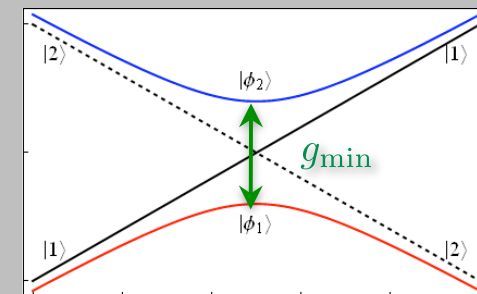
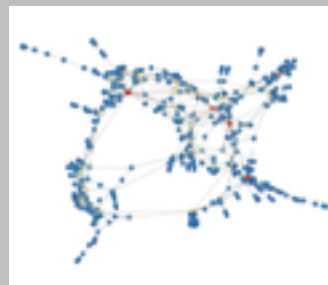
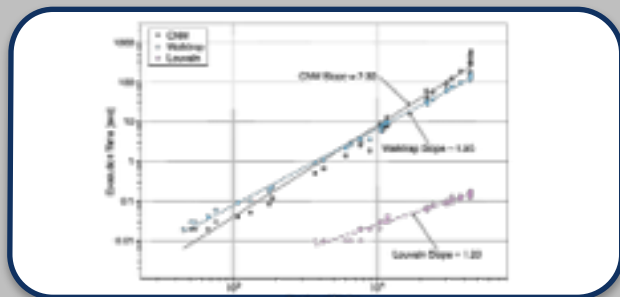


Exceptional service in the national interest



Benchmarking quantum annealing for community detection on synthetic social networks

Ojas Parekh

Sandia National Labs

AQC, 2014

A question?

Which is harder (pick a reasonable definition of “hard”)?

Finding an optimal solution
99% of the time

Finding a solution within
99% of optimal all the time

Which is more practically relevant?

A question?

Which is harder (pick a reasonable definition of “hard”)?

Finding an optimal solution
99% of the time

“Average”-case analysis,
rather than worst-case

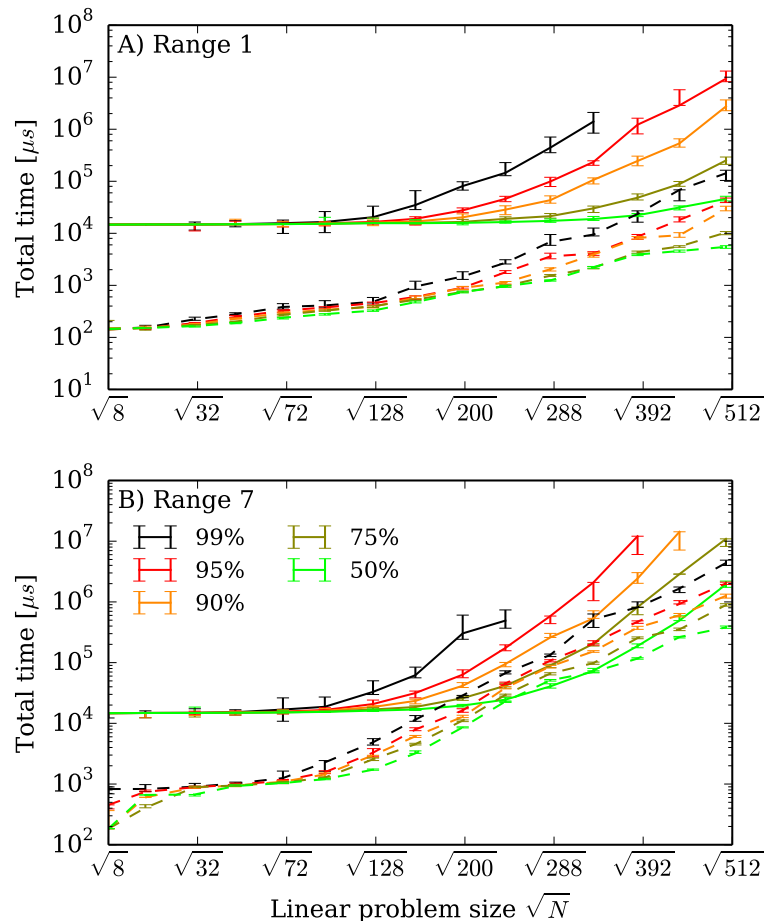
Finding a solution within
99% of optimal all the time

Approximation algorithm,
or approximation scheme

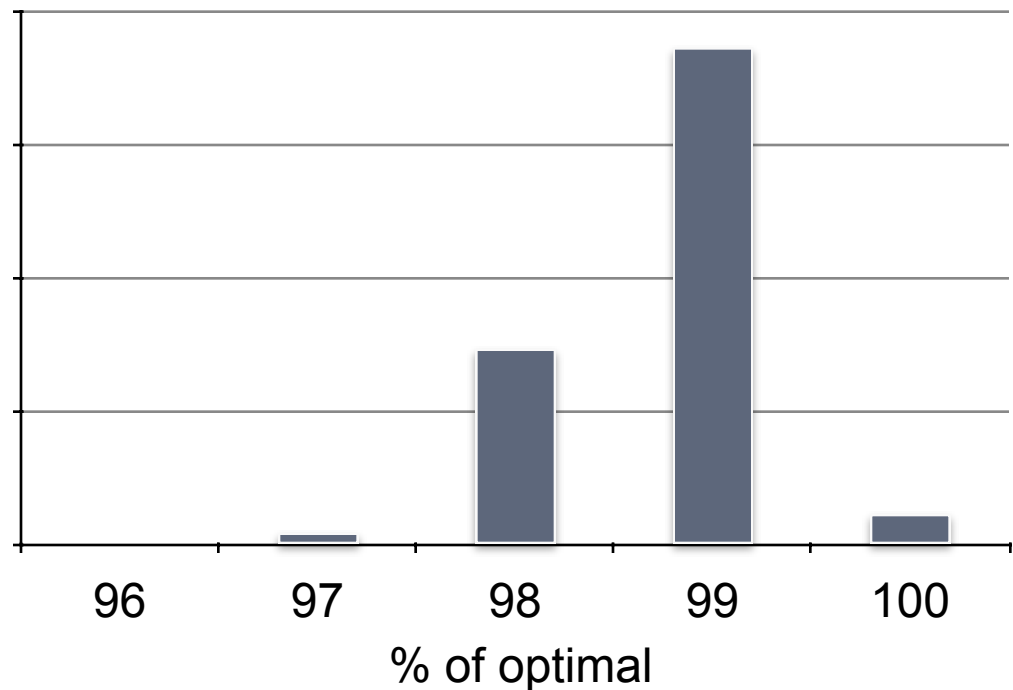
How should we measure success?

Optimal 99% of the time

Within 99% of optimal all of the time



55,000 random $\{-1, 1\}$ -weight instances
on 509-qubit D-Wave Two



Was always within 96% of optimal!

We ask

- What is an appropriate measure of success?
- What classical algorithm(s) should be used for comparison?
- How should one select appropriate benchmark instances?

