Reconfiguration: From statistical physics to graph theory

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Journées Structures Discrètes
ENS Lyon
Spin systems

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A spin configuration is a function \( \sigma : S \rightarrow \{1, \ldots, k\} \).

- Interactions between spins in \( S \) are modelized via an interaction matrix.
- If coefficients are in \( 0 - 1 \): representation with a graph:
  - 0 = no interaction = no link.
  - 1 = interaction = link.
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Spin configuration \( \Rightarrow \) (non necessarily proper) graph coloring.
Antiferromagnetic Potts model

$H(\sigma)$: number of monochromatic edges.

Edges with both endpoints of the same color.

Gibbs measure at fixed temperature $T$:

$$\nu_T(\sigma) = e^{-\frac{H(\sigma)}{T}}$$

Important points to notice:

• Free to rescale, $\nu_T$ is a probability distribution $P$ on the colorings.

• The probability $\downarrow$ if the number of monochromatic edges $\uparrow$.

• When $T \downarrow$, $P(c) \downarrow$ if $c$ has at least one monochromatic edge.

Limit of a $k$-state Potts model when $T \to 0$.

$\iff$ Only proper colorings have positive measure.
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$T = 5, 1, 0.2, 0.05$
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**Definition** (Glauber dynamics)

Limit of a \( k \)-state Potts model when \( T \to 0 \).

\( \iff \) Only **proper** colorings have positive measure.
Sampling spin configurations

In the statistical physics community, the following Monte Carlo Markov chain was proposed to **sample a configuration**:

- **Start** with an initial coloring $c$;
- **Choose** a vertex $v$ at random and a color $a$;
- **Recolor** $v$ with color $a$ if the resulting coloring is proper; otherwise do nothing;
- Repeat
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Questions:

- Can we generate any solution?
- How much time do we need to “sample a solution almost at random”?  


Reconfiguration graph

**Definition (k-Reconfiguration graph $C_k(G)$ of G)**

- **Vertices**: Proper $k$-colorings of $G$.
- **Create an edge** between any two $k$-colorings which differ on exactly one vertex.

All along the talk $k$ denotes the **number of colors**.
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![Diagram of two graphs with different colorings](attachment:image.png)
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**Remark 1.** Two colorings equivalent up to color permutation are distinct.

**Remark 2.**
All the \(k\)-colorings can be generated \(\iff\) The \(k\)-reconfiguration graph is connected.
Convergence of Markov chains

A Markov chain is **irreducible** if any solution can be reached from any other. ⇔ The reconfiguration graph is connected.

A chain is **aperiodic** if there exists $t_0$ such that $Pr(X_t = a)$ is positive for every $t > t_0$ and every state $a$.
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Every **ergodic** (aperiodic and irreducible) Markov chain converges to a **unique** stationnary distribution.
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**In our case:**

- $P(X_{t+1} = X_t) > 0$ ⇒ Irreducibility implies aperiodicity.
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Mixing time and Reconfiguration graph?

• Diameter of the Reconfiguration graph = $D$
  ⇒ Mixing time $\geq 2 \cdot D$. 
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**Mixing time and Reconfiguration graph ?**

- Diameter of the Reconfiguration graph = \( D \)
  \( \Rightarrow \) Mixing time \( \geq 2 \cdot D \).
- Better lower bounds? Look at the connectivity of the reconfiguration graph.
Main question in Statistical Physics

How many colors (in terms of the maximum degree $\Delta$) do we need to ensure that the chain is rapidly mixing?

We denote by $c(\Delta)$ the number of colors.
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- The chain is not always ergodic if $c \leq \Delta + 1$ (e.g. cliques).
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**Conjecture**

If $c \geq \Delta + 2$, the graph is $c(\Delta)$-mixing in time $O(n \log n)$. 
Informal definition

Two Markov chains \((X_t, Y_t)\) are coupled if:

- \(X_t\) without knowing \(Y_t = Y_t\) without knowing \(X_t\).
- But the chains might be “correlated” (in the sense that transitions in \(Y_t\) might depend on transitions of \(X_t\)).
Path coupling

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Theorem
If there exists a coupling defined only every \(X_t, Y_t\) that only differ on one vertex such that

\[ \mathbb{E}(d(X_{t+1}, Y_{t+1})) < \left(1 - \frac{1}{n}\right) \]

then the mixing time is \(\mathcal{O}(n \log n)\).

