Computation of point sets on the sphere with good separation, covering or polarization

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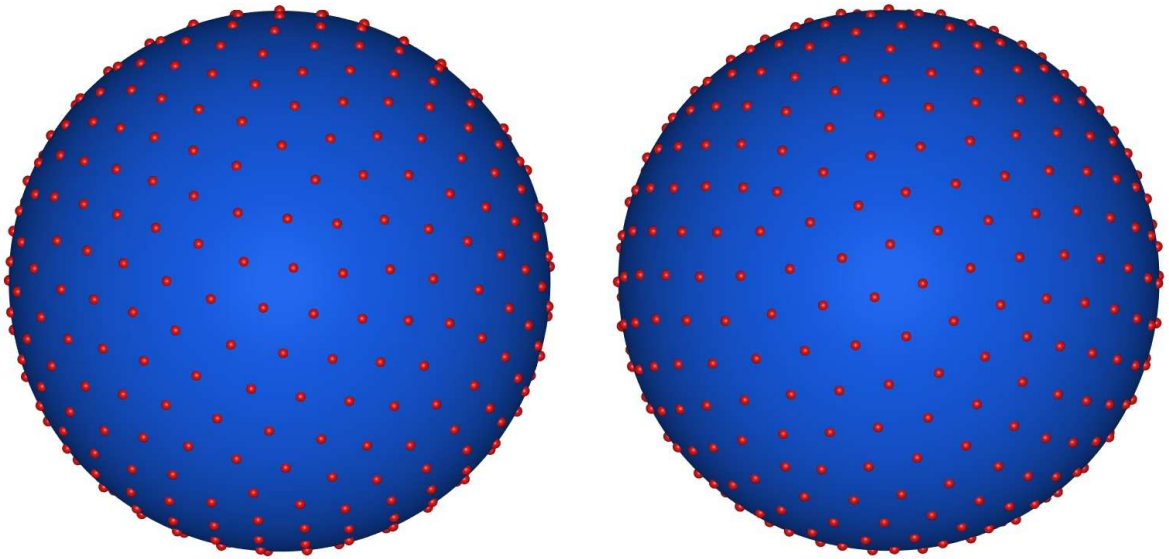


Good sets of 400 points for packing, covering $\mathbb{S}^2$

Outline

Unit sphere

Unit sphere

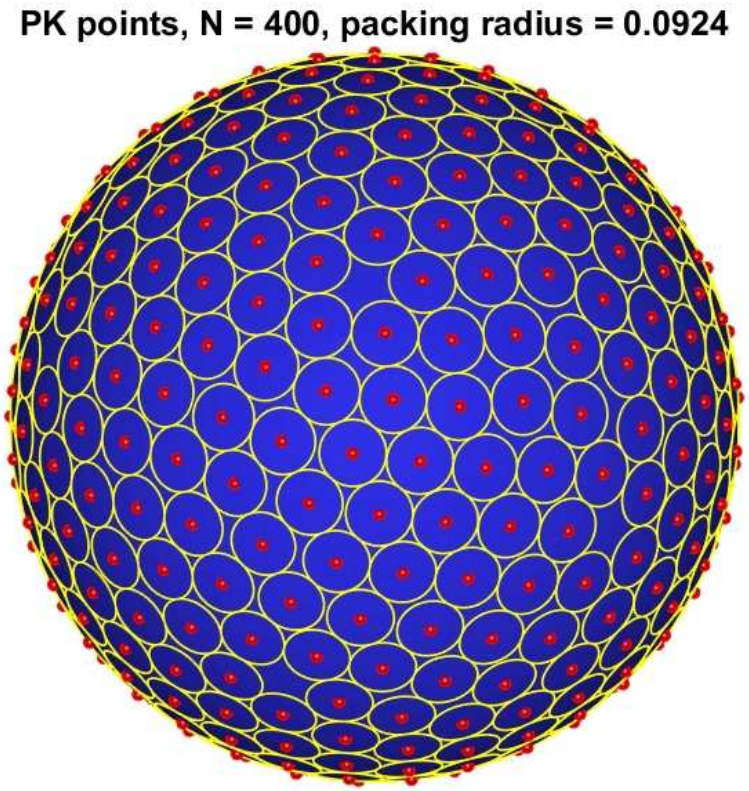
$$\mathbb{S}^d = \left\{ \boldsymbol{x} \in \mathbb{R}^{d+1} : |\boldsymbol{x}| = 1 \right\}$$

- Sets of distinct points $\mathcal{X}_N = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\} \subset \mathbb{S}^d$
  - $\boldsymbol{x} \cdot \boldsymbol{y} = \sum_{i=1}^{d+1} x_i y_i, \quad |\boldsymbol{x}|^2 = \boldsymbol{x} \cdot \boldsymbol{x}$
- Distance: : $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^d$
  - Euclidean distance $|\boldsymbol{x} - \boldsymbol{y}|^2 = 2(1 - \boldsymbol{x} \cdot \boldsymbol{y})$
  - Geodesic distance: $\text{dist}\,(\boldsymbol{x}, \boldsymbol{y}) = \arccos(\boldsymbol{x} \cdot \boldsymbol{y})$
  - $|\boldsymbol{x} - \boldsymbol{y}| = 2\sin(\text{dist}\,(\boldsymbol{x}, \boldsymbol{y})\,/2)$
- Spherical cap centre $\boldsymbol{z} \in \mathbb{S}^d$, radius α

$$\mathcal{C}\,(\boldsymbol{z}; \alpha) = \left\{ \boldsymbol{x} \in \mathbb{S}^d : \text{dist}\,(\boldsymbol{x}, \boldsymbol{z}) \leq \alpha \right\}$$

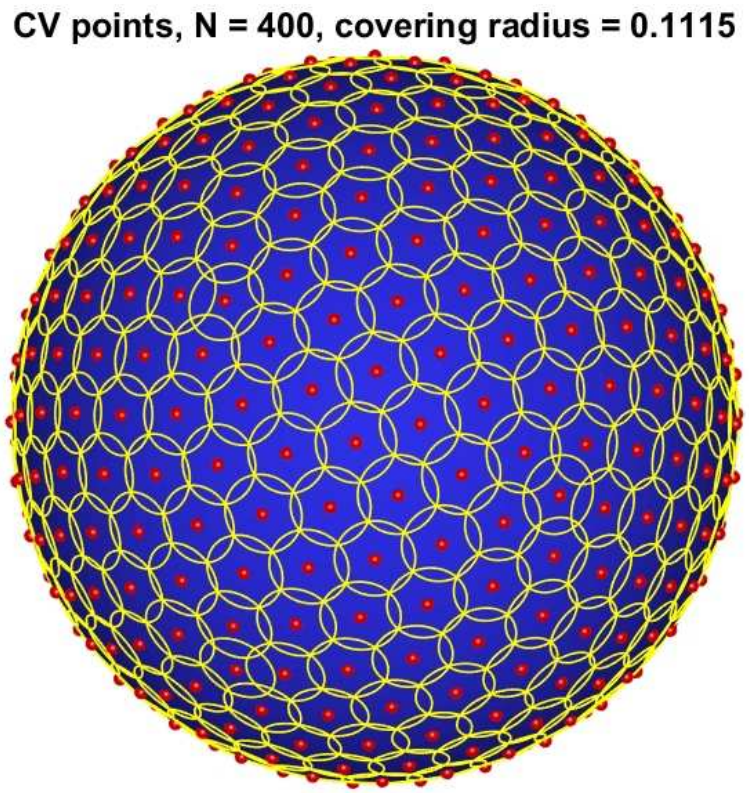
Packing/Separation

- Separation: $\delta(\mathcal{X}_N) := \min_{i \neq j} \text{dist}\,(\boldsymbol{x}_i, \boldsymbol{x}_j)$
- Packing radius $= \delta(\mathcal{X}_N)/2$
- Best packing: $\delta_N := \max_{\mathcal{X}_N \subset \mathbb{S}^d} \delta(\mathcal{X}_N) \sim c_d^{\text{sep}} N^{-1/d}$



