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Effect of dimensionality on site valence in percolation problems: a comparison of the triangular and simple cubic lattices

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Abstract. We present Monte Carlo and series analysis results for the distribution of valences of sites in percolating and non-percolating clusters for the triangular and simple cubic site percolation problems in order to explore the importance of dimensionality, at fixed lattice coordination number, on the degree of ramification of clusters.

1. Introduction

In order to explore the importance of dimensionality on the compactness of clusters in site percolation processes, we compare valence data for lattices in two and three dimensions *with the same coordination number Q*. Accordingly, we present series analysis and Monte Carlo results for the distribution of valences of sites in percolating and non-percolating clusters on the triangular and simple cubic lattices.

We have previously studied in detail the square lattice site problem (Gaunt *et al* 1980, Whittington *et al* 1980) and made a preliminary study of one aspect of the simple cubic site problem (Gaunt *et al* 1980). We have also investigated bond percolation on the square and simple cubic lattices and compared the results with calculations for the corresponding Bethe lattices (Whittington *et al* 1981). None of this work specifically compared lattices with the same coordination number in two and three dimensions, though Cherry and Domb (1980) calculated a 'coefficient of compactness' for the infinite cluster for the triangular and simple cubic site problems. Similar but less detailed information on the distribution of valences of sites has been used by Stanley *et al* (1981) in a discussion of the relevance of percolation concepts to the structure of liquid water.

If s is a randomly chosen occupied site on a lattice at occupation density p, and I is the set of occupied sites in infinite clusters, we define $P(p)$, the percolation probability, as

$$P(p) = \text{Prob}\{s \in I\}. \tag{1.1}$$

The probability that a site in a finite cluster has valence i is f_i^{F}, given by

$$f_i^{\mathrm{F}} = \text{Prob}\{s \in V_i | s \notin I\} \tag{1.2}$$

where V_i is the set of sites having valence i. Similarly, the probability that a site in an infinite cluster has valence i is given by

$$f_i^{\mathrm{I}} = \mathrm{Prob}\{s \in V_i | s \in I\}. \tag{1.3}$$

We have studied f_i^{F} and f_i^{I} using series expansion and Monte Carlo techniques. The results are presented in §§ 2 and 3 and discussed in § 4.

2. Non-percolating clusters

In order to derive high-density series expansions for f_i^{F} we note that (Whittington *et al* 1980)

$$\begin{aligned} f_i^{\mathrm{F}} &= \sum_{n,t} C(n, t, i) p^n q^t \Big/ \sum_{n,t,i} C(n, t, i) p^n q^t \\ &= \sum_{n,t} C(n, t, i) p^n q^t / p(1 - P(p)) \end{aligned} \tag{2.1}$$

where $C(n, t, i)$ is the number (per lattice site) of sites having valence i in clusters of n sites with perimeter t, and $q = 1 - p$. We have enumerated $C(n, t, i)$ for $n \leq 13$ for the triangular lattice and for $n \leq 11$ for the simple cubic lattice. As a check on the data we expand at low p where $P(p) = 0$ and

$$f_i^{\mathrm{F}} = \binom{Q}{i} p^i (1-p)^{Q-i} \qquad p \leq p_c. \tag{2.2}$$

The coefficients $(b_{i,k})$ of the corresponding high-density expansions

$$f_i^{\mathrm{F}}(q) = \sum_k b_{i,k} q^k \tag{2.3}$$

are given in tables A1 and A2 of the appendix. The additional terms given for f_0^{F} for the triangular lattice have been derived from the series for the percolation probability given by Sykes *et al* (1976). The mean valence of sites in finite clusters $\langle v(p) \rangle_{\mathrm{F}}$ is given by

$$\langle v(p) \rangle_{\mathrm{F}} = \sum_i i f_i^{\mathrm{F}} \tag{2.4}$$

which equals Qp for $p \leq p_c$ (Gaunt *et al* 1980) and, at high density, is given by

$$\begin{aligned} \langle v(q) \rangle_{\mathrm{F}} = {} & 6q^2 + 6q^3 + 6q^4 - 6q^5 + 6q^6 - 102q^7 \\ & + 312q^8 - 600q^9 + 1902q^{10} - 5634q^{11} + \ldots \end{aligned} \tag{2.5}$$

for the triangular lattice. For the simple cubic lattice the corresponding series has been given by Gaunt *et al* (1980) through q^{20}. At that time we added the caveat that the final two terms might contain small errors. In fact we have confirmed the coefficient of q^{19} but the value given for the coefficient of q^{20} does indeed contain a small error.

