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COMMENT

Isomorphisms for random sequential packing on lattices

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Abstract. Recently Nakamura reported results for two classes of random sequential packing problems on $n \times n$ square lattices. Non-overlapping squares covering a^2 cells are placed on the lattice either A allowing, or B forbidding contact. Here we demonstrate an exact isomorphism between these two classes, as well as a broader range of models (and their d -dimensional analogues). Nakamura first took the $n \rightarrow \infty$ infinite-lattice limit and then analysed convergence of the packing fraction, p (i.e. saturation or jamming coverage), to the $a \rightarrow \infty$ continuum limit (where A and B coincide). We obtain p values for model A with $n = \infty$ from the generalised Palasti conjecture (using exact $d = 1$ values), and develop a corresponding $a \rightarrow \infty$ asymptotic expansion; the corresponding p values for model B are obtained from isomorphism arguments. These facilitate analysis of Nakamura's results. Isomorphisms and continuum limit behaviour are also discussed for processes on other lattices.

Analysis of the hierarchical form of the master equations for $d \geq 1$ dimensional versions of these lattice packing processes reveals an empty cell shielding property (Evans *et al* 1983). This allows exact truncation solution of the $n = \infty$ infinite-lattice equations for $d = 1$ (Gonzalez *et al* 1974, Epstein 1979, Wolf *et al* 1984) and indicates appropriate approximate truncation procedures for $d > 1$. The latter have been implemented in $d = 2$ (with $n = \infty$) for model A with $a = 2$ (Nord and Evans 1985), but have limited utility (in their present form) for larger a . Recursive combinatorial techniques provide exact results for $d = 1$ with finite a and n , and therefore for various limits (MacKenzie 1962). They have seen little use for $d \geq 2$. There have been extensive computer simulations for model A in $d = 2$ with various a and n , and limiting behaviour has been extracted (Blaisdell and Solomon 1970). The most general continuum limit, which fixes $n/a \equiv L$ and lets $a, n \rightarrow \infty$, corresponds to a 'car parking problem' of randomly packing (aligned) non-overlapping unit-volume hypercubes into a hypercubic region with side length $L \geq 1$. Palasti (1960) conjectured (for $d = 2$ and $L = \infty$) that the $a = \infty$ continuum packing fraction equals the $d = 1$ value raised to the power d . There has been some analysis of generalised Palasti conjectures (GPC) covering finite ($L < \infty$) continuum cases, and both finite ($n < \infty$) and infinite ($n = \infty$) lattice cases (with $a < \infty$), for various $d > 1$ (Blaisdell and Solomon 1970). Here we utilise the latter for $d = 2$.

First, for points in d dimensions separated by a vector $l = (l_1, l_2, \dots, l_d)$, we introduce an appropriate distance measure, $\|l\| = \max_i (|l_i|)$, i.e. the l^∞ norm. We consider packing on d -dimensional periodic or infinite hypercubic lattices (with unit lattice vector) by non-overlapping hypercubes, each covering a^d cells, such that a hypercube cannot cover cells whose centres are within an (integer) distance, r , from the centres of previously filled cells (i.e. range r blocking). We denote the corresponding

packing fractions by $p(a|r)$, and shall denote cases $r=0, 1, 2, \dots$, as packing models A, B, C, ... (extending Nakamura's (1986) notation). Our central observation is that the process, for some specific a and r , is isomorphic to the packing of non-overlapping hypercubes covering $(a+r)^d$ cells, with range zero blocking† (see figure 1 for $d=2$).

Correspondingly, one has $a^{-d} p(a|r) = (a+r)^{-d} p(a+r|0)$, which allows us to obtain packing fraction results for models B, C, ..., trivially from those of A.

