# Tuning a TSP Algorithm

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**Outline**

Review of Recursive Generation

The Traveling Salesperson Problem

A Sequence of TSP Algorithms

Principles of Algorithm Engineering

# Recursive Generation

A technique for systematically generating all members of a class

Example: all subsets of the n integers 0, 1, 2, …, n-1

Representation? {1, 3, 4} or 01011 or …

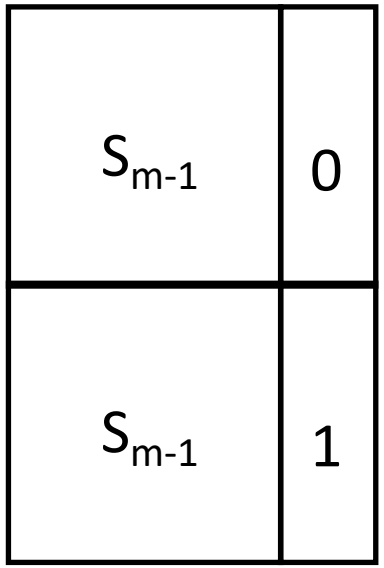
An Iterative Solution: binary counting

00000 00001 00010 00011 00100 … 11111

A Recursive Solution to Fill `p`

```
void allsubsets(int m)
{ if (m == 0) {
    visit();
  } else {
    p[m-1] = 0;
    allsubsets(m-1);
    p[m-1] = 1;
    allsubsets(m-1);
  }
}
```

$S_m$ =




000
100
010
110
001
101
011
111

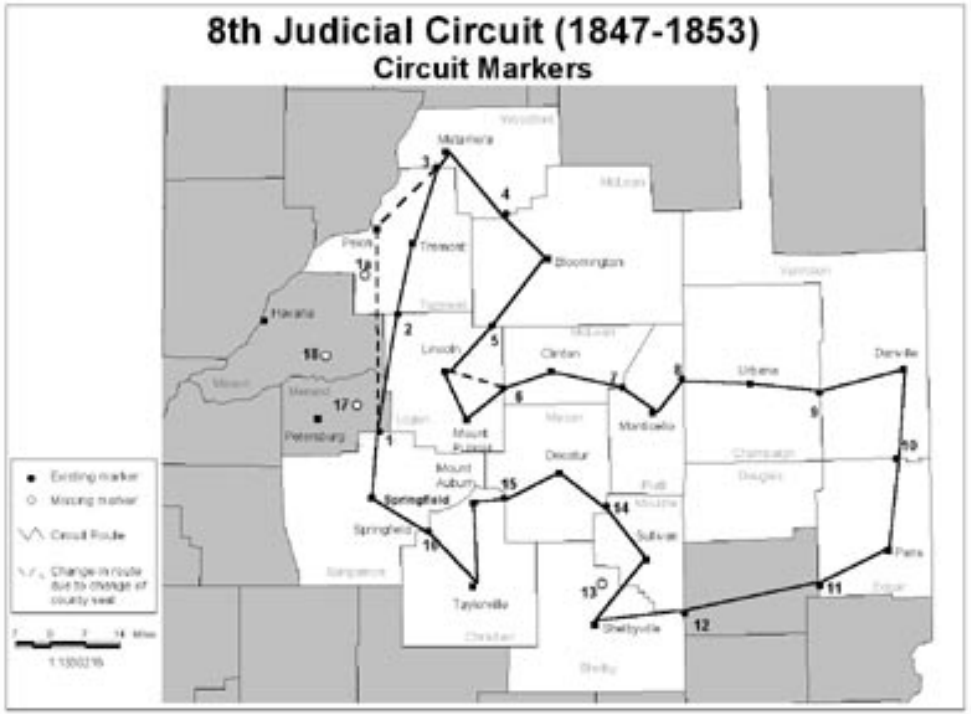
# The TSP

## The Problem

- Mr. Lincoln's Eighth Circuit
- Scheduling vehicles, drills, plotters
- Automobile assembly lines