As a further check on our data we have calculated the coefficients of $a_r(i)$ in

$$\sum_{n,t} C(n, t, i) p^n q^t \equiv \sum_r a_r(i) q^r \tag{2.6}$$

and compared with the values given by Cherry and Domb (1980), who obtained $a_r(i)$ to order $r = 14$ for the triangular lattice and $r = 24$ for the simple cubic lattice. Our values agree with theirs and, in addition, we have calculated for the triangular lattice three additional terms, which are given in table 1. Our results also confirm the values given by Gaunt *et al* (1980) for $a_{25}(i)$ for the simple cubic lattice.

Table 1. $a_r(i)$ for the triangular lattice.

r/i	1	2	3	4	5	6
15	−534	−375	−308	291	−204	−42
16	1098	948	1244	−642	720	138
17	−2088	−1692	−3582	1938	−1998	−450

We have formed a sequence of Padé approximants (Gaunt and Guttmann 1974) to the high-density series for $f_i^{\mathrm{F}}(q)$ and $\langle v(q)\rangle_{\mathrm{F}}$ and the results are given in figures 1, 2 and 3, together with the exact values for $p \leqslant p_c$.

Figure 1 shows the results for f_i^{F} for the triangular lattice, for which the convergence is not very good. For example we expect (Whittington *et al* 1980) that f_i^{F} is a continuous function of p although the matching of the high- and low-density branches in figure 1 is not convincing. However, we note that discontinuities in f_i^{F} at p_c would imply that $P(p)$ is discontinuous! The high-density branches for $i \geqslant 3$ are apparently monotonic. There is clear evidence of a maximum between $p = 0.60$ and 0.65 for $i = 1$. For $i = 2$ it is not possible to distinguish between monotonic behaviour and a shallow maximum at about $p = 0.55$. For $i = 0$ the behaviour is again monotonic.

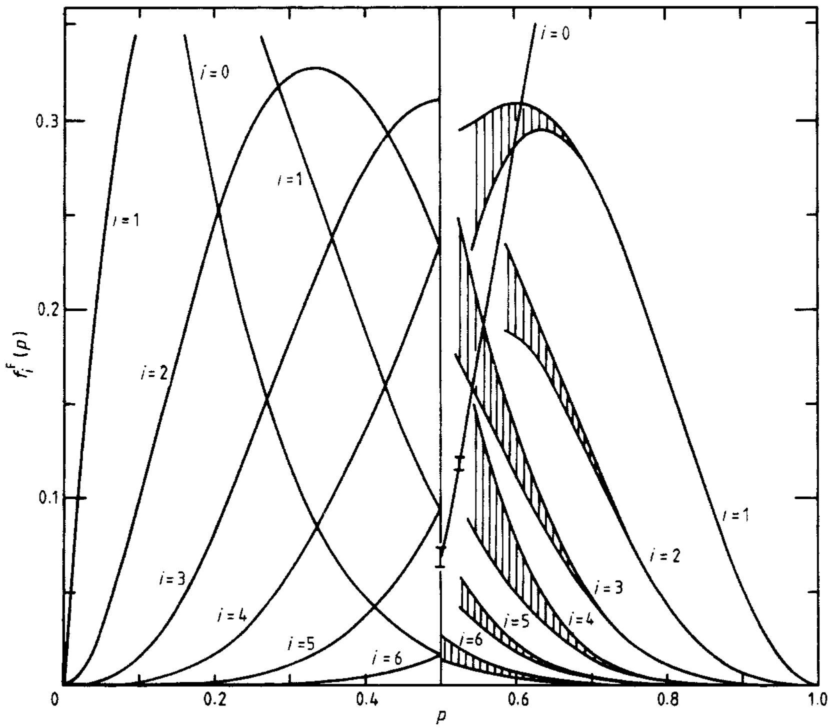

Figure 1. The p dependence of f_i^{F}, $i = 0, 1, 2, \ldots 6$, for the triangular site problem.

The Monte Carlo evidence is in general agreement with these conclusions. There is strong evidence of a maximum for $i = 1$, between $p = 0.6$ and 0.7 and, in the case of $i = 2$, the evidence for a shallow maximum at about $p = 0.55$ is stronger than from the series results.

