Point sets of minimal energy

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- the structure of polymers
- structure of ground states of particle systems
- viral morphology
- the arrangement of colloidal particles
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Idea: use this principle for generating Quasi-Monte Carlo point sets on manifolds, especially spheres.

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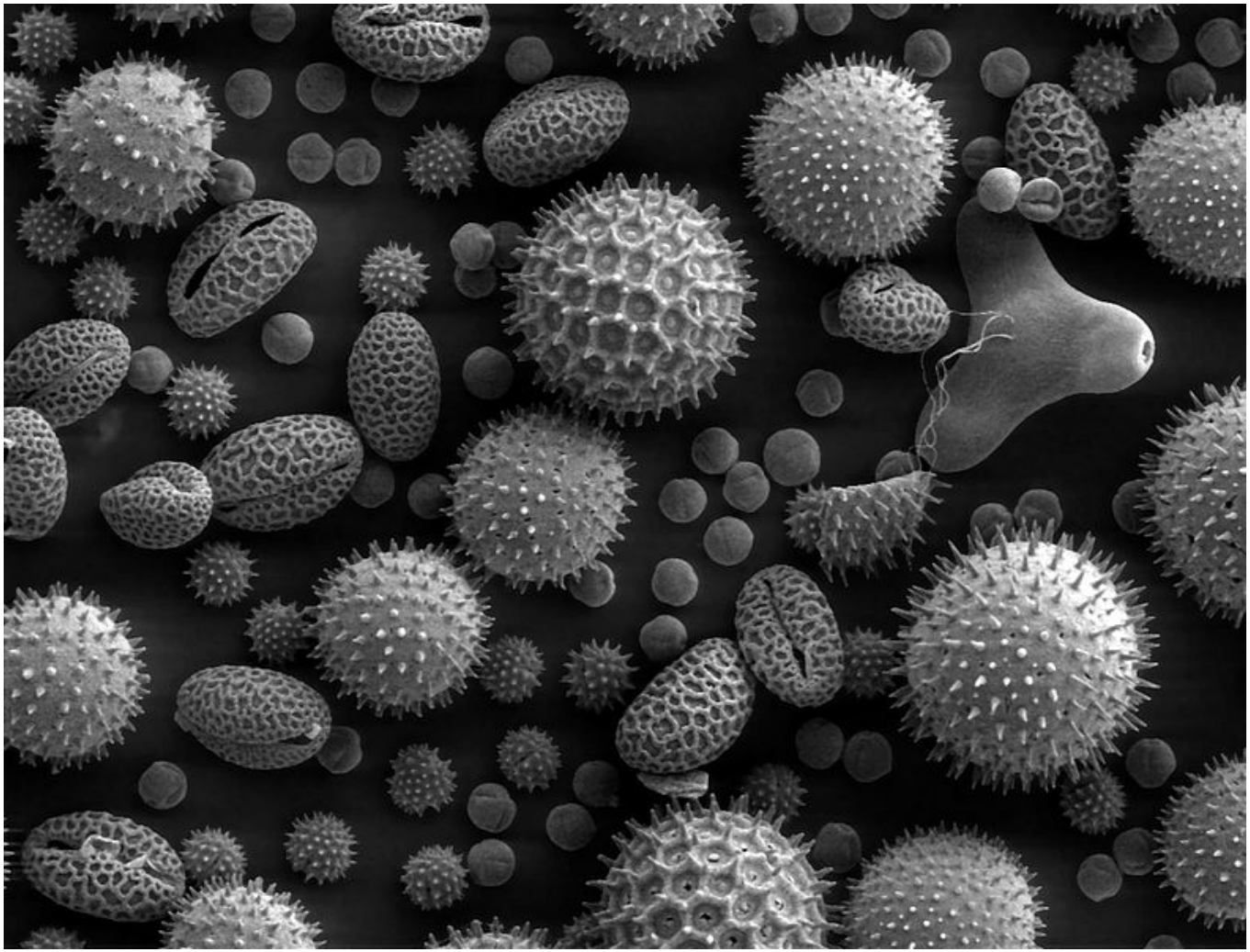
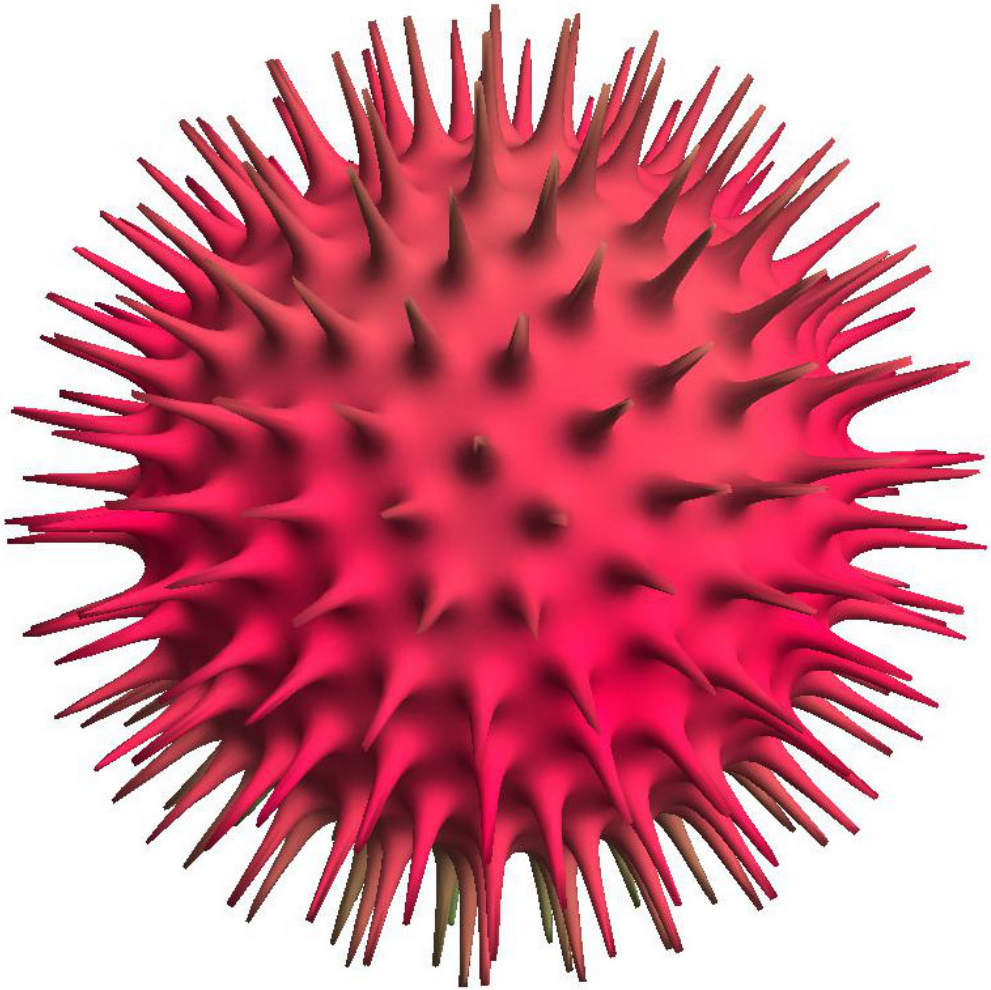
- sampling spacial directions

