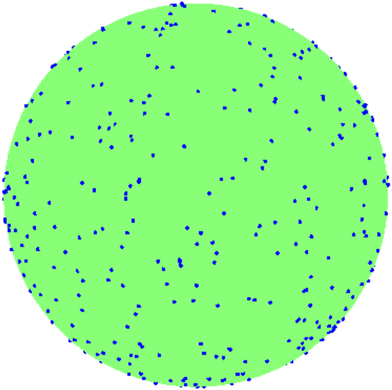
Random points on the sphere

C. Beltrán (U. Cantabria)
J. Marzo (U. Barcelona)
& J. Ortega-Cerdà (U. Barcelona)

"Well distributed" points on the sphere

$$\mathbb{S}^d = \{x = (x_1, \ldots, x_{d+1}) \in \mathbb{R}^{d+1} \ : \ x_1^2 + \cdots + x_{d+1}^2 = 1\}$$



529 random uniform points

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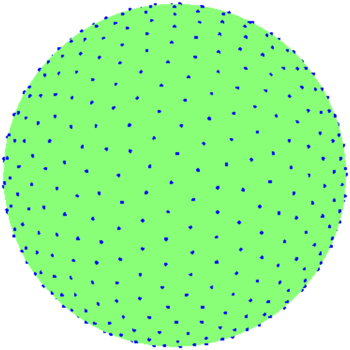

Rob Womersley web http://web.maths.unsw.edu.au/ rsw/Sphere/ 529 Fekete points

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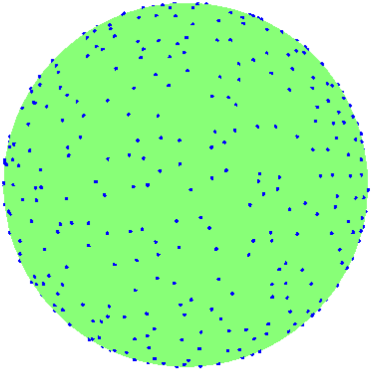
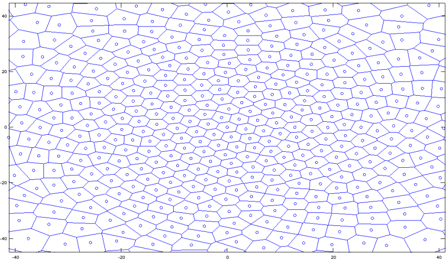
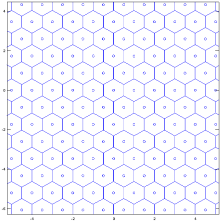


529 points points harmonic ensemble

Topological restriction

For large number of "well distributed" points, they appear to arrange according to hexagonal pattern slightly perturbed in order to fit in $\mathbb{S}^2$.





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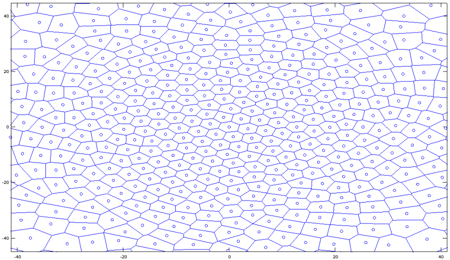

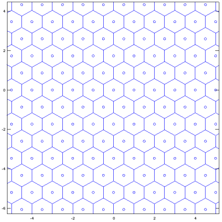

Euler characteristic formula $F - E + V = 2$.

Riesz energies

For a given collection of points $x_1, \ldots, x_n \in \mathbb{S}^d$ and $s > 0$ the **discrete s-energy** associated to the set $x = \{x_1, \ldots, x_n\}$ is

$$E_s(x) = \sum_{i \neq j} \frac{1}{\|x_i - x_j\|^s}.$$

Minimal s-energy

$$\mathcal{E}(s, n) = \inf_{x \in (\mathbb{S}^d)^n} E_s(x).$$

Discrete logarithmic energy and **minimal discrete logarithmic energy**

$$E_0(x) = \sum_{i \neq j} \log \frac{1}{\|x_i - x_j\|}, \quad \mathcal{E}(0, n) = \inf_x E_0(x).$$

- $0 < s < d$ Thomson problem: $d = 2$, $s = 1$ Coulomb (and generalizations).
- $s \to +\infty$ Tammes problem. Best packing.
- Logarithmic case $s = 0$, $d = 2$, (elliptic) Fekete points.
  - Sandier and Serfaty work about renormalized energies and its minimizers.
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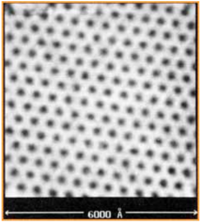
A. Abrikosov extended Ginzburg-Landau model for superconductivity to fit with some experimental measurements. In this extension he predicted the appearance of local defects of superconductivity called vortices. These vortices repel each other and arrange into a triangular lattice.



