The expected number of inversions after n adjacent transpositions

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A Markov chain

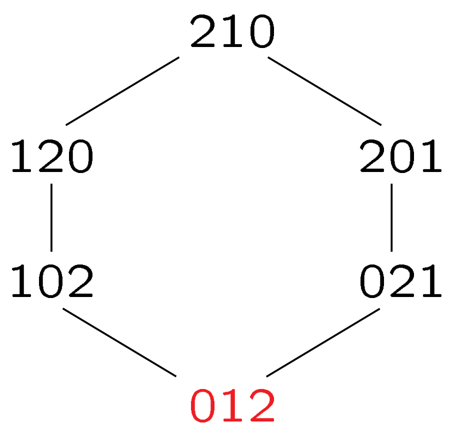
- Consider the symmetric group $\mathfrak{S}_{d+1}$ on the elements $\{0, 1, \ldots, d\}$.

- Start from the identity permutation $\pi^{(0)} = 012 \cdots d$.

- Apply an adjacent transposition, taken uniformly at random (probability $1/d$ for each).

- Repeat.

Example: $d = 2$



$\pi^{(0)} = 012$

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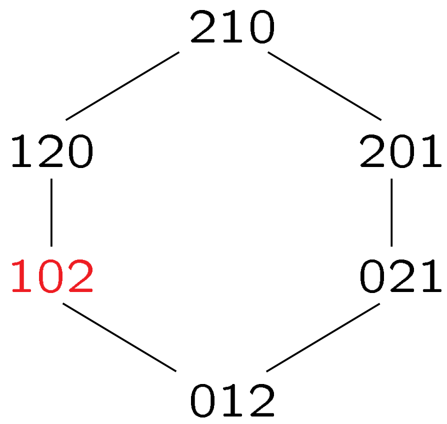

$\pi^{(1)} = 102$

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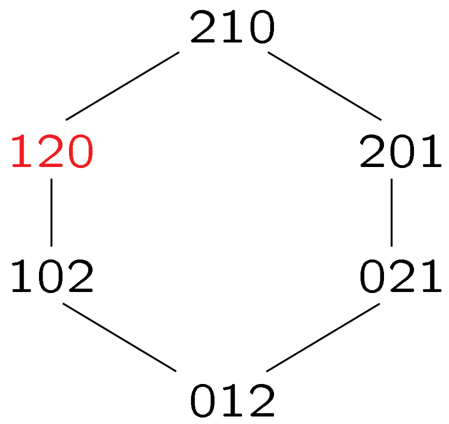

$\pi^{(2)} = 120$

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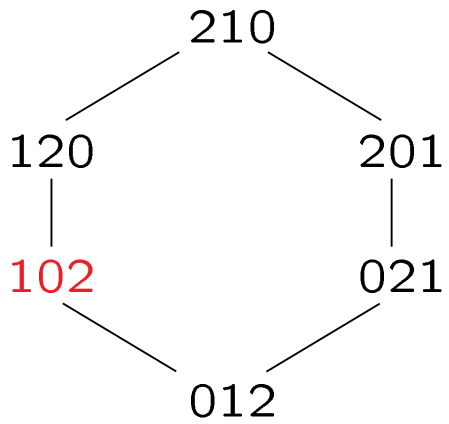

$\pi^{(3)} = 102$

A Markov chain

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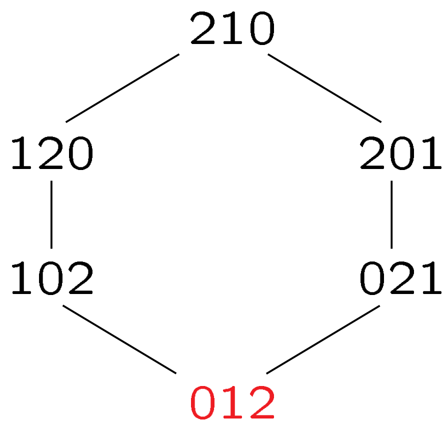

$\pi^{(4)} = 012$

A Markov chain

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- Repeat.