Problem definitions

- Ising:

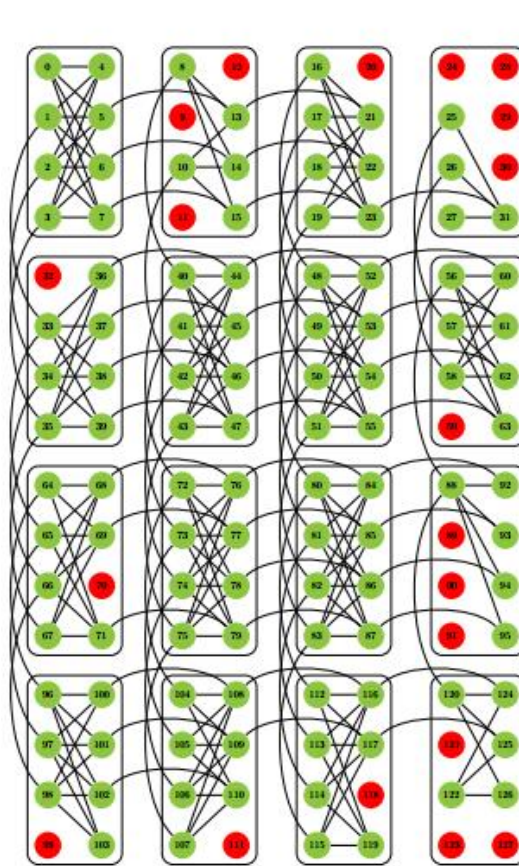
$$\min_{x_i \in \{-1, 1\}} \sum_{ij} J_{ij} x_i x_j + \sum_i h_i x_i$$

- Quadratic binary unconstrained optimization (QUBO):

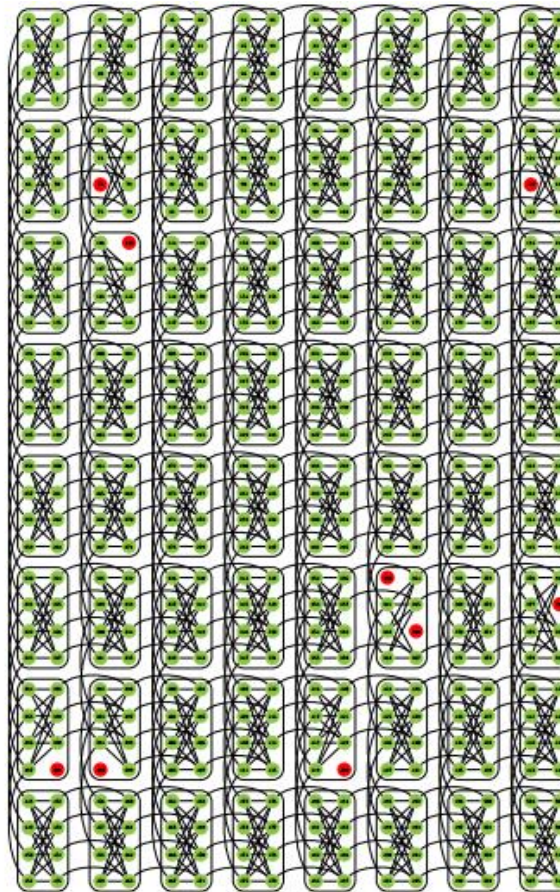
$$\min_{x_i \in \{0, 1\}} \sum_{ij} A_{ij} x_i x_j + \sum_i c_i x_i$$

Comparison of Rainier and Vesuvius chips

Rainier
108/128
spins



D-Wave One



Vesuvius
506/512
spins

D-Wave Two

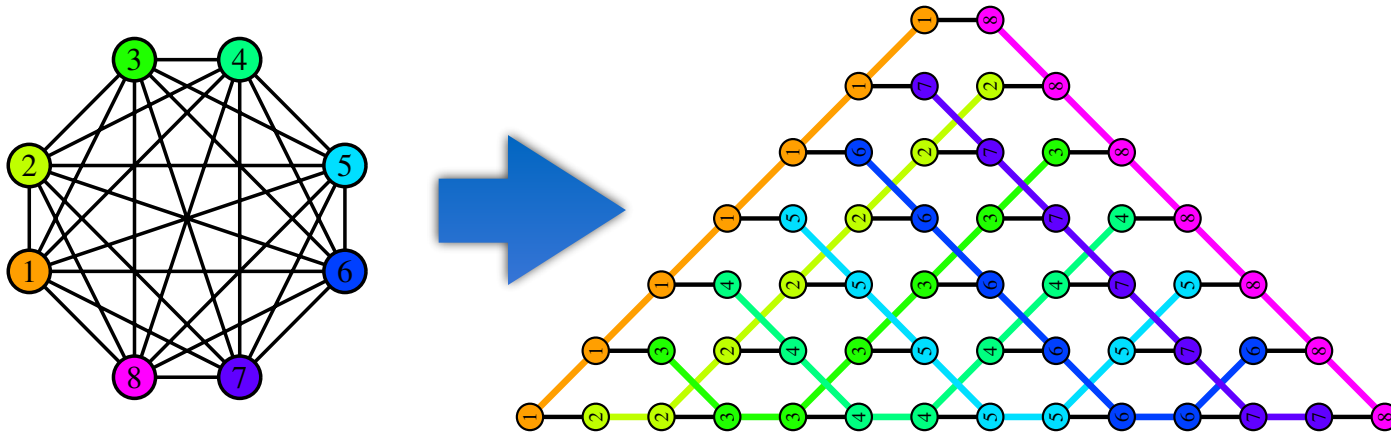
Images from D-Wave Systems: <http://www.dwavesys.com> .

Complexity of Ising on Chimera

- (Decision version) NP-complete even with no linear term and $\{-1, 0, 1\}$ weights [Barahona, 1982]
- We show NP-complete with no linear term and $\{-1, 1\}$ weights
 - Instances used in D-Wave benchmarking studies [with Benjamin Moseley at Washington University]
- Tree-width (path-width) is $\Theta(\sqrt{n})$, yielding $O(2^{\sqrt{n}})$ algorithm
 - “Subexponential” exact algorithm even though NP-hard
- Approximation complexity?
 - Polynomial-time approximation scheme (PTAS) [Saket, 2013, [arXiv:1306.6943](https://arxiv.org/abs/1306.6943)]
 - PTAS’s are rarely efficient; theory vs practice?
 - Efficient approx algorithm for say, getting within 75%?

