Statistics of lattice animals (polyominoes) and polygons

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Abstract

We have developed an improved algorithm that allows us to enumerate the number of site animals (polyominoes) on the square lattice up to size 46. Analysis of the resulting series yields an improved estimate, $\tau = 4.062570(8)$, for the growth constant of lattice animals and confirms to a very high degree of certainty that the generating function has a logarithmic divergence. We prove the bound $\tau > 3.90318$. We also calculate the radius of gyration of both lattice animals and polygons enumerated by area. The analysis of the radius of gyration series yields the estimate $\nu = 0.64115(5)$, for both animals and polygons enumerated by area. The mean perimeter of polygons of area n is also calculated. A number of new amplitude estimates are given.

The enumeration of lattice animals is a classical combinatorial problem of great interest both intrinsically and as a paradigm of recreational mathematics [1]. A lattice animal is a finite set of nearest neighbour sites on a lattice. The fundamental problem is the calculation of the number of animals, b_n, containing n sites. In the physics literature lattice animals are very often called *clusters* due to their very close relationship to percolation problems [2]. Series expansions for various percolation properties, such as the percolation probability or the average cluster size, can be obtained from the perimeter polynomials. These in turn can be calculated by counting the number of lattice animals $b_{n,m}$ according to their size n and perimeter m [3, 4]. Lattice animals have also been suggested as a model of branched polymers [5]. In mathematics, and combinatorics in particular, the term polyominoes is frequently used. A polymino is a set of lattice cells joined at their edges. So polyominoes are identical to site animals on the dual lattice. Furthermore, the enumeration of lattice animals has traditionally served as a benchmark for computer performance and algorithm design [6]–[12].

The enumeration of self-avoiding polygons is another classical combinatorial problem [13]. Most attention has been paid to the enumeration by perimeter, but enumeration by area is an equally interesting problem. (For polyominoes, the ordinary generating function of the number of polyominoes of perimeter n has zero radius of convergence [14] and hence is of rather less interest). Polygons enumerated by area are just the "hole-free" subset of polyominoes. There are exponentially fewer polygons than polyominoes [15], but on universality grounds one would

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expect the exponent ν characterising the radius of gyration to be the same for polyominoes and polygons enumerated by area. We confirm this expectation.

An algorithm for the calculation of $b_{n,m}$ has been published by Martin [6] and Redner [8]. It was used by Sykes and co-workers to calculate series expansions for percolation problems on various lattices. In particular Sykes and Glen [4] calculated $b_{n,m}$ up to $n = 19$ on the square lattice, and thus obtained the number of lattice animals, $b_n = \sum_m b_{n,m}$, to the same order. Redelmeier [7] presented an improved algorithm for the enumeration of lattice animals and extended the results to $n = 24$. This algorithm was later used by Mertens [10] to devise an improved algorithm for the calculation of $b_{n,m}$ and a parallel version of the algorithm appeared a few years later [11]. The next major advance was obtained by Conway [12] who used the finite lattice method with an associated transfer-matrix algorithm to calculate b_n and numerous other series up to $n = 25$ [16]. In unpublished work Oliveira e Silva [18] used the parallel version of the Redelmeier algorithm [11] to extend the enumeration to $n = 28$. In this work we use an improved version of Conway's algorithm to extend the enumeration to $n = 46$. We also calculate the the radius of gyration of lattice animals and square lattice polygons enumerated by area up to $n = 42$. Further, we also calculate the mean perimeter of polygons of area n. Instructions for the electronic retrieval of these series can be found at the end of this Letter.

The method we use to enumerate site animals and polygons on the square lattice is based on the method used by Conway [12] for the calculation of series expansions for percolation problems, and is similar to methods devised by Enting for enumeration of self-avoiding polygons [19] or the algorithm used by Derrida and De Seze to study percolation and lattice animals [20]. The number of animals that span rectangles of width W and length L are counted using a transfer matrix algorithm. A detailed description of the algorithm will appear elsewhere [21].

