Hamiltonian Cycle Problem and Cross Entropy: Passing Through the Nodes by Learning

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A Conference on the Occasion of R.Y. Rubinstein's 70th Birthday
Sønderborg, Denmark
14-18 July, 2008

The Hamiltonian Cycle Problem: An Introduction

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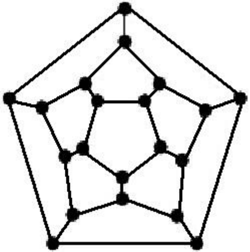
- With respect to this property - Hamiltonicity - graphs possessing a HC are called Hamiltonian.
- The name is due to the fact that Sir William Hamilton investigated the existence of such cycles on the dodecahedron graph.



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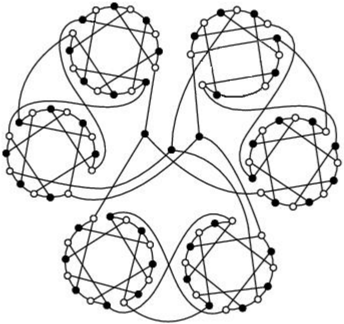
- Henceforth, a graph of order N will mean a simple N-vertex graph (without self-loops) that can be both:
  - symmetric - every edge admits two-way traffic, or
  - directed - digraph, with one-way traffic along each arc.
- The HCP is NP-complete and has become a challenge both in its own right and because of its close relationship to the famous Travelling Salesman Problem (TSP).
- An efficient solution of TSP would have an enormous impact in operations research, optimization and computer science.
- I claim that the underlying difficulty of the TSP is, perhaps, hidden in the Hamiltonian Cycle Problem and focus on the latter.

- Just to demonstrate the connection of HCP with “rare events”
- I claim that even some “simple” Hamiltonian Graphs, can be tough! For example, consider the “Horton94 Graph”.



Horton Graph

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- The standard, Horton graph is a 96-node cubic graph and is non-Hamiltonian. The "Horton94" graph is a simple 94-node modification (Ejov) which has only "a few" Hamiltonian cycles: (exactly?) 76, 800.
- This sounds like a lot, but there are 3^{94} possible sub-graphs. So, finding a Hamiltonian cycle "by chance", as percentage, is

$$\frac{76,800}{3^{94}} \times 100 = 1.08633 \times 10^{-38},$$

not terribly likely, is it?
- Like looking for a proverbial "needle in a haystack"...

- We consider a moving object tracing out a directed path on the graph Γ with its movement "controlled" by a function

$$f : \mathcal{V} = \mathcal{V}(\Gamma) = \{1, 2 \ldots, N\} \to \mathcal{A} = \mathcal{A}(\Gamma)$$

mapping the set of nodes of Γ into its set of arcs.

- We think of $\mathcal{V}$ as the state space of a controlled Markov chain, where for each state/node i, the action space

$$\mathcal{A}(i) := \{a | (i, a) \in \mathcal{A}\}$$

is in $1:1$ correspondence with the set of arcs emanating from that node or, equivalently, with the set of endpoints ("heads") of those arcs.

Stochastic, Dynamic, Embedding of the HCP

Example (1)

- Consider the complete graph Γ_4 on four nodes (with no self-loops). In a natural way, the Hamiltonian cycle

$$c_1 \ : \ 1 \to 2 \to 3 \to 4 \to 1$$

corresponds to the "deterministic (stationary) control"

$$\mathbf{f}_1 \ : \ \{1, 2, 3, 4\} \to \{2, 3, 4, 1\},$$

where $\mathbf{f}_1(2) = 3 \Leftrightarrow$ to the controller choosing arc $(2,3)$ in state 2 with probability 1.

- A Markov chain induced by $\mathbf{f}_1$ is given by the " zero-one" transition matrix

$$P(\mathbf{f}_1) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

an irreducible, stochastic matrix.

Example (1, cont.)