Mesh norm/Covering radius/Fill radius

- Covering radius: $h(\mathcal{X}_N) := \max_{\boldsymbol{x}\in\mathbb{S}^d} \min_{j=1,\ldots,N} \operatorname{dist}(\boldsymbol{x}, \boldsymbol{x}_j)$
- Mesh ratio: $\rho(\mathcal{X}_N) := \frac{2h(\mathcal{X}_N)}{\delta(\mathcal{X}_N)} \geq 1$
- Best covering: $h_N := \min_{\mathcal{X}_N\subset\mathbb{S}^d} h(\mathcal{X}_N) \sim c_d^{\mathrm{cov}} N^{-1/d}$



Riesz energy and sums of distances

$$E(s;\mathcal{X}_N) = \begin{cases} \displaystyle\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^s} & \text{if } s \neq 0; \\ \displaystyle\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \log\frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}, & \text{if } s = 0. \end{cases}$$

$$\mathcal{E}_{s,N} = \begin{cases} \displaystyle\min_{\mathcal{X}_N\subset\mathbb{S}^d} E(s;\mathcal{X}_N) & s > 0; \\ \displaystyle\max_{\mathcal{X}_N\subset\mathbb{S}^d} E(s;\mathcal{X}_N) & s \leq 0. \end{cases}$$

- Asymptotics ($N \to \infty$) for $s = 0$ (Log), $0 < s < d$, $s = d$, $s > d$
- $s > d$ uniformly distributed
- As $s \to \infty$ get best packing (separation)
- Borodachov, Hardin & Saff monograph

Polarization

- Function

$$U_s(\boldsymbol{x}, \mathcal{X}_N) := \text{sign}(s) \sum_{j=1}^{N} \frac{1}{|\boldsymbol{x} - \boldsymbol{x}_j|^s}.$$

- Polarization

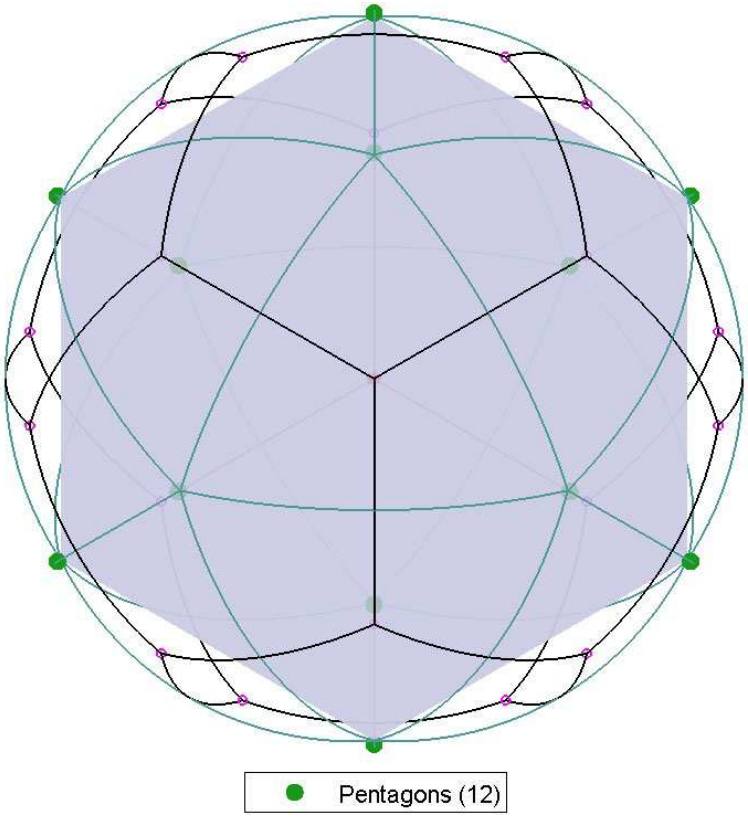
$$U_s^*(\mathcal{X}_N) = \min_{\boldsymbol{x} \in \mathbb{S}^d} U_s(\boldsymbol{x}, \mathcal{X}_N)$$

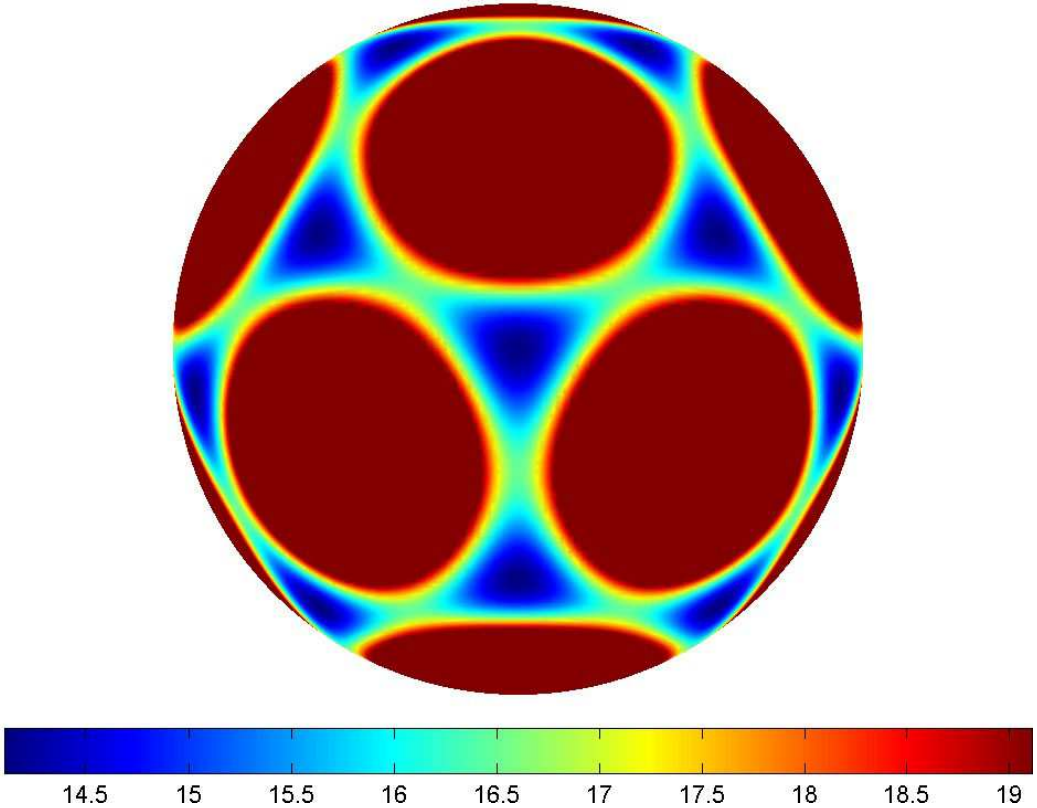
- Optimal set of N points $\mathcal{X}_N^*$ satisfy

$$M_{s,N} := \max_{\mathcal{X}_N \subset \mathbb{S}^d} U_s^*(\mathcal{X}_N) = \max_{\mathcal{X}_N \subset \mathbb{S}^d} \min_{\boldsymbol{x} \in \mathbb{S}^d} U_s(\boldsymbol{x}, \mathcal{X}_N).$$