The quantities and functions we consider in this Letter are: (i) the number of polygons of area n, denoted a_n, and the associated generating function, $A(y) = \sum a_n y^n$; (ii) the number of lattice animals b_n and the associated generating function, $\mathcal{A}(u) = \sum b_n u^n$; (iii) the first moment of the number $p_{n,m}$ of polygons of perimeter m and area n, $a_n \langle p \rangle_n = \sum_m m p_{n,m}$. Then $\langle p \rangle_n$ is the mean perimeter of polygons of area n. (iv) the mean-square radius of gyration of animals of area n, $\langle R_{\mathrm{a}}^2 \rangle_n$. (v) the mean-square radius of gyration of polygons of area n, $\langle R_{\mathrm{p}}^2 \rangle_n$. These quantities are expected to behave as

$$
\begin{aligned}
a_n &= A\kappa^n n^{-1}[1 + o(1)], \\
b_n &= B\tau^n n^{-1}[1 + o(1)], \\
a_n \langle p \rangle_n &= AC\kappa^n[1 + o(1)], \\
\langle R_{\mathrm{a}}^2 \rangle_n &= Dn^{2\nu_{\mathrm{a}}}[1 + o(1)], \\
\langle R_{\mathrm{p}}^2 \rangle_n &= En^{2\nu_{\mathrm{p}}}[1 + o(1)],
\end{aligned}
\tag{1}
$$

where κ is the reciprocal y_c^{-1} of the critical point of the polygon area generating function, and τ is the reciprocal u_c^{-1} of the critical point of the animal generating function. From numerical evidence [15] it is well-established that both the polygon area generating function and the animal generating function have a logarithmic singularity, hence the factor $1/n$ in the first two equations above. Similarly, it is generally believed [22] that $\langle p \rangle_n \sim n$, so the n-dependence vanishes to leading order in the third equation above.

The series studied in this Letter have coefficients which grow exponentially, with subdominant term given by a critical exponent. The generic behaviour is $G(x) = \sum_n g_n x^n \sim (1 - x/x_c)^{-\xi}$, and hence the coefficients of the generating function $g_n \sim \mu^n n^{\xi-1}$, where $\mu = 1/x_c$.

To obtain the singularity structure of the generating functions we first used the numerical method of differential approximants [23]. Combining the relationship (given above) between the coefficients in a series and the critical behaviour of the corresponding generating function with the expected behaviour (1) of the mean-square radius of gyration yields the following expectation for the animal generating functions:

$$\mathcal{A}(u) = \sum_n b_n u^n = A(u)\log(1 - \tau u), \tag{2}$$

$$\mathcal{R}_a^2(u) = \sum_n b_n \langle R_a^2 \rangle_n n^2 u^n = \sum_n r_n u^n \sim R(u)(1 - \tau u)^{-(2+2\nu_a)}. \tag{3}$$

Thus we expect these series to have a critical point, $u_c = 1/\tau$, and as stated previously the animal generating function is expected to have a logarithmic singularity. Similar expressions hold for the corresponding polygon area generating function, though with a different growth constant κ. The radius of gyration series are expected to diverge with exponents $2 + 2\nu_a$, and $2 + 2\nu_p$ respectively, though as we have argued above, we expect the exponents to be equal.

Estimates of the critical point and critical exponent were obtained by averaging values obtained from second order $[L/N; M; K]$ inhomogeneous differential approximants. In Table 1 we have listed the estimates obtained from this analysis. The error quoted for these estimates reflects the spread (basically one standard deviation) among the approximants. Note that these error bounds should *not* be viewed as a measure of the true error as they cannot include possible systematic sources of error. From this we see that the animal generating function has a singularity at $u_c = 0.246150(1)$, and thus we obtain the estimate, $\tau = 4.06256(2)$, for the growth constant. The exponent estimates are consistent with the expected logarithmic divergence. The central estimates of u_c obtained from the radius of gyration series are a little larger than, but nonetheless consistent with those from the animal generating function. From this analysis we see that this series has a divergence at u_c with an exponent $2 + 2\nu_a = 3.2840(8)$, and thus $\nu_a = 0.6420(4)$.

Once the conjectured exact value of the exponent has been confirmed we can obtain an improved estimate for the critical point. In figure 1 we have plotted estimates for the exponent vs the corresponding estimates for the critical point u_c as obtained from second order approximants to the animal generating function. From this figure we see that, as the estimates for the exponent approach 0, the estimates of u_c approach 0.2461497. From the spread among the approximants we obtain out final estimate $u_c = 0.2461496(5)$, and thus the growth constant $\tau = 4.062570(8)$. An earlier analysis, based on shorter series [15] gave $\tau = 4.062591(9)$. A similar analysis for the lattice tree generating function is given in [21], and there it is found that $\nu = 0.64115(5)$. The estimates of u_c obtained from differential approximants to the radius of gyration of animals is consistently larger than the above final estimate and this is probably the reason the estimate for ν_a is slightly larger than that obtained from trees. Further evidence of this can be found by looking at figure 2 where we have plotted the estimates of the exponent $2 + 2\nu_a$ vs u_c as obtained from the radius of gyration series for animals. Clearly as u_c decrease so does the exponent and as u_c approaches 0.2461497 the exponent gets closer to the estimate $2 + 2\nu_a = 3.2823(1)$ obtained [21] for lattice trees and the discrepancy is thus largely resolved. For this reason we claim that the most precise estimate for ν is the one obtained [21] from the tree series. Further evidence for this claim is given in [21].