- However, the union of two sub-cycles:

$$1 \to 2 \to 1 \text{ and } 3 \to 4 \to 3$$

corresponds to the deterministic control

$$\mathbf{f}_2 \; : \; \{1, 2, 3, 4\} \to \{2, 1, 4, 3\}$$

which identifies the Markov chain transition matrix

$$P(\mathbf{f}_2) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

containing two distinct ergodic classes.

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- Typically, the performance of a policy $\mathbf{f}$ is evaluated either by
  - a limiting average criterion

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  - a discounted criterion (for a "discount factor" $\beta \in [0,1)$)

$$\mathbf{v}_\beta(\mathbf{f}) = \sum_{t=0}^{\infty} \beta^t P(\mathbf{f})^t \mathbf{r}(\mathbf{f}) = [I - \beta P(\mathbf{f})]^{-1} \mathbf{r}(\mathbf{f}).$$

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- The immediate reward/cost vector $\mathbf{r}(\mathbf{f})$ will be set to

$$\mathbf{r}(\mathbf{f}) := (1, 0, \dots, 0)^T \text{ for all } \mathbf{f}.$$

Difficulties

- Such a controlled Markov chain (CMC, for short) has a multi-chain ergodic structure which complicates the analysis.
- This is essential because multiple ergodic classes correspond to sub-cycles in the original graph that are the "mother of all difficulties" in the TSP (and hence also in the HCP).

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- However, from Markov chains' perspective, there is an opportunity to parametrically differentiate between controls inducing the multi-chain and the uni-chain ergodic structures.
- Indeed, we have at least two ways of achieving such a differentiation.

Method 1: Perturbation

- Multiple chains are "disguised" with the help of a singular perturbation. For instance, we can replace $P(\mathbf{f}_2)$ with

$$P_\varepsilon(\mathbf{f}_2) = \begin{pmatrix} \varepsilon & 1-3\varepsilon & \varepsilon & \varepsilon \\ 1-3\varepsilon & \varepsilon & \varepsilon & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon & 1-3\varepsilon \\ \varepsilon & \varepsilon & 1-3\varepsilon & \varepsilon \end{pmatrix}.$$

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- This perturbation is singular as it alters the ergodic structure by changing the Markov chain $P(\mathbf{f}_2)$ to one that is irreducible. Its stationary distribution matrix is

$$P^*_\varepsilon(\mathbf{f}_2) = \begin{pmatrix} 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \end{pmatrix},$$

where $\pi^*_\varepsilon(\mathbf{f}_2) = (0.25, 0.25, 0.25, 0.25)$ is the unique invariant measure of $P_\varepsilon(\mathbf{f}_2)$.

Method 2: Discount

- Discount factor β is used to differentiate between the multi- and uni-chain cases.
- For instance,
  - for Hamiltonian cycle policy $\mathbf{f}_1$

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- Further, for a noose cycle control

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$$[\mathbf{v}_\beta(\mathbf{f}_3)]_1 = 1 + 0 + 0 + \ldots\ldots = 1.$$
- Since $\beta \in [0,1)$
$$\frac{1}{1-\beta^2} > \frac{1}{1-\beta^4} > 1.$$

Randomization

- Next, consider a Markov chain induced by a (stationary) randomized control.
- The latter is an $N \times N$ matrix $\mathbf{f}$ with entries representing probabilities $f(i, a)$ of choosing a possible arc a at state i whenever this state is visited; with $f(i, a) = 0$, whenever $a \notin \mathcal{A}(i)$.
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- Hitherto, we considered only special paths which our moving object can trace out in the graph Γ. These corresponded to the subspace $\mathcal{F}_D \subset \mathcal{F}_S$ of deterministic controls.
- Passing from $\mathcal{F}_D$ to $\mathcal{F}_S$ constitutes a "continuous relaxation" of the HCP.

Example (1, cont.)

