Extensive Simulations for Longest Common Subsequences

Finite Size Scaling, a Cavity Solution, and Configuration Space properties

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Abstract. Given two strings $X$ and $Y$ of $N$ and $M$ characters respectively, the Longest Common Subsequence (LCS) Problem asks for the longest sequence of (non-contiguous) matches between $X$ and $Y$. Using extensive Monte Carlo simulations for this problem, we find a finite size scaling law of the form $E(L_N)/N = \gamma_S + A_S/(N N) + ...$ for the average LCS length of two random strings of size $N$ over $S$ letters. We provide precise estimates of $\gamma_S$ for $2 \leq S \leq 15$. We consider also a related Bernoulli Matching model where the different entries of an $N \times M$ array are occupied with a match independently with probability $1/S$. On the basis of a cavity-like analysis we find that the length of a longest sequence of matches in that case behaves as $L_{NM}^B = \gamma_S(r) N$ where $r = M/N$ and $\gamma_S(r) = (2\sqrt{r}S - r - 1)/(S - 1)$. This formula agrees very well with our numerical computations. It provides a very good approximation for the Random String model, the approximation getting more accurate as $S$ increases. The question of the “universality class” of the LCS problem is also considered. Our results for the Bernoulli Matching model show very good agreement with the scaling predictions of [12] for Needleman-Wunsch sequence alignment. We find however that the variance of the LCS length has a scaling different from $V ar(L_N) \approx N^{2/3}$ in the Random String model, suggesting that long-ranged correlations among the matches are relevant in this model. We finally study the “ground state” properties of this problem. We find that the number $N_{LCS}$ of solutions typically grows exponentially with $N$. In other words, this system does not satisfy “Nernst’s principle”. This is also reflected at the level of the overlap between two LCSs chosen at random, which is found to be self averaging and to approach a definite value $q_S < 1$ as $N \to \infty$.

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1 Introduction

Let $X = (X_1, ..., X_N)$ and $Y = (Y_1, ..., Y_M)$ be two strings of characters. Here the $X_i$’s and $Y_j$’s are letters of a given alphabet, which will be assumed throughout this paper to be finite and of fixed size $S \geq 2$. The Longest Common Subsequence problem, which we shall refer to as the LCS problem, consists of finding a sequence of letters which appears as a subsequence of both $X$ and $Y$, and which is of maximal size. Equivalently one can ask for two sequences $1 \leq i_1 < ... < i_L \leq N$ and $1 \leq j_1 < ... < j_L \leq M$ such that $X_{i_k} = Y_{j_k}$, $1 \leq k \leq L$ and $L$ is maximal.

The length of a LCS can be viewed as a natural measure of the “proximity” of different strings of letters. It is an example of the “best sequence alignments” which are of use in biology, in tests for comparing long molecules such as proteins and nucleic acids [14,18,30].

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be the sum of the bonds’ weights along the path. Then clearly a LCS between \(X\) and \(Y\) may be constructed from any directed path of maximum weight joining the point \((0,0)\) to the point \((N,M)\). If we interpret the weight of a bond as a time required for the passage of that bond, we seek the maximum rather than the minimum passage time from \((0,0)\) to \((N,M)\), but this is of no significance here.

This paper is concerned with the stochastic version of the LCS problem, where one is given very long strings the letters of which are chosen at random, independently and uniformly in a given alphabet of size \(S\). This problem has retained much attention \(\text{(\cite{2})}\) (see also \(\text{\cite{3}}\) for a recent review). The main issue is to understand the large \(N\) behaviour of the LCS length of the \(N\) first letters of \(X\) and \(Y\). Let \(L_N\) be this number. Observing that the sequence \((L_N)\) is superadditive \((L_{N_1+N_2} \geq L_{N_1} + L_{N_2})\), and using the martingale difference method, one can prove in an elegant way \(\text{(\cite{22})}\) that with probability one (for infinite strings), \(L_N\) is asymptotic from below to \(\gamma_S N\), where \(0 < \gamma_S \leq 1\) is a constant whose exact value is unknown. It has also been proved \(\text{(\cite{2})}\) that the rate of convergence of the expected ratio \(E(L_N)/N\) to \(\gamma_S\) is at least as fast as \(O(\sqrt{\ln N/N})\).

In the passage time percolation picture the weights attached to the bonds are correlated random variables (for example the occupation numbers of the matches on the corners of any rectangle of the lattice are obviously correlated). We consider also a related model where each bond \(\{(i-1,j-1),(i,j)\}\) is given a weight 1 (resp. 0) independently of the others with probability 1/\(S\) (resp. 1-1/\(S\)). We shall refer to this model as the Bernoulli Matching model, and denote by \(L_N^B\) the maximum weight of a directed lattice path joining \((0,0)\) to \((N,N)\) (equivalently \(L_N^B\) is the maximum \(L\) for which there are sequences \(1 \leq i_1 < \ldots < i_L \leq N\) and \(1 \leq j_1 < \ldots < j_L \leq N\) such that \((i_k,j_k)\) is a match, \(1 \leq k \leq L\)). We let \(\gamma_S^B\) be the limit \(\lim_{N \to \infty} L_N^B/N\), which is shown to exist a.e. in exactly the same way as for \(\gamma_S\). Also we note that Alexander’s rate result \(\text{(\cite{4})}\) applies to \(E(L_N^B)/N\) as well.

Much effort have been made to get bounds on \(\gamma_S\) \(\text{(\cite{11,17,3})}\), but there are now negligible gaps between the known upper and lower bounds \(\text{\cite{3}}\). Estimations of \(\gamma_S\) based on numerical simulation are also available \(\text{\cite{11,17,30}}\) but apparently no attempt has been made to determine numerically the finite size corrections to the linear scaling law \(E(L_N^B) \sim \gamma_S N\).

This paper presents the results of extensive Monte Carlo simulations for the LCS problem, showing that the difference \(\gamma_S N - E(L_N)\) has a well defined asymptotic behaviour, allowing one to get precise estimates of \(\gamma_S\) by extrapolation. The same finite size scaling law appears to hold for the Bernoulli Matching model, and we have obtained corresponding estimates for \(\gamma_S\).

We further considered the case where the strings \(X\) and \(Y\) are of different sizes, \(N \neq M\). The relevant case occurs when \(N\) and \(M\) are large but comparable, namely \(N,M \to \infty\), the ratio \(r = M/N\) being fixed \((r > 0)\). Let \(L_N(r) = L_{N,[rN]}\) be the length of a LCS of \(X_1, \ldots, X_N\) and \(Y_1, \ldots, Y_{[rN]}\). Then with probability 1, one has \(\lim_{N \to \infty} L_N(r)/N = \gamma_S(r)\) where \(0 < \gamma_S(r) \leq 1\). Of course \(\gamma_S(1) = \gamma_S\), and the function \(\gamma_S(r)\) has the obvious symmetry property \(\gamma_S(1/r) = 1/r \gamma_S(r)\). In the picture of directed percolation \(r\) is given by \(\tan(\pi/4 + \phi)\) where \(\phi \in [-\pi/4, \pi/4]\) is the angle between the direction of interest and the first bisector, and the object of interest is the set of points which are “wet” at time \(t\), defined here to be the set \(C_t = \{(i,j) : L_{ij} \leq t\}\). As \(t \to \infty\) (for \(N\) and \(M\) infinite) the set \(C_t/t\) is asymptotically delimited by the curve of polar equation \(p(\phi) = \sqrt{1 + r(\phi)^2} \gamma_S(r(\phi))\).

The above symmetry property reflects the fact that \(C_t\) is asymptotically symmetric with respect to the first bissector. A percolation transition occurs in this problem when \(r = r_c = S\), namely \(\gamma_S(r) = 1\) for \(r \geq S\) while \(\gamma_S(r) < 1\) for \(r < S\). By symmetry we have another transition at \(r = 1/r_c = 1/S\), such that \(\gamma_S(r) = r\) for \(r \leq 1/S\) and \(\gamma_S(r) < r\) for \(r > 1/S\). Analogous comments apply to the Bernoulli Matching model. In that case we provide a simple analytic expression for the corresponding function \(\gamma_S^B(r)\), which is derived \(\text{(see section (3) below)}\) on the basis of a cavity-like analysis of the LCS problem. The cavity method is an approximation scheme generally considered to be appropriate for describing the mean field theory of disordered systems (such as spin glasses) \(\text{\cite{15}}\). The Bernoulli Matching model is not a mean field model however, but really a two dimensional percolation model, and by “cavity” we mean the following: First, the properties of the system can be computed by use of a recursion formula. This is equation \(\text{(\cite{1})}\) given below, which is valid for the Random String model as well as for the Bernoulli Matching model. Second, a decorrelation, or “clustering” property \(\text{\cite{12}}\) happens to hold in the Bernoulli Matching model, allowing the recursion formula to be solved at large \(N,M\) by use of a self-consistent approximation. This leads to an expression of \(\gamma_S^B(r)\) in very good agreement with our numerical results.

