Replica symmetry breaking for Ulam’s problem

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We study increasing subsequences (IS) for an ensemble of sequences given by permutation of numbers \( \{1, 2, \ldots, n\} \). We consider a Boltzmann ensemble at temperature \( T \). Thus each IS appears with the corresponding Boltzmann probability where the energy is the negative length \( -l \) of the IS. For \( T \to 0 \), only ground states, i.e. longest IS (LIS) contribute, also called Ulam’s problem. We introduce an algorithm which allows us to directly sample IS in perfect equilibrium in polynomial time, for any given sequence and any temperature. Thus, we can study very large sizes. We obtain averages for the first and second moments of number of IS as function of \( n \) and confirm analytical predictions. Furthermore, we analyze for low temperature \( T \) the sampled IS by computing the distribution of overlaps and performing hierarchical cluster analyses. In the thermodynamic limit \( n \to \infty \) the distribution of overlaps stays broad and the configuration landscape remains complex. Thus, Ulam’s problem exhibits replica symmetry breaking. This means it constitutes a model with complex behavior which can be studied numerically exactly in a highly efficient way, in contrast to other RSB-showing models, like spin glasses or NP-hard optimization problems, where no fast exact algorithms are known.

(Introduction) The mathematician Stanislaw Ulam was also a well-known pioneer in Computer simulations. One of the problems he studied numerically, back in the 1950s, was \( \{1\} \) the scaling of the length \( L \) of the longest increasing subsequence (LIS) \( \{2\} \) of random permutations of \( n \) numbers. Based on the knowledge \( \{3\} \) that the average length increases at least like the square root of \( n \), he proposed that the average length scales as \( \langle L \rangle = c\sqrt{n} \) with \( c \approx 1.7 \). In the meantime, \( \langle L \rangle = 2\sqrt{n} \) for \( n \to \infty \) has been proven \( \{4\} \). Also the distribution \( P(l) \) of maximum lengths has been studied analytically \( \{5, 7\} \) and it was found \( \{8\} \) that the central part is given by the Tracy-Widom distribution. This was confirmed numerically by large-deviations simulations \( \{9\} \), and also considered for other sequence ensembles \( \{10\} \). Furthermore, the expectation values of the number of IS of a certain length \( \{11\} \) and of all increasing subsequences (IS) \( \{12\} \) have been obtained analytically. The actual distribution of the number of LIS was obtained numerically over a large range of the support again by applying large-deviation algorithms \( \{13\} \).

As a tool, the calculation of LIS finds also applications outside mathematics, like in data analysis \( \{14\} \), financial fraud detection \( \{15\} \), or sequence alignment in bioinformatics \( \{16\} \).

In spite of these connections to many fields, to our knowledge, the behavior of IS and LIS was studied so far surprisingly only with respect to the length and to the exponentially growing number of increasing subsequences. Thus, we are not aware of any study, where the actual structure of the exponentially large IS configuration space has been studied.

Such questions with respect to phase-space organization lie at the heart of the statistical mechanics of complex systems like glasses, spin glasses, machine learning or optimization problems \( \{17, 25\} \). In particular one is interested whether the configuration space is rather simple, like for a ferromagnet, often coined as replica symmetric, or whether it is complex with a hierarchical organization of phase space coined as replica symmetry breaking (RSB), as it appears for mean-field spin glasses \( \{26\} \).

In most cases, analytical solutions cannot be obtained, so one has to use computer simulations \( \{27\} \). Unfortunately, all standard models where one knows or suspects that they exhibit a complex RSB-like behavior, like spin glasses, are numerically very hard to treat. Hence, only rather limited system sizes could be considered when performing equilibrium sampling, even when using special parallel computers like JANUS \( \{28\} \). Note that for combinatorial optimization problems like the Satisfiability problem, in some cases efficient algorithms exist \( \{29\} \). But they allow only to find some solution, i.e., this sampling is not controlled. Thus, these algorithms do not allow to sample the configuration space in equilibrium which is necessary to study the configuration-space structure. For this purpose one has to use Monte Carlo Markov-chain sampling, which requires equilibration and is slow therefore. Note, for directed polymers in random media, where indeed a fast polynomial sampling is possible \( \{30, 32\} \), recently a broad distribution of overlaps and a complex hierarchy of configurations was found \( \{33\} \), but this was the case only for ensembles which exhibit special correlations in the disorder, not the “natural” uncorrelated one.