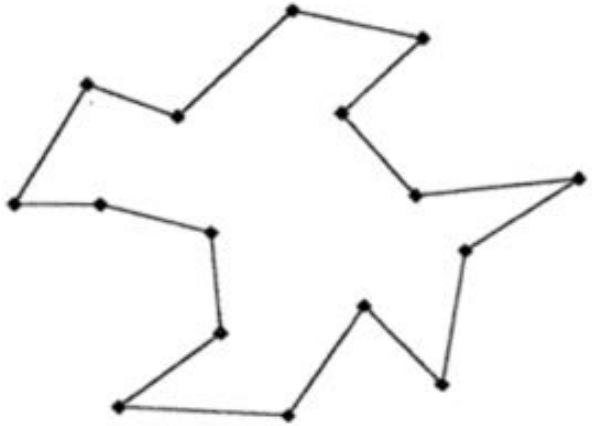
## A Prototypical Problem

- NP-Hard
- Held-Karp dynamic programming
- Approximation algorithms
- Kernighan-Lin heuristics



# A Personal History

## Shamos's 1978 Thesis



"In fact, the tour was obtained by applying the Christofides heuristic several times and selecting the best result. It is not known to be a shortest tour for the given set of points."

## A 1997 Exercise

Can simple code now solve a 16-city problem on faster machines?

## A 2016 Talk

What has changed in two more decades?

# This Talk

## Alternative Titles

- A case study in …
  - … implementing algorithms
  - … recursive enumeration
  - … algorithm engineering
  - … applying algorithms and data structures
- A master class in algorithms
- A sampler of performance engineering
- Two fun days of programming

## Non-Titles

- State-of-the-art TSP algorithms
- Experimental analysis of algorithms

# Representation Details

## Count of Cities

```
#define MAXN 20
int n;
```

## Permutation of Cities

```
int p[MAXN];
```

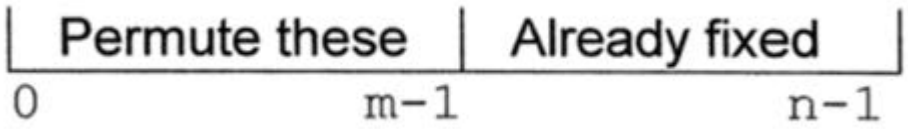
## Distances Between Cities

```
Typedef double Dist;
Dist d(int i, int j)
```

# Algorithm 1

## The Idea

Recursively generate all n! permutations
and choose the best




## Implementation

```
void search1(int m)
{ int i;
  if (m == 1)
    check1();
  else
    for (i = 0; i < m; i++) {
      swap(i, m-1);
      search1(m-1);
      swap(i, m-1);
    }
}
```

# Supporting Code

```
void check1()
{   int i;
    Dist sum = dist1(p[0], p[n-1]);
    for (i = 1; i < n; i++)
        sum += dist1(p[i-1], p[i]);
    save(sum);
}
void save(Dist sum)
{   int i;
    if (sum < minsum) {
        minsum = sum;
        for (i = 0; i < n; i++)
            minp[i] = p[i];
    }
}
void solve1()
{   search1(n);
}
```

Is this code correct?

# Run Time of Algorithm 1

## Analysis

Permutations: n!

Distance calculations at each: n

Total distance calculations: n x n!

## Experiments: Intel Core i7-6500U @ 2.50GHz (Default machine)

| N | Time |
|---|---|
| 8 | 0.05 secs |
| 9 | 0.34 secs |
| 10 | 3.97 secs |
| 11 | 45.47 secs |
| 12 | *9 minutes* |
| 13 | *2 hours* |

# Constant Factor Improvements

External to the Program

- Compiler optimizations
- Faster hardware

Internal Changes

- Modify the C code

# Compiler Optimizations

## An Experiment

| N | No Opt | -O3 |
|---|---|---|
| | | |
| 9 | 0.34 secs | |
| 10 | 3.97 secs | |
| 11 | 45.47 secs | |
| 12 | *9 min* | 19.81 secs |
| 13 | *2 hours* | *4.3 min* |

## gcc –O3

- Factor of ~25 on this machine
- Factor of ~6 on a Raspberry Pi 3
- Only full optimization shown from now on

# Faster Hardware

## Two Machines

1997: Pentium Pro @ 200MHz

2016: Intel Core i7-6500U @ 2.50GHz

| N | 1997 | 2016 |
|---|---|---|
| 10 | 20.9 secs | 0.12 secs |
| 11 | *4 min* | 1.62 secs |
| 12 | *48 min* | 19.81 secs |
| 13 | *10 hrs* | *4.3 min* |

