

# Shuffling permutations by swapping random pairs

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## 1 Introduction

A classical newbie error in programming is to shuffle an array or permutation by applying successive random transpositions as follows: [C code]

```
// initialize the array, but we will work with 0...N-1 instead in C.
for (int i = 0; i < N; i++)
    a[i] = i;
// for a number of iterations K that should depend on N
for (int t = 0; t < K; t++)
{
    int i = random(0,N-1); // pick element i uniformly from {0,...,N-1}
    int j = random(0,N-1); // independently of i
    swap(a,i,j); // swap positions i and j in a.
}
return a;
```

This procedure does not produce a uniform permutation of the array, and must be calibrated in order to approximate one by choosing  $K$  sufficiently large in order to ensure a certain approximation of a uniform permutation.

The evolution of the previous algorithm is modeled by a Markov Chain: that is, the namely the transition probabilities depend only on the current state of the permutation. We explain this. Let  $\pi_k$  be the permutation of  $[N] := \{1, \dots, N\}$  at time  $k$  (a random variable), then the definition is:

- at time 0 we have  $\pi_0 = [1, 2, 3, \dots, N]$ .
- at time  $t + 1 \geq 1$  we throw a random pair  $(i, j) \in [N] \times [N]$ , uniformly, and we swap the contents of positions  $i$  and  $j$ , namely  $\pi_{t+1}(k) := \pi_t(k)$  for  $k \neq i, j$  and  $\pi_{t+1}(i) := \pi_t(j)$ ,  $\pi_{t+1}(j) := \pi_t(i)$ . In this case we write  $\pi_{t+1} = (i, j)[\pi_t]$  to denote that we swap the entries.

Then  $(\pi_t)_t$  is a Markov Chain in which  $\Pr(\pi_{t+1} = \nu \mid \pi_t = \sigma) = 0$  if  $\nu$  and  $\sigma$  differ in more than two entries, if  $\nu = \sigma$  we have  $\Pr(\pi_{t+1} = \nu \mid \pi_t = \pi) = 1/N$ , and  $\Pr(\pi_{t+1} = \nu \mid \pi_t = \sigma) = 2/N^2$  if they differ in exactly two entries. Thus  $p_{\sigma, \nu} = \Pr(\pi_{t+1} = \nu \mid \pi_t = \sigma)$  depends only on the permutations  $\sigma$  and  $\nu$ .

**Important.** If the random pair  $(i, j)$  is chosen, the effect is the same as applying the transposition  $(\pi(i) \ \pi(j))$ . Thus we view the problem as shuffling by transpositions: at each time we choose  $(i, j) \in [N] \times [N]$  uniformly at random and apply the transposition  $(i \ j)$ .

We want to study the convergence of the distribution of  $\pi_t$  to the uniform distribution over all permutations. Let  $Q_k$  be the distribution after  $k$  steps, while we let  $U$  be the uniform distribution. Recall that, if we define the transition matrix  $P = [p_{\sigma, \nu}]_{\sigma, \nu \in S_N}$ , then  $Q_k = Q_0 P^k$ , where  $Q_0$  is thought of as a line vector  $Q_0 \in \mathcal{M}_{1 \times n!}(\mathbb{R})$ .

**Definition 1. (Total Variation Distance)** The total variation distance between to distributions  $P$  and  $Q$  over the same finite set of states  $S$  is defined by

$$\|Q - P\|_{\text{TV}} = \frac{1}{2} \sum_{s \in S} |Q(s) - P(s)|.$$

Equivalently,  $\|Q - P\|_{\text{TV}} = \max_{S' \subseteq S} |Q(S') - P(S')|$ , the maximum difference.

We are going to prove that the cut-off happens around  $K = \Theta(N \log N)$ , more precisely:

**Theorem 2.** *As  $N \rightarrow \infty$ , if  $K \ll (N/2) \log N$  we have  $\liminf \|Q_K - U\|_{\text{TV}} \geq 1 - e^{-1}$ , while, if  $K \gg 2N \log N$  we have  $\|Q_K - U\|_{\text{TV}} \rightarrow 0$ .*

The first statement tells us that  $\frac{N}{2} \log N$  shuffles are necessary, while the second one tells us that a bit more than  $2N \log N$  are enough. In this note we give a simple proof of this fact, based on the ideas in [1]. More precise results exist. In fact, it is known that the exact cut-off happens around  $\frac{1}{2}N \log N$ , see [2] for more.

