Recovering a Hidden Hamiltonian Cycle via Linear Programming

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Joint work with
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Mathematical problem: Hidden Hamiltonian cycle model

- Observe: a weighted undirected complete graph on \( n \) vertices with weighted adjacency matrix \( W \)
- Latent: a Hamiltonian cycle \( C^* \)
- Edge weight

\[
W_{e \text{ ind.}} \sim \begin{cases} 
  P & e \in C^* \\
  Q & e \notin C^*
\end{cases}
\]
Mathematical problem: Hidden Hamiltonian cycle model

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  \[ W_{e \text{ ind.}} \sim \begin{cases} 
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- Goal: observe $W$, recover $C^*$ with high probability
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• Goal: observe $W$, recover $C^*$ with high probability

Remarks:
• $P, Q$ depends on the graph size $n$
• For this talk, $Q = N(0, 1)$ and $P = N(\mu, 1)$, so that

\[ W = \mu \cdot \text{adj matrix of } C^* + \text{noise} \]

“signal”

• Hidden Hamiltonian cycle planted in Erdös-Rényi graph

[Broder-Frieze-Shamir '94]
1. Reconstitute chromatin in vitro upon naked DNA
2. Produce cross-links by fixing chromatin with formaldehyde

Chicago datasets generate cross-links among contigs [Putnam et al. '16]

On average more cross-links exist between adjacent contigs
Ordering DNA contigs with Chicago cross-links

Reduces to traveling salesman problem (TSP)

Find a path (tour) that visits every contig exactly once with the maximum number of cross-links

DNA Scaffolding

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Ordering DNA contigs with Chicago cross-links

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Key challenges for DNA scaffolding with Chicago data

- Computational: TSP is NP-hard in the worst-case
- Statistical: spurious cross-links between contigs that are far apart
Key challenges for DNA scaffolding with Chicago data

- Computational: TSP is NP-hard in the worst-case
- Statistical: spurious cross-links between contigs that are far apart

Key questions:

- How to efficiently order hundreds of thousands of contigs?
- How much noise can be tolerated for accurate DNA scaffolding?
Mathematical model for DNA scaffolding

Chicago dataset [Putnam et al. '16]
Mathematical model for DNA scaffolding

Chicago dataset [Putnam et al. '16]
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Chicago dataset [Putnam et al. '16]

Simulated Poisson data
Mathematical model for DNA scaffolding

Chicago dataset [Putnam et al. ’16]  
Simulated Poisson data
Maximum likelihood estimator reduces to TSP

\[ \hat{X}_{TSP} = \arg \max_X \langle L, X \rangle \]

s.t. \( X \) is the adjacency matrix of some Hamiltonian cycle

where \( L \) is the log likelihood ratio matrix \( L_{ij} = \log \frac{dP}{dQ}(W_{ij}) \). For Gaussian or Poisson, simply take \( L = W \).
What is known information-theoretically

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**Theorem (Sharp threshold)**

- If \( \mu^2 < 4 \log n \), exact recovery is information-theoretically impossible
- If \( \mu^2 > 4 \log n \), MLE succeeds in exact recovery
What is known algorithmically

- **Spectral methods** fails miserably:
  - $\mu \gg n^{2.5}$ (spectral gap of cycle is too small)
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- **Thresholding**:
  - $\mu > \sqrt{8 \log n}$

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Recovery Threshold for TSP LP
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- **Thresholding**:
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- **Greedy merging** [Motahari-Bresler-Tse '13]:
  - $\mu > \sqrt{6 \log n}$
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- **Greedy merging** [Motahari-Bresler-Tse '13]: 
  - $\mu > \sqrt{6 \log n}$
- **This talk**: **linear programming** achieves sharp threshold

\[
\begin{align*}
\frac{\mu^2}{\log n} > 4 : & \quad \text{LP succeeds} \\
\frac{\mu^2}{\log n} < 4 : & \quad \text{Everything fails}
\end{align*}
\]
In general

Threshold are determined by Rényi divergence of order $\rho > 0$ from $P$ to $Q$:

$$D_\rho(P\|Q) \triangleq \frac{1}{\rho - 1} \log \int (dP)^\rho (dQ)^{1-\rho}.$$

