An Algebraic Approach to Geometrical Optimization

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One of the top 10 algorithms of the 20th century [6] is the *simplex algorithm for linear programming* (LP). It allows one to maximize or minimize a linear function of several variables, subject to linear constraints. A simple example is illustrated in figure 1: minimize the objective function $x-2y$ subject to $0 \le x$, $0 \le y$, $2x+y \le 5$, and $-4x+4y \le 5$. Conceptually, one envisions the polygonal region determined by the constraints and notes that since the objective is linear, its optimal value must occur at a corner of this region. Thus checking a finite number of cases suffices to solve such problems; this is the basis for LP, which works even more efficiently by examining a relatively small set of corners.

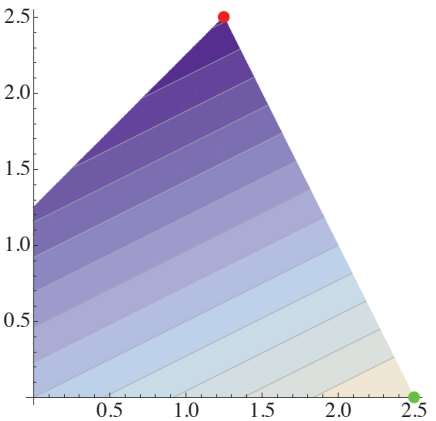

Figure 1. A linear function defined on a polygonal region is optimized at a corner of the region. Here the minimum is shown in red and the maximum in green.

LP works extremely well in practice, allowing us to minimize a linear function subject to linear constraints even when the number of variables (and constraints) is in the thousands.

An important variant is *integer linear programming* (ILP), where we are working not in the realm of rational (or approximate real) numbers, but in the integers. An ILP problem asks for the integer values of the variables that minimize or maximize a linear objective function subject to constraints of linear inequalities. The range of applications of ILP is huge; here we will show how it can be used on some traveling salesman-type problems.

The Traveling Salesman Problem

For the traveling salesman problem (TSP), where one wants the shortest cycle that visits all points in a given planar set, we can use 0-1 valued variables x_{ij} for each pair of points (i.e., each *edge* in the complete graph on the point set), the intent being that a value of 1 means that the tour should include the edge. The main constraint is the degree constraint, which forces each point to appear in precisely two edges of the final tour. Thus, the ILP formulation is:

Input: n points P_i in the plane, with distance d_{ij} defined to be $|| P_i - P_j ||$.

Variables: x_{ij} for each pair i,j with $i<j$.

Objective: $\sum d_{ij} x_{ij}$.

Constraints: $x_{ij} \in \{0,1\}$, and the degree constraints:

for each i, $\sum_{j=1}^{i-1} x_{ji} + \sum_{j=i+1}^{n} x_{ij} = 2$.

This is a simple system with roughly n^2 variables and n constraints. The catch is that a solution in integers might not yield the desired single cycle: Any union of two or more disjoint cycles will satisfy the degree constraints, and such unions will likely show up in the answer. We would like to add constraints guaranteeing that no cycle with fewer than n points exists, but the number of such constraints—just under 2^n—is too large. Following instead the "if it's not broken, don't fix it" strategy, we can fix (i.e., break) the cycles as they show up, as opposed to trying to break them all in advance. So we find the cycles C_1, C_2, ... that arise in an ILP solution, and for each $C = C_k$, add the cycle-killing constraint that requires at least two edges connecting C to its complement:

$$\sum_{i\in C, j\notin C, i<j} x_{ij} + \sum_{i\in C, j\notin C, j<i} x_{ji} \geq 2.$$

Now a remarkable thing happens: this process generally converges in only a few steps. For n up to 100 or a little larger, this allows us to find the optimal TSP tour.

Here is an example. For points at the rough centers of the lower 48 states, the optimal tour is shown in yellow in figure 2 (the blue edges show additional state adjacencies, but a general TSP tour is not restricted to going from a state to an adjacent one).