We finally investigated the “configuration space” properties of this problem, which are most easily accessible by constructing what we call the LCS graph of given strings \(X\) and \(Y\). This structure is defined in section \(\text{(4)}\). It can be computed in a very efficient way, and it gives a direct access to properties of the set of LCSs of \(X\) and \(Y\), enabling one to compute such quantities as:

i) The total number \(N_{\text{LCS}}\) of LCSs of \(X\) and \(Y\).

ii) The average overlap between two LCSs chosen at random among the set of LCSs of \(X\) and \(Y\).

iii) The distribution of the distance between two successive matches in a LCS. By distance we mean here the Manhattan distance \(|i_1 - i_2| + |j_1 - j_2|\) for given points \((i_1,j_1), (i_2,j_2)\).

iv) The mean square “displacement” with respect to the first bissector, of the matches along a LCS, where (following \(\text{\cite{12}}\)) the displacement coordinate of a point \((ij)\) is defined to be \(i - j\).

These type of computations are of interest because they provide informations on the structure of the set of solutions which in other systems may be very difficult to obtain. For example our computations show that typi-
cal random strings have many common subsequences of maximum length. Their number typically grows exponentially with $N$, i.e. the ground state entropy of this system is not zero. We provide estimates of this entropy and of the typical overlap between two randomly chosen LCSs for several values of $S$. Properties such as iv) are of physical interest as they depend on long-ranged correlations among the matches in a LCS, and they characterize the “universality class” of the LCS problem. This question has been recently analysed by Hwa and Lässig [12] who showed that the percolation formulation of the LCS problem (and more generally of Needleman-Wunsch sequence alignment described below) can be treated in the continuum limit as a model of directed polymer in a quenched random medium. In this analogy each directed path on the above defined lattice is assigned an energy $-W$, where $W$ is the weight of the path. The statistics of these paths is taken to be the Boltzmann-Gibbs distribution [25]. The LCS length then corresponds to the ground state energy of the “bridge” from $(0,0)$ to $(N,M)$. In the case of the Bernoulli Matching model, this leads to a complete characterization of the universality class of the model: The continuum limit is described by the well studied 2D-directed path (or equivalently the 1D-random walk) in a Gaussian random potential. The fluctuations of $L_N^2$ and of the “displacement” $i-j$ along the optimal paths are governed by exactly known universal exponents $\omega = 1/3$ and $\zeta = 2/3$ respectively. Hence $\text{Var}(L_N^2)$ should grow asymptotically as $N^{2/3}$ and the mean square displacement as $N^{4/3}$. Our numerical results agree very well with these predictions. The question of the universality class of the Random String model is more subtle, as this model involves long ranged correlations in the disorder. Hwa and Lässig provide evidence that these correlations are not relevant in the continuum limit for a range of the defining parameters of Needleman-Wunsch alignment. In the regime corresponding to the LCS problem (which was not considered in [12]), our results only partly supports the above predictions: The measured mean square displacement for the Random String model show no deviation from the superdiffusive $N^{4/3}$ scaling. The behaviour of $\text{Var}(L_N)$ is close to, but significantly different from $N^{2/3}$, suggesting that correlations among the matches in the Random String model are relevant to the universality class of the LCS problem. It should not be considered a surprise that the scaling relation $\omega = 2\zeta - 1$ appears invalidated by our results. This scaling relation is known to be intimately connected with Galilean invariance [4]. In the formulation of the Random String LCS problem as a 1D-random walk, long-range temporal correlations are present in the random potential, and Galilean invariance is broken. What is surprising is that only the fluctuations of the ground state energy show a scaling affected by these correlations. This is left to the reader as an interesting open question.

We close this introduction by explaining the position of the LCS problem with respect to sequence alignment methods in molecular biology. The purpose of these methods is to provide efficient tools for the detection of relevant similarities among DNA molecules or among proteins. Relevance refers here to finding the functional and evolutionary relationships between these molecules, and is a main biological issue. This problem is the source of a rich interplay between biology and computational sciences (see [29] for reviews). Even if determining what is the “best alignment” of two sequences for biological purposes remains in part a matter of art, standard comparison algorithms are widely used by biologists. These algorithms are very useful to confront a newly discovered DNA molecule or protein to the huge existing databases of known molecules (and then to infer the possible functional properties of the new molecule). The LCS problem corresponds to a class of alignment algorithms discovered by Needleman and Wunsch [16], which provided the first systematic tool for taking into account the insertions and deletions which naturally occurs in the evolution of biological sequences. To describe this approach consider again the percolation formulation of the LCS problem. An alignment of the strings $X$ and $Y$ is viewed as a directed path on the the lattice defined above, tracing a possible “evolution” from $X$ to $Y$: Each diagonal bond (ending at $(ij)$) on the path represents a substitution of the letter $Y_j$ to the letter $X_i$ (if $(ij)$ is a match $X_i$ is left unchanged). Horizontal and vertical bonds represents respectively deletions and insertions, also termed as indel operations, or “gaps”. In this way each directed path from $(0,0)$ to $(N,M)$ corresponds to a well defined sequence of edit operations transforming $X$ into $Y$ (or equivalently $Y$ into $X$), which is the usual definition of an “alignment”. A given path $\gamma$ is assigned a score $W(\gamma)$, which is defined (in the simplest version of the model) by weighting each substitution along $\gamma$ with a matching function $s(X_i,Y_j)$, and each gap with a penalty $-\delta (\delta > 0)$. A common choice for $s(X_i,Y_j)$ is to assign a score 1 to a match $X_i = Y_j$ and a penalty $-\mu (\mu > 0)$ to a mismatch $X_i \neq Y_j$. The optimal alignments are determined by maximisation of the score $W(\gamma)$. We are then facing a longest path problem very similar to the LCS problem. In particular the optimal score $W_{NM}$ from $(0,0)$ to $(N,M)$ can be computed in an efficient way using a straightforward adaptation of the dynamic programming algorithm of section 3. Needleman-Wunsch sequence alignment is a global alignment method, since the whole strings $X$ and $Y$ are aligned together. The optimal alignments are invariant by multiplying the matching function and the gap penalty by any positive constant. Moreover the numbers $N_+$, $N_-$, and $N_g$ of matches, mismatches, and gaps respectively along any directed path from $(0,0)$ to $(N,M)$ are related by $2N_+ + 2N_- + N_g = N + M$. Hence with the above choices the number of independent parameters is reduced to one: It is equivalent to maximize $W(\gamma) = N_+ - \mu N_- - \delta N_g$ or to maximize $\tilde{W}(\gamma) = N_+ - \epsilon N_g$, where $\epsilon = (\delta - \mu / 2) / (1 + \mu)$. As $N,M \to \infty$ the modified optimal score behaves as $\tilde{W}_{NM} \sim a(\epsilon,r)N$ ($r = M/N$), where $a(\epsilon,r)$ is a monotonous decreasing (demonstrably continuous) function of $\epsilon$. For $\epsilon \leq -1/2$ the problem is trivial and $\tilde{W}_{NM} = -(N+M)e$. When $-1/2 < \epsilon < 0$, it is always advantageous to change a mismatch for two gaps (an insertion followed by a deletion). We may then
assume \(2N_+ + N_{\text{gaps}} = N + M\) and the problem reduces to maximizing \(N_+\), i.e. to the LCS problem. In this region \(a(\epsilon, r)\) interpolates linearly from its value at \(\epsilon = -1/2\) to its value at \(\epsilon = 0\). The case \(\epsilon = 0\) corresponds exactly to the LCS problem: Mismatches and gaps are then equivalent as regards to the score. Since gaps and mismatches are known both to occur during evolution, and are not equivalent energetically, the biologically relevant region clearly lies within \(\epsilon > 0\). Hence the LCS problem represents a natural (even if unrealistic) limit case of Needleman-Wunsch sequence alignment. It must be pointed out that for biological purposes (in particular for detecting weak similarities between rather remote sequences), local rather than global alignment is often required. A powerful approach to local alignment is Smith-Waterman algorithm \([22]\), which maximizes the score \(W(\gamma)\) over all pairs of substrings (i.e. contiguous segments) of \(X\) and \(Y\). In the percolation picture, the end points of the paths associated with local alignments are no longer fixed. The gap and mismatch penalties are then really different parameters and strongly influence the optimal alignments. In fact for random sequences Smith-Waterman alignment undergoes a phase transition from global to local alignment \([13, 21]\). For small \(\delta\) and \(\mu\), more precisely as long as \(\delta\) and \(\mu\) are such that the optimal score \(W_{NM}\) obtained by global alignment is positive, we recover essentially Needleman-Wunsch alignment: For large \(N, M\), the optimal Smith-Waterman score \(H_{NM}\) satisfies \(H_{NM} \approx W_{NM}\) with high probability. Note that the case \(\delta = 0\) reduces as before to the LCS problem. For sufficiently high gap and mismatch penalties, global alignment leads to a negative score \(W_{NM}\) growing linearly with \(N, M\) in absolute value. A positive score can be achieved only by small gaps taking advantage of the local fluctuations in the density of matches. This is the genuinely local phase, where \(H_{NM}\) grows only logarithmically with \(N, M\). Clearly the LCS problem is no more relevant to this phase. For example the exponential proliferation of solutions occurring in the LCS problem, relevant to the global phase, is replaced in the local phase by a small number of well characterized optimal and suboptimal alignments \([23]\). The transition line between the global and the local phases, which separates the regions of positive and negative linear growth of the global score \(W_{NM}\), is easily determined from the knowledge of \(a(\epsilon, r)\) defined above. Interestingly, the neighborhood of this transition line is found empirically to be a most relevant \((\delta, \mu)\)-region for biological purposes \([27]\). Hence the value \(a(0, r) = \gamma_S(r)\) provides some valuable information thanks to the monotonicity of \(a(\epsilon, r)\). More importantly, even if the biological relevance of purely global alignments is for the present difficult to address, clearly it is of interest to understand their statistical properties \([14]\). As the LCS problem corresponds in some sense to the “most” global case of sequence alignment, it deserves particular attention.