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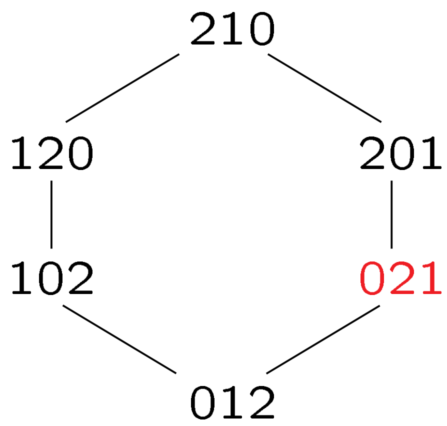


$\pi^{(5)} = 012$

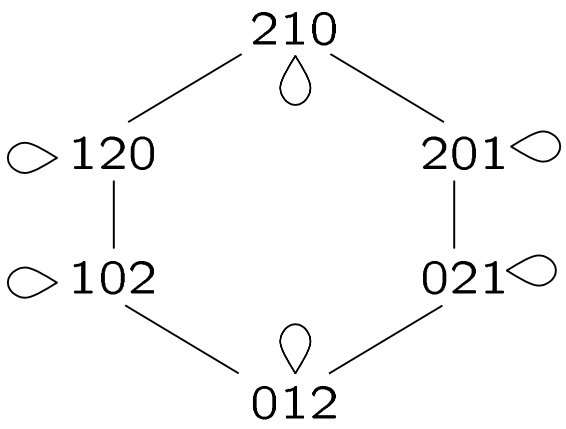
Periodicity

This chain, $\pi^{(0)}, \pi^{(1)}, \pi^{(2)}, \ldots$ is periodic of period 2: it takes an even number of steps to return to a point.

$$
\begin{tikzcd}
 & 210 \arrow[dl, no head] \arrow[dr, no head] & \\
120 \arrow[d, no head] & & 201 \arrow[d, no head] \\
102 \arrow[dr, no head] & & 021 \arrow[dl, no head] \\
 & 012 &
\end{tikzcd}
$$

An aperiodic variant

This chain, $\pi^{(0)}, \pi^{(1)}, \pi^{(2)}, \ldots$ is periodic of period 2: it takes an even number of steps to return to a point.



• Do nothing with probability $1/(d+1)$, and otherwise apply an adjacent transposition chosen uniformly

This chain is aperiodic, irreducible and symmetric, and thus converges to the uniform distribution on $\mathfrak{S}_{d+1}$.

Motivations

• 1980 $\to$ 2012: Random walks in finite groups (Aldous, Diaconis, Letac, Saloff-Coste, Wilson...)

Tools: coupling techniques, representation theory...

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• More recently: Computational biology (N. Beresticky, Durrett, Eriksen, Hultman, H. Eriksson, K. Eriksson, Sjöstrand...)

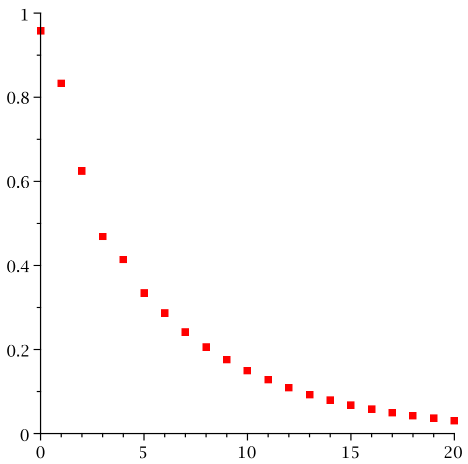
A transposition: a gene mutation

What do we ask? What do we expect?

