Hidden Hamiltonian Cycle Recovery via Linear Programming

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Joint work with
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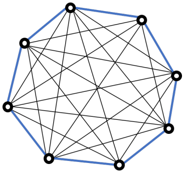
Mathematical problem: Hidden Hamiltonian cycle model

- Given a weighted undirected complete graph on n vertices
- 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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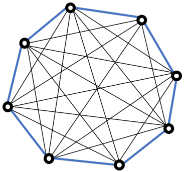

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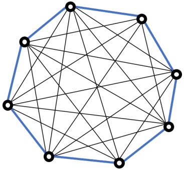

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Remarks:

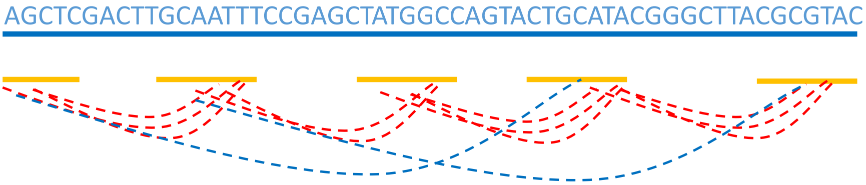
- For this talk, $Q = N(0,1)$ and $P = N(\mu, 1)$, so that

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

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

Motivation: Link information in Chicago datasets

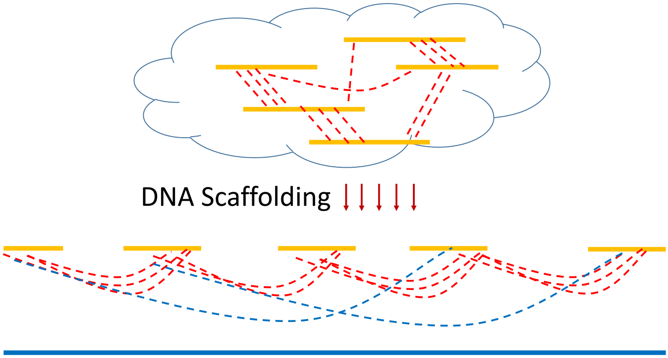
1. Reconstitute chromatin in vitro upon naked DNA
2. Produce cross-links by fixing chromatin with formaldehyde



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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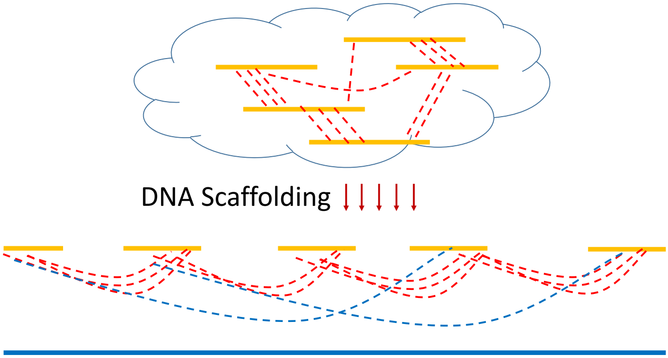

Reduces to traveling salesman problem (TSP)

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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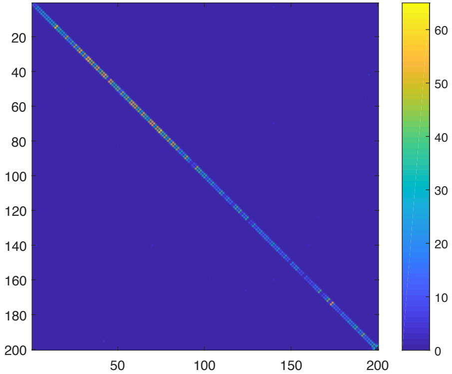
Key questions:

- 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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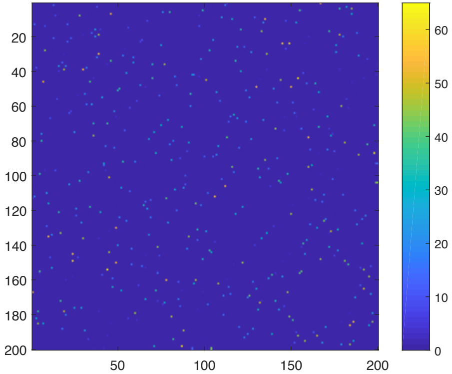

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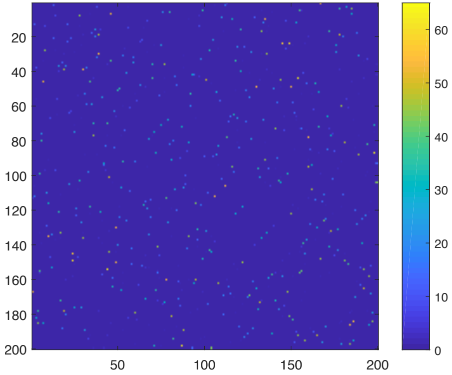

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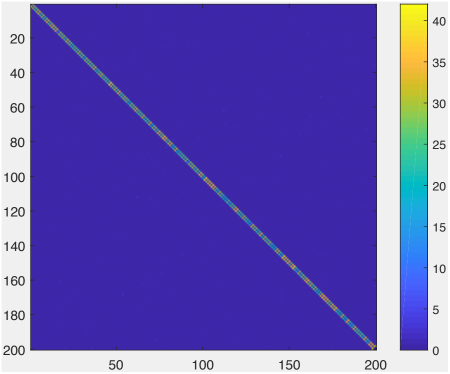

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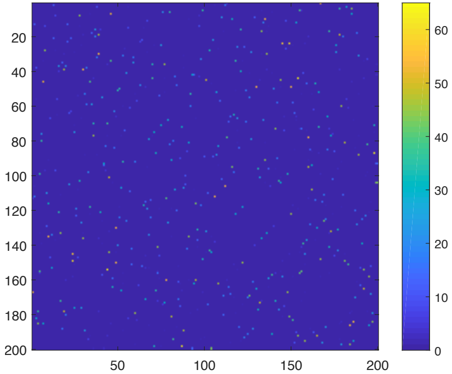

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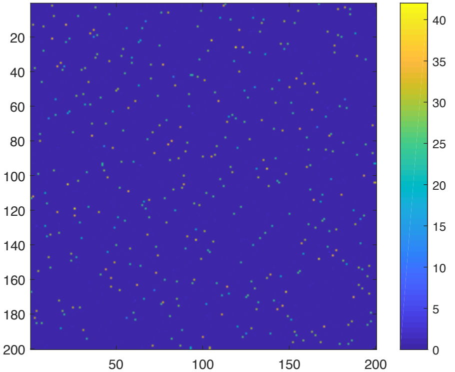

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What is known information-theoretically

Maximum likelihood estimator reduces to TSP

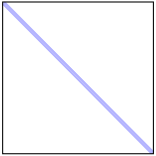
$$\widehat{X}_{\rm TSP} = \arg\max_{X} \ \langle W, X \rangle$$

$$\text{s.t.} \quad X \text{ is the adjacency matrix of some Hamiltonian cycle}$$

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

- Spectral methods fail miserably:
  - $\mu \gg n^{2.5}$ (spectral gap of cycle is too small)

$W = \mu$  $+$ Gaussian noise

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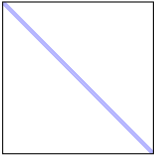
$W = \mu$  + Gaussian noise

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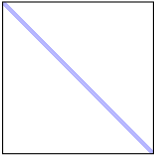
$W = \mu$  + Gaussian noise

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- Greedy merging [Motahari-Bresler-Tse '13]: $\mu > \sqrt{6 \log n}$

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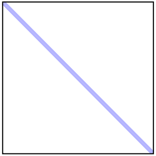
$W = \mu$  + Gaussian noise