Here we introduce an algorithm which allows one to count the number of IS for any given length \( l \) as well as sampling IS exactly for any given distribution which depends only on the IS length \( l \), in particular for any given length the sampling is uniform. Both calculation of the numbers and the sampling can be performed in polynomial time, which allows us to treat large systems exactly. We study the sequence ensemble of random permutations, which does not exhibit correlations and is the classical and most-studied ensemble for IS and LIS. Our results indicate that the structure of the configuration space exhibits properties of replica-symmetry breaking, i.e., a broad distribution of overlaps and a hierarchical clustering of configurations, even in the thermodynamic limit \( n \to \infty \).

Next, we present all necessary definitions and introduce the algorithms. Then we show our results and finish by a summary and discussion.

(Definitions and Algorithms) Let \( \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n) \) be a sequence of \( n \) distinct numbers. A subsequence \( \lambda = \{\sigma_{i_1}, \sigma_{i_2}, \ldots, \sigma_{i_l}\} \)
(σ₁, σ₂, ..., σᵢ) of length \( l = l(\lambda) \) fulfills \( 1 \leq i₁ < i₂ < ... < iₙ \leq n \) and is called increasing if \( σ_{i_j} < σ_{i_{j+1}} \) for all \( j = 1, ..., l - 1 \). To calculate the longest among all possible IS, the patience sort algorithm \([4]\) is a popular choice which runs in polynomial time. Recently, an extension was proposed \([13]\), which allows one to calculate the number of LIS. Here, we introduce a further extension and variant of the algorithm, which enables one to count all IS and sample them efficiently and exactly for any desired probability distribution which depends on the IS length \( l \).

Let \( H \) be a precedence matrix, which encodes possible joint occurrences of entries \( σ_i \) and \( σ_j \) in an IS \( λ \), i.e.,

\[
H_{i,j} = \begin{cases} 
1 & \text{if } i < j \text{ and } σ_i < σ_j \\
0 & \text{else.} 
\end{cases}
\]  

(1)

Note that the matrix \( H \) can be efficiently stored as a graph with neighbor lists. To set up \( H \), we run an extended variant of patience sort, which gives also the length \( L \) of the LIS and allows us to restrict the number of candidates \( i, j \) which have to be checked whether one has to assign \( H_{i,j} = 1 \). Still, this requires \( O(n²) \) steps.

To count IS and LIS, we denote by \( Ψ_j \) the number of IS of length \( l \) which end at position \( j \). Clearly, each single entry of \( σ \) represents an IS of length \( l = 1 \), i.e., we have \( Ψ_1 = 1 \) for \( i = 1, ..., n \). Now, IS of length \( l > 1 \) can be constructed by selecting a final entry \( σ_j \) preceding an IS of length \( l - 1 \) where all entries are smaller than \( σ_j \) and appear before position \( j \). For the number of IS this turns into

\[
Ψ_j = \sum_{i<j} H_{i,j} Ψ_i^{l-1} \quad \text{for } l = 2, \ldots, L
\]  

(2)

which can be computed in a convenient way recursively, i.e., by dynamic programming in \( O(n²L) \). The total number of IS of length \( l \) is given by \( Ψ_l = \sum_j Ψ_j^l \), where we also include the empty subsequence \( Ψ^0 \). The total number of IS is given by \( Ψ = \sum_{l=0}^L Ψ_l \).

To sample an IS for given length \( l \), one starts by sampling the final entry \( j \) which appears with probability \( Ψ_j^l / Ψ_l \). Next, the preceding entry \( i \) is sampled among all possible predecessors \( i < j \), i.e., where \( H_{i,j} = 1 \). Each possible entry \( i \) is selected with probability \( Ψ_i^{l-1} / Ψ_l \). This is continued iteratively for length \( l - 2, l - 3 \), etc., always given the just sampled entry, until length \( 0 \) is reached. This algorithm takes \( O(nl) \) steps.