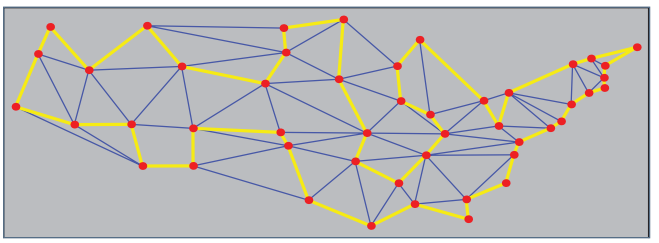

Figure 2. The shortest tour visiting the centroids of the lower 48 states.

Figure 3 shows what happened. In the first ILP iteration, three cycles arose. Destroying them by adding three new constraints, two new cycles arise. Adding two more cycle-killing inequalities and running ILP again leads to a single cycle: the optimal TSP tour. It is surely remarkable that five cycle-breaking constraints give a system strong enough to exclude all cycles; in other words, the system using five cycle-breaking inequalities is equivalent to the system using about 100 trillion inequalities that one would naively need to exclude all undesirable cycles.

Note that these three iterations conceal a tremendous number of calls to LP. If the simple branch-and-bound strategy of the sidebar on page 26 were used, each of the three ILP calls would require solving about 2,000 LP problems.

Progress on the TSP in recent years has been amazing. The *Concorde* program can solve giant problems and is available to the public [8]. The new book by Cook [5; see also *tsp.gatech.edu*] is a wonderful summary of the history of and modern work on the TSP.

The *Whole Earth Problem* (shortest TSP tour through about 2 million cities) is now known to have an optimal tour of length between 7,512,218,268 and 7,515,788,188 meters. Thus, the distance of the true best tour is not less than 99.95 percent of the length of the best tour known (current best tour due to Keld Helsgaun of Denmark, October 2011; images and more information at *tsp.gatech.edu/world*).

The Routing Problem

An important TSP-variant is the *routing problem.*

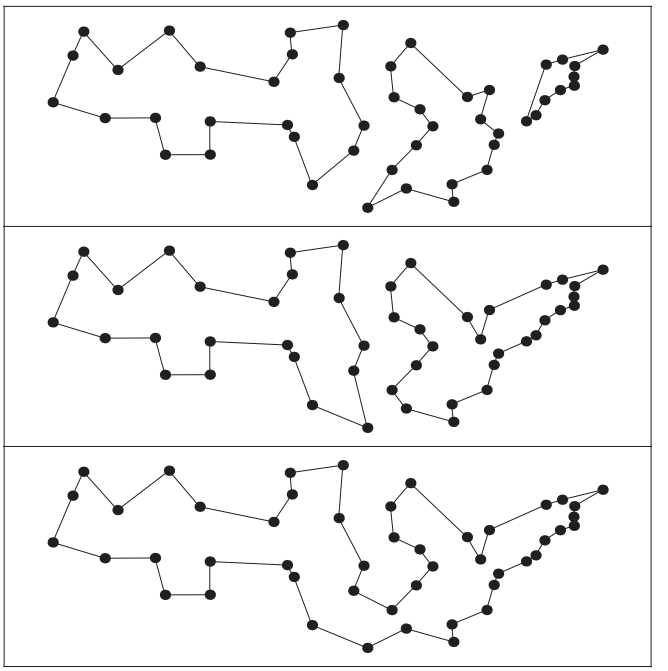

Figure 3. The results of the three ILP calls for the traveling salesman problem for the lower 48 states.

Suppose we have a graph derived from a map with edges corresponding to roads or walkways. We want to find the shortest route that visits all vertices. Indeed, this problem arose when a student asked me to help him find the shortest route through all the recycle bins on our campus. We can use the identical ILP-plus-cycle-breaking approach, provided we modify the setup as follows. The variables and constraints are as in the TSP, but the objective is defined in two cases. For each graph edge P_iP_j, the distance is taken to be its length; but when the pair ij does not correspond to an edge, we use the shortest-path distance in the graph from P_i to P_j. Finding shortest paths is very fast by Dijkstra's or related algorithms, so this adds almost no time to the process. The shortest tour might involve legs ij that are not edges in the graph; in such cases, we replace the nonedge by the corresponding shortest-path in the graph.

