Rare Event Sampling Using Multicanonical Monte Carlo Method

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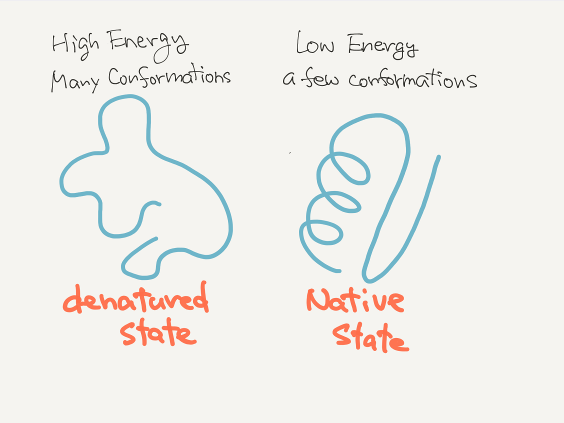
Outline

- Introduction: What is the Rare Event?
- Markov Chain Monte Carlo (Metropolis)
- Multicanonical MC
- Wang-Landau method
- Example: 2D Ising Model
- Application: Magic Square
- Multi-Self-Overlap Ensemble

Introduction

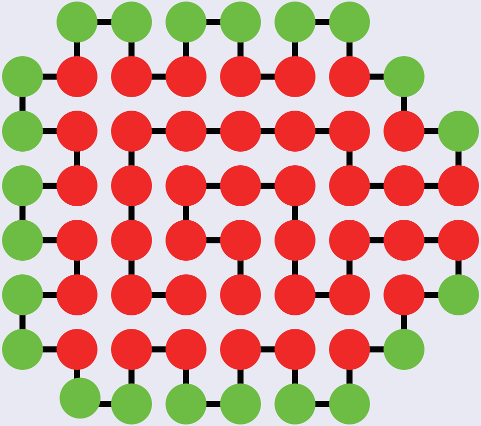
What is rare event?

Example: Protein folding



The native state is rare!

Lattice protein model (HP model)



A Red-Red contact gives energy -1. This conformation is one of the native ones

Purpose

- Sample the rare configuration using Monte Carlo method
- Count the number of such configurations
  - Degeneracy of the ground states / Residual entropy
- Free-energy landscape

Point to consider

- Random sampling is useless
  - Almost all the sampled conformations are high energy random ones.

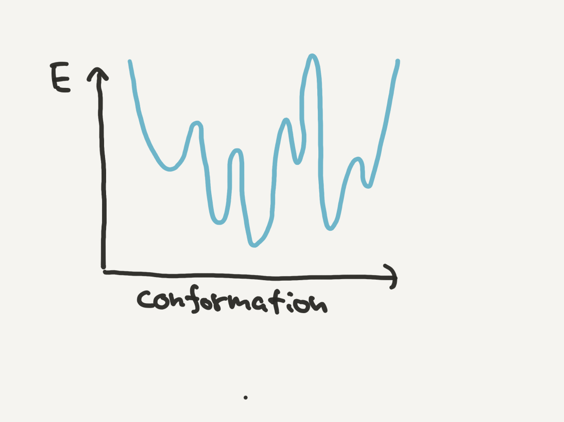
One step further

- Importance sampling
  - Apply bias to sample the desired conformations

Solution

- Markov chain Monte Carlo method at temperature T (MCMC or Metropolis method)
  - MCMC at low T will generate low energy states.

Problem of rough energy landscape



How to overcome the energy barrier

Optimization method

- If we only need some of the low-energy states, we can use numerical optimization methods

example

- Simulated annealing (SA)
- Genetic algorithm (GA)

Capables and uncapables of optimization methods

1. capables
   - generate some low-energy states
     - search for ground states
2. uncapables
   - count the number of the low-energy states
   - finite-temperature properties
     - free-energy landscape

Solution

Rare-event samplinc by multicanonical MC

Markov Chain Monte Carlo (Metropolis method)

Canonical ensemble

- Appearance probability of the microscopic state i at $\beta = 1/k_B T$

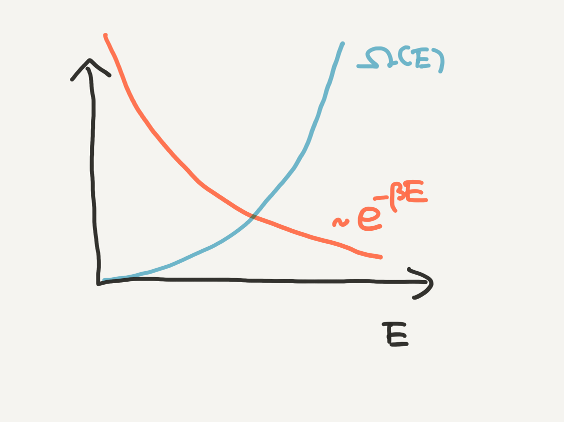
$$P_i \propto e^{-\beta E_i}$$

(Boltzman weight)