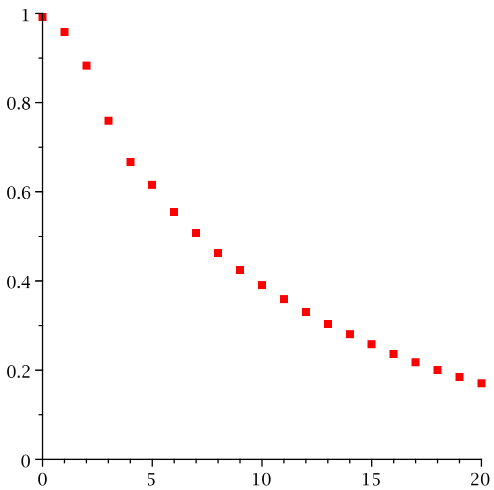
- Mixing time: How much time does it take to "reach" the uniform distribution?

The total variation distance between the distribution at time n and the uniform distribution on $\mathfrak{S}_{d+1}$:

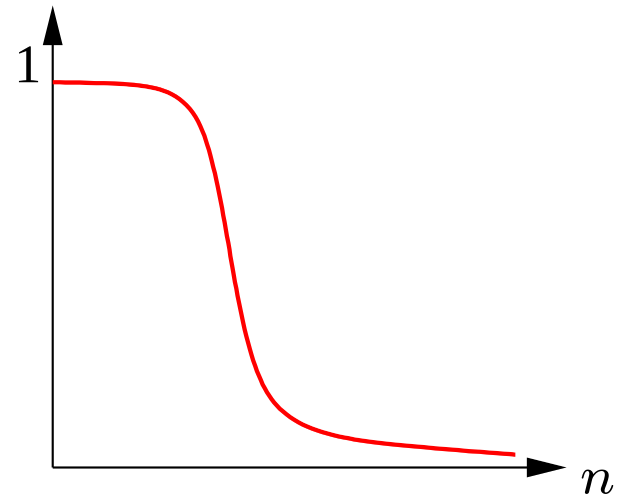
$d = 3$



$d = 4$



d large



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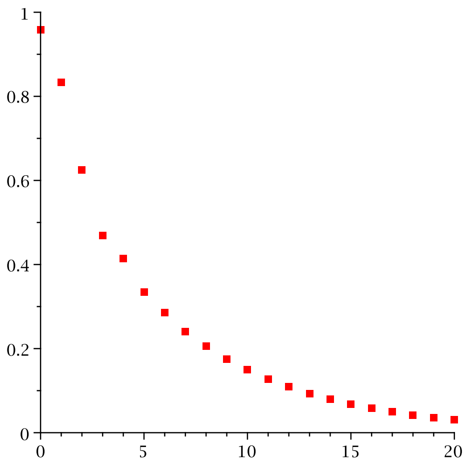

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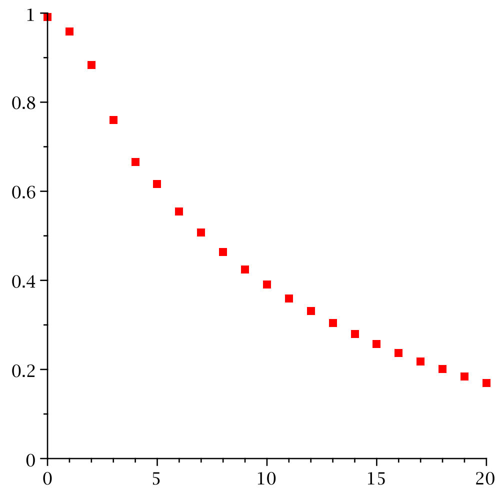