Using this value of the exponent ν, and the estimate of u_c cited above, we repeated the amplitude analysis of the animal series cited in [15]. Now however we have 46 terms. In [15] we

found evidence that $b_n \sim \tau^n/n[d_0 + d_1/n + d_2/n^{\Delta_2} + d_3/n^{\Delta_3} + \cdots]$ with $\Delta_n = n$. With the longer series we in fact find that $\Delta_2 = 1.5$ and $\Delta_3 = 2$, with subsequent values of Δ_k presumably increasing by $1/2$. We note that this is consistent with the known correction-to-scaling exponent for polygons enumerated by perimeter, $\Delta = 1.5$ [24]. By fitting to this form we estimate $d_0 = 0.316915(10)$, $d_1 = -0.276(2)$, $d_2 = 0.335(10)$, and $d_4 = -0.25(5)$. The errors quoted tacitly assume that the critical point is correct. A similar analysis for the radius of gyration series displays evidence of a similar confluent term, and we find the data can be effectively fitted by the following asymptotic form: $n^2 b_n \langle R_a^2 \rangle_n \sim \tau^n n^{2\nu+1}[e_0 + e_1/n + e_2/n^{\Delta_2} + e_3/n^{\Delta_3} + \cdots]$. That is to say, the same confluent exponent is observed, and the amplitudes may be estimated as: $e_0 = 0.0599(2)$, $e_1 = -0.190(8)$, and $e_2 = 0.5(1)$. The quality of the fit was less satisfactory than the corresponding fit to the total number of animals, and only three amplitudes can be quoted with any confidence. Combining these, we find $\langle R_a^2 \rangle_n \sim n^{2\nu}[f_0 + f_1/n + f_2/n^{3/2}]$ where $f_0 = 0.1890(12)$, $f_1 = -0.435(26)$ and $f_2 = 1.4(4)$.

For square lattice polygons enumerated by area, the series to 42 terms is given in [15]. The differential approximants are summarised in Table 2, and on the basis of these, and a subsequent analysis that assumes that the critical exponent is zero, we estimated the connective constant to be $\kappa = 3.97094397(9)$. An amplitude analysis, also given in [15] gave

$$a_n \sim \kappa^n/n[0.408105 - 0.547/n + 0.63/n^2 + o(1/n^2)].$$

Here there is no evidence of a correction-to-scaling term $\Delta = 1.5$, though there is some evidence of a weaker non-analytic correction, perhaps consistent with $\Delta = 2.5$.

The differential approximant analysis for the radius of gyration series is also summarised in Table 2, and displays similar features to that for animals, just discussed. Using the quoted value for κ, a biased differential approximant analysis of the generating function

$$\mathcal{R}_p^2(y) = \sum_n a_n \langle R_p^2 \rangle_n n^2 y^n = \sum_n r_n y^n \sim R(y)(1 - \kappa y)^{-(2+2\nu_p)}$$

similar to that described above for lattice animals, gave mainly defective approximants, though almost all exponent estimates were clustered around $2 + 2\nu_p = 3.283$ or $\nu_p = 0.6415$. This is very close to the estimate obtained for both polyominoes and lattice trees, cited above. Accordingly, we conjecture that the three exponents are the same, and we take the seemingly most precise value, $\nu = 0.64115$ as found for lattice trees, as our preferred value.

Using this value of the exponent, and the estimate of κ cited above, we repeated the amplitude analysis *mutatis mutandis* described above in our analysis of animals. A similar fit to the radius of gyration series also showed evidence of a correction-to-scaling term $\Delta = 1.5$, and we found: $n^2 a_n \langle R_p^2 \rangle_n \sim \kappa^n n^{2\nu+1}[0.08488 - 0.457/n + 0.77/n^{1.5} + 0.3/n^2 + \cdots]$. Errors in the amplitude estimates are expected to be confined to the last quoted digit. Combining these results we find $\langle R_a^2 \rangle_n \sim n^{2\nu}[g_0 + g_1/n + g_2/n^{3/2}]$ where $g_0 = 0.2080$, $g_1 = -0.840$ and $g_2 = 1.9$.