2 The average length of a Longest Common Subsequence.

There are several algorithms for computing the LCS length of two strings \(X = (X_1, \ldots, X_N)\) and \(Y = (Y_1, \ldots, Y_M)\). The best known is based on a dynamic programming approach as follows. For \(i, j \geq 1\), let \(L_{ij}\) be the length of a LCS of \((X_1, \ldots, X_i)\) and \((Y_1, \ldots, Y_j)\). We call the matrix \((L_{ij})\) the LCS matrix of the given instance. The strategy consists of using the fact that \(L_{ij}\) can be readily computed if \(L_{i-1,j-1}, L_{i-1,j}\) and \(L_{i,j-1}\) are known. Indeed one has \(L_{ij} = L_{i-1,j-1} + 1\) when \(X_i = Y_j\), and \(L_{ij} = \max(L_{i-1,j}, L_{i,j-1})\) when \(X_i \neq Y_j\). In short

\[
L_{ij} = \max(L_{i-1,j}, L_{i,j-1}, L_{i-1,j-1} + \delta_{X_i,Y_j}).
\] (1)

This recurrence relation, with the obvious initial conditions \(L_{ij}, 0 \leq i, j \leq N\) subject to the constraints

\[
L_{ij} \geq L_{i-1,j-1} + \delta_{X_i,Y_j}, L_{ij} \geq L_{i-1,j}, L_{ij} \geq L_{i,j-1},
\] (2)

and \(L_{i,0} = L_{0,j} = 0\).

The time required to compute the LCS matrix of \(X\) and \(Y\) using (1) is given essentially by the product \(NM\). Of course the whole LCS matrix contains more information than needed to construct a LCS of \(X\) and \(Y\) or to compute their LCS length. More involved algorithms focus attention on subsets of the set of matches of \(X\) and \(Y\), i.e. the set of points \((ij)\) such that \(X_i = Y_j\). These algorithms may achieve much better time bounds in some special cases. However no algorithm is known for the LCS problem which achieve a significantly better time bound than \(O(NM)\) in the general case, or even in average when \(X\) and \(Y\) are two random strings over an alphabet of size \(S \geq 2\). The fastest known algorithm is described in \([13]\).

Moreover relation (1) is highly suited for a finite size scaling analysis of the LCS length, as it may be easily implemented in order to compute in time \(O(N^2)\) and space \(O(N)\) the whole profile of values \(L_i = L_{i,j}, 1 \leq i \leq N\) for any given instance. Indeed, to compute the \(i^{th}\) line of the LCS matrix it is not necessary to have stored all the previous lines, since only the \((i-1)^{th}\) line is needed. This property also makes the computation of the LCS matrix parallelisable to some extent, and a significant speed up is obtained in the case of very long strings by implementing (1) on a parallel machine.
2.1 Finite size behaviour of $E(L_N)$.  

In order to measure the finite size behaviour of the average LCS length, we made a direct Monte Carlo evaluation of $E(L_N)$ for all $N$ up to a certain number and over large samples of random strings. Namely we computed averages of $L_N$ over $10^3$ instances for $N \leq 1500$, and over $10^4$ instances for $1500 \leq N \leq 10^4$. We then extrapolated these estimates to the large $N$ limit by using a $\chi^2$ analysis. In order to check the extrapolation procedure we performed a second series of experiments on a parallel computer, over smaller samples of $30$ to $50$ instances, but for problem sizes up to $N = 10^5$.

We found that a very reliable extrapolation to the large $N$ limit is obtained if one assumes a finite size behaviour of the form

$$
\frac{E(L_N)}{N} = \gamma_S + \frac{A_S}{\ln N \sqrt{N}} + \epsilon_N.
$$

Here $A_S$ is a negative constant and $\epsilon_N$ represents further corrections which we expect to be at most $O(1/N)$. To extract the precise asymptotic behaviour (if any) of $\epsilon_N$ would certainly require improvement on the precision of our finite size estimates. The statistical precision we had on $E(L_N)$, up to $N \leq 10^4$, was better than $0.002\%$, and further improvement would have been very time consuming. By using a best fit of our $N \leq 1500$ estimates based on (4) with $\epsilon_N$ of the form $\epsilon_N = K/(N \ln^\alpha N)$ ($K$ and $\alpha$ being constants) we get a surprisingly good extrapolation up to values of $N$ of order $10^5$, which one would not be able to obtain by using another form than (4).

However the form chosen for $\epsilon_N$ remains somewhat arbitrary. Since the estimation of $\gamma_S$ and $A_S$ should be more precise when extrapolating from larger values of $N$, we performed a second series of extrapolations, using the finite size estimates obtained for $1500 \leq N \leq 10^4$. For these values of $N$, the term $\epsilon_N$ is much less significant, and a linear extrapolation of $E(L_N)$ as a function of $x = 1/(\ln N \sqrt{N})$ is already very precise. Figure (5) reproduces our results in the cases $S = 2$, $S = 3$ and $S = 15$. The solid curves in these figures are best fits of our $1500 \leq N \leq 10^4$ estimates to a linear function of $1/(\sqrt{N} \ln N)$. In this way we obtained the estimates of $\gamma_S$ and $A_S$ which are given in table (5) a) for $2 \leq S \leq 15$.

To obtain error bars on these estimates one should use a $\chi^2$ analysis (6). However this method underestimates the true error here. Indeed, $\chi^2$ analysis leads to errors for the fitting parameters which decrease as $1/\sqrt{n}$ for $n >> 1$, $n$ being the number of degrees of freedom, that is the number of independent datas in the fit. Since we computed for each instance a whole profile, the averaged points in figure (5) are not independent: There are correlations in the sequence $(L_i)$, $1 \leq i \leq N$, which results in a smoothing of the averaged profile, or equivalently in a reduction of the “effective” number of independent datas in the fit. Moreover these correlations are long-ranged, which makes it uneasy to measure an effective number of degrees of freedom. We thus relied on a semi-empirical method, by measuring the range over which the fitting parameters varied for different choices of $\epsilon_N$. Typically we obtained in this way an “error” less than $0.01\%$ on $\gamma_S$ and $5\%$ on $A_S$. In fact $\epsilon_N$ happens to be only slightly larger than the precision of our finite size estimates for $1500 \leq N \leq 10^4$. We thus expect the above procedure to provide a faithful (slightly overestimated) measure of the true error on our estimates. Rather than quoting semi-empirical error bars, table (6) gives the results obtained by making respectively the choices a) $\epsilon_N = 0$, b) $\epsilon_N \sim B_S/N$ and c) $\epsilon_N \sim B_S/(N \ln N)$. Note that the cases b) and c) agree to a better accuracy together than with case a). To determine the precise form of the “second order” corrections however clearly more precise computations would be needed.