Pollen grains



Potential function of a point distribution



Quantify evenness

For every point set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ of *distinct* points, we assign several qualitative measures that describe aspects of even distribution.

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For every point set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ of *distinct* points, we assign several qualitative measures that describe aspects of even distribution.
Then we can try to minimise or maximise these measures for given N.

Combinatorial measures

- discrepancy

$$D_N(X_N) = \sup_C \left| \frac{1}{N} \sum_{n=1}^{N} \chi_C(\mathbf{x}_n) - \sigma(C) \right|$$

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$$\delta_N(X_N) = \sup_{\mathbf{x} \in S^d} \min_k |\mathbf{x} - \mathbf{x}_k|$$

- separation

$$\Delta_N(X_N) = \min_{i \neq j} |\mathbf{x}_i - \mathbf{x}_j|$$

Analytic measures

- error in numerical integration

$$I_N(f, X_N) = \left| \sum_{n=1}^{N} f(\mathbf{x}_n) - \int_{S^d} f(\mathbf{x})\, d\sigma_d(\mathbf{x}) \right|$$

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- Worst-case error for integration in a normed space H:

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- Worst-case error for integration in a normed space H:

$$I_N(X_N, H) = \sup_{\substack{f \in H \\ \|f\|=1}} I_N(f, X_N)),$$

- (generalised) energy:

$$E_g(X_N) = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \tilde{g}(\|\mathbf{x}_i - \mathbf{x}_j\|),$$

where g denotes a positive definite function.