- LP works when

$$D_{1/2}(P\|Q) - \log n \to \infty$$

optimal under mild assumptions
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- LP works when
  $$D_{1/2}(P\|Q) - \log n \to \infty$$
  optimal under mild assumptions
- Thresholding works when
  $$D_{1/2}(P\|Q) - 2 \log n \to \infty$$
- Greedy works when
  $$D_{1/3}(Q\|P) - \log n \to \infty$$
Convex relaxations of TSP
\[ \hat{X}_{\text{TSP}} = \arg \max_X \langle W, X \rangle \]

s.t. \[ \sum_j X_{ij} = 2, \ \forall i \]
\[ X_{ij} \in \{0, 1\} \]
\[ \sum_{i \in I, j \notin I} X_{ij} \geq 2, \ \forall \emptyset \neq I \subset [n] \]
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- The last constraint: subtour elimination
\[ \hat{X}_{\text{SUB}} = \arg \max_X \langle W, X \rangle \]

s.t. \[ \sum_j X_{ij} = 2, \quad \forall i \]
\[ X_{ij} \in [0, 1] \]
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- Replacing the integrality constraint with box constraint: \textbf{SUBTOUR LP} relaxation [Dantzig-Fulkerson-Johnson '54, Held-Karp '70]
- Exponentially many linear constraints, nevertheless solvable using interior point method
\[ \hat{X}_{F2F} = \arg \max_{X} \langle W, X \rangle \]

\[
\text{s.t. } \sum_{j} X_{ij} = 2, \quad \forall i
\]

\[ X_{ij} \in [0, 1] \]

- Further dropping subtour elimination constraints \( \implies \) Fractional 2-factor (F2F) LP
\[ \hat{X}_{F2F} = \arg \max_X \langle W, X \rangle \]

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- Further dropping subtour elimination constraints \( \implies \) Fractional 2-factor (F2F) LP
- Extensively studied in worst case [Boyd-Carr '99, Schalekamp-Williamson-van Zuylen '14]
  - The integrality gap \( \frac{2F}{F_{2F}} \leq \frac{4}{3} \) for metric TSP (min formulation)
\[ \hat{X}_{\text{F2F}} = \arg \max_X \langle W, X \rangle \]

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  - The integrality gap \(\frac{2F}{F_{\text{F2F}}} \leq \frac{4}{3}\) for metric TSP (min formulation)
- What is the integrality gap whp in our random instance?
Theorem

If $\mu^2 - 4 \log n \to \infty$, then $\hat{X}_{F2F} = X^*$ with high probability.
Optimality of Fractional 2-Factor LP

Theorem

If $\mu^2 - 4 \log n \to \infty$, then $\hat{X}_{F2F} = X^*$ with high probability.

Remarks

- The integrality gap is 1 whp!
- Achieving the IT-limit $\mu^2 = 4 \log n$
Max-Product Belief Propagation

\[ m_{i \rightarrow j}(t) = w_{ij} - 2\text{nd max}_{\ell \neq j} \{ m_{\ell \rightarrow i}(t - 1) \} \]

\[ m_{i \rightarrow j}(0) = w_{ij} \]

After \( T \) iterations, for each vertex \( i \), keep the two largest incoming messages \( m_{\ell \rightarrow i}(T) \) and delete the rest.

- BP is exact provided the solution is integral [Bayati-Borgs-Chayes-Zecchina '11]
- It can be shown that \( T = O(n^2 \log n) \) whp
SDP relaxations for TSP

Add more constraints to F2F LP

- SDP1 [Cvetković et al ’99]: PSD constraint based on second largest eigenvalue of cycle

\[
X \preceq \frac{2}{n} J + 2 \cos \frac{2\pi}{n} \left( I - \frac{1}{n} J \right)
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SDP relaxations for TSP

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- provably weaker than Subtour LP [Goemans-Rendl ’00]
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- **SDP2** [Zhao et al '98]: Quadratic Assignment Problem

  \[
  \langle W, X \rangle = \langle W, \Pi X_0 \Pi^T \rangle = \left\langle W \otimes X_0, \text{vec}(\Pi)\text{vec}(\Pi)^T \right\rangle
  \]

  \(\text{fixed cycle}\)

  \(\text{relax..}\)
SDP relaxations for TSP

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\[ \langle W, X \rangle = \langle W, \Pi X_0 \Pi^\top \rangle = \left\langle W \otimes X_0, \text{vec}(\Pi)\text{vec}(\Pi)^\top \right\rangle \]

- decision variable: \( n^2 \times n^2 \) matrix
- provably stronger than SDP1 [de Klerk et al '08]
Different relaxations

F2F LP succeeds $\implies$ all other relaxations succeed.