In models A, B, C, ..., permanent (unfillable) gaps between the edges of adjacent hypercubes (of side length a) can have width up to $(a-1)/a$, $(a+1)/a$, $(a+2)/a, \dots$, times the hypercube side length, respectively (cf unity for the continuum limit). Thus we expect the packing fraction for model A (B, C, ...) to approach its continuum limit, p^* , for finite or infinite $L = n/a$, from above (below), and the difference should scale like a^{-1} (with $O(a^{-2})$ corrections) as $a \rightarrow 0$. Thus we write $p(a|0) \sim p^* + k_{1,0}a^{-1} + k_{2,0}a^{-2} + \dots$, with $k_{1,0} > 0$, and then isomorphism arguments imply that $p(a|r) \sim p^* + k_{1,r}a^{-1} + k_{2,r}a^{-2} + \dots$, where $k_{1,r} = -drp^* + k_{1,0}$, $k_{2,r} = \frac{1}{2}d(d+1)r^2p^* - (d+1)rk_{1,0} + k_{2,0}, \dots$

We now compare Nakamura's packing fraction results for $d=2$ infinite lattices with those from the corresponding GPC (for model A), augmented with isomorphism arguments (for models B, C, ...). GPC results are obtained from numerical integration of exactly truncated $d=1$ infinite lattice ($n = \infty$) hierarchy equations for random a -mer filling (Gonzalez *et al* 1974, Epstein 1979). Exact GPC values for $p^* \approx 0.558\ 902\ 65$ and $k_{1,0} \approx 0.323\ 232\ 31$ can be extracted (cf Blaisdell and Solomon 1970), and an estimate of $k_{2,0} \approx -0.0071$ follows from Mackenzie's work. We find that $p^* + k_{1,0}a^{-1}$ gives a very accurate estimate of the GPC $p(a|0)$ for $a \geq 10$; Mackenzie's correction does not help here, but instead, choosing $k_{2,0} = 0.1011$ (and neglecting only $O(a^{-3})$ terms) reproduce the GPC $p(a|0)$ to eight decimal places for $a \geq 100$, and results in an underestimation for $a = 70, 50, 30, 20, 15$ and 10 by only $1, 5, 38, 149, 346$ and 1252 ($\times 10^{-8}$), respectively (and thus is essentially exact).

In figure 2, we have plotted first and second order asymptotic GPC behaviour for packing models A-D with $a \geq 10$. Exact B, C and D GPC values (shown) deviate only slightly from the above second-order behaviour. Upon these plots, we have superimposed Nakamura's model A(B) simulation results for $a = 10, 15, 20$ and 30 , together with values obtained from these by isomorphism arguments for models B, C and D (A, C and D). It appears that Nakamura's results for model A are more reliable than

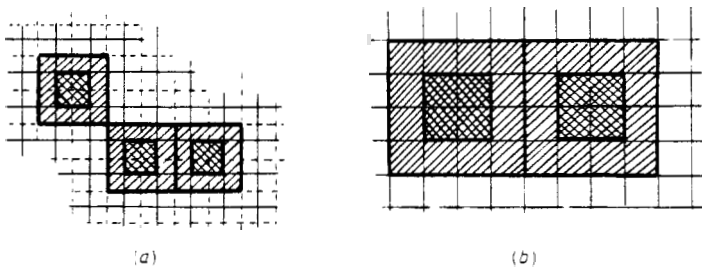


Figure 1. Examples of $d=2$ isomorphisms for the packing of squares covering a^d cells (i.e. squares of side length a lattice vectors) with range r blocking (in the l^∞ norm). (a), $(a, r) = (1, 1)$ and $(2, 0)$; (b), $(a, r) = (2, 2)$ and $(4, 0)$.

† This isomorphism has been noted previously for $d=1$ (Wolf *et al* 1984) and $d=2$ with $a=r=1$ (Nord and Evans 1985).

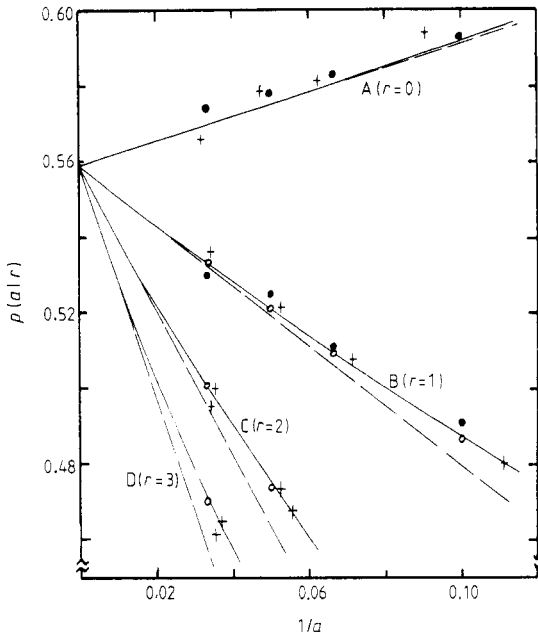


Figure 2. Comparison of Nakamura's results for packing fractions (●); results obtained from Nakamura's by isomorphism arguments (+); and results obtained from the generalised Palasti conjecture (GPC) and its large- a asymptotic expansion (---, first order; —, second order, ○, exact).