H. F. Hess et al. Bell Labs Phys. Rev. Lett. 62, 214 (1989)

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$$an \le \mathcal{E}(0, n) - \left(\frac{1}{2} - \log 2\right) n^2 + \frac{n}{2} \log n \le An, \quad n \to \infty.$$

Brauchart, Hardin and Saff conjectured that

$$\mathcal{E}(0, n) = \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n}{2} \log n + Cn + o(n), \quad n \to \infty,$$

and

$$C = 2 \log 2 + \frac{1}{2} \log \frac{2}{3} + 3 \log \frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.055605...$$

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Betermin and Sandier show that C exists and both conjectures are equivalent.

$s = 0$ elliptic Fekete points (Smale 7th problem)

$$E_0(x) - \mathcal{E}(0, n) \leq c \log n.$$

Asymptotic behavior of the Riesz energies when $n \to \infty$

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Asymptotic behavior of the Riesz energies when $n \to \infty$

We want computable examples. Random configurations...but sets of independent uniformly random points exhibit clumping.

Determinantal point process (Macchi 70's)

Let μ be the normalized Lebesgue surface measure in a space X, in our case $X = \mathbb{S}^d$, $\mu(X) = 1$.

Given a function (kernel) $K : X \times X \longrightarrow \mathbb{C}$ such that:

- $K(x, y) = \overline{K(y, x)}$
- Reproducing property

$$\int_X K(x, y)K(y, z)d\mu(y) = K(x, z)$$

- Trace

$$\int_X K(x, x)d\mu(x) = n$$

Then

$$f(x_1, \ldots, x_n) = \frac{1}{n!} \det(K(x_i, x_j))_{1\leq i,j\leq n}$$

is a density function in X.

Determinantal point process

Take $\phi_1, \ldots, \phi_n$ ON system in $L^2(X)$ then

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Example:
Circular unitary ensemble (CUE). For $X = \mathbb{S}^1$, take $\phi_k(\theta) = e^{ik\theta}$ then $K(x,y) = \frac{\sin\left((n+\frac{1}{2})(\theta-\phi)\right)}{\sin\left(\frac{1}{2}(\theta-\phi)\right)}$ defines the density

$$f(\theta_1, \ldots, \theta_n) = \frac{1}{n!} \prod_{j<k} |e^{i\theta_k} - e^{i\theta_j}|^2.$$

Weyl and Dyson: the eigenvalues of $n \times n$ unitary matrices drawn according to the Haar measure have a CUE distribution.

Random matrix theory, Quantum physics, Machine learning...

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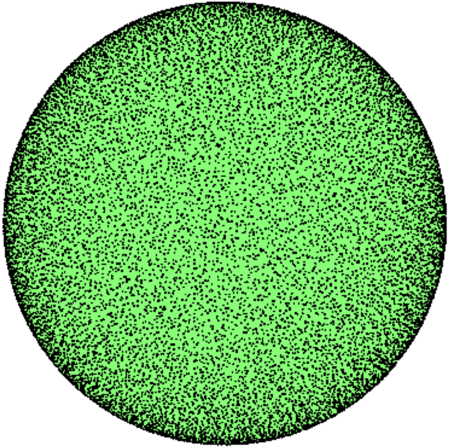
Spherical ensemble in $\mathbb{S}^2$: generalized eigenvalues of random $n \times n$ matrices A, B with independent complex Gaussian entries (i.e. eigenvalues of $A^{-1}B$).
It is a determinantal process (Krishnapur) in the plane and by the stereographic projection defines a point process in $\mathbb{S}^2$ with density

$$f(p_1, \ldots, p_n) = \prod_{j<k} |p_j - p_k|^2, \quad p_i \in \mathbb{R}^3.$$

Alishashi-Zamani (15).



$25281 = 159^2$ points from the spherical ensemble

The harmonic ensemble in $\mathbb{S}^d$

Let Π_L be the space of spherical harmonics of degree at most L in $\mathbb{S}^d$ (i.e. polynomials in $\mathbb{R}^{d+1}$ of degree at most L restricted to $\mathbb{S}^d$).

