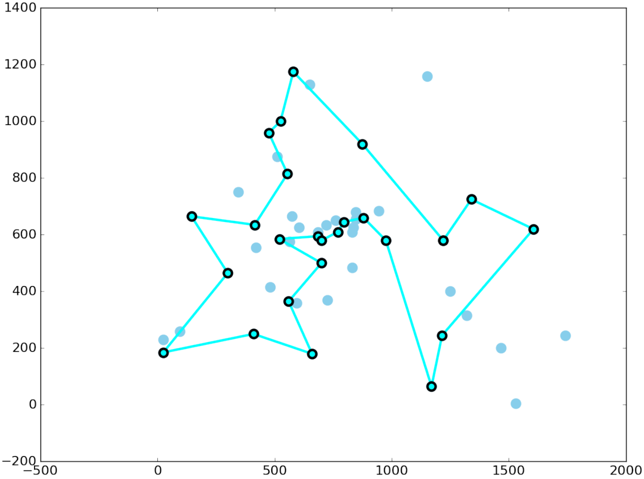
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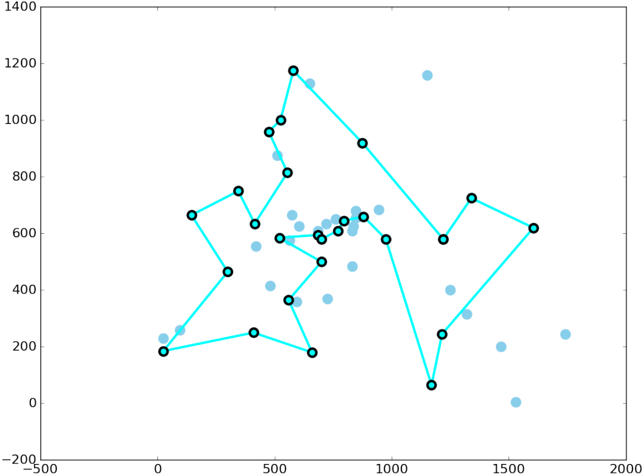

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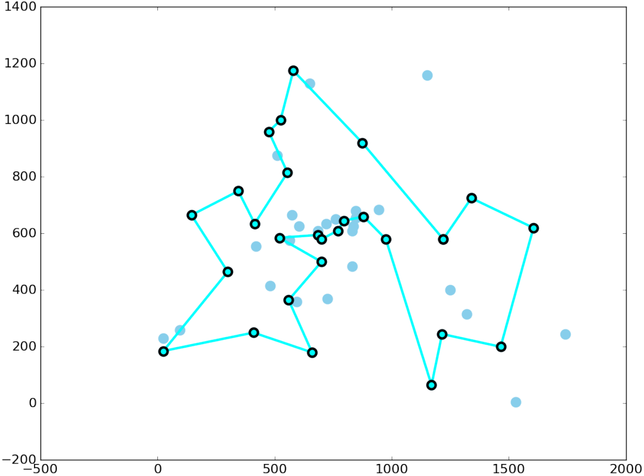

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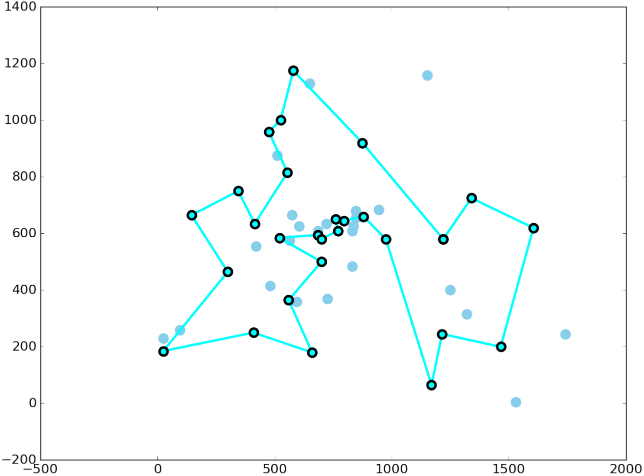

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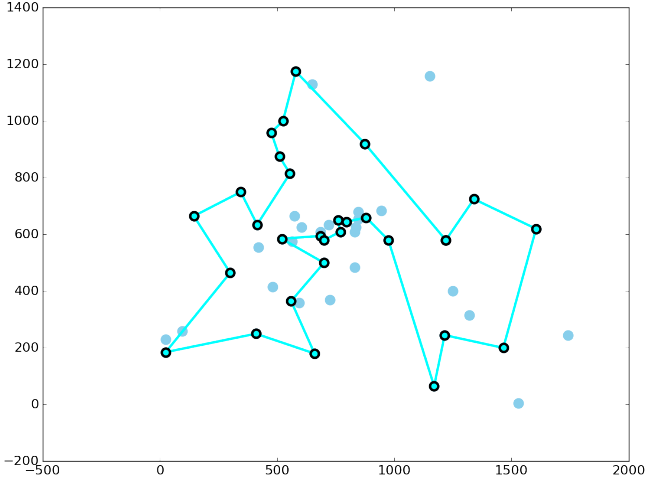

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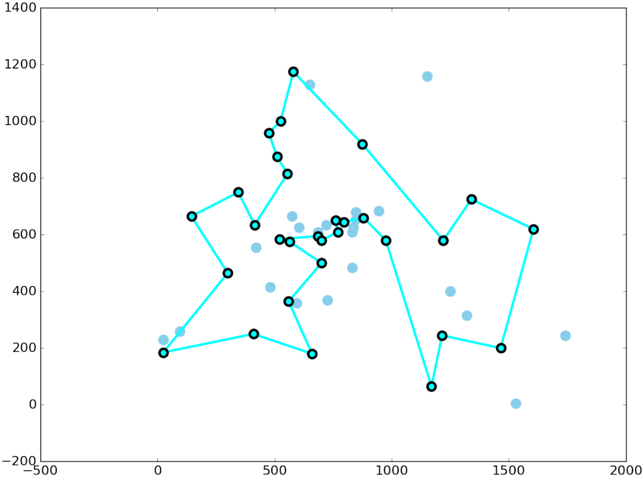

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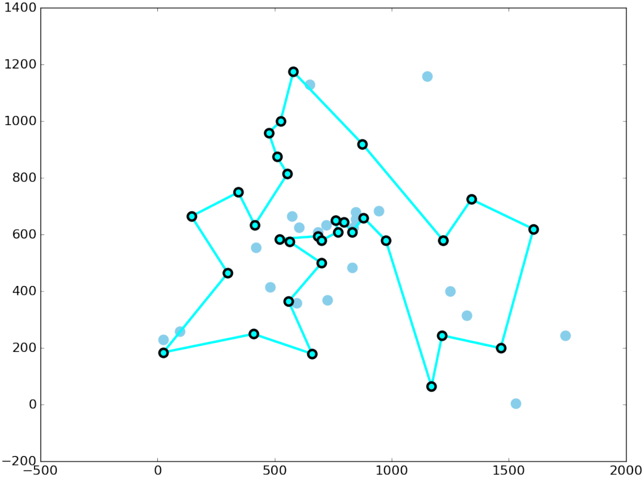

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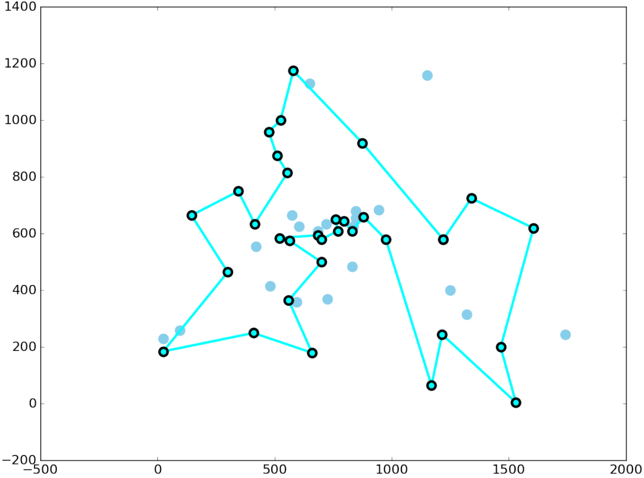

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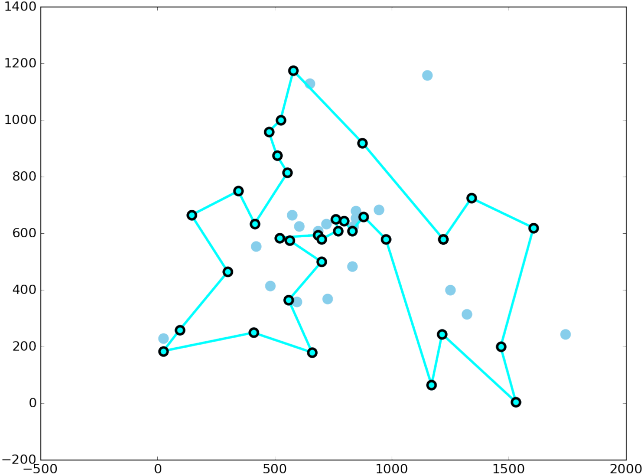

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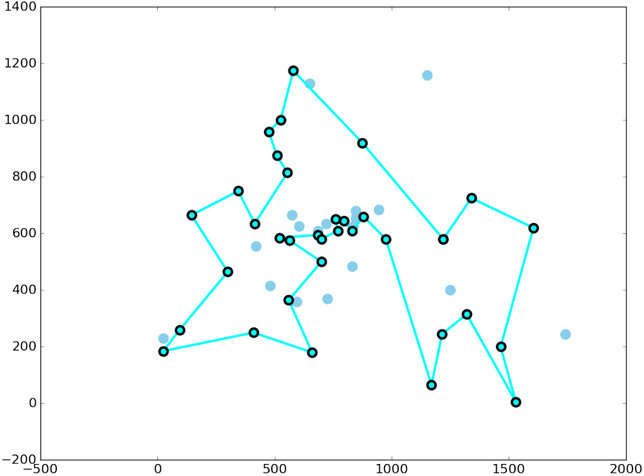

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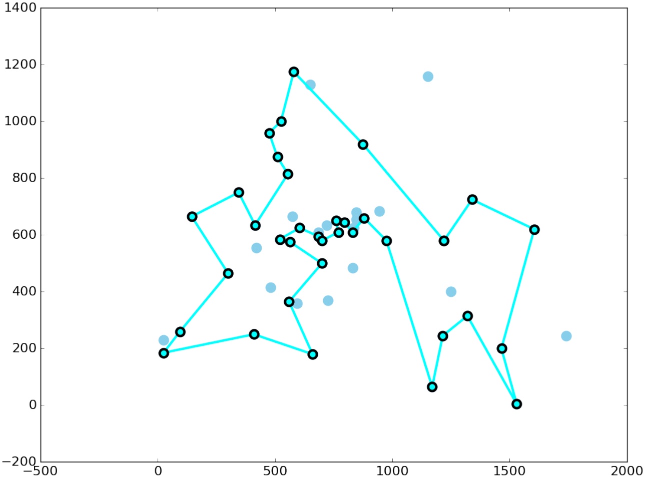

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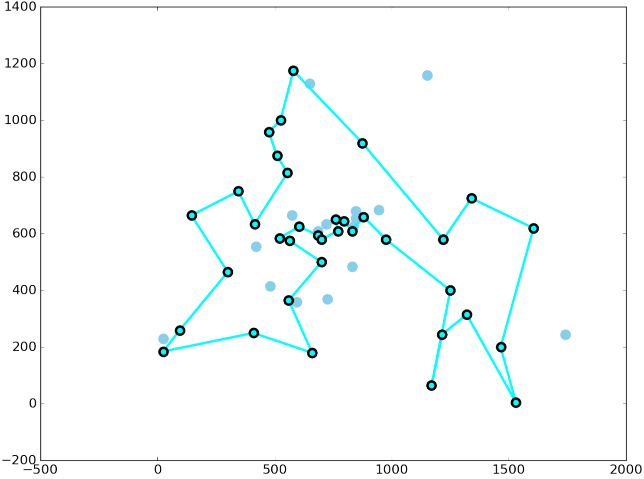

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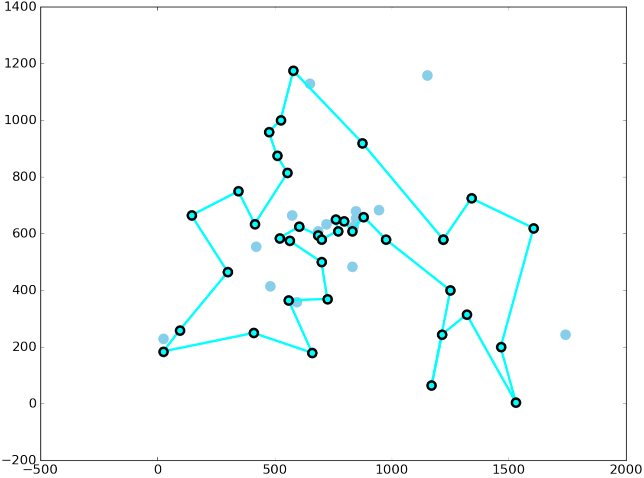

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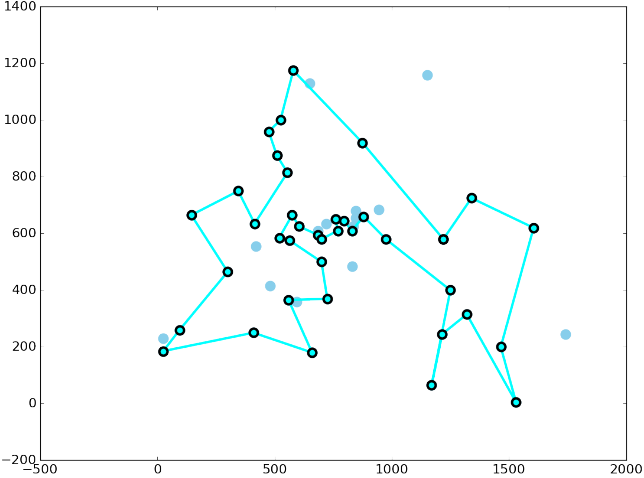

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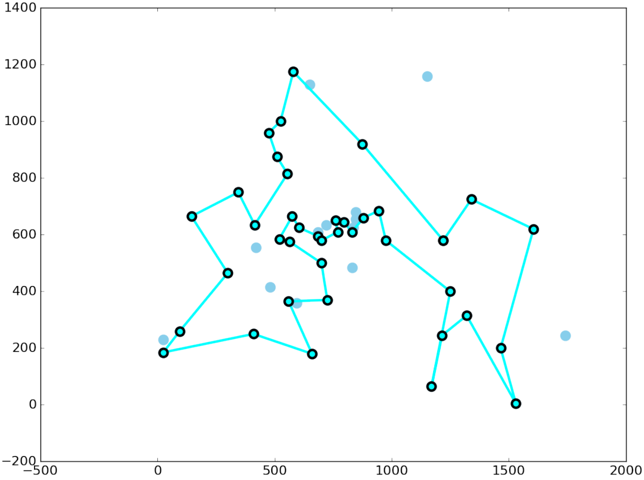

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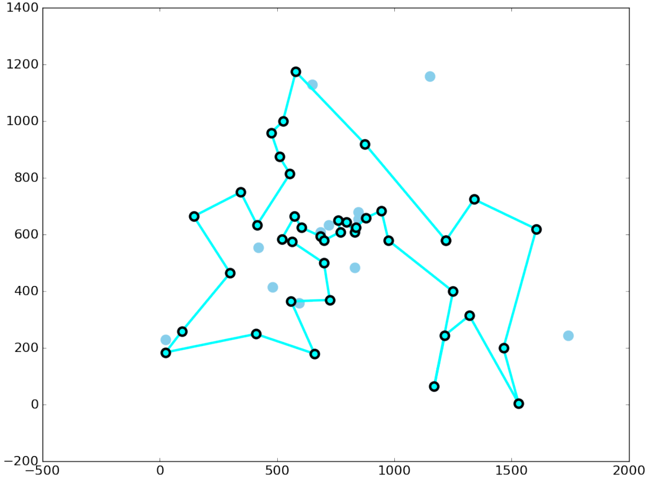