The corresponding results for the simple cubic lattice are shown in figure 2. The convergence is much better for this lattice and it is possible to find extrapolants of the high-density branches which essentially match the low-density branches at p_c. The error bars shown in the diagram represent the spread in the extrapolated values from the last few approximants. The qualitative behaviour is the same as for the triangular lattice except for $i = 2$ where the curve is now monotone. The evidence for a maximum for $i = 1$ is again strong.

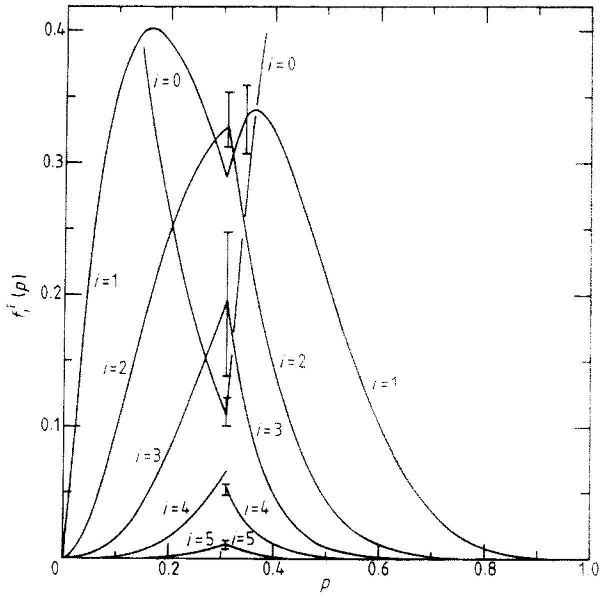

Figure 2. The p dependence of f_i^F, $i = 0, 1, 2, \ldots 6$, for the simple cubic site problem.

For ease of comparison we have plotted the data for $\langle v(p)\rangle_F$ for both lattices in figure 3. The convergence is again better for the simple cubic lattice for which the high-density mimic functions essentially match the low-density branch at p_c. The curves are qualitatively similar to those found for the square site, square bond and simple cubic bond problems (Gaunt *et al* 1980, Whittington *et al* 1981).

3. Percolating clusters

The high-density series for f_i^I can be derived from the series for f_i^F and $P(q)$, using the relation (Whittington *et al* 1980)

$$\binom{Q}{i} p^i q^{Q-i} = P f_i^I + (1-P) f_i^F. \tag{3.1}$$

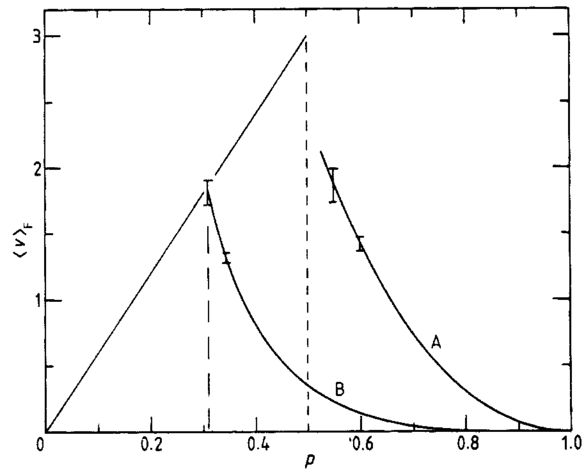

Figure 3. Comparison of the p dependence of $\langle v(p)\rangle_F$ for the triangular (A) and simple cubic (B) site problems.

Writing

$$f_i^I(q) = \sum_k c_{i,k} q^k \tag{3.2}$$

the coefficients $c_{i,k}$ are presented in tables A3 and A4 in the appendix, through orders q^{17} for the triangular lattice and q^{25} for the simple cubic lattice. All of these coefficients are new. The corresponding series for the mean valence of sites in infinite clusters are

$$\langle v(q)\rangle_I = 6 - 6q + 6q^6 - 6q^7 + 30q^8 - 42q^9 + 120q^{10} - 228q^{11} + 504q^{12} - 1092q^{13} + 2562q^{14} - 5934q^{15} + 14088q^{16} - 34164q^{17} + \ldots \tag{3.3}$$

for the triangular lattice, and

$$\langle v(q)\rangle_I = 6 - 6q + 6q^6 - 6q^7 + 30q^{10} - 66q^{11} + 42q^{12} + 162q^{13} - 510q^{14} + 606q^{15} + 288q^{16} - 2448q^{17} + 4848q^{18} - 5940q^{19} + 7032q^{20} - 13068q^{21} + 23844q^{22} - 21120q^{23} - 34680q^{24} + 189000q^{25} + \ldots \tag{3.4}$$

for the simple cubic lattice.

