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

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

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- Goal: observe $W$, recover $C^*$ with high probability
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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"
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
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Key challenges for DNA scaffolding with Chicago data

- Computational: TSP is NP-hard in the \textit{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

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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
What is known information-theoretically

Maximum likelihood estimator reduces to TSP

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

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 \( L = W \).
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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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- **Thresholding**:
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- **Greedy merging** [Motahari-Bresler-Tse '13]:
  - $\mu > \sqrt{6 \log n}$
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- **This talk**: **linear programming** achieves sharp threshold

\[
\frac{\mu^2}{\log n} > 4 : \quad \text{LP succeeds} \\
\frac{\mu^2}{\log n} < 4 : \quad \text{Everything fails}
\]
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. \[ \sum_{j} X_{ij} = 2, \ \forall i \]

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

\[ \sum_{i \in I, j \notin I} X_{ij} \geq 2, \ \forall \emptyset \neq I \subset [n] \]
Integer Linear Programming reformulation of TSP

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

subject to:
\[ \sum_{j} X_{ij} = 2, \ \forall i \]
\[ X_{ij} \in \{0, 1\} \]
\[ \sum_{i \in I, j \notin I} X_{ij} \geq 2, \ \forall \emptyset \neq I \subset [n] \]

- The last constraint: subtour elimination
\[ \hat{X}_{\text{SUB}} = \arg \max_X \langle W, X \rangle \]

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

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

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

- Further dropping subtour elimination constraints \[ \rightarrow \text{Fractional 2-factor (F2F) LP} \]
\[ \hat{X}_{F2F} = \arg \max_X \langle W, X \rangle \]
\[ \text{s.t. } \sum_j X_{ij} = 2, \forall i \]
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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)
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- Extensively studied in worst case \([\text{Boyd-Carr '99, Schalekamp-Williamson-van Zuylen '14}]\)
  - The integrality gap \( \frac{2F}{F_{2F}} \leq \frac{4}{3} \) for metric TSP (min formulation)
- What is the integrality gap whp in our random instance?
Optimality of Fractional 2-Factor LP

**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 \( \mu^2 - 4 \log n \rightarrow \infty \), 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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- **SDP2** [Zhao et al '98]: Quadratic Assignment Problem

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

fixed cycle

relax..
SDP relaxations for TSP

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  \[ \langle W, X \rangle = \langle W, \Pi X_0 \Pi^\top \rangle = \langle W \otimes X_0, \text{vec}(\Pi)\text{vec}(\Pi)^\top \rangle \]
  
  ▶ decision variable: \( n^2 \times n^2 \) matrix
  ▶ provably stronger than SDP1 [de Klerk et al '08]
Different relaxations

F2F LP

Subtour LP

TSP

SDP 2

SDP 1

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

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Recovery Threshold for TSP LP
- **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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- **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)
Dual approach

- KKT conditions (Farkas’ lemma): \( \hat{X}_{F2F} = X^* \iff \exists u \in \mathbb{R}^n \) (dual certificate):

\[
\begin{align*}
u_i + u_j & \leq W_{ij}, \quad \text{for } i \sim j \text{ in } C^* \\
u_i + u_j & \geq W_{ij}, \quad \text{for } i \not\sim j \text{ in } C^*
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- One feasible choice of dual:

  $$u_i = \frac{1}{2} \min\{W_{ij} : j \sim i\}$$
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- This certificate shows correctness if $\mu^2 > 6 \log n$ (same as greedy merging)
Synthetic data experiment

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
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  ▶ F2F polytope is not integral: fractional vertices exist
  ▶ Characterization [Balinski ’65]: for any vertex $X$ of F2F polytope
    • Half integrality
      $$X_{ij} \in \{0, 1/2, 1\}$$
Primal approach

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    • 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):
    \[
    \{ x \in \mathbb{R}^{(\binom{n}{2})} : Ax = 21 \}
    \]
    - \( A \) 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

$$x = (\underbrace{x_S}_{\text{fractional}}, \underbrace{x_{Sc}}_{\text{integral}})$$

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

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

$$A_S x_S = b'$$
Why half integral?

Extremal feasible solution $x$ is of the following form

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

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:

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

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

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

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

$$w(G_X) = \sum_i w(F_i), \quad F_i \in \mathcal{F}$$
1. **Encode the solution**: for any extremal point $X$, represent $2(X - X^*)$ as a bicolored multigraph $G_X$

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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

$X^*$: true cycle

$G_{X}^*$ is always balanced: red degree = blue degree
Step 1: Bicolored multigraph representation

$X$: extremal solution

$G_X$ is always balanced: red degree = blue degree
Step 1: Bicolored multigraph representation

$X$: extremal solution

$G_X$
Step 1: Bicolored multigraph representation

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

**key observation**

\[ G_X \text{ is always balanced: red degree } = \text{ blue degree} \]
Theorem (Kotzig ’68)

Every connected balanced bicolored multigraph has an alternating Eulerian circuit.
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

\( \mathcal{U} \): 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
Step 2: Edge decomposition

$\mathcal{U}$: collection of graphs recursively constructed

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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.

\begin{align*}
\begin{array}{c}
1 \quad 9 \quad 10 \quad 5 \\
\text{3} & \quad \text{8} & \quad \text{7} & \quad \text{6} \\
\end{array}
\end{align*}

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$H$ \quad $F$
Graph homomorphism $\phi : H \to F$ is a vertex map that preserves edges and edge multiplicity.

Lemma (Decomposition)

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

$$\mathcal{F} = \{ F : V(F) \subset [n], H \to F \text{ for some } H \in \mathcal{U} \}$$
Graph homomorphism $\phi : H \rightarrow F$ is a vertex map that preserves edges and edge multiplicity.

**Lemma (Decomposition)**

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

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

*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 \( 1 - n^{-\Theta(k+\ell)} \),

\[ \max_{F \in \mathcal{F}_{k,\ell}} \left( w(F) - \mathbb{E}[w(F)] \right) \leq (1 + \epsilon) (2k + \ell) \sqrt{\log n} \]
Step 4: Probabilistic arguments

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**Lemma**

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

**Remarks**

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

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

- 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


Yihong Wu (Yale)
Conclusion and remarks

Future work

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

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  - small-world graphs
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- More realistic models
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  - small-world graphs
- Smarter rounding algorithm in practice

References

Yihong Wu (Yale) Recovery Threshold for TSP LP
Conclusion and remarks

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

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