Approaches to problem embedding

- Embedding is hard: $O(n^n)$ vs $O(2^n)$
- Even harder when optimizing # qubits
- Choi: worst case $O(n^2)$ qubits for n vars
 - Requires (linearly) large coupler weights



Limits of reducing to Chimera

- Can we do better than a quadratic blowup in qubits?
- Probably not, due to Exponential Time Hypothesis
 - Problems like Max-Cut on general graphs are conjectured to require $O(2^n)$ time
 - But we have a $O(2^{\sqrt{n}})$ time algorithm for Chimera Ising
 - So in some sense quadratic factor is artifact of Chimera
- Weights make this worse: Choi embedding assumes (linearly) large weights
- Reduction better than $O(n^2)$ for Max-Cut on bounded-degree graphs would improve best-known classical algorithm
 - Applies to **any** reduction, not just minor embeddings

Max-Cut as model problem

- NP-complete on bipartite graphs with weights $\{-1,1\}$
 - Replace each edge by a path of +1 and -1 edge
- Max-Cut essentially equivalent to Ising problem
 - Can use an apex vertex to model linear term
- We give reduction from weighted QUBO to unweighted QUBO
 - Unroll and optimize existing chain of reductions
 - Weights are a significant barrier in D-Wave benchmarking
- Our reduction only incurs linear blowup on bounded-degree graphs
 - However, does not preserve Chimera structure

Weighted QUBO as 3-SAT

x_1, \dots, x_n



$$\Phi_1(\vec{x}, \vec{y}) = \bigwedge_{ij \in E} (\overline{y_{ij}} \vee x_i \vee x_j) \wedge (\overline{y_{ij}} \vee \overline{x_i} \vee \overline{x_j}) \wedge (y_{ij} \vee x_i \vee \overline{x_j}) \wedge (y_{ij} \vee \overline{x_i} \vee x_j)$$

$$y_{ij} = x_i \oplus x_j$$



y_1, \dots, y_m

k, w_1, \dots, w_m



Adder circuit: $\sum_i w_i y_i \geq k ?$



$\{0, 1\}$

$$\Phi_2(\vec{y}, \vec{w}, k)$$

$$\Phi = \Phi_1 \wedge \Phi_2$$

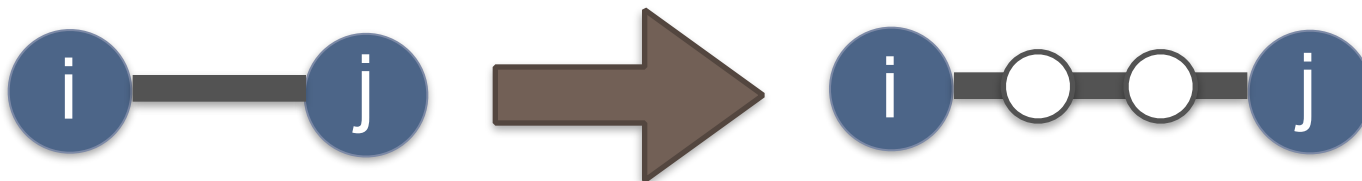
3-SAT as Unweighted Ising

- Standard reduction from 3-SAT to Independent Set
- Usual Ising formulation of Independent Set:

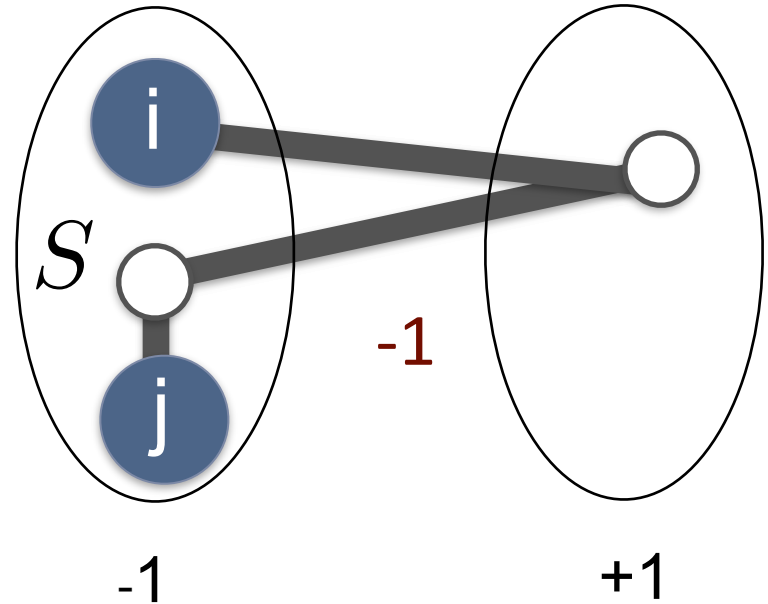
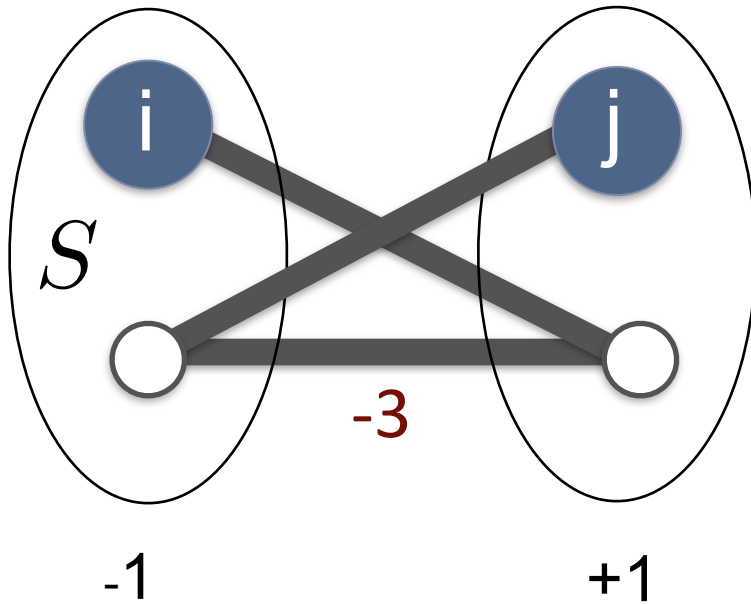
$$\min_{x_i \in \{-1, 1\}} \sum_{ij \in E} x_i x_j - \sum_{i \in V} d_i x_i$$

- New formulation on graph where each edge replaced by 3-path circumvents linear weights above:

$$\min_{x_i \in \{-1, 1\}} \sum_{ij \in E'} x_i x_j - \sum_{i \in V'} x_i$$



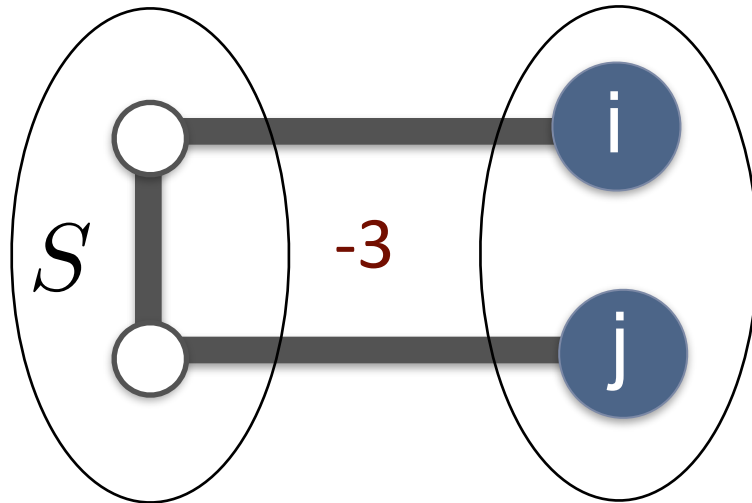
Independent set as Ising



WLOG: -1 side is an independent set

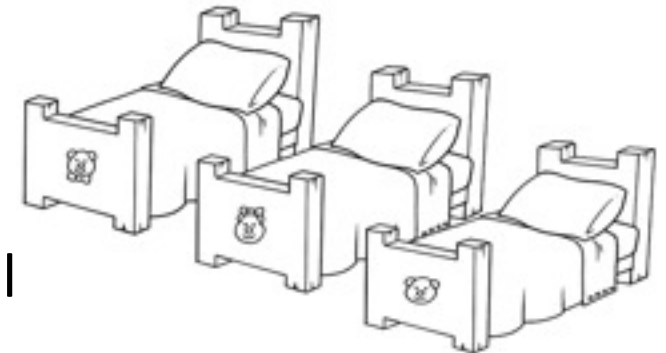
Objective value:

