Growth of Quasicrystals by a Relaxation Process

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Tilings are often used as a toy model for quasicrystals, with the ground states corresponding to the tilings satisfying some local properties (matching rules). In this context, a challenging problem is to provide a theory for quasicrystals growth. We consider here one of the proposed theories, namely a relaxation process. One assumes that the entropy of a tiling increases with the number of tilings which can be formed with the same tiles, while its energy is proportional to the ratio of satisfied matching rules. Then, by starting from an entropically stabilized tiling at high temperature and by decreasing the temperature, the phason flips which decrease (resp. increase) the energy would become more and more favoured (resp. inhibited). Ideally, the tiling eventually satisfies all the matching rules, and thus shows a quasicrystalline structure.

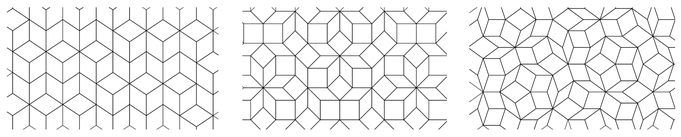
General Settings

Canonical tilings

Canonical $n \to d$ *tiling*: covering of $\mathbb{R}^d$ by interior-disjoint *tiles*:

$$\left\{\vec{x} + \lambda_1\vec{v}_{i_1} + \ldots + \lambda_d\vec{v}_{i_d} \,|\, 0 \leq \lambda_1, \ldots, \lambda_d \leq 1\right\},$$

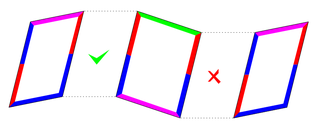
where $\vec{v}_1, \ldots, \vec{v}_n$ are non-colinear vectors of $\mathbb{R}^d$ and $n > d \geq 1$.



Physically, a tile model a stable local configuration of atoms, while tilings model the possible global configurations. Quasicrystals correspond to some particular non-periodic "straight" tilings.

Matching rules

Tile's *decoration*: real function (color) defined over its boundary. Two decorated tiles *match* if their decorations take the same value in each intersecting point (if any).

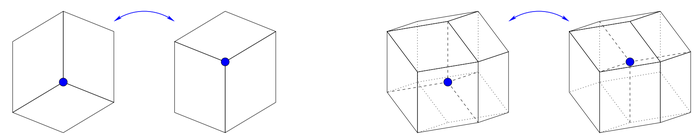


Set τ of decorated tiles $\rightsquigarrow$ set X_τ of tilings, in which tiles match. Interesting case: tilings in X_τ model quasicrystals.

Physically, matching rules model short-range interactions between atoms, with the energy being proportional to the ratio of matching tiles (tilings in X_τ thus model ground states).

Flips

If a vertex x of a $n \to d$ tiling belongs to exactly $d+1$ tiles, then performing a *flip* around $\vec{x}$ consists in translating each of these tiles by the vector which belongs to the d other tiles.



Physically, a flip models a local rearrangement of atoms.

Flips act over tilings, with the tiles proportions being conserved. The question whether two tilings with identical tiles proportions can be connected by a sequence of flips (*ergodicity*) is not trivial.

Relaxation Process

The stability of a material at temperature T is governed by the minimization of its free energy $F = E - TS$. Usually, the internal energy E of a finite decorated tiling is defined by the number of its mismatches, while its entropy S is defined by the logarithm of the number of different tilings which can be obtained by rearranging tiles. We then model the evolution of a tiling with the temperature by the following Markov chain $(x_t)_{t\in\mathbb{N}}$:

1. The temperature parameter T starts from a very high initial value T_0 and varies in a specified way (*temperature schedule*) up to reach zero.
2. We start from a finite decorated $n \to d$ tiling x_0 whose tiles do not necessarily all match, but can do it up to some rearrangement (which do not modify the covered subset of $\mathbb{R}^d$).
3. Given $x = x_t$ and $T > 0$, we choose uniformly at random a flippable vertex of x and we denote by y the tiling obtained by performing this flip. We then choose uniformly at random $\alpha \in [0, 1]$, and we set $x_{t+1} := y$ or $x_{t+1} := x$, depending whether or not α is lower than
$$\frac{\exp(-E(y)/T) \times F(x)}{\exp(-E(x)/T) \times F(y)},$$
where $E(z)$ and $F(z)$ respectively denotes the number of mismatches and the number of flippable vertices of a tiling z.