Other concepts

- designs:

$$\frac{1}{N}\sum_{n=1}^{N} f(\mathbf{x}_n) = \int_{S^d} f(\mathbf{x})\, d\sigma(\mathbf{x})$$

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  for all polynomials of degree $\leq t$.

- L^2-discrepancy:

$$\int_0^{\pi} \int_{S^d} \left| \frac{1}{N}\sum_{n=1}^{N} \chi_{C(\mathbf{x},t)}(\mathbf{x}_n) - \sigma_d(C(\mathbf{x},t)) \right|^2 d\sigma_d(\mathbf{x})\, dt$$

Discrepancy

Discrepancy is the most classical measure for the difference of two distributions

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It is rather difficult to compute explicitly, even for moderate values of N.

Estimates for discrepancy

Thus estimates for $D_N(X_N)$ are of interest (PG 1991, X.-J. Li & J. Vaaler, 1999), Erdős-Turán type inequality

$$D_N^C(X_N) \leq C_d \left(\frac{1}{M} + \sum_{k=1}^{M} \frac{1}{k} \sum_{j=1}^{Z(d,k)} \left| \frac{1}{N} \sum_{n=1}^{N} Y_{k,j}(\mathbf{x}_n) \right| \right)$$

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F. J. Narcowich, X. Sun, J. D. Ward, and Z. Wu (2010), LeVeque-type inequality:

$$D(X_N) \leq B(d) \left(\sum_{\ell=0}^{\infty} \ell^{-(d+1)} \sum_{m=1}^{Z(d,\ell)} \left(\frac{1}{N} \sum_{n=1}^{N} Y_{\ell,m}(\mathbf{x}_n) \right)^2 \right)^{\frac{1}{d+2}}.$$

Irregularities

On the other hand the theory of irregularities of distributions developed by K. F. Roth, W. Schmidt, J. Beck, W. Chen, ... gives a lower bound

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This is essentially best possible. Namely, for every N there exists a point set X_N such that

$$DN(X_N) \leq CN^{-\frac{1}{2}-\frac{1}{2d}} \log N.$$

The construction of this point set is probabilistic.

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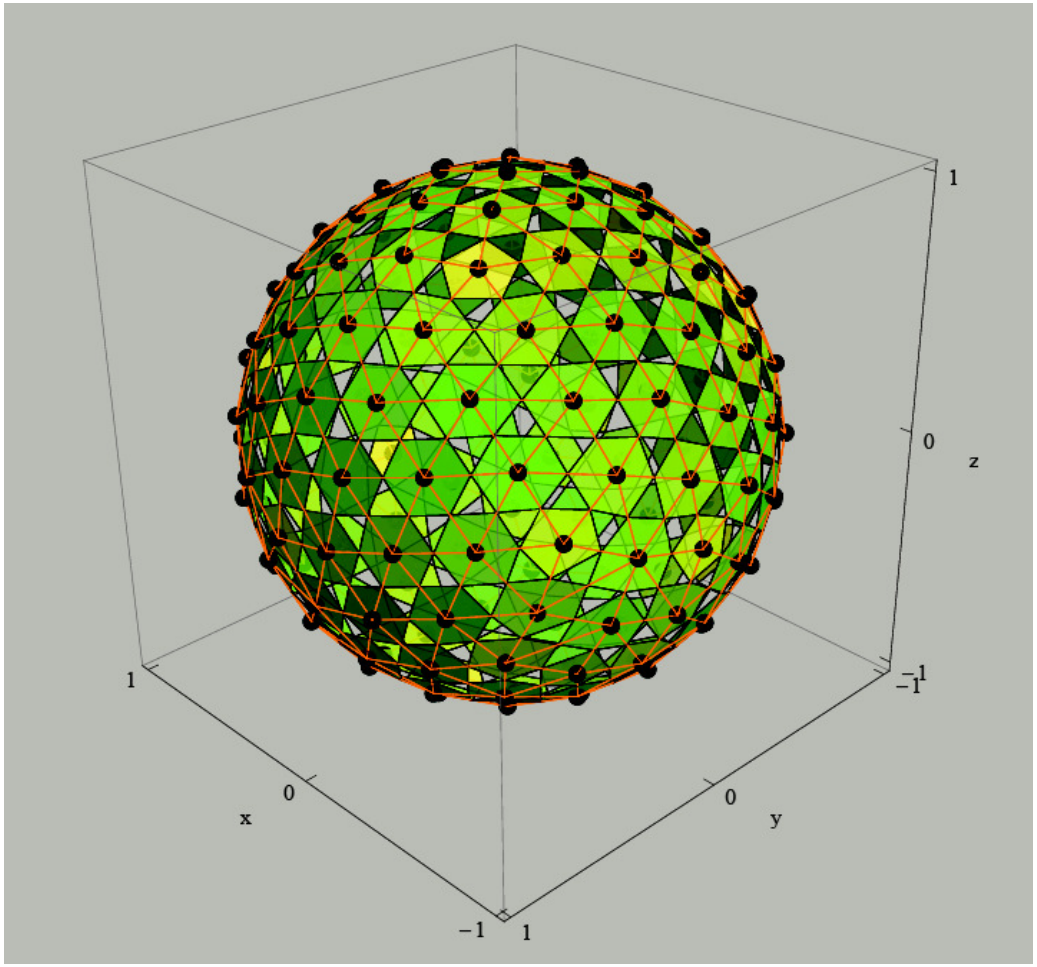
- if $g(1-t) = \Omega(t^{-s/2})$ for $s \geq d$ the energy functional is called *super-singular*.