$$-|S| + (|V| - |S|) - 3|E| = |V| - 2|S| - 3|E|$$



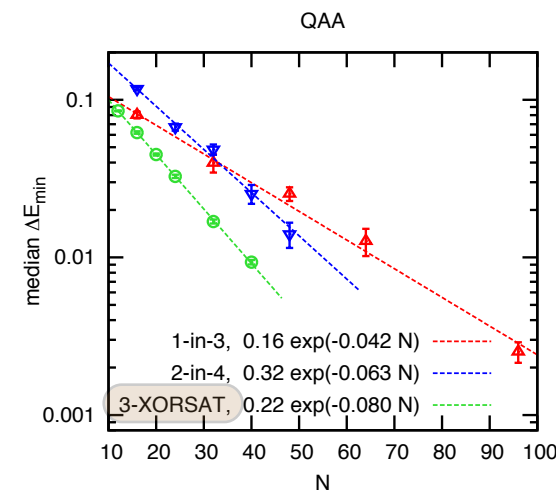
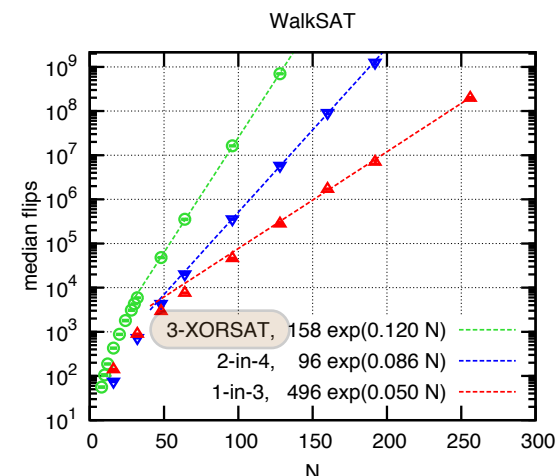
Instance selection: challenges

- Desire scalable family of related instances
- Real world often lacks well-defined optimality
- Random instances too easy or hard
- Known hard instances may be artificial
- Fairness to all benchmark algorithms
- Resources: time, memory, etc.



Picking the right algorithm

- Random Ising instances on D-Wave hardware
 - $\{-1,1\}$ coupler values
 - Are such instances hard?
 - Hen and Young observed problem in P may appear hard (3-XORSAT in figure)
[[Phys. Rev. E 84, 061152 \(2011\)](#)]
 - Random vs hard instances is a tricky issue



Configuration matters

- Random instances on D-Wave hardware
 - $\{-1,1\}$ coupler values
 - D-Wave Two finds optimal in 0.5 sec, while classical algorithms scale poorly [McGeoch and Wang, [Conf. Computing Frontiers 2013](#): 23]
 - Claimed 3600x speedup
 - We observe classical Integer Program solvers match performance with appropriate model [also Dash, [arXiv:1306.1202v2](#) (2013)]
 - Speedup vanishes with proper configuration/usage
 - QUBO vs Ising
 - Random instance with linear term appear easy for former but hard for latter!

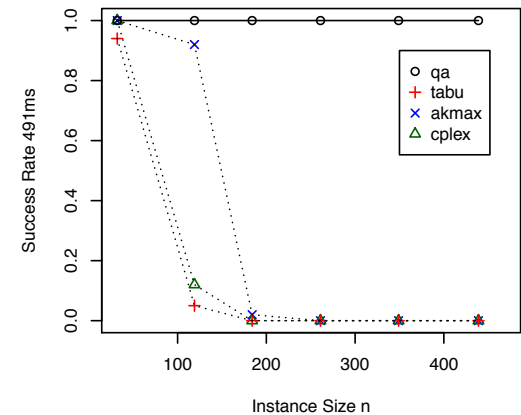


Figure 1: Success rates: proportion of best solutions found in 491ms CPU time (tabu, amax, cplex software) and exclusive access time (QA hardware).

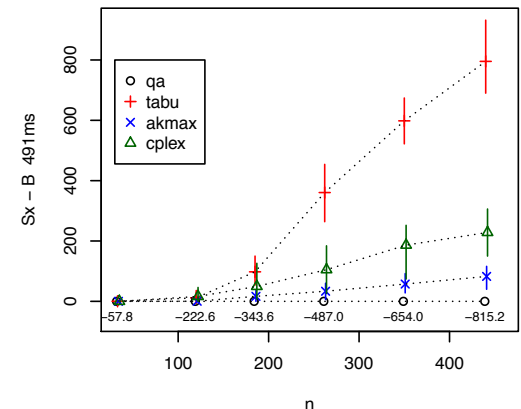
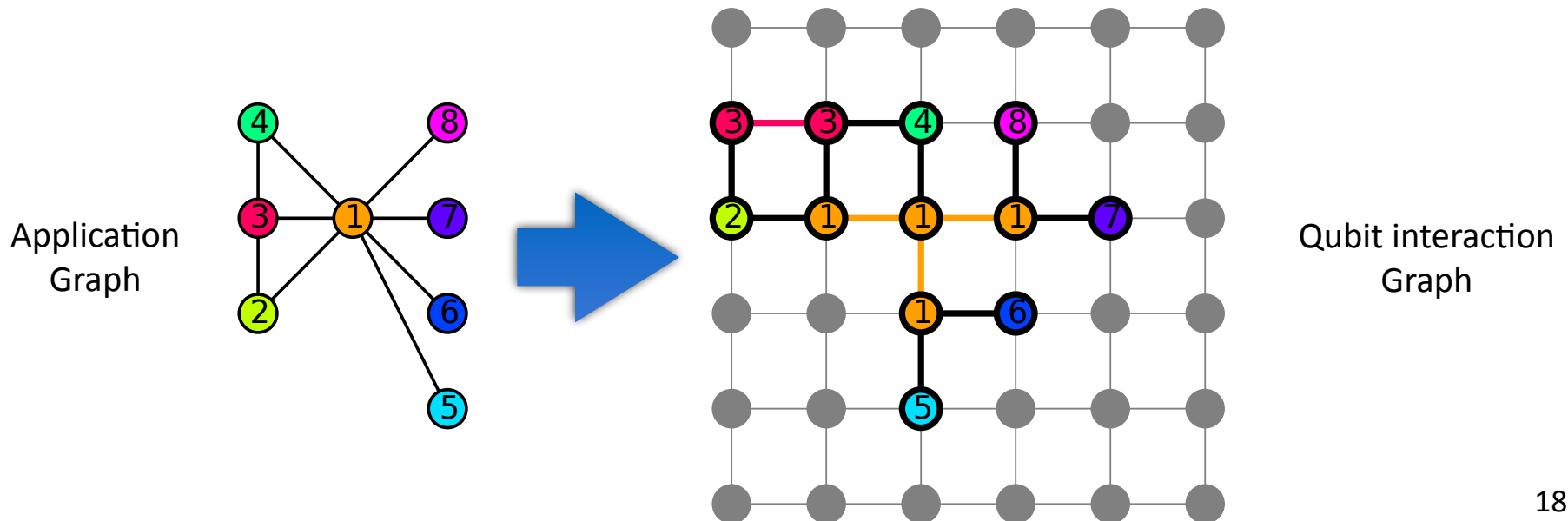