Speedup of about 150

x12 due to clock speed; x12 due to wider data and deeper pipes

# Constant Factor Improvements: Internal

## Faster computation

- Change doubles to floats or (scaled) ints
- Measure and use fastest size (short, int, long)

## Avoid recomputing math-intensive function

- Algorithm 1

```
Dist geomdist(int i, int j) {
    return (Dist) (sqrt(sqr(c[i].x-c[j].x) +
                        sqr(c[i].y-c[j].y)));
}
```

- Algorithm 2
  - Precompute all $n^2$ distances in a table

```
#define dist2(i, j) distarr[i][j]
```

- Speedup of about 2.5 or 3

# Algorithm 3

## Idea

Reduce distance calculations by examining fewer permutations

Fix last city in the permutation

## Code

```
void solve3()
{ search2(n-1);
}
```

## Analysis

Permutations: (n-1)!

Distance calculations at each: n

Total distance calculations: n x (n-1)! = n!

# Algorithm 4

Don’t recompute sum; carry along a partial sum instead

```
void solve4()
{ search4(n-1, ZERO);
}

void search4(int m, Dist sum)
{ int i;
  if (m == 1)
    check4(sum + dist2(p[0], p[1]));
  else
    for (i = 0; i < m; i++) {
      swap(i, m-1);
      search4(m-1, sum + dist2(p[m-1], p[m]));
      swap(i, m-1);
    }
 }

void check4(Dist sum)
{ sum += dist2(p[0], p[n-1]);
  save(sum);
}
```

Reduces n x (n-1)! to ~(1+e) x (n-1)!

# Summary of Four Algorithms

| | Alg 1 | Alg 2 | Alg 3 | Alg 4 |
|---|---|---|---|---|
| n | n x n! | n x n! | n x (n-1)! | (1+e) x (n-1)! |
| 10 | 0.83 | 0.25 | 0.02 | |
| 11 | 10.28 | 3.22 | 0.28 | 0.25 |
| 12 | *120* | 33.50 | 3.47 | 2.59 |
| 13 | *1560* | *430* | 34.84 | 21.02 |

Seconds on an AMD E-450 at 1.65GHz

All run times are for initial members of one sequence uniform on the unit square

# Perspective on Factorial Growth

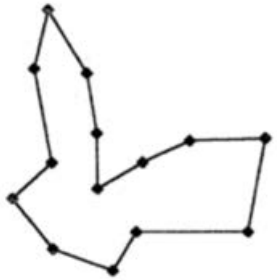
Each factor of n allows us to increase the problem size by 1 in about the same wall-clock time

Fast machines, great compilers and code tuning allow us to solve problems into the teens

14 cities in 5 minutes

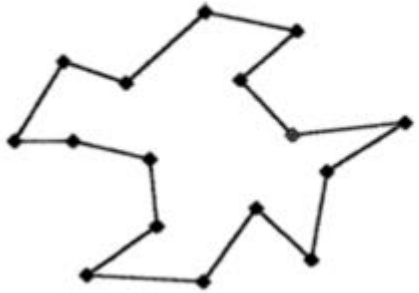
Lincoln's: 447.4

Opt: 399.1

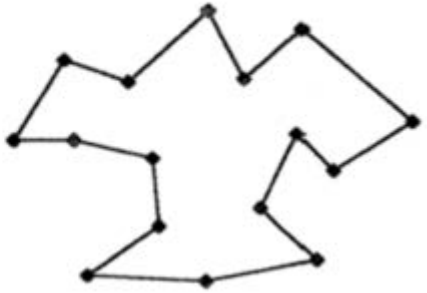


16 cities in 16 hours

Thesis: 237.11



Opt: 236.08



But can we ever analyze, say, all permutations of a deck of cards?

# Exponential Growth

## Definition of "Growing Exponentially"

- Popular usage: "growing real fast, looks like"
- Mathematics: $c^n$ for some base c and time period for n

## Factorial Growth

- By Stirling's approximation,
  - $\ln n! = n \ln n - n + O(\ln n)$
  - $\lg n! \sim n \lg n - 1.386\, n$
- So $n! \sim 2^{(n \lg n - 1.386\, n)} \sim 2^{(n \lg n)} \sim (n / e)^n$
- Factorial grows faster than *any* exponential function

## How Big is 52!?

- $52! \sim 8.0658 \times 10^{67} \sim 2^{225}$

# 52! in Everyday Terms

Set a timer to count down $52! = 8.0658 \times 10^{67}$ nanoseconds.