## 2 Model and definitions

As mentioned, what we have is clearly a Markov Chain. This chain is actually Ergodic and, thus the distribution  $Q_k$  converges to its unique stationary distribution, which can easily be checked to be the uniform distribution  $U$ .

### 2.1 Ergodic Theorem

We recall that a Markov Chain is irreducible if and only if there is a path of nonzero probability between any two states (in both senses). This ensures that all states are reachable.

Second, a Markov Chain is aperiodic if and only if the greatest common divisor of the lengths of all cycles is one. By coprimality, this condition implies that there exists some  $L$  such that, for all  $k \geq L$  there is a path of length  $k$  (with strictly positive) between every pair of states, or even from a state to itself.

Both conditions together ensure the convergence to a **unique** stationary distribution, see e.g., [4]. Observe that these conditions can be verified from the transition matrix  $P$ , and do not involve the initial distribution  $\mu_0$ . Let us write  $\mu_t = \mu_0 P^t$ .

**Theorem 3.** *If a Markov Chain is both irreducible and aperiodic, then there is only one stationary distribution  $\mu_\infty$ , moreover, starting from any initial distribution  $\mu_0$  we have  $\mu_t \rightarrow \mu_\infty$ .*

In the case of our Markov Chain it is easy to verify that the uniform distribution is a stationary distribution. We remark that, since  $(a, b)[s]$  is the only state such that  $(a, b)[(a, b)[s]] = s$ ,

$$\mu_{t+1}(s) = \sum_{(a,b) \in [N] \times [N]} \mu_t((a,b)[s]) \frac{1}{N^2}.$$

Trivially we have

$$\frac{1}{N!} = \frac{1}{N^2} \sum_{(a,b) \in [N] \times [N]} \frac{1}{N!},$$

the uniform distribution is stationary. Since it is clear that the chain is irreducible and aperiodic, we have the convergence to the uniform distribution.

## 3 The coupon collector: a lower bound

A very simple lower bound we can produce for our problem is the following: surely, if some position  $i$  has not yet been swapped we have  $\pi_t(i) = i$ . Such an  $i$  is said to be a fixed-point of the permutation  $\pi_t$ . It is important to note (and we are not going to prove it here) that the set of permutations without fixed points  $\mathcal{D}_N$  satisfies  $|\mathcal{D}_N|/|S_N| \rightarrow e^{-1}$ .

Unfortunately, if  $K \leq (1 - \varepsilon) \frac{N}{2} \log N$ , we are going to show that  $\Pr(\pi_K \in \mathcal{D}_N) \rightarrow 0$ . This means that

$$\|Q_K - U\|_{\text{TV}} = \max_{A \subseteq S_N} |Q_K(A) - U(A)| \geq |Q_K(\mathcal{D}_N) - U(\mathcal{D}_N)| \rightarrow e^{-1}.$$

Hence we are far from converging to  $U$ .

In order to prove that there exists some  $i$  that has not yet been discovered by time  $K$ , we use the Coupon Collector Problem. The connection is simple: each  $i \in \{1, \dots, N\}$  is a coupon, and each pair  $(i, j)$  corresponds to drawing two new random coupons in the Coupon Collector Problem.

### 3.1 The coupon collector problem

The coupon collector problem reads as follows:

Suppose we had to collect a collection of  $N$  distinct coupon's. At the beginning we have zero coupons. Each time we buy a coupon, we obtain a coupon among those  $N$  uniformly at random. How long does it take to complete the full collection?

The answer is actually not that difficult. Let  $C = C_N$  be the necessary number of coupon's we have to buy.

**Notation 4.** Let us denote by  $X = \text{Geom}(q)$  a generic geometric random variable that is 1 based, i.e.  $\Pr(X = j) = q(1 - q)^{j-1}$  for  $j \in \mathbb{Z}_{>0}$ . Unless otherwise stated, all of the geometrics are independent rv.

With this notation we note that  $C_N = \text{Geom}(1) + \text{Geom}((N - 1)/N) + \dots + \text{Geom}(1/N)$ . The following is an immedaite consequence of  $\mathbb{E}[\text{Geom}(p)] = \frac{1}{p}$  for  $p > 0$ .