2.2 The variance of $L_N$ and the universality class of the LCS problem.

It has been observed long ago by Chvatal and Sankoff (7) that the variance of the LCS length is numerically very small. These authors even conjectured that $\text{Var}(L_N)$ might be $o(N^{2/3})$. It has been suggested by Talagrand (in the context of longest increasing subsequences (24)), that the smallness of $\text{Var}(L_N)$ may be related to the fact that the number of LCSs of two random sequences is very large. The only known general bound is however $\text{Var}(L_N) = O(N)$, an immediate consequence of the concentration inequality (7). Anyway the work of Hwa and Lässig (12) provides a theoretical answer to the conjecture of Chvatal and Sankoff: The LCS problem falls into the universality class of a model of directed polymer in a 2D random potential. The variance of $L_N^B$ in the Bernoulli Matching model should grow as $N^{2/3}$. For the Random String model we must be cautious with this prediction, but it should provide at least a first approximation. The scaling behaviour of the variance of the LCS length is shown in figure (8), both for the Random String model and for the Bernoulli Matching model, and for different values of $S$. We see as expected a very good agreement with the scaling law $\text{Var}(L_N^B) \approx N^{2/3}$ for the Bernoulli Matching model. The results for the Random String model are more interesting: The scaling of $\text{Var}(L_N)$ is slightly, but clearly different from $N^{2/3}$. The correlations among the matches should be expected to be more and more relevant as $N$ grows, since $2N$ independent variables are involved in $L_N$ against $N^2$ in $L_N^B$. In fact our results suggest that something like a crossover occurs from a small $N$ scaling regime where $\text{Var}(L_N) \approx N^{2/3}$ to an asymptotic scaling regime where $\text{Var}(L_N) \approx N^{2\omega'}, \omega' > 1/3$. Note that this asymptotic regime seems not completely reached on figure (8) which includes estimates for $N$ up to $10^4$. Hence the “small $N$” regime is rather extended. As is apparent on the figure, it becomes more and more extended as $S$ increases, and the asymptotic regime is more and more difficult to reach. For this reason it is difficult to tell if the exponent $\omega'$ depends on $S$ or not. It is also difficult to tell if the numerical dependancies of $\text{Var}(L_N^B)$ and $\text{Var}(L_N)$ respectively on $S$ remain reversed in the asymptotic regime. As is seen on figure (8A) however, our datas for $S = 2$ and $S = 4$ are
Fig. 1. Extrapolation of the $N \leq 10^4$ estimates for $E(L_N)/N$ to the large $N$ limit for $S = 2, 3$ and 15. The solid curves represent best fits to a linear function of $x = 1/(\ln N \sqrt{N})$. Estimates of $E(L_N)/N$ for $2.10^4 \leq N \leq 10^5$, not taken into account in the extrapolation, are also included.
Table 1. Results of an extrapolation of our finite size estimates (1500 ≤ N ≤ 10^4) based on [1] with different choices of ε_N. a) ε_N = 0; b) ε_N ∼ B_5/N; c) ε_N ∼ C_5/(N ln N). The numbers in parentheses represent statistical errors obtained by χ^2 analysis, in units of the last written digit.

| S  | γ_S     | A_S    | B_S    | S  | γ_S     | A_S    | B_S    |
|----|---------|--------|--------|----|---------|--------|--------|
| 2  | 0.812282(2) | -1.6276(5) | -     | 9  | 0.493582(3) | -1.734(2) | -     |
| 3  | 0.716734(3)  | -1.665(2)  | -     | 10 | 0.474702(2) | -1.742(1)  | -     |
| 4  | 0.654304(11) | -1.677(7)  | -     | 11 | 0.458028(2) | -1.724(1)  | -     |
| 5  | 0.607452(4)  | -1.710(3)  | -     | 12 | 0.435166(3) | -1.721(2)  | -     |
| 6  | 0.570625(3)  | -1.729(2)  | -     | 13 | 0.427843(3) | -1.694(2)  | -     |
| 7  | 0.540500(9)  | -1.726(3)  | -     | 14 | 0.417665(3) | -1.728(2)  | -     |
| 8  | 0.515228(3)  | -1.710(3)  | -     | 15 | 0.406604(4) | -1.745(3)  | -     |

a)

| S  | γ_S     | A_S    | C_S    | S  | γ_S     | A_S    | C_S    |
|----|---------|--------|--------|----|---------|--------|--------|
| 2  | 0.812386(4) | -1.765(5) | 0.59(2) | 9  | 0.493596(13) | -1.73(2) | 0.10(9) |
| 3  | 0.716377(11) | -1.67(2)  | 0.03(8) | 10 | 0.474696(9) | -1.73(2) | -0.05(7) |
| 4  | 0.654487(7)  | -1.692(5) | 0.77(3) | 11 | 0.458017(9) | -1.71(2) | -0.09(7) |
| 5  | 0.607495(20) | -1.78(3)  | 0.33(12) | 12 | 0.443176(2) | -1.73(2) | 0.06(9) |
| 6  | 0.570655(12) | -1.78(2)  | 0.25(8) | 13 | 0.427918(10) | -1.59(2) | -0.51(7) |
| 7  | 0.540500(9)  | -1.72(2)  | -0.06(7) | 14 | 0.417627(13) | -1.67(2) | -0.3(1)  |
| 8  | 0.515173(10) | -1.64(2)  | -0.42(8) | 15 | 0.406654(16) | -1.82(2) | 0.34(12) |

b)

2.3 Computations for the Bernoulli Matching model.

We have performed similar Monte Carlo simulations for the Bernoulli Matching model. For computational reasons (generating two pseudo-random strings of size N is faster than a whole N × N matrix), we restricted extensive computations to sizes N ≤ 1500. We nevertheless performed a limited set of computations at sizes up to N = 10^5, in order to check the validity of [1] in that case. We found that this finite size scaling law applies to the mean value E(L^B_N)/N as well. Using the same method as above we obtained the estimates of γ^B_S which are quoted in table [1] for 2 ≤ S ≤ 15. These are not as precise as the corresponding estimates for the Random String model, since the extrapolation was restricted to smaller values of N. However we estimate the precision on γ^B_S to be better than 0.1%. More interestingly, we found that the values of γ^B_S are very well reproduced by the simple expression

$$\gamma^B_S = 2/(1 + \sqrt{S}),$$

a formula which had already been conjectured by Steele [21,22]. In fact Steele made his conjecture for the original LCS problem, at a time where precise numerical estimates of γ_S where not available, but it happens to be valid for the Bernoulli Matching model.

A short discussion may be instructive. Let A_k be the event that there exists a sequence of matches of length k. Then the length of a longest sequence of matches is

$$L = \sum_{k=1}^{N} 1_{A_k},$$

where 1_A is the indicator of set A in the sample space Ω of the model (be it the random string model or the
Fig. 2. Scaling of the variance of the LCS length. Random String model: Averages over $10^5$ instances for $1 \leq N \leq 1500$ and over $10^4$ instances for $1500 \leq 10^4$. Bernoulli Matching model: Averages over $10^4$ instances for $1 \leq N \leq 1500$. Dashed lines of slope $2/3$ give the expected scaling for the Bernoulli Matching model.

Table 2. Estimates of $\gamma_B$ for $2 \leq S \leq 15$. The extrapolation of $E(L^2_N)/N, N \leq 1500$, was based on $[1]$ with $\epsilon_N \sim C_S/(N \ln N)$ (values obtained for $A_S$ and $C_S$ are not reproduced). Precision on $\gamma_S$, estimated as the range of variation of our estimates for several choices $\epsilon_N \sim K_S/(N \ln^a N)^{-1}$, is about 0.05%. The conjectured values $2/(1 + \sqrt{S})$ for $\gamma_B$ are also quoted.

| $S$ | $\gamma^B_S$ | $2/(1 + \sqrt{S})$ | $S$ | $\gamma^B_S$ | $2/(1 + \sqrt{S})$ |
|-----|---------------|---------------------|-----|---------------|---------------------|
| 2   | 0.82860       | 0.828427            | 9   | 0.50047       | 0.5               |
| 3   | 0.73236       | 0.732051            | 10  | 0.48082       | 0.480506           |
| 4   | 0.66698       | 0.666667            | 11  | 0.46383       | 0.463225           |
| 5   | 0.61823       | 0.618034            | 12  | 0.44850       | 0.448018           |
| 6   | 0.58030       | 0.579796            | 13  | 0.43484       | 0.434259           |
| 7   | 0.54892       | 0.548584            | 14  | 0.42223       | 0.421793           |
| 8   | 0.52291       | 0.522408            | 15  | 0.41077       | 0.410426           |

Fig. 3. (A) Scaling of of $\text{Var}(L_N)$ for $10^4 \leq N \leq 2 \times 10^4$ in cases $S = 2$ and $S = 4$ (averages over 5000 random strings). The solid lines are best linear fits (slope 0.830 for $S = 2$ and 0.844 for $S = 4$). The dashed line has reference slope 2/3. (B) Histogram of the values of $X_N$ for $S = 2$ and $N = 500$ (averages over $10^4$ random strings). The solid curve corresponds to the normal distribution with mean 0 and unit variance.

Bernoulli Matching model. Hence the mean value $E(L)$ essentially depends on the behaviour of the probabilities $P(A_k)$: Using the martingale difference method (see e.g. [22]), one finds that

$$P(|L - E(L)| \geq k) \leq 2e^{-\frac{x_k^2}{2N}}$$  \hspace{1cm} (7)

hence $P(A_k) \geq 1 - 2 \exp(-(EL - k)^2/8N)$ for $k \leq E(L)$, and $P(A_k) \leq 2 \exp(-(k - EL)^2/8N)$ for $k \geq E(L)$.