The sampling can be easily extended to include any probability which depends on the length. Here we take a physical viewpoint by considering \( E = -l \) as energy within the canonical ensemble at temperature \( T \), i.e., by using probabilities \( \sim \exp(l/T) \). Thus, for an IS \( λ \) we have the probability given by

\[
p(λ) = \exp(l(λ)/T) / Z, \quad Z = \sum_λ Ψ_l^l \exp(l(T)) .
\]  

(3)

This includes in particular all LISs for \( T \to 0 \). Sampling an IS now consists of first drawing a length \( l \) according the probabilities \( Ψ_l^l \exp(l(T)) / Z \), and then uniformly sampling an IS of length \( l \) as explained before. Note that this approach is exact and direct, i.e., for each run of the algorithm an independently sampled configuration is returned. Our approach runs in polynomial time, such that we can treat rather large systems in perfect equilibrium.

(Results) We performed simulations \([27]\) for ensembles of permutations of \( n \) numbers in the range \( n = 128 \) to \( n = 8192 \). We studied for all sizes 10000 realizations of the disorder, i.e., independent permutations. For comparison, we also considered in some cases the ordered sequence \( σ^o = (1, 2, ..., n) \).

We start by considering the number \( Ψ \) of IS. The asymptotic behavior of the expectation value is analytically given by \([12]\)

\[
E(Ψ) = \frac{1}{2\sqrt{π}e} n^{-1/4} \exp(2\sqrt{n}) .
\]  

(4)

In Fig. 1 we compare the numerical average \( ⟨Ψ⟩ \) with the analytical result and find very good agreement, even for rather small system sizes. Note that the average is “annealed” in the sense that is represents an exponentially growing quantity, such that sequences with exceptionally large values of \( Ψ \) will dominate. This means, we need a rather large number of samples to observe agreement, as we do. This also indicates the correctness of our approach. We have also evaluated the second moment \( ⟨Ψ^2⟩ \) (not shown). Here the agreement with the analytical result \([12]\) is fair, i.e., a bit lower, due to the even stronger dominance of exponentially large but exponentially rare sequences. To find a good agreement here, one would have to obtain the distribution \( P(Ψ) \) down to the tails. This should be possible by using a large-deviation approach, as it has been used to obtain the distribution of the number of LIS \([13]\), but lies outside the scope of the present study.

Next, we analyze IS sampled in equilibrium according to Eq. (3) at a low temperature \( T = 0.2 \) for several sequence lengths \( n \). For independently sampled pairs \( λ(1), λ(2) \) of IS,
we calculate the similarity of the two IS via the overlap $q$.

Here, considering the IS as sets of the contained numbers, we use the Jaccard-Index \[34\] as given by

$$ q = \frac{|\lambda^{(1)} \cap \lambda^{(2)}|}{|\lambda^{(1)} \cup \lambda^{(2)}|}. \quad (5) $$

The distribution $P(q)$ of overlaps is shown for $T = 0.2$ in Fig. 2 for three sequence sizes $n$. Apparently the distribution is broad, even for large systems, indicating a complex configuration landscape.

To investigate whether this is true also in the thermodynamic limit, we have evaluated the width $\sigma_q$ of the distribution as function of system size $n$. The result for $T = 0.2$ is shown in Fig. 3. We fitted a power law $\sigma_q(n) = \sigma_q^\infty + an^{-b}$ and obtained the limiting value $\sigma_q^\infty = 0.073(10)$, which is significantly different from zero and shows that the distribution remains broad in the thermodynamic limit.

When evaluating $\sigma_q^\infty$ as function of $T$, see inset of Fig. 3, it appears to be nonzero for all temperatures in the studied range. Thus only a rather smooth decrease is visible, no sign of a transition, where one would expect a power-law decrease $\sim L^{-\eta}$ at and beyond the transition. This behavior we observe also for the average overlap (not shown here).

We also obtained the specific heat via the variance of the length by calculating $C = (\langle l^2 \rangle - \langle l \rangle^2) / (nT^2)$. Interestingly, the disorder-averaged $C(T)$ exhibits peaks near $T = 0.4$ for all system sizes, but the peak height decreases with growing system size $n$. Thus, this behavior provides also no sign for a phase transition. Note that a non-growing peak is obtained also when one considers just the single ordered sequence $\sigma^o$, where each number can independently be part of an IS with probability $p(T) = e^{1/T} / (e^{1/T} + 1)$. Thus, $\sigma^o$ represents $n$ independent paramagnets in a field, where the variance of the length is just the sum of the single-number variances $p(T)(1 - p(T))$ and therefore $C(T) = p(T) / (1 - p(T))^2$ is readily available \[35\]. This $C(T)$ exhibits also a peak at the same temperature $T \approx 0.4$. Thus, from the energetic point of view no phase transition is visible. This is maybe similar to spin glasses, where the transition to the RSB phase is also not visible when studying the specific heat \[19\].