Stand on the equator, and take one step forward every million years.

When you've circled the earth once, take a drop of water from the Pacific Ocean, and keep going.

When the Pacific Ocean is empty, lay a sheet of paper down, refill the ocean and carry on.

When your stack of paper reaches the moon, check the timer. You're about done.

Fact: the universe is about $26! = 4.03 \times 10^{26}$ nanoseconds old

Moral: we're going to have to ignore some of the possible tours.

# Puzzle Break

From Greg Conti

- Find all permutations of 1..9 such that each initial substring of length m is divisible by m
- For 1..3, 321 works but not 132

Two Main Approaches

- Thinking
- Computing
  - What structures?  What language?
- How to generate all n! permutations of a string?
  - Recursive search(left, right)
  - Start with left = “123456789”, right = “”; end when left == “”
  - search(“356”, “421978”) calls
    - search(“56”, “3421978”), search(“36”, “5421978”), search(“35”, “6421978”)

# An Awk Program

```
function search(left, right,   i) {
   if (left == "") {
      for (i = 1; i <= length(right); i++)
         if (substr(right, 1, i) % i)
            return
      print "   " right
   } else
      for (i = 1; i <= length(left); i++)
         search(substr(left, 1, i-1) substr(left, i+1), substr(left, i, 1) right)
}

BEGIN { search("123456789", "") }
```

About 3 seconds to find 381654729

# How To Make it Faster?

## Constant Factors

Don’t check for divisibility by 1; change language; …

## Pruning the Search – Lessons from 381654729?

Even digits in even positions

Odd digits in odd positions

Digit 5 in position 5

Old: $9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1 = 9! = 362880$

New: $4 \times 4 \times 3 \times 3 \times 1 \times 2 \times 2 \times 1 \times 1 = (4!)^2 = 576$

Code

```
digit = substr(left, i, 1)
if (((length(left) % 2)  == (digit % 2)) &&
    ((length(left) == 5) == (digit == 5)) )
     search2(substr(left, 1, i-1) substr(left, i+1), digit right)
```

# Lessons from the Break

Factorial grows very quickly

- We can never visit the entire search space

The key to speed is pruning the search

Some fancy algorithms can be implemented in very little code

# Algorithm 5

Don’t keep doing what doesn’t work; sum never decreases

Code

```
void search5(int m, Dist sum)
{ int i;
  if (sum > minsum)
    return;
  if (m == 1) {
  …
```

Experiments on an Intel Core i7-3630QM @ 2.40GHz

| | 12 | 13 | 14 | 15 | 16 | 17 |
|---|---|---|---|---|---|---|
| Alg 4 | 0.59 | 5.14 | 54.44 | | | |
| Alg 5 | 0.01 | 0.12 | 0.41 | 0.99 | 3.92 | 39.00 |

# Algorithm 6

A Better Lower Bound: Add MST of remaining points

Code

```
void search6(int m, Dist sum, Mask mask)
{ int i;
  if (sum + mstdist(mask | bit[p[m]]) > minsum)
    return;
  ...
      search6(m-1,
              sum + dist2(p[m-1], p[m]),
              mask & ~bit[p[m-1]]);
```

# Prim-Dijkstra MST Code

```
Dist mstdist(Mask mask)
{   int i, m, mini, newcity, n;
    Dist mindist, thisdist, totaldist;
    totaldist = ZERO;
    n = 0;
    for (i = 0; i < MAXN; i++)
        if (mask & bit[i])
            q[n++].city = i;
    newcity = q[n-1].city;
    for (i = 0; i < n-1; i++)
        q[i].nndist = INF;
    for (m = n-1; m > 0; m--) {
        mindist = INF;
        for (i = 0; i < m; i++) {
            thisdist = dist2(q[i].city, newcity);
            if (thisdist < q[i].nndist) {
                q[i].nndist = thisdist;
                q[i].nnfrag = newcity;
            }
            if (q[i].nndist < mindist) {
                mindist = q[i].nndist;
                mini = i;
            }
        }
        newcity = q[mini].city;
        totaldist += mindist;
        q[mini] = q[m-1];
    }
    return totaldist;
}
```

