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Random sampling of lattice paths with constraints, via transportation

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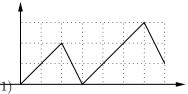
received 7th December 2009,

We discuss a Monte Carlo Markov Chain (MCMC) procedure for the random sampling of some one-dimensional lattice paths with constraints, for various constraints. We show that an approach inspired by *optimal transport* allows us to bound efficiently the mixing time of the associated Markov chain. The algorithm is robust and easy to implement, and samples an "almost" uniform path of length n in $n^{3+\varepsilon}$ steps. This bound makes use of a certain *contraction property* of the Markov chain, and is also used to derive a bound for the running time of Propp-Wilson's *Coupling From The Past* algorithm.

Keywords: lattice paths, random sampling, MCMC, discrete Ricci curvature

1 Lattice Paths with Constraints

We are interested in this paper in some families of one-dimensional lattices paths. We fix three integers n, a, b > 0, and consider the paths of length n, with steps +a/-b, that is, the words of n letters taken in the alphabet $\{a, -b\}$. Such a word $s = (s_1, s_2, \ldots, s_n)$ is identified to the path $S = (S_1, \ldots, S_n) := (s_1, s_1 + s_2, \ldots, s_1 + s_2 + \cdots + s_n)$. On the right, one sees the lattice path S = (1, 2, 0, 1, 2, 3, 1)



associated to the word s = (1, 1, -2, 1, 1, 1, -2). The problem we discuss here is to sample efficiently uniform (or *almost* uniform) paths in a sub-family A_n of paths, with Markov chains.

To illustrate the methods and the results, we focus on three particular sub-families.

- 1. Discrete *meanders*, denoted by \mathcal{M}_n , which are simply the non-negative paths: $S \in \mathcal{M}_n$ if for any $i \leq n$ we have $S_i \geq 0$. This example is mainly illustrative because the combinatorial properties of meanders make it possible to perform exact sampling very efficiently (an algorithm running in $\mathcal{O}(n^{1+\varepsilon})$ steps is given in [2], an order that we cannot obtain in the present paper).
- 2. Paths with walls; a path with a wall of height h between r and s is a path such that $S_i \geq h$ for any $r \leq i \leq s$ (see Fig. 1 for an example). These are denoted by $\mathcal{W}_n = \mathcal{W}_n(h,r,s)$, they appear in statistical mechanics as toy models for the analysis of random interfaces and polymers (see examples in [5]).

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3. Culminating paths, denoted by C_n , which are non-negative paths whose maximum is attained at the last step: for any i we have $0 \le S_i \le S_n$. They have been introduced in [2], motivated in particular by the analysis of some algorithms in bioinformatics.

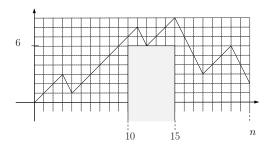


Fig. 1: A path of steps +1/-2, with a wall of height h=6 between i=10 and j=15.

Remark 1 The methods discussed here apply to any values of (a, b), but we have in mind the challenging case b > a: for our three families the ratio $\operatorname{card}(\mathcal{A}_n)/\operatorname{card}(\mathcal{P}_n)$ decreases exponentially fast, making impossible a naive rejection algorithm.

2 Sampling with Markov chains

In the sequel, we will consider Markov chains in a family A_n , where all the probability transitions are symmetric. For a modern introduction to Markov chains, we refer to [6]. Hence we are given a transition matrix $(p_{i,j})$ of size $|A_n| \times |A_n|$ with

$$p_{i,j} = p_{j,i}$$
 whenever $i \neq j$, $p_{i,i} = 1 - \sum_{j \neq i} p_{i,j}$.

Lemma 2 If such a Markov chain is irreducible, then it admits as unique stationnary distribution the uniform distribution $\pi = \pi(A_n)$ on A_n .

Proof: The equality $\pi(i)p_{i,j} = \pi(j)p_{j,i}$ holds for two any vertices i, j. This shows that the probability distribution π is reversible for $(p_{i,j})$, and hence stationnary. It is unique if the chain is irreducible.