- Consider the case where $\mathbf{f}_\lambda$ is obtained from the 2-cycle deterministic control $\mathbf{f}_2$ by the "controller" randomizing at node 4 as follows. He/she chooses:
    - arc $(4, 2)$ with probability $f(4, 2) = \lambda$, and
    - arc $(4, 3)$ with probability $f(4, 3) = (1 - \lambda)$.
- The resulting policy $\mathbf{f}_\lambda$ induces a MC

$$P(\mathbf{f}_\lambda) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \lambda & (1-\lambda) & 0 \end{pmatrix}.$$

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A convex control/policy space of a MDP, or
A convex frequency space of such a process.

Optimization in the Frequency Space

- The discounted frequency space is the set

$$X_\beta := \{\mathbf{x}(\mathbf{f}) | \mathbf{f} \in \mathcal{F}_S\}$$

of vectors $\mathbf{x}(\mathbf{f})$ whose entries are defined by

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- The map M is invertible and its inverse M^{-1} is defined by

$$M^{-1}(\mathbf{x})[i,a] = f_x(i,a) := \frac{x_{ia}}{\sum_a x_{ia}}.$$

- The above discounted frequency space X_β is actually a linear polytope characterized by the transportation-like constraints:

$$\sum_{i=1}^{N}\sum_{a=1}^{N}(\delta_{ij} - \beta p(j|i,a))x_{ia} = \delta_{1j},\ \forall j = 1, \ldots, N, \quad (1)$$

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Theorem (Feinberg, 2000)

At a control $\mathbf{f}$ *that is a Hamiltonian cycle,* $\mathbf{x} = \mathbf{x}(\mathbf{f})$ *satisfies*

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- Now, let

$$W := \{\mathbf{x} | (1) - (3) \text{ hold}\} = \{\mathbf{x} | A(\beta)\mathbf{x} = \mathbf{b};\ \mathbf{x} \geq \mathbf{0}\}.$$

Theorem (Chen & Filar, 1992; Feinberg, 2000)

Let $\mathbf{x} \in W$ *be such that for all* i *and* a*:*

$$M^{-1}(\mathbf{x})[i,a] = \mathbf{f}_x(i,a) := \frac{x_{ia}}{\sum_a x_{ia}} \in \{0,1\}.$$

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- So, HCP is equivalent to feasibility problem: Find $\mathbf{x}$ satisfying:

$$\sum_{i=1}^{N}\sum_{a=1}^{N}(\delta_{ij} - \beta p(j|i,a))x_{ia} = \delta_{1j},\ j = 1,\dots,N, \tag{4}$$

$$x_{ia} \geq 0 \ \forall\ i,a, \tag{5}$$

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$$\sum_{a \in A(1)} x_{1a} = \frac{1}{1-\beta^N}, \quad (6)$$

$$(\text{\& sadly})\ \frac{x_{ia}}{\sum_{a \in A(i)} x_{ia}} \in \{0,1\}\ \forall\ i, a. \quad (7)$$

- Meanwhile, in 1998, Jean Lasserre (CNRS) and I considered a version of the original question:

Does $\exists\ \mathbf{x} \in W$ such that $M^{-1}(\mathbf{x}) = \mathbf{f}_{\mathbf{x}}$ is a HC?

- Or, equivalently, does $\exists\ \mathbf{x}$ such that

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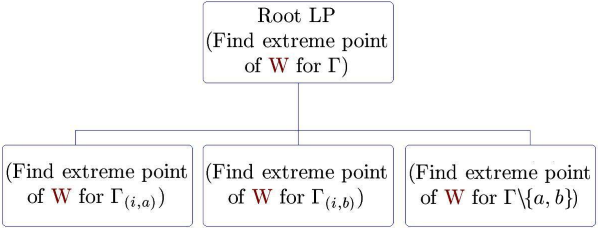
- We observed that if $\mathbf{x}$ is an extreme point of W, then either
  - $\mathbf{f_x} \in \mathcal{F}_D$ (and we're done), or
  - $\exists!$ node i and a pair of arcs $(i, a), (i, b)$ such that

$$\mathbf{f_x}(i, a)\ \&\ \mathbf{f_x}(i, b) > 0 \quad \Leftrightarrow \quad x_{ia}\ \&\ x_{ib} > 0.$$

Branch & Fix Algorithm

- Hence, we proposed - but did not implement - a "Branch & Fix" algorithm with the logical structure:



- Note that at each sub-node of this B& F tree we are solving the feasibility problem for a smaller graph.