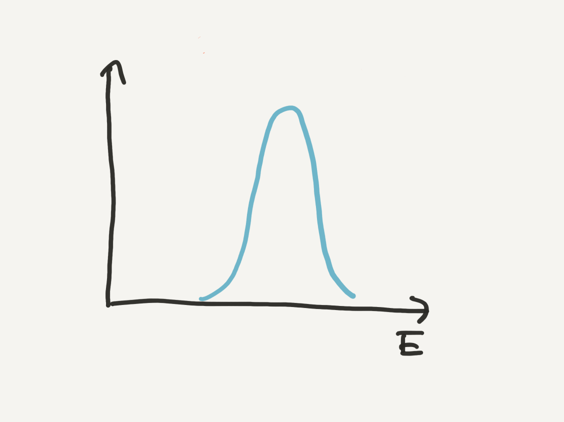
- Appearance probability of energy E

$$P(E) \propto \Omega(E) e^{-\beta E}$$

    - $\Omega(E)$: Number of states of energy E



Trade off of $\Omega(E)$ and the Boltzman weight



Energy distribution of the canonical ensemble

Markov Chain Monte Carlo

Sample microscopic states of temperature T using the computer simulations of a Markov chain

goal

Construct a Markov process that the average quantities (*e.g.* energy) in the steady state coincide with the thermal averages at temperature T

Markov process is defined by a set of the transition probability w_{ij} from jth microscopic state to ith states

requirement

1. $$0 \leq w_{ij} \leq 1$$
2. $$\sum_i w_{ij} = 1$$

Consider the probability distribution of microscopic state i at t-th step $P_i(t)$, then

$$\sum_i P_i(t) = 1$$

One step of evolution of the state according to the transition probability is

$$P_i(t+1) = \sum_j w_{ij} P_j(t)$$

In the vector and matrix notation

$$\vec{P}(t+1) = W\vec{P}(t)$$

W: Markov matrix
The large step limit

$$\vec{P}(\infty) = \lim_{n\to\infty} W^n \vec{P}(t_0)$$

Since the largest eigenvalue of the Markov matrix is 1, $\vec{P}_\infty$ is a steady state that satisfies

$$W\vec{P}(\infty) = \vec{P}(\infty)$$

requirement for W

Ergodicity

- System at an arbitrary state can reach all the states in finite steps
  - State space should be singly connected, otherwise the steady state is not uniquely determined.

Since the number of states is finite, the steady state is reached in a finite steps.

We require that the steady state coincides with the thermal equilibrium state

requirement

$$P_i(\infty) \propto \exp\left(-\frac{E_i}{k_B T}\right)$$

The following is the sufficient condition

Detailed balance

$$w_{ij} \exp\left(-\frac{E_j}{k_B T}\right) = w_{ji} \exp\left(-\frac{E_i}{k_B T}\right)$$

or

Detailed balance 2

$$\frac{w_{ij}}{w_{ji}} = \exp\left(\frac{-\Delta E_{ij}}{k_B T}\right)$$

where

$$\Delta E_{ij} \equiv E_i - E_j$$

The most widely used transition probability is

Metropolis transition probability

$$w_{ij} = \min\left[1, \exp\left(-\frac{\Delta E_{ij}}{k_B T}\right)\right]$$

Problem

The state space is usually astronomically huge

- In case of the two-state system with 1000 elements (very small considering today's computing power), the number of the microscopic states is $2^{1000} \simeq 10^{300}$. Thus the Markov matrix is $10^{300} \times 10^{300}$.