This lemma already provides us with a scheme for sampling an almost uniform path in A_n , without knowing much about A_n . To do so, we define a "flip" operator on paths. Fix an integer $i \in \{1, 2, \ldots, n-1\}$ and a path $S = (S_1, \ldots, S_n)$; let (s_1, \ldots, s_n) be the corresponding word.

The path $\phi(\mathbf{S},i,\uparrow)$ is defined as follows: if $(s_i,s_{i+1})=(-b,a)=$ then these two steps are exchanged into (a,-b)=. The n-2 other steps remain unchanged. For the case $i=n, \phi(\mathbf{S},n,\uparrow)$

is simply the path the path associated to the word

$$(s_1,\ldots,s_{n-1},a).$$

The path $\phi(\mathbf{S}, i, \downarrow)$ is defined the same way: if $(s_i, s_{i+1}) = \bullet$, it turns into \bullet . The path $\phi(\mathbf{S}, n, \uparrow)$ is the path associated to $(s_1, \ldots, s_{n-1}, -b)$.

For the family $\mathcal{A}_n = \mathcal{C}_n$, we have to take another definition of $\phi(\mathbf{S}, n, \uparrow)$ and $\phi(\mathbf{S}, n, \downarrow)$, if we want the chain to be irreducible. Notice that since the maximum is attained at n, the $\lceil b/a \rceil + 1$ last steps are necessarily

$$(a, a, ..., a)$$
 or $(-b, a, ..., a)$.

We thus define $\phi(\mathbf{S}, n, \uparrow)$ as the path obtained by changing the $\lceil b/a \rceil + 1$ last steps into (a, a, \ldots, a) (regardless of their initial values in \mathbf{S}) and $\phi(\mathbf{S}, n, \downarrow)$ as the path obtained by changing the $\lceil b/a \rceil + 1$ last steps into $(-b, a, \ldots, a)$

We are also given a probability distribution $\mathbf{p} = (p_i)_{1 \le i \le n}$, and we assume that $p_i > 0$ for each i. We will take a particular sequence \mathbf{p} later on, but at this point we can think of it as the uniform distribution in $\{1, \ldots, n\}$. We can now describe the algorithm.

Algorithm 1 MCMC: Approximate sampling of a path in A_n

```
initialize \mathbf{S} \in \mathcal{A}_n I_1, I_2, \dots \leftarrow i.i.d. r.v. with law \mathbf{p} \varepsilon_1, \varepsilon_2, \dots \leftarrow i.i.d. uniform r.v. in \{\uparrow, \downarrow\} for t=1 to T do if \phi(\mathbf{S}, I_t, \varepsilon_t) is in \mathcal{A}_n then \mathbf{S} \leftarrow \phi(\mathbf{S}, I_t, \varepsilon_t) end if end for
```

In words, this algorithm performs the Markov chain in A_n with transition matrix $P = (P_{\mathbf{R},\mathbf{S}})_{\mathbf{R},\mathbf{S}\in\mathcal{A}_n}$ defined as follows:

$$\begin{cases} P_{\mathbf{R},\mathbf{S}} &= p_i/2, \text{ if } \mathbf{S} = \phi(\mathbf{R},i,\varepsilon) \text{ for some } \varepsilon \text{ and } 0 \text{ otherwise,} \\ P_{\mathbf{R},\mathbf{R}} &= 1 - \sum_{\mathbf{S} \neq \mathbf{R}} P_{\mathbf{R},\mathbf{S}}. \end{cases}$$

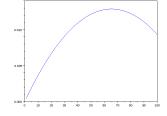
Proposition 3 Denote by S(t) the path sampled by the t-th run of the loop in Algorithm 1. When $t \to \infty$, the sequence S(t) converges in law to the uniform distribution in A_n .