A similar analysis of the first moment series was also made, and again we found evidence of a non-analytic correction-to-scaling term $\Delta = 1.5$. More precisely, we found

$$a_n \langle p \rangle_n \sim \kappa^n[0.75715 - 0.064/n + 0.07/n^{3/2} + O(1/n^2)],$$

so that

$$\langle p \rangle_n \sim 1.8552n + 2.33 + 0.17/\sqrt{n}.$$

Finally, we used the series to derive improved rigorous lower bounds for the growth constants of lattice animals and trees. Using concatenation arguments, Rands and Welsh [25] showed that if we define a sequence p_n such that

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$$b_{n+1} = p_{n+1} + p_n b_2 + \ldots p_3 b_{n-1} + p_2 b_n, \tag{4}$$

and construct the generating functions

$$\mathcal{A}^*(u) = 1 + \sum_{n=1}^{\infty} b_{n+1} u^n \tag{5}$$

and

$$\mathcal{P}(u) = \sum_{n=1}^{\infty} p_{n+1} u^n \tag{6}$$

then

$$\mathcal{A}^*(u) = 1 + \mathcal{A}^*(u)\mathcal{P}(u) \tag{7}$$

and $\mathcal{A}^*(u)$ is singular when $\mathcal{P}(u) = 1$. The coefficients in $\mathcal{P}(u)$ are obviously known correctly to the same order $N = 2W_{\max} - 1$ as $\mathcal{A}^*(u)$. If we look at the polynomial P_N obtained by truncating $\mathcal{P}(u)$ at order N then the unique positive zero, $1/\tau_N$, of $P_N - 1 = 0$ is a lower bound for τ. Using our extended series we find that $\tau \geq 3.903184\ldots$.

In conclusion, radically extended series for animals and polygons enumerated by area have been presented. Improved estimates of critical points and critical exponents have been made. The area generating function of both polyominoes and polygons is found to have a logarithmic singularity, while the radius of gyration exponent was estimated to be $\nu = 0.64115$. This value merits some discussion. Two dimensional lattice models frequently have rational critical exponents with typically one or two digit numerators and denominators. In this case the closest "small" rational fraction is $\frac{109}{170}$, a startlingly uncompelling one! However as the animal problem is not conformally invariant, we have no theoretical reason to expect a rational exponent, and our result certainly doesn't suggest one. Earlier, less precise estimates of ν have been given in [20], wherein the estimate $\nu = 0.6408(3)$ was made, and more recently in [26] the Monte Carlo estimate for lattice trees, $\nu = 0.642(10)$ is given. Several earlier, less precise Monte Carlo and series estimates are also referenced there, and the correction-to-scaling exponent is also studied, and the estimate $\Delta = 0.65 \pm 0.20$ given. However for the problems of both polyominoes and polygons, we find no evidence of any such singularity with exponent less than 1. This is reminiscent of the situation for the enumeration of polygons by perimeter, where for many years various methods of analysis yielded estimates in the range 0.5 to 1.5. Only with very long series [17] did it become clear that there were no such terms with exponent less than 1, and that the long-standing prediction of Nienhuis [24] that $\Delta = 1.5$ was completely correct. We suggest that something similar is the case here.

We have also obtained a more precise lower bound, $\tau > 3.90318$, on the polyomino connective constant.

Finally we should comment briefly on the amplitude estimates we have made. These may be summarised, following the definitions in 1, as $A = 0.408105(10)$, $B = 0.316915(10)$, $C = 1.8552(10)$, $D = 0.1890(12)$, and $E = 0.2080(2)$. For polygon enumeration by perimeter, there are a number of universal ratios [27] known. In the case considered here, where we enumerate by area, there are no published predictions. Many analogous relations would not exist, as in the perimeter case they depend on theorems following from conformal invariance. While certain products and quotients are suggestive, none are sufficiently compelling as to lead us to believe that they are worth publishing. We rather highlight this as an open problem, for which we provide useful test data.

E-mail or WWW retrieval of series

The series for the generating functions studied in this Letter can be obtained via e-mail by sending a request to I.Jensen@ms.unimelb.edu.au or via the world wide web on the URL http://www.ms.unimelb.edu.au/~iwan/ by following the instructions.