Solution

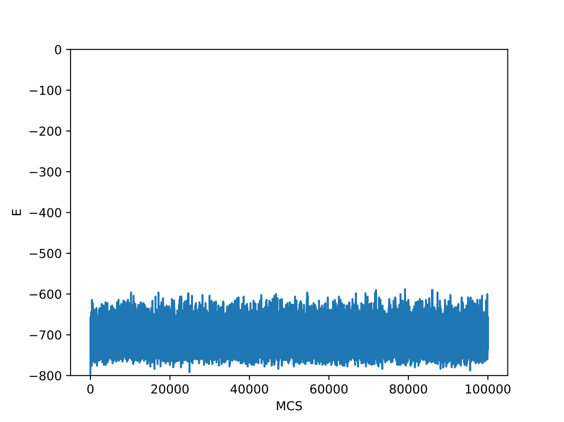
Instead of having the distribution vector $\vec{P}$, we carry a single microscopic state and follow its trajectory in the state spece by simulating the stochastic process.

Procedure

1. Prepare any initial state i
2. Make a candidate state j for the next step
3. Generate a random number R in $[0, 1]$ and compare to the transition probability w_{ji}
4. If $R \leq w_{ji}$, change the state to j. Otherwise, keep the state i.
5. Repeat many times

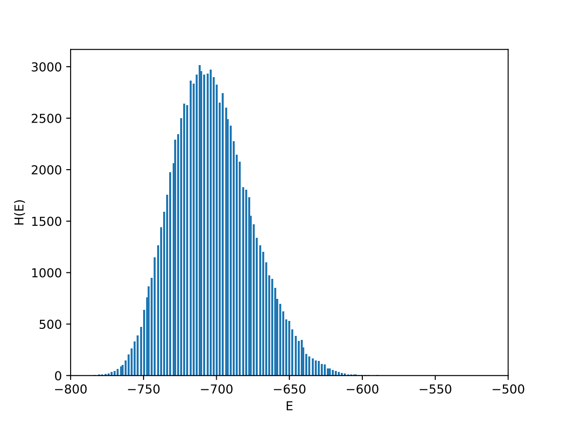
After sufficiently long steps, the system reaches the thermal equilibrium state. After that, the states obtained by the simulation are samples from the thermal equilibrium.

example: 2D Ising model (20×20)



Time series of energy ($\beta = 0.45$)

example: 2D Ising model (20×20)



Histogram of energy $(\beta = 0.45)$

Problem

- We cannot obtain the absolute probability P_i, because we do not know $\Omega(E)$.
- Only states in a narrow range of energy are sampled
  - Canonical ensemble

Multicanonical Monte Carlo method

purpose

Sample conformations from a wide range of energy using MCMC

- Multicanonical ensemble
  - Berg and Neuhaus (1991)
- Entropic sampling
  - Lee (1993)

idea

We can use any weight of function of energy, instead of Boltzman weight

$$P_i \propto e^{-f(E_i)}$$

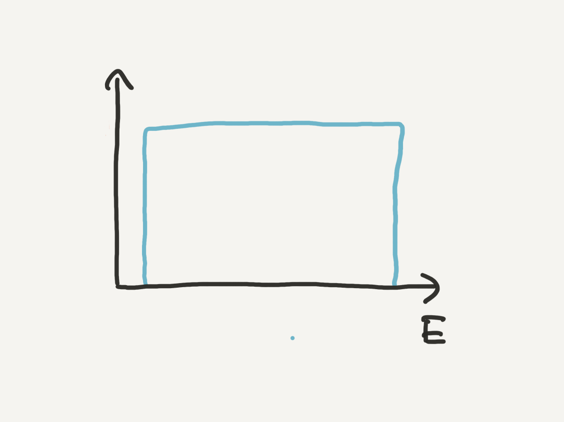
if we make the weight as

$$P_i \propto \frac{1}{\Omega(E_i)}$$

or

$$f(E_i) = \log \Omega(E_i) + const.$$

Then, energy distribution becomes constant (flat distribution)



Ideal energy distribution of multicanonical ensemble

Problem

$\Omega(E)$ is not known beforehand

Solution

Improve $f(E)$ step by step until it finally gives sufficiently flat distribution of energy

Multicanonical ensemble method consists of two stages

1. Preliminary run
   - Machine learning for determining $f(E)$
2. Measurement run
   - Long run for measuring physical quantities using fixed $f(E)$

In the original methods, E is divided into bins.

Original multicanonical ensemble

for ith bin

$$f(E) = \alpha_i + \beta_i E$$

- $\log \Omega(E)$ is approximated by a piecewise-linear function
  - assign different temperature to each bin (that is why it is called as multi-canonical

Entropic sampling

for ith bin

$$f(E) = \alpha_i$$

- multi-microcanonical ensemble

The entropic sampling is used in most cases, because it's simpler than the original multicanonical ensemble.