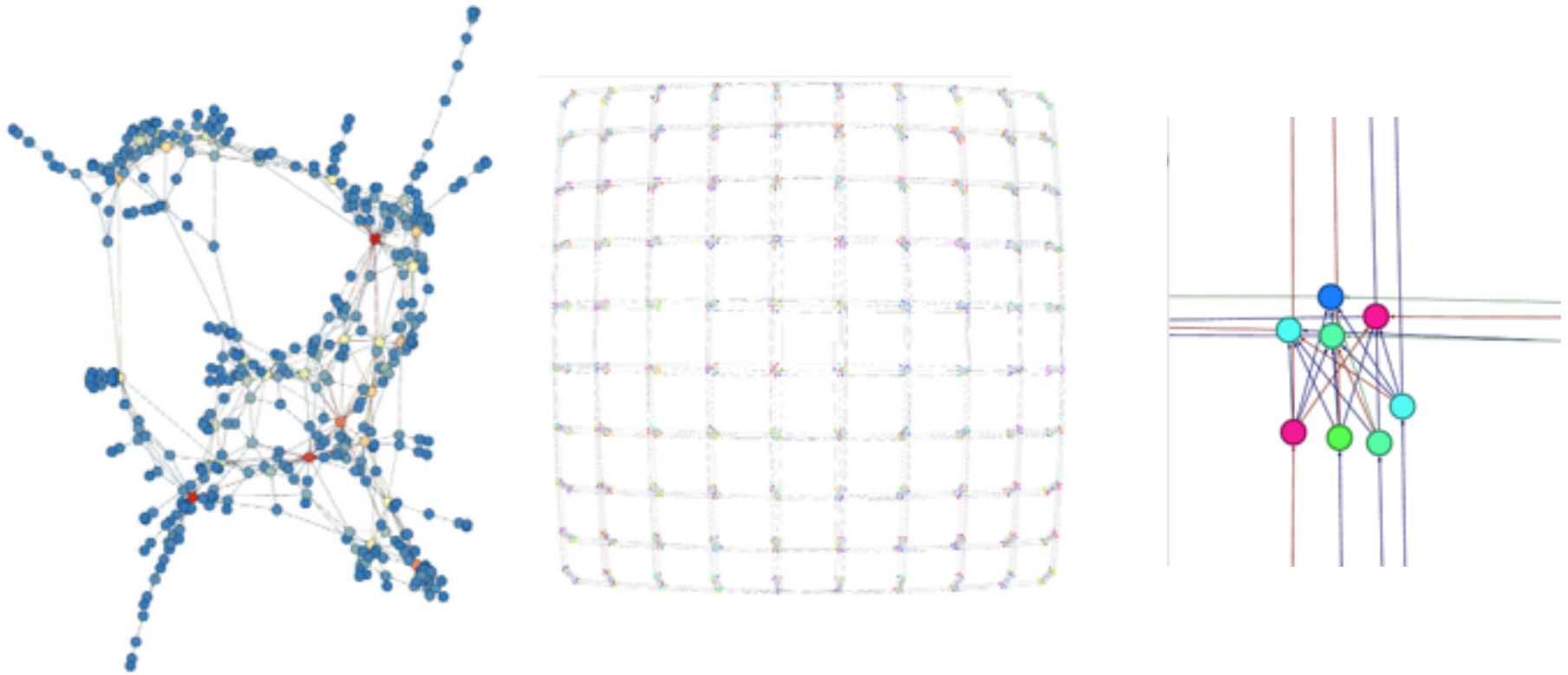
Figure 2: Differences between solution cost S_x in 491ms runtime, and best solution B for each input. Dotted lines connect means for each solver; vertical bars show the range of observations. The numbers at bottom are means B for each problem size.

Solving problems with D-Wave: challenges

- Application graph must be embedded within Chimera graph
 - Requires extra qubits; worst case approx n^2 qubits for n nodes
 - Very hard to determine a good embedding for a given graph
 - Typical approaches to embedding require large weights to force all qubits corresponding to a node have same spin
 - Efficiency: $\#(\text{Application graph nodes})/\#(\text{Qubits in Chimera graph})$



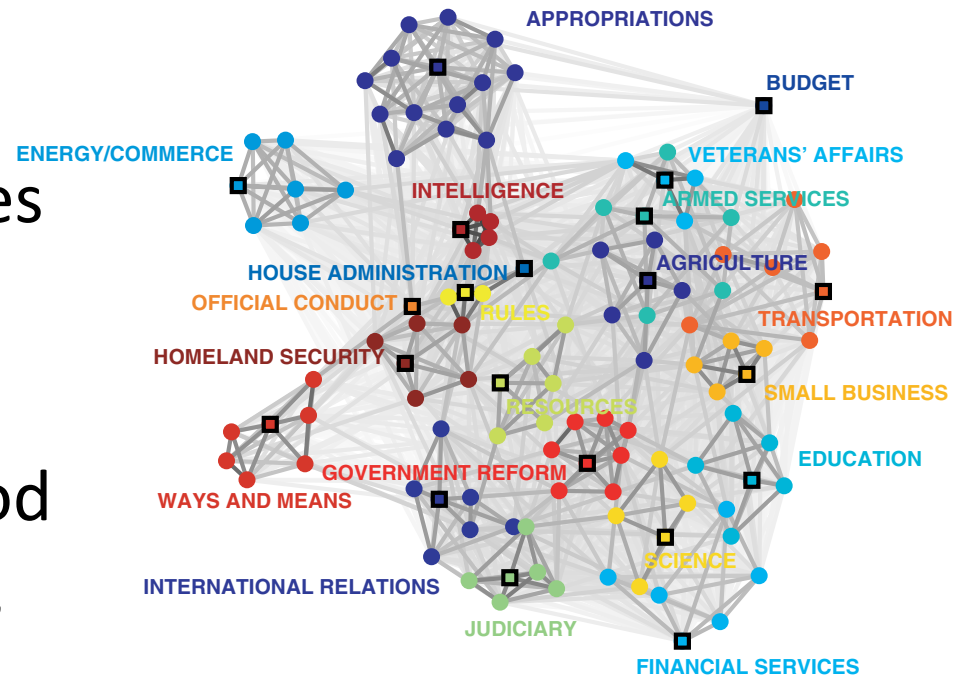
Complex networks on the Chimera graph



- New approach to circumvent embedding [with Jeremy Wendt]
- Generate complex network simultaneously while embedding it
- Efficiency for 512-node Chimera around 40% vs 6.25% worst case