- $M_{s,N} \geq \frac{\mathcal{E}_{s,N}}{N-1}$
- As $s \to \infty$ get best covering
- Erdélyi and Saff (2013), ..., Borodachov, Hardin & Saff monograph

Polarization N = 12, d = 2, s = 3



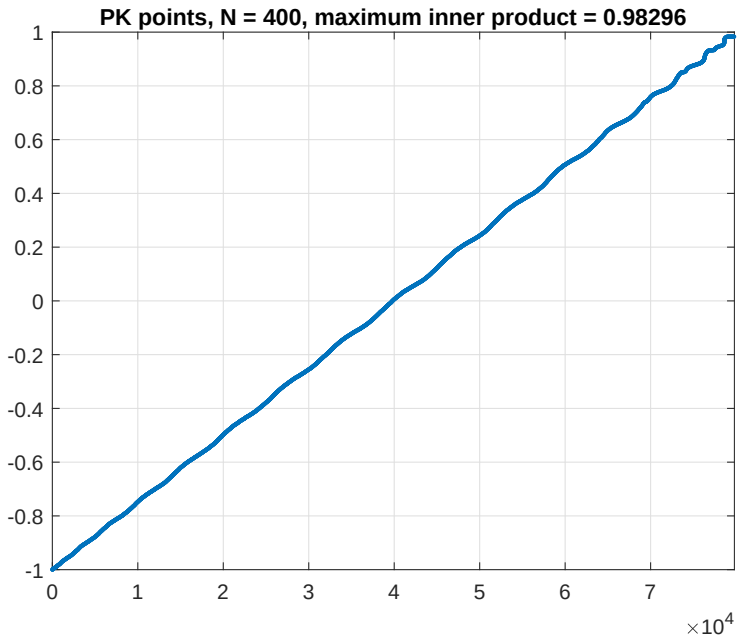


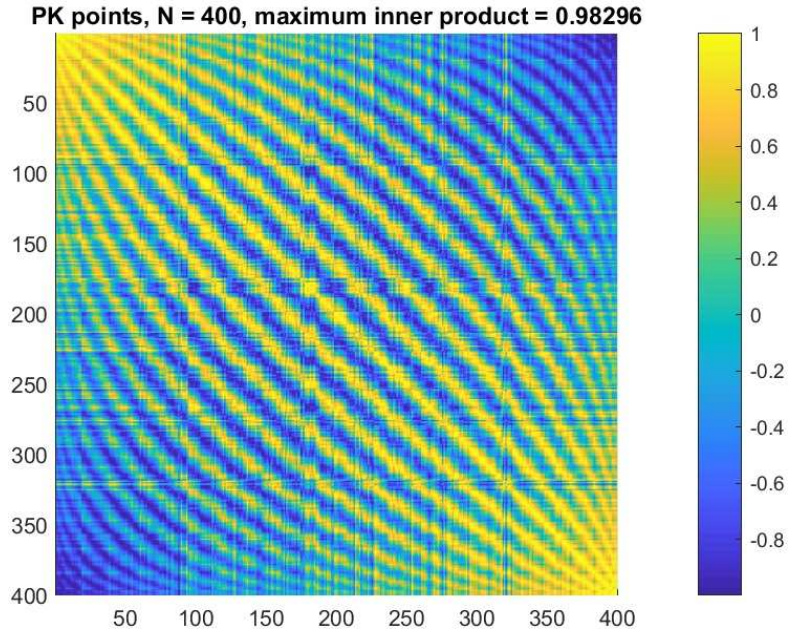
Parametrizations

- Criteria invariant under
  - rotation of point set
  - permutation of points
- Criteria depend only on
  - distance/angle/inner product between points, or
  - distance/angle/inner product with another point on $\mathbb{S}^d$
- Aim: always feasible $\mathcal{X}_N \subset \mathbb{S}^d$
- Spherical parametrization
  - For $\mathbb{S}^2$: polar angle $\theta \in [0, \pi]$, azimuthal angle $\phi \in [0, 2\pi)$
  - Derivative discontinuities at poles
  - Rotation to fix
    - first point at north pole ($\theta = 0$)
    - second point on prime meridian ($\phi = 0$)
  - Issues if using gradient differences to estimate second order information
- Minimax $\Longrightarrow$ derivative discontinuities/generalized gradients
  - eg. $|x| = \max(x, -x) = \min v \quad \text{s.t.} \quad v \geq x,\ v \geq -x$

Inner products

- Matrix of distinct points $X = [\boldsymbol{x}_1 \cdots \boldsymbol{x}_N] \in \mathbb{R}^{d+1 \times N}$
- Set $\mathcal{A}(\mathcal{X}_N) = \{z = \boldsymbol{x}_i \cdot \boldsymbol{x}_j \in [-1, 1), j > i\}, \quad |\mathcal{A}(\mathcal{X}_N)| \leq \frac{N(N-1)}{2}$
  - Best packing: $\min\limits_{\mathcal{X}_N \subset \mathbb{S}^d} \max\limits_{i \neq j} \boldsymbol{x}_i \cdot \boldsymbol{x}_j$
- Matrix of inner products $Z = X^T X \in \mathbb{R}^{N \times N}$
  - Z is symmetric, positive semi-definite $X \succeq 0 \implies$ SDP
  - $\text{diag}(Z) = \boldsymbol{e}$ where $\boldsymbol{e} = (1, \ldots, 1)^T \in \mathbb{R}^{d+1}$
  - $\text{rank}(Z) = d + 1 \implies$ fixed (low) rank correlation matrix





Best packing

- Best packing

$$\min_{\mathcal{X}_N \subset \mathbb{S}^d} \max_{i \neq j} \boldsymbol{x}_i \cdot \boldsymbol{x}_j$$