Wang-Landau method

Wang-Landau method

- Originaly proposed as an independent method from the multicanonical ensemble to estimate $\Omega(E)$
- Now it is considered as a method for preliminary run to determine $f(E)$
  - Applicable only to the entropic sampling
- Non-Markovian process
  - Transition probability changes at each step

Wang and Landau (2001)

idea

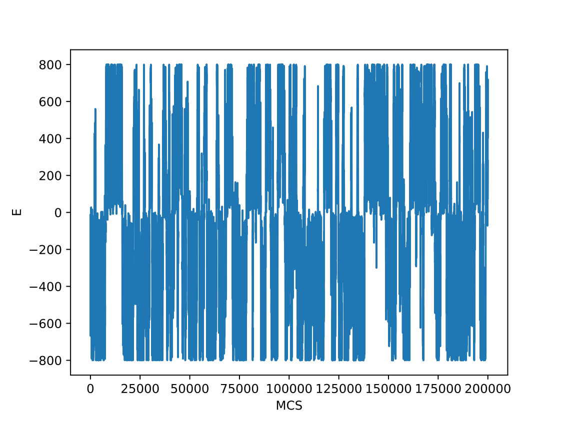
- When a conformation having energy E is visited, weight for E is reduced.
  - Visited energy is made to be more difficult to appear
- After many steps the energy histogram becomes flat and the weight is close to the multicanonical weight

procedure

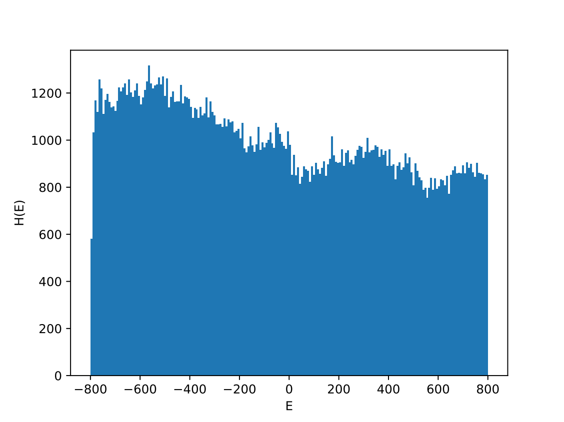
1. Initialize: set $f(E) = 1$ for all E
2. Run: When E_n is visited, $f(E_n) \to f(E_n) + df$
    - This step is repeated until the energy histogram is sufficiently flat
3. Reduce df (e.g. division by 2), reset the histogram, and repeat the whole procedure until df becomes sufficiently small

Finally, $f(E)$'s are determined.

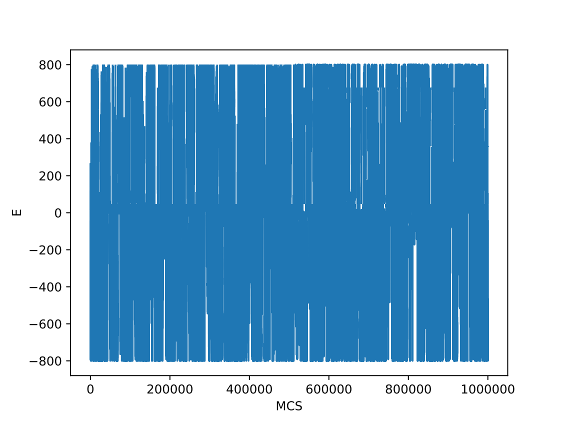
Example: 20×20 Ising model



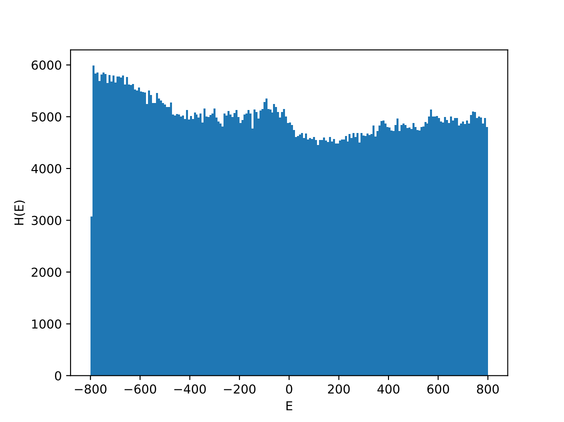
Time series of energy for the last run of Wang-Landau method