**Proposition 5.** The expected number of coupons we have to buy is  $\mathbb{E}[C_N] = N \cdot H_N$  where  $H_N = \frac{1}{1} + \frac{1}{2} + \dots + \frac{1}{N}$  are the Harmonic numbers. Moreover  $\mathbb{E}[C_N] \sim N \log N$ .

### 3.2 Cocentration on the expected value

In this case not only is  $\mathbb{E}[C_N] \sim N \log N$  but also  $C_N$  behaves like  $N \log N$  with high probability. We will use the convergence (or equivalent) in probability.

**Definition 6.** Let  $X_n$  be a sequence of positive random variables. We say that  $X_n \rightarrow L$  in probability if and only if, for every fixed  $\varepsilon > 0$  we have  $\Pr(|X_n - L| \geq \varepsilon) \rightarrow 0$  as  $n \rightarrow \infty$ .

**Definition 7.** Let  $X_n$  be a sequence of positive random variables and let  $(e_n)$  be a sequence of real numbers. We say that  $X_n \sim e_n$  if and only if  $X_n/e_n$  tends to one in probability.

To prove concetration we use Chebyshev's inequality: if the random variable  $X$  has finite first and second moments, for any  $\delta > 0$ ,

$$\Pr(|X - \mathbb{E}[X]| \geq \delta) \leq \frac{\sigma(X)}{\delta}, \quad \sigma(X) = \sqrt{\text{Var}(X)} = \sqrt{\mathbb{E}[(X - \mathbb{E}[X])^2]}.$$

The following lemma is a direction application of Chebyshev's inequality by picking  $\delta = \varepsilon \mathbb{E}[X_n]$ :

**Lemma 8.** Let  $X_n$  be a sequence of positive random variables such that  $e_n := \mathbb{E}[X_n]$  tends to infinity. If  $\mathbb{E}[X_n^2] \sim e_n^2$  we have that  $X_n \sim e_n$  in probability.

To better deal with the moments of our random variables  $C_N$ , we consider the probability generating functions. Observe that if  $X$  is a random variable taking values in the positive integers:

$$F_X(z) = \sum_k \Pr(X = k)z^k,$$

and then  $F'_X(1) = \mathbb{E}[X]$  and  $F''_X(1) = \mathbb{E}[X(X - 1)]$ .

In the case of  $C_N$  we simply have, due to the independence of each of the geometric random variables,

$$F(z) = F_N(z) = \prod_{i=1}^{N-1} \frac{zp_i}{1 - z(1 - p_i)}.$$

We show that we have the concentration in a more general setting for sums of geometric random variables:

**Lemma 9.** For each  $n$ , define  $(p_n(i))$  for  $i = 1, \dots, m(n)$  satisfying  $p_n(i) \in (0, 1]$ , where we suppose  $m(n) \rightarrow \infty$ . Let  $S_n = \sum_{i=1}^{m(n)} \text{Geom}(p_n(i))$ , then  $S_n \sim \mathbb{E}[S_n]$  in probability.

**Proof.** The PGF of  $S_n$  is

$$F(z) = F_n(z) = \prod_{i=1}^{m(n)} \frac{z p_n(i)}{1 - z(1 - p_n(i))}.$$

Observe that  $F'(z) = m(n) \frac{F(z)}{z} + F(z) \sum_{i=1}^{m(n)} \frac{(1 - p_n(i))}{1 - z(1 - p_n(i))}$ . Thus  $F'(1) = \sum_{i=1}^{m(n)} \frac{1}{p_n(i)}$ . We note that the expected value is  $\mathbb{E}[S_n] = \sum_{i=1}^{m(n)} \frac{1}{p_n(i)} \geq m(n) \rightarrow \infty$ .