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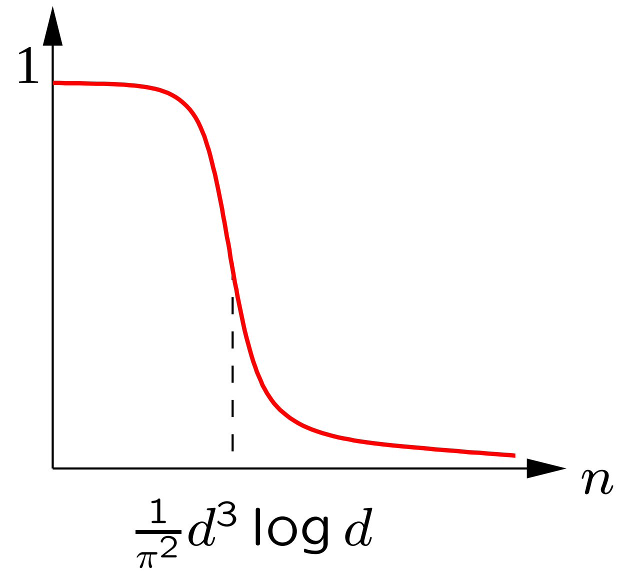

[Aldous 83, Diaconis & Saloff-Coste 93, Wilson 04]

What do we ask? What do we expect?

- Focus on observables, for instance the inversion number $\mathcal{I}_{d,n} = \mathrm{inv}(\pi^{(n)})$.

The expected value of the inversion number, $\mathsf{I}_{d,n} := \mathbb{E}(\mathcal{I}_{d,n})$:

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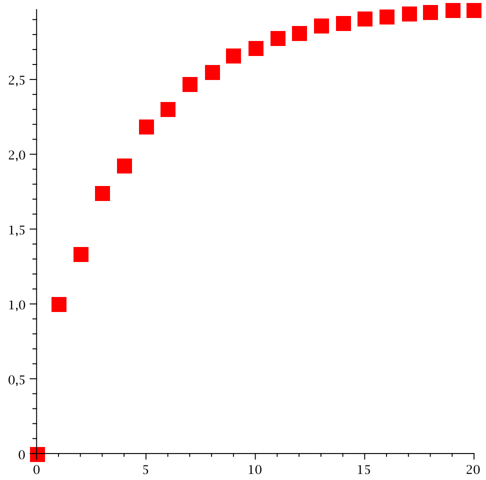

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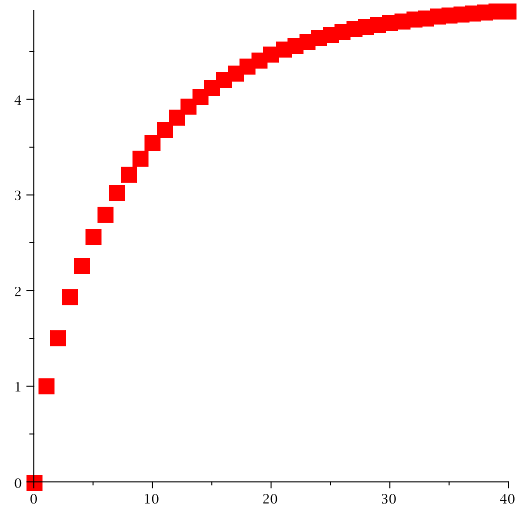

$\Longrightarrow$ Estimate the number of transpositions (mutations) that have occurred, and hence the evolutionary distance between species.

Of particular interest: what happens before mixing.

A formula for the expected inversion number

Theorem: The expected number of inversions after n adjacent transpositions in $\mathfrak{S}_{d+1}$ is

$$\mathsf{I}_{d,n} = \frac{d(d+1)}{4} - \frac{1}{8(d+1)^2} \sum_{k,j=0}^{d} \frac{(c_j + c_k)^2}{s_j^2 s_k^2} \, {x_{jk}}^n,$$

where

$$c_k = \cos \alpha_k, \quad s_k = \sin \alpha_k, \quad \alpha_k = \frac{(2k+1)\pi}{2d+2},$$

and

$$x_{jk} = 1 - \frac{4}{d}(1 - c_j c_k).$$

Remark: For d large enough ($d \geq 8$), $\mathsf{I}_{d,n}$ increases, as n grows, to $\frac{d(d+1)}{4}$, which is the average inversion number of a random permutation in $\mathfrak{S}_{d+1}$.