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Theoretical analysis of convex relaxation
Primal approach vs Dual approach: high level

- **Dual argument:**
  - Construct *dual witness* that certify the ground truth whp (KKT conditions)

- **Primal argument:**
  - No feasible solution other than the ground truth has a better objective value whp
  - Key: for LP, can restrict to extremal points (vertices of the feasible polytope)
Primal approach vs Dual approach: high level

• **Dual argument:**
  ▶ Construct dual witness that certify the ground truth whp (KKT conditions)
  ▶ Successful in proving SDP relaxation attaining sharp threshold for graph partitions: community detection, densest subgraph, etc
  [Abbe-Bandeira-Hall ’14, Hajek-W-Xu ’14,’15, Bandeira ’15, Perry-Wein ’15]
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Dual approach

- KKT conditions (Farkas’ lemma): $\hat{X}_{F2F} = X^* \iff \exists u \in \mathbb{R}^n$ (dual certificate):
  
  $u_i + u_j \leq W_{ij}$, for $i \sim j$ in $C^*$
  
  $u_i + u_j \geq W_{ij}$, for $i \not\sim j$ in $C^*$
Dual approach

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- One feasible choice of dual:
  
  $$
  u_i = \frac{1}{2} \min \{W_{ij} : j \sim i\}
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Dual approach

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• One feasible choice of dual:

$$u_i = \frac{1}{2} \min \{ W_{ij} : j \sim i \}$$

• This certificate shows correctness if $\mu^2 > 6 \log n$ (same as greedy merging)
Planted Hamiltonian cycle model with Gaussian weights $(n = 1000)$

- **F2F**
- **Belief Propagation**
- **Greedy Merging**
- **Simple Thresholding**

- **Simple Thresholding limit:** $\mu^2 = 8 \log n$
- **Merge greedy limit:** $\mu^2 = 6 \log n$
- **IT limit:** $\mu^2 = 4 \log n$
Primal approach

• Show whp for all extremal points $X \neq X^*$:

$$\langle W, X \rangle < \langle W, X^* \rangle$$

• F2F polytope:

$$\left\{ X \in [0, 1]^{n \times n} : \sum_{j=1}^{n} X_{ij} = 2 \right\}$$

• The proof heavily exploits the characterization of extremal points

▶ F2F polytope is not integral: fractional vertices exist

▶ Characterization [Balinski '65]: for any vertex $X$ of F2F polytope

• Half integrality $X_{ij} \in \{0, \frac{1}{2}, 1\}$

• $\frac{1}{2}$'s form disjoint odd cycle connected by path of $1$'s.
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    • $1/2$'s form disjoint odd cycle connected by path of 1's.
Why half integral?

Usual proofs:

- combinatorial proof [Lovasz-Plummer ’86, Schrijver ’04]
- linear-algebraic proof
  - F2F polytope (in adjacency vector):
    \[
    \{ x \in \mathbb{R}^{(n \choose 2)} : Ax = 21 \}
    \]
  - $A$ is $n \times \binom{n}{2}$ zero-one matrix: $A_{ie} = 1_{\{i \in e\}}$
  - Each column of $A$ has exactly two 1’s
Extremal feasible solution $x$ is of the following form

$$x = \left( \begin{array}{c} x_S \\ x_{S^c} \end{array} \right)$$

for some $S \subset \binom{n}{2}$ of size $n$, where
- $x_S$ is the solution to the following linear system:

$$A_S x_S = b'$$

Cramer's rule:

$$x_S^i = \frac{\text{det}(A_S(i))}{\text{det}(A_S)}$$

where $A_S(i)$ is obtained by substituting the $i$th column by $b'$, hence $\text{det}(A_S(i)) \in \mathbb{Z}$. 