Branch & Fix Algorithm

- However, we were suspicious that the B & F tree would grow so fast that the method would be essentially a brute force enumeration of all subgraphs of Γ (all deterministic controls).
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- The preliminary results were surprisingly good and we're beginning to understand why!

Graph	Branches	Time
Hamiltonian (24 N 72 A)	394	0:04
Dodecahedron (20 N 60 A)	65	0:01
Chess8 (64 N 336A)	1097	0:38
NH: Petersen (10 N 30 A)	154	0:01
NH: Coxeter (28 N 84 A)	41268	8:23

- Even $41,268 \ll 3^{28} = 22,876,792,454,961$; right?!

- At each sub-problem in B & F, we find an extreme point of $W = \{\mathbf{x} | A(\beta)\mathbf{x} = \mathbf{b};\ \mathbf{x} \geq \mathbf{0}\}$ for that sub-problem and check if:

$$\mathbf{f_x} \in \mathcal{F}_D \iff \frac{x_{ia}}{\sum_a x_{ia}} \in \{0, 1\} \quad \forall i, a \ ?$$

    - If answer YES, $\mathbf{f_x}$ is a HC.
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- Well, $\mathbf{f_x} \in \mathcal{F}_S$ and $\mathbf{x}$ satisfies:

$$\sum_{a \in \mathcal{A}(1)} x_{1a} = \frac{1}{1 - \beta^N}. \tag{8}$$

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- Recall the inequality (for $\beta \in [0, 1)$ and $k < N$)

$$\frac{1}{1 - \beta^k} > \frac{1}{1 - \beta^N} > 1.$$

- How does $\mathbf{f}_{\mathbf{x}} \in \mathcal{F}_S$ "fool us" and manage to satisfy (8)?

Proposition (Nguyen, 2007)

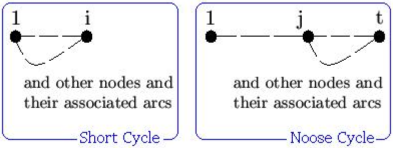
If an extreme point $\mathbf{x}$ of W induces a randomized control

$$\mathbf{f_x} \in \mathcal{F}_S \text{ and } \sum_{a \in \mathcal{A}(1)} x_{1a} = \frac{1}{1-\beta^N} \text{ holds,}$$

then $\exists$ a short-cycle control $\mathbf{f}_2$ and a noose-cycle policy $\mathbf{f}_3$ and $\lambda \in (0,1)$ such that

$$\mathbf{f_x} = \lambda \mathbf{f}_2 + (1-\lambda)\mathbf{f}_3.$$

Also, $\mathbf{f}_2$ & $\mathbf{f}_3$ coincide except at one node.



- So, perhaps, it's not so easy for $\mathbf{f_x}$ to "pretend" to be a HC......Certainly, it cannot be done by mixing just any two deterministic controls.....

A Faster Heuristic

- Here the cut frequency space is constrained further

$$
\begin{aligned}
\sum_{i=1}^{N} \sum_{a \in A(i)} (\delta_{ij} - \beta p(j|i,a))\, x_{ia} &= \delta_{1j}(1-\beta^N), \ \forall\, j, \\
\sum_{a \in A(1)} x_{1a} &= 1, \\
\text{box-constraints } \beta^{N-1} \le \sum_{a \in A(i)} x_{ia} &\le \beta, \ \forall\ i \neq 1, \\
x_{ia} &\ge 0, \ \forall\, i, a.
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- The new x_{ia}'s are the old x_{ia}'s multiplied by $(1-\beta^N)$.
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- The new x_{ia}'s are the old x_{ia}'s multiplied by $(1-\beta^N)$.
- The box-constraints can be narrowed by increasing $\beta \uparrow 1$.
- We still need

