Recovering a Hidden Hamiltonian Cycle via Linear Programming

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Joint work with
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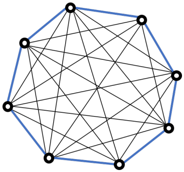
Mathematical problem: Hidden Hamiltonian cycle model

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

$$W_e \overset{\text{ind.}}{\sim} \begin{cases} P & e \in C^* \\ Q & e \notin C^* \end{cases}$$



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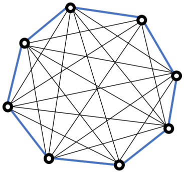

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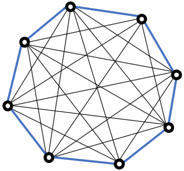

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Remarks:

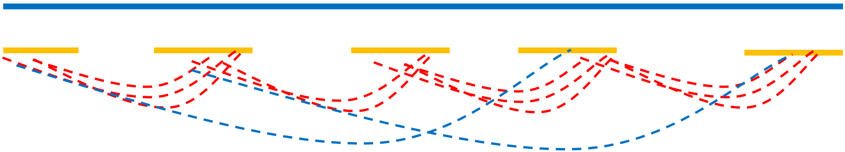
- P, Q depends on the graph size n
- For this talk, $Q = N(0,1)$ and $P = N(\mu, 1)$, so that

$$W = \mu \cdot \underbrace{\text{adj matrix of } C^*}_{\text{“signal”}} + \text{noise}$$

- Hidden Hamiltonian cycle planted in Erdös-Rényi graph [Broder-Frieze-Shamir '94]

Link information in Chicago datasets

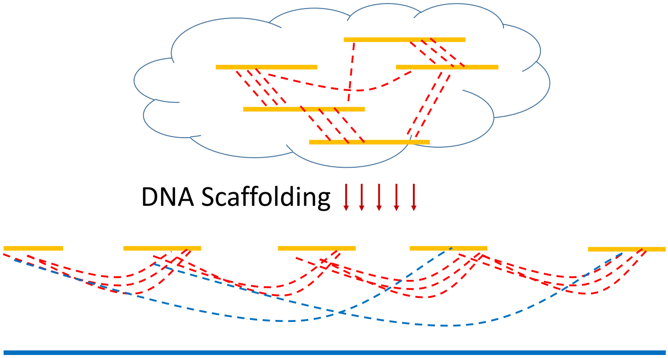
1. Reconstitute chromatin in vitro upon naked DNA
2. Produce cross-links by fixing chromatin with formaldehyde



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



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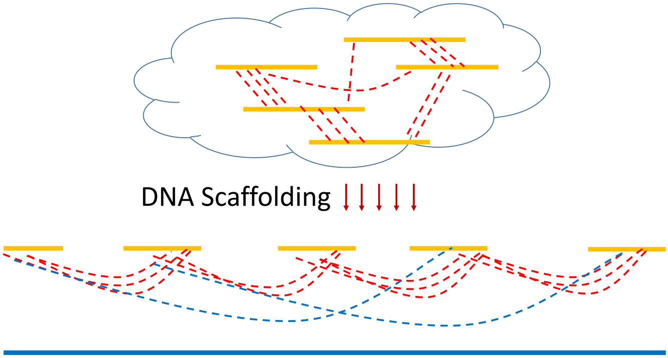

Reduces to traveling salesman problem (TSP)

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

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

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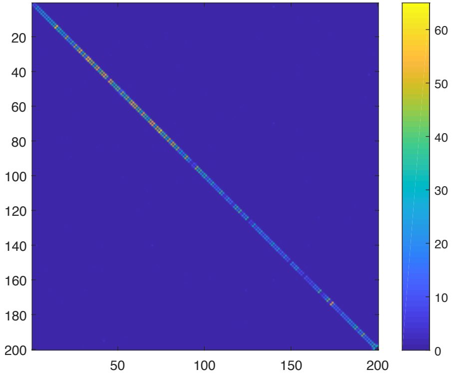
Key questions:

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

Mathematical model for DNA scaffolding



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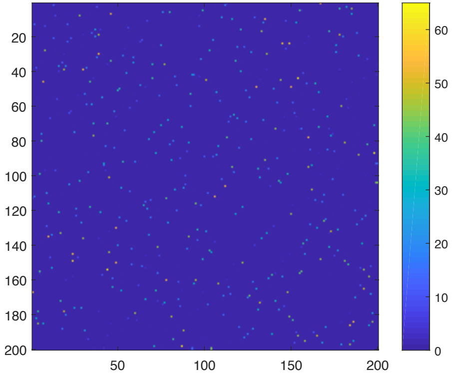

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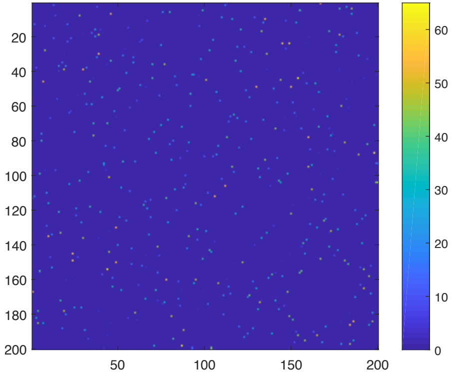

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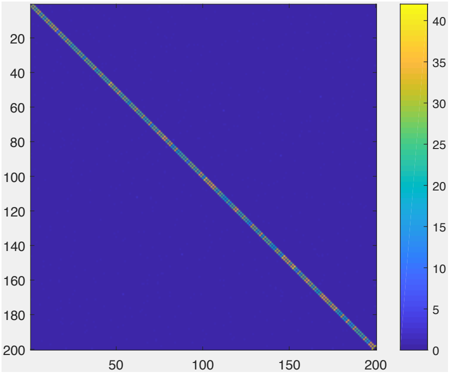
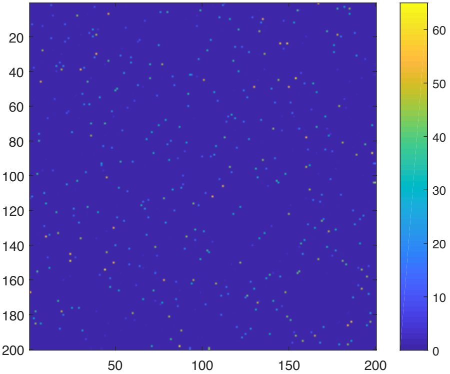


Simulated Poisson data

Mathematical model for DNA scaffolding



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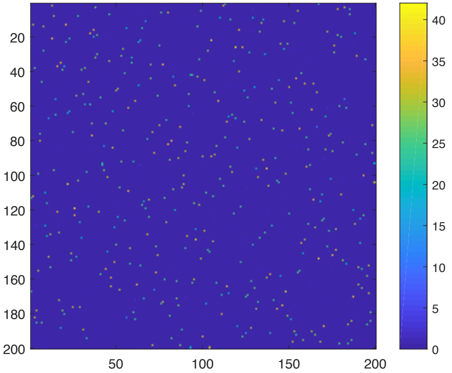

Simulated Poisson data

What is known information-theoretically

Maximum likelihood estimator reduces to TSP

$$\widehat{X}_{\mathrm{TSP}} = \arg\max_{X} \ \langle L, X \rangle$$
$$\text{s.t.} \quad X \text{ is the adjacency matrix of some Hamiltonian cycle}$$

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

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- Spectral methods fails miserably:
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- This talk: **linear programming** achieves sharp threshold

$\frac{\mu^2}{\log n} > 4:$	LP succeeds
$\frac{\mu^2}{\log n} < 4:$	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

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

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- 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

Integer Linear Programming reformulation of TSP

$$
\begin{aligned}
\widehat{X}_{\mathrm{TSP}} = \arg\max_{X} \; & \langle W, X \rangle \\
\text{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

Subtour LP

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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

F2F LP

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- Extensively studied in worst case [Boyd-Carr '99,Schalekamp-Williamson-van Zuylen '14]
  - The integrality gap $\frac{\text{2F}}{\text{F2F}} \leq \frac{4}{3}$ for metric TSP (min formulation)

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  - The integrality gap $\frac{\mathrm{2F}}{\mathrm{F2F}} \leq \frac{4}{3}$ 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* $\widehat{X}_{\mathrm{F2F}} = X^*$ *with high probability.*

