D:wave
The Quantum Computing Company™

Driving to the 48 USA State Capitals:
Programming the D-Wave QPU

North Carolina State University
Joel M. Gottlieb
February 6, 2018

Overview

- *Review* **(Scott Pakin and D-Wave)**
- **qbsolv**
- **7-city Traveling Salesman Problem**
- **48-city Traveling Salesman Problem**
- **Summary**

Review: Programming Model

QUBIT		Quantum bit which participates in annealing cycle and settles into one of two possible final states:
COUPLER		Physical device that allows one **qubit** to influence another **qubit**
WEIGHT		Real-valued constant associated with each **qubit**, which influences the **qubit's** tendency to collapse into its two possible final states; controlled by the programmer
STRENGTH		Real-valued constant associated with each **coupler**, which controls the influence exerted by one **qubit** on another; controlled by the programmer
OBJECTIVE		Real-valued function which is minimized during the annealing cycle

$$Obj(a_i, b_{ij}; q_i) = \sum_i a_i q_i + \sum_{ij} b_{ij} q_i q_j$$

The system **samples** from the q_i that minimize the objective

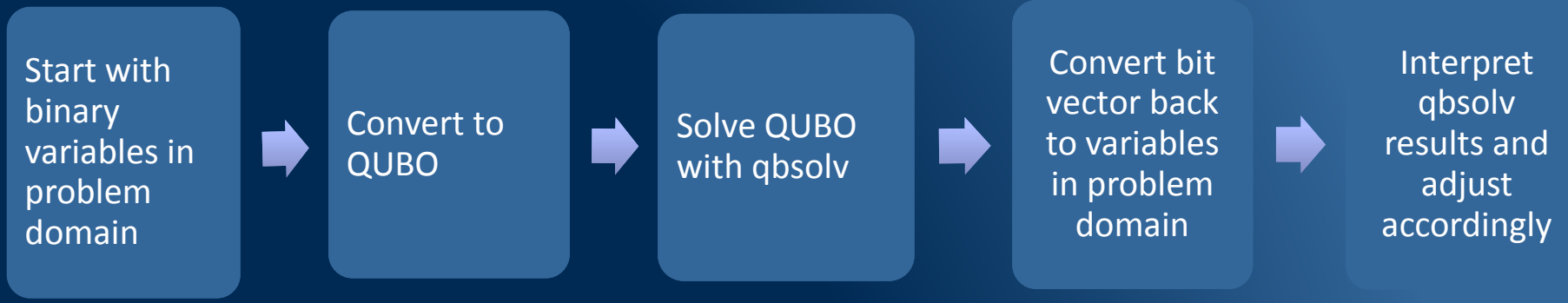
Review: The overall process

- Need to map problems into binary variables
- Need to map the binary variable expressions into linear terms and pair quadratic terms
  - QUBO: Quadratic Unconstrained Binary Optimization
- Run the QUBO on the D-Wave QPU
- Interpret the results
- Revisit the mapping…

QUBOs can be found in many fields

- Optimization
  - Recent: financial portfolio management
  - Recent: hospital re-admission statistics (Medicare funding)
  - Recent: bioinformatics / Multiple Sequence Alignment
  - Recent: nuclear power plant failure scenario analysis
  - Mathematical problems like Minimum Vertex Cover
  - Job-shop scheduling, other graph problems (Map Coloring, vertex set color)
- Sampling (from probability distribution)

Application example flow



Overview

- Review (from Scott Pakin and D-Wave)
- *qbsolv*
- 7-city Traveling Salesman Problem
- 48-city Traveling Salesman Problem
- Summary

The need for qbsolv

- Many problems require many more qubits or couplers than are available with the current chip.
- Examples:
  - Portfolio Optimization example requires 63-variable complete graph, but 2000Q does not go beyond ~50-qubit complete graph with direct embedding
  - 48-city Traveling Salesman requires complete graph, and it might be possible on the 2000Q, but the needed embedding would have very long chains, which do not perform well
  - Traffic flow optimization example using 418 cars (with 3 routes each) require almost 2000 highly-connected variables, too many to fit directly on the 2000Q chip.