Another formula for the expected inversion number [Eriksen 05]

$$\mathsf{I}_{d,n} = \sum_{r=1}^{n} \frac{1}{d^r}\binom{n}{r} \sum_{s=1}^{r} \binom{r-1}{s-1}(-4)^{r-s} g_{s,d}\, h_{s,d},$$

with

$$g_{s,d} = \sum_{\ell=0}^{d} \sum_{k\geq 0} (-1)^k (p-2\ell)\binom{2\lceil s/2\rceil - 1}{\lceil s/2\rceil + \ell + k(d+1)}$$

and

$$h_{s,d} = \sum_{j\in\mathbb{Z}} (-1)^j \binom{2\lfloor s/2\rfloor}{\lfloor s/2\rfloor + j(d+1)}.$$

Based on [Eriksson & Eriksson & Sjöstrand 00]

Beresticky & Durrett 08: “it is far from obvious how to extract useful asymptotic from this formula”.

Combinatorialists could not throw in the sponge!

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The expected inversion number: asymptotics

Three regimes, as d and n tend to ∞

• When n is "small", each step of the chain increases the inversion number with high probability. For example,

$$\mathrm{inv}(\pi^{(1)}) = 1, \qquad \mathbb{P}\left(\mathrm{inv}(\pi^{(2)}) = 2\right) = 1 - \frac{1}{d}, \qquad \mathbb{P}\left(\mathrm{inv}(\pi^{(n)}) = n\right) = 1 - O\left(\frac{1}{d}\right).$$

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• When n is "large", the expected inversion number must approach its limit value $d(d+1)/4 \sim d^2/4$.

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• An intermediate regime?

Small times: linear and before

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$$\frac{\mathsf{I}_{d,n}}{n} = 1 + O(n/d).$$

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- Linear regime. If $n \sim \kappa d$,

$$\frac{\mathsf{I}_{d,n}}{n} = f(\kappa) + O(1/d)$$

where

$$\begin{aligned} f(\kappa) &= \frac{1}{2\pi\kappa}\int_0^\infty \frac{1-\exp(-8\kappa t^2/(1+t^2))}{t^2(1+t^2)}dt \\ &= \sum_{j\geq 0}(-1)^j \frac{(2j)!}{j!(j+1)!^2}(2\kappa)^j. \end{aligned}$$

The function $f(\kappa)$ decreases from $f(0)=1$ to $f(\infty)=0$.

Large times: cubic and beyond

- Super-cubic regime. If $n \gg d^3$,

$$\frac{\mathsf{I}_{d,n}}{d^2} \to \frac{1}{4}.$$

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- Super-cubic regime. If $n \gg d^3$,

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- Cubic regime. If $n \sim \kappa d^3$,

$$\frac{\mathsf{I}_{d,n}}{d^2} \sim g(\kappa)$$

where

$$g(\kappa) = \frac{1}{4} - \frac{16}{\pi^4} \left(\sum_{j \geq 0} \frac{e^{-\kappa\pi^2(2j+1)^2/2}}{(2j+1)^2} \right)^2.$$

The function $g(\kappa)$ increases from $g(0) = 0$ to $g(\infty) = 1/4$.

The intermediate regime

- If $d \ll n \ll d^3$,

$$\frac{\mathsf{I}_{d,n}}{\sqrt{dn}} \to \sqrt{\frac{2}{\pi}}.$$

Remark. For a related continuous time chain, the normalized inversion number $\mathcal{I}_{d,n}/\sqrt{dn}$ converges in probability to $\sqrt{2/\pi}$ [Berestycky & Durrett 08]

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Where are the inversions? [Eriksson *et al.* 00]

For $i \le j$, let $p_{i,j}^{(n)}$ be the probability that there is an inversion at time n in the positions i and $j+1$:

$$p_{i,j}^{(n)} = \mathbb{P}(\pi_i^{(n)} > \pi_{j+1}^{(n)}).$$

- The expected number of inversions at time n is

$$\mathsf{I}_{d,n} = \sum_{0 \le i \le j < d} p_{i,j}^{(n)}.$$

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  - If $i = j$ and the nth transposition has switched the ith and $i+1$st values:

$$\left(1 - p_{i,j}^{(n-1)}\right) \frac{1}{d}$$

  - etc.