Figure 4 shows the best route through all the vertices in a map derived from our campus; seven cycle-breaking steps were used. Note the out-and-back section in the center. Such would be forbidden in a TSP route.

Shortest Hamiltonian Cycle

Often the routing problem is confused with the problem of finding the shortest *Hamiltonian cycle* (a cycle through the graph that travels on edges, visits each vertex, and never duplicates an edge). A first important distinction is that not all graphs have a

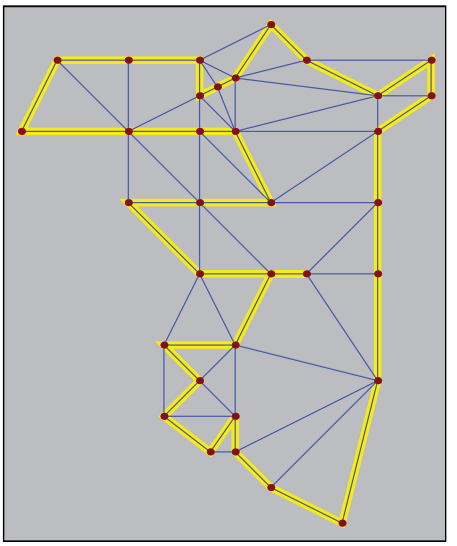

Figure 4. The yellow route, of total distance 63.18, is the shortest way to visit all the vertices and return to the start, always staying on graph edges.

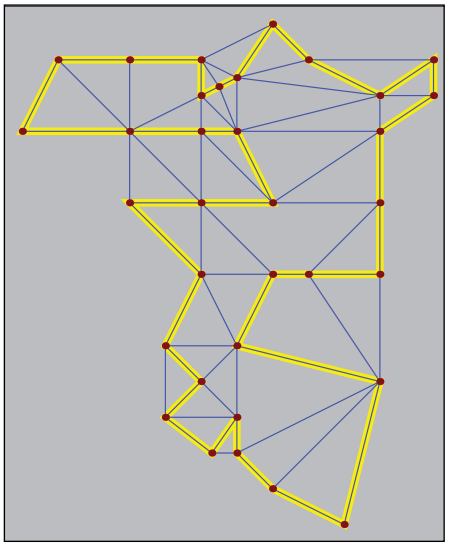

Figure 5. The yellow cycle is the shortest Hamiltonian cycle through the campus map; its length is 63.54, a little longer than the route in figure 4.

Hamiltonian cycle. But many planar graphs do (Tutte [11] proved that every 4-connected planar graph is Hamiltonian). If a Hamiltonian cycle exists, we can easily find the shortest one. The ILP becomes much simpler since we need variables only for the edges in the graph, of which there are most $6n$ by Euler's formula. So we have a system with about n variables and n constraints; we can therefore handle larger sets than the TSP or routing problems (which use about n^2 variables). Figure 5 shows the best Hamiltonian cycle through our campus.

While an ILP approach cannot be used on *very* large problems, we can find some nice Hamiltonian tours in medium-sized graphs. Figure 6 shows an example