$\Rightarrow$ Each column of $A_S$ has two 1's
Why half integral?

Extremal feasible solution $x$ is of the following form

$$x = (\underline{x_S}, \underline{x_{Sc}})$$

for some $S \subset \binom{[2]}{n}$ of size $n$, where

- $x_S$ is the solution to the following linear system:

$$A_S x_S = b'$$

- Cramer’s rule:

$$(x_S)_i = \frac{\det(A_S^{(i)})}{\det(A_S)}$$

- $A_S^{(i)}$ is obtained by substituting the $i$th column by $b'$, hence $\det(A_S^{(i)}) \in \mathbb{Z}$.

- Each column of $A_S$ has two 1’s $\implies \det(A_S) \in \{0, \pm 1, \pm 2\}$ [Balinski '65]
Proof of correctness for F2F LP
Encode the solution: for any extremal point $X$, represent $2(X - X^*)$ as a bicolored multigraph $G_X$

$$w(G_X) = \langle W, 2(X - X^*) \rangle$$
Proof Outline

1. **Encode the solution**: for any extremal point $X$, represent $2(X - X^*)$ as a bicolored multigraph $G_X$

   $$w(G_X) = \langle W, 2(X - X^*) \rangle$$

2. **Divide and conquer**: decompose $G_X$ as edge-disjoint union of graphs in some family $\mathcal{F}$

   $$w(G_X) = \sum_i w(F_i), \quad F_i \in \mathcal{F}$$
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$$w(G_X) = \sum_i w(F_i), \quad F_i \in \mathcal{F}$$

3. **Counting**: Show that whp $w(F) < 0$ for all $F \in \mathcal{F}$
Step 1: Bicolored multigraph representation

\[ X^* : \text{true cycle} \]
Step 1: Bicolored multigraph representation

$X$: extremal solution
Step 1: Bicolored multigraph representation

\[ \frac{1}{2} \]

X: extremal solution

\[ G_X \]
Step 1: Bicolored multigraph representation

\[ X: \text{extremal solution} \]

\[ G_X \]

**key observation**

\( G_X \) is always balanced: red degree = blue degree
Step 2: Edge decomposition

Theorem (Kotzig ’68)

Every connected balanced bicolored multigraph has an alternating Eulerian circuit.

Remarks

- An Eulerian circuit may traverse a double edge twice
- "Dumbbell" structure
Step 2: Edge decomposition

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“Dumbbell” structure
Step 2: Edge decomposition

\[ U \]: collection of graphs recursively constructed

1. Start with an even cycle in alternating colors

2. **Blossoming procedure**: At each step, contract an edge in any cycle and attach a flower (path of double edges followed by an alternating odd cycle)

Obtained by starting with an 10-cycle and blossoming 4 times
Step 2: Edge decomposition

\( \mathcal{U} \): collection of graphs recursively constructed

1. Start with an even cycle in alternating colors

2. **Blossoming procedure**: At each step, contract an edge in any cycle and attach a **flower** (path of double edges followed by an alternating odd cycle)

Obtained by starting with an 10-cycle and blossoming 4 times

However, not every \( G_X \) is of this form...
• Graph homomorphism $\phi : H \rightarrow F$ is a vertex map that preserves edges and edge multiplicity
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\[
\begin{array}{cccc}
1 & 2 & 9 & 10 \\
3 & 11 & 8 & 7 \\
4 & 12 & 6 & 5 \\
\end{array}
\xrightarrow{\phi}
\begin{array}{cccc}
1 & 2 & 9 & 10 \\
3 & 4 & 8 & 7 \\
4 & 1 & 6 & 5 \\
\end{array}
\]

**Lemma (Decomposition)**

Every balanced bicolored multigraph $G$ with edge multiplicity at most 2 can be decomposed as an union of elements in

\[
\mathcal{F} = \{ F : V(F) \subset [n], H \rightarrow F \text{ for some } H \in \mathcal{U} \}
\]

\[
\begin{array}{cccc}
1 & 2 & 5 \\
4 & 3 & 6 \\
\end{array}
\xrightarrow{\text{decompose}}
\begin{array}{cccc}
1 & 2 & 2 & 5 \\
4 & 3 & 3 & 6 \\
\end{array}
\]
• Graph homomorphism $\phi : H \rightarrow F$ is a vertex map that preserves edges and edge multiplicity

```
1  9  10  5
3  8  7  6

H

1  9  10  5
3  8  7  6

F

\phi
```