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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 determined by Battacharyya distance (a.k.a. Rényi divergence of order $\frac{1}{2}$):

$$B(P,Q) \triangleq -2\log \int \sqrt{\mathrm{d}P\mathrm{d}Q}$$

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Threshold determined by Battacharyya distance (a.k.a. Rényi divergence of order $\frac{1}{2}$):

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LP succeeds when

$$\boxed{B(P,Q) - \log n \to +\infty}$$

optimal under mild assumptions

Convex relaxations of TSP

Integer Linear Programming reformulation of TSP

$$
\begin{aligned}
\widehat{X}_{\rm 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

$$\widehat{X}_{\rm SUB} = \arg\max_{X} \; \langle W, X \rangle$$

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

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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

$$\widehat{X}_{\mathrm{F2F}} = \arg\max_{X} \langle W, X \rangle$$
$$\text{s.t.} \quad \sum_j X_{ij} = 2, \quad \forall i$$
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- Further dropping subtour elimination constraints $\Longrightarrow$ Fractional 2-factor (F2F) LP

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- How it performs in our random instance?

Optimality of Fractional 2-Factor LP

Theorem (Bagaria-Ding-Tse-Wu-X. '18)

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

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Remarks

- Achieving the IT-limit $\mu^2 = 4\log n$

Belief propagation

Max-Product Belief Propagation

$$m_{i\to j}(t) = w_{ij} - \underset{\ell\neq j}{\text{2nd}\max}\left\{m_{\ell\to i}(t-1)\right\}$$
$$m_{i\to j}(0) = w_{ij}$$

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

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- BP is exact provided the optimal solution of F2F is integral [Bayati-Borgs-Chayes-Zecchina '11]
- It can be shown that $T = O(n^2 \log n)$ whp

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)

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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):

$$\begin{aligned} u_i + u_j &\le W_{ij}, \quad \text{for } i \sim j \text{ in } C^* \\ u_i + u_j &\ge W_{ij}, \quad \text{for } i \not\sim j \text{ in } C^* \end{aligned}$$

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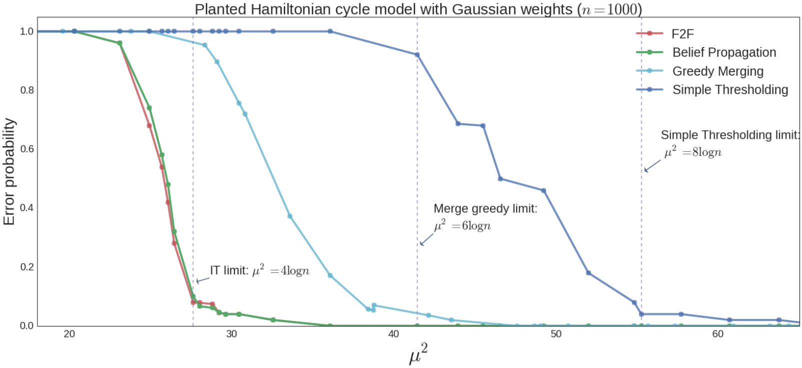
- This certificate shows correctness if $\mu^2 > 6 \log n$ (same as greedy merging)

Synthetic data experiment



Primal approach

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

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- F2F polytope:

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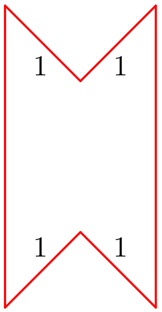
3. Counting: Show that whp $w(F) < 0$ for all $F \in \mathcal{F}$

Step 1: Bicolored multigraph representation



X^*: true cycle

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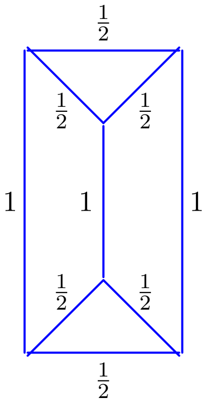

