A LIMIT THEOREM FOR MATCHING RANDOM SEQUENCES ALLOWING DELETIONS¹

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We consider a sequence matching problem involving the optimal alignment score for contiguous sequences, rewarding matches by one unit and penalizing for deletions and mismatches by parameters δ and μ , respectively. Let M_n be the optimal score over all possible choices of two contiguous regions. Arratia and Waterman conjectured that, when the score constant $a(\mu, \delta) < 0$,

$$P\bigg(\frac{M_n}{\log n}\to 2b\bigg)=1$$

for some constant b. Here we prove the conjecture affirmatively.

1. Introduction. Let A_1,A_2,\ldots and B_1,B_2,\ldots be two independent sequences of i.i.d. random variables such that A_i and B_i have the same distribution on a finite number set $\{0,1,\ldots,\tau\}$. Let $I=(A_{g+1},\ldots,A_{g+i})$ and $J=(B_{h+1},\ldots,B_{h+j})$ with $1\leq g+1\leq g+i\leq n$ and $1\leq h+1\leq h+j\leq n$. The alignment score S(I,J) is defined to be

(1.1)
$$S(I,J) = \max \left\{ -\delta(i-l+j-l) + \sum_{k=1}^{l} s(A_{a(k)}, B_{b(k)}) \right\},$$

where the maximum is taken over all alignments, given by increasing sequences

$$g = a(0) \le a(1) < a(2) < \cdots < a(l) \le a(l+1) = g+i+1$$

and

$$h = b(0) \le b(1) < b(2) < \dots < b(l) \le b(l+1) = h+j+1.$$

In particular, if we restrict a(0) = g, $a(1) = g + 1, \ldots$, a(l) = g + l and b(0) = h, $b(1) = h + 1, \ldots$, b(l) = h + l, the corresponding score is called the nonalignment score or the score without deletions. The score function s(x, y) for aligned pairs is 1 if x = y and $-\mu$ if $x \neq y$. In words, each match is rewarded by 1, each mismatch is penalized by μ and each deletion by δ . Let $S_n = S(A_1, \ldots, A_n, B_1, \ldots, B_n)$. That is, $I = A_1, \ldots, A_n$ and $J = B_1, \ldots, B_n$. By a standard subadditive argument (see [2]), it is easy to see that, for

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 $\mu, \delta \geq 0$, there exists a nonrandom constant $a(\mu, \delta)$ such that

(1.2)
$$\lim_{n\to\infty} \frac{S_n}{n} = a(\mu, \delta) \quad \text{a.s. and in } L_1.$$

Here $a(\mu, \delta)$ is called the *score constant*. On the other hand, denote the *large deviation rate* by

$$(1.3) r(q) = \lim_{n \to \infty} \frac{-\log P(S_n \ge qn)}{n} = \inf \left\{ \frac{-\log P(S_n \ge qn)}{n} \right\},$$

where log means the natural logarithm. The limit in (1.3) exists and equals the infimum also using the subadditive property. Let M_n be the optimal aligned score over all possible choices of two contiguous regions I and J for $I \subset \{A_1, \ldots, A_n\}$ and $J \subset \{B_1, \ldots, B_n\}$. Formally,

$$(1.4) M_n = \max_{I,J} S(I,J).$$

Let $b = \max_{q \ge 0} q/r(q)$. It can be proved by applying the Borel-Cantelli lemma along a suitable skeleton in Lemma 2 in [2] that, if $a(\mu, \delta) < 0$, then

$$(1.5) b \le \liminf \frac{M_n}{\log n} \le \limsup \frac{M_n}{\log n} \le 2b \quad \text{a.s.}$$

On the other hand, it was also proved in [2] that, if $a(\mu, \delta) > 0$,

$$\lim_{n\to\infty}\frac{M_n}{n}=a(\mu,\delta)\quad\text{a.s. and in }L_1.$$

The phenomenon of the two different behaviors of M_n is called a *phase transition*. When $a(\mu, \delta) < 0$, one of the most important problems is to decide whether $M_n/(\log n)$ converges. In fact, Arratia and Waterman conjectured that $M_n/(\log n)$ converges to 2b in probability. Note that it was verified in [1] that the conjecture is true for the nonaligned case. Furthermore, Dembo, Karlin and Zeitouni [3] gave a more general discussion for the nonaligned case. In the following theorem we prove that the conjecture is true for any δ and μ .