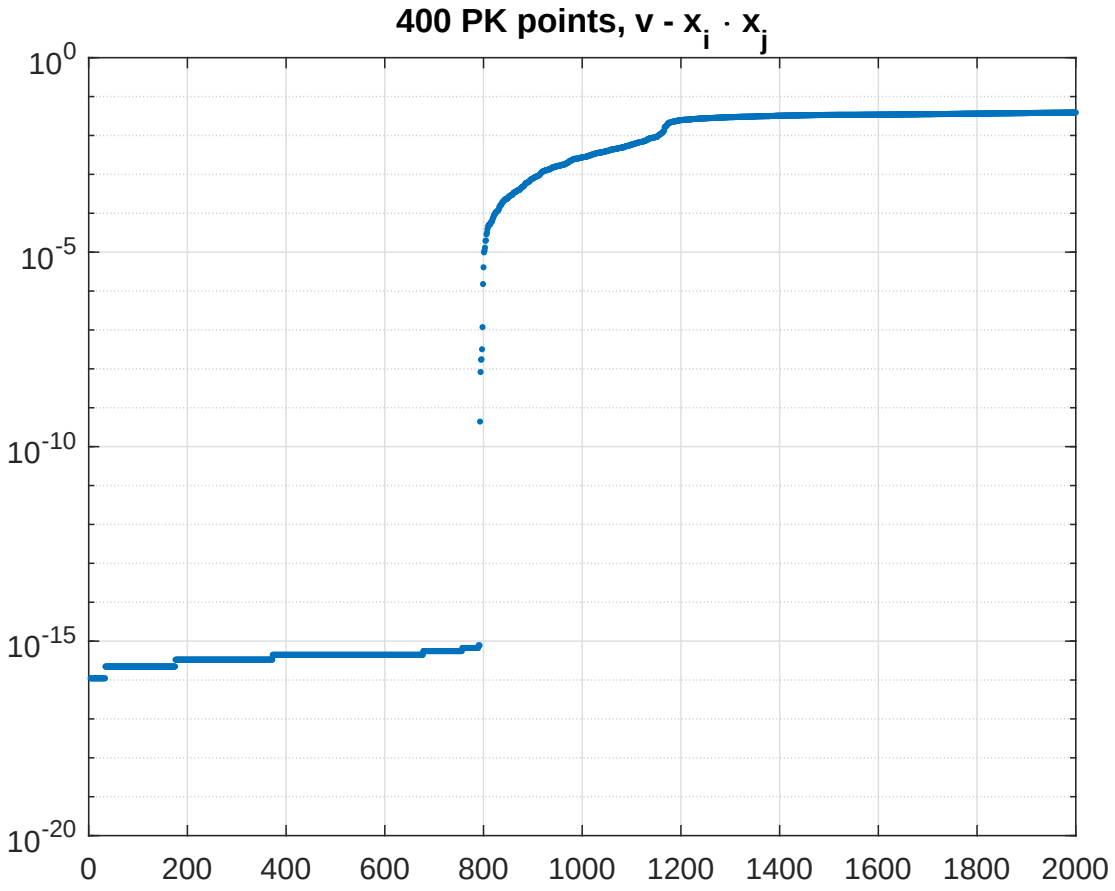
  - Finite minimax problem: convert to

$$\begin{array}{ll} \text{Minimize} & v \\ \mathcal{X}_N \subset \mathbb{S}^d & \\ \text{Subject to} & v \geq \boldsymbol{x}_i \cdot \boldsymbol{x}_j, \quad 1 \leq i < j \leq N \end{array}$$

  - Number of variables $n = Nd - \frac{d(d+1)}{2}$
  - Vertex solution/strongly unique local minimum
    - $n+1$ active constraints/inner products achieving max
    - Positive Lagrange multipliers for active constraints/0 in interior of generalized gradient
  - Fewer active constraints $\Longrightarrow$ curvature critical
  - More active constraints $\Longrightarrow$ degeneracy

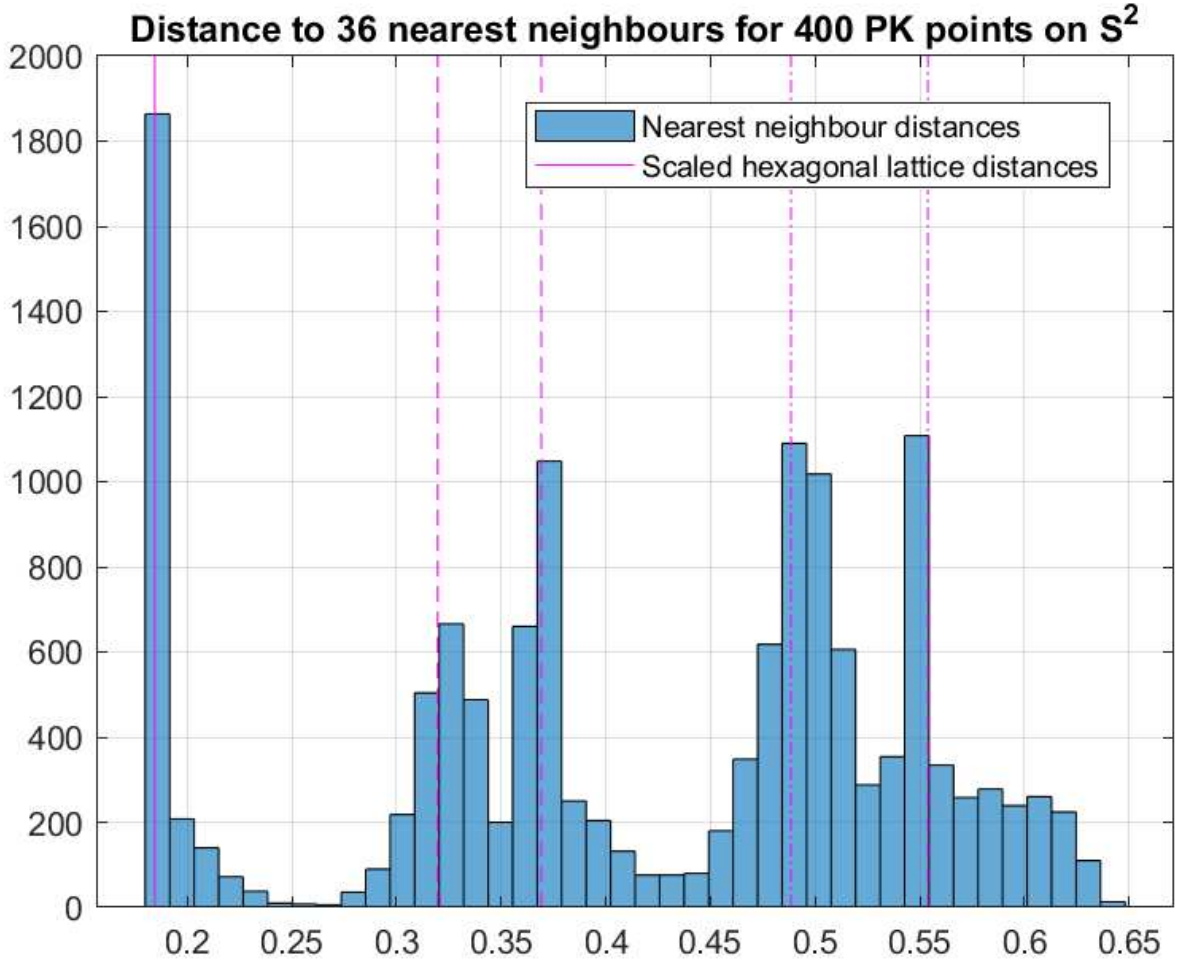
Largest inner products

- PK points on $\mathbb{S}^2$, $N = 400$, Number of variables $n = 797$
- Number active inner products: $\boldsymbol{x}_i \cdot \boldsymbol{x}_j > v - \epsilon$
  $\epsilon = 10^{-15} \Longrightarrow 792$, $\epsilon = 10^{-6} \Longrightarrow 798$, $\epsilon = 10^{-5} \Longrightarrow 801$