qbsolv

- Hybrid quantum/classical QUBO solver (tabu = classical heuristic solver)
- Designed for problems too large and/or too dense to run on D-Wave quantum computer
- Divides problems into chunks, and iterates on sub-QUBOs (similar to HFS algorithm)
- Open-source: https://github.com/dwavesystems/qbsolv
- Can be used standalone, or with 128-qubit simulator, or with QPU
- Produces a single bitstring solution representing the final states of all the binary variables

Motivating Algorithm

- "A Multilevel Algorithm for Large Unconstrained Binary Quadratic Optimization", Wang, Lu, Glover, and Hao [2012]

- Principles
  - Identify the *backbone* of the QUBO; *i.e.*, the variable settings that are correlated for all valid answers, or, contribute the most to a local optimum
  - Select subQUBOs by most/least impact of each variable in determining the optimum
  - Solve the subQUBOs with a solver known to run effectively at smaller scale
  - Propagate subQUBO answer out to original variables in full QUBO
  - Iterate above steps until no further improvement

How qbsolv works

- Hybrid algorithm:
  - Identify the significant rows and columns of the larger problem (What changes a lot with spin flips? What doesn't?)
  - Create a smaller representative QUBO of that subset
  - Execute that smaller QUBO on the D-Wave system (pre-computed embedding, speeds up run-time)
  - Use the answer to guide the larger solver (new starting point, closer to the minimum)

Example qbsolv Output

```
$ qbsolv -i bqp50.qubo1.qubo

50 Number of bits in solution

10111111101001111101001101011111011111110110110

-5176.00000 Energy of solution

0 Number of Partitioned calls

 0.21352 seconds of classic cpu time
```

Overview

- **Review (from Scott Pakin and D-Wave)**
- **qbsolv**
- *7-city Traveling Salesman Problem*
- **48-city Traveling Salesman Problem**
- **Summary**

7-city Traveling Salesman Problem

- A learning exercise

- We will explore:
  1. QUBO for leg variables
  2. City visit constraints
  3. Embedding and chain constraints
  4. Importance of parameters and problem construction

Problem Specifications

Optimization:

- Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?
- Given a length *L*, decide whether the list of cities and distances has any tour shorter than *L.*
- Symmetric TSP; Undirected graph, distances in miles; distances obtained from various Web sites .