**Lemma (Decomposition)**

*Every balanced bicolored multigraph $G$ with edge multiplicity at most 2 can be decomposed as an union of elements in*

$$\mathcal{F} = \{ F : V(F) \subset [n], H \rightarrow F \text{ for some } H \in \mathcal{U} \}$$

```
1  2  5
4  3  6

decompose

1  2  2  5
4  3  3  6
```

• It remains to show $\min_{F \in \mathcal{F}} w(F) < 0$ whp
Step 3: Counting

\[ \mathcal{F}_{k,\ell} = \{ F \in \mathcal{F} : E(F) \text{ consists of } k \text{ double edges and } \ell \text{ single edges} \} \]

**Lemma (Counting isomorphism classes)**

The number of distinct \( H \in \mathcal{U} \) with \( k \) double edges and \( \ell \) single edges is at most \( C^{k+\ell} \) for universal constant \( C \).

**Lemma (Counting homomorphisms)**

For each \( H \in \mathcal{U} \), there exists \( 0 \leq r \leq \ell/2 \)

- **Number of labelings for double edges:**

  \[ \leq (Cn)^{k/2+r/2} \]

- **Number of labelings for single edges conditioned on double edges**

  \[ \leq (Cn)^{\ell/2-r} \]
Step 4: Probabilistic arguments

\[ \mathcal{F}_{k,\ell} = \{ F \in \mathcal{F} : E(F) \text{ consists of } k \text{ double edges and } \ell \text{ single edges} \} \]

**Lemma**

For any \( k \geq 0 \) and \( \ell \geq 3 \). With probability at least \( 1 - n^{-\Theta(k+\ell)} \),

\[
\max_{F \in \mathcal{F}_{k,\ell}} (w(F) - \mathbb{E}[w(F)]) \leq (1 + \epsilon) (2k + \ell) \sqrt{\log n}
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**Remarks**

- Total: \( 2k + \ell \) edges, half red half blue. Weights on red edges \( \sim N(\mu, 1) \). Weights on blue edges \( \sim N(0, 1) \).

\[ w(F) \sim N(- (k + \ell/2)\mu, 4k + \ell) \]

- Proof: Counting \( \mathcal{F}_{k,\ell} \) and large deviation bounds
Real-data experiment

- 1000 DNA contigs of size 100 kbps
- 0.45 million Chicago cross-links
- Subsample each cross-link with probability $p$
Homosapiens [Putnam et al 16, Genome Research]
Aedes Aegypti (zika mosquito) [Dudchenko et al '16, Science]
Conclusion and remarks

\[ \mu^2 / \log n \]

- IT limit/F2F
- greedy
- thresholding

References
Conclusion and remarks

\[ \mu^2 / \log n \]

4 
IT limit/F2F

6 
greedy

8 
thresholding

Future work

- More realistic models
  - 2-NN graph: IT limit becomes \( \sqrt{2 \log n} \) not achieved by LP.

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4 \hspace{1cm} 6 \hspace{1cm} 8 \hspace{1cm} \mu^2 / \log n

IT limit/F2F \hspace{1cm} greedy \hspace{1cm} thresholding

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- More realistic models
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References

- Yihong Wu (Yale) Recovery Threshold for TSP LP
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Future work
- More realistic models
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References
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\[ \mu^2 / \log n \]

4 \hspace{2cm} 6 \hspace{2cm} 8

IT limit/F2F \hspace{2cm} greedy \hspace{2cm} thresholding

Future work

- More realistic models
  - 2-NN graph: IT limit becomes \( \sqrt{2 \log n} \) not achieved by LP.
  - small-world graphs
- Smarter rounding algorithm in practice
- Reduction from/to Hamiltonian cycle and path more elegantly

References


Yihong Wu (Yale)

Recovery Threshold for TSP LP