Community detection

- Find natural communities or clusters in complex network
- Many measures of a good cluster (e.g., modularity, conductance)

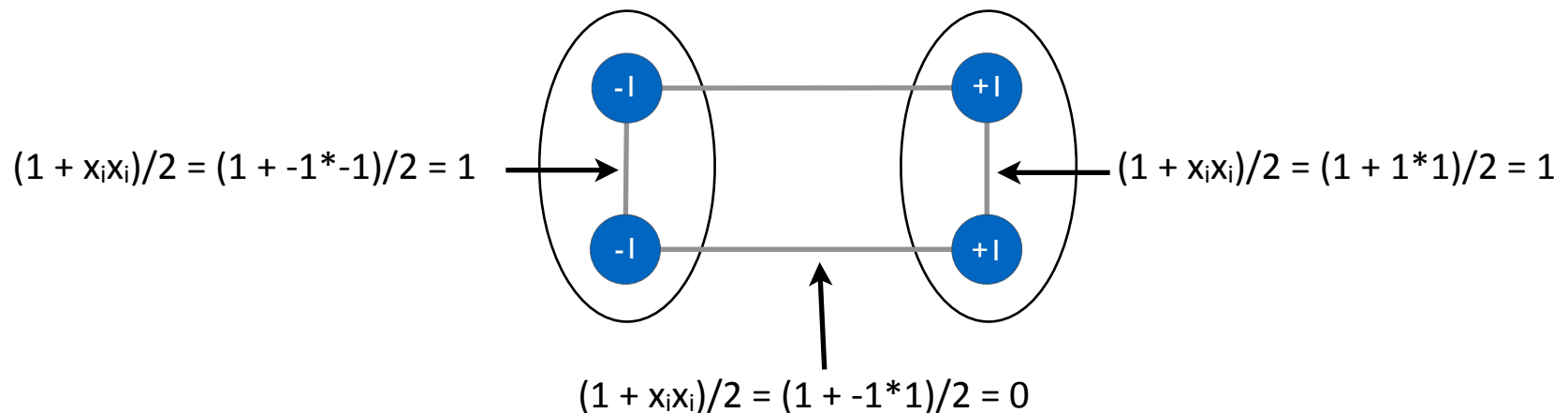


2003-2004 House Committees
“Communities in Networks”, AMS

Community detection via Ising

- Modularity

- Measures strength of a partition of a graph into clusters/communities
- Fraction of edges within clusters minus expected number within clusters for a random graph with a given degree distribution
- Example: partitioning into 2 clusters
 - Each node i assigned $x_i = -1$ or $x_i = +1$, based on cluster in which it lives
 - $(1 + x_i x_j)/2$ indicates edges within clusters



Community detection via Ising

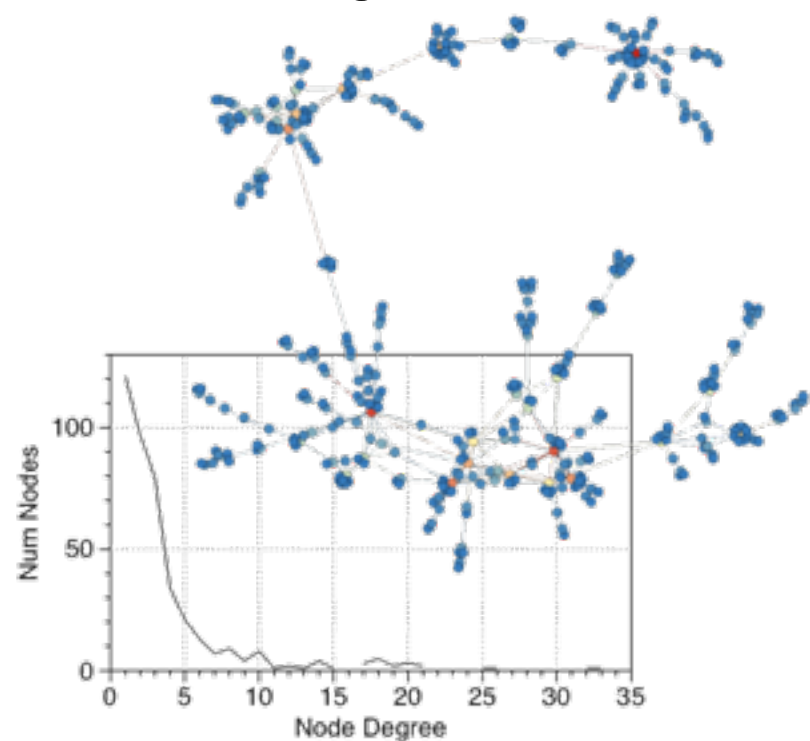
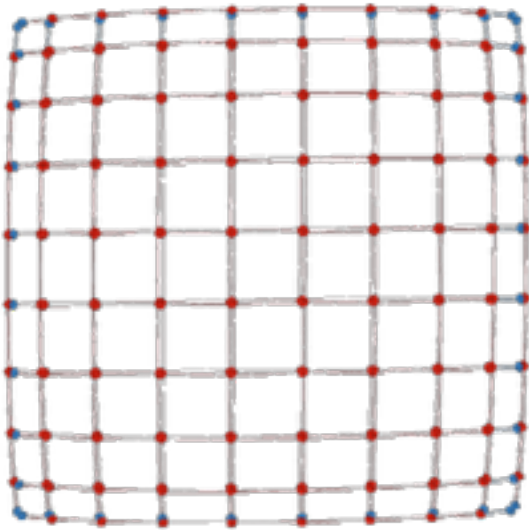
● Modularity

- Fraction of edges within clusters minus expected number within clusters for a random graph with a given degree distribution
- Example: partitioning into 2 clusters
 - Each node i assigned $x_i = -1$ or $x_i = +1$, based on cluster in which it lives
 - $(1 + x_i x_j)/2$ indicates edges within clusters
- QUBO formulation for finding 2-clustering that maximizes modularity
 - m - number of edges
 - a_{ij} - 1 if edge ij is in the graph; 0 otherwise
 - d_i - degree of node i , i.e., number of edges incident to i
- Note: this QUBO implementation requires a dense graph

$$\sum_{i,j} \left(a_{ij} - \frac{d_i d_j}{2m} \right) \frac{1 + x_i x_j}{2} = \underbrace{\sum_{i,j} \frac{1}{2} \left(a_{ij} - \frac{d_i d_j}{2m} \right)}_{\text{Constant term}} + \sum_{i,j} \underbrace{\frac{1}{2} \left(a_{ij} - \frac{d_i d_j}{2m} \right)}_{(i,j) \text{ entry of QUBO matrix}} x_i x_j$$