Theorem 1. For each μ and δ , if $a(\mu, \delta) < 0$, then

(1.6)
$$\lim_{n\to\infty}\frac{M_n}{\log n}=2b\quad a.s.$$

REMARK 1. Here we prove that the theorem holds on a finite number set. We can also show that the theorem holds on Polish alphabets by the same proof of the theorem and Theorem 4' in [3]. On the other hand, the theorem also holds for a more general score function s(x, y).

REMARK 2. Amir Dembo pointed out that the same proof of the theorem carries over to generalized scoring and gapping, repeats in a sequence, and matching Markov chains (see the detailed definitions in [2]).

2. Proof of the theorem. The proof is based on Theorem 3 in [3]. For a positive integer m, consider two independent sequences $\{X_i\}$ and $\{Y_i\}$ with

$$X_i = (A_{im+1}, \dots, A_{(i+1)m})$$
 and $Y_j = (B_{jm+1}, \dots, B_{(j+1)m})$.

Clearly, $\{X_i\}$ is i.i.d. and so is $\{Y_j\}$. Let X_i and Y_j have the probability laws π_X and π_Y on finite sets Γ_X and Γ_Y , respectively, where

$$\Gamma_X = \Gamma_Y = \{0, 1, ..., \tau\}^m = \{(x_1, ..., x_m) : x_i \in \{0, 1, ..., \tau\} \text{ for } i = 1, ..., m\}.$$
 Clearly,

$$\pi_X(X_i = \mathscr{X}) = P((A_{im+1}, \dots, A_{(i+1)m}) = \mathscr{X}),$$

$$\pi_Y(Y_i = \mathscr{Y}) = P((B_{im+1}, \dots, B_{(i+1)m}) = \mathscr{Y})$$

for $\mathscr{X} \in \Gamma_X$ and $\mathscr{Y} \in \Gamma_Y$. A general score $F: \Gamma_X \times \Gamma_Y \to \mathscr{R}$ is assigned to each pair (X_i, Y_i) and the maximal nonaligned segment score is

(2.1)
$$\mathcal{M}_n = \max_{0 \le i, j \le n-k; \ k \ge 0} \left\{ \sum_{l=1}^k F(X_{i+l}, Y_{j+l}) \right\}.$$

It was proved in [3] that, if

(2.2)
$$E_{\pi_Y \times \pi_Y} F < 0 \quad \text{and} \quad \pi_X \times \pi_Y (F > 0) > 0,$$

then

(2.3)
$$\frac{\mathscr{M}_n}{\log n} \to \gamma(\pi_X, \pi_Y).$$

Furthermore, if (2.2) holds, there exists a unique positive value θ such that

$$(2.4) E_{\pi_{\mathsf{X}} \times \pi_{\mathsf{y}}}[e^{\theta F}] = 1.$$

Let α denote the conjugate measure associated with θ , that is,

$$\frac{d\alpha}{d(\pi_X \times \pi_Y)} = e^{\theta F},$$

and let α_X and α_Y denote the marginals of α on Γ_X and Γ_Y , respectively. Dembo, Karlin and Zeitouni [3] also showed that, if

$$(2.5) H(\alpha|\pi_X \times \pi_Y) \ge 2 \max\{H(\alpha_X|\pi_X), H(\alpha_Y|\pi_Y)\},$$

then

$$(2.6) \frac{\mathscr{M}_n}{\log n} \to \frac{2}{\theta},$$

where the relative entropy $H(\nu|\pi)$ is defined to be

$$H(\nu|\pi) = \sum_{i=1}^{K} \nu(b_i) \log \frac{\nu(b_i)}{\pi(b_i)}$$

for $\{b_1, \ldots, b_K\} = \Gamma_X \times \Gamma_Y$. Now we apply (2.6) to our purpose. Note that the score defined in (2.1) is nonaligned so that we have to choose some special F

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and use F to approximate the aligned score. Set

$$F(X_i, Y_i) = S(X_i, Y_i)$$
 [see (1.1) for the definition of S].

