Planar Voronoi cells and the failure of Aboav’s law

H.J. Hilhorst

Laboratoire de Physique Théorique, Bâtiment 210, Université de Paris-Sud, 91405 Orsay, France
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Aboav’s law is a quantitative expression of the empirical fact that in planar cellular structures many-sided cells tend to have few-sided neighbors. This law is nonetheless violated in the most widely used model system, viz. the Poisson-Voronoi tessellation. We obtain the correct law for this model: Given an \( n \)-sided cell, any of its neighbors has on average \( m_n \) sides where \( m_n = 4 + 3(\pi/n)^{1/2} \ldots \) in the limit of large \( n \). This expression is quite accurate also for nonasymptotic \( n \) and we discuss its implications for the analysis of experimental data.

Two empirical rules play a key role in studies of planar cellular systems: Lewis’ law and Aboav’s law. Both are statements about the statistics of a cell’s most prominent properties, viz. its area and its number of sides. Lewis’ law \(^1\) says that the average area \( A_n \) of an \( n \)-sided cell increases with \( n \) as \( A_n = a_0(n-n_0)/\lambda \), where \( a_0 \) and \( n_0 \) are constants, and \( \lambda \) is the two-dimensional cell density. Aboav \(^2\) noticed that many-sided cells tend to have few-sided neighbors and vice versa. He expressed this correlation in terms of the average \( m_n \) of the number of sides of a cell that neighbors an \( n \)-sided cell. Aboav’s law, also called the Aboav-Weaire \(^3\) law, asserts that

\[
m_n = a + \frac{b}{n}, \tag{1}
\]

where \( a \) and \( b \) are constants. This law is in widespread use \(^2, 6, 7, 8, 9, 10, 11, 12, 13, 14\) in the analysis of experimental data on cellular structures.

In nature, planar cellular systems come in a wide variety. They include biological tissues \(^1, 4, 5\), polycrystals \(^2\), cells formed by particles trapped at a water/air interface \(^3\), cells in surface-tension driven Bénard convection \(^5\), in two-dimensional soap froths \(^8\), and in magnetic liquid froths \(^3\).

Alternatively, the cellular structure may appear when the data are subjected to the Voronoi construction \(^10\). Examples are hard disks on an air table \(^11\), a binary liquid during late stage coarsening \(^12\), two-dimensional colloidal aggregation \(^13\), nanostructured cellular layers \(^14\), and studies of two-dimensional melting \(^15\).

Many of these cellular systems, in spite of all their diversity, closely obey Lewis’ law from \( n \approx 5 \) up; also in many, Aboav’s law appears to hold with good accuracy in the full experimentally accessible range, i.e. from \( n = 3 \) to \( n \) typically between 9 and 12. Fitting \(^10\) to experimental data leads to values for the coefficient \( a \) ranging from 4.6 to 5.3 and for \( b \) from 7.0 to 8.5. This observed similarity of behavior, sometimes called “universality,” is generally attributed to the strong geometrical constraints that accompany a division of the plane into convex cells; by contrast, physical or biological mechanisms are believed only to lead to corrections. It is of obvious interest to subtract from the experimental data any purely geometrical effect that one can isolate in order to identify the mechanisms at work that cause the corrections.

Although Lewis’ and Aboav’s laws arose initially merely as good descriptions of the available data, several “derivations” have since conferred to them the status of theoretical truths valid for all \( n \) and embodying a purely geometrical theory. Most attempts \(^10\) to derive these laws apply maximum entropy principles to a hypothesized entropy functional \(^17\). A critique of this usage of the maximum entropy method is due to Chiu \(^18\), who has shown that no firm conclusions can be drawn from it. In any case, none of these derivations connects either Lewis’ or Aboav’s law by a first principle calculation to a microscopic model of planar cellular structure.

First-principle approach. – The simplest microscopic model of a planar cell model is the Poisson-Voronoi (PV) tessellation: It is obtained by constructing the Voronoi cells \(^10\) of a configuration of randomly and uniformly distributed point centers in the plane, for convenience often called “seeds” (but without the implication that they are material). The PV tessellation is therefore a natural candidate for the purely geometrical theory, and certainly the easiest one to handle.