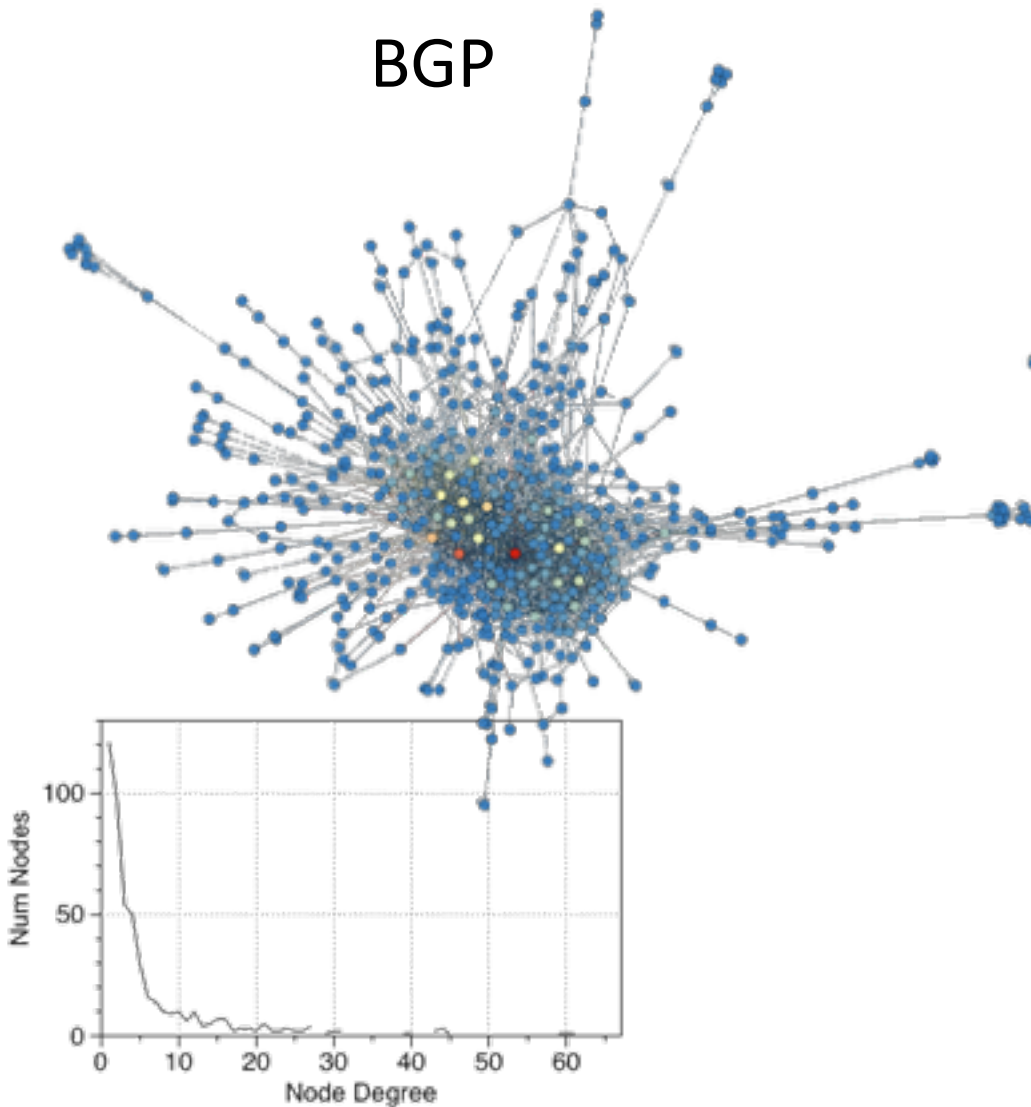
Generating complex networks on a Chimera graph

- Mapping arbitrary graph to Chimera is hard
- Instead, alter Chimera graph to have “real-world” properties
 - Merge nodes to increase node degree
 - Remove edges between nodes to decrease degree