# More Experiments

## Algorithms 5 and 6

| N | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 |
|---|---|---|---|---|---|---|---|---|---|
| Alg 5 | 0.95 | 4.03 | 40.00 | | | | | | |
| Alg 6 | | 0.00 | 0.02 | 0.03 | 0.05 | 0.06 | 0.22 | 0.20 | 2.39 |

## Algorithm 6

| N | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|---|---|
| Alg 6 | 2.39 | 0.75 | 1.81 | 5.56 | 8.97 | 13.36 | 7.67 | 13.73 |

# Algorithms 7 and 8

Cache MST distances rather than recomputing them

Algorithm 7: Store all (used) distances in a table of size $2^n$

```
nmask = mask | bit[p[m]];
if (mstdistarr[nmask] < 0.0)
  mstdistarr[nmask] = mstdist(nmask);
if (sum + mstdistarr[nmask] > minsum)
  return;
```

Algorithm 8: Store them in a hash table

```
if (sum + mstdistlookup(mask | bit[p[m]]) > minsum)
  return;
```

# Hash Table Implementation

```
Dist mstdistlookup(Mask mask)
{ Tptr p;
  int h;
  h = mask % MAXBIN;
  for (p = bin[h]; p != NULL; p = p->next)
    if (p->arg == mask)
      return p->val;
  p = (Tptr) malloc(sizeof(Tnode));
  p->arg = mask;
  p->val = mstdist(mask);
  p->next = bin[h];
  bin[h] = p;
  return p->val;
}
```

# Experiments

## Algorithms 6 and 8

| N | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|---|---|---|---|---|---|---|---|---|---|
| Alg 6 | 13.44 | 12.69 | 40.39 | | | | | | |
| Alg 8 | 0.50 | 0.45 | 1.41 | 1.88 | 5.33 | 2.31 | 2.44 | 48.52 | 7.59 |

# Algorithm 9

Sort edges to visit nearest city first, then others in order

```
for (i = 0; i < m; i++)
  unvis[i] = i;
for (top = m; top > 0; top--) {
  mindist = INF;
  for (j = 0; j < top; j++) {
    thisdist = dist2(p[unvis[j]], p[m]);
    if (thisdist < mindist) {
      mindist = thisdist;
      minj = j;
    }
  }
  swap(unvis[minj], m-1);
  search9(m-1,
          sum + dist2(p[m-1], p[m]),
          mask & ~bit[p[m-1]]);
  swap(unvis[minj], m-1);
  unvis[minj] = unvis[top-1];
}
```