Energy

For $s > 0$ consider the Riesz-energy functional of X_N

$$E_s(X_N) = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \|\mathbf{x}_i - \mathbf{x}_j\|^{-s}$$

and find its minimal value and the corresponding point sets for given N.



Minimal energy point configuration provided by J. Brauchart

Energy continued

For $0 < s < d$ classical potential theory asserts that the discrete distribution measures of minimal energy point sets

$$\frac{1}{N}\sum_{n=1}^{N}\delta_{\mathbf{x}_n}$$

weakly tend to the unique minimiser of the continuous energy functional

$$E(\mu) = \int_{S^d}\int_{S^d} \|\mathbf{x}-\mathbf{y}\|^{-s}\, d\mu(\mathbf{x})\, d\mu(\mathbf{y}),$$

the surface measure σ.

Energy continued

This gives

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n) = \int_{S^2} f(\mathbf{x})\, d\sigma(\mathbf{x})$$

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Minimal energy points give good behaviour for numerical integration and discrepancy.

Energy continued

Furthermore, for $d-2 \leq s < d$ the point sets X_N of minimal energy are well separated:

$$\min_{i \neq j} \|\mathbf{x}_i - \mathbf{x}_j\| \geq \frac{C}{N^{\frac{1}{d}}}$$

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For $0 < s < d$ the minimal value of the energy satisfies (G. Wagner)

$$C_s N^2 - c_s^{(1)} N^{1+\frac{s}{d}} \leq \min_{X_N} E_s(X_N) \leq C_s N^2 - c_s^{(2)} N^{1+\frac{s}{d}}$$

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for positive constants $c_s^{(1)}$ and $c_s^{(2)}$ with

$$C_s = \int_{S^2} \int_{S^2} \|\mathbf{x} - \mathbf{y}\|^{-s} \, d\sigma(\mathbf{x}) \, d\sigma(\mathbf{y}).$$

Energy continued

It is conjectured that

$$\lim_{N\to\infty} \frac{\min_{X_N} E_s(X_N) - C_s N^2}{N^{1+\frac{s}{d}}}$$

exists. The conjectured value of the limit is given in terms of the zeta-function of a lattice.

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This conjecture reflects the fact that on S^2 locally the numerical examples of minimal energy configurations show a hexagonal structure.
Furthermore, in the plane the hexagonal lattice minimises the corresponding energy functional.