\(d(X, Y)\) = Hamming distance
= number of vertices on which they differ
Example 1

Let $v$ be the vertex on which $X_t$ and $Y_t$ differ.

**Coupling:**

If vertex $u$ and color $c$ are chosen in $X_t$, we make the same choice in $Y_t$. 
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**Analysis:**
Assume that \( k \geq 3\Delta + 1 \).
\[
\mathbb{P}(d(X_{t+1}, Y_{t+1}) = 0) > \frac{1}{n} \cdot \frac{2\Delta + 1}{3\Delta + 1}.
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\[\Rightarrow \quad \mathbb{E}(d(X_{t+1}, Y_{t+1}) = 1 - \frac{1}{(3\Delta+1)n}.\]

\[\Rightarrow \quad \text{The chain is rapidly mixing if } k > 3\Delta.\]
Example 2

\( v = \) Unique vertex on which \( X_t \) and \( Y_t \) differ.

**Coupling :**

- If \( u \in N(v) \) and \( c \) color of \( v \) in \( X_t \) is chosen in \( X \).
  \( \Rightarrow \) Choose \( v \) and \( c' \) color of \( v \) in \( Y_t \).

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- In all the other cases, perform the same.
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**Analysis :**

Assume that \( k \geq 2\Delta + 1 \).

\[ P(d(X_{t+1}, Y_{t+1}) = 0) > \frac{1}{n} \cdot \frac{\Delta+1}{2\Delta+1}. \]

\[ P(d(X_{t+1}, Y_{t+1}) = 2) \leq \frac{\Delta}{n} \cdot \frac{1}{2\Delta+1}. \]
Example 2

$\nu = \text{Unique vertex on which } X_t \text{ and } Y_t \text{ differ.}$

**Coupling :**

- If $u \in N(\nu)$ and $c$ color of $\nu$ in $X_t$ is chosen in $X$.
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- In all the other cases, perform the same.

**Analysis :**

Assume that $k \geq 2\Delta + 1$.

$\mathbb{P}(d(X_{t+1}, Y_{t+1}) = 0) > \frac{1}{n} \cdot \frac{\Delta+1}{2\Delta+1}.$

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$\Rightarrow \mathbb{E}(d(X_{t+1}, Y_{t+1}) = 1 - \frac{1}{(2\Delta+1)n}.$

$\Rightarrow \text{The chain is rapidly mixing if } k > 2\Delta.$
Relation with enumeration

**Theorem**

If the reconfiguration is connected then there exists a *polynomial delay algorithm* that enumerate all the solutions.

An algorithm is *polynomial delay* if it enumerates all the solutions and the delay between two solutions is polynomial in $n$. 
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**Sketch of the proof**:
- Diameter of the reconfiguration graph polynomial $\Rightarrow$ BFS.
- Non-polynomial diameter $\Rightarrow$ Be careful.
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**Sketch of the proof**:

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**Remark**:
The algorithm might need an exponential space!
Main questions in Comb. / Alg.

- Can we transform any coloring into any other?
  
  *Is the reconfiguration graph connected?*
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  \textit{Given two vertices of the reconfiguration graph, are they in the same connected component?}
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• If the answer is positive, how many steps do we need?
  *What is the diameter of the reconfiguration graph?*
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- If the answer is positive, how many steps do we need?
  *What is the diameter of the reconfiguration graph?*

- Can we efficiently find a short transformation (from an algorithmic point of view)?
  *Can we find a path between two vertices of the reconfiguration graph in polynomial time?*
Main question in CS

**Conjecture (Cereceda)**

The \((k + 2)\)-recoloring diameter of any \(k\)-degenerate graph is \(\mathcal{O}(n^2)\).