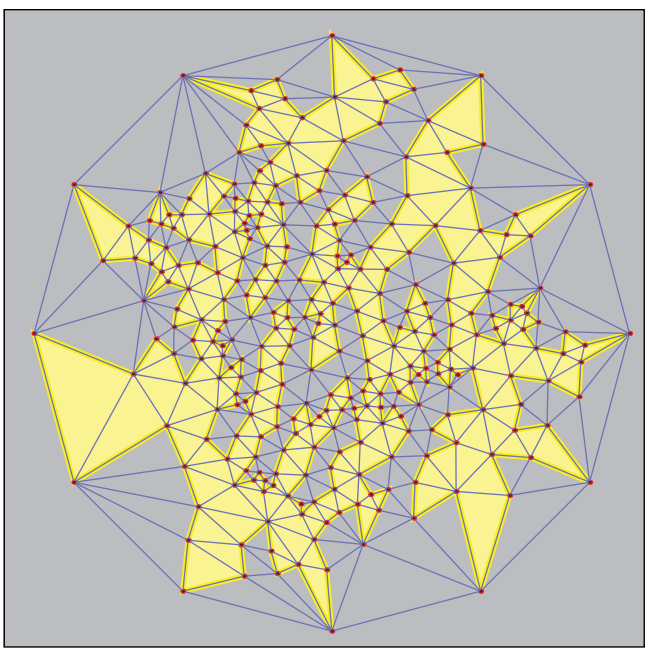

Figure 6. The shortest Hamiltonian tour in this 300-vertex planar graph is the boundary of the yellow polygon, found by ILP.

in a 300-vertex graph; computing time was about one minute, with 10 iterations of cycle-breaking.

Other Applications

There are many applications of ILP to real-world problems. One intriguing area is the logistics of arranging kidney exchanges [1, 4]. When a patient and donor are incompatible, they can enter a protocol for kidney exchanges where donor$_1$ gives a kidney to patient$_2$ and donor$_2$ gives one to patient$_1$. Three-way exchanges are also feasible, though less desirable than two-way exchanges. So the setup is a directed graph where each vertex is a donor-patient pair, with a directed edge from one pair to another if the second patient is compatible with the first donor. One then wants to decompose this graph into 2-cycles and 3-cycles so that the maximum number of exchanges is performed and the number of 3-cycles is minimized.

For modest-sized graphs, this can be done with ILP. Set up a variable P_{ij} for each possible pair exchange and a triple T_{ijk} for each possible triple exchange. Constraints are: (1) all variables are either 0 or 1; and (2) conservation of kidneys: for each i,

$$\sum x \le 1$$

where x runs through all P and T variables that involve i. The objective function is

$$2\sum P_{ij} + 3\sum T_{ijk}.$$

Once the optimal number E of exchanges is found, one can redo the ILP to minimize the number of triples, but with the additional constraint that the number of exchanges is E.

In a recent discrete applied mathematics course,

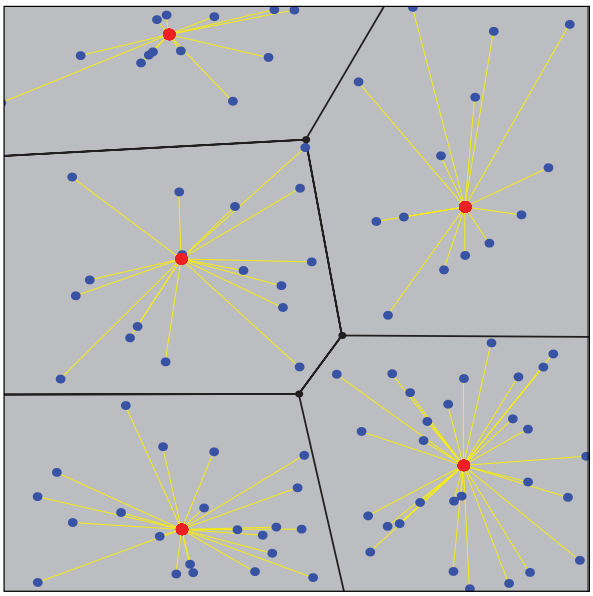

Figure 7a.