The Cities

A = Albuquerque, NM

B = Boston, MA

C = Charlotte, NC

D = Detroit, MI

E = Evanston, IL

F = Frankfort, KY

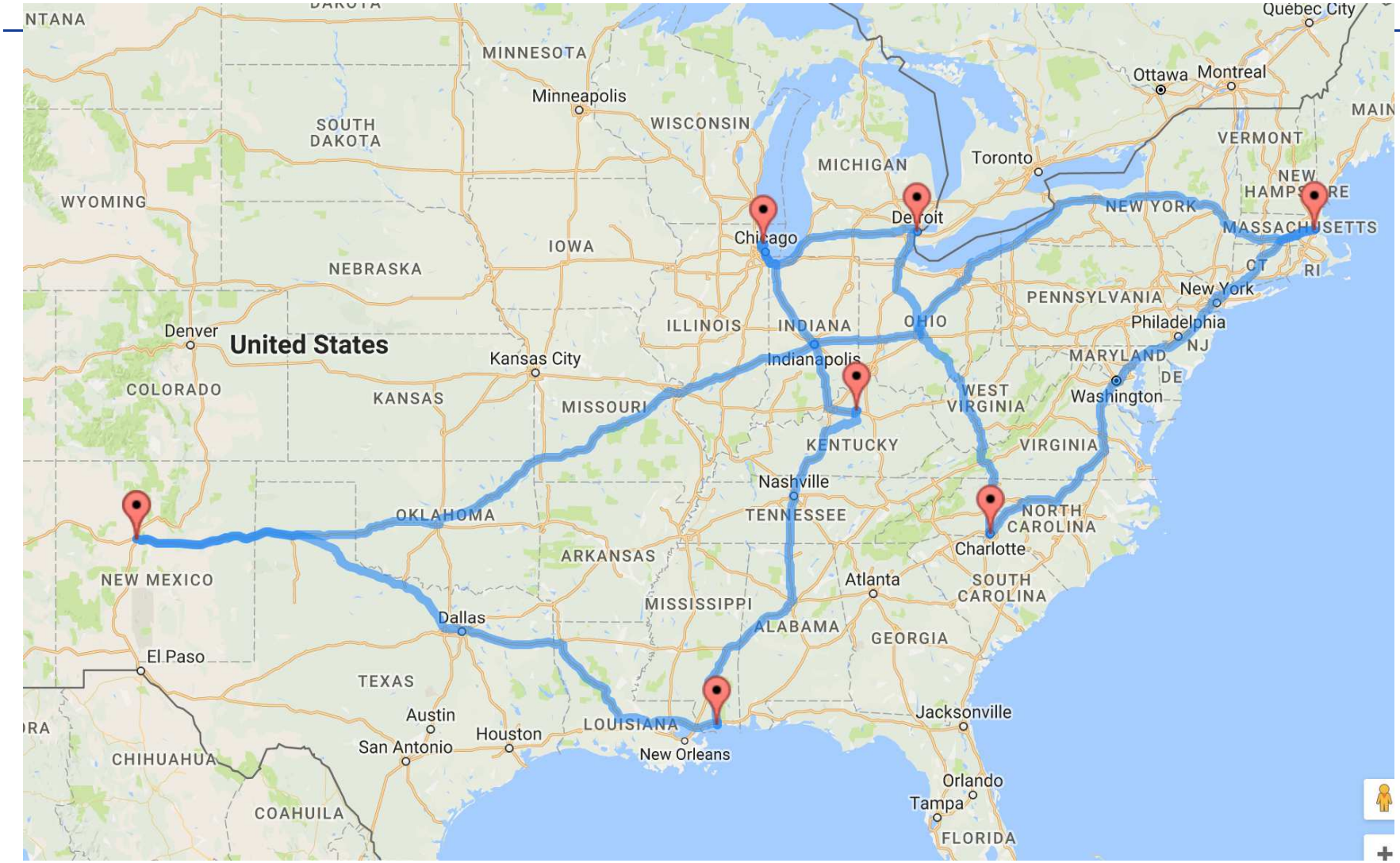
G = Gulfport, MS

(Distances found in file tsp7.b)

Example path:

Path = (A->B) + (B->C) + (C->D) + (D->E) + (E->F) + (F->G) + (G->A)

Map of Alphabetical Order Path



D-Wave
The Quantum Computing Company™

QUBO: Leg Variables

Binary Variable *ab*:

1 if the trip includes the segment A -> B

0 if the trip does not include A->B

Distances between cities A and B denoted by *Dab*

Distance to Minimize:

*Dab * ab + Dac * ac + Dad * ad + … + fg * Dfg*

How do we convert this into a QUBO?

Converting into a QUBO

- Each city must be visited exactly twice – once arriving, and once departing.

  For city A, we must have:

  $$ab + ac + ad + ae + af + ag - 2 = 0$$

  For City B,

  $$ab + bc + bd + be + bf + bg - 2 = 0$$

  And so on, up to city G.

The QUBO to minimize:

$$Dab * ab + Dac * ac + Dad * ad + \ldots + fg * Dfg + \gamma((ab+ac+ad+\ldots-2)**2 + (ab + bc + bd + be + bf + bg - 2)**2 + \ldots)$$

Algebraic results: expanding the equation

- Groups of terms of the form:

  *- 3 * vertex * ab*: favor visiting the path A->B

- Groups of terms of the form:

  *2 * vertex * ab * ag*: penalize visiting the paths A->B and A->G (some of these will be selected)

- There are seven explicit **dw** assert statements (which help identify valid solutions):

  assert:vertex:ab + ac + ad + ae + af + ag – 2

- *vertex* is a Lagrangian multiplier; needs to be weighed against the inter-city distances

Steps to run the 7-city TSP (write a run script)

- Prepared tsp7.b (parameter file) and tsp7.q (QUBO file) by hand
- Embed the problem onto the 128-qubit simulator using the **dw embed** command (the default embedder algorithm tries to find a way to map the needed logical qubits onto available physical qubits)
- Try a value of *vertex* and a value of *param_chain*, another adjustable parameter (controls the chain strength in the embedding)
- Run **dw bind** to bind the parameter values in the B file to the QUBO
- Run **dw exec** to run the problem on the simulator (or QPU)
- Run **dw val** to interpret and validate the output