Proof: We have to check that the chain is aperiodic and irreducible. Aperiodicity comes from the (many) loops. Irreducibility will follow from Lemma 5.

We fix now the distribution (p_i) . Instead of $p_i = 1/n$, we will use the weights defined by (see the plot of $i \mapsto p_i$ for n = 100 on the right):

$$p_i := \frac{4i}{n(n+1)} - \kappa_0 \frac{i(i+1)}{2} \quad (\text{ for } i = 1, \dots, n), \tag{1}$$

where $\kappa_0 = \frac{6}{n(n+1)(n+2)} \sim 6n^{-3}$. We leave the reader check that $(p_i)_{i \leq n}$ is indeed a probability distribution.



The reason for which we use this particular distribution will appear in the proof of Proposition 6. We will need at the time the following relation: for each $1 \le i \le n-1$,

$$2p_i - p_{i-1} - p_{i+1} = \kappa_0. (2)$$

Remark 4 There are obviously many other Markov chains which are reversible with respect to the uniform measure, and some of them may seem more natural to the reader. However, such Markov chains are in general neither monotonous (see later Section 4) nor of positive Ricci curvature (Section 3). The latter condition is essential for our purpose.

2.1 Analysis of Algorithm 1

We could deduce from a brief glance at Algorithm 1 that the time-complexity is always linear in T, but we have to pay attention to what is hidden behind each run of the for loop.

- If $I_t < n$, the time needed for the test " $\phi(\mathbf{S}, I_t, \varepsilon_t)$ is in \mathcal{A}_n " can be considered as constant, since we only have to compare 0, S(i), S(n).
- If $I_t = n$, the new value S(n) is compared with the maximum of S, which can be done in O(n). Fortunately, this occurs with probability $p_n = O(n^{-1})$, so that the time-complexity of each loop is, in average, a O(1).

For Algorithm 1 to be efficient, we need to know how S(T) is close in law to π . This question is related to the spectral properties of the matrix P. In particular, the speed of convergence is governed by the spectral gap (i.e. $1 - \lambda$, where λ is the largest of the modulus of the eigenvalues different from one, see [8] for example), but this quantity is not known in general. Some geometrical methods [4] allow to bound from below $1 - \lambda$, but they assume a precise knowledge of the structure of the graph defined by the chain P. It seems that such results do not apply here.

Instead, we will study the metric properties of the chain P with respect to a natural distance on A_n , and show that it satisfies a certain *contraction property*.

3 Error estimates with contraction

Going back to a more general setting, we consider a Markov chain in a finite set V, endowed with a metric d. For a vertice $x \in V$ and a transition matrix P, we denote by $P\delta_x$ (resp. $P^t\delta_x$) the law of the Markov chain associated to P at time 1 (resp. t), when starting from t. For t, t, the main assumption

made on P is that there exists a coupling between $P\delta_x, P\delta_y$ (that is, a random variable (X_1, Y_1) with $X_1 \stackrel{\text{law}}{=} P\delta_x, Y_1 \stackrel{\text{law}}{=} P\delta_Y$) such that

$$\mathbb{E}\left[d(X_1, Y_1)\right] \le (1 - \kappa)d(x, y),\tag{3}$$

for some $\kappa > 0$, which is called the *Ricci curvature* of the chain, by analogy with the Ricci curvature in differential geometry⁽ⁱ⁾. If the inequality holds, then it implies that P admits a unique stationnary measure π and that, for any x,

$$\parallel P^t \delta_x - \pi \parallel_{\text{TV}} \le (1 - \kappa)^t \text{diam}(V), \tag{4}$$

where $\operatorname{diam}(V)$ is the diameter of the graph with vertices V induced by the Markov chain and $\|\cdot\|_{\mathrm{TV}}$ stands, as usual, for the *Total Variation distance*

$$\| \mu_1 - \mu_2 \|_{\text{TV}} := \sup_{A \subset V} |\mu_1(A) - \mu_2(A)|.$$

Hence, a positive Ricci curvature gives the exponential convergence to the stationnary measure, with an exact (again, exact means non-asymptotic) bound. In many situations, a smart choice for the coupling between X_1, X_2 gives a sharp rate of convergence in (4) (see [9]).