Previously (Whittington *et al* 1980, 1981) we have characterised the degree of ramification of infinite clusters by a parameter $\mu(q)$ given by

$$\mu(q) = \sum_{i=1}^{Q} (i-2) f_i^I(q) \Big/ \sum_{i=3}^{Q} (i-2) f_i^I(q), \tag{3.5}$$

and the first few terms in the series are

$$\mu(q) = 1 - 1\tfrac{1}{2}q^5 - \tfrac{3}{4}q^6 - 1\tfrac{1}{8}q^7 - \tfrac{3}{16}q^8 - 1\tfrac{25}{35}q^9 + \ldots \tag{3.6}$$

for the triangular lattice, and

$$\mu(q) = 1 - 1\tfrac{1}{2}q^5 - \tfrac{3}{4}q^6 - 1\tfrac{1}{8}q^7 - 1\tfrac{11}{16}q^8 - 2\tfrac{17}{32}q^9 + \ldots \tag{3.7}$$

for the simple cubic lattice, where we omit higher-order terms since the fractions are

$$ {}^{?}q^{3}-2q^{4}-4q^{5}-2q^{6}+12q^{8} $$
$$ +18q^{9}+84q^{10}+50q^{11}+416q^{12}-178q^{13}+\ldots. \qquad (3.9) $$

rmed Padé approximants to all of these series. In Whittington *et al* (1981) ɘd detailed calculations of f_i^{I} for the Bethe approximation with $Q=6$ and :s are in remarkably good agreement with both Monte Carlo and series ɔoth the triangular and simple cubic lattices. The plots for the Bethe and ˌattices are indistinguishable above $p=0.65$ while even at $p_c(=\frac{1}{2})$ the .eviation, which occurs for $i=1$, is only 0.02. For the simple cubic lattice the ndistinguishable from the Bethe approximation for $p>0.45$ and, at the maximum deviation, again for $i=1$, is 0.04. Of course, this implies that r the simple cubic and triangular lattices are superimposable for $p>0.65$, ›uch as $\langle v(q)\rangle_{\mathrm{I}}$ and $\mu(q)$ will also be well approximated by the Bethe results. ɔare the structures of the percolating clusters, at and above the percolation n different lattices, we define a reduced density variable

$$ \rho=(p-p_c)/(1-p_c). \qquad (3.10) $$

› and 5 we show the dependence of $\langle v\rangle_{\mathrm{I}}$ and μ on ρ. For comparison we ults for the $Q=6$ Bethe approximation (Whittington *et al* 1981) and the c bond problem (Whittington *et al* 1981).

ults are in accord with one's qualitative expectations. For p large we expect

$$ \langle v(p)\rangle_{\mathrm{I}}\simeq Qp $$
$$ \simeq Qp_c+Q(1-p_c)\rho \qquad (3.11) $$

ˌt all occupied sites are members of infinite clusters. This approximation is ›r $\rho>0.45$ in every case shown in figure 4. The Bethe results are a much ·oximation to the three-dimensional lattice than to the two-dimensional for the simple cubic lattice, the mean valence is lower for the bond problem : site problem, since site clusters are section graphs of the lattice. In a similar wer for the bond problem than for the site problem, as expected, since the ɔh on a vertex set contains all cycles present in any subgraph on this vertex ɘgree of *ramification* decreases monotonically with increasing ρ for each at fixed ρ, is less for the site problem than for the bond problem and is less in sions than in three, for fixed Q. Even at p_c the infinite cluster on the attice is very compact as measured by the value of μ ($\mu(p_c)\simeq 0.94$) and the ɘ in the cluster has more than three neighbours ($\langle v(p_c)\rangle_{\mathrm{I}}\simeq 3.13$).

ue of μ for the square site problem (from (3.9) or Whittington *et al* (1980)) is ll ρ, than for the triangular site problem so that increasing Q apparently