A recursion for the inversion probabilities

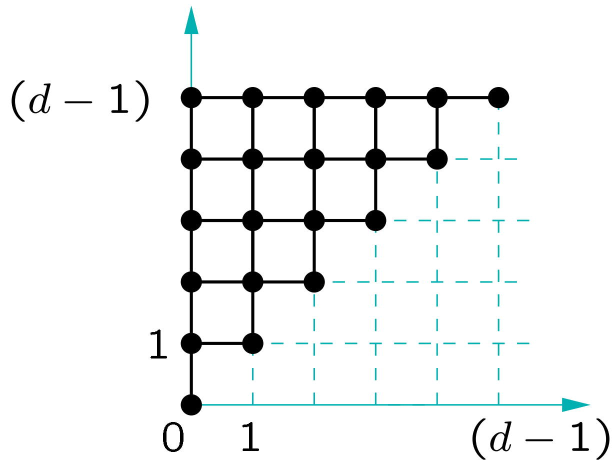
Lemma. The inversion probabilities $p_{i,j}^{(n)}$ are characterized by:

$$p_{i,j}^{(0)} = 0 \quad \text{for} \quad 0 \le i \le j < d,$$

and for $n \ge 0$,

$$p_{i,j}^{(n+1)} = p_{i,j}^{(n)} + \frac{1}{d} \sum_{(k,\ell) \leftrightarrow (i,j)} \left(p_{k,\ell}^{(n)} - p_{i,j}^{(n)} \right) + \frac{\delta_{i,j}}{d} \left(1 - 2p_{i,j}^{(n)} \right),$$

where $\delta_{i,j} = 1$ if $i = j$ and 0 otherwise, and the neighbour relations $\leftrightarrow$ are those of the following graph:



$\rightsquigarrow$ A (weighted) walk in a triangle.

A functional equation for the GF of the inversion probabilities

Let $P(t; u, v)$ be the generating function of the numbers $p_{i,j}^{(n)}$:

$$P(t; u, v) \equiv P(u, v) := \sum_{n \geq 0} t^n \sum_{0 \leq i \leq j < d} p_{i,j}^{(n)} u^i v^j.$$

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The above recursion translates as

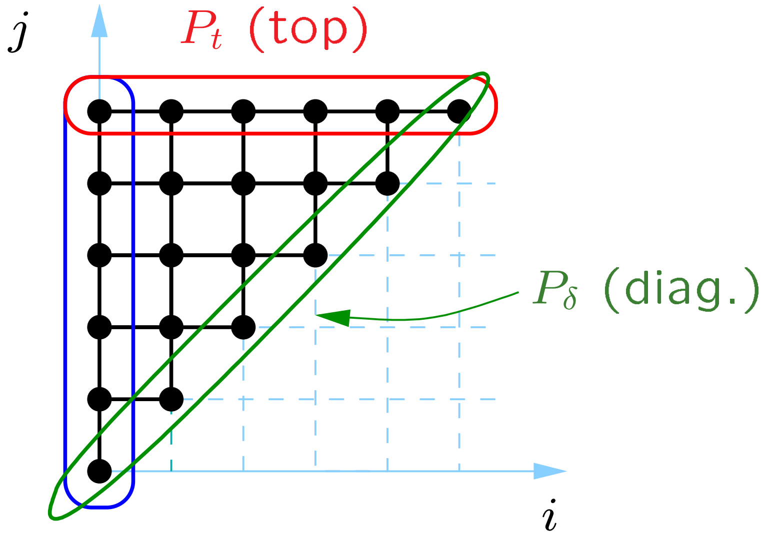
$$\left(1-t+\frac{t}{d}(4-u-\bar{u}-v-\bar{v})\right)P(u,v) =$$

$$\frac{t}{d}\left(\frac{1-u^d v^d}{(1-uv)(1-t)} - (\bar{u}-1)P_\ell(v) - (v-1)v^{d-1}P_t(u) - (u+\bar{v})P_\delta(uv)\right),$$

where $\bar{u} = 1/u$, $\bar{v} = 1/v$, and the series P_ℓ, P_t and P_δ describe the numbers $p_{i,j}^{(n)}$ on the boundaries of the graph:

P_ℓ (left)

$$P_\ell(v) \equiv P_\ell(t;v) = P(t;0;v)$$



Back to the inversion number

We are interested in

$$\mathsf{I}_m(t) = \sum_{n\geq 0} \mathsf{I}_{d,n} t^n = P(t;1,1),$$

which, according to the functional equation, may be rewritten

$$\mathsf{I}_m(t) = \frac{t}{(1-t)^2} - \frac{2tP_\delta(1)}{d(1-t)}.$$

◁ ◁ ◇ ▷ ▷

$$P(t;u,v) \equiv P(u,v) := \sum_{n\geq 0} t^n \sum_{0\leq i\leq j<d} p_{i,j}^{(n)} u^i v^j.$$

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$$\frac{t}{d}\left(\frac{1-u^d v^d}{(1-uv)(1-t)} - (\bar{u}-1)P_\ell(v) - (v-1)v^{d-1}P_t(u) - (u+\bar{v})P_\delta(uv)\right),$$

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What a beautiful equation!

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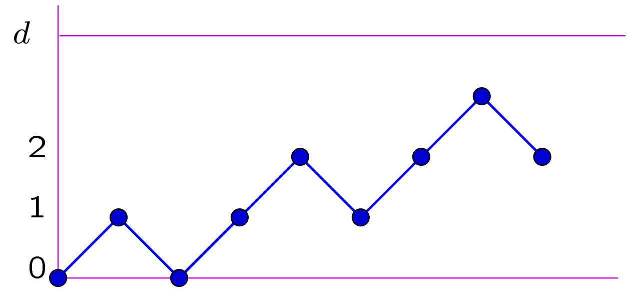
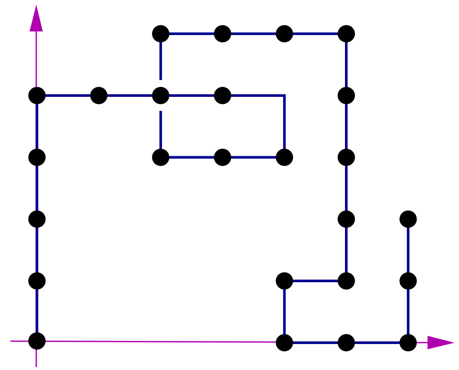
Analogies with:



- Walks with steps ± 1 in a strip of height d:

$$(1 - t(u+\bar{u}))P(u) = 1 - t\bar{u}P_0 - tu^{d+1}P_d$$



- Walks in the quarter plane

$$(1 - t(u + \bar{u} + v + \bar{v}))P(u,v) =$$
$$1 - t\bar{u}P(0,v) - t\bar{v}P(u,0)$$

- and others...

The ingredients of the solution

$$\left(1 - t + \frac{t}{d}(4 - u - \bar{u} - v - \bar{v})\right) P(u, v) =$$
$$\frac{t}{d}\left(\frac{1 - u^d v^d}{(1 - uv)(1 - t)} - (\bar{u} - 1)P_\ell(v) - (v - 1)v^{d-1}P_t(u) - (u + \bar{v})P_\delta(uv)\right)$$

- Cancel the kernel $\left(1 - t + \frac{t}{d}(4 - u - \bar{u} - v - \bar{v})\right)$ by coupling u and v

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- Exploit the symmetries of this kernel, which is invariant by $(u,v) \mapsto (\bar{u}, v)$ $(u,v) \mapsto (u,\bar{v})$, $(u,v) \mapsto (\bar{u},\bar{v})$ (the reflection principle)

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- Plus one more coupling between u and v.