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By Christoffel-Darboux formula the reproducing kernel of Π_L

$$K_L(x,y) = \frac{\pi_L}{\binom{L+\frac{d}{2}}{L}} P_L^{(1+\lambda,\lambda)}(\langle x,y\rangle), \quad x,y \in \mathbb{S}^d,$$

where $\lambda = \frac{d-2}{2}$ and the Jacobi polynomials are $P_L^{(1+\lambda,\lambda)}(1) = \binom{L+\frac{d}{2}}{L}$.
By definition

$$P(x) = \langle P, K_L(\cdot,x)\rangle = \int_{\mathbb{S}^d} K_L(x,y)P(y)d\mu(y), \text{ for } P \in \Pi_L.$$

Then

$$\dim \Pi_L = \pi_L = \frac{2}{\Gamma(d+1)} L^d + o(L^d),$$

and $K_L(x,x) = \pi_L$ for every $x \in \mathbb{S}^d$.

The harmonic ensemble in $\mathbb{S}^d$

The harmonic ensemble is the determinantal point process in $\mathbb{S}^d$ with π_L points a.s. induced by the kernel

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We study diferent aspects of this process:

- Expected Riesz energies
- Linear statistics and spherical cap discrepancy
- Separation distance
- Energy optimality among isotropic processes

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For any measurable $f : \mathbb{S}^d \times \mathbb{S}^d \to [0, \infty)$ we have

$$\mathbb{E} \left(\sum_{i \neq j} f(x_i, x_j) \right) = \int_{(\mathbb{S}^d)^2} \left(K(x,x)K(y,y) - |K(x,y)|^2 \right) f(x,y) d\mu(x) d\mu(y).$$

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Continuous s-energy for the normalized Lebesgue measure is $(0 < s < d)$

$$V_s(\mathbb{S}^d) = \int_{\mathbb{S}^d}\int_{\mathbb{S}^d}\frac{1}{\|x-y\|^s}\,d\mu(x)\,d\mu(y) = 2^{d-s-1}\frac{\Gamma\left(\frac{d+1}{2}\right)\Gamma\left(\frac{d-s}{2}\right)}{\sqrt{\pi}\,\Gamma\left(d-\frac{s}{2}\right)}.$$

It is known that (Alexander, Stolarsky, Wagner, Kuijlaars, Saff, Brauchart) for $d \geq 2$ and $0 < s < d$ there exist constants $C, c > 0$ such that

$$-cn^{1+s/d} \leq \mathcal{E}(s, n) - V_s(\mathbb{S}^d)n^2 \leq -Cn^{1+s/d},$$

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Conjecture (BHS) : there is a constant $A_{s,d}$ such that

$$\mathcal{E}(s,n) = V_s(\mathbb{S}^d)n^2 + \frac{A_{s,d}}{\omega_d^{s/d}} n^{1+s/d} + o(n^{1+s/d}).$$

Furthermore, when $d = 2, 4, 8, 24$

$$A_{s,d} = |\Lambda_d|^{s/d} \zeta_{\Lambda_d}(s),$$

where $|\Lambda_d|$ stands for the co-volume and $\zeta_{\Lambda_d}(s)$ for the Epstein zeta function of the lattice Λ_d. Here Λ_d denotes the triangular lattice for $d = 2$, the root lattices D_4 for $d = 4$ and E_8 for $d = 8$ and the Leech lattice for $d = 24$.

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Recall that in the logarithmic case the constant exist.

Computing the expected energy

$K_L(x, y)$ reproducing kernel of the space of polynomials of degree at most L in $\mathbb{S}^d$

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with

$$K_L(x,y)=C_L P_L^{(1+\lambda,\lambda)}(\langle x,y\rangle),$$

then

$$\int_{\mathbb{S}^d}\frac{|K_L(x,N)|^2}{\|x-N\|^s}d\mu(x)=C_{L,s,d}\int_{-1}^{1}P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{\lambda-\frac{s}{2}}(1+t)^{\lambda}\,dt.$$

From Erdélyi-Magnus-Oberhettinger-Tricomi 54

Jacobi polynomials (cont'd) $m,\ n = 0,\ 1,\ 2,\ \ldots$

(20)	$\int_{-1}^{1} (1-x)^{\tau}(1+x)^{\beta} P_n^{(\alpha,\beta)}(x)\, P_m^{(\rho,\sigma)}(x)\, dx$ $= \dfrac{2^{\beta+\tau+1}\,\Gamma(\alpha-\tau+n)\,\Gamma(\beta+n+1)\,\Gamma(\rho+m+1)\,\Gamma(\tau+1)}{m!\,n!\,\Gamma(\rho+1)\,\Gamma(\alpha-\tau)\,\Gamma(\beta+\tau+n+2)}$ $\times\ {}_4F_3(-m, \rho+\sigma+m+1, \tau+1, \tau-\alpha+1; \rho+1, \beta+\tau+n+2, \tau-\alpha-n+1; 1)$ $\mathrm{Re}\,\beta > -1, \quad \mathrm{Re}\,\tau > -1$