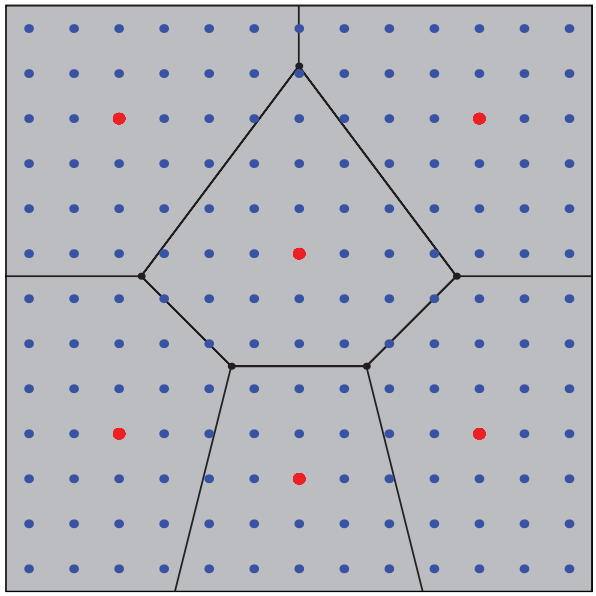

Figure 7b.

Optimal solutions to the facilities location problem with (a) 100 random points and five hosts, and (b) 169 uniformly placed points and six hosts.

all student projects involved ILP. It was used on the *facilities location problem* (explained below), the kidney exchange problem, the problem of determining whether a soccer team is eliminated from the playoffs where wins earn three points and draws one point (this is known to be *NP*-complete [2, 7]), the assignment of students to classes, and the problem of finding a maximum matching in a general graph. For the last, there is a much faster algorithm (the blossom algorithm of Edmonds), but ILP is useful as a check on a blossom implementation.

In the facilities location problem (also known as the *k-median problem*), one is given n points in the plane and wishes to choose k of them to act as hosts, the idea being that if each point is moved to the nearest host, the total of the $n-k$ distances is minimized. For an ILP, use 0-1 variables x_{ij} to indicate that person i will travel to the house of person j, who is a host, and y_j to pick out the hosts. Then the constraints are: $0 \le x_{ij} \le y_j \le 1$, which indicates that person i can go only to the house of a host;

Further Reading

There are various commercial and open-source ILP solvers (e.g., *CBC* or *Symphony* by COIN-OR [3]). I use *Mathematica,* which has good LP and ILP capabilities via its `Minimize` and `Maximize` functions.

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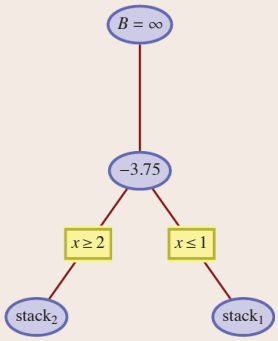
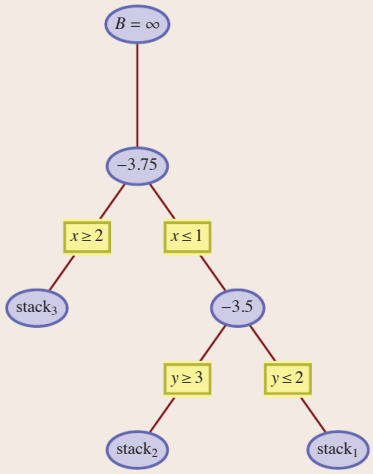
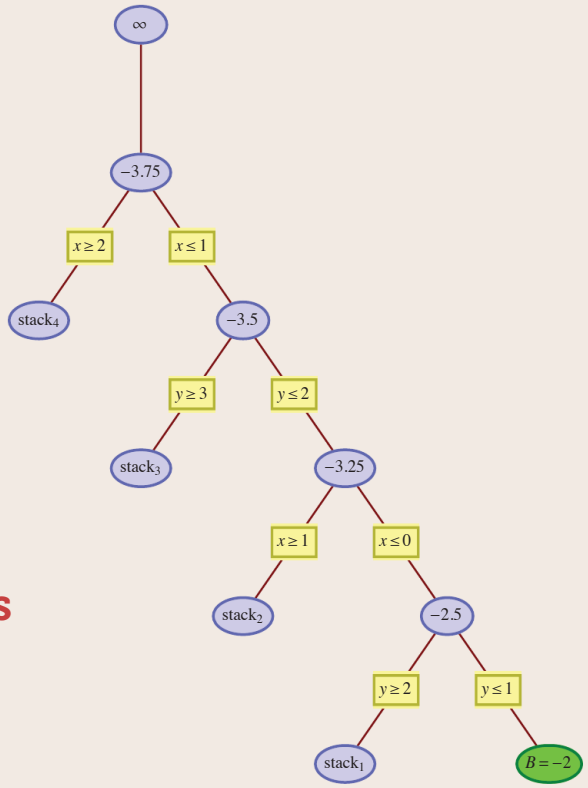
11. W. T. Tutte, A theorem on planar graphs, *Transactions of the American Mathematical Society* **82** (1956) 99–116.