# Experiments

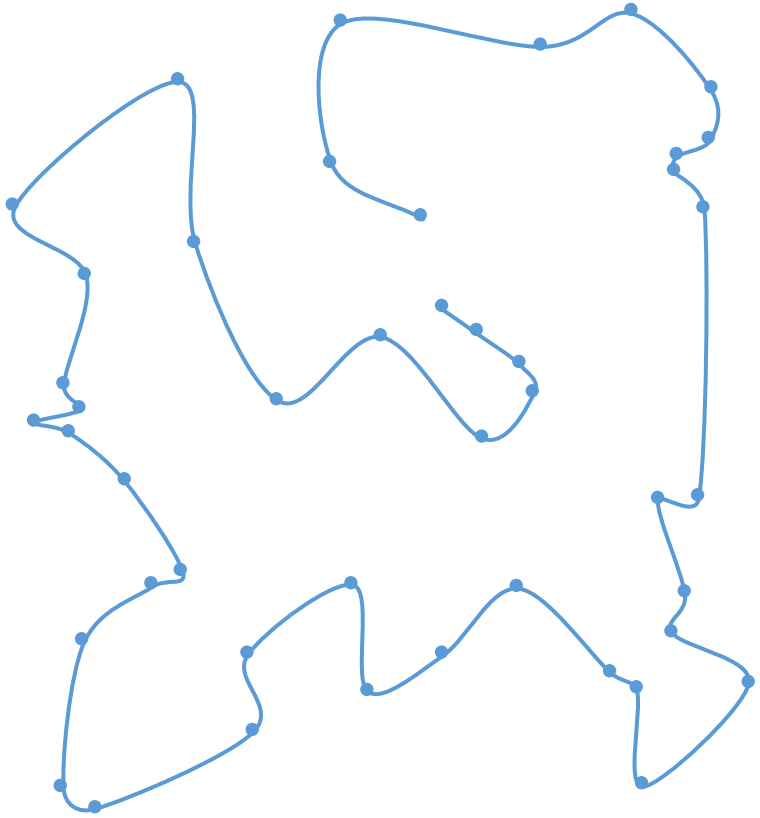
## Algorithms 8 and 9

| N | 38 | 39 | 40 | 41 | 42 | 43 | 44 |
|---|---|---|---|---|---|---|---|
| Alg 8 | 8.27 | 11.08 | 25.84 | 93.61 | 55.20 | 41.95 | |
| Alg 9 | 4.41 | 0.86 | 3.44 | 10.80 | 12.69 | 10.39 | 21.19 |

In 1997, stopped at n=30 and 305.66 seconds

# A 45-City Tour

42 seconds on a 2.50GHz Core i7



# How Far Can Algorithm 9 Go?

| N | Seconds | |
|---|---|---|
| 40 | 3.59 | |
| 41 | 11.33 | |
| 42 | 12.17 | |
| 43 | 11.62 | |
| 44 | 23.49 | |
| 45 | 41.89 | |
| 46 | 183.70 | My Thanksgiving 2016 Cyclefest |
| 47 | 1036.28 | When to think and when to run programs? |
| 48 | 1199.11 | |
| 49 | 7815.83 | |
| 50 | 2172.03 | |
| 51 | 6537.12 | |
| 52 | 11254.17 | = 3hrs 7 min |

# Complete Code: 160 Lines of C

```
/* tspfastonly.c -- Cut tsp.c down to only final algorithm 9 */

#include <stdio.h>
#include <time.h>
#include <math.h>
#include <stdlib.h>

/* Globals: points and perm vectors; edge operations */
#define MASKTYPE long
#define MAXN 60
#define MAXBIN 9999991
typedef double Dist;

int n = 0;
typedef struct point {
    float x;
    float y;
} Point;
Point c[MAXN];
int p[MAXN], minp[MAXN];
Dist minsum;

Dist distarr[MAXN][MAXN];
float sqr(float x) { return x*x; }
Dist geomdist(int i, int j)
{   return (Dist) (sqrt(sqr(c[i].x-c[j].x)
                      + sqr(c[i].y-c[j].y)));
}
#define dist2(i, j) (distarr[i][j])

// Search algs
void swap(int i, int j)
{   int t = p[i]; p[i] = p[j]; p[j] = t; }

void check4(Dist sum)
{   sum += dist2(p[0], p[n-1]);
    int i;
    if (sum < minsum) {
        minsum = sum;
        for (i = 0; i < n; i++)
            minp[i] = p[i];
    }
}

typedef MASKTYPE Mask;
Mask bit[MAXN];
struct link {
    int city;
    int nnfrag;
    Dist nndist;
} q[MAXN];

Dist mstdist(Mask mask)
{   int i, m, mini, newcity, n;
    Dist mindist, thisdist, totaldist;
    n = 0;
    for (i = 0; i < MAXN; i++)
        if (mask & bit[i])
            q[n++].city = i;
    newcity = q[n-1].city;
    for (i = 0; i < n-1; i++)
        q[i].nndist = 1e35;
    for (m = n-1; m > 0; m--) {
        mindist = 1e35;
        for (i = 0; i < m; i++) {
            thisdist = dist2(q[i].city, newcity);
            if (thisdist < q[i].nndist) {
                q[i].nndist = thisdist;
                q[i].nnfrag = newcity;
            }
            if (q[i].nndist < mindist) {
                mindist = q[i].nndist;
                mini = i;
            }
        }
        newcity = q[mini].city;
        totaldist += mindist;
        q[mini] = q[m-1];
    }
    return totaldist;
}

typedef struct tnode *Tptr;
typedef struct tnode {
        Mask arg;
        Dist val;
        Tptr next;
} Tnode;
Tptr bin[MAXBIN];

Dist mstdistlookup(Mask mask)
{       Tptr p;
        int h;
        h = mask % MAXBIN;
        for (p = bin[h]; p != NULL; p = p->next)
                if (p->arg == mask)
                        return p->val;
        p = (Tptr) malloc(sizeof(Tnode));
        p->arg = mask;
        p->val = mstdist(mask);
        p->next = bin[h];
        bin[h] = p;
        return p->val;
}

void search9(int m, Dist sum, Mask mask)
{   int i;
    if (sum + mstdistlookup(mask | bit[p[m]]) > minsum)
        return;
    if (m == 1) {
        check4(sum + dist2(p[0], p[1]));
    } else {
        int j, minj, unvis[MAXN], top;
        Dist mindist, thisdist;
        for (i = 0; i < m; i++)
            unvis[i] = i;
        for (top = m; top > 0; top--) {
            mindist = 1e35;
            for (j = 0; j < top; j++) {
                thisdist = dist2(p[unvis[j]], p[m]);
                if (thisdist < mindist) {
                    mindist = thisdist;
                    minj = j;
                }
            }
            swap(unvis[minj], m-1);
            search9(m-1,
            sum + dist2(p[m-1], p[m]), mask & ~bit[p[m-1]]);
            swap(unvis[minj], m-1);
            unvis[minj] = unvis[top-1];
        }
    }
}

void solve9()
{   int i, j;
    Mask mask;
    for (i = 0; i < n; i++)
        for (j = 0; j < n; j++)
            distarr[i][j] = geomdist(i, j);
    for (i = 0; i < MAXN; i++)
        bit[i] = (Mask) 1 << i;
    for (i = 0; i < MAXBIN; i++)
    bin[i] = NULL;
    mask = 0;     // mask is a bit vector
    for (i = 0; i < n; i++) {
        mask |= bit[i];
        p[i] = i;
    }
    minsum = 1e35;
    search9(n-1, 0.0, mask);
}

void main()
{   int i;
    FILE *fp;
    fp = fopen("rand60.txt", "r");
    while (fscanf(fp, "%f %f", &c[n].x, &c[n].y) != EOF)
        n++;
    n = 25;
    solve9();
    for (i = 0; i < n; i++)
         printf("%3d\t%10.8f\t%10.8f\n", minp[i],
                c[minp[i]].x, c[minp[i]].y);
}
```