The choice of this transition is very difficult to compute, but it is clearly related to the behaviour of the random variable $N_k(\omega)$ defined as the number of sequences of matches of length $k$ for a given instance $\omega$. Clearly

$$P(A_k) \leq E(N_k) = S^{-k} \left(\frac{N}{k}\right)^2.$$  \hspace{1cm} (8)

Setting $k = xN$ for $0 \leq x < 1$ and using Stirling formula, it is found $[22]$ that $E(N_k)$ has a transition from exponentially growing to exponentially decreasing behaviour at a value $x = \hat{x}_S$ given by the solution to $x(1-x)^{(1-x)/x} = S^{-1/2}$. Hence $\hat{x}_S$ is an upper bound for $\gamma_S$ and $\gamma^B_S$. It is not very accurate: One has $\hat{x}_2 \approx 0.9$, and as $S \to \infty$, $\hat{x}_S \sim e/\sqrt{S}$ which is not what one would expect from $[22]$. The reason of this failure is that $N_k$ is not a self-averaging
quantity, so that its mean value does not reproduce well its typical behaviour. Consider then the “entropy” \( \ln(N_k + 1) \). This is a self-averaging quantity from which \( \gamma_S = \ln(N_k + 1) \) can be computed as the smallest number \( 0 < \gamma < 1 \) such that \( x > \gamma \) implies
\[
\lim_{N \to \infty} E \ln(N_{x,N} + 1) / N = 0. \tag{9}
\]
Clearly the function \( f(x) = \lim_{N \to \infty} N^{-1} E \ln(N_{x,N} + 1) \) is singular at \( x = \gamma \). From the results of section 4, we even expect \( f(x) \) to be discontinuous at \( x = \gamma \). Fortunately, computing \( E \ln(N_k + 1) \) is still a difficult problem.

Steele suggested another approach to the problem \( [23] \), which consists of looking at the maximum of \( N_k(\omega) \). The location \( k_{\max} \) of this maximum is a self-averaging quantity which may be expected to be comparable in a simple way with the LCS length: A plausible guess is that with probability one, \( k_{\max} / L \to 1/2 \) as \( N \to \infty \). Assuming this we must maximize \( f(x) \) defined above, and the situation is not much better than before. But now the approximation of replacing \( N_k \) by its mean value does work much better: \( E(N_k) \) has a sharp maximum at \( k \sim xS \). Hence quite surprisingly, \( 2xS \) is a really good estimate for \( \gamma_S \), and it happens to give the correct value of \( \gamma_S^B \). We have no explanation for this observation, but we remark that a similar computation can be done for the related Longest Increasing Subsequence (LIS) Problem. Given a sequence of distinct numbers \( x_1, ..., x_N \) this problem asks for a sequence \( 1 \leq i_1 < ... < i_k \leq N \) such that \( x_{i_1} < ... < x_{i_k} \) and \( k \) is maximal. When the \( x \)'s are i.i.d. random variables uniformly distributed in \([0, 1]\), it is known that the expected length of a LIS is asymptotic to \( \gamma_{IS} \sqrt{N} \) where \( \gamma_{IS} = 2 \tag{26} \). Now let \( A_k^{(IS)} \) be the number of increasing subsequences of length \( k \) of \( x_1, ..., x_N \), so that
\[
E(A_k^{(IS)}) = \binom{N}{k} / k!. \tag{10}
\]
Using Stirling formula, one finds that \( E(A_k^{(IS)}) \) has a transition from a rapidly growing to a rapidly decreasing behaviour at \( k \sim c \sqrt{N} \), and presents a sharp maximum at \( k \sim x_{IS} \sqrt{N} \) where \( x_{IS} = 1 \). Hence \( \gamma_{IS} = 2x_{IS} \) and the above approximation is actually exact in this case.

As a byproduct, expression \( [3] \) provides a consistent mean to check the validity of the finite size scaling \( [4] \) for the Bernoulli Matching model. Indeed we can measure directly the scaling in \( N \) of the quantity
\[
a_S(N) = \sqrt{N}(\gamma_S^B N - E(L_S^B)). \tag{11}
\]
As is shown in figure \( [4] \), \( \ln a_S(N) \) has a near linear dependence on \( \ln(\ln N) \) with a slope consistent with \(-1\), as is expected by assuming the validity of \( [4] \).

3 The case \( N \neq M \) and a cavity solution.

There is still another way to study the asymptotic behaviour of \( E(L_N) \), which consists of working directly with the recurrence relation \( [1] \). This point of view has the advantage that it enables one to study the case \( M \neq N \) in a natural way, leading to a generalization of \( [1] \) to the case where \( N, M \to \infty \), the ratio \( r = M/N \) being fixed.

In order to find the asymptotics of \( [1] \) it is convenient not to work with \( L_{ij} \) directly, but rather (as in \( [13] \)) with the differences \( \nu_{ij} \) and \( \mu_{ij} \) defined by
\[
\nu_{ij} = L_{ij} - L_{i-1,j}, \mu_{ij} = L_{ij} - L_{i,j-1}, \quad 1 \leq i, j \leq N. \tag{12}
\]
The recurrence relations for \( \nu_{ij} \) and \( \mu_{ij} \) are readily seen to be
\[
\nu_{ij} = \max(0, \epsilon_{ij} - \mu_{i-1,j}, \nu_{i,j-1} - \mu_{i-1,j}) \quad \mu_{ij} = \max(0, \epsilon_{ij} - \nu_{i,j-1}, \mu_{i,j-1} - \nu_{i,j-1}) \tag{13}
\]
with boundary conditions \( \nu_{i,0} = \nu_{0,i} = \mu_{i,0} = \mu_{0,i} = 0 \). In the Random String model we have \( \epsilon_{ij} = \delta_{X_j,Y_i} \), whereas in the Bernoulli Matching model the \( \epsilon \)'s are i.i.d. Bernoulli variables with \( P(\epsilon_{ij} = 1) = 1 - P(\epsilon_{ij} = 0) = 1/S \). We consider relations \( [13] \) as a kind of exact cavity equations \( [13] \) for the LCS problem. The LCS length \( L_N \) can be retrieved by summing the \( \nu \)'s and \( \mu \)'s along the first bissector. To be precise
\[
L_N = \sum_{i=1}^{N} (\nu_{ii} + \mu_{i-1,i}) = \sum_{i=1}^{N} (\mu_{ii} + \nu_{i,i-1}). \tag{14}
\]
When $N \neq M$, $M/N = r$, we view $L_{NM}$ as a sum along a path “as straight as possible” in the direction defined by $r$, e.g. a path zigzagging along the straight line joining the points $(0,0)$ and $(N,M)$ in such a way as to keep as close as possible from this line.

A simple, but important observation is that the variables $\nu_{ij}$ and $\mu_{ij}$ can take only the values 0 and 1. Hence let us introduce the probabilities

$$p_{ij} = P(\nu_{ij} = 1), \quad p'_{ij} = P(\mu_{ij} = 1).$$

(15)

As $i$ and $j \to \infty$, it is natural to expect that $p_{ij}$ and $p'_{ij}$ have limits depending only on the ratio $r = j/i$. We denote these limits respectively by $p(r)$ and $p'(r)$ (or $p$ and $p'$ for short).

For a given $r > 0$, $L_{N,[rN]}$ is a sum of $N$ terms $\nu_{ij}$ and $rN$ terms $\mu_{ij}$, along a path “close” to the straight line from $(0,0)$ to $(N,[rN])$. Hence the limit $\gamma_S(r) = \lim_{N \to \infty} E(L_{N,[rN]})/N$ must be given by

$$\gamma_S(r) = p(r) + rp'(r).$$

(16)

Now a relation between $p(r)$ and $p'(r)$ can be readily obtained from (13) if we assume that for large $i$ and $j$, the occupation numbers $\nu_{ij}$ and $\mu_{ij}$ are nearly independent variables. It turns out that this decorrelation property holds true in the Bernoulli Matching model. It can be justified on the basis of a transfert matrix method for this percolation problem which will be presented elsewhere.

In the limit $i,j \to \infty$ we are thus led to the following self-consistent equations:

$$p_{ij} = 1 - p'_{i-1,j} - (1 - 1/S)(1 - p_{i,j-1})(1 - p'_{i-1,j}),$$

$$p'_{ij} = 1 - p_{i-1,j} - (1 - 1/S)(1 - p_{i,j-1})(1 - p'_{i-1,j}).$$

(17)

If we now let $p(r) = \lim_{i \to \infty} p_{i,[r]}$ and $p'(r) = \lim_{i \to \infty} p'_{i,[r]}$ and note that $p_{i,[r]} = 1 - p_{i,[r]} - 1/i(d/dr)p(r)$ and $p'_{i,[r]} = 1 - p_{i,[r]} - 1/i(d/dr)p'(r)$, then taking the sum and the difference in (17) leads to

$$1 = p + p' + (S - 1)pp'$$

(18)

and

$$\frac{d}{dr}p(r) + r\frac{d}{dr}p'(r) = 0.$$  

(19)

These last two equations determine the functions $p(r)$ and $p'(r)$ completely. A simple computation gives now

$$p(r) = \frac{\sqrt{rS} - 1}{S - 1}, \quad p'(r) = \frac{\sqrt{S/r} - 1}{S - 1}. $$

(20)

Note that the relation $p'(r) = p(1/r)$ is obvious from symmetry considerations. It must be also remarked that (20) is only satisfied for $1/S \leq r \leq S$ (although (18) and (19) are valid for all $r$ except $r = S$ and $r = 1/S$): The LCS problem has a percolation transition when one of the two strings is $S$ times larger than the other. Suppose for instance $r = M/N = S$. Consider the sequence of matches $(1, j_1), (2, j_2), \ldots$, where $j_1$ is the smallest integer $j \geq 1$ such that $(1, j)$ is a match, $j_2$ is the smallest integer $j > j_1$ such that $(2, j)$ is a match, and so on. The differences $j_{k+1} - j_k$ are independent random variables with mean value $S$. By the law of large numbers, $j_k$ is asymptotic to $KS$ as $k \to \infty$. It follows that the length of this sequence of matches, restricted to the integer points $(ij)$ such that $j \leq M$, is asymptotic to $M/S = N$ as $N \to \infty$.