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Remarks

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

Belief propagation

Max-Product Belief Propagation

$$m_{i\to j}(t) = w_{ij} - \underset{\ell\neq j}{\text{2nd}\max}\{m_{\ell\to i}(t-1)\}$$

$$m_{i\to j}(0) = w_{ij}$$

After T iterations, for each vertex i, keep the two largest incoming messages $m_{\ell\to i}(T)$ 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

$$\langle W, X\rangle = \langle W, \Pi \underbrace{X_0}_{\substack{\text{fixed}\\\text{cycle}}} \Pi^\top\rangle = \left\langle W \otimes X_0, \underbrace{\text{vec}(\Pi)\text{vec}(\Pi)^\top}_{\text{relax..}}\right\rangle$$

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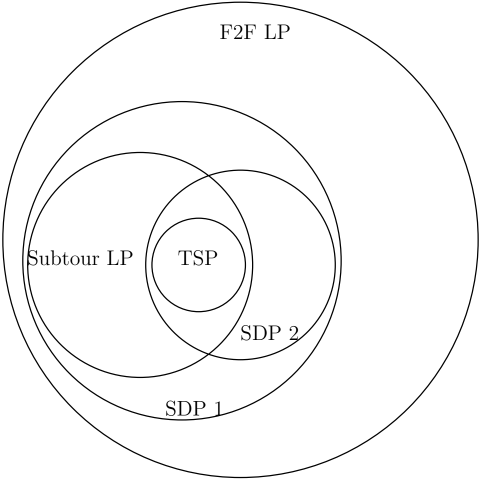
  - decision variable: $n^2 \times n^2$ matrix
  - provably stronger than SDP1 [de Klerk et al '08]

Different relaxations



F2F LP succeeds $\Longrightarrow$ all other relaxations succeeed.

Theoretical analysis of convex relaxation

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- Dual argument:
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  - Key: for LP, can restrict to **extremal points** (vertices of the feasible polytope)

Dual approach

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

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u_i + u_j &\le W_{ij}, &\quad \text{for } i \sim j \text{ in } C^* \\
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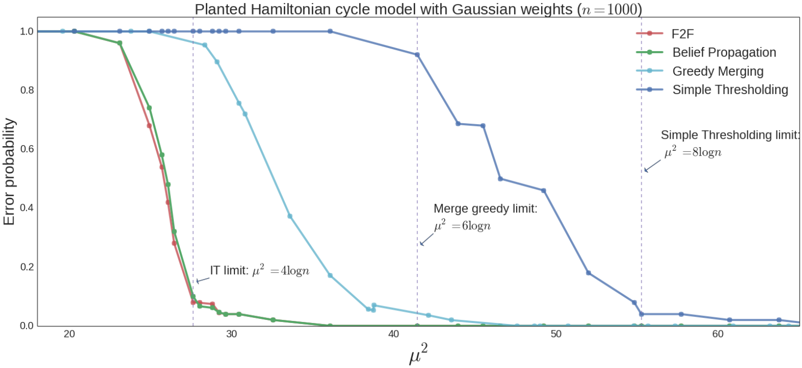
- This certificate shows correctness if $\mu^2 > 6 \log n$ (same as greedy merging)

Synthetic data experiment



Primal approach

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

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- F2F polytope:

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

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  - Characterization [Balinski '65]: for any vertex X of F2F polytope
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Why half integral?

Usual proofs:

- combinatorial proof [Lovasz-Plummer '86, Schrijver '04]
- linear-algebraic proof
  - F2F polytope (in adjacency vector):

$$\{x \in \mathbb{R}^{\binom{n}{[2]}} : Ax = 2\mathbf{1}\}$$

  - A is $n \times \binom{n}{2}$ zero-one matrix: $A_{ie} = \mathbf{1}_{\{i \in e\}}$
  - Each column of A has exactly two 1's

Why half integral?