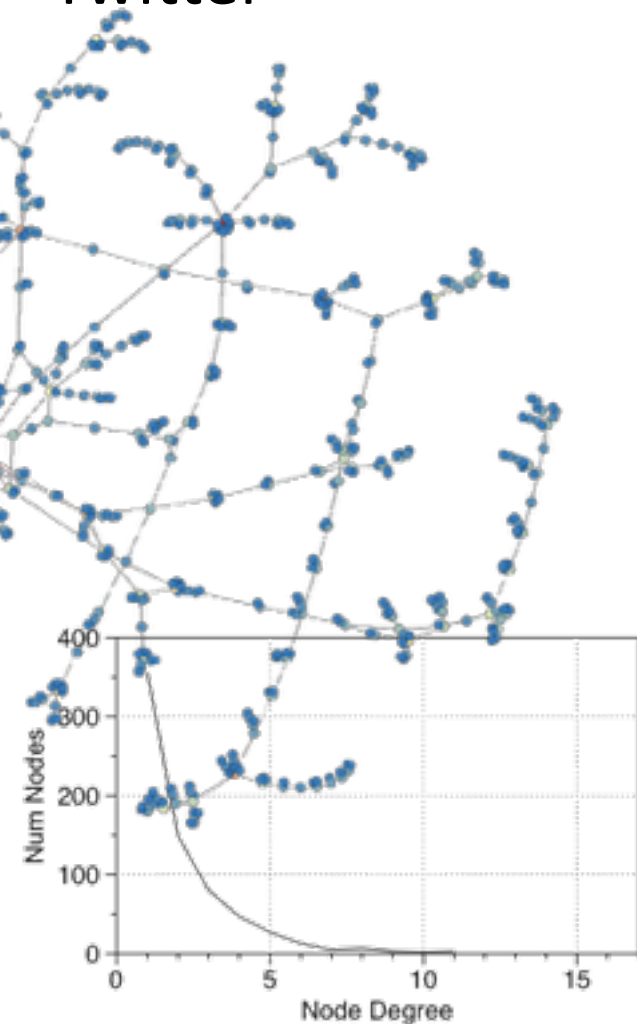


Real-world complex networks

BGP

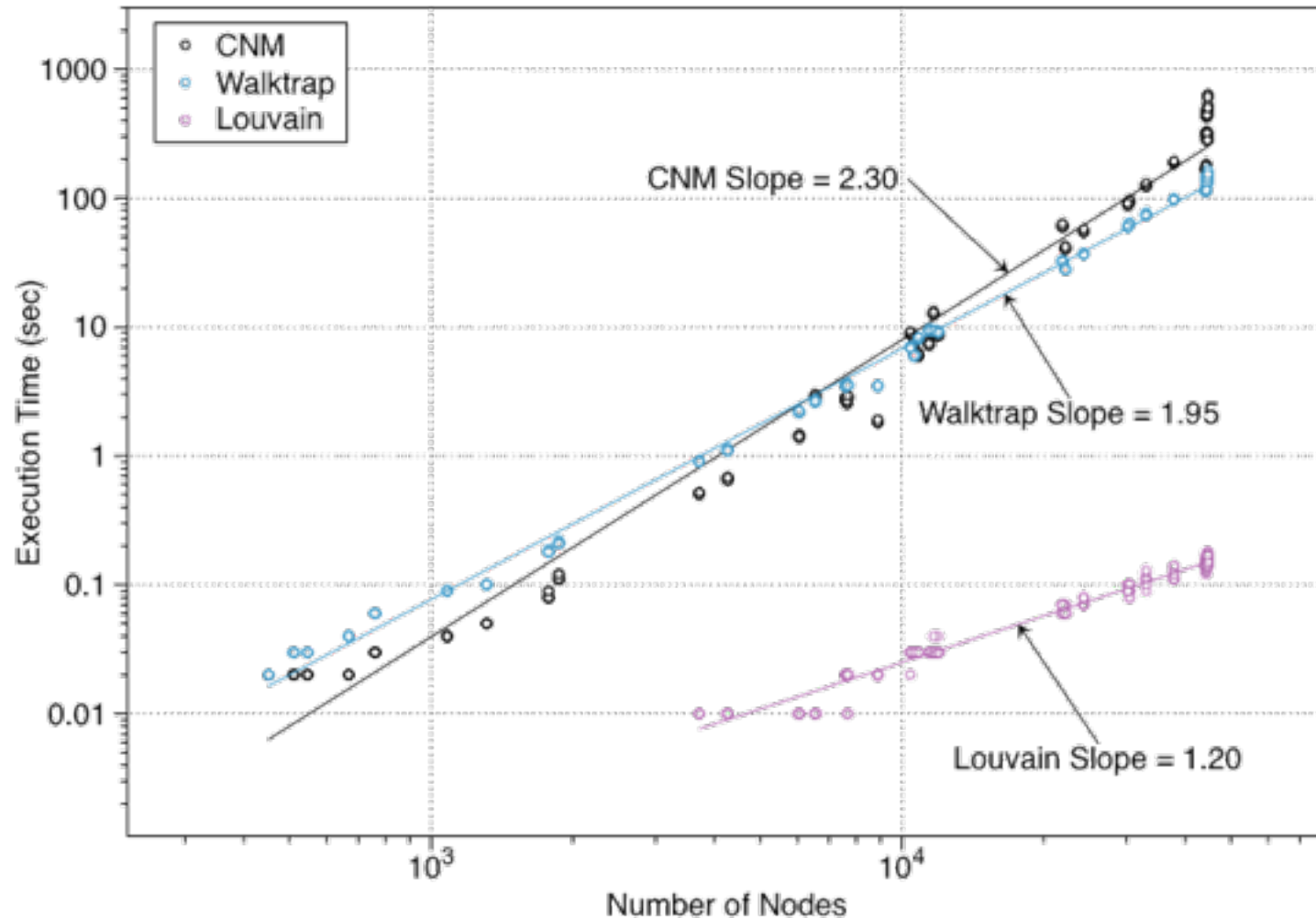


Twitter



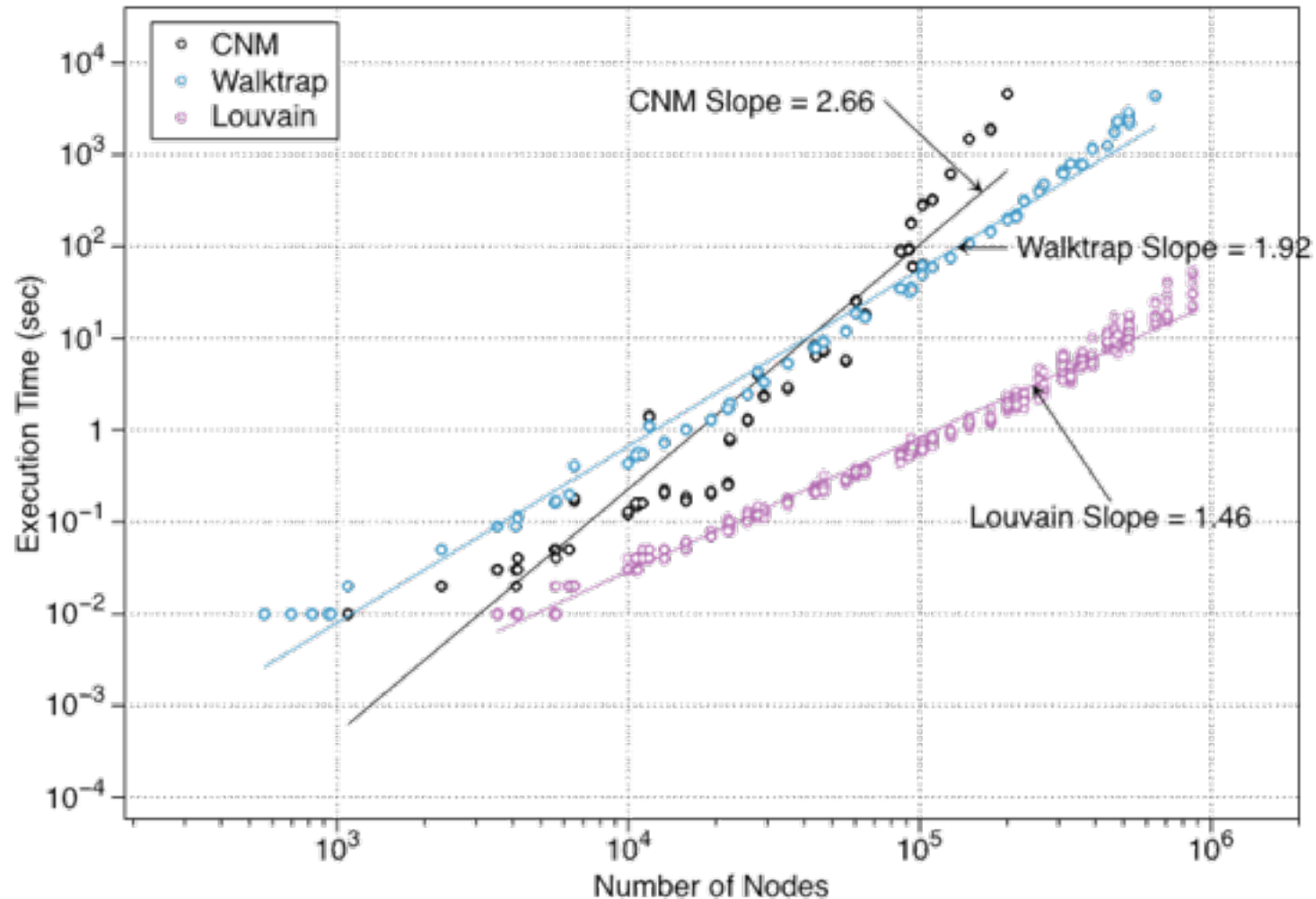
Classical Community Detection

- BGP Execution Time



Classical Community Detection

- Twitter Execution Time



Conclusion: We asked

- What is an appropriate measure of success?
 - Awareness of artificially hard problems for “natural” problems where close is good enough
 - Should try properly leverage hardness in defining success
- What classical algorithm(s) should be used for comparison?
 - Must select proper algorithm and configuration
 - Achieving fairness is tough when comparing an infant technology like quantum vs one honed over decades
- How should one select appropriate benchmark instances?
 - Balance between real-world, random, and hard is challenging