Hence for $r \geq S$ we have $\gamma_S(r) = \gamma_S^B(r) = 1$ (and also $\gamma_S(1/r) = \gamma_S^B(1/r) = 1$ by symmetry). This means that when $i$ is large and $j \geq Si$, $\gamma_{ij}$ is nearly equal to $i$, hence for each $i' < i$ and $j' \geq j$ we have $\nu_{ij} = 1$ and $\mu_{ij} = 0$ with high probability. In other words, $r \geq S$ implies $p(r) = 1$ and $p'(r) = 0$, and by symmetry, $p(1/r) = 0$ and $p'(1/r) = 1$. From (20) and (16) we find the expression of the function $\gamma_S^B(r)$ of the Bernoulli Matching model for $1/S \leq r \leq S$:

$$\gamma_S^B(r) = \frac{2\sqrt{rS} - r - 1}{S - 1}. $$

(21)

Note that the transition of $\gamma_S^B(r)$ at $r = S$ and $r = 1/S$ is “second order”, that is $d^2\gamma_S^B/dr^2 = p'(r)$ is continuous and $d^2\gamma_S^B/dr^2(r)$ is discontinuous at $r = S$ and $r = 1/S$.

Figure 5 shows the confrontation of equation (21) to a Monte Carlo computation of the Bernoulli Matching model for $S = 2$ and $S = 15$.

We have plotted, for several values of $t$, the “curves” delimiting the set $C_t/t$ in the two dimensional $(x,y)$ plane, where $C_t = \{(ij) : 1 \leq i, j \leq N, \gamma_{ij} \leq t\}$. As $t \to \infty$, the boundary of $C_{t}/t$ approaches asymptotically the curve of parametric equation $r \to (1/\gamma_S^B(r), r/\gamma_S^B(r))$. This is the solid curve which we have plotted using (21). Figure 6 reproduces for comparison the results of analogous computations made for the Random String model. Note that as $S$ increases, the differences between the results for the Bernoulli Matching model and the random string model are less and less significant, and it is reasonable to expect that $\gamma_S(r)$ is asymptotic to $\gamma_S^B(r)$ as $S \to \infty$. Numerically the convergence is rather rapid: the quantity $S(\gamma_S^B - \gamma_S)$ shows a maximum at $S \approx 11$ after which it happens to decrease. Such a phenomenon has already been observed and interpreted in other combinatorial optimisation problems, and it would be of interest to have a theoretical understanding of the large $S$ behaviour of $\gamma_S^B - \gamma_S$. We leave this question open for future work.

4 Configuration space properties of the LCS problem.

In this section we study generic properties of the set of solutions of the LCS problem, that is average properties of the set of all LCSs of two random strings.

A most direct computational access to these properties is provided by what we shall call the LCS graph of a given instance. Given any strings $X$ and $Y$ of length $N$, this graph is defined as follows. The vertices are the LCS matches, that is the set of points $(ij)$, $1 \leq i, j \leq N$ such that $X_i = Y_j$ and $(ij)$ occurs in at least a LCS of $X$ and $Y$. Two LCS matches are incident in the LCS graph if
they occur as successive matches (regardless the order) in the same LCS.

It is a nice feature of the LCS problem that this structure may be computed in a very efficient way. To a large part, this circumstance is due to the directed nature of the problem, which greatly simplifies the structure of the set of solutions.

4.1 Construction of the LCS graph.

Since the construction we have used is rather simple we shall not give a precise algorithm, but rather indicate the main steps, together with the main observations which enable an efficient implementation.

Given integer points \((i_1,j_1)\) and \((i_2,j_2)\) we write \((i_1,j_1) \prec (i_2,j_2)\) if \(i_1 < i_2\) and \(i_2 < j_2\). Suppose the LCS matrix of \(X\) and \(Y\) is computed, and let \(L\) be the length of a LCS of \(X\) and \(Y\). Following the terminology of [2], we call an integer point \((i,j)\) such that \(X_i = Y_j\) a match of rank \(k\) if \(k\) is the length of a LCS of \(X_1, \ldots, X_i\) and \(Y_1, \ldots, Y_j\). It is then easy to construct, for each \(1 \leq k \leq L\), a list \(M(k)\) of the matches of rank \(k\) of \(X\) and \(Y\). It is convenient to have the members \((i,j)\) of \(M(k)\) ordered lexicographically, in such a way that \(i\) increasing while \(j\) is decreasing. Then setting \(M(k) = \{(i_1,j_1), \ldots, (i_m, j_m)\}\), one sees that \((i_1, \ldots, i_m)\) is an increasing sequence, while \((j_1, \ldots, j_m)\) is a decreasing sequence. The reason for this is that given any two members \((i,j)\) and \((i',j')\) of \(M(k)\) we have \(i < i' \Rightarrow j \geq j'\), since otherwise \((i,j)\) and \((i',j')\) would not be of the same rank. This property is important for an efficient construction of the LCS graph.

The lists \(M(k)\) are the basic data in the construction of the LCS graph. Remark that the members of \(M(L)\) are...
obviously LCS matches, hence these must be included as vertices of the LCS graph. If \( P \) is a match of rank \( k < L \), then \( P \) is a LCS match if and only if there is a LCS match \( Q \) of rank \( k + 1 \) such that \( P < Q \). Remark also that, by definition, a LCS match of rank \( k \) may be connected only to LCS matches of rank \( k - 1 \) or \( k + 1 \) in the LCS graph. If \( P \) is a LCS match of rank \( k > 1 \), and \( Q \) is a LCS match of rank \( k - 1 \), then \( P \) and \( Q \) are connected if and only if \( Q < P \). We will denote by \( M_{LCS}(k) \) the list of the LCS matches of rank \( k \), ordered in the way which is inherited from the ordering of \( M(k) \).

We construct the LCS graph in \( L \) stages numbered \( k = L, L - 1, \ldots, 1 \). Stage \( L \) consists of inserting all matches of rank \( L \) as vertices of the LCS graph. Once all the LCS matches of rank \( k \) have been inserted, stage \( k \) consists of selecting the members of \( M(k) \) which belong to \( M_{LCS}(k) \), and then to insert the required edges connecting \( M_{LCS}(k) \) to \( M_{LCS}(k + 1) \).

Using remarks made previously and exploiting the way \( M(k) \) and \( M_{LCS}(k + 1) \) have been ordered, it is easy to see that the selection of the members of \( M_{LCS}(k) \) from those of \( M(k) \) at stage \( k \) may be performed in \( O(m_k + l_{k+1}) \) steps, \( m_k \) and \( l_{k+1} \) being the cardinality of \( M(k) \) and \( M_{LCS}(k + 1) \) respectively. Hence the detection of the whole set of LCS matches takes at most \( O(m) \) steps in this construction, \( m = \sum_k m_k \) being the total number of matches of \( X \) and \( Y \). The main part of the computation is devoted to the insertion of the edges in the LCS graph. The number of operations (comparisons and insertions) needed to determine the edges connecting \( M_{LCS}(k) \) and \( M_{LCS}(k + 1) \), once these lists are known, is of order \( O(l_k) \). Since there is no obvious bound for \( l_k \) better than \( m_k \), and no obvious bound for \( m_k \) better than \( 2N \), we obtain a bound for the time required to compute the LCS graph which is \( O(LN^2) \).

However when \( X \) and \( Y \) are random strings from a finite alphabet, the typical values of \( l_k \) happen to be much smaller than \( m_k \), and the typical time required by the above construction is in fact much smaller than \( O(LN^2) \).

### 4.2 Computations of the LCS graph.

We performed a series of Monte Carlo computations in order to study some of the basic properties of the set of LCSs of two random strings. We concentrated our study on different quantities which can be easily computed once the LCS graph is constructed.

Probably the most basic quantity which characterizes the set of LCSs is its cardinality \( N_{LCS} \). Figure (a) reproduces the estimated average and variance of the ground state entropy \( S_N = \ln N_{LCS} \) in case \( S = 2 \), computed over \( 10^4 \) random instances and for values of \( N \) ranging from 100 to 1000. It is rather striking on this figure that \( E(S_N) \) grows linearly with \( N \). We expect the random variable \( \ln N_{LCS} \) to be self-averaging, and this is confirmed by the measured behaviour of its variance, whose growth is also nearly linear. We observed this behaviour for all the values of \( S \) we considered.

Hence we found that the number of LCSs of two typical random strings is very large. \( N_{LCS} \) typically grows exponentially with \( N \), with a well defined exponential factor \( \alpha_S \), which we define, assuming the limit indeed exists, as

\[
\alpha_S = \lim_{N \to \infty} \frac{E(S_N)}{N} \quad (22)
\]

Also we define (provided the limit exists)

\[
\beta_S = \lim_{N \to \infty} \frac{\text{Var}(S_N)}{N} \quad (23)
\]

Using best linear fits we obtained rather precise estimates of \( \alpha_S \) and \( \beta_S \), which are quoted in table (a) for several values of \( S \).