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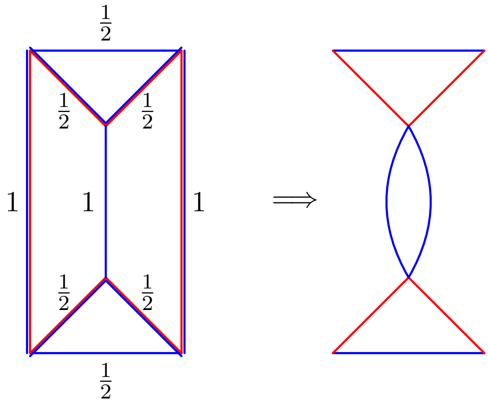

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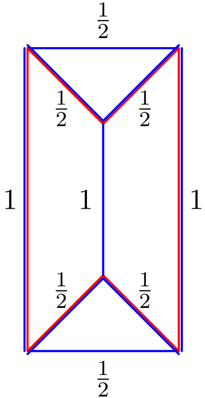
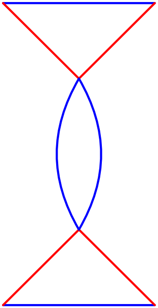


$\Longrightarrow$



X: 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.

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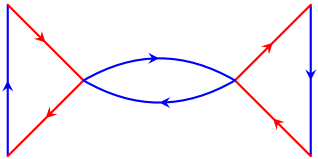
Remarks

- An Eulerian circuit may traverse a double edge twice

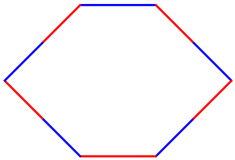


"Dumbbell" structure

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** (alternating path of double edges followed by an alternating odd cycle)



Obtained by starting with an 10-cycle and blossoming 3 times

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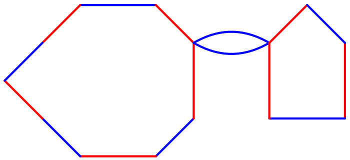

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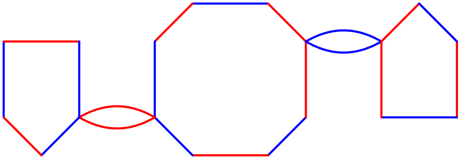

Obtained by starting with an 10-cycle and blossoming 3 times

Step 2: Edge decomposition

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

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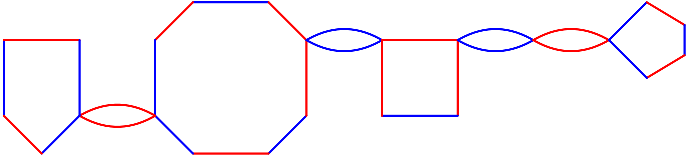

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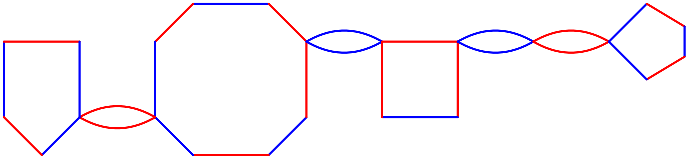

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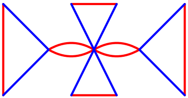
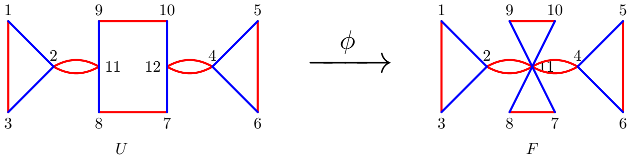
However, not every G_X is of this form...