Minimal energy point sets

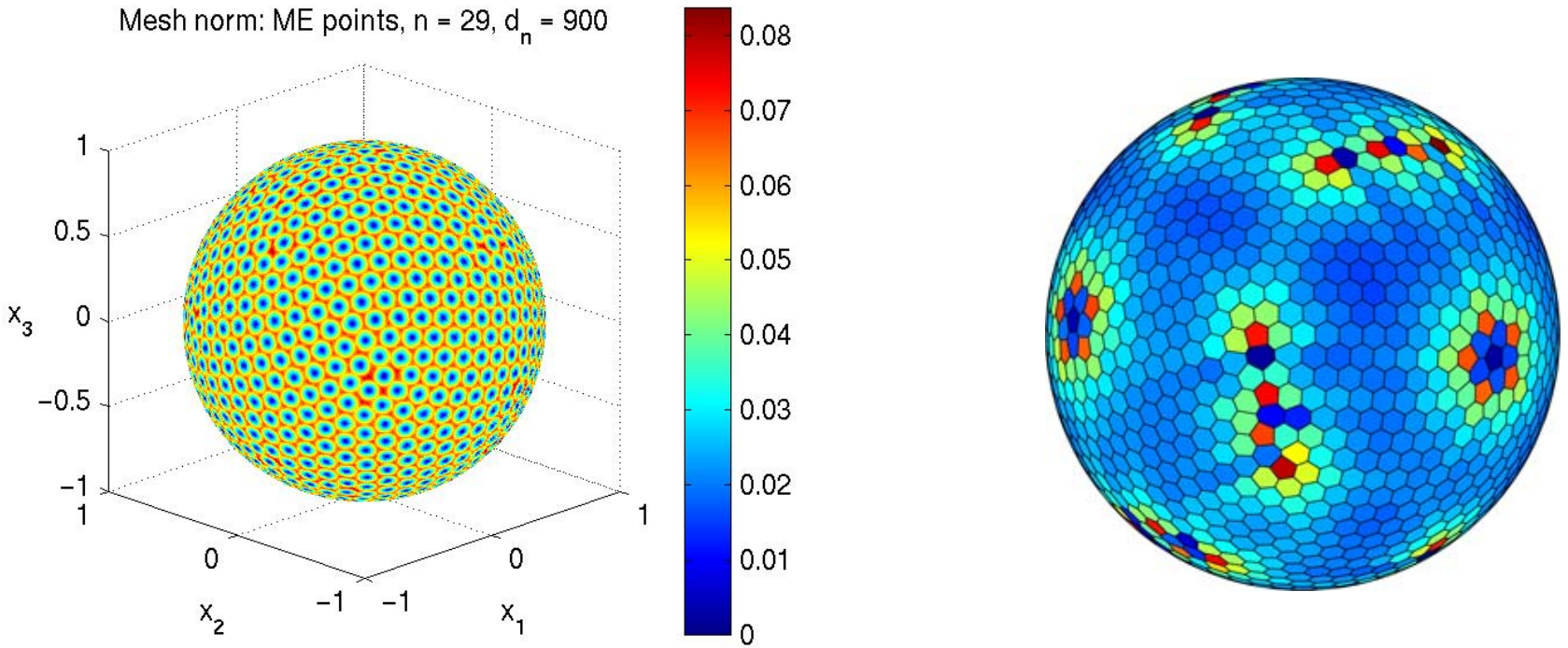

Figure: Mesh function and Voronoi cells for minimal energy point sets

Energy and numerical integration

Let $0 < s < d$. For f with $|f(\mathbf{x}) - f(\mathbf{y})| \leq C|\mathbf{x} - \mathbf{y}|$ (PG & S. Damelin)

$$I_N(f, X_N) \leq 24C\frac{1}{m} + \max_{1 \leq k \leq m} \left(\frac{2k+1}{\omega_d a_k(\delta)}\right)^{\frac{1}{2}} \|f\|_2 \times \left(\frac{1}{N^2}E_s(X_N) + \frac{1}{N}\delta^{-s} - a_0(\delta)\right)^{\frac{1}{2}},$$

where

$$\frac{1}{(1+\delta-\cos(t))^s} = \sum_{k=0}^{\infty} a_k(\delta) P_k(\cos(t)).$$

Super-singular energy

For $s \geq d$ potential theoretic methods are no more applicable, since the energy integral

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diverges for all measures μ.
The case $s = d$ could still be managed by taking the limit $s \to d-$; this was used by M. Götz and E. Saff to obtain asymptotic uniform distribution for $N \to \infty$.