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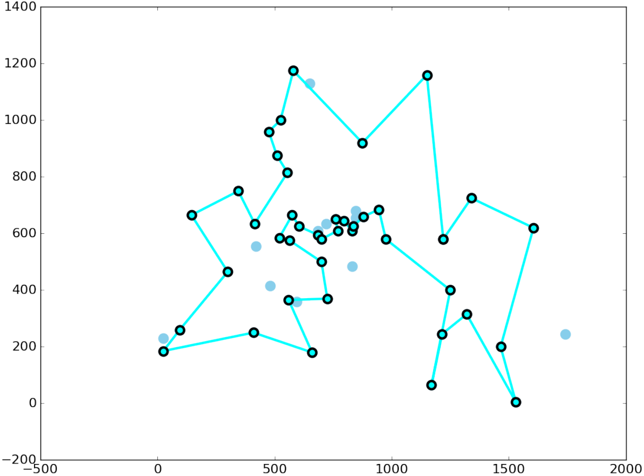

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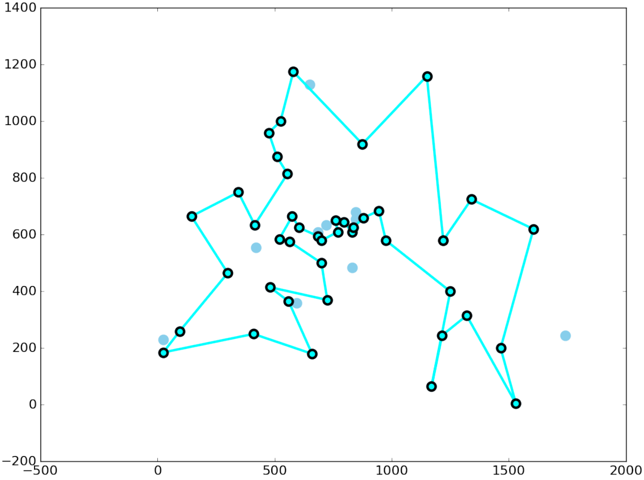

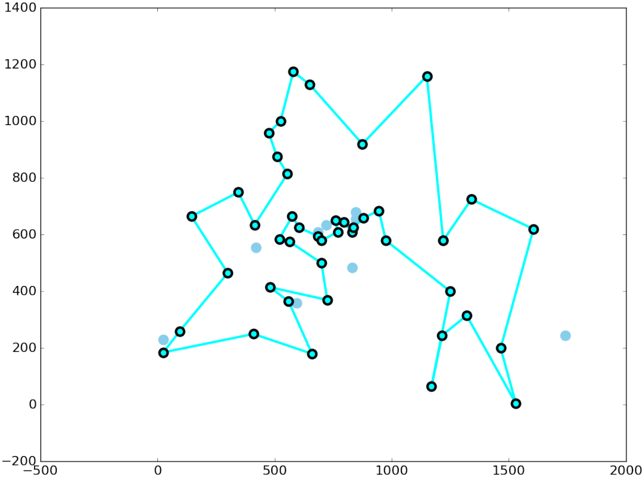
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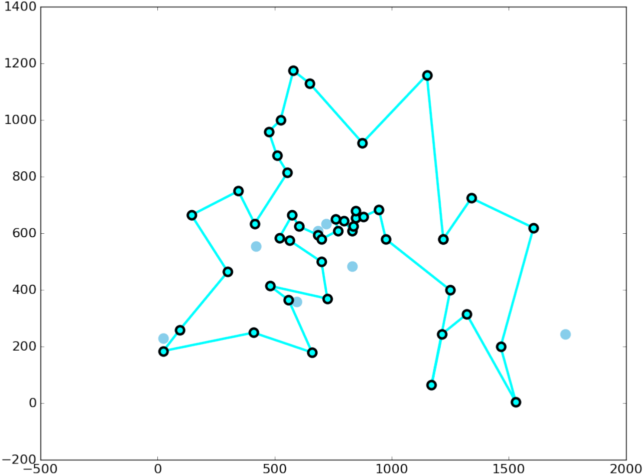

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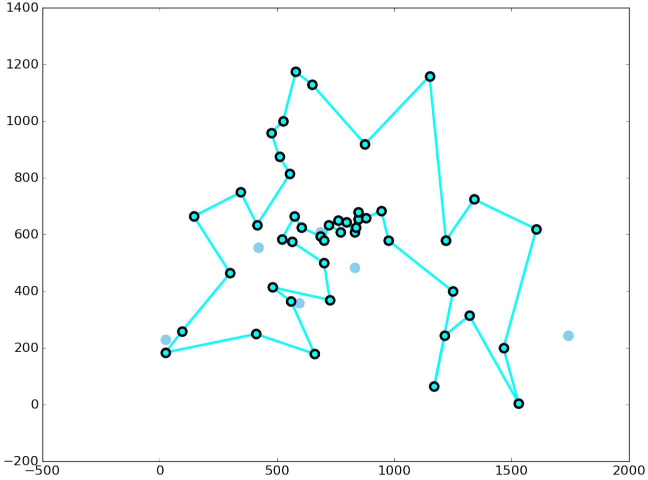

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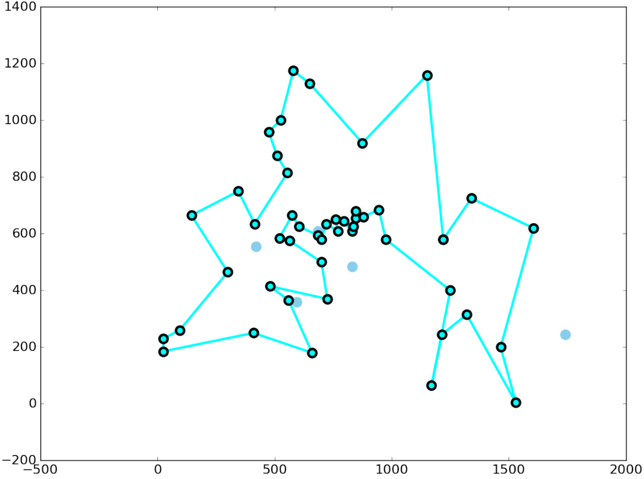

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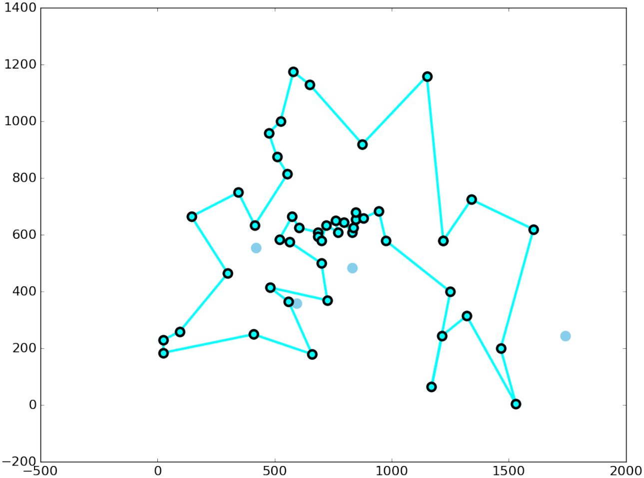

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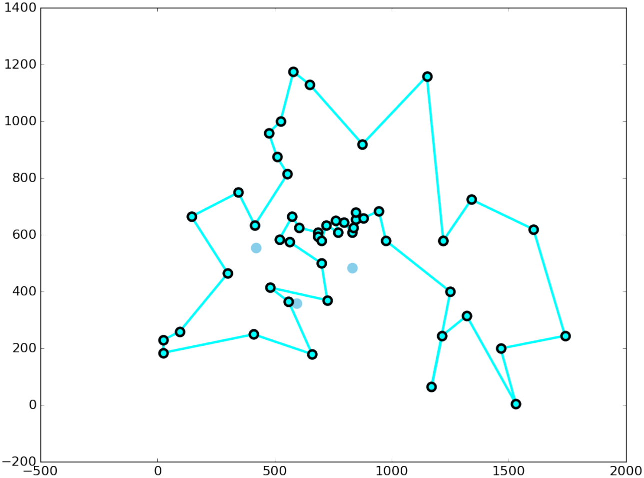

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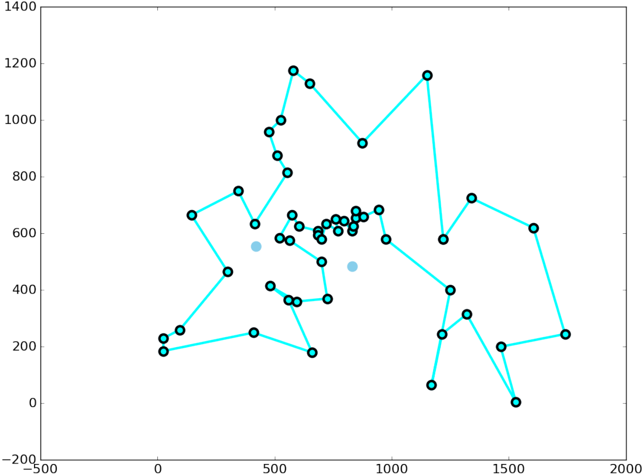

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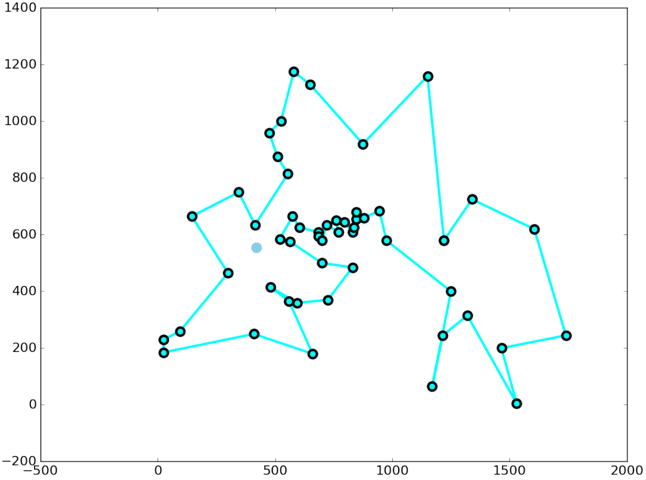

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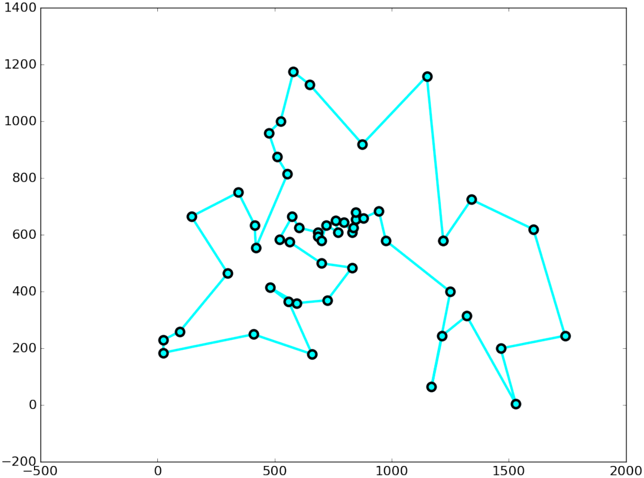


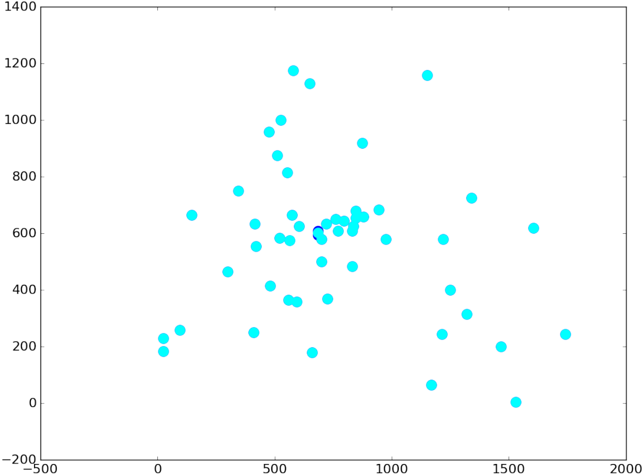
How does the pair-center algorithm work?

The pair-center tour algorithm is a contribution of my own for this course (still haven't found it on the internet). It is a deterministic algorithm:

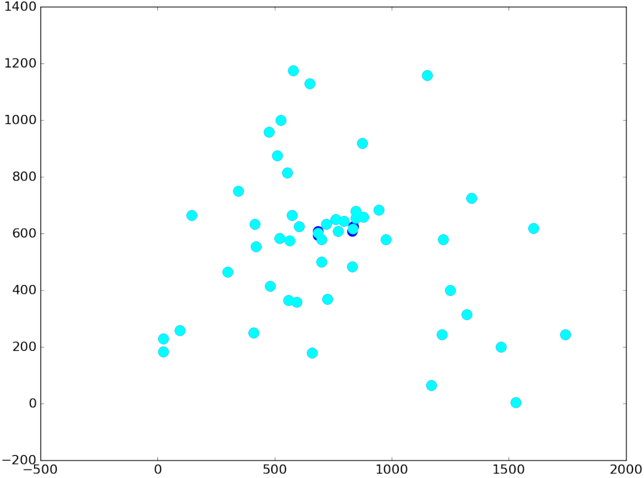
- with a bottom-up construction build a binary tree by replacing the/a closest pair of points by their center
- with a top-down construction build the tour by inserting the corresponding pairs in the best possible way

The runtime is in $\mathcal{O}(n^2)$, I guess (implemented is $\mathcal{O}(n^3)$ and a $\mathcal{O}(n^2)$ version with more sophisticated data structures).
Can you prove a worst case bound for the tour length? Recently I've improved to $\mathcal{O}(n\mathrm{polylog}(n))$ with practical runtime in the order of $n \log n$ and error below 5%.

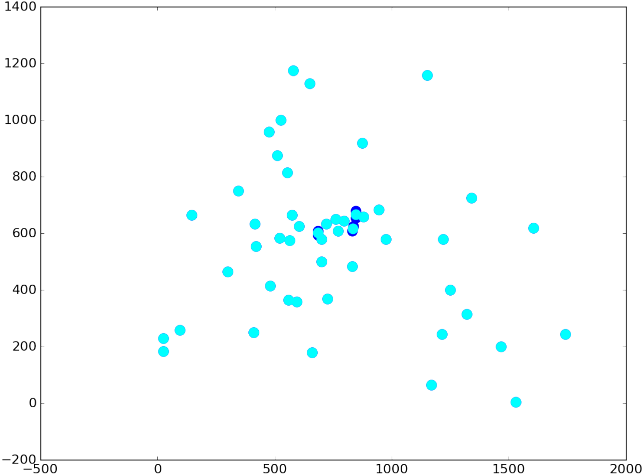
animation of the pair-center tour algorithm



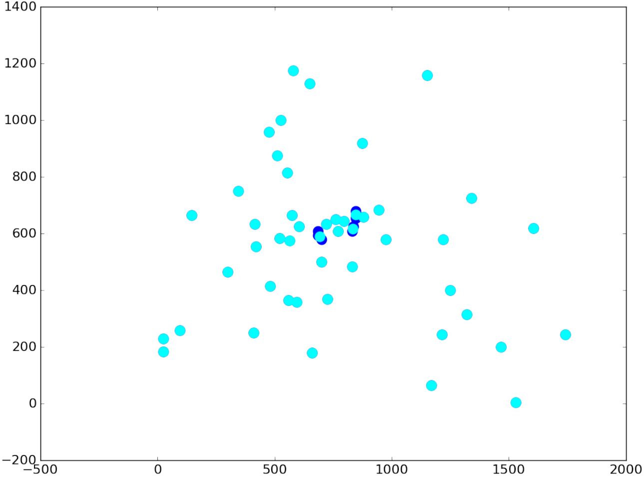
animation of the pair-center tour algorithm



animation of the pair-center tour algorithm



animation of the pair-center tour algorithm



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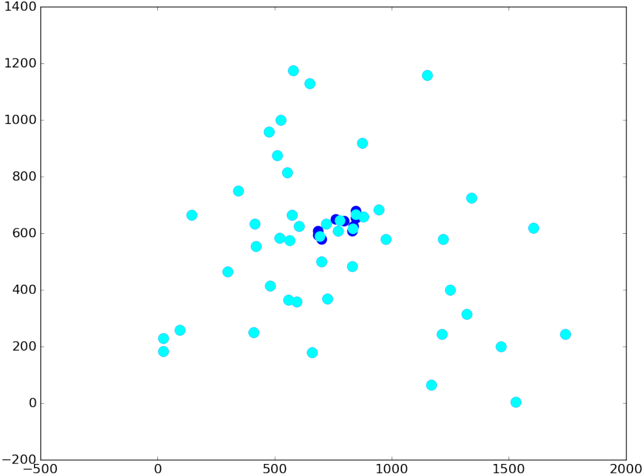