MST

Hash

Sort

# Each Algorithm in under a Minute

| | | | |
|---|---|---|---|
| 1. | Simple | N = 11 | 20 secs |
| 2. | Store precomputed distances | 12 | 8 |
| 3. | Fix starting city | 13 | 35 |
| 4. | Accumulate distance | 13 | 21 |
| 5. | Prune search | 17 | 40 |
| 6. | Add MST of remaining cities | 32 | 40 |
| 7. | Store MST distances | -- | -- |
| 8. | Store MST distances in hash table | 40 | 26 |
| 9. | Visit cities sorted by distance | 45 | 42 |

# Possible Additional Improvements

- Constant Factor Speedups
  - Faster machines
  - Code tuning as before
  - Better hashing: larger table, remove `malloc`
- Better Pruning
  - Better starting tour
  - Better bounds: MST Length + Nearest Neighbor to each end
  - Earlier pruning tests
- Better Sorting
  - Tune insertion sort; better algorithms
  - Precompute all sorts
    - Sort once for each city
    - Select subsequence using mask

# Components

## Incremental Software Development

- Total of 580 lines of C

## Algorithmic Techniques

- Recursive permutation generation
- Store precomputed results: distances, MST lengths
- Partial sums
- Early cutoffs

## Algorithms and Data Structures

- Vectors, strings
- Sets: Arrays and bit vectors
- Minimum Spanning Trees (MSTs)
- Hash tables
- Insertion sort

# Code Tuning Rules

Space-for-Time 2: Store precomputed results

- Interpoint distances in a matrix; table of MST lengths

Space-for-Time 4: Lazy evaluation

- Compute all $n^2$ distances but only compute MSTs as needed

Logic Rule 2: Short-circuiting monotone functions

- Prune search when length exceeds best so far

Logic Rule 3: Reordering tests

- Sort cities to visit closest first

Expression Rule 5: Exploit word parallelism

- Bit mask represents a set of cities

From *Writing Efficient Programs*, 1982

# Performance Tools Behind the Scenes

Driver to make experiments easy

- Variety of input data: real, uniform, annular, random symmetric matrices, …
- Count critical operations: distances, MSTs, …

Software profilers

Cost models

Spreadsheet as a “lab notebook”

- Graphs of performance
- Curve fitting