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$$\times\ {}_4F_3(-m, \rho+\sigma+m+1, \tau+1, \tau-\alpha+1; \rho+1, \beta+\tau+n+2, \tau-\alpha-n+1; 1)$$

$\operatorname{Re}\beta > -1, \quad \operatorname{Re}\tau > -1$

For integer $p, q \geq 0$ and complex values a_i, b_j the **generalized hypergeometric function** is

$$ {}_pF_q(a_1, \ldots, a_p; b_1, \ldots, b_q; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n \ldots (a_p)_n}{(b_1)_n \ldots (b_q)_n} \frac{z^n}{n!}, $$

where $(\cdot)_n$ is the rising factorial or **Pochhammer symbol**

$$ (x)_n = \frac{\Gamma(x+n)}{\Gamma(x)}. $$

In our case for $n = \pi_L \sim L^d$ we get

$$ {}_4F_3\left(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d-\frac{s}{2}+L, -\frac{s}{2}-L; 1\right) $$

$$ = \sum_{k=0}^{L} \frac{(-L)_k (d+L)_k (\frac{d-s}{2})_k (-\frac{s}{2})_k}{(\frac{d}{2}+1)_k (d-\frac{s}{2}+L)_k (-\frac{s}{2}-L)_k} \frac{1}{k!}. $$

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When s is even

$$
\left(-\frac{s}{2}\right)_k = (-1)^k \left(\frac{s}{2}-k+1\right)_k = (-1)^k \frac{\Gamma\left(\frac{s}{2}+1\right)}{\Gamma\left(\frac{s}{2}-k+1\right)} = 0,
$$

if $k > s/2$.

We have

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and we get for $L \to \infty$ (for $\alpha \in \mathbb{R}$ $\Gamma(n+\alpha) \sim \Gamma(n) n^{\alpha}$)

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$$

$$
= {}_2F_1\left(\frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1; 1\right) = \frac{\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(1+s\right)}{\Gamma\left(1+\frac{s}{2}\right)\Gamma\left(1+\frac{d+s}{2}\right)},
$$

by Gauss theorem.

Theorem

Let $x = (x_1, \ldots, x_n)$ where $n = \pi_L$ be drawn from the harmonic ensemble. Then, for $0 < s < d$,

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The general case (and the limiting cases) are more difficult: we improve the constants or match the order (s=d).
For $d = 2$ the BHS conjecture is

$$\mathcal{E}(s,n) = V_s(\mathbb{S}^2)n^2 + \frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}n^{1+s/2} + o(n^{1+s/2}),$$

where $\zeta_{\Lambda_2}(s)$ is the zeta function of the triangular lattice (Dirichlet L-series).

d=2

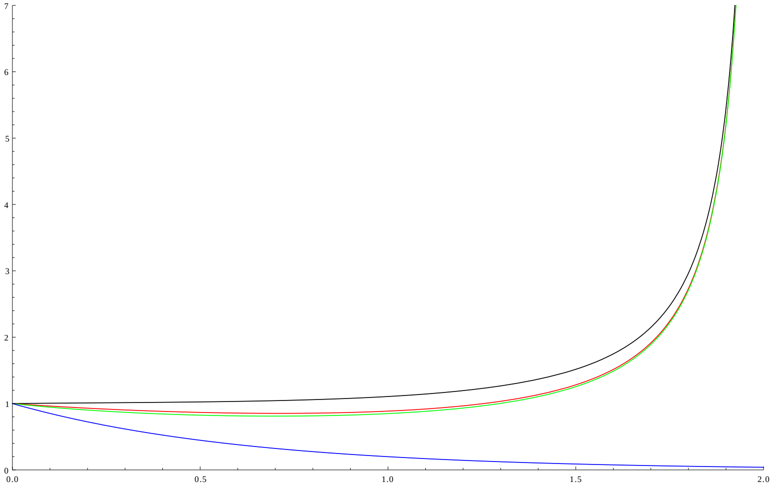

Figure : Graphic of $-\frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}$ in black, $2^{-s}\Gamma(1-\frac{s}{2})$ (spherical) in red, the constant $C_{s,2}$ (harmonic) in green and $1/(2\sqrt{2\pi})^s$ in blue.

Optimality

Could we find the best determinantal process? i.e. the kernel such that the expected energy is minimal?

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Theorem (Shirai-Takahashi)

In a determinantal process, the number of points that fall in a compact set $D \subset X$ has the same distribution as a sum of independent random variables Bernouilli(λ_i^D), where λ_i^D are the eigenvalues of the integral operator defined by the kernel $K(x, y)$ restricted to D.