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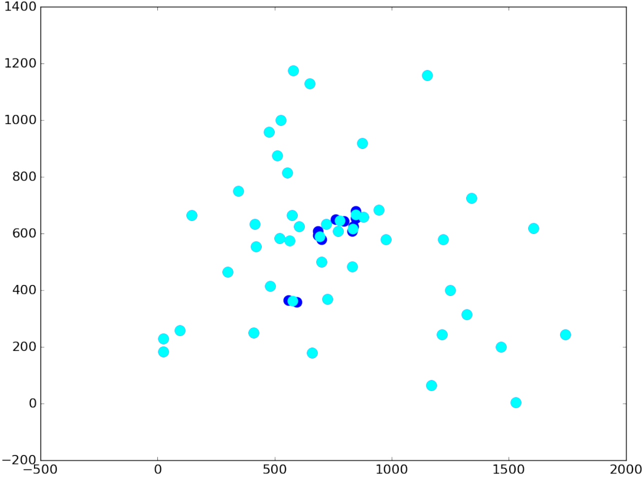

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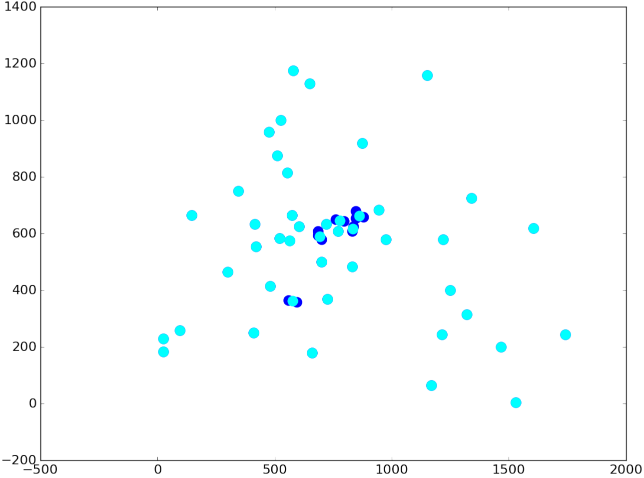

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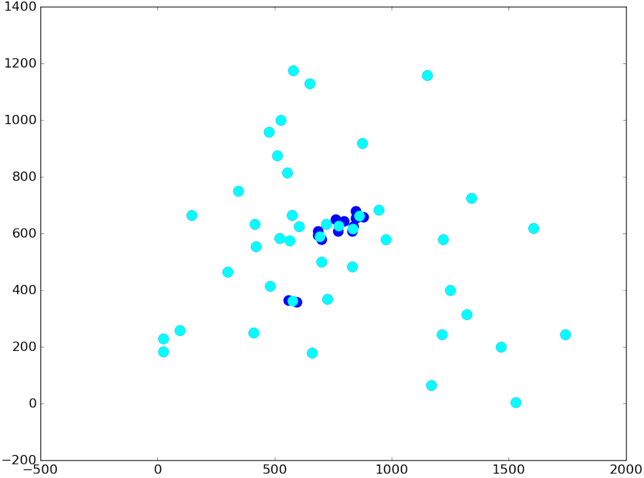

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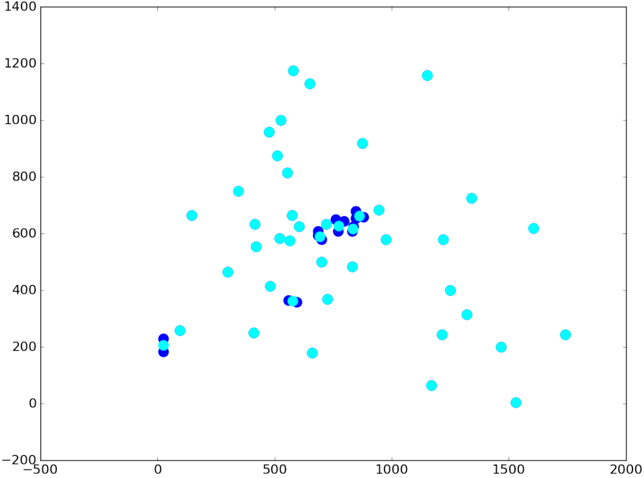

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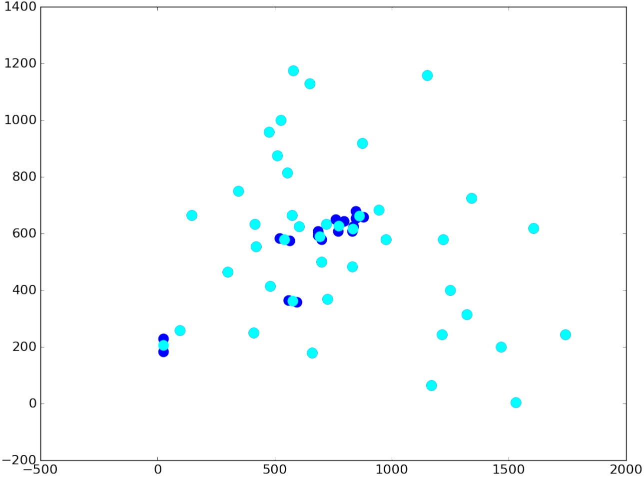

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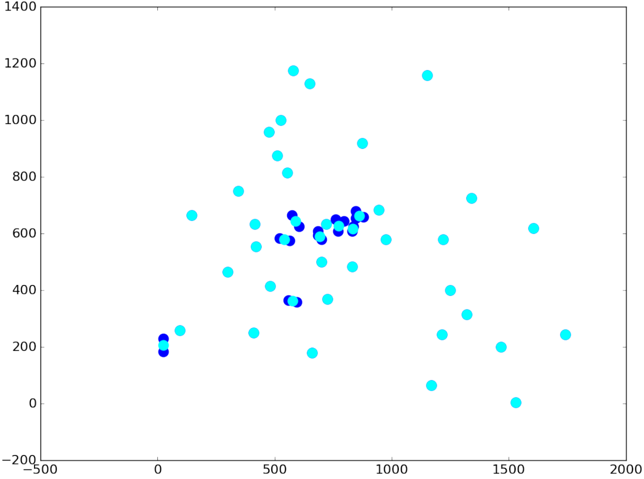

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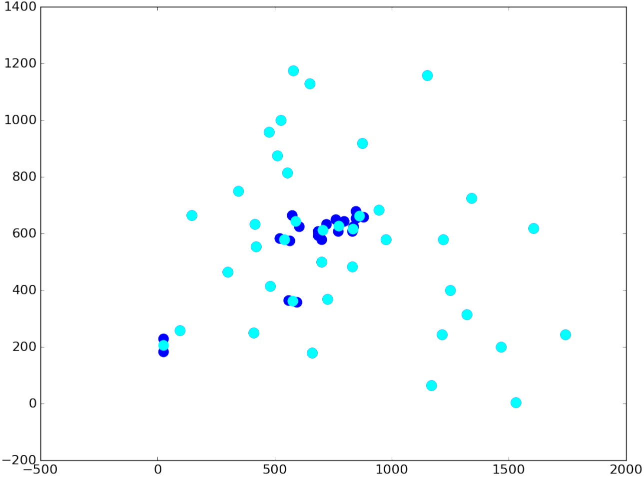

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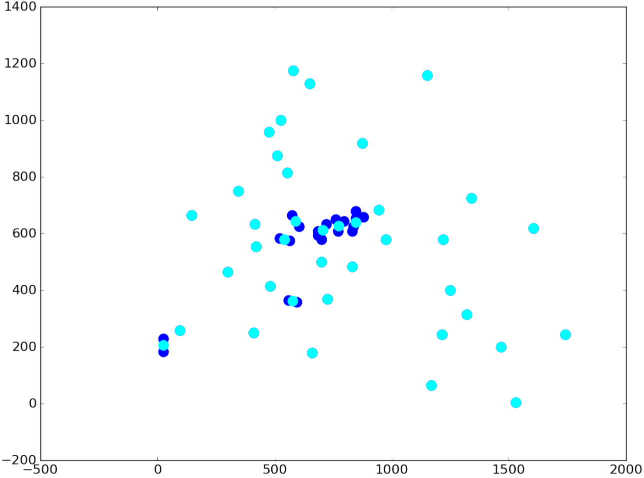

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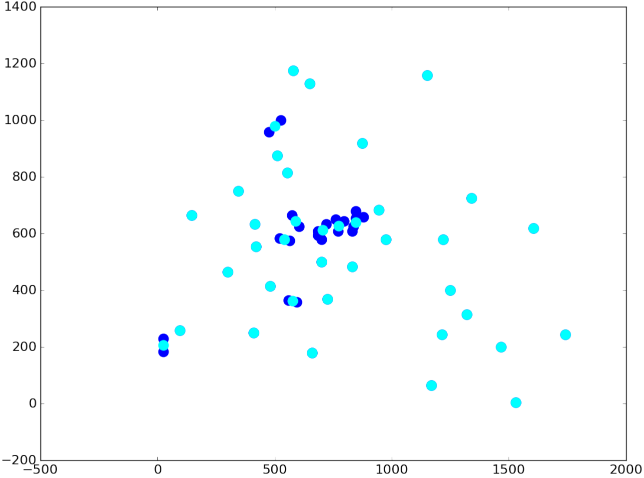

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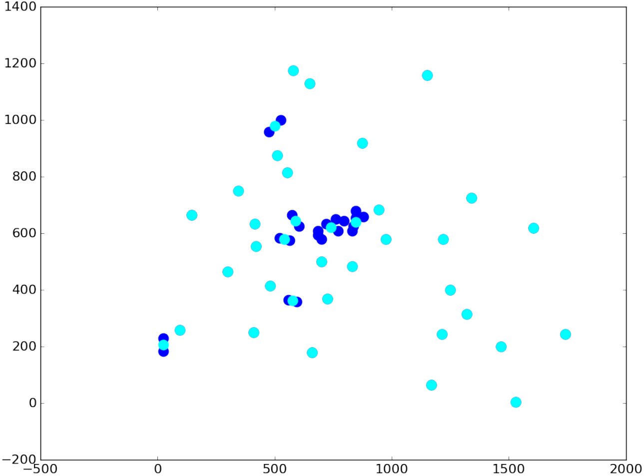

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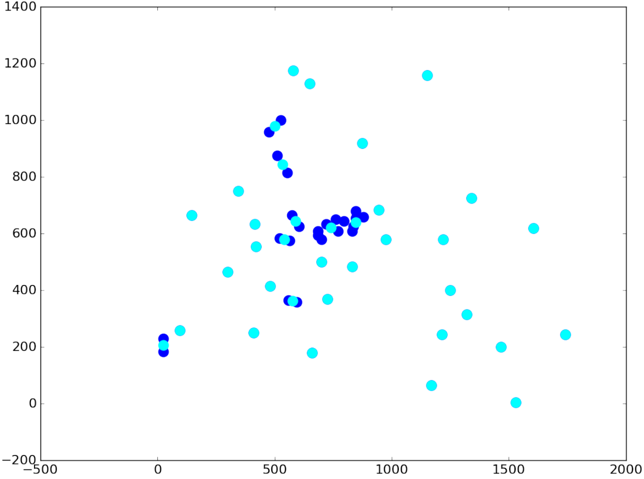

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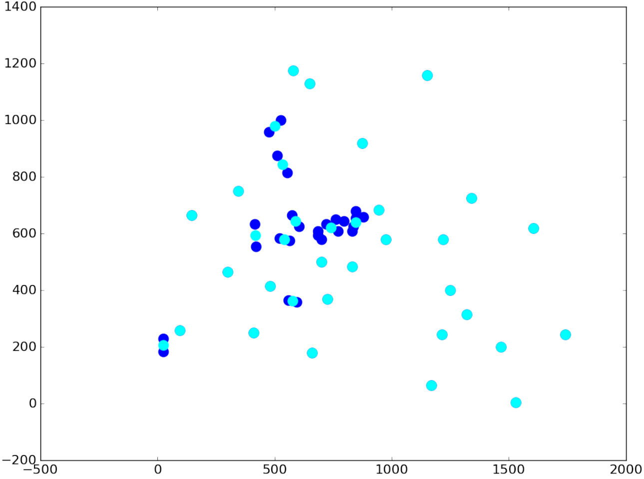

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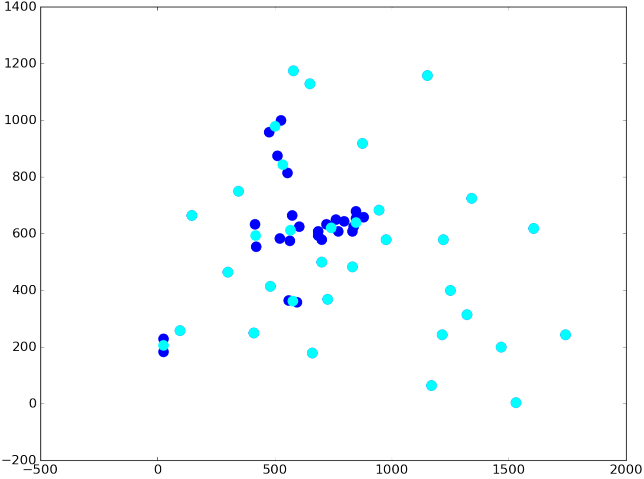

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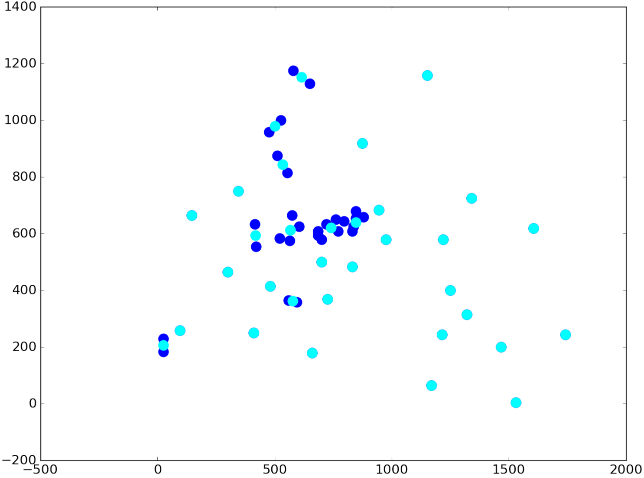

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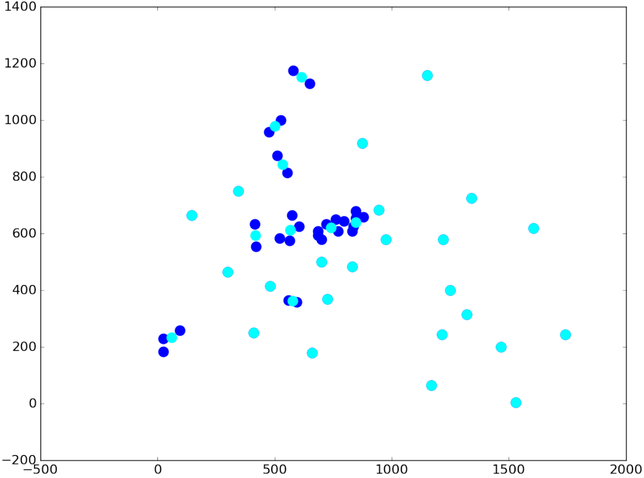

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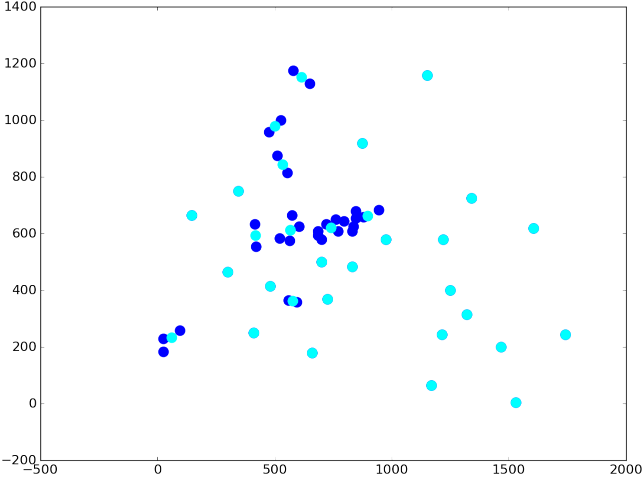