those for B (the $a = 30$ B value seems particularly low) and, furthermore, that linear extrapolation of these A values to $a = \infty$ should be more reliable (and justifiable) than for the B values. This is consistent with the result of Jodrey and Tory (1980) for $p^* = 0.562\ 10 \pm 0.000\ 56$. Finally, we remark on the uniformly high accuracy of the GPC for small a . (Compare Nakamura's p values with the squares of the $d = 1$ results of Gonzalez *et al* (1974). In particular, compare the GPC $p(2|0) = 0.747\ 645 \dots$ with the recent computer simulation result $0.747\ 88 \pm 0.000\ 11$ of Nord (1986).)

We now describe a number of other packing problems between which isomorphisms exist.

(I) We can change the above distance measure to $\|I\| = \sum_i |I_i|$, i.e. the l^1 norm. This leads to consideration of packing on a hypercubic lattice (with unit lattice vector) of hyperdiamond shaped blocks of $N(a)$ cells with centres within a distance $a - 1$ from a central one, and with range r blocking (defined by the l^1 norm). See figure 3(a) for $d = 2$ where $N(a) = 2a^2 - 2a + 1$. In the continuum limit ($a \rightarrow \infty$), this problem reduces to the one described above.

(II) Analogous packing problems can be considered on a hexagonal lattice, where the distance between two cells is defined as the number of links (between adjacent cell centres) in the shortest connecting path. Here we consider packing of blocks of $N(a) = 3a^2 - 3a + 1$ cells whose centres are within a distance $a - 1$ of a central one, and with range r blocking (see figure 3(b)). In the continuum limit ($a \rightarrow \infty$), this problem reduces to the packing of (aligned) hexagons in the plane.

(III) For a triangular lattice, consider the packing of hexagonal shaped blocks of $N(a) = 6a^2$ cells (the hexagon side length is a -lattice vectors) with range r blocking (see figure 3(c)). For the latter, the distance between edges of different hexagons

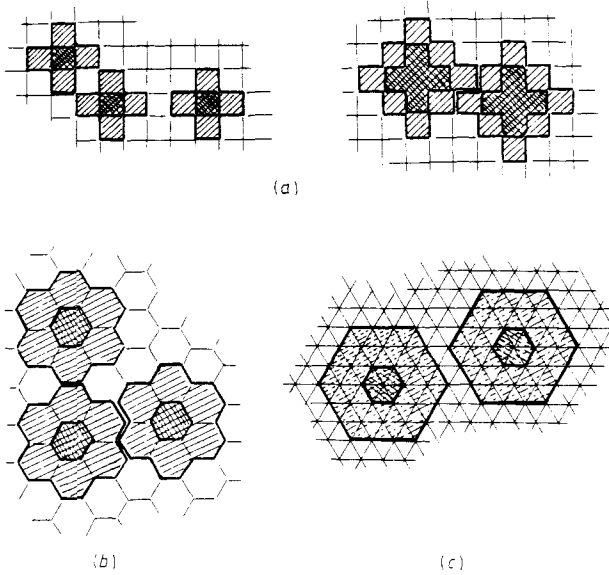


Figure 3. Examples of $d = 2$ isomorphisms for packing models (I(a), $(a, r) = (1, 3)$ and $(2, 1)$ (left); $(a, r) = (2, 2)$ and $(3, 0)$ (right)), II(b), $(a, r) = (1, 2)$ and $(2, 0)$) and III(c), $(a, r) = (1, 5)$ and $(3, 1)$), involving various objects (blocks of cells) of 'linear size' a , with range r blocking (in l^1 type norms).