The statistical properties of the PV tessellation have been studied analytically and by Monte Carlo methods (see Ref. \(^10\) for a review). Nonetheless, a first principle derivation of expressions for \( A_n \) and \( m_n \) has long seemed forbiddingly difficult. Numerically it is known \(^10, 19, 20, 21, 22\) that Aboav’s law is not exactly valid for the Poisson-Voronoi tessellation: Whereas Eq. \(^1\) predicts \( nm_n \) to be linear in \( n \), this quantity shows in fact a very small but distinct downward curvature for the PV tessellation. To accommodate this discrepancy modifications of Aboav’s law have been suggested, in particular, by Boots and Murdoch \(^19\) and by LeCaër and Ho \(^20\). The former authors write \( m_n = A + Bn^{-1} + Cn^{-2} \), which was later found to be true exactly for a class of graphs in field theory \(^22\).

A recent letter \(^24\) has achieved a step forward in the statistical mechanics of planar Voronoi tessellations. It opens up the possibility for an expansion in powers of \( n^{-\frac{1}{2}} \) of all quantities of interest related to the \( n \)-sided Voronoi cell; an immediate result was that Lewis’ law holds with coefficient \( a_0 = \frac{1}{4} \) for asymptotically large \( n \).
respectively. All solid line segments separate Voronoi cells. To each of them proportional to its own power of \( n \), we extend and interpret, we establish the following

\[ n \approx 100 \]  

The incipient piecewise parabolic structure of \( \Gamma_1 \) is discernible.

**Aboav’s law.** – Whereas Lewis’ law refers to a single cell, Aboav’s deals with the intrinsically more difficult problem of correlations between cells. Here we track down the implications of the \( n^{\frac{1}{2}} \) expansion for Aboav’s law. We consider an \( n \)-sided cell with \( n \) very large. Cells with very many sides are extremely rare, but if one occurs, then its environment must look as depicted in Fig. 1, where the \( n \)-sided cell of a “central” seed at \( O \) is surrounded by \( n \) strongly elongated first neighbor cells containing seeds \( F_i \). Independent evidence for such a geometry comes from work by Lauritsen et al. [22], who Monte Carlo simulated a Hamiltonian favoring the appearance of many-sided cells.

In Fig. 1 at least four different length scales play a role, each of them proportional to its own power of \( n \). Heavily relying on the work of Ref. [24], which for the present purpose we extend and interpret, we establish the following list of scales:

(i) The perimeter \( \Gamma_0 \) of the central cell typically runs within an annulus of center \( O \), of radius \( R_c = (n/4\pi\lambda)^{\frac{1}{2}} \), and of width of order 1. Hence for \( n \rightarrow \infty \) the perimeter tends towards a circle of radius \( R_c \). Consequently in that limit the first neighbors \( F_i \) will be on a circle of radius \( 2R_c \).

(ii) Two successive vertices on the perimeter of the central cell have an average distance \( \ell_{\text{vert}} = 2\pi R_c/n = (\pi/n\lambda)^{\frac{1}{2}} \). Consequently, two successive first neighbor seeds \( F_i \) and \( F_{i+1} \) have an average distance \( 2\ell_{\text{vert}} \).

(iii) Locally the positions of the vertices of the central cell are strongly aligned: Their radial coordinates have rms deviations of order \( n^{\frac{1}{2}} \) with respect to the locally averaged radius. For the purpose of the present discussion we may set these deviations equal to zero; their smallness implies that for \( n \rightarrow \infty \) the perimeter of the central cell becomes a smooth curve. Similar statements hold for the curve, not drawn in the Fig. 1, that links the successive first neighbors.

(iv) In the region to the right of the heavy solid line \( \Gamma_1 \), which is occupied by second and further neighbors, the seed density has its “background” value, \( \lambda \), i.e., is of order \( n^{0.2} \).

On the basis of this picture we reason as follows. The perimeter of the central cell carries a vertex line density \( \rho_{\text{vert}} = 1/\ell_{\text{vert}} = (n\lambda/\pi)^{\frac{1}{2}} \), which for \( n \rightarrow \infty \) tends to infinity. In spite of this diverging line density the surface density \( \lambda \) of the seeds to the right of the curve \( \Gamma_1 \) stays of order \( n^0 \). It follows that the central cell will have \( \sim n^{\frac{1}{2}} \) second neighbor cells and that each second neighbor \( S_j \) will be adjacent to \( \sim n^{\frac{1}{2}} \) first neighbor cells \( F_i \) (where we call the cells by the names of their seeds). Fig. 1 shows that under these circumstances each first neighbor \( F_i \) is most likely to have itself four neighbors, \( \text{viz.} \) the central \( n \)-sided cell, a single second neighbor cell, and two other first neighbors, \( F_{i-1} \) and \( F_{i+1} \).