Another quantity reflecting the “size” of the set of LCSs of two random strings is the typical overlap of two LCSs. Viewing a LCS of \( X \) and \( Y \) as a sequence of integer points we define the overlap of two LCSs \( \sigma_1 = (Q_1, \ldots, Q_L) \)
and \( \sigma_2 = (P_1, ..., P_L) \) as the quantity

\[
q = q(\sigma_1, \sigma_2) = \frac{1}{T} \sum_{k=1}^{L} \delta(Q_k, P_k).
\]

(24)

where \( \delta(Q_k, P_k) = 1 \) if \( Q_k = P_k \) and 0 otherwise. \( q(\sigma_1, \sigma_2) \) is analogous to the order parameter used in the theory of spin glasses \([13]\). The quantity \( L(1 - q(\sigma_1, \sigma_2)) \) should be regarded as a kind of Hamming distance in the space of LCSs of \( X \) and \( Y \). The object of interest here is the empirical distribution of \( q(\sigma_1, \sigma_2) \) for \( \sigma_1 \) and \( \sigma_2 \) ranging over the set of LCSs of \( X \) and \( Y \). We denote by \(< q > \) and \(< q^2 > \) the first and second moment of the overlap under this distribution. It is not difficult to see that

\[
< q > = \frac{1}{L} \sum_{k=1}^{L} \sum_{Q \in M_{LCS}(k)} P_1(Q)^2
\]

(25)

where

\[
P_1(Q) = \frac{N_{LCS}(Q)}{N_{LCS}}
\]

(26)

and \( N_{LCS}(Q) \) is the number of LCSs of \( X \) and \( Y \) of which the integer point \( Q \) is a member. Hence the average overlap \(< q > \) can be easily computed for any given instance of \( X, Y \) once the LCS graph is constructed. Also we have

\[
< q^2 > = \frac{1}{L^2} \sum_{k=1}^{L} \sum_{Q \in M_{LCS}(k)} \sum_{Q' \in M_{LCS}(l)} P_2(Q, Q')^2
\]

(27)

where

\[
P_2(Q, Q') = \frac{N_{LCS}(Q, Q')}{N_{LCS}^2}
\]

(28)

and \( N_{LCS}(Q, Q') \) is the number of LCSs of \( X \) and \( Y \) of which points \( Q \) and \( Q' \) are members. It is still elementary to compute \(< q^2 > \), but more computationally lengthy due to the above double summation.

We denote the averages of \( < q > \) and \( < q^2 > \) over the random strings \( X \) and \( Y \) simply by \( E(q) \) and \( E(q^2) \). Figure \([6]\) presents the results of a Monte Carlo computation of \( E(q) \) and \( Var(q) = E(q^2) - (E(q))^2 \) in the case \( S = 2 \). This figure shows that \( E(q) \) has a nearly \( 1/\sqrt{N} \) convergence to a limit value \( q_S \) as \( N \to \infty \). Not surprisingly in view of the fact that \( N_{LCS} \) grows exponentially with \( N \), we find that \( q_S < 1 \). Estimates of \( q_S \) based on a \( 1/\sqrt{N} \) extrapolation of our finite size results are given in table \([3]\).

It is also seen on figure \([6]\) that the variance of the overlap decreases with \( N \) roughly as \( 1/N \). Hence we conclude that the overlap \( q(\sigma_1, \sigma_2) \) of two randomly chosen LCSs happens to be self-averaging, i.e. \( q(\sigma_1, \sigma_2) \) becomes non random (and equal to \( q_S \)) in the limit \( N \to \infty \). This is in fact not surprising: the space of LCSs of two random strings is not very far from having a product structure and the quantity \( (1 - q(\sigma_1, \sigma_2)) \) is a kind of (normalized) Hamming distance on this space. In the conventional wisdom of statistical mechanics, we would say that, although there is some pathology in this system from a physical point of view (it does not satisfy “Nernst’s principle”), it presents no replica symmetry breaking.

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**Table 3.** The exponential growth factor of the number of LCSs of two random strings and the average overlap between two LCSs.

| \( S \) | \( a_S \) | \( b_S \) | \( q_S \) |
|-------|-------|-------|-------|
| 2     | 0.2458(8) | 0.232(2) | 0.6753(8) |
| 3     | 0.2302(4) | 0.171(1) | 0.6782(8) |
| 4     | 0.2086(3) | 0.145(2) | 0.6851(7) |
| 5     | 0.1903(2) | 0.125(2) | 0.6921(7) |
| 10    | 0.1365(2) | 0.0885(1) | 0.7138(10) |
| 15    | 0.1100(1) | 0.0711(1) | 0.7264(8) |
We also considered quantities which are of interest to describe the "shape" of the LCS graph. Two such quantities are the distribution of the distance between two successive matches of a LCS, and the distribution of the number of LCS matches of a given rank. More precisely, we let \( P(d, X, Y) \) be the empirical distribution, over the set of LCSs of \( X \) and \( Y \), of the distance between two successive LCS matches:

\[
P(d, X, Y) = \frac{1}{L-1} \sum_{k=1}^{L-1} \sum_{Q \in M_{LCS}(k)} \frac{N_{LCS}(Q, d)}{N_{LCS}}.
\]  

Here \( N_{LCS}(Q, d) \) is the number of LCS \( \sigma = (Q_1, \ldots, Q_L) \) of \( X \) and \( Y \) such that \( Q_k = Q \) for some \( k < L \), and \( |Q_{k+1} - Q_k| = d \) (the distance between two points is taken to be Manhattan distance \(|(i_1, j_1) - (i_2, j_2)| = |i_1 - i_2| + |j_1 - j_2|\)). We define \( P_S(d, N) \) as the average of \( P(d, X, Y) \) over random \( S \)-ary strings of size \( N \). Also we let \( \Pi(m, X, Y) \) be the empirical distribution of the cardinality of \( M_{LCS}(k) \) over \( 1 \leq k \leq L \), i.e.

\[
\Pi(m, X, Y) = \frac{1}{L} \sum_{k=1}^{L} \delta(l_k, m),
\]  

\( l_k \) being the number of LCS matches of rank \( k \), and we let \( \Pi_S(m, N) \) be the average of \( \Pi(m, X, Y) \) over \( X \) and \( Y \). It is natural to expect that \( P_S(d, N) \) has a limit \( P_S(d) \) as \( N \to \infty \). It is not so obvious that the same holds for \( \Pi_S(m, N) \). We found numerically that both \( P_S(d, N) \) and \( \Pi_S(l, N) \) approach well defined distributions as \( N \) grows. Figure (9) reproduces graphically \( P_S(d) \) for \( S = 2, 4, 10 \) and 15. As \( S \) increases the maximum of \( P_S(d) \) becomes more and more pronounced and is displaced to the right, as is expected from the relation \( \sum_{d \geq 0} dP_S(d) = 2/\gamma_S \). The asymptotic shape of \( \Pi_S(m) \) appears to depend much less drastically on \( S \) so we give only the results obtained for \( S = 2 \) and \( S = 4 \) (figure (10)). Numerically it is found that the typical number of LCS matches of a given rank remains bounded as \( N \) grows.

This contrasts with the behaviour of the diameter of the sets \( M_{LCS}(k) \) (in the Manhattan distance). This behaviour is shown in figure Figure (11), where are plotted the quantities \( D_S(N) \) and \( V_S(N) \), defined to be respectively the mean and variance over random \( S \)-ary strings of size \( N \) of

\[
D_S(X, Y) = \frac{1}{L} \sum_{k=1}^{L} diam(M_{LCS}(k)).
\]  

Clearly \( D_S(N) \) appears to grow with \( N \). In fact from heuristic scaling arguments, we expect \( D_S(N) \) to be of the same order as the finite size corrections to the linear scaling of \( E(LN) \). If we are confident in (10), this means that \( D_S(N) \) should grow asymptotically as \( \sqrt{N}/\ln N \). Fortunately this is what we find from a \( \chi^2 \) analysis: The solid curve in figure (11)(A) is a best fit of our estimates to a function of the form \( C_1 + C_2 \sqrt{N}/\ln N \). The corresponding \( \chi^2 \) value is 12.74 for a number of degrees of freedom of 15.

Fig. 9. The distribution \( P_S(d) \) of the distance between two successive LCS matches, for \( S = 2, 4, 10, 15 \) (averages over \( 10^4 \) random strings in each case). Each figure show results for different values of \( 100 \leq N \leq 1500 \) superposed in order to visualize the collapse toward a limit value.
Fig. 10. The distribution $\Pi_S(m)$ of the number of LCS matches of a given rank for $S = 2$ and $S = 15$ (averages over $10^4$ random strings in each cases).

Fig. 11. Behaviour of (A) the mean $D_S(N)$ and (B) the variance $V_S(N)$ of the width of the LCS graph (averages over $10^4$ random 15-ary strings).