3.1 Metric properties of P

To apply the Ricci curvature machinery, we endowe each A_n with the L^1 -distance

$$d_1(S, S') = \frac{1}{a+b} \sum_{i=0}^{n} |S_i - S'_i|.$$

(Notice that $|S_i - S_i'|$ is always a multiple of a + b.) For our purpose, it is fundamental that this metric space is *geodesic*.

Lemma 5 (Families A_n **are geodesic)** Each A_n , equipped with the distance d_1 , is geodesic in the following sense: for two any $S, T \in A_n$ with $d_1(S, T) = k$, there exist k + 1 paths $S_0 = S, S_1, \ldots, S_k = T$ in A_n such that for each i

- $d_1(S_i, S_{i+1}) = 1$;
- S_i and S_{i+1} are neighbours in the Markov chain P.

This implies in particular that P is irreducible and that the diameter of P is smaller than $\max_{S,T} d_1(S,T) \le n(n+1)/2$.

Proof of Lemma 5: The proof goes by induction on k. We fix $S \neq T$ (and denote by s, t the corresponding words); we want to decrease $d_1(S,T)$ by one, by applying the operator $\phi(\cdot,i,\varepsilon)$ with proper i,ε . We denote by $i_0 \in \{1,\ldots,n\}$ the first index for which $S \neq T$:

$$S_0 = T_0, S_1 = T_1, \dots, S_{i_0-1} = T_{i_0-1}, S_{i_0} \neq T_{i_0}.$$

The Ricci curvature is actually the largest positive number such that (3) holds, for all the couplings of $P\delta_x$, $P\delta_y$; here we should rather say that Ricci curvature is larger than κ .

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For instance we have $T_{i_0} = S_{i_0} + a + b$. Let j be the left-most peak in T in $\{i_0 + 1, i_0 + 2, \dots, n\}$; if such a peak exist. Then $S' := \phi(\mathbf{T}, j, \downarrow)$ is also in \mathcal{A}_n : it is immediate for the three families $\mathcal{M}_n, \mathcal{W}_n, \mathcal{C}_n$. We have $d_1(S, S') = k - 1$.

If there does not exist a peak in T after i_0 , then $(t_{i_0+1},t_{i_0+2},\ldots,t_n)=(a,a,\ldots,a)$. Hence we try to increase the final steps of S by one. To do so, we chose $S':=\phi(\mathbf{S},n,\uparrow)$ if $S\neq\phi(\mathbf{S},n,\uparrow)$, or $S'=\phi(\mathbf{S},j,\uparrow)$ where j is the position of the right-most valley otherwise.

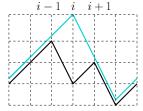
We will show that P's Ricci curvature w.r.t. this distance is (at least) of order $1/n^3$.

Proposition 6 For the three families \mathcal{M}_n , \mathcal{C}_n , \mathcal{W}_n , the Ricci curvature of the associated Markov chain, with weights defined as in (1), is larger than κ_0 .

Proof of Proposition 6:

Fix \mathbf{S} , \mathbf{T} in $\mathcal{A}_n \in \{\mathcal{M}_n, \mathcal{C}_n, \mathcal{W}_n\}$, we assume first that \mathbf{S} , \mathbf{T} are neighbours, for instance $\mathbf{T} = \phi(\mathbf{S}, i, \uparrow)$ for some i. Let $(\mathbf{S}^1, \mathbf{S}^2)$ be the random variable in $\mathcal{A}_n \times \mathcal{A}_n$ whose law is defined by

$$(\mathbf{S}^1, \mathbf{S}^2) \overset{(\text{law})}{=} (\phi(\mathbf{S}, \mathcal{I}, E), \phi(\mathbf{T}, \mathcal{I}, E)),$$



where \mathcal{I} is a r.v. $\{1, \dots, n\}$ with distribution \mathbf{p} and E is uniform in $\{\uparrow, \downarrow\}$. In other words, we run one loop of Algorithm 1 simultaneously on the both paths.