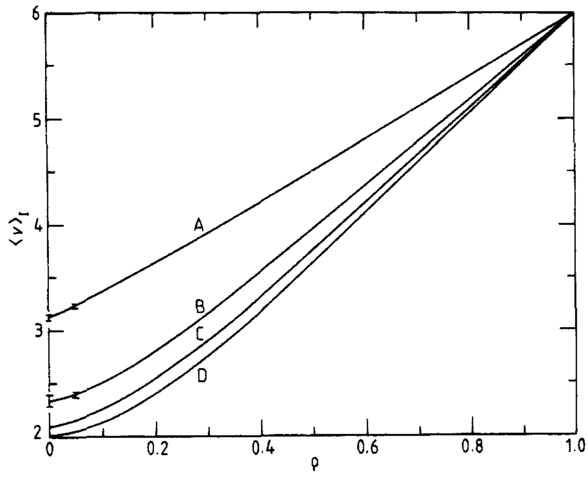

Figure 4. Comparison of the ρ dependence of $\langle v \rangle_I$ for the triangular site (A), simple cubic site (B), simple cubic bond (C) and the $Q=6$ Bethe approximation (D).

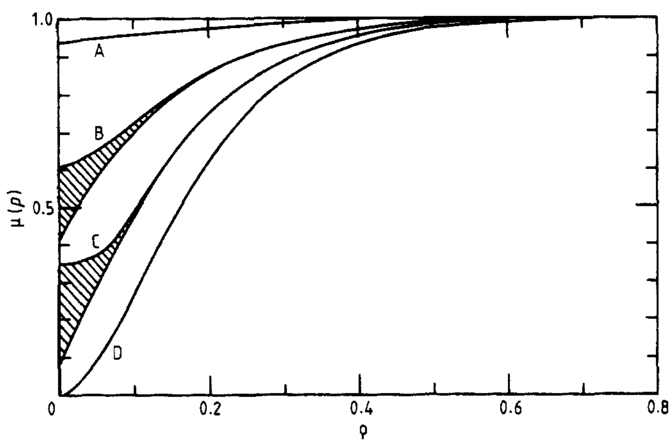

Figure 5. Comparison of the ρ dependence of the compactness parameter μ for the triangular site (A), simple cubic site (B), simple cubic bond (C) and the $Q=6$ Bethe approximation (D).

increases the compactness of the infinite cluster. This result is not unexpected and is borne out by calculations in the Bethe approximation.

The coefficient of compactness λ (Cherry and Domb 1980) is related to $\langle v \rangle_I$ by

$$\lambda = \{\tfrac{1}{2}\langle v \rangle_I - 1\}/\{\tfrac{1}{2}Q - 1\}. \tag{3.12}$$

Outside the critical region the agreement between our estimates of λ and those of Domb and Cherry is excellent. At the critical point our estimates of λ are 0.28 (triangular), 0.08 (cubic site), 0.02 (cubic bond) and exactly zero (Bethe approximation). Cherry and Domb estimate 0.07 for the cubic site problem, and a value between 0.3 and 0.35 for the triangular site problem.

4. Discussion

The high-density branches of f_i^{F} are rather difficult to determine accurately because of poor convergence of the Padé approximants although, if one accepts the arguments for continuity, it is possible to get a good idea of the qualitative behaviour, even just above p_c. The series for $\langle v\rangle_{\mathrm{F}}$ are rather better behaved, because of the pre-averaging.

For the infinite cluster data, the convergence is very good. At fixed p the Bethe approximation is excellent. The results essentially coincide for $p > p_c + 0.15$ and the agreement is still surprisingly good even at p_c. However, this comparison, at fixed p, approximates the incipiently percolating cluster(s) on a lattice with infinite clusters in the corresponding Bethe approximation at a density well above the critical density. The use of the reduced density variable ρ avoids this problem, since it takes into account the differing values of p_c.

The two compactness parameters, λ (or equivalently $\langle v\rangle_{\mathrm{I}}$) and μ, assign the same order to the degree of ramification of the infinite clusters in all cases considered.

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Appendix

Coefficients in the high-density expansions of f_i^{F} and f_i^{I} for the triangular and simple cubic lattices.