Energy histogram for the last run of Wang-Landau method



Time series of energy for the measurement run

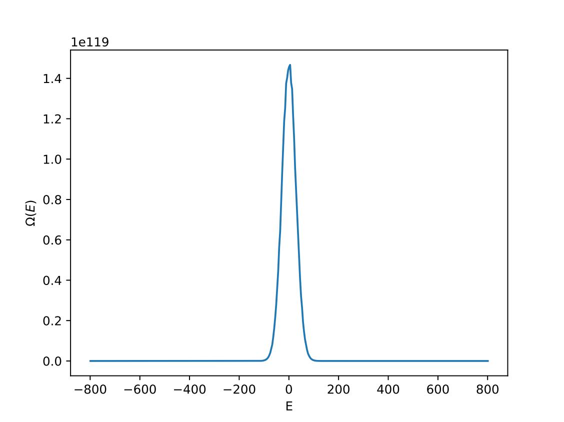


Energy histogram for the measurement run

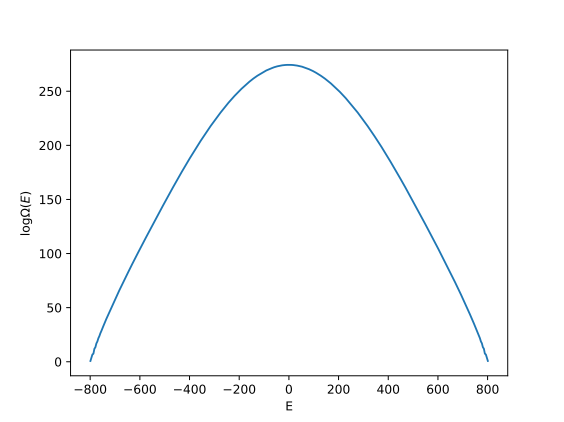
From the obtained energy histogram $H(E)$, $\Omega(E)$ is estimated as

$$\Omega(E) \propto H(E)e^{f(E)}$$

(Histogram reweighting method)



$\Omega(E)$ estimated from $H(E)$ and $f(E)$



$\log \Omega(E)$ estimated from $H(E)$ and $f(E)$

If the total number of the conformations is known as N, the number of conformations having the energy E_n as

$$N\frac{H(E_n)e^{f(E_n)}}{\sum_E H(E)e^{f(E)}}$$

Result

The estimated number of the ground state is 2.07

- cf. exact value, 2

Application to non-physical problems

Idea

Multicanonical ensemble with Wang-Landau method can be applied to sample rare states of non-physical systems, if an appropriate energy function (cost function) is defined

Example: The magic square

- Placing the numbers from 1 to n^2 in a square array using each number once, if all the sums of the numbers in each row, column and diagonal give the same value, the array makes a magic square
- Magic squares are numerous but rare

Then how rare?

- Count the number of the magic squares by the multicanonical method

Making rare conformations randomly

- Define the magicness

$$E = \sum_{row,column,diagonal} |sum - M|$$

  where M is the desired sum.
  - $E = 0$ if the array is a magic square, and $E > 0$ otherwise
  - Magic squares are the ground states of this system
- Considering E as the energy and estimate the appearance probability by the multicanonical method
  - Since the total number of the conformations is known, the number of the magic square is estimated

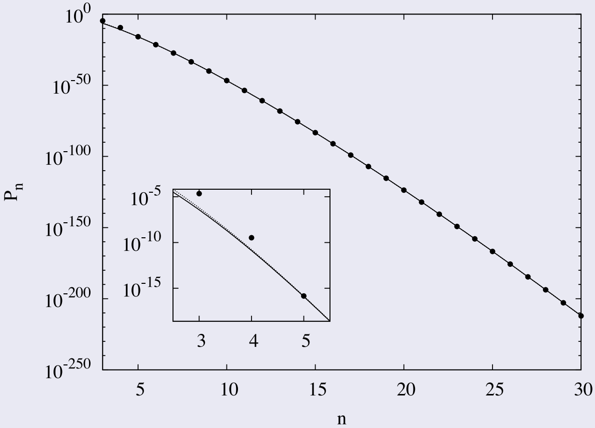
An example of 30 $\times$ 30 magic square