(determined by the path involving the shortest number of steps between adjacent lattice sites) cannot be less than r . The continuum limit ($a \rightarrow \infty$) here is the same as for II.

For any of I, II or III, we denote the process for specific a and r by $\mathbb{P}(a|r)$, and its packing fraction by $p(a|r)$. Then for each of these classes, we have that $\mathbb{P}(a|2r')$ ($\mathbb{P}(a|2r'+1)$) is isomorphic to $\mathbb{P}(a+r'|0)$ ($\mathbb{P}(a+r'+1)$) (see figure 3). Correspondingly, one has that $N(a)^{-1}p(a|2r') = N(a+r')^{-1}p(a+r'|0)$ and $N(a)^{-1}p(a|2r'+1) = N(a+r')^{-1}p(a+r'+1)$. Arguments used previously apply here to show that $p(a|0)$ ($p(a|r > 0)$) approach their continuum limit ($a \rightarrow \infty$) values above (below).

Note that the above isomorphisms connect only processes with even (or odd) blocking range r . It is possible to relate processes of opposite parity r on (the mutually dual) hexagonal (II) and triangular (III) lattices. Specifically, one has that $\mathbb{P}_{III}(a|1)$ is isomorphic to $\mathbb{P}_{II}(a+1|0)$ so, e.g., $\mathbb{P}_{III}(a|2r'+1)$ is isomorphic to $\mathbb{P}_{II}(a+r'+1|0)$; similarly $\mathbb{P}_{II}(a|1)$ is isomorphic to $\mathbb{P}_{III}(a|0)$ so, e.g., $\mathbb{P}_{II}(a|2r'+1)$ is isomorphic to $\mathbb{P}_{III}(a+r'|0)$ (see figure 4). Corresponding relationships between packing fractions follow immediately.

Finally we describe some isomorphisms between the cell packing processes considered above and certain site filling processes. Clearly packing of hypercubes covering a^d cells is isomorphic to filling hypercubic blocks of a^d sites (cf Nord and Evans 1985) (or of smaller blocks of a'^d sites with a compensating l^∞ -type range $a - a'$ blocking). Cell filling models I, II and III can be readily related to single-site filling processes with an appropriate blocking range. Here, for the latter, distances must be determined from the path involving the shortest number of steps between adjacent sites. Then (i) $\mathbb{P}_I(a|r)$, (ii) $\mathbb{P}_{II}(a|r)$ and (iii) $\mathbb{P}_{III}(a|r)$ are isomorphic to single-site filling on (i) hypercubic, (ii) triangular and (iii) triangular lattices with range (i) $2a+r-2$, (ii) $2a+r-2$ and (iii) $2a+r-1$ blocking, respectively.

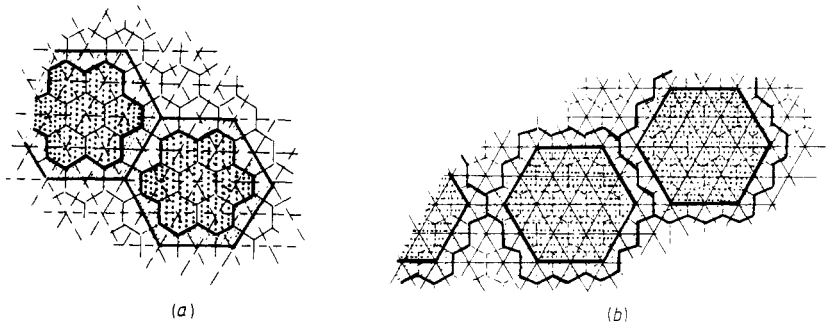


Figure 4. Examples of isomorphisms between packing models (II and III) on hexagonal and triangular lattices (respectively) with range 0 and 1 blocking. (a), $(a, r) = (2, 1)_{II}$ and $(2, 0)_{III}$; (b), $(a, r) = (2, 1)_{III}$ and $(3, 0)_{II}$.

In summary, we have described exact isomorphisms between various random sequential packing or filling processes (on periodic or infinite lattices). These were used to facilitate analysis of the continuum limit in Nakamura's square packing models. (Only infinite n/a was considered, but the finite case could similarly be treated.) The GPC was particularly useful here, but lacks an analogue for packing of non-square (or non-hypercubic) blocks of cells.

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