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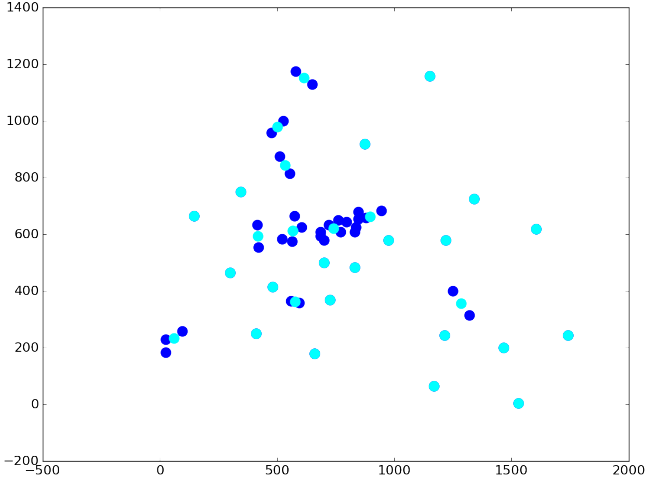

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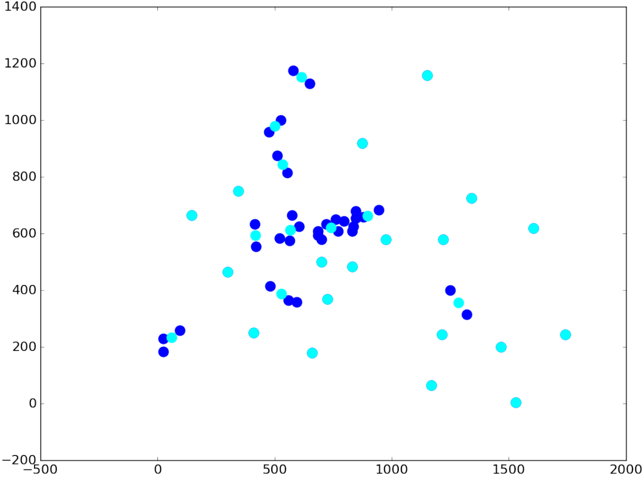

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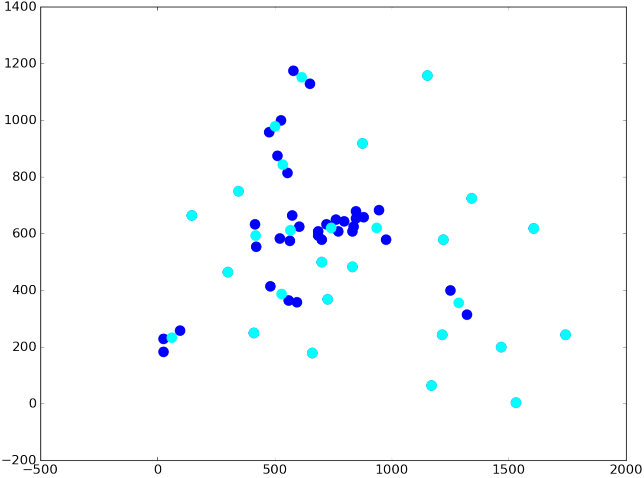

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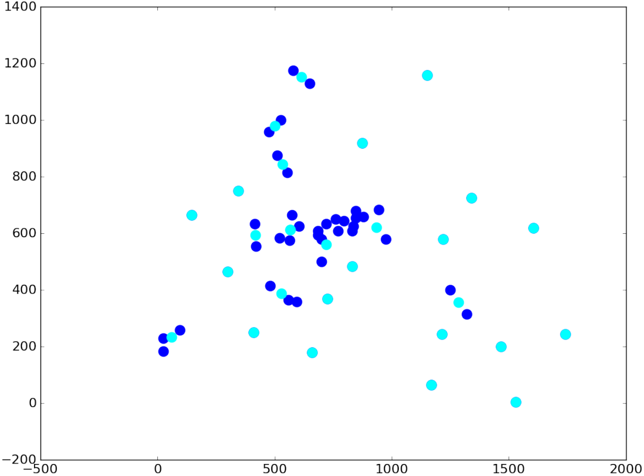

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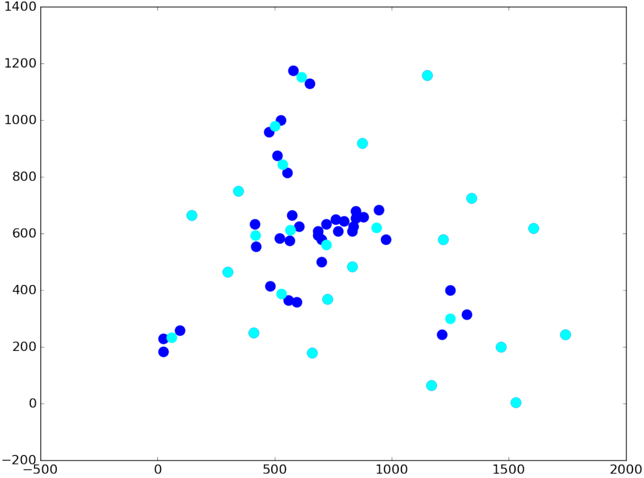

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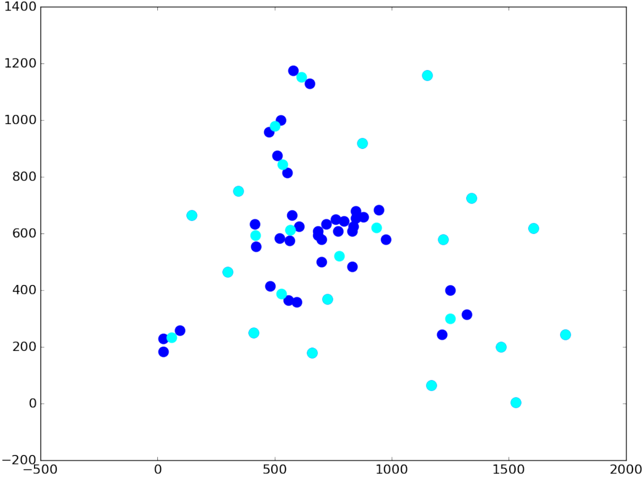

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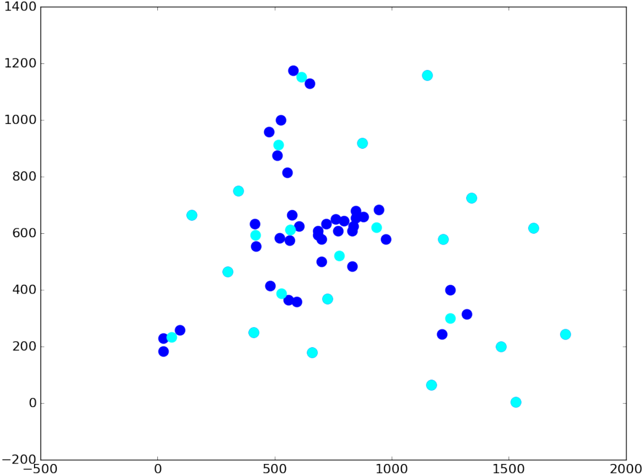

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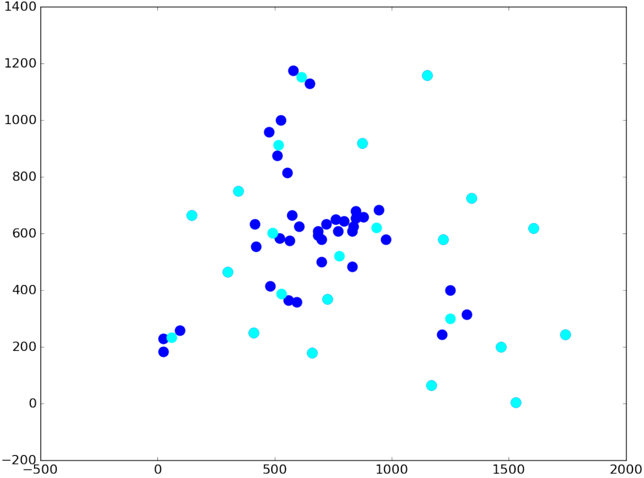

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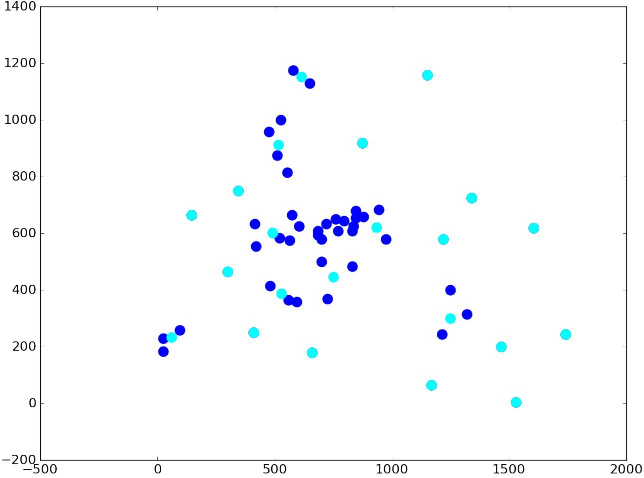

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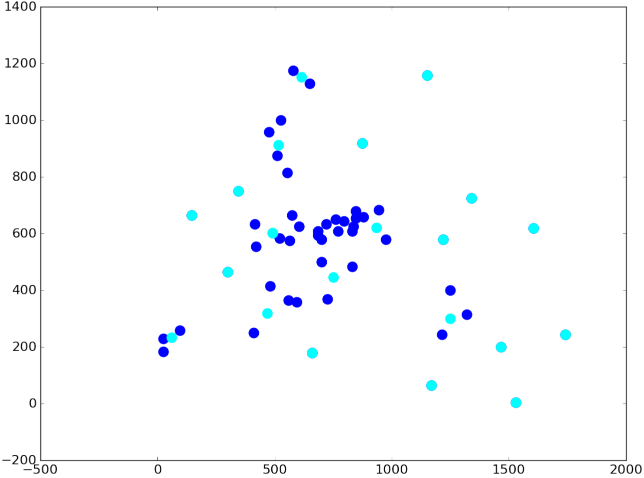

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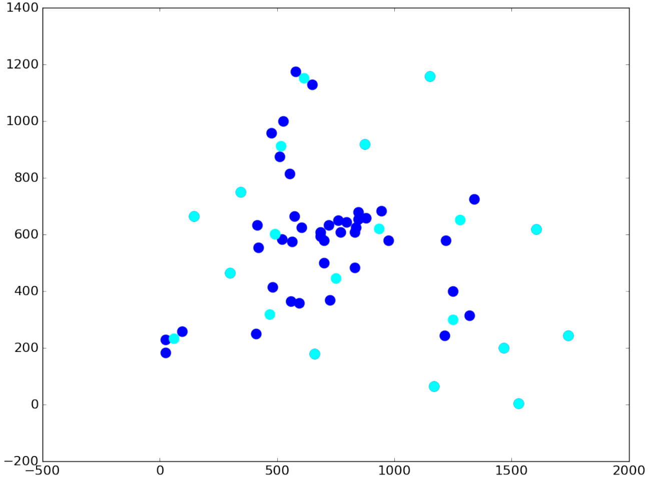

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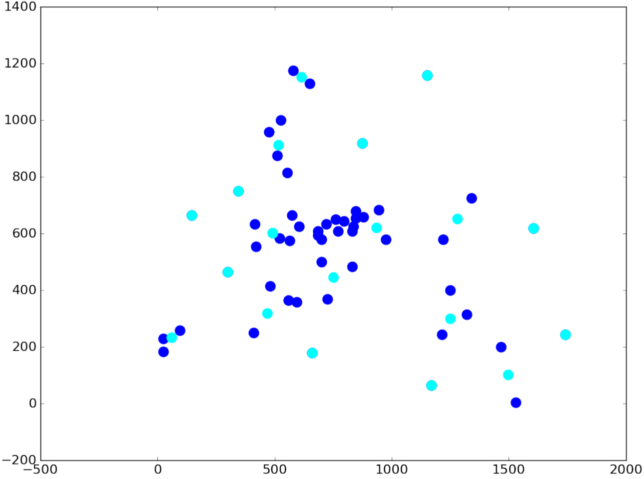

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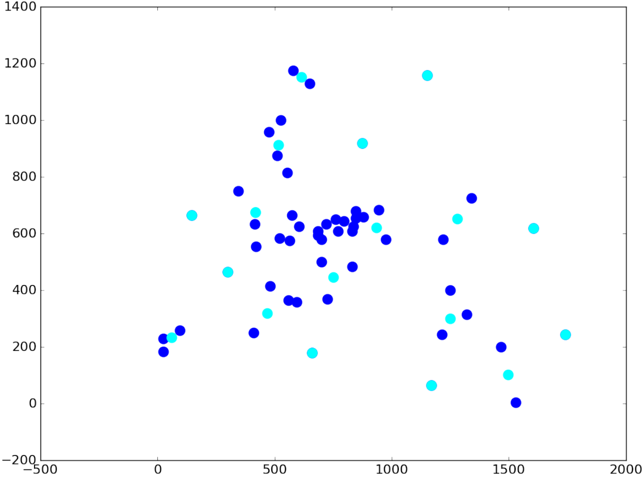

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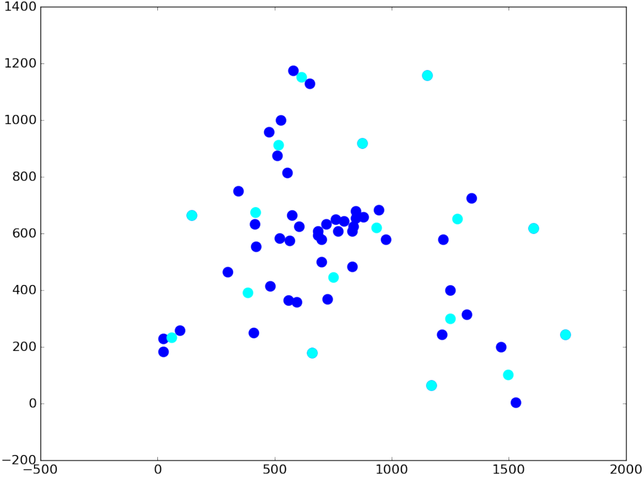

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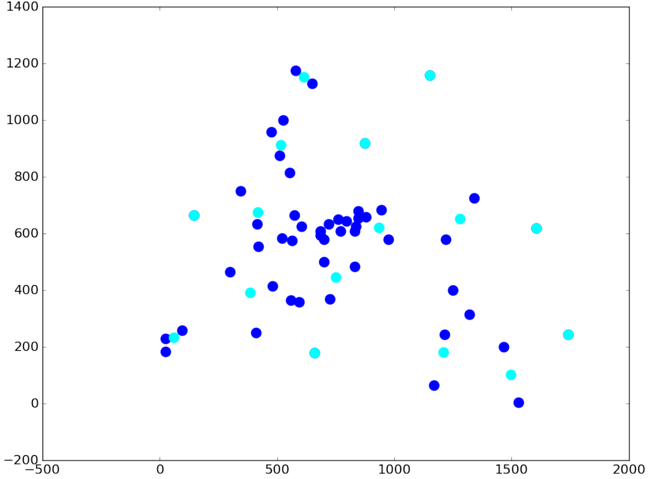

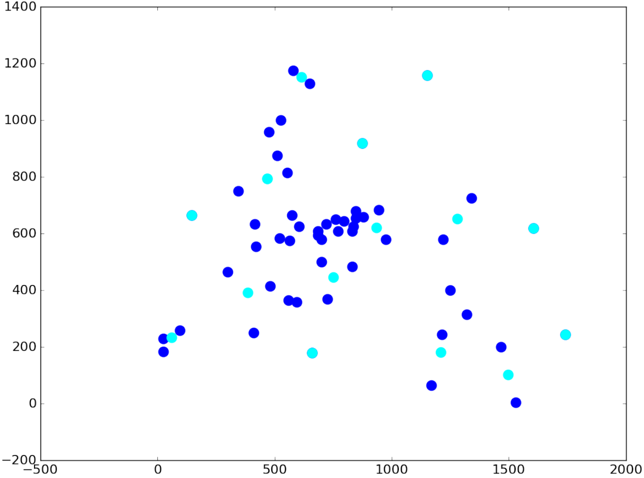
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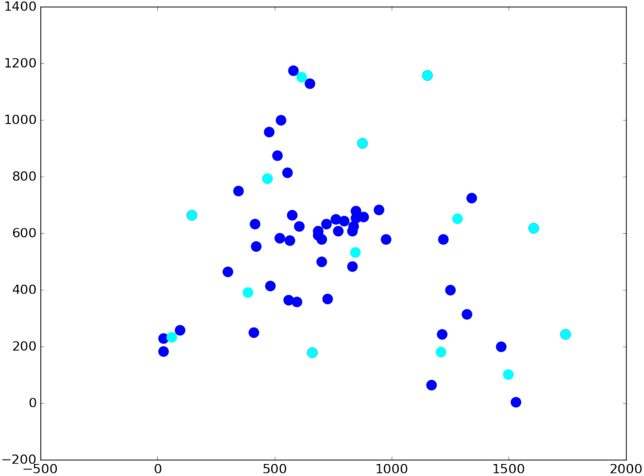