Extremal feasible solution x is of the following form

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

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

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- Cramer's rule:

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

  - $A_S^{(i)}$ is obtained by substituting the ith colum 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

Proof Outline

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

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

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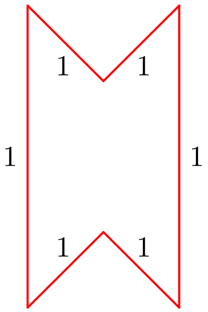
$$w(G_X) = \sum_i w(F_i), \quad F_i \in \mathcal{F}$$

3. Counting: Show that whp $w(F) < 0$ for all $F \in \mathcal{F}$

Step 1: Bicolored multigraph representation



X^*: true cycle

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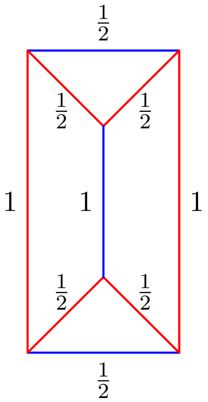
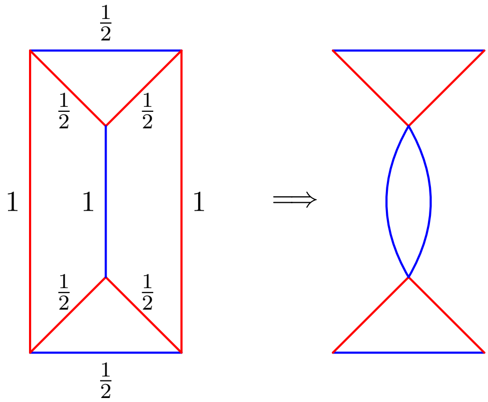


X: extremal solution

Step 1: Bicolored multigraph representation



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G_X

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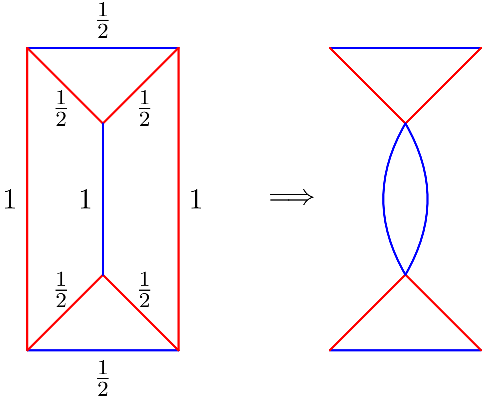
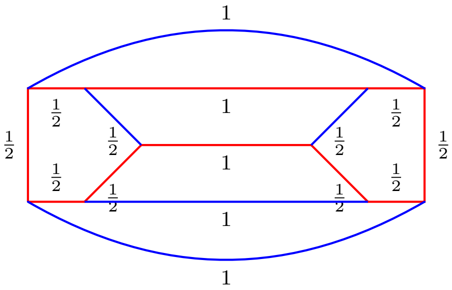


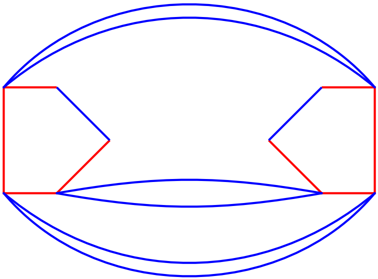
X: extremal solution $\qquad$ G_X

key observation

G_X is always balanced: red degree = blue degree



$\Downarrow$



Step 2: Edge decomposition

Theorem (Kotzig '68)

Every connected balanced bicolored multigraph has an alternating Eulerian circuit.

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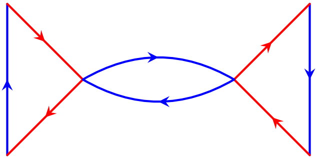
Remarks