We now focus on the exceptional \( F_i \) that have five neighbors due to their being adjacent to two second neighbors \( S_j \) and \( S_{j+1} \). An example is the cell marked \( F_1 \) in Fig. 1, which is adjacent to both \( S_1 \) and \( S_2 \). Let us denote by \( f_5 \) the fraction of first neighbors that are 5-sided. In view of the scaling relations that precede we expect that \( f_5 = cn^{-\frac{1}{2}} + \ldots \), where \( c \) is a numerical coefficient and the dots indicate terms of higher order in \( n^{-\frac{1}{2}} \). Any 6- and higher-sided \( F_i \) will contribute only to these dot terms. Hence we have

\[
m_n = 4(1-f_5) + 5f_5 = 4 + cn^{-\frac{1}{2}} + \ldots \tag{2}
\]

We next consider the solid line \( \Gamma_1 \) in Fig. 1, which separates the central seed’s first from its second neighbors. In the large \( n \) limit the curve linking successive first neighbor seeds becomes a circle which may locally be replaced with a straight line. In Fig. 2 this same straight line is represented by the \( x \) axis and the region of space containing the second and further neighbors by the half-plane \( y > 0 \). The second and further neighbor seeds are uniformly distributed in the upper half plane with the background density \( \lambda \). Since the first neighbors \( F_i \) are dense on the \( x \) axis, the curve \( \Gamma_1 \) now divides the half-plane \( y > 0 \) into a lower part of points closer to the \( x \) axis than to any of the seeds, and its complement. Hence the function \( y = \Gamma_1(x) \) is piecewise parabolic; its incipient parabolic segments are discernible in Fig. 1. To each cusp of \( \Gamma_1(x) \) corresponds a 5-sided first neighbor cell. Let \( \ell_{\text{cusp}} \) be the average distance between the abscissae
The inverse square root decay and the limiting value $m_{\infty} = 4$ of Eq. (3) are in contradistinction to Aboav’s law (1). This equation explains for the first time the downward curvature observed [19, 20, 21, 22] in the $m$ vs. $n$ curves for the PV tessellation.

**Data analysis.** – We cannot assess a priori the applicability of Eq. (3) to $m_n$ data in the range of $n$ covered by experiments and simulations. We have plotted in a new way in Fig. 3 the Monte Carlo data for $m_n$ due to Boots and Murdoch [19]. The dotted curve shows the best two-parameter fit to the data provided by Aboav’s law (1); it is obtained for $a = 5.251$ and $b = 5.755$ [10] and is generally taken as evidence that this law fails for the PV tessellation. The dashed line in Fig. 3 represents the right hand side of Eq. (3) with the dot terms neglected. It appears that in the regime of the data our zero-parameter asymptotic result is numerically only slightly more off than Aboav’s two-parameter law [21]. This high degree of accuracy is remarkable in view of the fact that Eq. (3) rests on an expansion around the improbable event of a large $n$-sided cell. But more importantly, there is full compatibility between our dashed line and the downward trend of the data for $n$ larger than about 10. One may attempt to improve our Eq. (3) by including higher order terms in $n^{-1/2}$ in the series, the simplest possibility being

$$m_n = 4 + 3 \sqrt{\frac{\pi}{n}} + \ldots, \quad n \to \infty. \quad (3)$$

Dashed line: Our zero-parameter exact asymptotic result (3), Dotted line: Best two-parameter fit with Aboav’s law (1).