$$x_{ia} x_{ib} = 0 \quad \text{for all } i, \ \ a \ne b.$$

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A Faster Heuristic

- A recent heuristic simply searches for a feasible solution of the above using the simplex-based OPL-CPLEX.
- Preliminary results were very encouraging.
- In particular, two well known "difficult" graphs, listed on the University of Heidelberg's web site successfully solved.

Graph	Time
8x8 Knight's Tour Problem (64 nodes, 336 arcs)	1 sec
Perturbed Horton Graph (94 nodes, 282 arcs)	2 sec
20x20 Knight's Tour Problem (400 nodes, 2736 arcs)	11 min
1000-node Heidelberg Graph (1000 nodes, 3996 arcs)	24 min
2000-node Heidelberg Graph (2000 nodes, 7992 arcs)	46 hrs

- A choice of β strongly influences the numerical performance.

Optimization in the Policy Space

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Theorem (Birkhoff-von Neumann)

The set of all $N \times N$ doubly stochastic matrices is the convex hull of permutation matrices.

Theorem (Borkar, Ejov & Filar, 2004)

Given a graph and the $\varepsilon-$perturbed Markov Decision Process, let $\mathcal{DS}$ be the space of doubly stochastic controls. Define the r.v.

$$\tau_1 := \textit{ first hitting time of the home node } 1.$$

The Hamiltonian Cycle Problem reduces to "merely" minimizing the variance of τ_1, namely,

$$\min_{\mathbf{f} \in \mathcal{DS}} E_1 \left[(\tau_1 - N)^2 | \mathbf{f} \right].$$

- This is an, interesting, optimization problem that we are tackling, with Walter Murray's help, by interior point methods.
- Could (should?) it be also tackled by cross-entropy methods?

Connection with Cross-Entropy Methods

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$$\min \left\{ \gamma : \ \frac{1}{n} \sum_{j=1}^{n} \exp^{\frac{-L(\tau_j)}{\gamma}} \geq \rho \right\},$$

for a fixed ρ. Denote the initial solution by γ_1^*.

Step 2.

- Use the same n tours $\tau_1, \tau_2, \ldots, \tau_n$ associated with P_0.
- Calculate P_1^* and P_1 by applying the following equations:

$$
\begin{aligned}
p_{1,ia}^* &= \frac{\sum\limits_{1 \le j \le n : \{ia\} \in \tau_j} e^{\frac{-L(\tau_j)}{\gamma_1^*}}}{\sum_{j=1}^{n} e^{\frac{-L(\tau_j)}{\gamma_1^*}}}, \\
P_1 &= (1-\alpha) P_0 + \alpha P_1^*,
\end{aligned}
$$

where α is the smoothing parameter chosen from $(0, 1)$.

Step 3.

- Generate n new tours $\tau_1, \tau_2, \ldots, \tau_n$ from P_1.
- Repeat Step 1 and Step 2 again with P_0 and P_1^* replaced with P_1 and P_2^*, respectively.
- Denote the final solution by P_2 and the corresponding solution at stage t by P_t.

CE Algorithm

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Step 4.

- Let $\mathcal{L}_t$ denote the length of the shortest tour up to stage t.
- If for any $t > r$ and some r, say $r = 5$,

$$\mathcal{L}_t = \mathcal{L}_{t-1} = \ldots = \mathcal{L}_{t-r},$$

then repeat Step 3 and STOP, else repeat Steps 2 - 4 again.

CE Algorithm

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CE Algorithm

- Convergence: It is shown in Margolin 2005 and Costa et al 2007 that similar Cross-Entropy algorithms converge to an optimum solution in finite number of steps with probability one.
- However, it is possible that the stopping criterion of Step 4 may require many iterations to satisfy.
- Is it possible that some insights from preceding results could be used in conjunction with this CE algorithm?