We want to show that S^1 , S^2 are, in average, closer than S, T. Three cases may occur: **Case 1.** $\mathcal{I} = i$ This occurs with probability p_i and, no matter the value of E, we have $S^1 = S^2$.

<u>Case 2. $\mathcal{I} = i - 1$ or i + 1.</u> We treat the case i - 1. Since **S** and **T** coincide everywhere but in i, we have necessarily one of these two cases:

- there is a peak in S at i-1 and neither peak nor valley in T at i-1 (as in the figure on the right);
- there is a valley in **T** at i-1 and neither peak nor valley in **S** at i-1.

In the first case for instance, then we may have $d_1(\mathbf{S}^1, \mathbf{S}^2) = 2$ if $E = \downarrow$, while the distance remains unchanged if $E = \uparrow$. The case $\mathcal{I} = i + 1$ is identical. This shows that with a probability smaller than $p_{i-1}/2 + p_{i+1}/2$ we have $d_1(\mathbf{S}^1, \mathbf{S}^2) = 2$.

Case 3. $\mathcal{I} \neq i-1, i, i+1$ In this case, **S** and **T** are possibly modified in \mathcal{I} , but if there is a modification it occurs in the both paths. It is immediate for the families $\mathcal{M}_n, \mathcal{W}_n$, less apparent for \mathcal{C}_n . In the latter we have to check that if $\phi(\mathbf{T}, \mathcal{I}, \uparrow)$ is in \mathcal{C}_n , so is $\phi(\mathbf{S}, \mathcal{I}, \uparrow)$. But this is true because we have $\max_j S_j = S_n = T_n$. Hence a flip in **S** at \mathcal{I} does not violate the *maximum-at-last-position* condition, because it does not violate this condition for **T**.

Thus, we have proved that when S, T only differ at i

$$\mathbb{E}\left[d_1(\mathbf{S}^1, \mathbf{S}^2)\right] \le 2 \times (p_{i-1}/2 + p_{i+1}/2) + 0 \times p_i + 1 \times (1 - p_i - p_{i-1}/2 - p_{i+1}/2)$$

$$\le (1 - \kappa_0) \times 1 = (1 - \kappa_0)d_1(S, T).$$
(5)

What makes Ricci curvature very useful is that if this inequality holds for pairs of neighbours then it holds for any pair, as noticed in [3]. Take indeed k paths $S_0 = S, S_1, \ldots, S_k = T$ as in Lemma 5 and apply the triangular inequality for d_1 :

$$\mathbb{E}\left[d_1(\phi(S, \mathcal{I}, E), \phi(T, \mathcal{I}, E))\right] \le \sum_{i=0}^{k-1} \mathbb{E}\left[d_1(\phi(S_i, \mathcal{I}, E), \phi(S_{i+1}, \mathcal{I}, E))\right]$$

$$\le (1 - \kappa_0)k = (1 - \kappa_0)d_1(S, T).$$

Remark 7 It is easy to exhibit some S, T such that inequality (5) is in fact an equality. In the case where $p_i = 1/n$, this equality reads $\mathbb{E}\left[d_1(\mathbf{S}^1, \mathbf{S}^2)\right] = d_1(S, T)$, and we cannot obtain a positive Ricci curvature (though, this does not prove that there does not exist **one** coupling for which we would get a $\kappa > 0$ in the case $p_i = 1/n$.).

Together with Eq. (4), this gives a first non-trivial result : for each A_n , Algorithm 1 returns a good approximation of π as soon as $T \gg n^3$.

3.2 Related works

Bounding mixing times via a contraction property over the transportation metric is a quite standard technique, the main ideas dating back to Dobrushin (1950's). A modern introduction is made in [8]. For geodesic spaces, this technique has been developed in [3] under the name *path coupling*.