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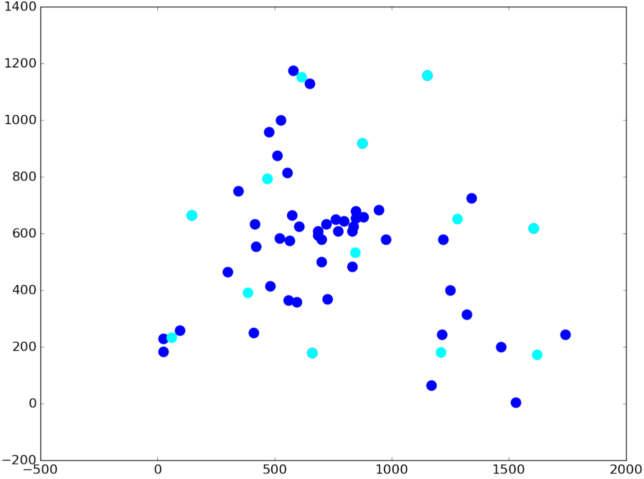

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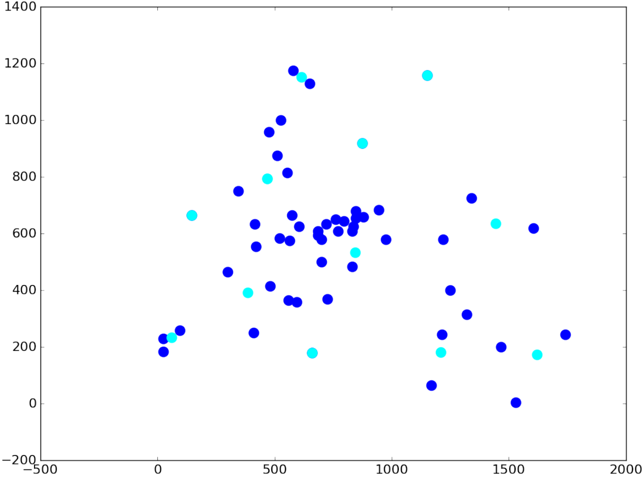

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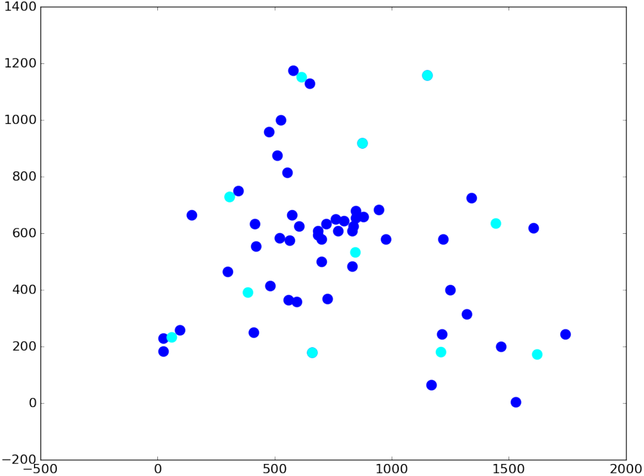

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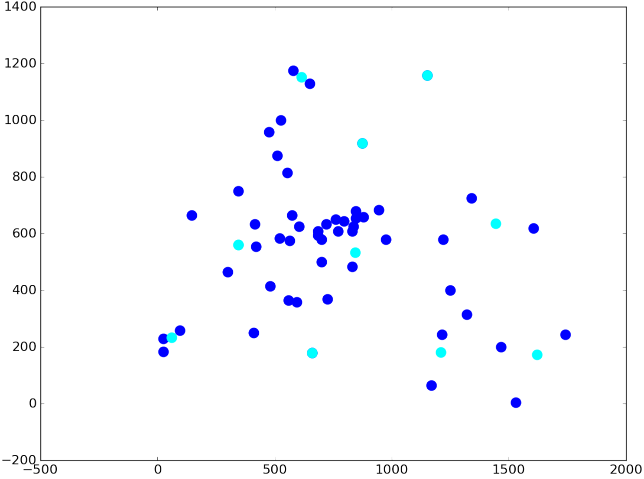

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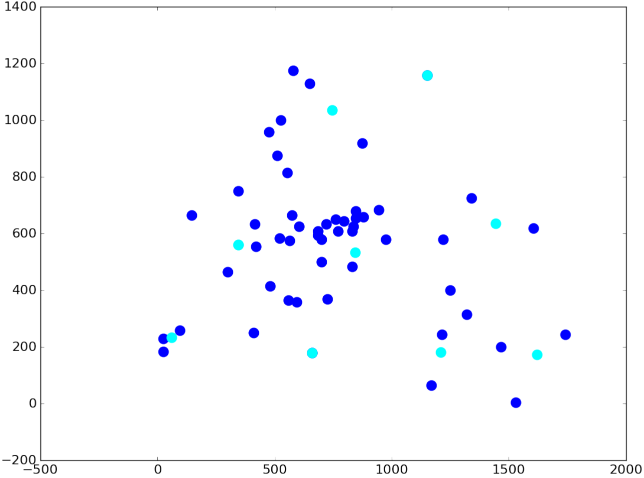

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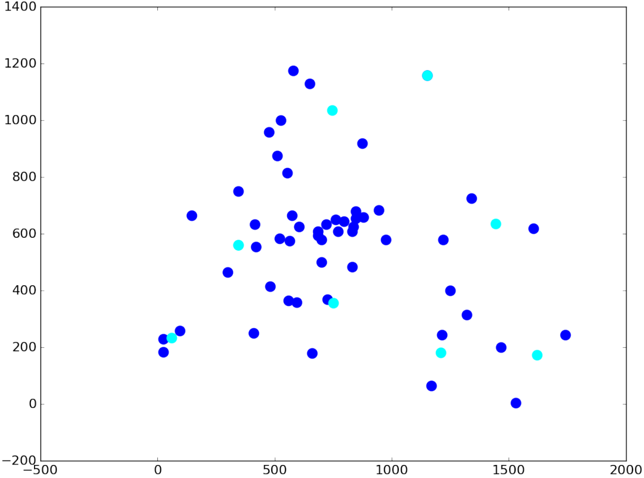

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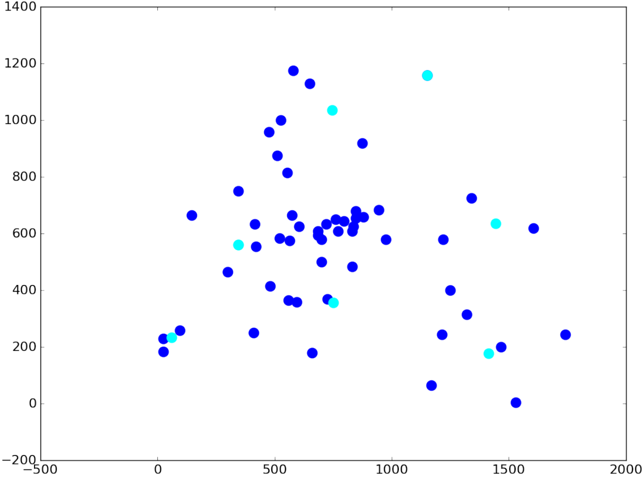

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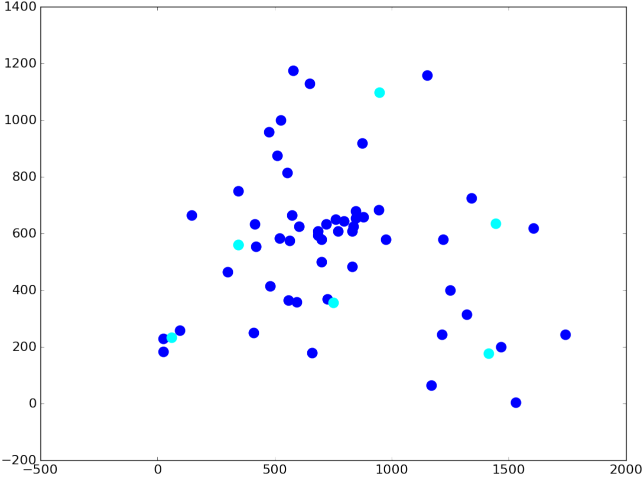

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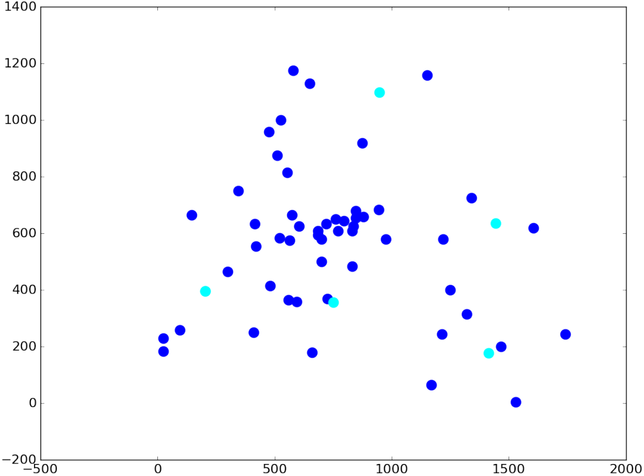

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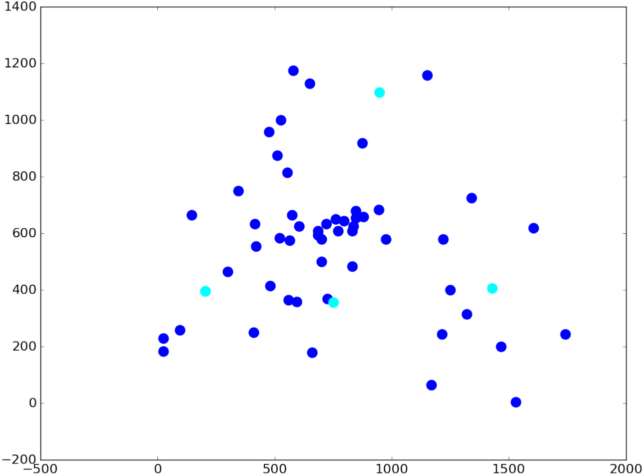

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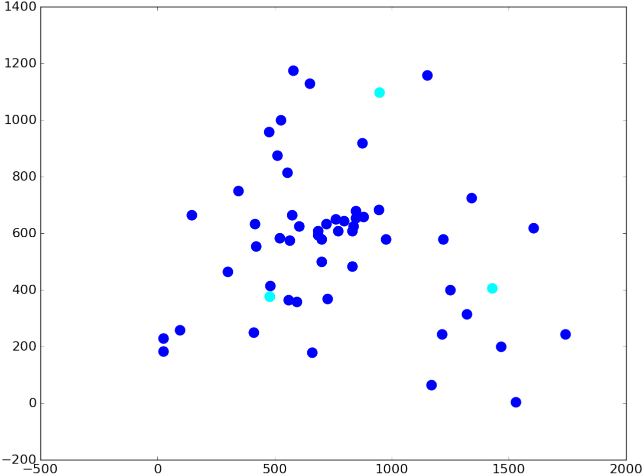

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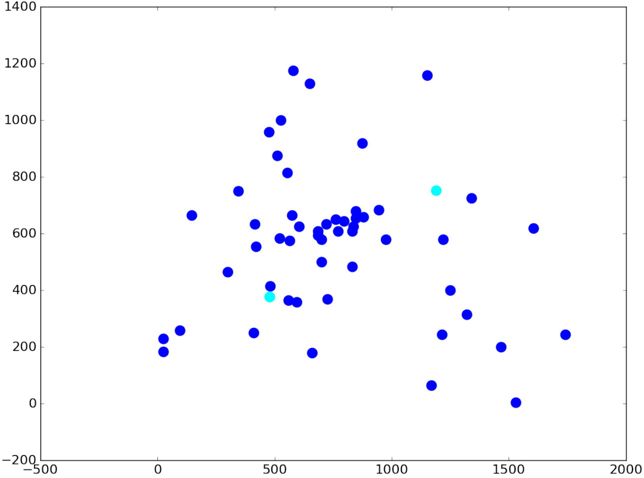

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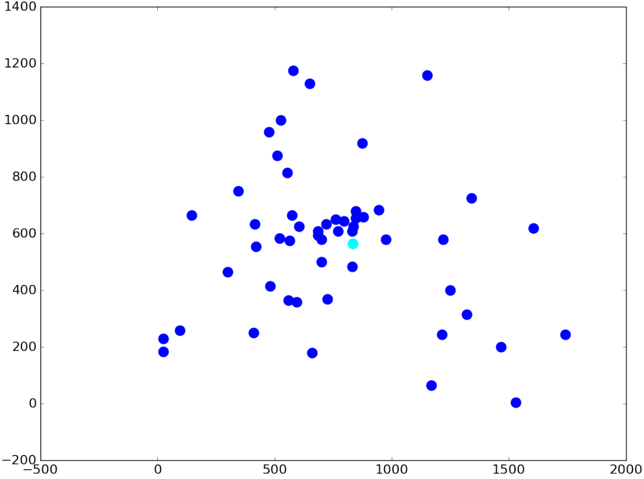

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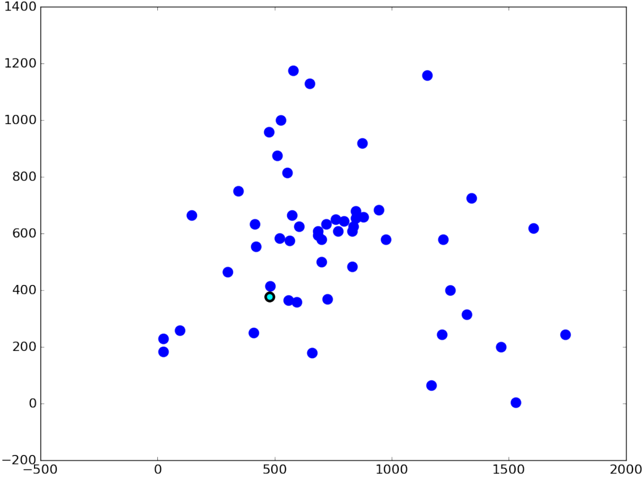

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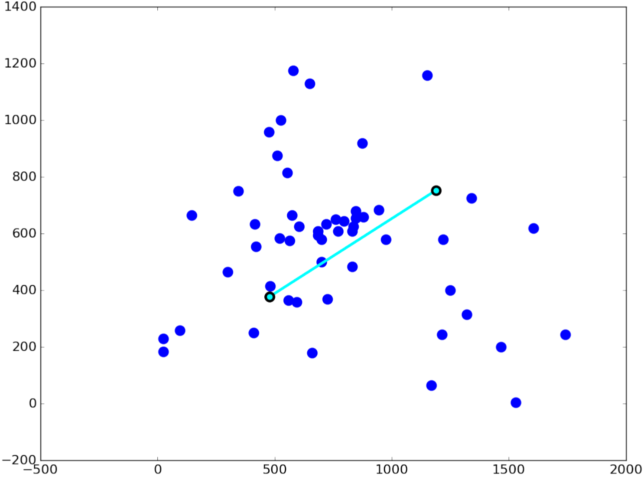

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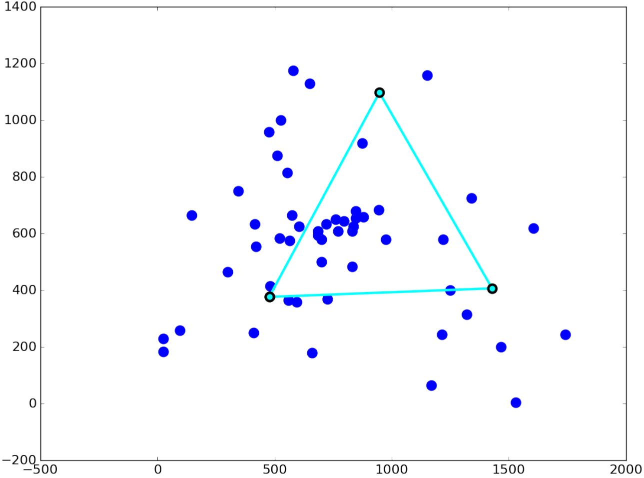