Acknowledgements

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Table 1: Estimates for the critical point u_c and exponents $1-\theta_\mathrm{a}$ and $1+\theta_\mathrm{a}+2\nu_\mathrm{a}$ obtained from second order inhomogeneous differential approximants to the series for the generating functions of lattice animals and their radius of gyration. Also listed are the corresponding estimates for polygons. L is the order of the inhomogeneous polynomial.

L	u_c	$1-\theta_\mathrm{a}$	u_c	$1+\theta_\mathrm{a}+2\nu_\mathrm{a}$
Square lattice site animals
0	0.246149987(43)	-0.000523(46)	0.246150539(87)	3.28413(11)
2	0.24614992(14)	-0.00043(14)	0.24615046(10)	3.28402(28)
4	0.24615007(15)	-0.00055(16)	0.24615037(22)	3.28394(30)
6	0.24614999(24)	-0.00046(25)	0.24615068(16)	3.28426(22)
8	0.24615001(15)	-0.00052(13)	0.24615067(25)	3.28432(44)
10	0.24614997(22)	-0.00044(28)	0.24615055(31)	3.28417(56)

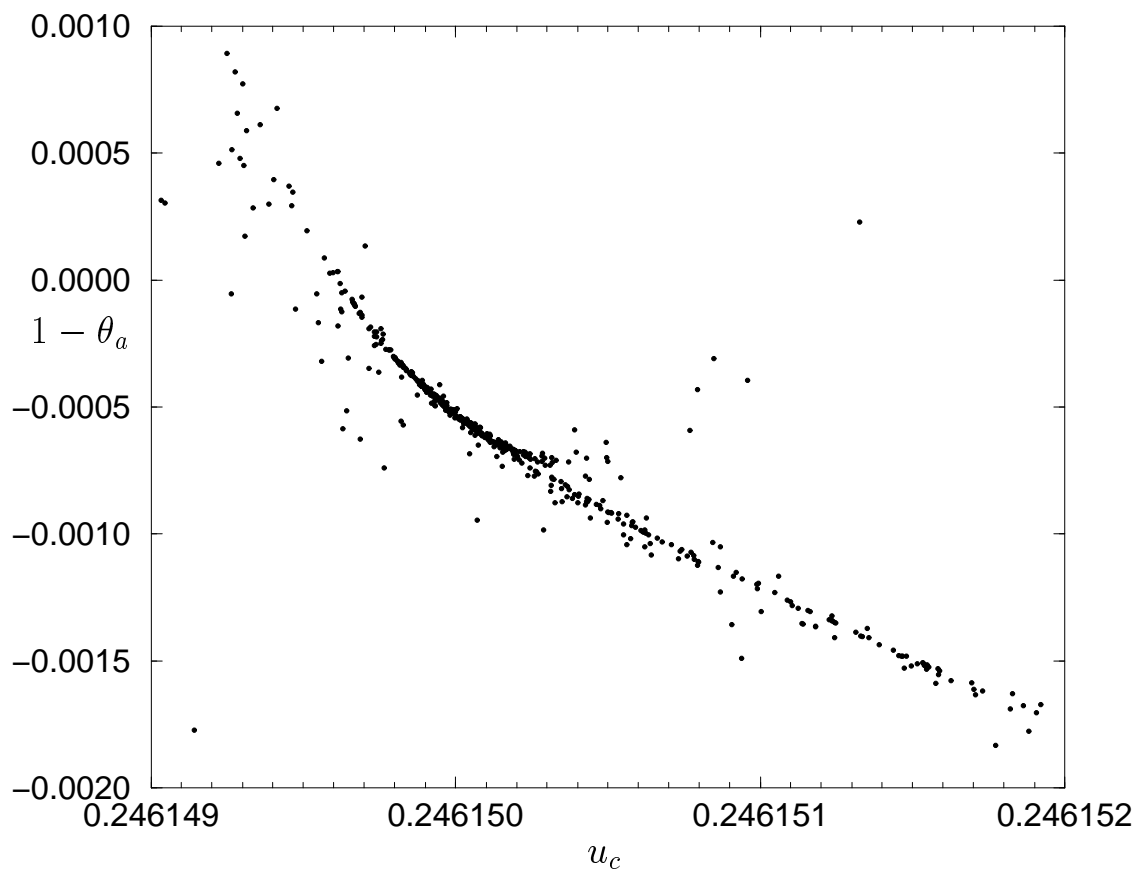| L	y_c	$1-\theta_\mathrm{p}$	y_c	$1+\theta_\mathrm{p}+2\nu_\mathrm{p}$
Square lattice polygons enumerated by area
0	0.251829311(24)	-0.000022(23)	0.25183133(81)	-3.2847(13)
2	0.251829340(20)	-0.000051(19)	0.25183043(73)	-3.28439(88)
4	0.251829349(52)	-0.000059(53)	0.25183052(62)	-3.2846(12)
6	0.251829314(12)	-0.000025(12)	0.2518302(11)	-3.2841(16)
8	0.251829320(18)	-0.000031(19)	0.25183035(50)	-3.28432(62)
10	0.251829319(12)	-0.000029(12)	0.2518298(19)	-3.2836(28)

