Simulated annealing for
Graph Golf

Toru Koizumi

Graduate School of Information Science and Technology
The University of Tokyo
Introduction and my result
Graph Golf

• Given number of vertex \( (n) \) and degree \( (d) \),
  • find the small diameter graph,
  • and minimize Average Shortest Path Length (ASPL, \( l \)).

\( n = 8, d = 3 \)

Diameter = 2
ASPL = 1.571 (opt.)
Graph Golf

• Average Shortest Path Length (ASPL, \( l \)) has a theoretical lower bound (\( L \)).
  • “ASPL gap” (\( l - L \geq 0 \))

• For general graph with small \( n \), we may be able to find a optimal solution (\( l = L \)).

• I am a beginner → Target to ‘Deepest Improvement’
• I focused on these three problems.

<table>
<thead>
<tr>
<th>Order $n$</th>
<th>Degree $d$</th>
<th>Length $r$</th>
<th>Diam. $k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>72</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>256</td>
<td>5</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>256</td>
<td>10</td>
<td>3</td>
<td></td>
</tr>
</tbody>
</table>

• I thought $(n=72, d=4)$ is the easiest but actually $(n=256, d=10)$ is the easiest.
I got optimal solution for \((n=256, d=10)\) 6/22

<table>
<thead>
<tr>
<th>Rank</th>
<th>Author</th>
<th>Diam. (k)</th>
<th>ASPL (l)</th>
<th>Diam. gap</th>
<th>ASPL gap</th>
<th>Info.</th>
<th>Date (UTC)</th>
<th>Week</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Haruishi masato</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-08-13 09:05:21</td>
<td>33</td>
</tr>
<tr>
<td>1</td>
<td>thai9cdb</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-07-29 13:08:27</td>
<td>30</td>
</tr>
<tr>
<td>★ 1</td>
<td>Toru Koizumi</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-06-12 01:36:40</td>
<td>24</td>
</tr>
<tr>
<td>★ 1</td>
<td>Toru Koizumi</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-06-12 01:33:30</td>
<td>24</td>
</tr>
<tr>
<td>★ 1</td>
<td>Toru Koizumi</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-06-11 14:52:50</td>
<td>24</td>
</tr>
<tr>
<td>★ 1</td>
<td>Toru Koizumi</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-06-11 14:50:46</td>
<td>24</td>
</tr>
<tr>
<td>★ 1</td>
<td>Toru Koizumi</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-06-11 14:48:06</td>
<td>24</td>
</tr>
<tr>
<td>★ 1</td>
<td>Toru Koizumi</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-06-11 14:42:56</td>
<td>24</td>
</tr>
<tr>
<td>★ 1</td>
<td>Teruaki Kitasuka, Masahiro Iida</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-05-15 09:40:41</td>
<td>20</td>
</tr>
<tr>
<td>★ 1</td>
<td>Masahiro Nakao</td>
<td>3</td>
<td>2.56863</td>
<td>0</td>
<td>0.00000</td>
<td></td>
<td>2018-05-15 05:11:20</td>
<td>20</td>
</tr>
</tbody>
</table>
My approach
• Random graph has a ASPL that is not bad but far away from optimal solution.

Distribution of ASPL (random graph, n=256, d=10)

Theoretical lower bound (2.56863)
Search for optimal graph

• Random search cannot achieve optimal graph
  • Probability is $\sim 10^{-530}$ (n=256, d=10)

• Adopt simulated annealing
  ? The Neighbors of a state
  ? Probability distribution
  ? Transition probabilities
  ? Cooling schedule
The Neighbors of a state

- The neighbors of an optimal solution must be good solutions

- Should(?) consider the constraint of degree
  - Every vertex has $d$ edges

- 2-opt is the simplest choice
• Most popular choice: canonical ensemble

• Preparation: normalize graph related values
  • Unit of ASPL $k := \frac{2}{n(n-1)}$
  • ASPL gap $E(G) := \text{ASPL}(G) - \text{ASPL}_{\text{lower bound}}$
    • $\frac{E(G)}{k} \in \mathbb{Z}_{\geq 0}$

• The probability distribution

$$p(T; G) \propto e^{-\frac{E(G)}{kT}}$$
Transition probability

• Use Metropolis-Hastings algorithm
• One of the transition probability for realizing $p(T; G)$

$$A(T; G, G') = \begin{cases} 1 & \text{for } E(G) \geq E(G') \\ e^{-\frac{E(G')-E(G)}{kT}} & \text{for } E(G) < E(G') \end{cases}$$
Cooling schedule

• Most popular way: Exponential cooling
• This is a bad choice.
• Why?
• Number of state $W(E) := \#\{G|E(G) = E\}$
• Entropy $S(E) := k \log W(E)$

$\left(\frac{\partial S}{\partial E}\right)_V = \frac{1}{T}$

(V is always constant because we are calculating on canonical ensemble)
Entropy of graph (n=256, d=10)
Entropy of graph (n=256, d=10)

\[ T=1 \iff \left( \frac{\partial S}{\partial E} \right) = 1 \]

\[ T=5 \iff \left( \frac{\partial S}{\partial E} \right) = 0.2 \]
Entropy of graph (n=256, d=10)

T=1 ⇔ \( \frac{\partial S}{\partial E} = 1 \)

T=5 ⇔ \( \frac{\partial S}{\partial E} = 0.2 \)
$E$ vs $\left( \frac{\partial S}{\partial E} \right)$ and $T$ \hspace{1cm} (n=256, d=10)

- How far should we lower the temperature?

- $T = \frac{1}{\left( \frac{\partial S}{\partial E} \right)} \sim 0.26$ at $E = 0$

→ calculate with $T \sim 0.26$
Why not exponential cooling

• Using exponential cooling takes very long time to achieve an optimal solution because there are very few $E \sim 0$ states.

• It is better to quickly cool down when $E$ is small.
Annealing results

- According to theory,
  - $T \geq 0.30$ cannot achieve optimal solution.
  - $T \leq 0.25$ can achieve optimal solution
In fact,

- (n=256, d=10) problem is very easy
- Even greedy method (in other words, simulated annealing with $T=0$) can achieve optimal solution
Conclusion

- Simulated annealing is simple (but insufficient) way to find optimal solution
- Some configurations can be diverted general purpose one
  - 2-opt
  - Canonical ensemble
  - Metropolis-Hastings algorithm
- It is better to quickly cool down where it is close to optimal solution
Appendix: Entropy of graph (n=72, d=4)