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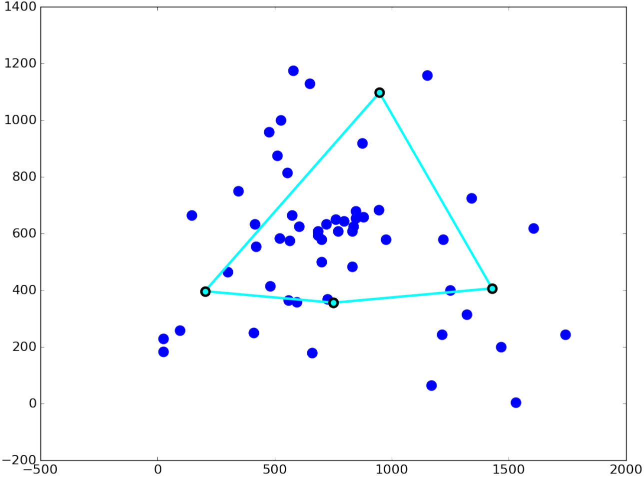

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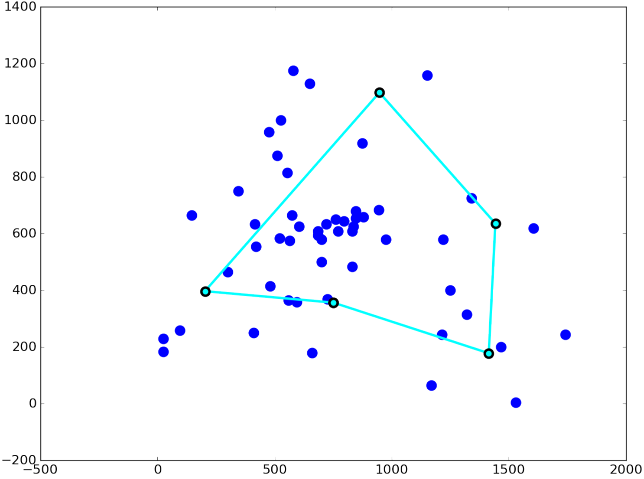

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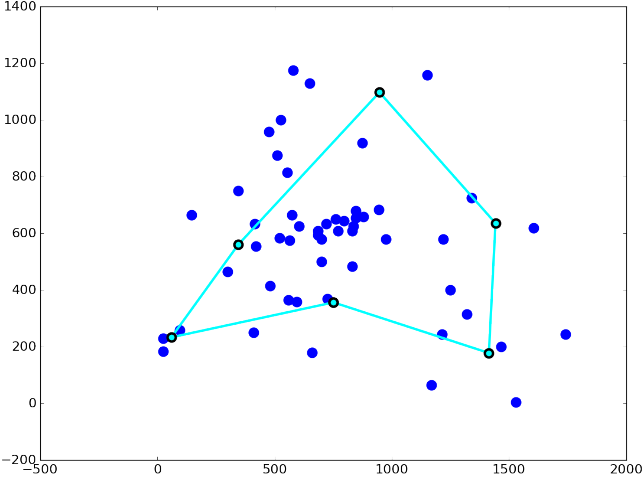

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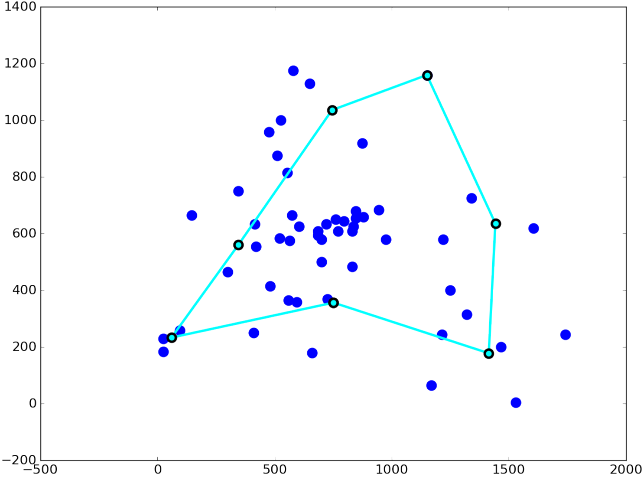

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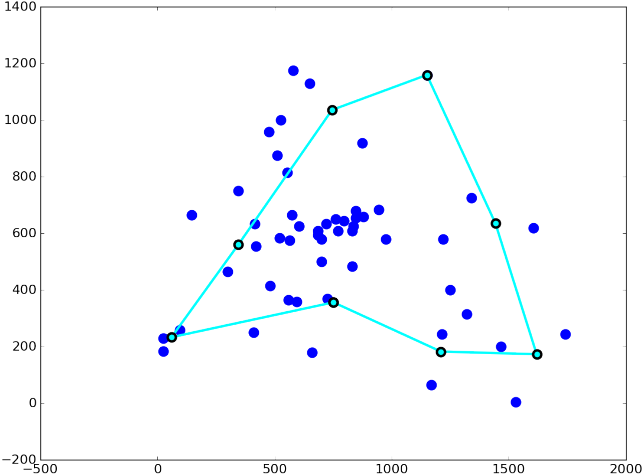

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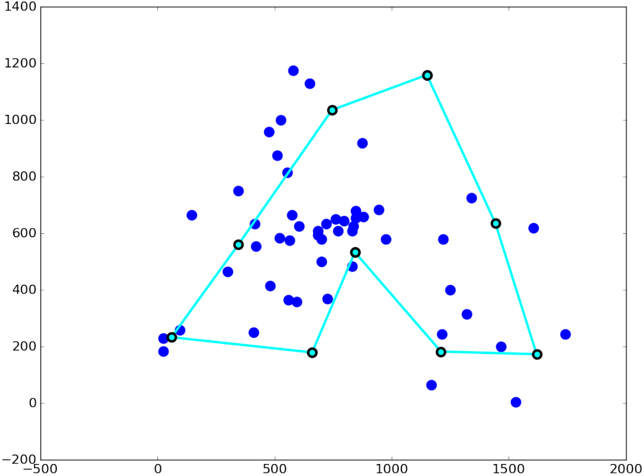

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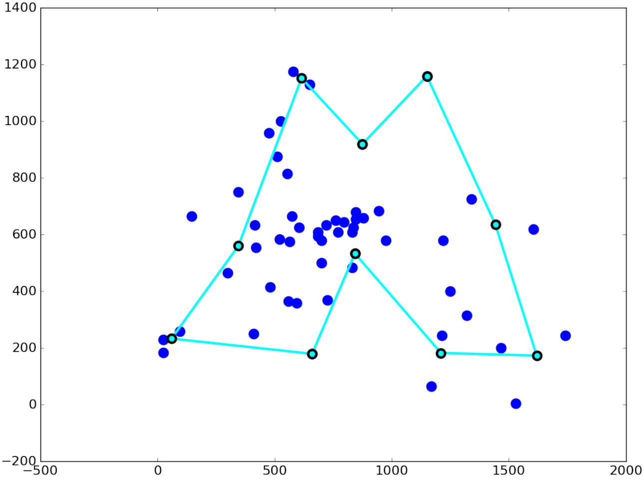

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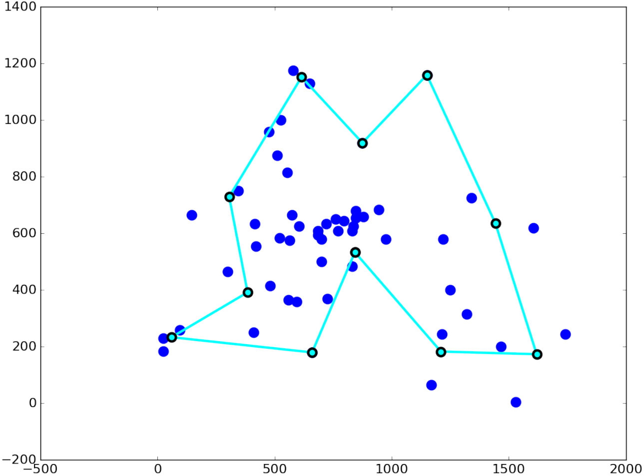

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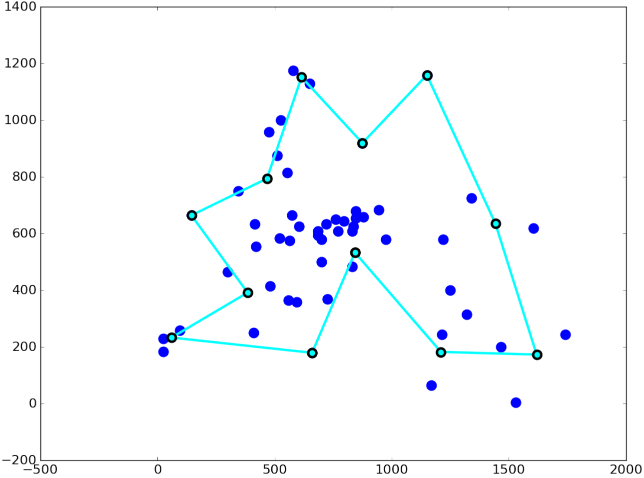

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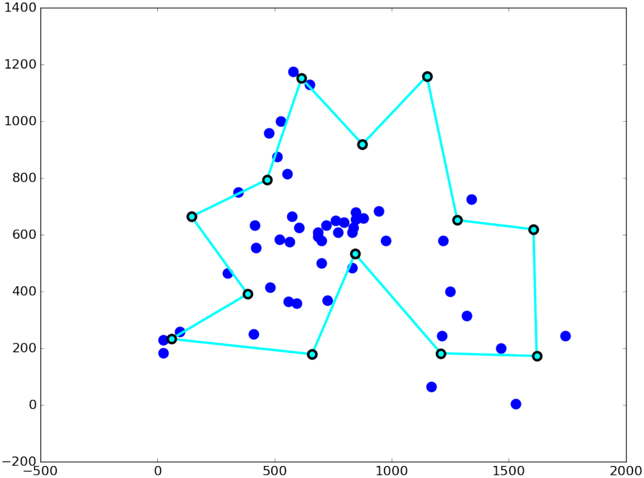

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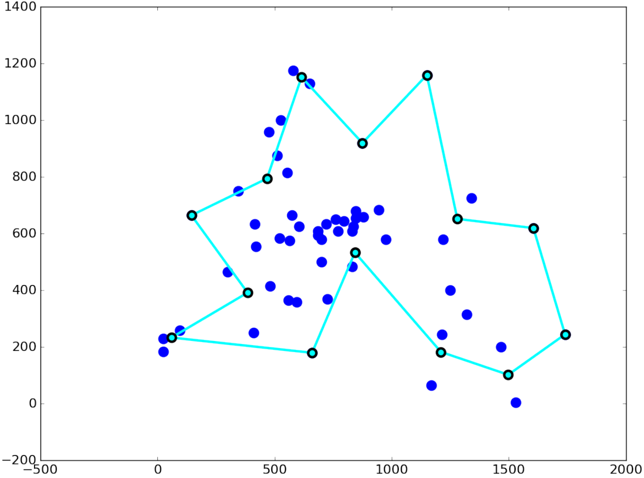

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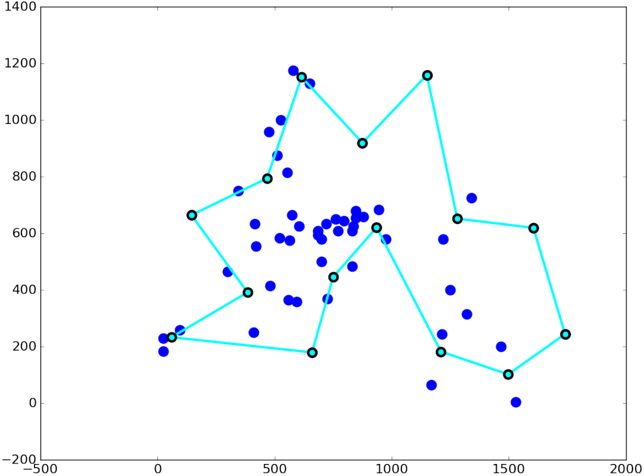

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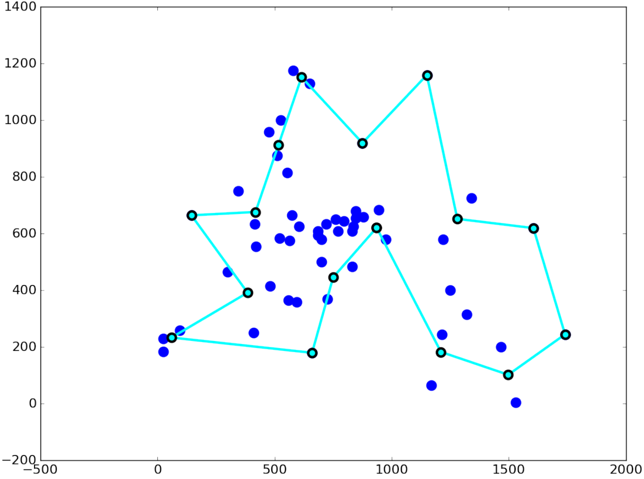

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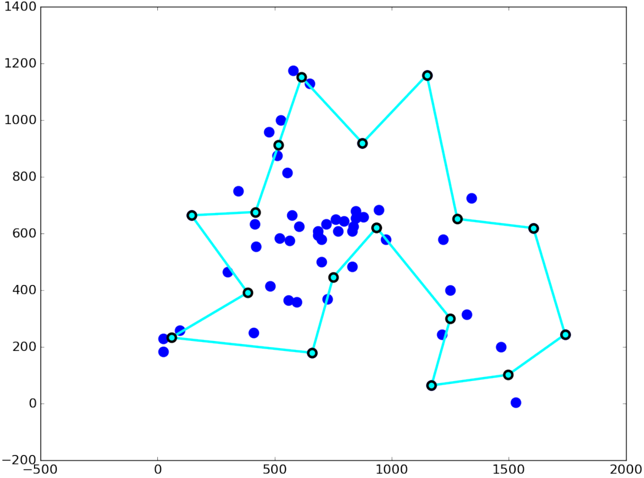

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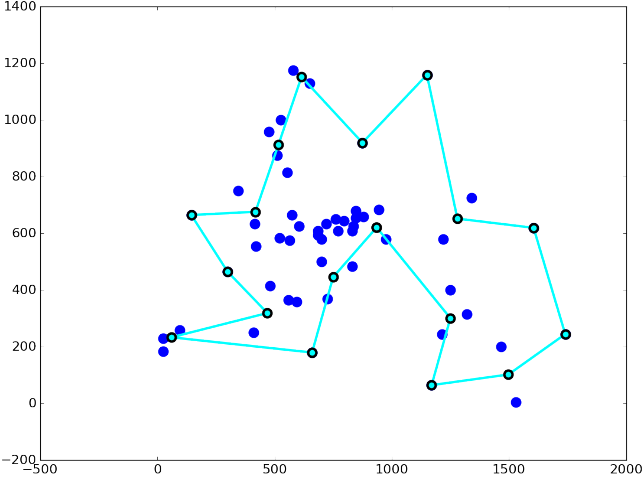

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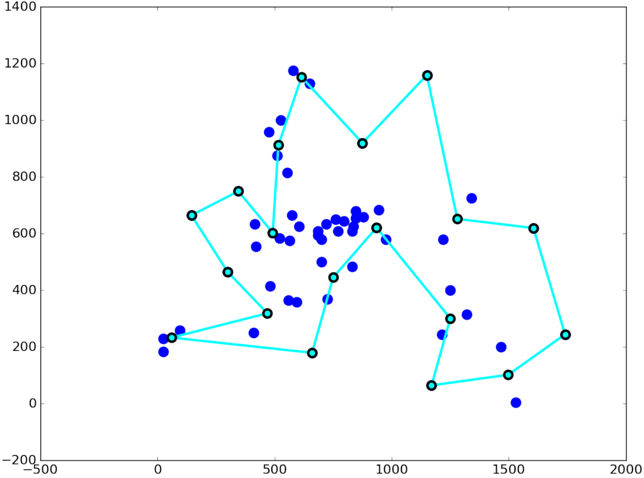