Figure 1: Estimates for the critical exponent $1 - \theta_\mathrm{a}$ vs. the critical point u_c as obtained from second order differential approximants to the series for the generating function of site animals on the square lattice.
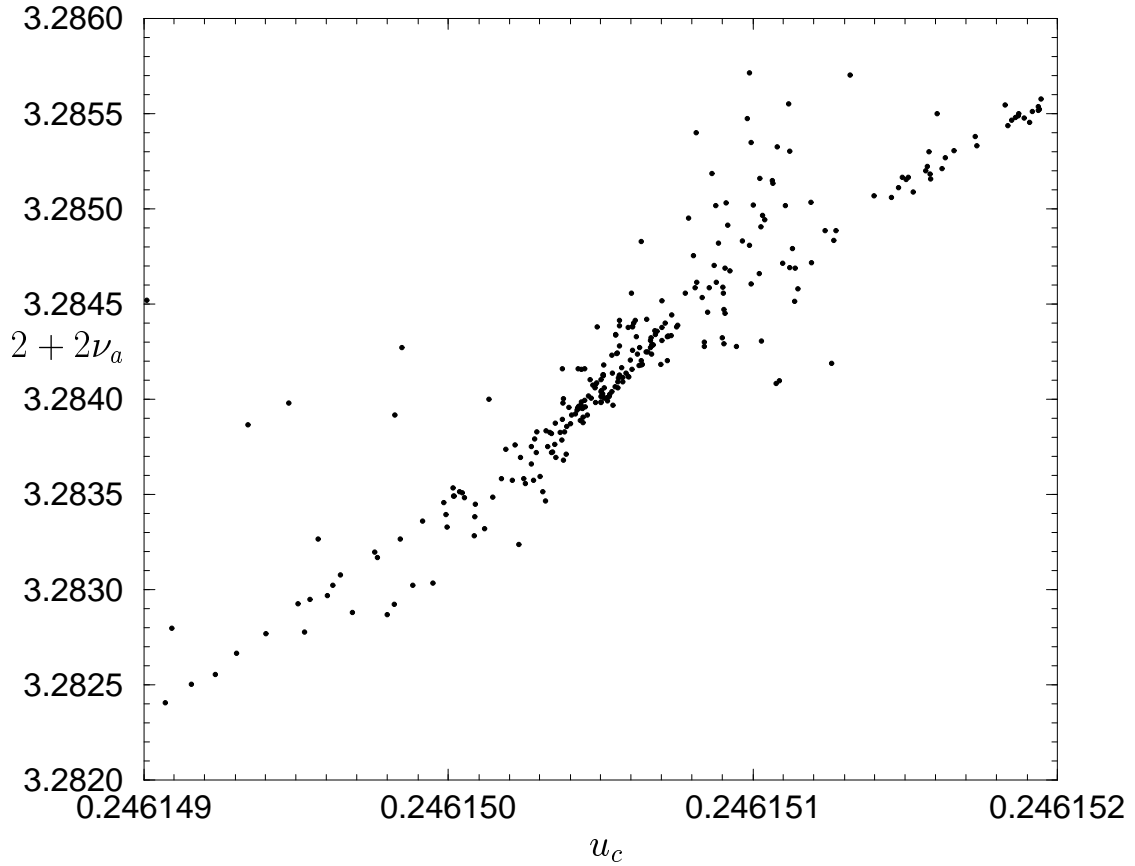
Figure 2:   Estimates for the critical exponent $2 + 2\nu_{\mathrm{a}}$ vs. the critical point u_c as obtained from second order differential approximants to the series for the generating function of the radius of gyration of site animals on the square lattice.