- An Eulerian circuit may traverse a double edge twice

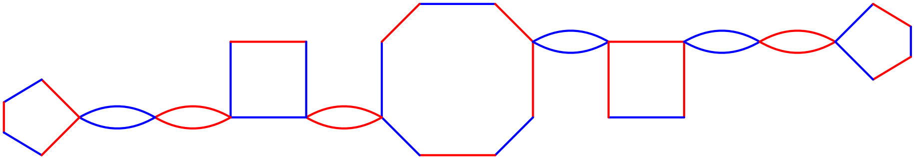


"Dumbbell" structure

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

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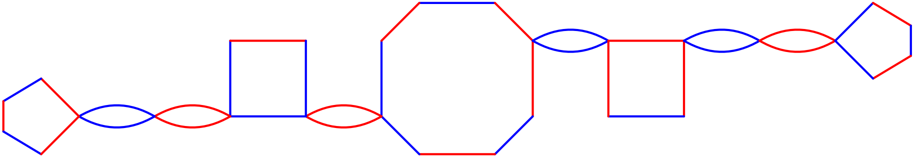
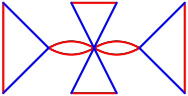
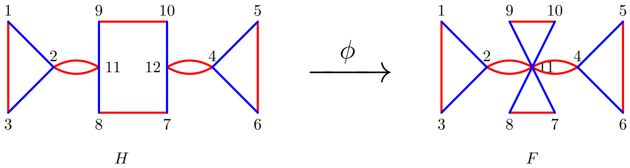


Obtained by starting with an 10-cycle and blossoming 4 times

However, not every G_X is of this form...



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



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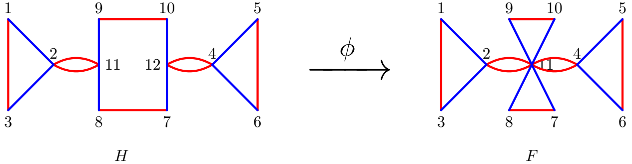
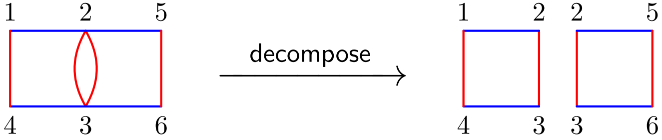


Lemma (Decomposition)

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

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



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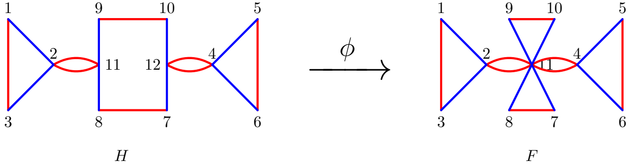

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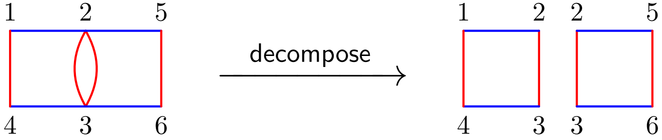

- It remains to show $\min_{F \in \mathcal{F}} w(F) < 0$ whp

Step 3: Counting

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

Lemma (Counting isomorphism classes)

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

Lemma (Counting homomorphisms)

For each $H \in \mathcal{U}$, there exists $0 \le r \le \ell/2$

- *Number of labelings for double edges:*

$$\le (Cn)^{k/2+r/2}$$

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

$$\le (Cn)^{\ell/2-r}$$

Step 4: Probabilistic arguments

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

Lemma

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

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

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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 $\sim N(0,1)$.

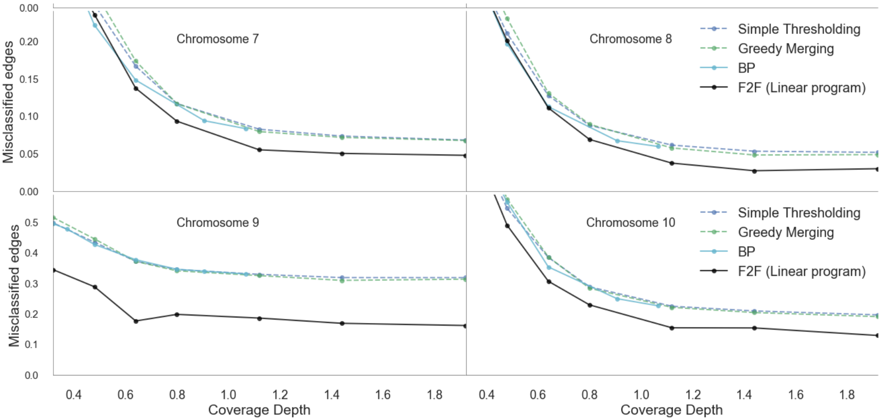
$$w(F) \sim N(-(k + \ell/2)\mu, \mathbf{4}k + \ell)$$