A graph is \(k\)-degenerate if there exists an order \(v_1, \ldots, v_n\) such that for every \(i\), \(v_i\) has at most \(k\) neighbors after it in the order.
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\[
\begin{tikzpicture}[scale=0.8]
  \foreach \i in {1,...,6} { \node (v\i) at (90 + 360/6 * \i:2) {}; }
  \foreach \i in {1,2,3,4,5,6} { \foreach \j in {\i,...,6} { \path (v\i) edge (v\j); } }
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Any \((k + 2)\)-coloring can be transformed into any other by recoloring at most \((k + 1)^n\) times each vertex.
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- Delete a vertex of degree at most \(k\).
- Apply induction on the remaining graph.
Proof scheme

**Theorem (Cereceda '07)**

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Proof scheme

**Theorem (Cereceda ’07)**

The $(k + 2)$-recoloring diameter of any $k$-degenerate graph is at most $n \cdot (k + 1)^n$.

**Lemma**

Any $(k + 2)$-coloring can be transformed into any other by recoloring at most $(k + 1)^n$ times each vertex.

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![Diagram of two graphs](image-url)
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Number of recolorings?

When do we need to recolor the leftmost vertex?

- Each time a neighbor is recolored.

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- In the last round: +1 recoloring.

The total number of recolorings is at most \((k + 1)^n\).
Cereceda’s conjecture

**Conjecture** (Cereceda)

The \((k + 2)\)-recoloring diameter of any \(k\)-degenerate graph is \(O(n^2)\).
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**Known results:**
- [Bonamy et al.] True for \(k = 1 \iff \) Trees.
- Open for \(k = 2\) and \(\Delta = 4\).
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\(d\)-degenerate

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\frac{d + 1}{d + 1}
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Chordal graphs
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Chordal graphs  Not Conn.  \(O(n^2)\)
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Theorem (Bonamy et al.)

The 3-recoloring diameter of the path $P_n$ is $\Omega(n^2)$. 

Claim: A recoloring performs the following: 

- If $c(v_{i+1}) = c(v_i) - 1$ ⇒ Write $\rightarrow$. 
- If $c(v_{i+1}) = c(v_i) + 1$ ⇒ Write $\uparrow$. 

The surface is only modified by “one” at each step. 

Claim: $\Omega(n^2)$ steps are needed to transform 123....123 into 132....132.
Theorem (Bonamy et al.)

The 3-recoloring diameter of the path $P_n$ is $\Omega(n^2)$.

Sketch of the proof

- If $c(v_{i+1}) = c(v_i) - 1 \Rightarrow$ Write $\rightarrow$.
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Lower bound

**Theorem** (Bonamy et al.)

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**Sketch of the proof**

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**Claim:** A recoloring performs the following:

$$
\begin{array}{c}
  a + 1 \\
  a \\
  a \\
\end{array}
\begin{array}{c}
  a \\
  a \\
  a - 1 \\
\end{array}
\Rightarrow \text{The surface is only modified by “one” at each step.}

**Claim:** $\Omega(n^2)$ steps are needed to transform $123\ldots123$ into $132\ldots132$. 
Going below \((\Delta + 2)\) colors

Impossible to sample - count \((\Delta + 1)\)-colorings?

A coloring is frozen if all the colors appear in the (closed) neighborhood of all the vertices.

Theorems:

- \([\text{Feghali, Johnson, Paulusma}]\) A \(O(n^2)\) recoloring sequence exists between any pair of non-frozen \((\Delta + 1)\)-colorings (when \(\Delta \geq 3\)).

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What does “close” mean?

At the beginning of the talk (a long time ago...).

“At each step, change the color of a single vertex”
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Recoloring via Kempe chains

**Theorem (Mohar)**

We can generate all the $(\Delta + 1)$-colorings using Kempe chains.
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We can generate all the $\Delta$-colorings of any graph using Kempe chains.

Counter-example proposed by Jan van den Heuvel (2013)

21/22
Recoloring via Kempe chains

**Theorem (Mohar)**

We can generate all the \((\Delta + 1)\)-colorings using Kempe chains.

**Theorem (Bonamy, B., Feghali, Johnson 2017+)**

We can generate all the \(\Delta\)-colorings of any graph except the 3-prism using Kempe chains.

Counter-example proposed by Jan van den Heuvel (2013)
Conclusion

Relation with other fields:

- **Sampling.** Connectivity? Diameter? Huge connectivity?

More questions:

- A connected reconfiguration graph with exponential diameter.
- Understand better what "not connected" means.

Thanks for your attention!
Conclusion

Relation with other fields:

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