At fixed T, this is just a Metropolis-Hasting algorithm which draws samples from the Boltzmann distribution. Moreover, under some conditions (Random Tiling Hypothesis), the initial tiling x_0 has maximal entropy among tilings with the same number of tiles (hence is stable at $T = T_0$).

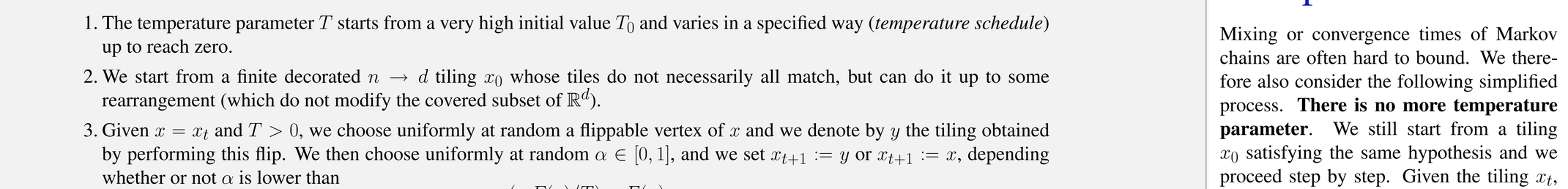
Does this process converge towards a mismatch-free tiling? At which rate?
How does it depends on the temperature schedule? Which one is optimal?

Simplified Process

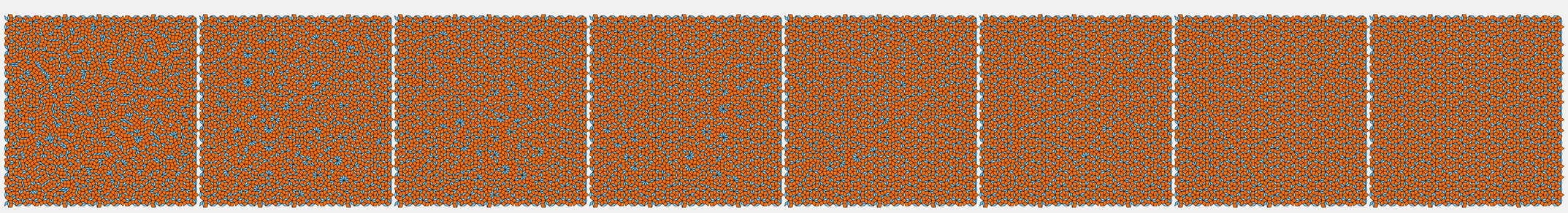
Mixing or convergence times of Markov chains are often hard to bound. We therefore also consider the following simplified process. **There is no more temperature parameter**. We still start from a tiling x_0 satisfying the same hypothesis and we proceed step by step. Given the tiling x_t, **we choose uniformly at random a flip which does not increase the number of mismatches**. If there is no such flip, the process stops. Otherwise, x_{t+1} is the tiling obtained by performing this flip. In other words, flip probability obeys to a $0-1$ law.

It experimentally similarly runs, but faster and without noise. However, there is yet no result for ergodicity with forbidden flips.

Two Examples



Snapshots (each 600 flips) of the evolution under the simplified process of an initial random canonical $3 \to 2$ tiling made of 4914 tiles. It converges towards a periodic dimer tiling.
The total number of flips to correct a tiling of n tiles is conjectured to be at most $O(n^3)$, and $O(n^{3/2})$ in average.



Snapshots (each 5000 flips) of the evolution under the simplified process of an initial random canonical $5 \to 2$ tiling made of 3500 tiles. It converges towards a Penrose tiling.
The total number of flips to correct a tiling of n tiles is conjectured to be at most $O(n^3)$, and $O(n^{3/2})$ in average.