- Proof: Counting $\mathcal{F}_{k,\ell}$ and large deviation bounds

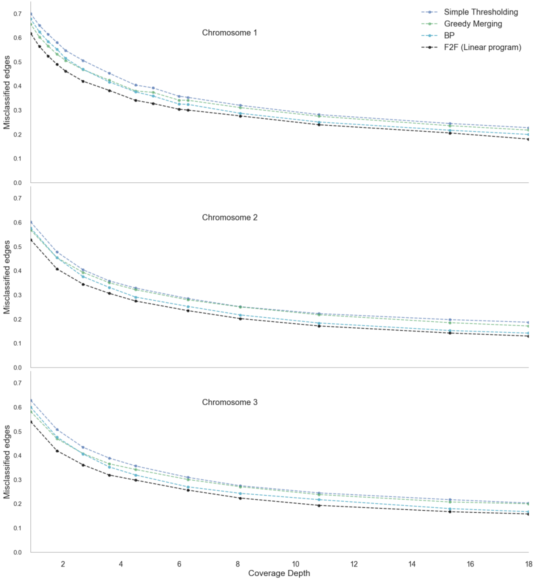
Real-data experiment

- 1000 DNA contigs of size 100 kbps
- 0.45 million Chicago cross-links
- Subsample each cross-link with probability p

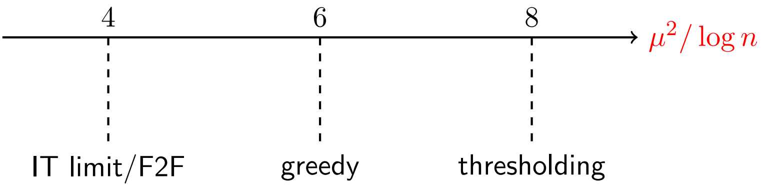
Homosapiens [Putnam et al 16, Genome Research]



Aedes Aegypti (zika mosquito) [Dudchenko et al '16, Science]



Conclusion and remarks



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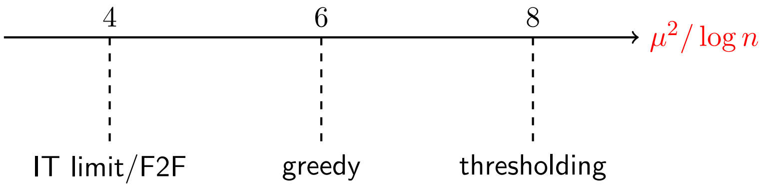
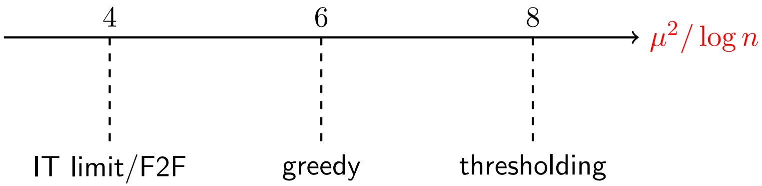


Future work

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



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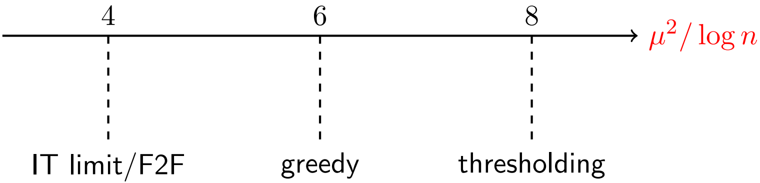

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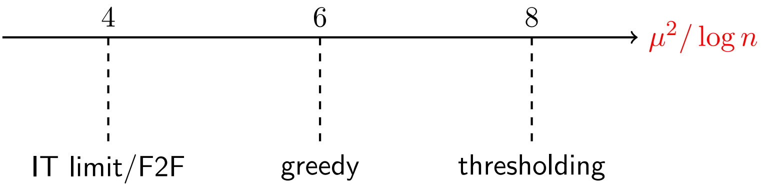

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- More realistic models
  - 2-NN graph: IT limit becomes $\sqrt{2 \log n}$ not achieved by LP.
  - small-world graphs
- Smarter rounding algorithm in practice
- Reduction from/to Hamiltonian cycle and path more elegantly

References

- Vivek Bagaria, Jian Ding, David Tse, W. & Jiaming Xu (2018). *Hidden Hamiltonian Cycle Recovery via Linear Programming*, https://arxiv.org/abs/1804.05436