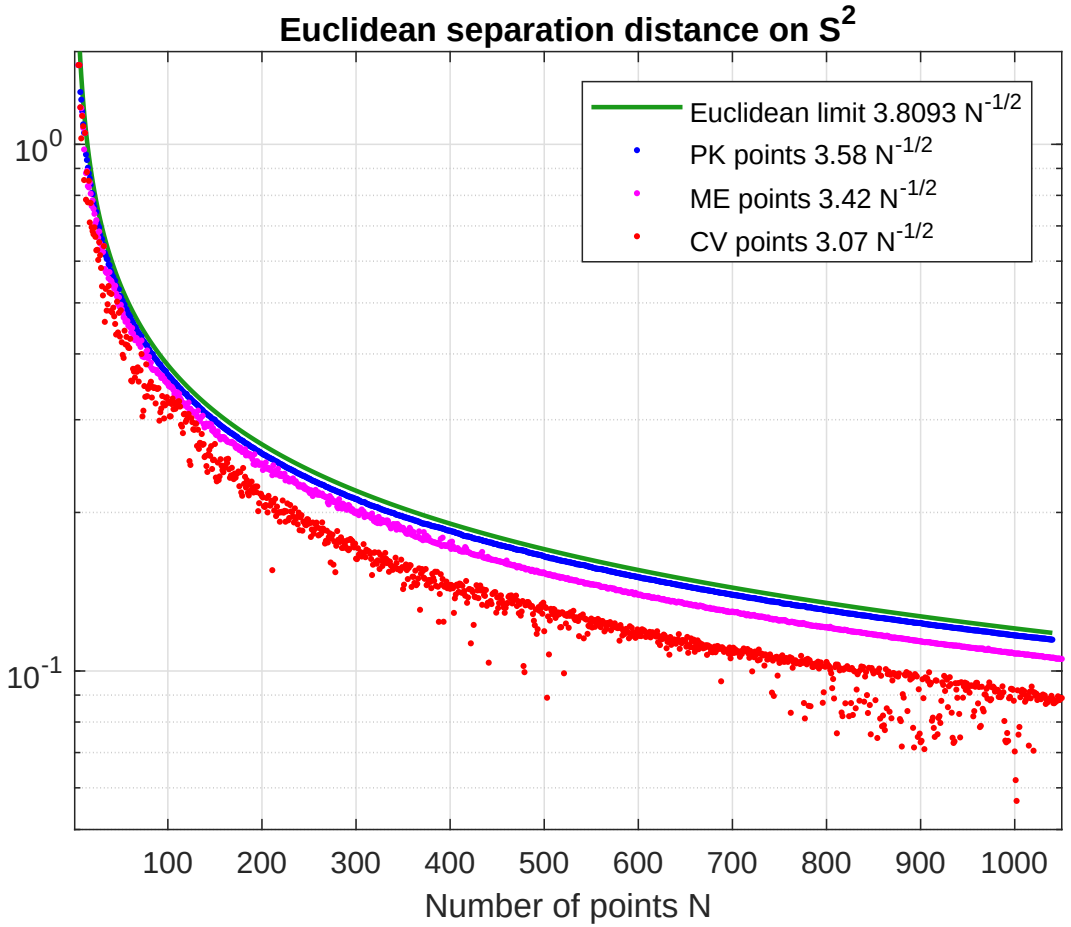
Nearest neighbour distances

- PK points on $\mathbb{S}^2$, $N = 400$



Good separation for $N = 4, ..., 1050$

- PK points: Good packing
- ME points: Low Riesz $s = 1$ (Coulomb) energy (Kuijlaars, Saff, Sun, 2007)
- CV points: Good covering



Best covering

- Best covering

$$\max_{\mathcal{X}_N \subset \mathbb{S}^d} \min_{\boldsymbol{x} \in \mathbb{S}^d} \max_{j=1,\ldots,N} \boldsymbol{x} \cdot \boldsymbol{x}_j$$

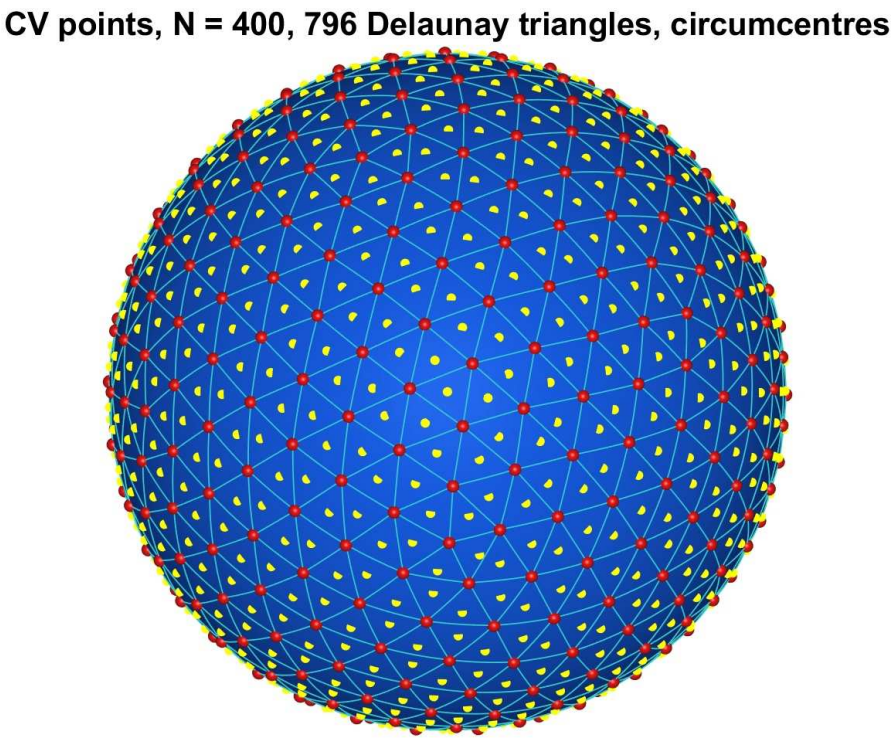
  - Continuous maximin problem: convert to finite problem
  - Facets $\mathcal{F}(\mathcal{X}_N)$ of convex hull of $\mathcal{X}_N$
    - Facet $F \in \mathcal{F}(\mathcal{X}_N) \Longrightarrow$ set of $d+1$ elements of $\{1, \ldots, N\}$
    - $2N-4$ Delaunay triangles for $\mathcal{X}_N \subset \mathbb{S}^2$
  - Circumcentres $\boldsymbol{c}(F)$ of facet $F \in \mathcal{F}(\mathcal{X}_N)$
    - $\boldsymbol{c}(F)$ equidistant from $d+1$ vertices determining facet F
    - Solve $B\boldsymbol{u} = \boldsymbol{e}, \quad B = [\boldsymbol{x}_i^T, i \in F], \quad \boldsymbol{e} = (1, \ldots, 1)^T \in \mathbb{R}^{d+1}$
    - $\Longrightarrow z(F) = 1/\|\boldsymbol{u}\|_2, \quad \boldsymbol{c}(F) = z(F)\boldsymbol{u}$
- Best covering: Finite maximin problem

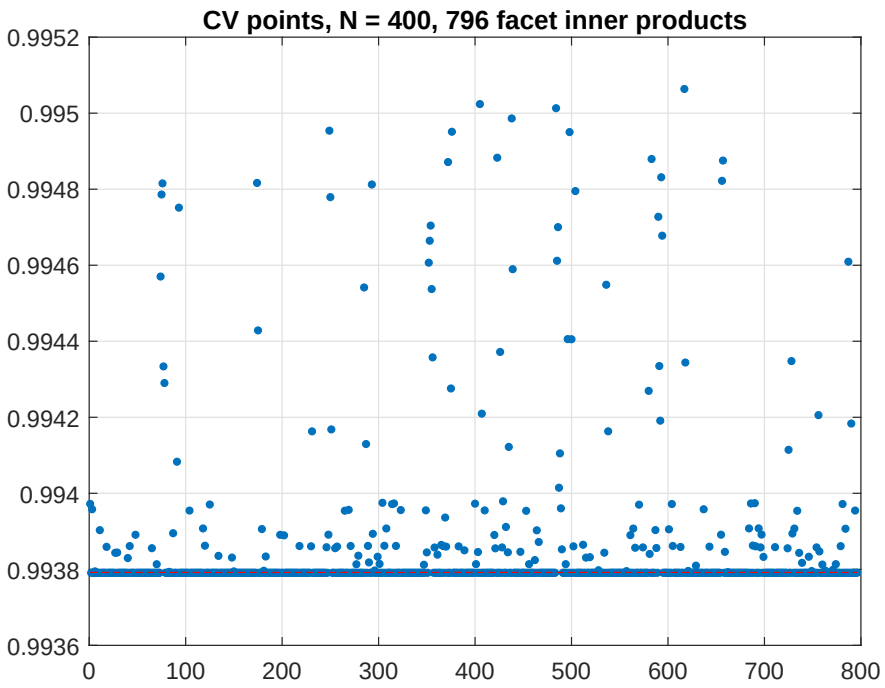
$$\max_{\mathcal{X}_N \subset \mathbb{S}^d} \min_{F \in \mathcal{F}(\mathcal{X}_N)} z(F)$$