If $a(\mu, \delta) < 0$, by (1.2) and our definition, with a large m,

(2.7)
$$E_{\pi_X \times \pi_Y} F = ES_m < \frac{a(\mu, \delta)m}{2} < 0,$$

$$\pi_X \times \pi_Y (F > 0) \ge P(A_1 = B_1, \dots, A_m = B_m) > 0.$$

It follows from (2.7) and (2.3) that

(2.8)
$$\frac{\mathscr{M}_n}{\log n} \to \gamma(\pi_X, \pi_Y)$$

for our special definition of $\{X\}$ and $\{Y\}$. It also follows from (2.1) that

$$(2.9) M_n \le M_{nm},$$

where mn is the product of m and n. On the other hand, by a standard information inequality (see (13) in [3])

(2.10)
$$H(\alpha|\pi_X \times \pi_Y) \ge H(\alpha_X|\pi_X) + H(\alpha_Y|\pi_Y).$$

Note that $\Gamma_X = \Gamma_Y = \{0, 1, ..., \tau\}^m$, $\pi_X = \pi_Y$ and $F(\mathcal{X}, \mathcal{Y}) = F(\mathcal{Y}, \mathcal{X}) = S(\mathcal{X}, \mathcal{Y}) = S(\mathcal{Y}, \mathcal{X})$ so that $\alpha_X = \alpha_Y$. By (2.10), (2.5) holds. It follows from (2.10) and (2.6) that, for the m satisfying (2.7),

(2.11)
$$\frac{\mathscr{M}_n}{\log n} \to \frac{2}{\theta} \quad \text{as } n \to \infty,$$

where θ , which may depend on m, is a positive constant such that $E_{\pi_X \times \pi_Y}[e^{\theta F}] = 1$. For a given $\varepsilon > 0$, it follows from Theorem 2 in [2] that we can pick q' > 0 such that

$$r(q') > 0$$
 and $b < \frac{q'}{r(q')} + \varepsilon$.

Furthermore, by (1.3), we can also pick m large such that

$$(2.12) P(F \ge q'm) = P(S_m \ge q'm) \ge \exp[(-r(q') - \varepsilon)m].$$

Note that $\theta > 0$ so that, by (2.12),

(2.13)
$$1 = E_{\pi_X \times \pi_Y} \exp(\theta F) \ge \exp(\theta q' m) P(F \ge q' m)$$
$$\ge \exp[m(\theta q' - r(q') - \varepsilon)].$$

Note also that $m \ge 1$ and q' > 0 so that

$$(2.14) 0 < \theta \le \frac{r(q') + \varepsilon}{q'}.$$

By (2.9), (2.11) and (2.14), we choose a large n such that, for the m satisfying (2.7) and (2.13),

(2.15)
$$\frac{M_{nm}}{\log n} \ge \frac{\mathscr{M}_n}{\log n} \ge \frac{2}{\theta} - \varepsilon \ge 2(b - \varepsilon) \frac{r(q')}{r(q') + \varepsilon} - \varepsilon.$$

Note that $r(q') \ge r(0)$ and r(0) is a positive constant which does not depend on n, m and ε so that, by (2.15),

(2.16)
$$\frac{M_{nm}}{\log n} \ge 2(b-\varepsilon) \left(1 - \frac{\varepsilon}{r(0)}\right) - \varepsilon.$$

For any t = nm + k with k < m, note that

$$M_{nm} \leq M_t \leq M_{n(m+1)}$$

so that, for the m satisfying (2.7) and (2.13) by (2.16),

$$\begin{aligned} \liminf_{t} \frac{M_{t}}{\log t} &\geq \liminf_{n} \frac{M_{nm}}{\log[n(m+1)]} \\ &= \liminf_{n} \frac{M_{nm}}{\log n} \geq 2(b-\varepsilon) \left(1 - \frac{\varepsilon}{r(0)}\right) - \varepsilon \quad \text{a.s.} \end{aligned}$$

The theorem holds by (1.5) and (2.17). \square

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