693	635	356	574	785	77	125	49	805	469	427	663	151	163	767	579	702	233	183	13	312	129	755	537	634	588	523	782	238	568
506	128	483	831	390	303	61	210	549	596	240	725	268	707	277	794	194	366	58	873	419	336	498	618	119	342	378	865	586	795
715	530	323	87	601	389	224	735	866	587	683	88	684	613	348	566	259	405	880	862	146	130	821	97	722	358	85	624	16	71
254	429	354	686	792	790	69	21	799	875	765	893	585	786	114	511	616	545	676	215	65	2	159	157	304	267	494	333	140	819
694	293	212	623	154	305	768	843	840	869	508	173	817	841	223	83	82	479	554	270	175	728	445	272	852	739	399	11	220	43
103	414	514	98	249	363	538	751	375	359	745	811	110	828	80	166	882	242	655	217	847	836	243	539	505	611	23	133	899	379
55	513	519	756	306	139	377	758	898	391	192	803	352	60	137	464	101	209	150	576	653	877	698	416	213	897	639	640	289	437
752	885	520	661	800	219	704	727	70	669	57	229	53	93	250	4	555	394	132	291	204	597	116	127	816	814	516	625	881	754
170	200	463	78	879	450	134	364	736	155	542	614	284	280	730	829	860	42	779	660	380	544	251	347	478	331	521	647	723	44
592	895	552	395	299	492	226	310	695	468	448	59	871	17	349	633	237	236	748	451	187	629	457	541	180	246	646	529	760	367
160	535	503	241	273	603	848	216	452	214	426	844	729	766	509	761	258	607	33	413	102	853	374	868	10	560	225	369	531	232
446	495	397	796	780	466	425	700	184	673	567	256	563	547	222	462	441	610	682	92	757	124	351	486	387	675	7	30	76	818
262	191	341	753	685	837	350	138	688	645	206	824	257	227	827	261	604	546	812	551	265	421	564	515	50	838	108	288	153	308
485	99	487	810	708	571	230	600	235	526	423	724	195	689	344	118	434	743	309	699	136	64	636	659	317	637	622	476	424	115
595	606	197	826	643	851	371	477	105	383	896	205	208	703	734	444	145	74	443	63	773	605	820	48	248	161	677	31	858	325
791	594	889	415	656	874	275	131	274	500	121	96	91	435	5	630	490	863	393	54	575	631	706	740	433	438	411	301	75	628
572	830	120	244	798	338	510	793	330	807	744	148	3	292	589	430	79	870	386	298	891	287	147	453	697	578	581	1	626	73
340	422	774	38	353	253	228	95	747	185	26	612	189	196	804	252	770	701	608	81	409	279	559	320	772	867	787	886	295	667
141	149	307	678	117	396	591	297	319	168	584	239	527	525	582	650	662	62	732	617	467	642	318	550	737	165	447	454	558	834
857	496	282	15	169	480	403	384	410	381	719	18	769	536	162	883	856	172	177	716	573	158	41	570	72	876	850	854	112	524
710	181	556	504	784	311	615	456	123	286	731	107	835	749	56	94	203	188	501	90	711	801	808	528	313	255	861	126	593	439
171	859	315	329	497	522	360	822	40	475	580	802	720	266	322	32	449	872	283	143	417	37	733	561	218	436	679	652	553	370
548	491	408	202	234	100	28	599	776	14	285	658	900	775	709	334	182	789	783	771	718	326	460	540	674	22	362	156	231	440
19	296	324	27	142	717	759	276	489	372	144	36	644	484	260	420	657	839	24	892	598	888	68	507	632	245	671	855	518	712
690	314	428	373	122	641	649	442	190	741	687	455	532	327	332	51	746	376	66	39	672	461	221	691	474	458	781	278	388	890
281	609	809	470	714	207	849	357	401	186	365	619	167	602	823	488	878	84	788	471	638	174	864	193	89	25	52	368	680	264
742	499	763	402	45	577	583	696	670	152	9	302	46	47	825	726	176	832	762	884	135	721	300	198	565	400	271	269	557	361
668	104	407	666	179	199	842	86	412	385	337	534	321	113	845	713	263	346	316	493	382	459	109	665	846	502	211	651	664	797
111	533	431	465	355	418	692	620	8	806	404	201	750	35	778	705	406	543	590	833	339	482	345	738	343	20	67	764	398	335
392	290	481	472	6	627	681	562	29	178	654	777	894	813	512	432	328	247	12	887	569	294	648	34	815	164	621	517	473	106

How rare

- The number of 30×30 magic squares is 6.6×10^{2056}
- Probability that a random arrangement of numbers 1 to 900 makes a magic number is 7.8×10^{-213}

Kitajima and MK (2015)



Probability that a random arrangement of the number 1 to n^2 makes a magic number