Tree 1. The first call to LP leads to two subproblems via a branch on x.



Tree 2. The second call to LP leads to two more, via a branch on y.



Tree 3. The fourth call to LP leads to an integer solution with value −2.

How Integer Linear Programming Works

The simplex method for linear programming (LP) is fast and robust, so we can approach an *integer* linear programming (ILP) problem by repeated calls to LP, adding new constraints each time. Here we will illustrate a basic idea known as *branch-and-bound*.

We wish to optimize a linear function subject to a set of linear constraints, and we wish to find a solution among only *integer* values of the variables. A simple example from [10] will convey the idea. Suppose we wish to minimize the function $x - 2y$ subject to the constraints $x, y \in \mathbb{N}$, $2x + y \leq 5$, and $-4x + 4y \leq 5$.

We begin by using LP to solve the system in the space of rational (or approximate real) numbers. See figure 1 on page 22. If the LP solution occurs at integer values of the variables, we are done. Here LP finds the minimum value -3.75 at $x = 1.25$ and $y = 2.5$. We then choose a variable, say x, and set up two new LP problems: one with the additional constraint that $x \geq 2$, and the other with the constraint that $x \leq 1$. That is, we are pushing x toward the nearest integers. These two problems are placed on a "to do" *stack* of LP problems. The first tree figure shows the state of the system at this point.

We repeat this process many times, sending the problem at the top of the stack to LP: whenever it produces a solution where one or more variables is a noninteger, say $x = q$, we *branch* into two subproblems, one with the new constraint that $x \geq \lceil q \rceil$, the other with the new constraint that $x \leq \lfloor q \rfloor$.

The subproblems form a tree, which can have thousands of vertices. There are some choices we must make: the order in which the two new problems are placed on the stack and the choice of branching variable. We might choose the variable whose value is closest to an integer or farthest from an in-