Differentiating again,

$$F''(1) = m(n) \sum_{i=1}^{m(n)} \frac{1}{p_n(i)} - m(n) + \left( \sum_{i=1}^{m(n)} \frac{1}{p_n(i)} \right) \left( \sum_{i=1}^{m(n)} \frac{1 - p_n(i)}{p_n(i)} \right) + \sum_{i=1}^{m(n)} \frac{(1 - p_n(i))^2}{p_n(i)}.$$

Which we can simplify to:

$$F''(1) = -m(n) + \left( \sum_{i=1}^{m(n)} \frac{1}{p_n(i)} \right)^2 + \sum_{i=1}^{m(n)} \frac{(1 - p_n(i))^2}{p_n(i)}.$$

Here we note that  $\sum_{i=1}^{m(n)} \frac{(1 - p_n(i))^2}{p_n(i)} \leq \sum_{i=1}^{m(n)} \frac{1}{p_n(i)} = o\left(\left(\sum_{i=1}^{m(n)} \frac{1}{p_n(i)}\right)^2\right)$  and similarly  $m(n) = o\left(\left(\sum_{i=1}^{m(n)} \frac{1}{p_n(i)}\right)^2\right)$  too. Thus  $\mathbb{E}[S_n(S_n - 1)] = \mathbb{E}[S_n^2] - \mathbb{E}[S_n] = F''(1) \sim \left(\sum_{i=1}^{m(n)} \frac{1}{p_n(i)}\right)^2 = (\mathbb{E}[S_n])^2$ .  $\square$

**Corollary 10.** For any fixed  $\varepsilon > 0$ ,  $\Pr((1 - \varepsilon)N \log N \leq C_N \leq (1 + \varepsilon)N \log N) \rightarrow 1$ .

### 3.3 Coupon collector and fixed points in the process

In the case of the Coupon Collector much more is known. The following is a classical inequality:

**Proposition 11.**  $\Pr(C_N \geq N \log N + \theta N) \leq e^{-\theta}$  for every  $\theta \in \mathbb{R}$ .

**Proof.** Remark that  $\Pr(C_N \geq M)$ , for  $M$  integer, is the probability that at least one of the coupons is missing at time  $M$ . Let  $A_i(M)$  be the event that coupon  $i$  is missing. Observe that  $\Pr(A_i(M)) = \left(1 - \frac{1}{N}\right)^M$ .

By the union bound:

$$\Pr(C_N \geq M) = \Pr\left(\bigcup_{i=1}^N A_i(M)\right) \leq \sum_{i=1}^N \Pr(A_i(M)) = N \times \left(1 - \frac{1}{N}\right)^M.$$

Since  $1 + x \leq e^x$  for all  $x \in \mathbb{R}$ , we deduce  $N \times \left(1 - \frac{1}{N}\right)^M \leq N e^{-M/N}$ . Being  $C_N$  an integer, we deduce that  $\Pr(C_N \geq N \log N + \theta N) = \Pr(C_N \geq \lceil N \log N + \theta N \rceil)$  and the result follows.  $\square$

Actually, this inequality can be made more precise by using more terms from the so-called Bonferroni inequalities (the partial sums of the inclusion-exclusion provide bounds). That is the idea behind the proof of the following result from Erdős and Rényi [3].

**Theorem 12.**  $\Pr(C_N < N \log N + \theta N) \rightarrow \exp(-e^{-\theta})$  as  $N \rightarrow \infty$ , for every  $\theta \in \mathbb{R}$ .

The distribution function  $\theta \mapsto \exp(-e^{-\theta})$  is known as a Gumbel distribution.

## 4 Uniform stopping rule: an upper bound

### 4.1 Strong uniform time and convergence

Aldous and Diaconis introduced in [1] the concept of *strong uniform time*. A uniform stopping time  $T$  for  $(\pi_t)$ , is a stopping time, i.e.,  $\{T \leq t\}$  can be determined from our knowledge at time  $t$ , such that  $\Pr(\pi_t = \sigma \mid T = t) = 1/N!$ , i.e., that the distribution when the stopping time  $T$  tells us to stop  $\mu(\sigma) = \Pr(\pi_t = \sigma \mid T = t)$  is uniform.

Of course, here we have adapted the definition to our context, but it extends easily to other contexts. The key interest of a strong uniform time is the following bound (see Lemma 1 in [1]):

**Proposition 13.** *Let  $T$  be a uniform stopping time and let  $U$  be the uniform distribution, then  $\|Q_k - U\|_{\text{TV}} \leq \Pr(T > k)$ .*

That is, the total variation distance between  $Q_k$ , the distribution of  $\pi_k$ , and the uniform distribution  $U$  is at most  $\Pr(T > k)$ .