FIG. 2: The $x$-axis represents a continuum of first neighbors. The upper half-plane is randomly filled with seeds of uniform density $\lambda$ (here $\lambda = 1$). The piecewise parabolic curve $y = \Gamma_1(x)$ separates the region of the half-plane closer to the $x$ axis than to any of the random seeds from its complement. The abscissae of the cusps of $\Gamma_1$ have a density of $\frac{\lambda}{n}$ on the $x$ axis. Solid and open squares represent second and further neighbors, respectively. Note that the horizontal and vertical scales are different.

of two successive cusps of $\Gamma_1(x)$. Then it is clear that $f_5 = 2\ell_{\text{vert}}/\ell_{\text{cusp}}$. The determination of $\ell_{\text{cusp}}$ for given seed density $\lambda$ in the upper half plane is a problem in statistics that yields $\ell_{\text{cusp}} = 2/(3\lambda^{3/2})$ [20]. Using the expression for $\ell_{\text{vert}}$ found above we therefore have that $f_5 = 2(\pi/n\lambda)^{3/2} \times 3\lambda^{3/2}/2 = 3(\pi/n)^{3/2}$, whence $c = 3\pi^{3/2}$. Substituting this in (2) we conclude that for the Poisson-Voronoi tessellation $m_n$ is exactly given by

$$m_n = 4 + 3\sqrt{\frac{\pi}{n}} + \ldots, \quad n \to \infty. \quad (3)$$

The upper half-plane is randomly filled with seeds of uniform density $\lambda$ (here $\lambda = 1$). The piecewise parabolic curve $y = \Gamma_1(x)$ separates the region of the half-plane closer to the $x$ axis than to any of the random seeds from its complement. The abscissae of the cusps of $\Gamma_1$ have a density of $\frac{\lambda}{n}$ on the $x$ axis. Solid and open squares represent second and further neighbors, respectively. Note that the horizontal and vertical scales are different.

FIG. 3: The two-cell correlation $m_n$ as a function of $n$. Open squares: Simulation values due to Boots and Murdoch [19]. Dotted line: Best two-parameter fit with Aboav’s law (1). Dashed line: Our zero-parameter exact asymptotic result (3), which in this representation is a constant equal to $3\pi^{3/2}$.
To show how such a discussion might proceed, we consider briefly and heuristically an example from class (ii) above, viz. the Voronoi tessellations associated with hard core particles of finite diameter \( a \). The preceding analysis of the large \( n \) limit goes through as long as \( n \lesssim n^* \), where the crossover value \( n^* \) is determined by the condition that the distance between adjacent first neighbors become comparable to the particle diameter. This gives \( 2\pi R_c \sim n^* a \), whence \( n^* \sim \pi/(\lambda a^2) \). For \( n \gtrsim n^* \) the repulsion between the particles combined with the condition that they be locally aligned imposes that the radius of the central cell grows as \( R_c \sim na \) and hence that \( f_5 \) must saturate at a value \( f_5 = c_0 a \lambda^{\frac{1}{2}} \) where \( c_0 \) is an unknown numerical coefficient. Upon assuming that this knowledge may be expressed with the aid of a scaling function \( M \) we obtain for hard core particles of diameter \( a \) the relation \( m_n = 4 + a \lambda^{\frac{1}{2}} M(n \lambda a^2) \), valid in the scaling limit \( n \to \infty \), \( \lambda a^2 \to 0 \) with \( x = n \lambda a^2 \) fixed, and where the scaling function \( M \) satisfies \( M(0) = c_0 \) and \( M(x) \approx 3(\pi/\lambda x)^{\frac{1}{2}} \) for \( x \to \infty \). Hence for hard core particles the limiting value \( m_\infty \) of \( \lambda \) is changed, but the \( n^{-\frac{1}{2}} \) decay law remains. Future work will have to deal with this and other instances of deviations from PV statistics.

**Conclusion.** – The simplest and most widely used model of a cellular structure – the Poisson-Voronoi tessellation – does not obey the most widely used law – Aboav’s law \([1]\) – governing the two-cell correlations. We have shown that for the PV tessellation the \( n^{-1} \) decay of Aboav’s law should in fact be replaced with an \( n^{-\frac{1}{2}} \) decay. Experimental data of sufficient precision and/or covering a large enough range should be able to distinguish between the two and thereby shed light on the question of the universality classes and of the underlying cell formation mechanisms. We therefore advocate that experimental results be analyzed not only by Aboav’s two-parameter fit \([1]\), but also by the simpler one-parameter formula \([4]\), of which the first two terms have a firm theoretical basis.

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* Electronic address: Henk.Hilhorst@th.u-psud.fr

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