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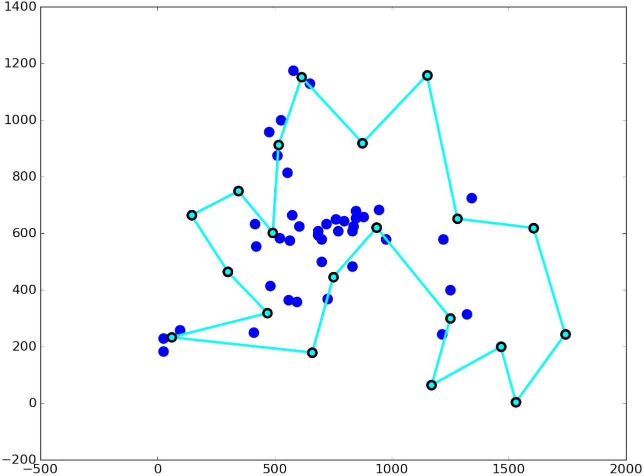

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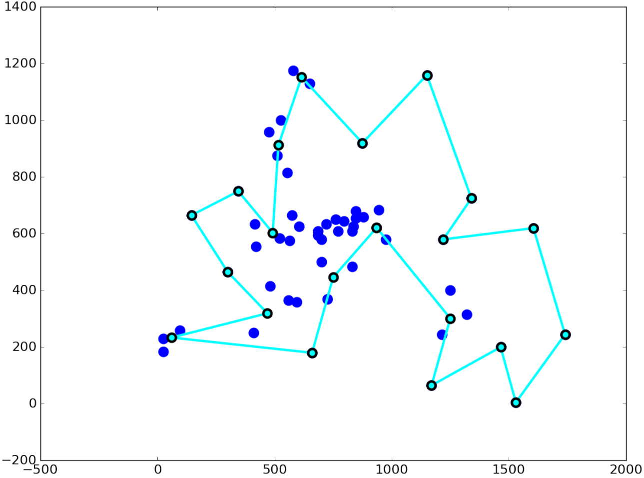

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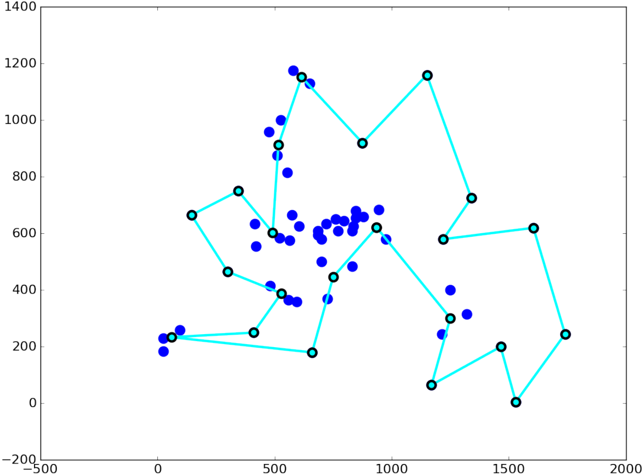

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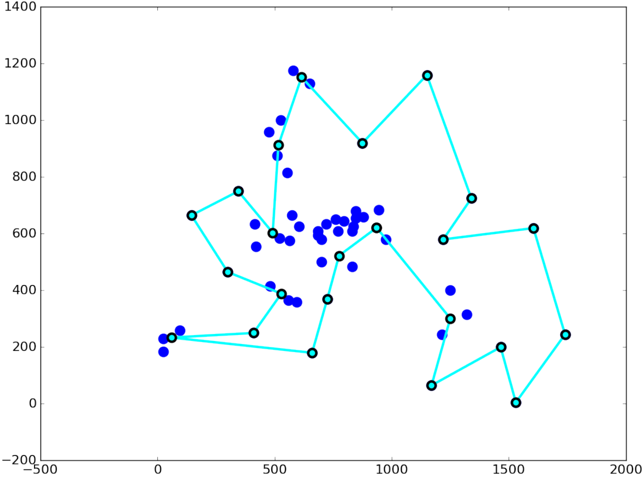

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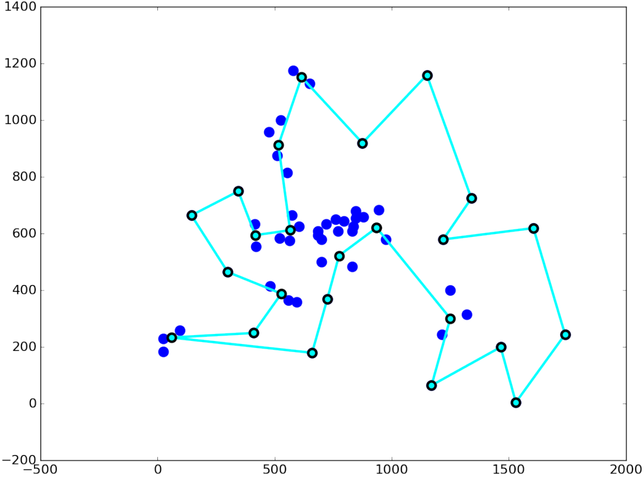

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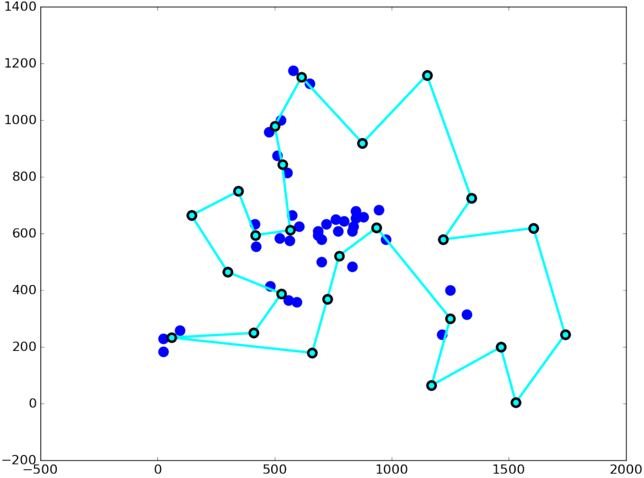

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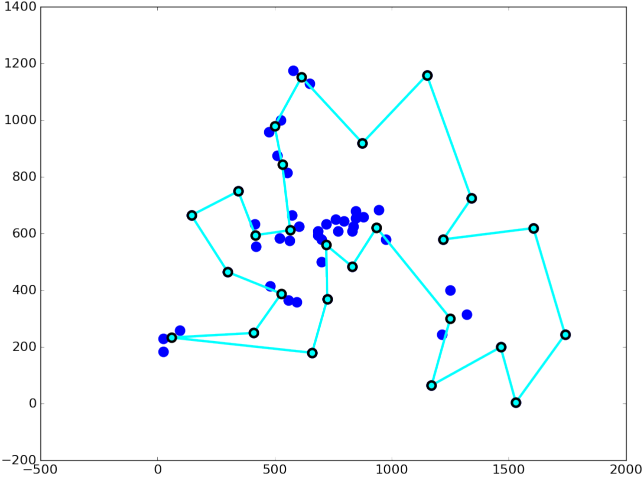

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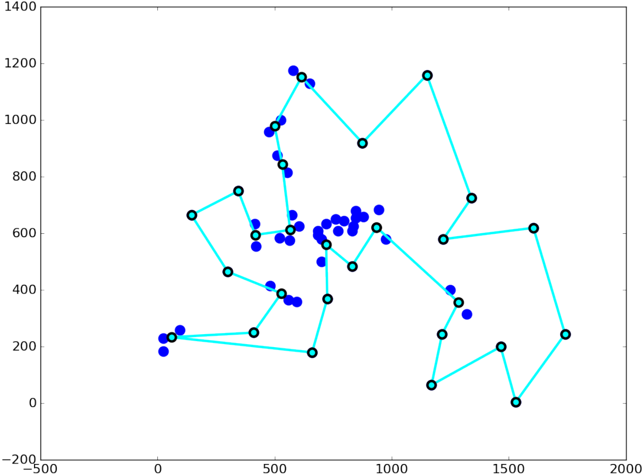

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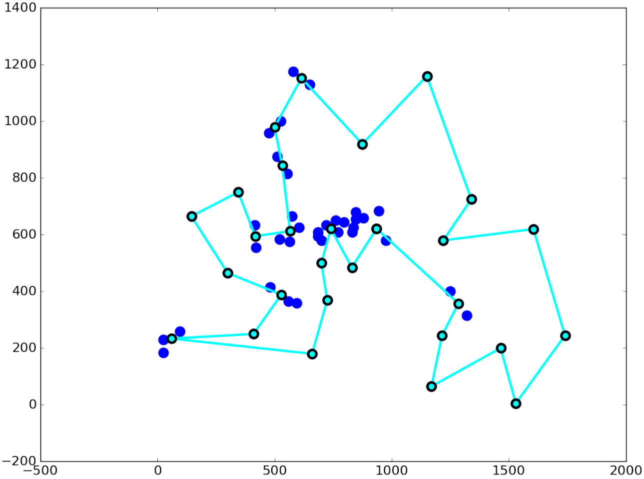

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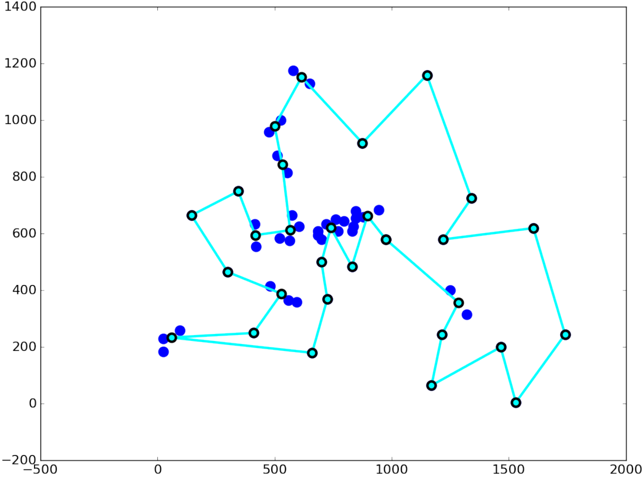

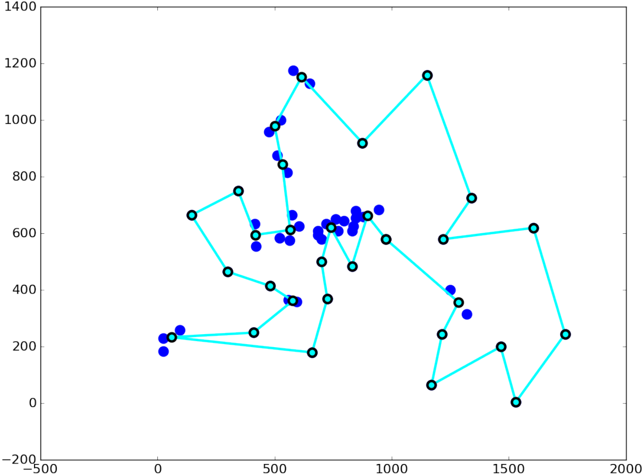
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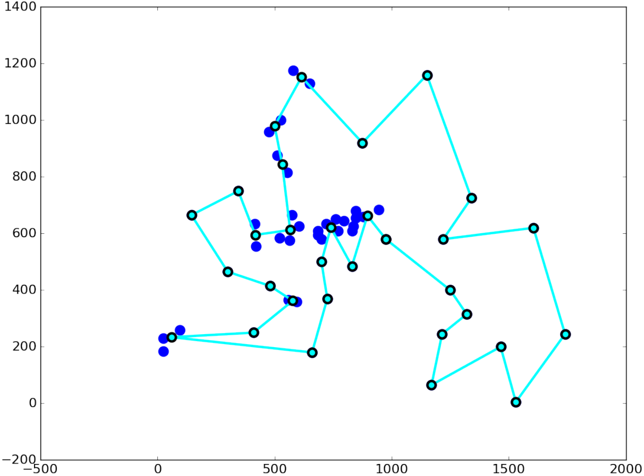
animation of the pair-center tour algorithm



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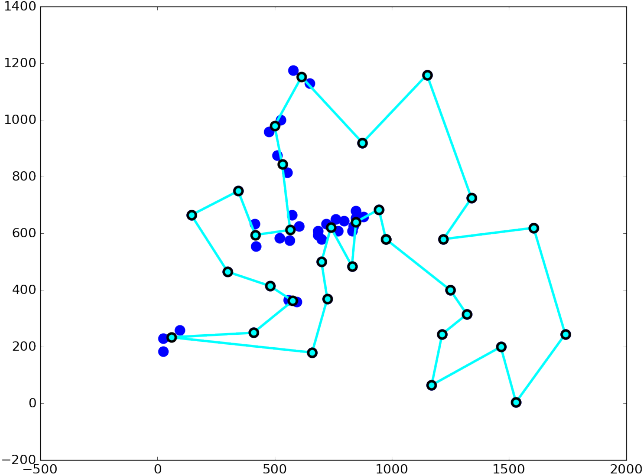

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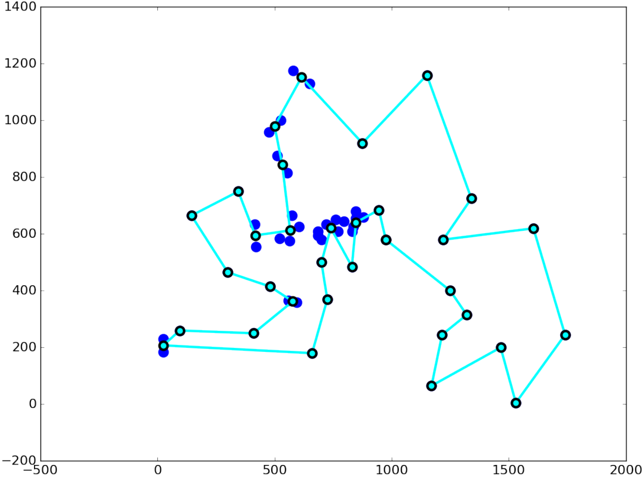

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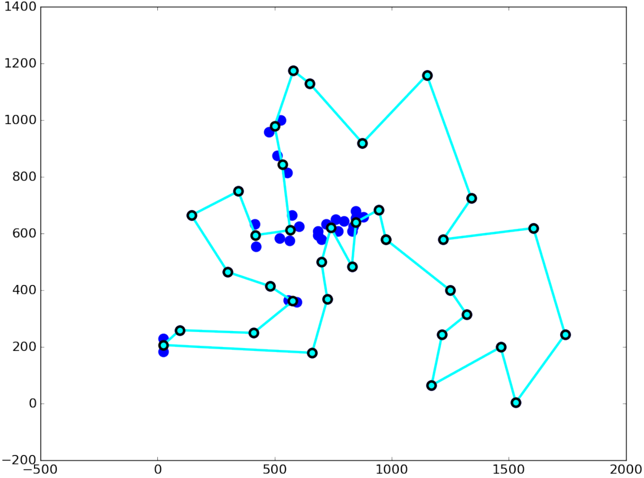

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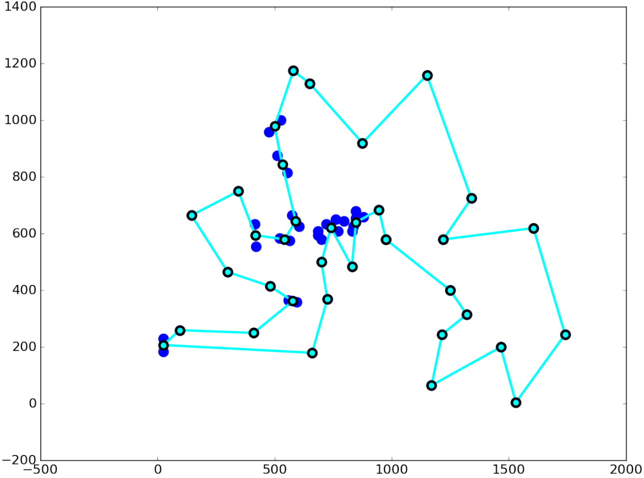

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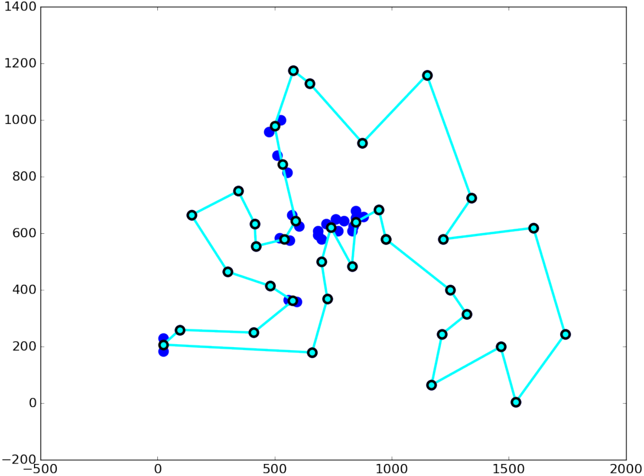