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One obtains an explicit expression of $P_\delta(q)$ at every $q\neq -1$ such that $q^{d+1}=-1$, and this is enough to reconstruct the whole polynomial $P_\delta(u)$ (and in particular, $P_\delta(1)$) by interpolation.

The final result

The generating function $\mathsf{I}_d(t) = \sum_{n \geq 0} \mathsf{I}_{d,n} t^n$ is

$$\mathsf{I}_d(t) = \frac{d(d+1)}{4(1-t)} - \frac{1}{8(d+1)^2} \sum_{k,j=0}^{d} \frac{(c_j + c_k)^2}{s_j^2 s_k^2} \frac{1}{1 - t x_{jk}}$$

with

$$c_k = \cos \alpha_k, \quad s_k = \sin \alpha_k, \quad \alpha_k = \frac{(2k+1)\pi}{2d+2},$$

and

$$x_{jk} = 1 - \frac{4}{d}(1 - c_j c_k).$$

Perspectives

- Other generators (ex: all transpositions [Sjöstrand 10], transpositions $(0, i)$, block transpositions...)

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Thank you!

Around the mixing time (super-cubic regime)

Assume $n \sim \kappa d^3 \log d$.

- If $\kappa < 1/\pi^2$, there exists $\gamma > 0$ such that

$$\mathsf{I}_{d,n} \leq \frac{d(d+1)}{4} - \Theta(d^{1+\gamma}),$$

- If $\kappa > 1/\pi^2$, there exists $\gamma > 0$ such that

$$\mathsf{I}_{d,n} = \frac{d(d+1)}{4} - O(d^{1-\gamma}).$$

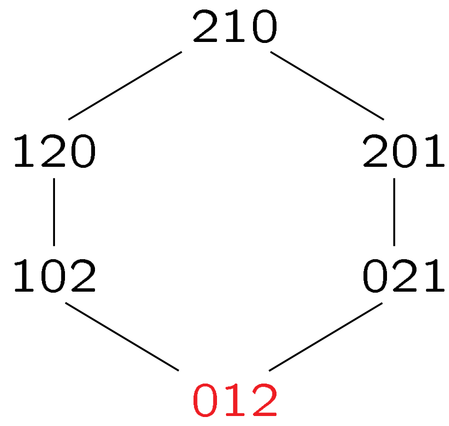
- For the critical value $\kappa = 1/\pi^2$, the following refined estimate holds: if $n \sim 1/\pi^2 d^3 \log d + \alpha d^3 + o(d^3)$, then

$$\mathsf{I}_{d,n} = \frac{d(d+1)}{4} - \frac{16d}{\pi^4} e^{-\alpha\pi^2}(1 + o(1)).$$

What do we ask? What do we expect?

Let $Q = (Q_{\sigma,\tau})$ be the transition matrix of the chain:

$$Q = \begin{pmatrix} 0 & 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 0 & 1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \end{pmatrix}$$



- Then for all $\sigma \in \mathfrak{S}_{d+1}$,

$$\sum_{n\geq 0} \mathbb{P}\left(\pi^{(n)} = \sigma\right) t^n = \sum_{n\geq 0} Q^n_{\mathrm{id},\sigma}\, t^n = \left((1-tQ)^{-1}\right)_{\mathrm{id},\sigma}$$

is a rational series in t.

- The GF of the expected inversion number

$$\sum_{n\geq 0} \mathbb{E}(I_{d,n}) t^n = \sum_{n\geq 0} \left(\sum_{\sigma\in\mathfrak{S}_{d+1}} \mathrm{inv}(\sigma) \mathbb{P}\left(\pi^{(n)} = \sigma\right) \right) t^n = \sum_{\sigma\in\mathfrak{S}_{d+1}} \mathrm{inv}(\sigma) G_\sigma(t)$$

is rational as well.