Parameter explorations

- Earlier, we mentioned *vertex* and *param_chain*, the adjustable parameters
- *Vertex* controls the strength of obeying the constraints
- *Param_chain* controls the strength of chains in the embedding
- When running the problem, parameter space must be explored, to find largest possible number of solutions

	1300	1400	1500
4500			
4750			
5000			

Looking at the lowest-energy solution

- **dw val –s 1 tsp7.sol** produces output that looks like this:

  **** SOLUTION 1 ****

  ab <== 0

  af <== 1

  ag <== 1

  bc <== 1

  …

  VALID: Y

  SAMPLES: 4

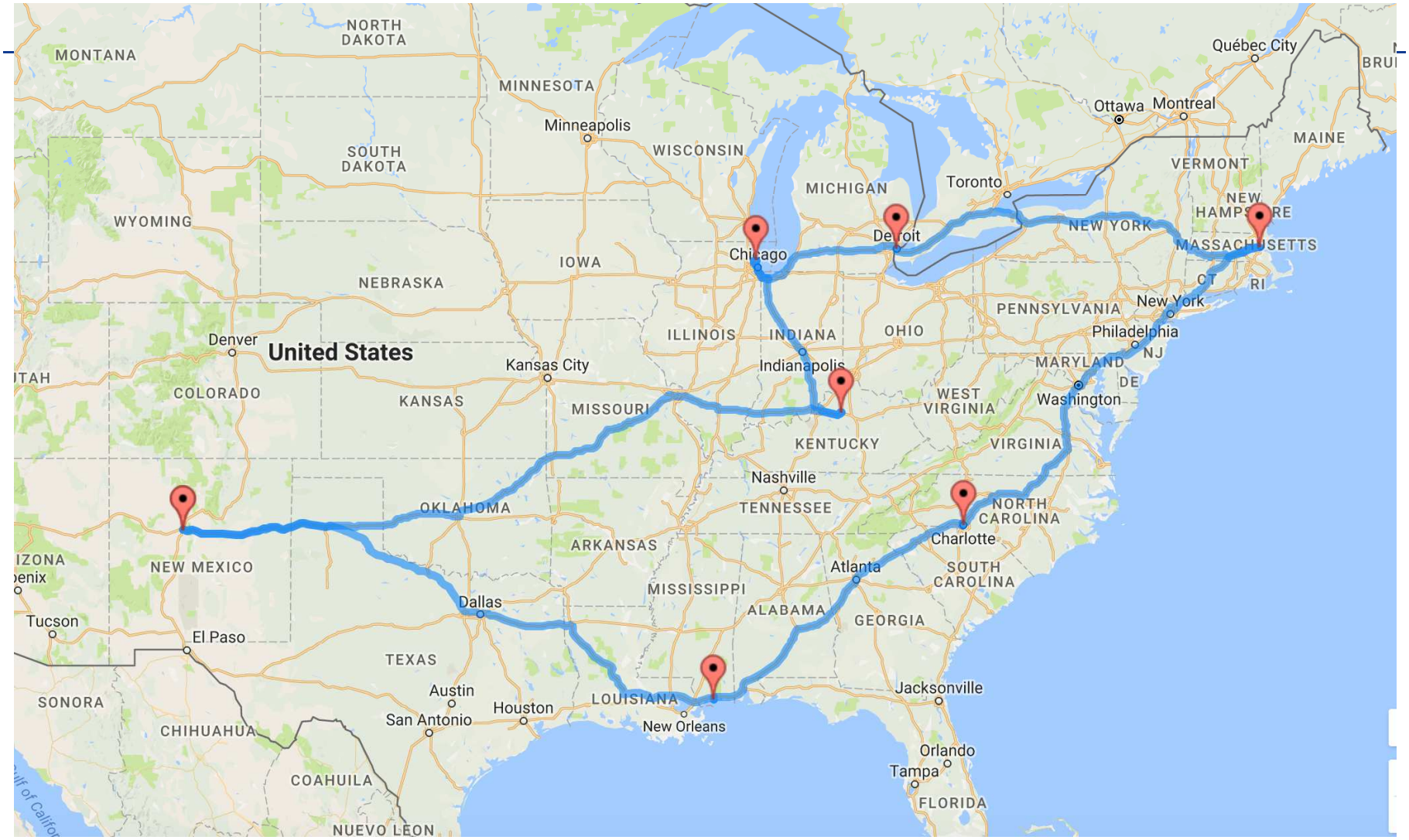
  OBJECTIVE: -33778.00

  And we get the path:

  af + ef + de + bd + bc + cg + ag

  a -> f -> e -> d -> b -> c -> g -> a

A map of the lowest-energy solution



D-Wave
The Quantum Computing Company™

Interpreting the energy

The path: *af + ef + de + bd + bc + cg + ag*

Adding up the miles: 5422 miles

dw tells us the energy is -33778

For each vertex, there will be two nonzero terms of the form:

*-3 * vertex * af = -3 * vertex*

And one term of the form:

*2 * vertex * af * ag = 2 * vertex*

Thus: *-4 * vertex* per 7 cities => *-28 * vertex*

*Energy = Total Mileage – 28 * vertex*

(for vertex = 1400, this equality works)

An interesting issue

A valid solution and different path*:*

ae ag bc bd cf df eg

Notice: A -> E -> G -> A

This is called a **subloop**: the path split into a 3-loop and a 4-loop

- Subloops are not prevented by “visit twice” constraint
- Subloops are not desirable solutions; we would have to write many more constraints to eliminate them

- The Lucas formulation (Permutation matrix) rules out subloops (next section)

Conclusions from 7-city TSP

- **dw** can be used as part of overall toolbox, start to finish
- Good problem for exploring Lagrangian parameters, understanding solutions, how QUBO construction affects solutions (subloop problem).
- Good problem for understanding chains and embedding
- Has quick physical interpretation of solution
- Good problem for understanding what the QPU does, what its inputs are, and what it returns

Overview

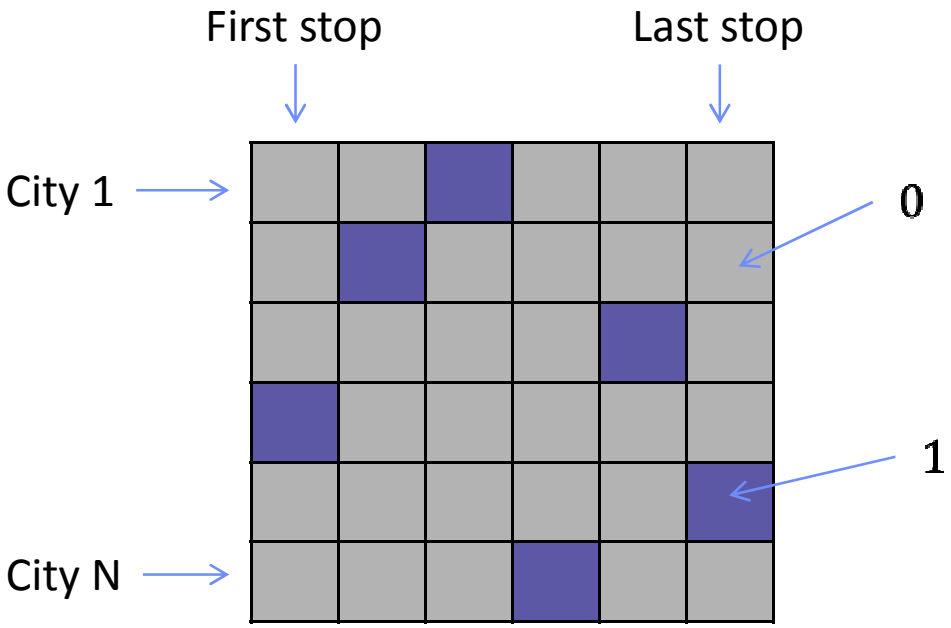
- **Review (from Scott Pakin and D-Wave)**
- **qbsolv**
- **7-city Traveling Salesman Problem**
- *48-city Traveling Salesman Problem*
- **Summary**

48-city Problem Specifications

- Symmetric TSP; undirected graph; distances in miles
- Driving distances obtained from Google Maps
- We can reduce the complexity of the problem by 1- assume last city visited is alphabetically last city (Cheyenne, WY)
- Andrew Lucas paper: https://arxiv.org/pdf/1302.5843.pdf

First approach: QUBO (ref. Andrew Lucas)

QUBO approach means building a **permutation matrix** of 0's and 1's and then introducing quadratic terms to include distances:



Tour represented: city 4 ➡ city 2 ➡ city 1 ➡ city 6 ➡ city 3 ➡ city 5

QUBO (continued)

For each row and column, we introduce a constraint via the following QUBO terms:

$$Constraint = A\left(-1+\sum_{i=1}^{N} x_{1,i}\right)^2$$ ← For row 1

$$Constraint = A\left(-1+\sum_{j=1}^{N} x_{j,1}\right)^2$$ ← For column 1

Distance from the first city visited to the second city visited is computed like this:

$$Distance = B\sum_{i=1}^{N}\sum_{j=1}^{N} d_{i,j}x_{i,1}x_{j,2}$$ ← From 1st to 2nd city

Algebraic results

- QUBO approach requires boolean variables to encode a tour, but "last city visited" assumption provides reduction
- Constant term (2N-2)A: one for each row + column, reduced
- Each variable gets a term -2A multiplied by it (e.g. -2A) to incentivize visiting it on a particular step (e.g., city 1, step i)
- Pairwise terms penalize cities being visited twice, or visited on same step (e.g. 2A or 2A)
- Distance terms penalize following an edge between two cities (the distance term raises the overall energy) (e.g. B)
- "Last city visited" assumption leads to diagonal terms B and B (last and first have to get to Cheyenne)

Python program generate_qubo.py

- Number of cities N is input, cannot go beyond 48, but easy to extend
- Divided through by B, so that there is only one adjustable parameter A
- Read in the inter-city distances from state_capitals.txt, and create distance matrix
- Diagonal terms will be -2A, except when we need to include “last city visited” reduction effect
- qbsolv requires off-diagonal terms to have i < j
- Use QUBO_details library to write QUBO

Looking at the 48-city QUBO

- For N = 48, with the reduction, (N-1)^2 Boolean variables (2209)
- A set to 8500 (required: larger than biggest inter-city distance)
- Most of the diagonals are -17000 (-2 * A), but some have the distance added in, to the last city ("How far from here to Cheyenne?")
- Many of the off-diagonal terms are 17000 (2 * A) as well
- The last off-diagonal term is (2207,2208), as we expect

Python program interpret_lucas.py

- Read in the inter-city distances from state_capitals.txt, and create distance matrix
- Read in the names of the cities
- Read in the qbsolv output
- Associate the result bitstring with binary variables to compute the city tour
- Output a city tour for eventual drawing on Google Maps
- Useful for debugging QUBO/energy

Python program generate_map.py

- Read in the city tour from the previous step
- Read in an HTML template for generating Google USA map
- Insert the city tour into the HTML template
- Write out an HTML page which can be displayed, containing the Google map of the route!

The solution – meh

A possible “Optimal solution” from Randal Olson

- Randal Olson from the University of Pennsylvania wanted to drive all 48 state capitol buildings
- Genetic algorithm
- Olson’s Web page indicates his route is 13,310 miles, but he focuses on state capitol buildings
- http://www.randalolson.com/2016/06/05/computing-optimal-road-trips-on-a-limited-budget/

Randal Olson's solution – way better

D-Wave
The Quantum Computing Company™

Insights

- Why didn't we get the better solution?
- Notice that the difference between "good" and "bad" solutions is less than 1% of the overall energy – why is this?
- Some problems are mathematically not great for the D-Wave
- Only N-1=47 1's can be turned on; the qbsolv algorithms are more effective with larger numbers of bitflips (I need to try this the other way)
- For your problems, focus initially on special cases which can be intuitively understood (TSP with 4 cities, etc.)
- Use post-qbsolv code to test solutions for consistency (for example, introduce additional parameters and establish that the solutions don't change)

Overview

- Review (from Scott Pakin and D-Wave)
- qbsolv
- 7-city Traveling Salesman Problem
- 48-city Traveling Salesman Problem
- *Summary*

Summary

- Hybrid classical/quantum approach to using D-Wave
- “Toolbox” approach: Python, dw, qbsolv, simulator, (hardware)
- Problem has understandable graphical representation
- “This problem is not particularly large, but hard.”
- The goal: you can formulate your client’s problems into QUBO and then run them, even if solutions are not immediately optimal
- The post-qbsolv code is vital for at least three reasons:
  - Interpreting the bitstrings and understanding the solutions
  - Debugging the math of converting the problem to QUBO
  - Debugging the code representing the QUBO