Nexus Between HCP and CE

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Since - for the HCP - not all arcs are available in a given graph, we "fill-it-in" with artificial arcs that have sufficiently high costs that they will be identifiable.

So, we solve a "TSP" and claim that the graph is (very likely) non-Hamiltonian, if the minimal tour is "too long".

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- Insert artificial arcs to make the given graph a complete one with no self-loops.

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$$\begin{cases} l_{ia} \sim U(0, \omega), & \text{if } (i, a) \text{ is an authentic arc,} \\ l_{ia} \sim U(\mu, \mu + \sigma), & \text{otherwise.} \end{cases}$$
Here, $\omega, \mu,$ and σ are arbitrary positive real numbers and the only restriction is $\omega \ll \mu$.

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Here, $\omega, \mu,$ and σ are arbitrary positive real numbers and the only restriction is $\omega \ll \mu$.
- Since all the lengths are generated from some continuous distributions, the total length $L(\tau)$ of a typical tour τ is a continuous random variable.

- Hence, for two distinct tours τ_i and τ_j, we will have
$$\Pr(L(\tau_i) = L(\tau_j)) = 0.$$

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- Set up the initial transition probability matrix as below:

$$p_{0,ia} := \begin{cases} \frac{1}{|A(i)|} - \frac{N-1-|A(i)|}{|A(i)|}\varepsilon, & \text{if } (i,a) \text{ is an authentic arc,} \\ \varepsilon, & \text{otherwise.} \end{cases}$$

Here, $\varepsilon > 0$ and is sufficiently small.

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$$t := t + 1.$$

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- Construct updated matrix P_t with the best m generated tours as in Step 2 of the CE algorithm.
- If t is "large enough" AND P_t is "not close enough" to being Hamiltonian, STOP; and claim that the graph is (likely) non-Hamiltonian.

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- If Γ^* is a tour, the original graph is Hamiltonian.
- If Γ^* is not a tour, return to Step 1 and update the transition matrix.

Numerical Results

- Many Hamiltonian graphs in the range of $6 - 324$ nodes have been tested with the above algorithm. In all cases, Hamiltonian cycles were found.

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- Many Hamiltonian graphs in the range of $6 - 324$ nodes have been tested with the above algorithm. In all cases, Hamiltonian cycles were found.

- When the size of graph was small, say less than 50 nodes, often termination occurred in Step 2 by generating a Hamiltonian cycle randomly.

- However, for the larger graphs, in most tests, the algorithm terminated in Step 4 by solving the proposed LP model.

Theoretical Explanation

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- Let Λ_t be a transition matrix (obtained from P_t by suitable adjustment) comprising of values of λ_{ia} at iteration t, that is, coefficients of objective function of the linear program proposed in the Step 4.

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- Let Λ_t be a transition matrix (obtained from P_t by suitable adjustment) comprising of values of λ_{ia} at iteration t, that is, coefficients of objective function of the linear program proposed in the Step 4.
- Consider Λ^* as the coefficient matrix associated with a deterministic policy that corresponds to θ^*, that is, elements of Λ^* which coincide with the arcs in θ^* are equal to 1 and the others are equal to 0.

Theoretical Explanation

Proposition

There exists $\delta > 0$ such that, if $\|\Lambda_t - \Lambda^*\| \leq \delta$, then an optimal solution of the linear program given in Step 4 is associated with a deterministic policy corresponding to the shortest tour θ^*.

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Corollary

It can be shown that depending on the graph structure and for β near 1 that,

$$O(N^{-1}) \leq \delta \leq \frac{3}{7}.$$

Finally: Is HCP's NP-completeness an "anomaly"?

- For 18-node cubic graphs of which 39, 635 are Hamiltonian and 1, 666 are non-Hamiltonian ($t = 20$)