The configuration space structure was further analyzed by applying the agglomerative clustering approach of Ward \[36\]. The hierarchical structure obtained by the clustering can be visualized by a tree, usually called dendrogram, where each branching corresponds to a subspace of configurations, see Fig. 5. The sequence of configurations as located in the leafs defines a partial order. This order can be used to display the
matrix of the pair-wise overlaps or distances where the order of the rows and columns is exactly given by the leaf order. The resulting matrix for 200 samples IS ($T = 0.2$) of one random permutation of length $n = 8192$ is displayed in Fig. 5. One observes a hierarchical structure given by two major clusters, visible by dark squares, i.e., similar configurations, which are subdivided into sub clusters, with relatively smaller similarities on the off diagonals, respectively.

The extend of the hierarchical structure can be made quantitative by calculating the cophenetic correlation

$$\kappa \equiv [d \cdot d_c]_P - [d][d_c]_P,$$

where $d = 1 - q$ is the distance corresponding to overlap value $q$. The cophenetic distance $d_c$ between two states is measured on the dendrogram as the distance of the two largest clusters that contain only one of the states, respectively. $[\ldots]_P$ denotes the combined average over the sampled IS and the disorder ensemble. Thus, this $\kappa$ measures the correlation between the original distance $d$ of two states and the distance $d_c$ imposed by the clustering, i.e., the degree of hierarchical structure. In Fig. 6 $\kappa$ is shown as function of $n$. By fitting a power law $\kappa(n) = \kappa_\infty + a n^{-b}$ we obtained $\kappa_\infty = 0.23(4)$. This means, the IS landscape of permutations exhibits also in the thermodynamic limit a nested hierarchical structure, like it has been found for problems exhibiting RSB as mean-field spin glasses or some hard combinatorial optimization problems \[39\].

(Summary and Discussion) The original problem of Ulam is to find the longest increasing subsequence for random permutations. With so far known algorithms it was possible to generate one LIS, but in a statistically uncontrolled way. To study the structure of configurations for LIS and IS for permutations, we have introduced an algorithm which allows for exact and direct sampling of increasing subsequences in polynomial time. For the uncorrelated and most natural ensemble of permutations, we study the annealed mean and second moment of the number of IS, which agree with the analytical calculations very well. We study the structure of the configuration space and find a broad distribution of overlaps and a hierarchical structure. By extrapolating to infinitely long sequences, we show that this persists in the thermodynamic limit, thus the model exhibits replica symmetry breaking. This model is, to our knowledge, the first one which at the same time exhibits RSB and for which a polynomial exact sampling algorithm is available. This is in strong contrast to known complex but computationally hard problems like mean-field spin glasses and NP-hard optimization problems. Thus, Ulam’s problem provides an ideal test bed to study other phenomena of interest in the field of complex disordered systems. In particular one can address the non-equilibrium behavior, the scaling of excitations, the coupling of replicas, or an extended model obtained by the introduction of additional quenched disorder, obtained by assigning individual local lengths for the numbers. It could also be of interest to consider ensembles with correlation or structure, in the spirit of a recent work on directed polymers in random media \[33\]. Furthermore, this study might motivate or help to identify other models with complex RSB behavior which can also be treated by polynomial algorithms.

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Note2, the clustering approach [37, 38] operates on a set of $M$ sampled configurations by initializing a set of $M$ clusters each containing one configuration. One maintains pairwise distances between all clusters, which are initially the distances $d = 1 − q$ between the configurations, obtained from the overlaps $q$. Then iteratively two clusters exhibiting the currently shortest distance between them are selected and merged to one single cluster, thereby reducing the cluster number by one. For this new merged cluster, an updated distance to all other still existing clusters have to be obtained. Here the update is done with the approach of Ward [37], which has been used previously for the analysis of disordered systems [39–41], for more details see there. The merging process is iterated until only one cluster is left.

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