Super-singular energy and discrepancy

For the discrepancy of a point set minimising the energy for $s = d$ an estimate of the form

$$D_N^C(X_N) = \mathcal{O}\left(\sqrt{\frac{\log\log N}{\log N}}\right)$$

could be given (PG & S. Damelin).

Super-singular energy continued

The case $s > d$ was open for a longer period of time. In 2005 D. Hardin and E. Saff could show that for $s > d$ the point sets of minimal energy are asymptotically uniformly distributed.

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- For any rectifiable manifold M the minimal energy point sets are asymptotically uniformly distributed with respect to the normalised Hausdorff measure on M.

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They could even prove more:

- For any rectifiable manifold M the minimal energy point sets are asymptotically uniformly distributed with respect to the normalised Hausdorff measure on M.
- There exists a constant $C(s, d)$ such that

$$\lim_{N\to\infty} \frac{E_s(X_N)}{N^{1+\frac{s}{d}}} = \frac{C(s,d)}{\mathcal{H}(M)^{\frac{s}{d}}}$$

The constant $C(s, d)$ is again conjectured to be expressible in terms of the zeta-function of a lattice.

Super-singular energy continued

As opposed to the case $s < d$ the energy for $s > d$ mostly depends on local (short range) interactions between the points. This provides a heuristic explanation of why the approaches for $s < d$ are not applicable for the singular case.

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On the other hand the dominance of the short range interactions allows to show separation results for minimal energy point sets by an easy argument

$$\delta_N(X_N) = \min_{i \neq j} \|\mathbf{x}_i - \mathbf{x}_j\| \geq \frac{C}{N^{\frac{1}{d}}}.$$

Super-singular energy continued

For $s \to \infty$ the problem of minimising the s-energy becomes the problem of maximising the minimal distance $\delta_N(X_N)$, the problem of best packing.

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In the plane the problem of best packing is solved by the hexagonal lattice, which supports the conjecture about the constant $C(s, 2)$.

Non-singular energy

For every positive definite zonal function

$$g(t) = \sum_{k=0}^{\infty} Z(d,k) a_k P_k(t)$$

the corresponding energy functional of a set X_N is defined by

$$E_g(X_N) = \sum_{i,j=1}^{N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle).$$

Non-singular energy continued

As in the potential-theoretic case minimal energy configurations for $N \to \infty$ tend to the unique minimiser of the energy integral

$$I_g(\mu) = \iint_{S^d \times S^d} g(\langle \mathbf{x}, \mathbf{y} \rangle)\, d\mu(\mathbf{x})\, d\mu(\mathbf{y})$$

amongst all Borel probability measures; the normalised surface measure σ_d on S^d

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in the sense

$$\frac{1}{N} \sum_{i=1}^{N} \delta_{\mathbf{x}_i} \rightharpoonup \sigma_d.$$

Example

For a reproducing kernel Hilbert space H with kernel K take $g = K$. Then the worst case integration error satisfies

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Minimising the worst case integration error gives asymptotically uniformly distributed point sets.

Interpretation of L^2-Discrepancy

"Random Functions"

If $g(1)$ exists we can define a stochastic process by the covariance matrix

$$(g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle))_{i,j}\,.$$

Then the mean square of the integration error (with respect to the measure defined by the process) satisfies

$$\int_{C(S^d)} \left(\frac{1}{N} \sum_{n=1}^{N} y(\mathbf{x}_n) - \int_{S^d} y(\mathbf{x})\, d\sigma(\mathbf{x}) \right)^2 d\lambda(y) = \frac{1}{N^2} E_g(X_N) - a_0.$$

Example

For instance, the process can be chosen in a way that $\frac{1}{N^2} E_g(X_N) - a_0$ equals the usual L^2-discrepancy

$$\int_0^\pi \int_{S^d} \left(\frac{1}{N} \sum_{n=1}^{N} \chi_{B(\mathbf{x},r)}(\mathbf{x}_n) - \sigma(B(\mathbf{x},r)) \right)^2 d\sigma(\mathbf{x}\, dr.$$

The process can be given explicitely by

$$Y(\mathbf{x}) = \sum_{n=0}^{\infty} \sum_{k=1}^{Z(d,n)} A_{n,k}\, Y_{n,k}(\mathbf{x}),$$

where the $A_{n,k}$'s are independent normal random variables with mean 0 and variance $\frac{a_n}{Z(d,n)}$.