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- We need that for any $x_1, \ldots, x_k \in \mathbb{S}^d$ the matrix

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  is nonegative definite (sphere version of Bochner theorem).
- If we want n points a.s. in $\mathbb{S}^d$ then all the eigenvalues must be 1 (projection kernel).

Schoenberg theorem (42)

We must have

$$K(x,y) = K(\langle x,y\rangle), \quad K(t) = \sum_{k=0}^{\infty} a_k C_k^{d/2-1/2}(t),$$

where $C_k^{d/2-1/2}$ is a Gegenbauer polynomial and the $a_k \in \left[0, \frac{2k+d-1}{d-1}\right]$ satisfy:

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To have a projection kernel with with n points we take

$$a_k \in \left\{0, \frac{2k+d-1}{d-1}\right\} \text{ with } \sum_{k=0}^{\infty} a_k \binom{d+k-2}{k} = n. \quad (*)$$

Theorem

For $s = 2$, $d \geq 3$ *and* $(a_0, a_1, a_2, \dots)$ *such that* $(*)$ *we have*

$$\mathbb{E}_{x \in (\mathbb{S}^d)^n}(E_2(x)) = V_2(\mathbb{S}^d) \left(n^2 - \sum_{\ell=0}^{\infty} a_\ell \binom{d+\ell-2}{\ell} \left(a_\ell + 2 \sum_{j>\ell} a_j \right) \right)$$

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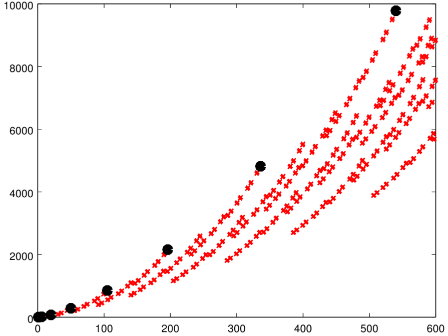

$d = 4$

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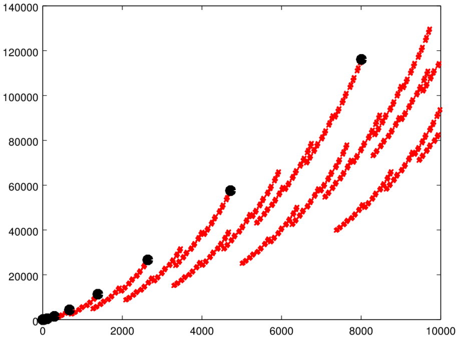

$d = 6$

Theorem

Let K_a and K_b be two kernels with coefficients $a = (a_0, a_1, \ldots)$ and $b = (b_0, b_1, \ldots)$ satifying conditions $(*)$. Let $\mathbb{E}_a$ and $\mathbb{E}_b$ denote respectively the expected value of

$$E_2(x) = \sum_{i \neq j} \frac{1}{\|x_i - x_j\|^2},$$

when $x = (x_1, \ldots, x_n)$ is given by the determinantal point process associated to K_a and K_b. Assume that for every $i, j \in \mathbb{N}$ we have:

$$\text{if } i < j, a_i = 0 \text{ and } a_j > 0 \text{ then } b_i = 0. \tag{1}$$

Then, $\mathbb{E}_a \leq \mathbb{E}_b$, with strict inequality unless $a = b$. In particular, the harmonic kernel is optimal since (1) is trivially satisfied in that case.

Example. The harmonic kernel is optimal ($d = 3$)

We have

$$n = \pi_L = \sum_{k=1}^{L+1} k^2 = \frac{(2L+3)(L+2)(L+1)}{6} \in \{5, 14, 30, 55, 91, 140 \ldots\}$$

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For example:

$$1{+}4{+}9{+}16{=}\mathbf{30}{=}1{+}4{+}25$$
$$1{+}4{+}9{+}16{+}25{+}36{=}\mathbf{91}{=}1{+}9{+}81$$

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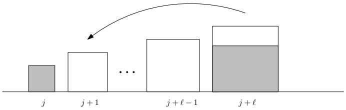

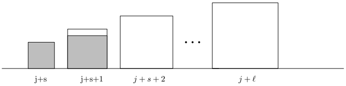

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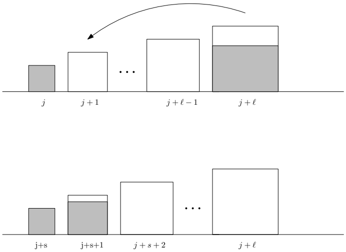

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