  - where $z(F) = \boldsymbol{c}(F) \cdot \boldsymbol{x}_j$ for each $j \in F$
  - small changes in $\mathcal{X}_N$ can change set of facets $\mathcal{F}(\mathcal{X}_N)$ (eg. square)

Circumcentres

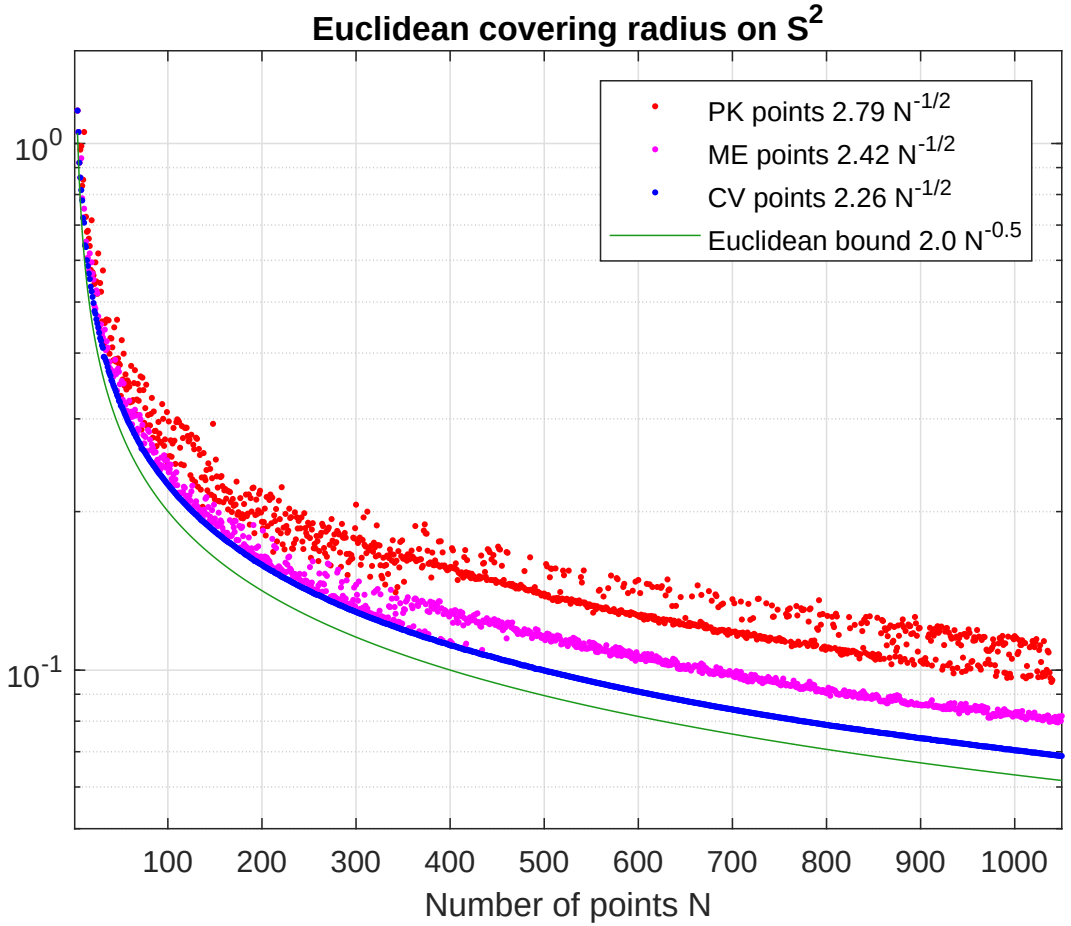
- CV points on $\mathbb{S}^2$, $N = 400$
  - $2N - 4 = 796$ facets F (Delaunay triangles)
  - 604 facets within 10^{-6} of minimum inner product





Good Covering for $N = 4, ..., 1050$

- PK points: Good packing
- ME points: Low Riesz $s = 1$ (Coulomb) energy (Damelin, Maymeskul, 2005)
- CV points: Good covering



Consistency checks

- Separation/Packing
  - If you remove one of the points achieving the minimum separation, the separation cannot get worse
  - $\delta_{N-1} \geq \delta_N$
- Covering/Mesh norm
  - If you add a point at the circumcentre of one of the facets achieving the maximum distance (deep hole) then covering radius cannot get worse
  - $h_{N+1} \leq h_N$
- Only (good) local optima; no guarantee of global optimality
  - Try a variety of starting point sets
  - Try starting from a point set obtained by deleting/adding a point
  - Try starting from local perturbations of a point set
  - Points sets with special structure (symmetry) hard to find
  - ...

Best polarization

- Optimal polarization, parameter $s > 0$

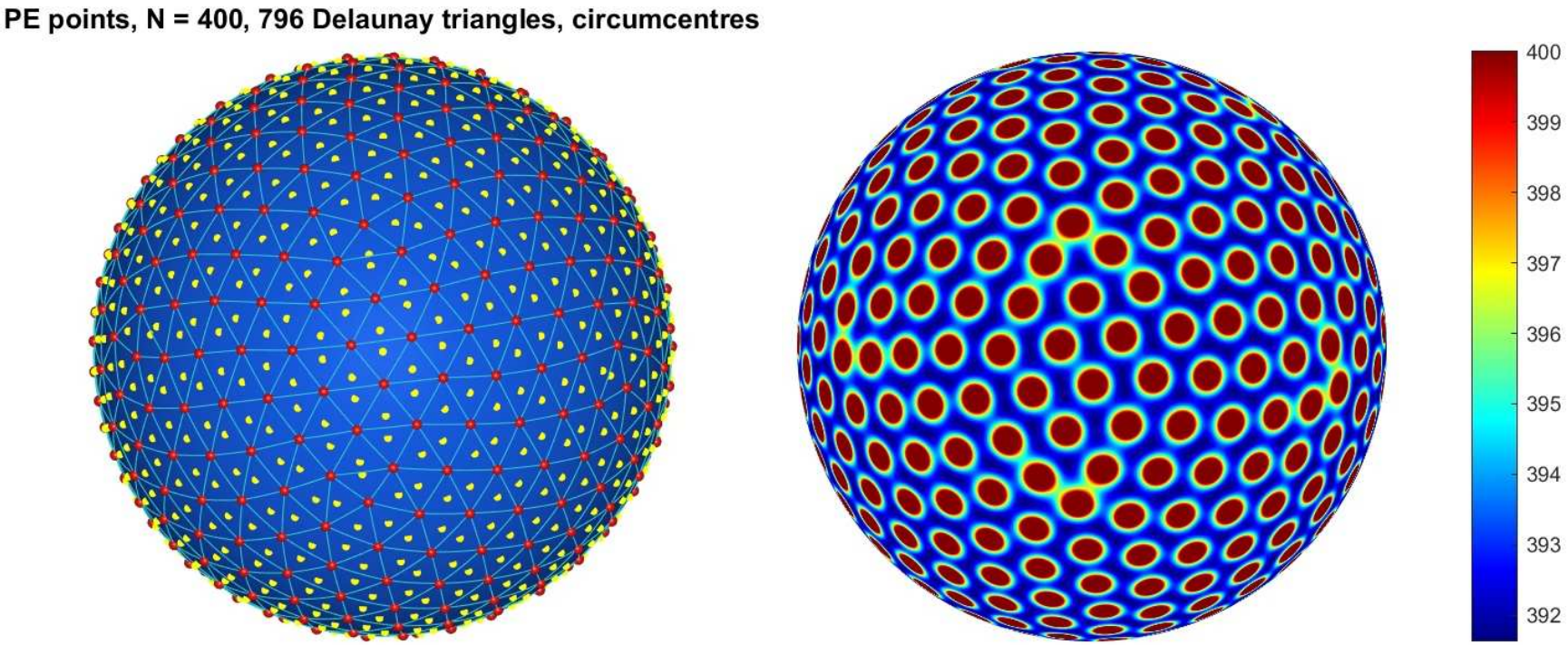
$$\max_{\mathcal{X}_N \subset \mathbb{S}^d} \min_{\boldsymbol{x} \in \mathbb{S}^d} \sum_{j=1}^{N} \frac{1}{|\boldsymbol{x} - \boldsymbol{x}_j|^s}$$