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



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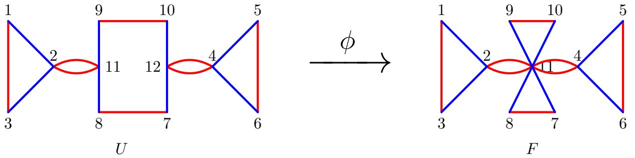
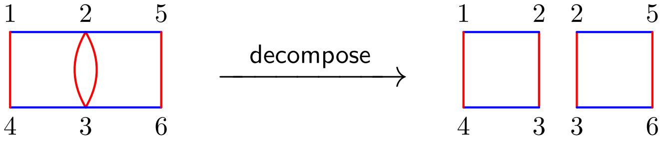


Lemma (Decomposition)

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

$$\mathcal{F} = \{F : U \to F \text{ for some } U \in \mathcal{U}\}$$



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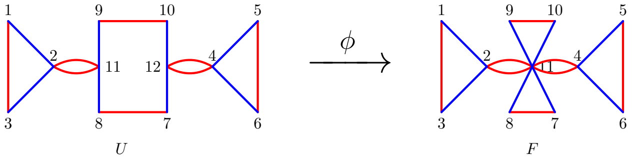

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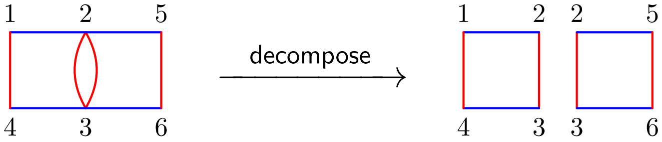

- It remains to show $\min_{F \in \mathcal{F}} w(F) < 0$ whp

Step 3: Counting and large deviation 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

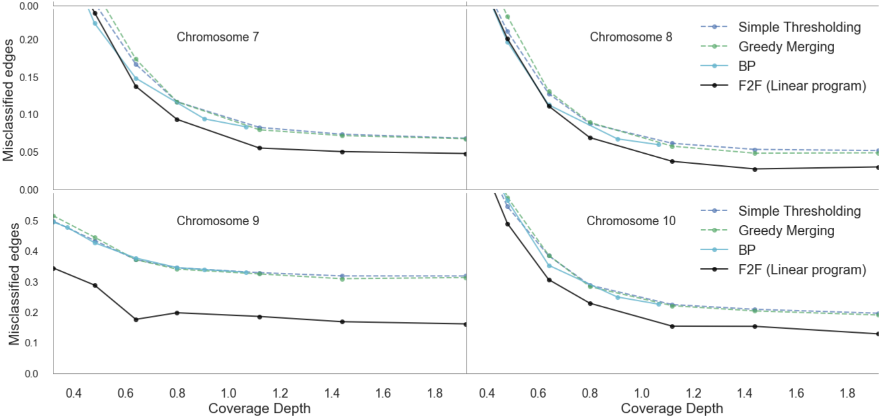
- Total: $2k + \ell$ edges, half red half blue.
- Weights on red edges $\sim \mathcal{N}(-\mu, 1)$; weights on blue edges $\sim \mathcal{N}(0, 1)$

$$w(F) \sim \mathcal{N}\left(-\frac{2k+\ell}{2}\mu,\ \mathbf{4}k + \ell\right)$$

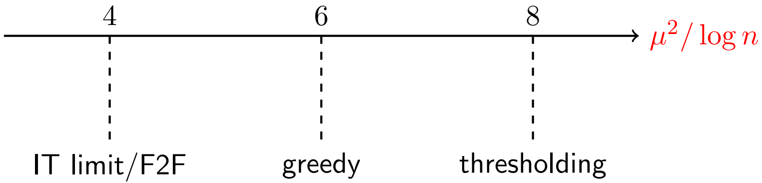
Real-data experiment

- 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]



Conclusion and remarks



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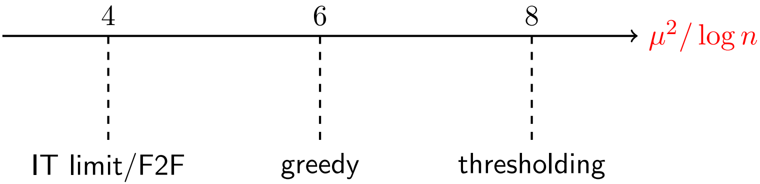

References

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