Table A1. Coefficients $b_{i,k}$ in high-density expansions of $f_i^{\mathrm{F}}(q)$ for triangular lattice (see equation (2.3)).

k	$b_{0,k}$	$b_{1,k}$	$b_{2,k}$	$b_{3,k}$	$b_{4,k}$	$b_{5,k}$	$b_{6,k}$
0	1						
1	0						
2	−6	6					
3	0	−6	6				
4	9	−18	3	6			
5	6	12	−30	6	6		
6	−3	6	9	−22	3	6	1
7	0	42	0	−30	−6	−6	0
8	−93	−48	72	96	−57	24	6
9	98	84	−42	−128	126	−108	−30
10	12	−672	−12	450	−93	270	45
11	552	1482	−300	−1308	306	−576	−156
12	−1802						
13	1944						
14	−570						
15	−1938						
16	2499						

Table A2. Coefficients $b_{i,k}$ in high-density expansions of $f_i^F(q)$ for simple cubic lattice (see equation (2.3)).

k	$b_{0,k}$	$b_{1,k}$	$b_{2,k}$	$b_{3,k}$	$b_{4,k}$	$b_{5,k}$	$b_{6,k}$
0	1						
1	0						
2	0						
3	0						
4	−6	6					
5	6	−6					
6	0	0					
7	−36	24	12				
8	99	−78	−21				
9	−122	108	6	8			
10	−81	6	87	−12			
11	792	−516	−276	−12	12		
12	−2 006	1 440	504	100	−45	6	1
13	2 658	−2 034	−444	−204	60	−30	−6
14	417	−210	−612	228	102	60	15
15	−11 992	9 456	3 084	96	−648	12	−8
16	32 200	−26 550	−5 802	−1084	1713	−408	−69
17	−40 674	36 414	2 898	2580	−2910	1398	294
18	−19 053	5 718	17 652	−3208	2658	−3054	−713
19	221 968	−165 450	−63 690	−936	2148	4740	1220

Table A3. Coefficients $c_{i,k}$ in expansions of $f_i^I(q)$ for triangular lattice (see equation (3.2)).

k	$c_{1,k}$	$c_{2,k}$	$c_{3,k}$	$c_{4,k}$	$c_{5,k}$	$c_{6,k}$
0						1
1					6	−6
2				15	−30	15
3			20	−60	60	−20
4		15	−60	90	−60	15
5	6	−30	60	−60	30	−6
6	−6	15	−20	15	−6	2
7	0	0	0	0	6	−6
8	−6	0	0	15	−30	21
9	6	−6	20	−60	96	−56
10	−18	12	−66	180	−240	132
11	30	−36	174	−426	552	−294
12	−66	78	−394	957	−1 218	643
13	120	−162	894	−2 100	2 658	−1 410
14	−246	324	−1 986	4 599	−5 868	3 177
15	498	−702	4 402	−10 212	13 470	−7 456
16	−1020	1518	−10 128	23 745	−32 166	18 051
17	2088	−3624	24 594	−57 174	78 786	−44 670

Table A4. Coefficients $c_{i,k}$ in expansions of $f_i^{\mathrm{l}}(q)$ for simple cubic lattice (see equation (3.2)).

k	$c_{1,k}$	$c_{2,k}$	$c_{3,k}$	$c_{4,k}$	$c_{5,k}$	$c_{6,k}$
0						1
1					6	−6
2				15	−30	15
3			20	−60	60	−20
4		15	−60	90	−60	15
5	6	−30	60	−60	30	−6
6	−6	15	−20	15	−6	2
7	0	0	0	0	6	6
8	0	0	0	15	−30	15
9	0	0	20	−60	60	−20
10	−6	15	−60	90	−60	21
11	12	−30	60	−60	66	−48
12	−6	15	−20	105	−222	128
13	−24	−12	120	−450	546	−180
14	42	111	−480	915	−534	−54
15	0	−276	732	−420	−858	822
16	−120	198	192	−2 565	4 074	−1 779
17	204	624	−3 228	7 608	−6 600	1 392
18	−24	−2 316	6 820	−8 835	1 746	2 609
19	−378	3 450	−4 764	−4 560	17 442	−11 190
20	240	−795	−11 028	38 928	−49 824	22 479
21	1368	−8 100	41 016	−84 804	85 188	−34 668
22	−4050	21 036	−72 584	126 249	−122 484	51 833
23	5298	−32 586	97 632	−177 252	186 582	−79 674
24	−1830	45 822	−142 128	286 593	−286 260	97 803
25	−6276	−79 506	241 744	−427 362	289 896	−18 496

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