## 4.2 Perfectly stopping our Markov Chain

We define an increasing family of sets as follows:

- Let  $S_0 = \{1\}$  (the choice of 1 is arbitrary and not important).
- Given  $S_t$  we define  $S_{t+1}$  as follows. First,  $S_t \subseteq S_{t+1}$ . If the next random pair  $(a_{t+1}, b_{t+1})$  satisfies  $a_{t+1} \in S_t$  then  $b_{t+1}$  is added to  $S_{t+1}$ . Else if  $a_{t+1} = b_{t+1}$ , then add  $a_{t+1}$  to  $S_{t+1}$ .

The invariant is the following: the restriction of  $\pi_t$  to  $S_t$  is a uniform permutation. This is easily proven by induction. As  $S_t$  increases in size, at some point we obtain  $S_t = [N]$ .

We define our stopping time as follows:

$$T(\omega) = \inf \{t: S_t(\omega) = [N]\}.$$

**Proposition 14.** *[ $T$  is a strong uniform time]  $\Pr(\pi_k = \sigma \mid T = k)$  is uniformly distributed in  $\sigma$ .*

**Proof.** Suppose that  $\pi_k|_{S_k}$  is a uniform permutation for some  $k$ , we will show that this also holds for  $k+1$ . This is obvious if  $S_k = S_{k+1}$ , so suppose  $S_{k+1}$  has some new element  $j$ .

This means that the random pair  $(a_{k+1}, b_{k+1})$  was either  $(a, j)$  with  $a$  in  $S_k$  or it was  $(j, j)$ . Remark that all of these transpositions have equal probability of being produced. Most importantly, as  $j$  has the same probability of being swapped with any element in  $S_{k+1} = S_k \cup \{j\}$  we conclude that the resulting permutation (given that  $\pi_k|_{S_k}$  is a uniform permutation for some  $k$ ) is also uniform  $\pi_{k+1}|_{S_{k+1}}$ .  $\square$

**Remark 15.** It is possible to produce a perfect random permutation by keeping  $S_t$  and thus perfectly stopping our permutation. Of course, no one does this in practice, and there are much better ways to produce permutations.

## 4.3 Concentration of the stopping time

In this section we prove that the stopping time is concentrated around its expected value  $\mathbb{E}[T] \sim 2N \log N$ . Let us start by calculating the expected value. The probability of discovering a new number at time  $t+1$ , given that  $|S_t| = i$  is given by

$$p_i = \frac{i(N-i) + (N-i)}{N^2} = \frac{(i+1)(N-i)}{N^2},$$

independently of the past.

Thus we have

$$T = \sum_{i=1}^{N-1} \text{Geom}(p_i)$$

for certain independent geometric random variables.

**Proposition 16.** *The expected value satisfies  $\mathbb{E}[T] \sim 2N \log N$  as  $N \rightarrow \infty$ .*

**Proof.** It suffices to check that  $\mathbb{E}[T] = \sum_{i=1}^{N-1} \frac{1}{p_i} = \sum_{i=1}^{N-1} \frac{N^2}{(i+1)(N-i)} = N \sum_{i=1}^{N-1} \left( \frac{1}{i+1} + \frac{1}{N-i} \right)$ . Here we remark that  $H_{N-1} = \sum_{i=1}^{N-1} \frac{1}{N-i}$ , while  $\sum_{i=1}^{N-1} \frac{1}{i+1} = H_N - 1$ .  $\square$

Now, applying Lemma 9 we deduce the following corollary.

**Corollary 17.** *For any fixed  $\varepsilon > 0$ ,  $\Pr(T \geq (1 + \varepsilon)2N \log N) \rightarrow 0$ .*

Finally, Proposition 13 proves that  $\|Q_K - U\|_{TV} \rightarrow 0$  for  $K \geq (2 + \varepsilon)N \log N$ , for any  $\varepsilon > 0$ , completing the proof of our theorem.

## 5 Conclusions

The method proposed at the beginning is not very good; it requires  $\Theta(N \log N)$  random numbers from  $[N]$ . A simple algorithm that is efficient, and a perfect simulation, is the following [known as Knuth's shuffle or the Fisher-Yates shuffle]

```
// initialize the array, but we will work with 0...N-1 instead.
for (int i = 0; i < N; i++)
    a[i] = i;
// for each position choose one of the not-chosen elements
for (int i = 0; i < N; i++)
{
    int pos = random(i, N-1); // pick uniformly at random from {i, ..., N-1}
    swap(a, i, pos); // swap positions i and pos in a.
}
return a;
```

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