The Markov chain P on lattice paths has been in fact already introduced⁽ⁱⁱ⁾ by D.Wilson [11] for lattice paths with a fixed end-point (as a first step for the sampling of random tilings), with uniform weights $p_i = 1/n$. The author also proves a mixing time of order $n^3 \log n$, by computing the deviations of a kind of Fourier transform of the heights of the paths. It is not apparent to us that this method goes through for paths with our kinds of constraints (when the end-point is not fixed).

4 Coupling From The Past with P

Propp-Wilson's Coupling From The Past (CFTP) [10] is a very general procedure for the exact sampling of the the stationnary distribution of a Markov chain. It is efficient if the chain is monotonous with respect to a certain order relation \leq on the set V of vertices, with two extremal points denoted $\hat{0}$, $\hat{1}$ (*i.e.* such that $\hat{0} \leq x \leq \hat{1}$ for any vertice x). This is the case here for our three families, with the partial order

$$\mathbf{S} \preceq \mathbf{T}$$
 iff $S_i \leq T_i$ for any i .

For the family \mathcal{M}_{10} with a=1,b=-2 for instance, we have

$$\begin{split} \hat{0} &= \hat{0}_{meanders} = (1,1,-2,1,1,-2,1,1,-2,1), \\ \hat{1} &= \hat{1}_{meanders} = (1,1,1,1,1,1,1,1,1). \end{split}$$

It is easy to check that for each n families C_n and W_n also admit extremal points $\hat{0}, \hat{1}$. We describe in Algorithm 2 CFTP in our context.

⁽ii) It is considered in [11] 2d-paths from (0,0) to (x,y) with steps East/North. These are, up to a linear transformation, one-dimensional paths of length x+y with steps +x/-y, starting and ending at zero.

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Algorithm 2 CFTP: Exact sampling of a path in A_n

```
\begin{split} \mathbf{S} &\leftarrow \hat{\mathbf{0}}, \mathbf{T} \leftarrow \hat{\mathbf{1}} \\ &\dots, I_{-2}, I_{-1} \leftarrow \text{i.i.d. r.v. with law } \mathbf{p} \\ &\dots, \varepsilon_{-2}, \varepsilon_{-1} \leftarrow \text{i.i.d. uniform r.v. in } \{\uparrow, \downarrow\} \\ &\tau = 1 \\ \textbf{repeat} \\ &\mathbf{S} \leftarrow \hat{\mathbf{0}}, \mathbf{T} \leftarrow \hat{\mathbf{1}} \\ &\mathbf{for} \ t = -\tau \ \text{to } 0 \ \mathbf{do} \\ &\mathbf{if} \ \phi(\mathbf{S}, I_t, \varepsilon_t) \ \text{is in } \mathcal{A}_n \ \mathbf{then} \ \mathbf{S} \leftarrow \phi(\mathbf{S}, I_t, \varepsilon_t) \\ &\mathbf{if} \ \phi(\mathbf{T}, I_t, \varepsilon_t) \ \text{is in } \mathcal{A}_n \ \mathbf{then} \ \mathbf{T} \leftarrow \phi(\mathbf{T}, I_t, \varepsilon_t) \\ &\mathbf{end for} \\ &\tau \leftarrow 2\tau \\ &\mathbf{until } \mathbf{S} = \mathbf{T} \end{split}
```

We refer to ([6],Chap.10) for a very clear introduction to CFTP, and we only sketch here the reason why this gives indeed an exact sampling of the stationnary distribution.

- The output of the algorithm (if it ever ends!) is the state of the chain P which has been running "since time $-\infty$ ", and thus has attained stationnarity.
- The exit condition S = T ensures that it is not worth running the chain from T steps earlier, since the trajectory of any lattice path $\hat{0} \leq R \leq \hat{1}$ is "sandwiched" between those of $\hat{0}, \hat{1}$, and therefore ends at the same value.