$$\sum y_j = k,$$

which specifies exactly k hosts; and for each i,

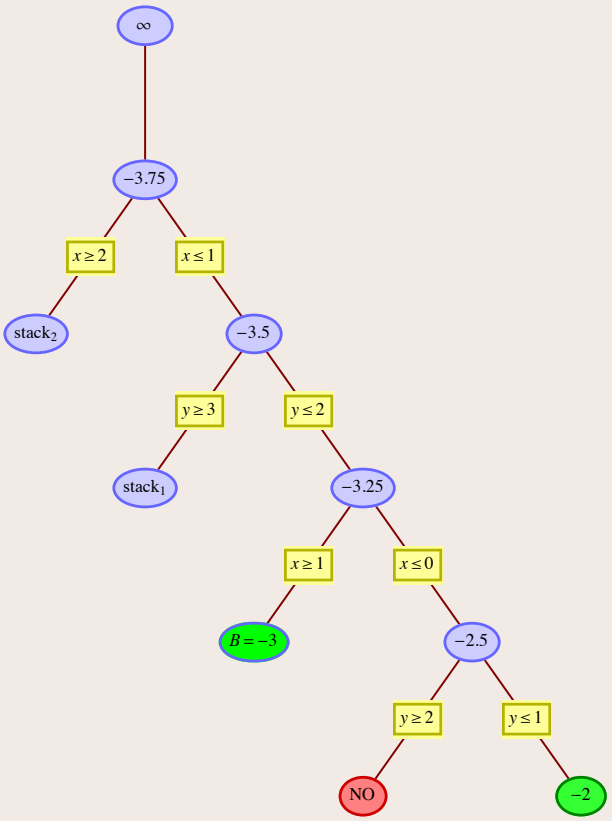
$$\sum x_{ij} = 1,$$

which asserts that person i goes to exactly one host. The objective is just

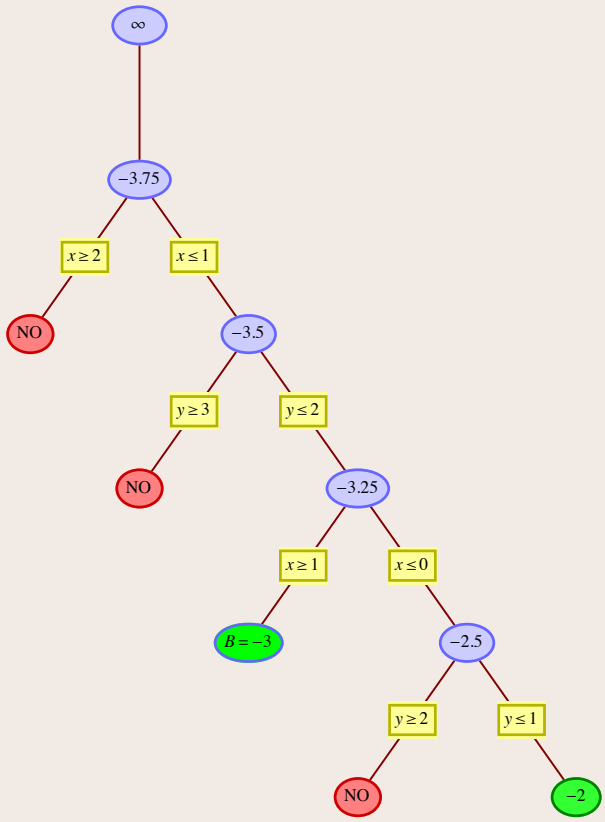
$$\sum d_{ij} x_{ij}$$

where d_{ij} is the distance matrix. Figure 7a shows the solution for a random set of 100 points, with five hosts.

Having code to do this allows one to investigate some interesting mathematical problems. Suppose we have houses at *every* point in the unit square (the *continuous* facilities location problem). Where should k hosts be placed so as to minimize the average of the travel distances? This is an open question (see [10] for important work on the topic). Figure 7b shows the results of an ILP experiment with $k = 6$, using 169 uniformly spaced points. The ILP involves more than 28,000 variables $(169^2 + 169)$, but yields the optimal



Tree 4. The current best of -2 makes the problem atop the stack unworthy of pursuit.



Tree 5. The fifth call to LP leads to an integer solution with value −3, which defeats the last two remaining problems on the stack and solves the problem.

teger. Another important subtlety is whether to work with rationals or approximate reals (terminating decimals). In this example, the tree is explored in a depth-first fashion from right to left.

Eventually one of the problems is solved with integer values for *all* the variables, and the minimum value B (best-so-far) is recorded. In tree 3, $B = -2$ is shown in green.

At this point, we take advantage of the fact that the objective $x - 2y$ assumes an *integer* value when both variables are integers. This means that only values of -3 or less are candidates for improving on our current best-so-far. As subsequent problems on the stack are sent to LP, rather than branch, we *ignore* any nodes where LP returns a value greater than -3. These dead-end nodes are shown in red. Once the green -2 is found, there is no need to explore the next node (the $y \geq 2$ branch). Then a green -3 is found, telling us that the last two red nodes are dead ends. The answer is therefore -3, realized at $(x, y) = (1, 2)$.

For situations such as the traveling salesman problem, where the objective has real coefficients, one can scale up all the input points, assumed rational, by a large integer and round all distances to the nearest integer. ■

solution in only eight seconds. Such approximations lead to patterns that might well correspond to the optimal placement in the continuous case. In Figure 7 the black lines are the *Voronoi diagram* of the hosts: the "polygons of nearness" for each host.

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