For comparison, the $\chi^2$ value achieved from a best fit to $C_1 + C_2\sqrt{N}$ is of 37.7, which is much too large. This numerical test provides another support to the reliability of (4). Note however that the fluctuations of $D_S(X, Y)$ are far from negligible, as the variance of $D_S(X, Y)$ shows a near linear growth.

The asymptotic distributions $P_S(d)$ and $\Pi_S(m)$ provide useful informations on the local properties of the LCS graph, but they tell nothing about the universality class of the LCS problem. Results for the mean square “displacement” $i - j$ along the LCS graph are presented in figure (12). One way to measure this quantity would be to generate a given LCS in a sequential way and to perform averages along this LCS. Since we are able to perform exact averages over the set of LCSs, we use here a more “static” definition: For a given instance, the mean square displacement along a LCS chosen at random is given by

$$<(i - j)^2> = \frac{1}{L} \sum_{k=1}^{L} \sum_{Q \in M_{LCS}(k)} P_1(Q)(i - j)^2$$  \hspace{1cm} (32)

where $P_1(Q)$ is defined as before and we have set $Q = (ij)$. We then estimate $E((i - j)^2)$ as an average over a large number of random strings of $< (i - j)^2 >$ computed for each instance. The price to pay for exact computations is mainly a limitation on the size $N$ of our instances. It is seen on figure (12) however that the scaling behaviour $E((i - j)^2) \approx N^{4/3}$ is reached rather fast, both for the Bernoulli matching model and for the Random String model. We cannot exclude the possibility of a crossover at $N \gg 1500$ for the Random String model. But then the asymptotic scaling regime of $E((i - j)^2)$ would be attained at much larger values of $N$ than for $\text{Var}(L_N)$, which seems unlikely.

5 Concluding remarks.

This article has been devoted to the presentation of a thorough investigation of the LCS Problem by means of numerical simulations. One of our main findings is that the finite size behaviour of the average LCS length $E(L_N)$ is very well reproduced by (4). This form provides a numeri-
Fig. 12. Scaling of the average “displacement” $E((i-j)^2)$ along the LCS graph, for the Random String model (RS) ($100 \leq N \leq 1500$) and for the Bernoulli Matching model (B) ($100 \leq N \leq 1000$). Averages are over $10^4$ instances in each case, with $S = 2$. The $N^{3/5}$ scaling is visualized by the dashed line of slope $4/3$.

A further interesting question concerns the applicability of the cavity-like method used to derive (21). What makes this method work for the Bernoulli Matching model is that a remarkable decorrelation property holds in this percolation problem (10). It would be interesting to find other percolation problems where such a decorrelation property occurs. This would provide simple means to obtain analytical information on the passage time constants of such models.

We finally investigated average properties of the set of solutions, and the “universality class” of the LCS problem. We were rather surprised to find that the number of common subsequences of maximal size of two typical random strings grows exponentially with the size of the strings. It follows that two (randomly) given LCSs are to a large extent distinct, as confirmed by the study of their typical overlap. We also found that the long ranged correlations in the Random String model appear to be relevant to the universality class of the model, as is seen from the large $N$ behaviour of $\text{Var}(L_N)$. One may wonder why this has not been observed in Needleman-Wunsch sequence alignment (4). A plausible reason (pointed out in (12)) is that introducing a gap penalty in the model results in binding more tightly the optimal paths to the first bissector. This should reduce the effect of correlations and extend the “small $N$” scaling regime to larger values of $N$. In particular for biological purposes only the small $N$ regime is likely to be relevant. An exciting issue is the possible occurrence of a phase transition in the gap parameter of Needleman-Wunsch alignment.

Another interesting question is whether a proliferation of solutions is specific to random sequences and subsequences, or if such phenomenon is of relevance to other percolation situations. As already said, the smallness of the variance of $L_N$ is probably related to the large number of LCSs of two random sequences. Smallness of the variance of the passage time from $(0,0)$ to $(0,N)$ is also observed in usual first passage percolation on $\mathbb{Z}^2$. In fact these models (a famous example of which is the Eden model) are known to fall into the universality class of directed polymers in random media. One may expect to find in these models a large number of quasi optimal paths with typical overlaps smaller than one.

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References
1. K. Alexander, The rate of convergence of the mean length of the longest common subsequence, The Annals of Applied Probability, 4–4 (1994), pp. 1074–1082.
2. A. Apostolico and C. Guerra, The Longest Common Subsequence Problem Revisited, Algorithmica, 2 (1987), pp. 315–336.
3. R. Arratia and M. Waterman, A Phase Transition for the Score in Matching Random Sequences Allowing Deletions, The Annals of Applied Probability, 4–1 (1994), pp. 200–225.
4. P. Bevington and D. Robinson, Data Reduction and Error Analysis for the Physical Sciences, McGraw-Hill, New York, 1994.
5. J. H. Boutet de Monvel, Markov Chain Approximations to the LCS Problem, In preparation, (98).
6. J. H. Boutet de Monvel and O. C. Martin, Mean Field and Corrections for the Euclidean Minimum Matching Problem, Physical Review Letters, 79–1 (1997), pp. 167–170.
7. V. Chvatal and D. Sankoff, Longest Common Subsequences of two Random Sequences, Journal of Applied Probability, 12 (1975), pp. 306–315.
8. V. Dancik, Expected Length of Longest Common Subsequences, Thése, University of Warwick, 1994.
9. V. Dancik and M. Paterson, Upper bounds for expected length of a longest common subsequence of two random sequences, in STACS94. Lecture Notes in Computer Science 775, 1994, pp. 306–315. Springer, New York.
10. J. Deken, Some Limit Results for Longest Common Subsequences, Discrete Mathematics, 26 (1979), pp. 17–31.
11. D. Drasdo, T. Hwa, and M. Lässig, Scaling Relations and Similarity Detection in Sequence Alignment with Gaps, (1998), pp. –. cond-mat/9802023.
12. T. Hwa and M. Lässig, Similarity-Detection and Localization, Physical Review Letters, 76 (1996), pp. 2591–2595. cond-mat/9712081.
13. W. Masek and M. Paterson, A Faster Algorithm for Computing String Edit Distances, Journal of Computer and Science Systems, 20 (1980), pp. 18–31.
14. E. Medina, T. Hwa, and M. Kardar, Burgers equations with correlated noise: Renormalization-group analysis and applications to directed polymers and interface growth, Physical Review A, 39–6 (1989), pp. 3053–3075.
15. M. Mézard, G. Parisi, and M. A. Virasoro, eds., Spin Glass Theory and Beyond, World Scientific, Singapore, 1987.
16. S. Needleman and C. Wunsch, A General Method Applicable to the Search for Similarities in the Amino Acids Sequence of Two Proteins, Journal of Molecular Biology, 48 (1970), pp. 443–453.
17. W. T. Rhee, On rates of convergence for common subsequences and first passage time, The Annals of Applied Probability, 5–1 (1995), pp. 44–48.
18. D. Sankoff, R. Cedergren, and G. Lapalme, Frequency of insertion-deletion, transversion, and transition in evolution of 5S ribosomal RNA, Journal of Molecular Evolution, 7–2 (1976), pp. 133–149.
19. D. Sankoff and J. Kruskal, Time Warps, String Edits, and Macromolecules: The theory and practice of sequence comparison, Addison Wesley, Reading, Mass, 1983.
20. T. Smith and M. Waterman, Identification of common molecular subsequences, Journal of Molecular Biology, 147 (1981), pp. 195–197.
21. M. Steele, Long Common Subsequences and the proximity of two random strings, SIAM Journal on Applied Mathematics, 42–4 (1982), pp. 731–737.
22. M. Steele, Probability Theory and Combinatorial Optimization, SIAM Philadelphia, ISBN 0-89871-380-3, 1997.
23. M. Steele, private communication, (1998).
24. M. Talagrand, A New Look at Independence, The Annals of Probability, 24–1 (1996), pp. 1–34.
25. E. Ukkonen, Algorithms for Approximate String Matching, Information and Control, 64 (1985), pp. 100–118.
26. A. Versik and S. Kerov, Asymptotics of the Plancherel Measure of the Symmetric Group and the Limiting Shape of Young Tables, Soviet Math. Dokl., 18–2 (1977), pp. 527–531.
27. M. Vingron and M. Waterman, Sequence Alignment and Penalty Choice, Journal of Molecular Biology, 325 (1994), pp. 1–12.
28. R. Wagner and M. Fisher, The string to string correction problem, J. Assoc. Comput. Mach., 21 (1974), pp. 168–173.
29. M. Waterman, ed., Mathematical methods in DNA Sequences, CRC press, Boca Raton, FL., 1989.
30. M. Waterman, Estimating statistical significance of sequence alignments, Philosophical Transactions of the Royal Society of London B, 344 (1994), pp. 383–390.
31. M. Zhang and T. Marr, Alignment of Molecular Sequences Seen as Random Path Analysis, Journal of theoretical Biology, 174 (1995), pp. 119–129.