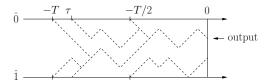


Fig. 2: A sketchy representation of CFTP : trajectories starting from $\hat{0}$, $\hat{1}$ at time -T/2 don't meet before time zero, while those starting at time -T do.

Proposition 8 Algorithm 2 ends with probability 1 and returns a exact sample of the uniform distribution over A_n . This takes in average $O(n^3(\log n)^2)$ time units.

Proof (sketch of): It is shown in [10] that Algorithm 2 returns exact sampling in $\mathcal{O}(t_{\mbox{mix}}\log H)$ runs of the chain , with

$$t_{\text{mix}} := \left\{ t \ge 0 \; ; \; \sup_{v \in V} \| P^t \delta_v - \pi \|_{\text{TV}} \le e^{-1} . \right\},$$

where $\|\cdot\|_{\text{TV}}$ stands, as usual, for the *Total Variation distance*; H is the length of the longest ordered chain of states between $\hat{0}$ and $\hat{1}$. It is a consequence of the proof of Lemma 5 that $H = \mathcal{O}(n^2)$. About

 t_{mix} , we have, for instance by ([8], p.189),

$$t_{\text{mix}} \leq \frac{1}{\kappa_0} \left(\log(\text{diam}V) + 1 \right),$$

hence $t_{\min} = \mathcal{O}(n^3 \log n)$. Recall that under Section 2.1, each test in Algorithm 2 takes, in average, $\mathcal{O}(1)$ time units.

5 Concluding remarks and simulations

1. We show in Fig.3 simulations of the three kinds of paths, for n=600. The final height of the culminating path is very low (about 30), it would be interesting to use our algorithms to investigate the behavior of this height when $n \to \infty$; this question was left open in [2].

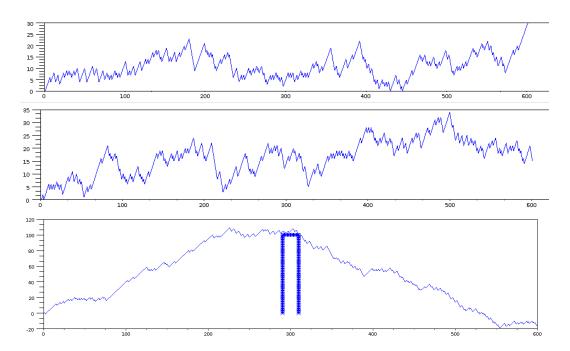


Fig. 3: (Almost) uniform paths of length 600. From top to bottom: a culminating path, a meander, a path with wall (shown by an arch).

2. One may wonder to what extent this work applies to other families A_n of paths. The main assumption is that the family of paths should be a geodesic space w.r.t. distance d_1 . This is true for example if the following condition on A_n is fulfilled:

$$(R, T \in \mathcal{A}_n \text{ and } R \leq S \leq T) \Rightarrow S \in \mathcal{A}_n.$$

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3. A motivation to do sampling of random paths is to make and test guesses for some functionals of these paths, taken in average over \mathcal{A}_n . Consider a function $f: \mathcal{A}_n \to \mathbb{R}$, we want an approximate value of $\pi(f) := \operatorname{card}(\mathcal{A}_n)^{-1} \sum_{s \in \mathcal{A}_n} f(s)$, if the exact value is out of reach by calculation. We estimate this quantity by

$$\hat{\pi}(f) := \frac{1}{T} \sum_{t=1}^{T} f(\mathbf{S}(t)),$$
(6)

(recall that S(t) is the value of the chain at time t). For Algorithm 1 to be efficient in practice, we have to bound

$$\mathbb{P}\left(|\pi(f) - \hat{\pi}(f)| > r\right),\tag{7}$$

for any fixed r > 0, by a non-asymptotic (in T) quantity. This can be done with ([7], Th.4-5), in which one can found concentration inequalities for (7). The sharpness of these inequalities depends on κ and on the geometrical structure of \mathcal{A}_n .

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