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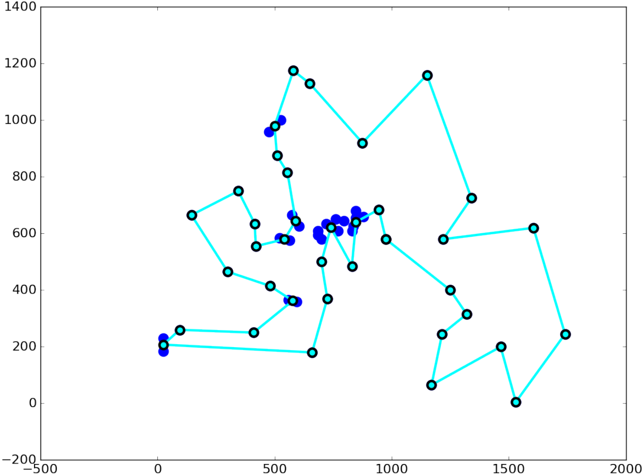

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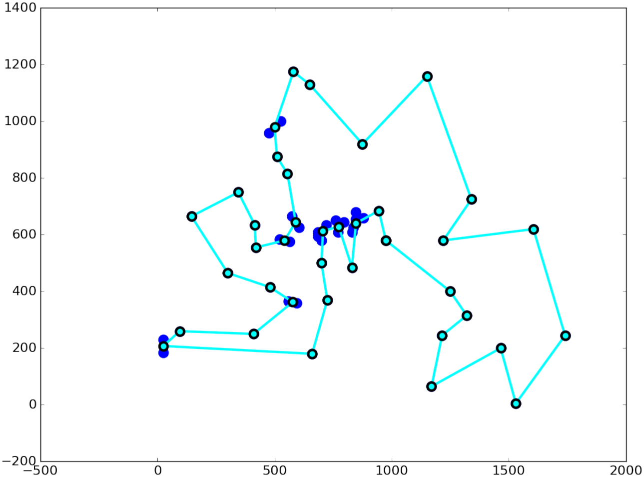

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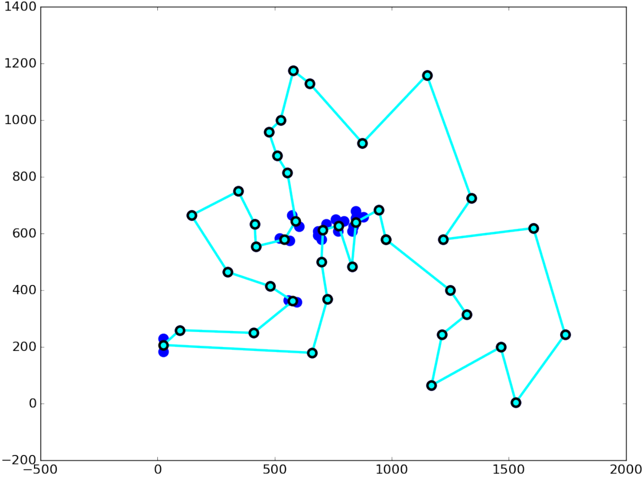

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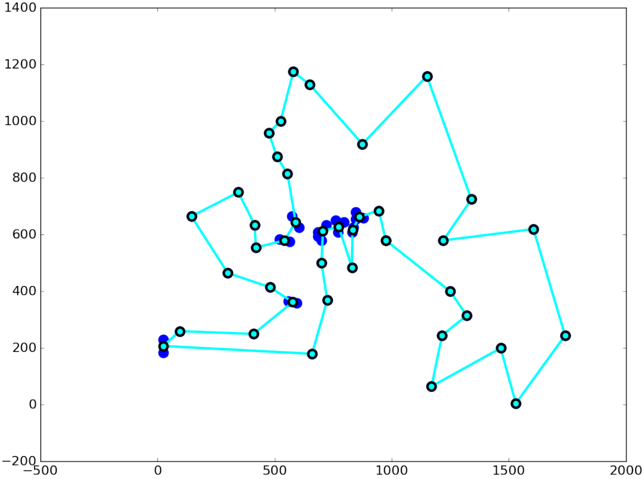

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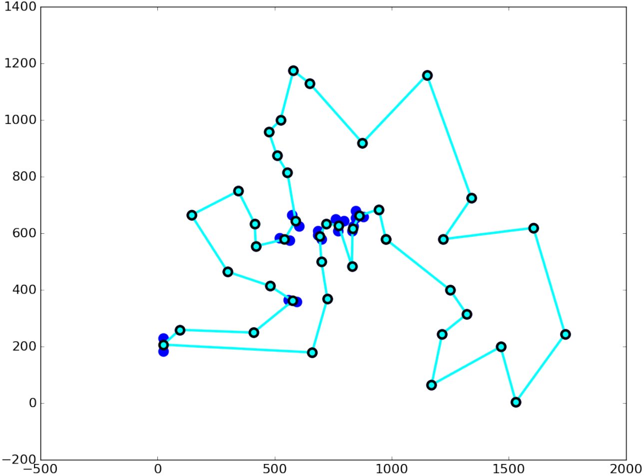

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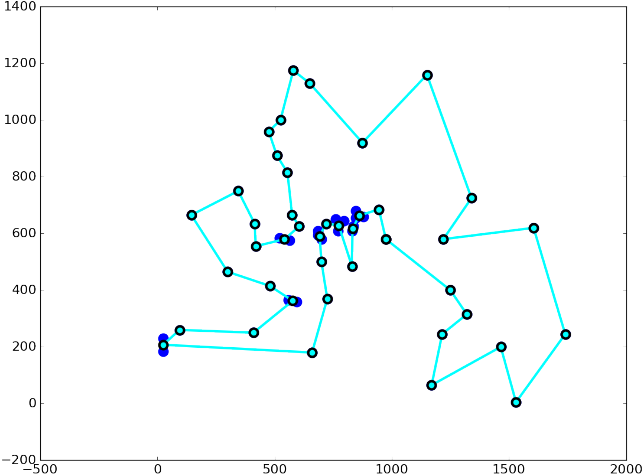

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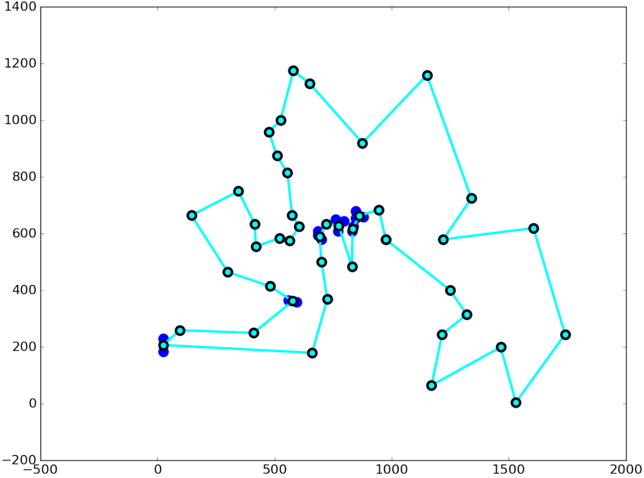

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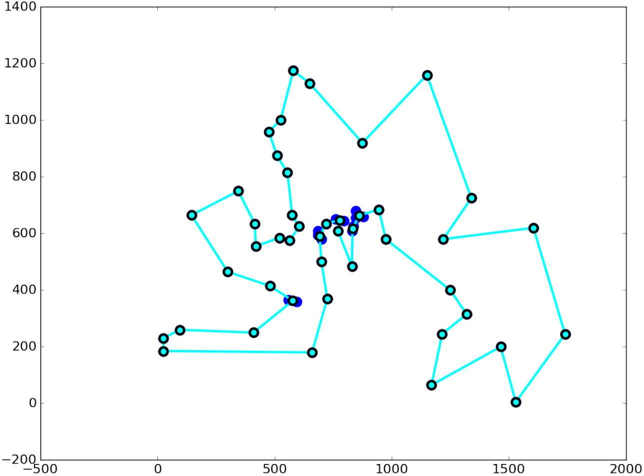

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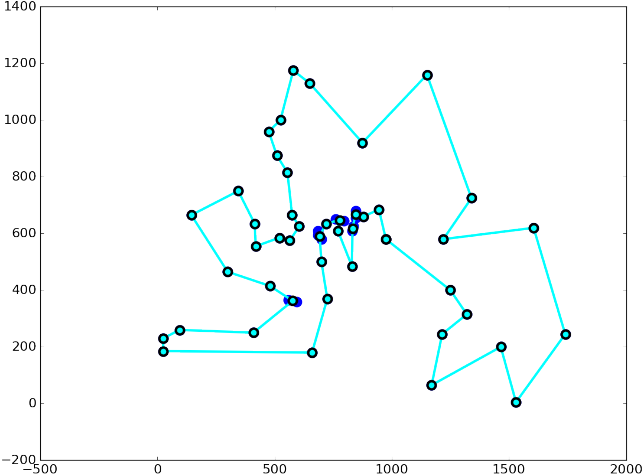

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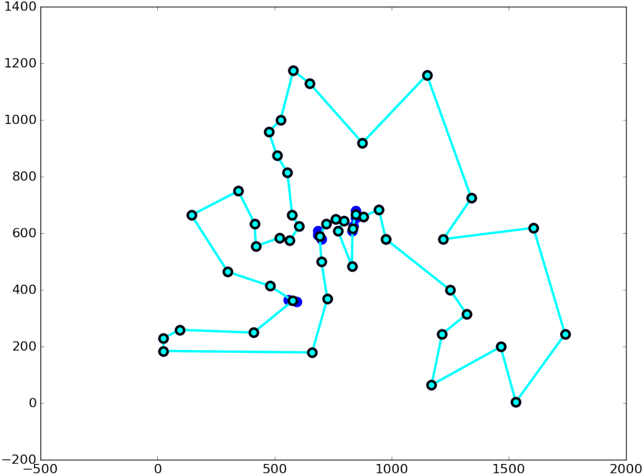

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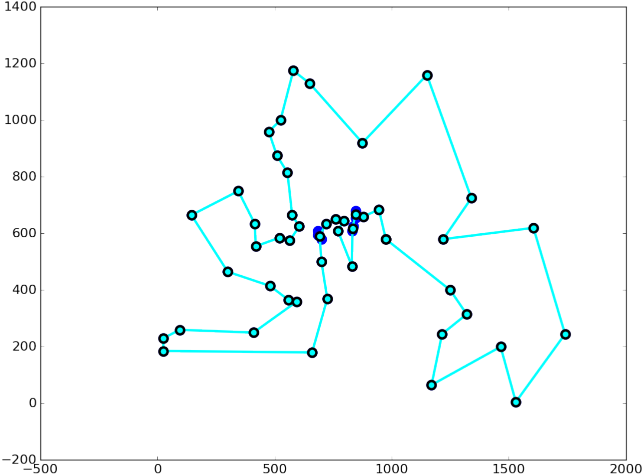

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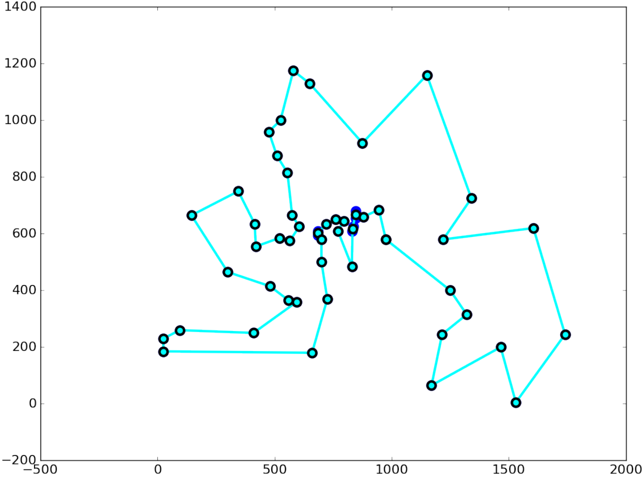

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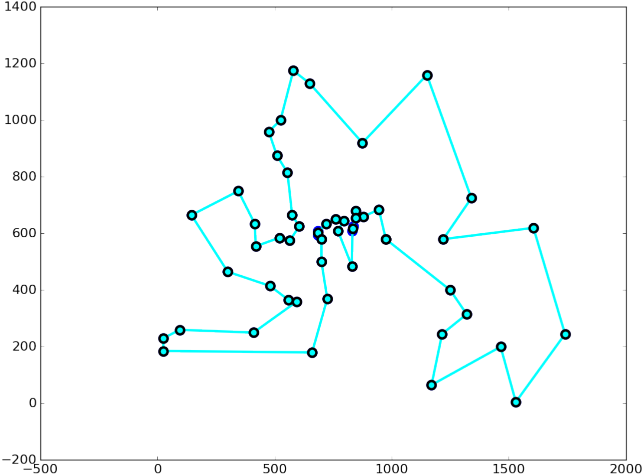

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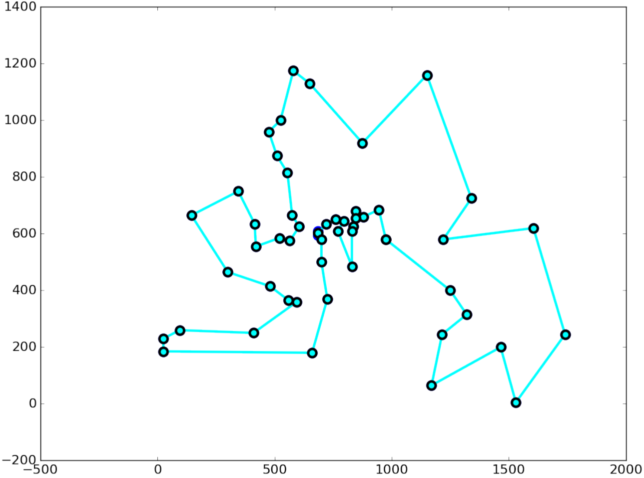

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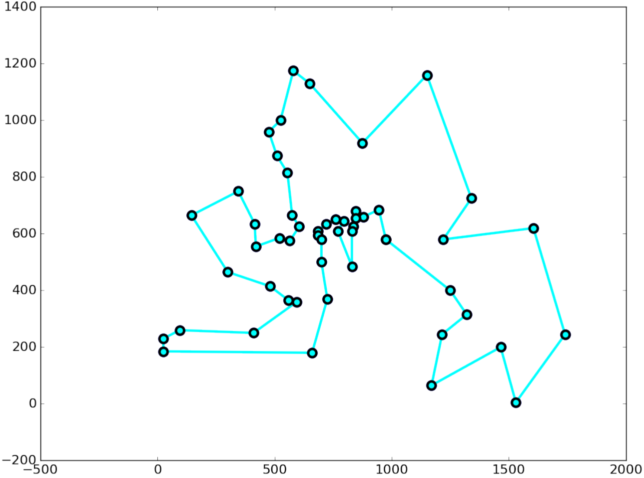

the TSP length-line sum-up

length of tour

L_{CN}	closest-neighbor tour (can be large, 1974)
$2 \cdot L_{opt}$	minimum spanning tree algorithm (or quick tour)
$1.5 \cdot L_{opt}$	Christofides algorithm (best known, 1976)
L_{play}	playground for good heuristic algorithms
L_{opt}	optimal tour length, Bellman-Held-Karp algorithm (1962)
L_{HKB}	*Held-Karp bound* $((L_{opt} - L_{HKB})/L_{opt} \approx 0.01$*, 1971)*
L_{MDB}	*minimal distance bound (possible* $L_{MDB} = L_{opt}$*)*
0	absolute minimum

How does the genetic algorithm work?

A genetic algorithm is a bio-inspired probabilistic algorithm:

- initialize a set of individuals
- while *stopping criterium* not met
  - evaluate fitness of the individuals (in search space)
  - generate off-springs (mutation and crossover, in the encoding space)
  - generate a new generation, i.e., a subset of parents plus off-springs (selection)
- report best individual generated in the process

You'll work with this approach in the lab hours.

additional information

additional information and benchmark instances can be found at:

- http://comopt.ifi.uni-heidelberg.de/software/TSPLIB95/ or
- https://www.math.uwaterloo.ca/tsp/data/index.html
- almost a counterexample of how to implement GA for TSP https://jaketae.github.io/study/genetic-algorithm/
- we use the work at https://github.com/guofei9987/scikit-opt

parallelization

- Monte Carlo algorithms, and hence, evolutionary algorithms are often quite easy to parallelize.
- We will not talk about parallelization in this course, however, it's an important issue in order to achieve good performance on modern systems.