  - Continuous maximin problem: convert to finite problem
  - Find all local minimizers $\boldsymbol{x}$ achieving (close to) global minimum $U_s^*(\mathcal{X}_N)$ of $U_s(\boldsymbol{x}, \mathcal{X}_N) := \sum_{j=1}^{N} \frac{1}{|\boldsymbol{x}-\boldsymbol{x}_j|^s}$
  - Assumption: Local minimizers achieving global minimum satisfy second order sufficient conditions, so are isolated
  - Finite set $\mathcal{M}_s(\mathcal{X}_N) = \{\boldsymbol{x}^* \in \mathbb{S}^d : U_s(\boldsymbol{x}^*, \mathcal{X}_N) = U_s^*(\mathcal{X}_N)\}$
  - Finite maximin problem

$$\begin{array}{ll} \text{Maximize} & v \\ \mathcal{X}_N \subset \mathbb{S}^d & \\ \text{Subject to} & v \leq U_s(\boldsymbol{x}^*, \mathcal{X}_N) \quad \text{for } \boldsymbol{x}^* \in \mathcal{M}_s(\mathcal{X}_N) \end{array}$$

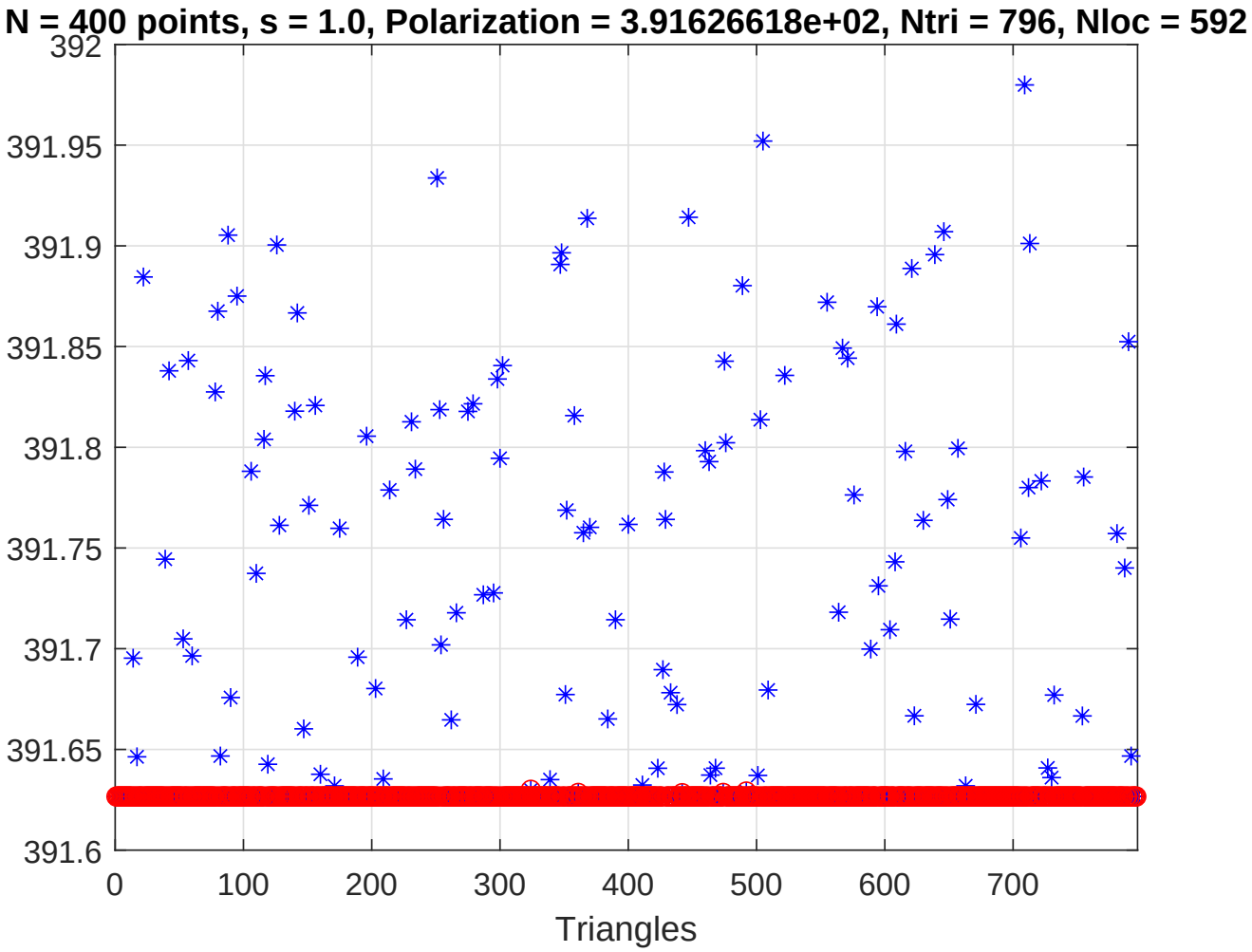
PE points, local minima

- PE points: Good polarization, $N = 400$

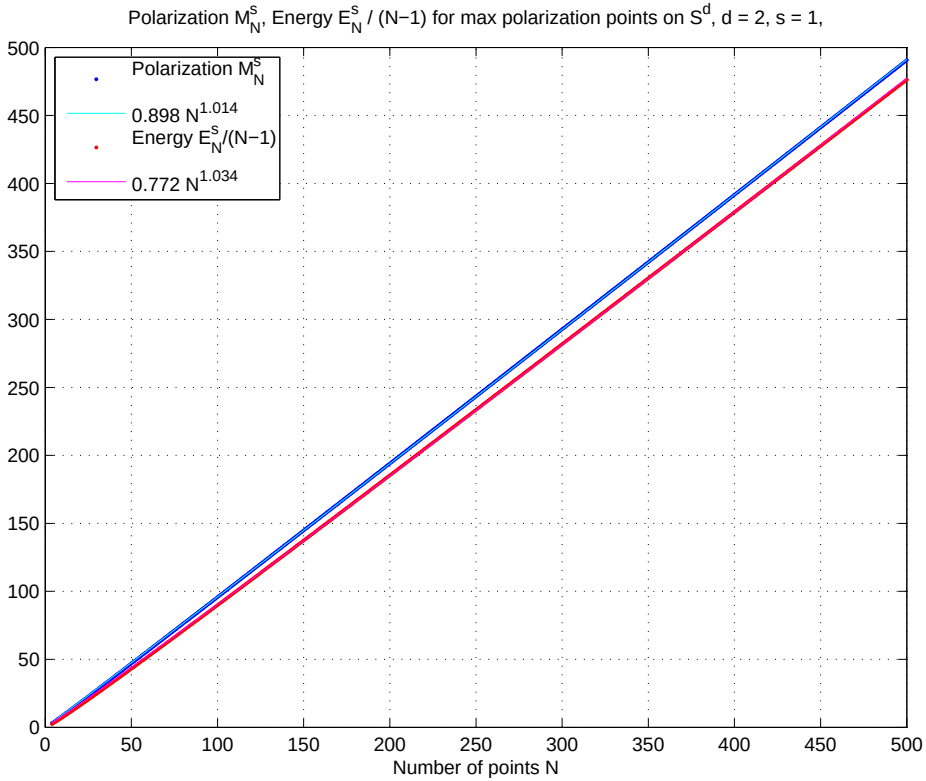


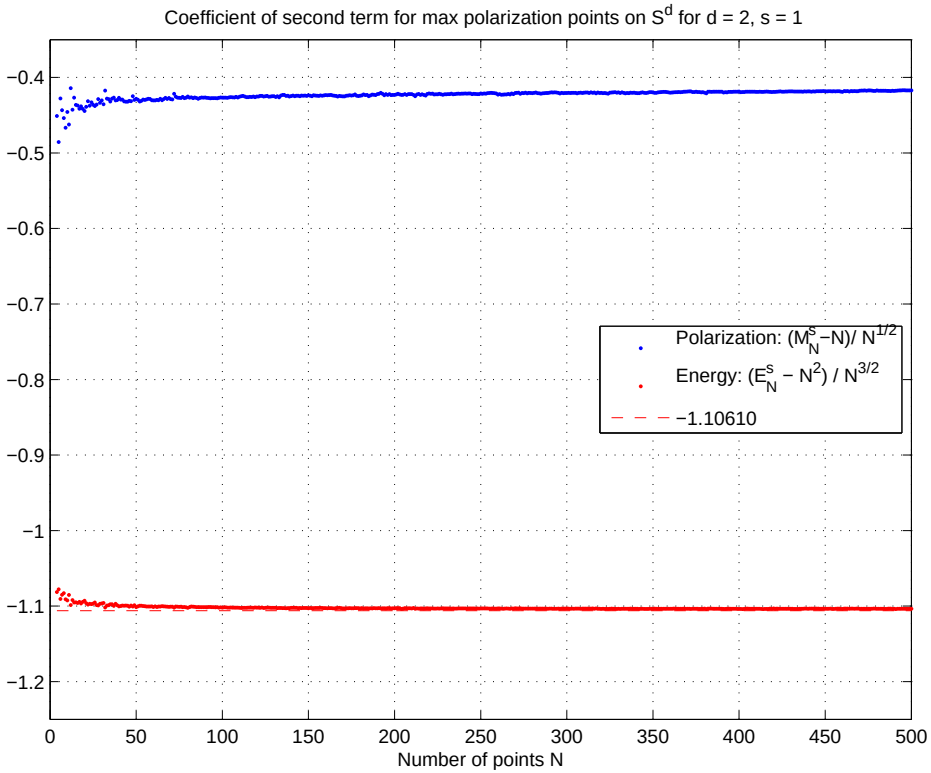
PE points, active local minima

- PE points: Good polarization, $N = 400$

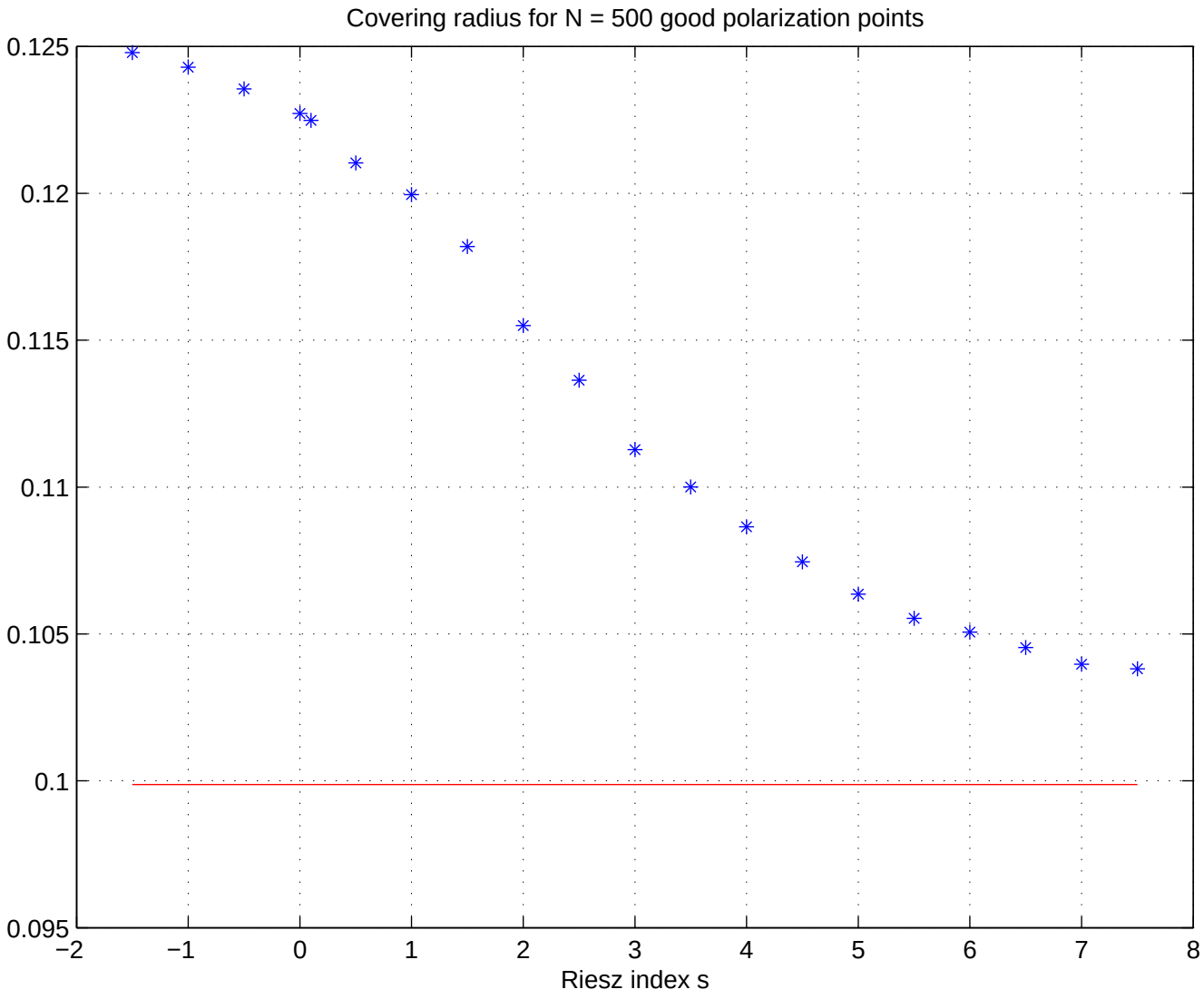


Good polarization $s = 1$, $N = 4, \ldots, 500$





Good polarization for increasing s



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Thank You