MINIMAL N-POINT DIAMETERS AND f-BEST-PACKING CONSTANTS IN $\mathbb{R}^d$

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Abstract. In terms of the minimal N-point diameter for $\mathbb{R}^d$, we determine, for a class of continuous real-valued functions f on $[0,+\infty]$, the N-point f-best-packing constant $\min\{f(\|x-y\|) : x,y \in \mathbb{R}^d\}$, where the minimum is taken over point sets of cardinality N. We also obtain asymptotic results (as $N \to \infty$) for this minimal diameter as well as for the f-best-packing constants.

Let f be a non-negative function on $[0,\infty)$ and $\omega_N = \{x_1, x_2, \ldots, x_N\}$ a collection of N distinct points in Euclidean space $\mathbb{R}^d$. Set

$$\delta_d^{\omega_N}(f) := \min_{\substack{x,y\in\omega_N \\ x\neq y}} f(\|x-y\|),$$

where $\|\cdot\|$ denotes the Euclidean norm. In this article we investigate the *N-point f-best-packing constant*

$$\delta_d(N;f) := \sup_{\substack{\omega_N\subset\mathbb{R}^d \\ \#\omega_N=N}} \delta_d^{\omega_N}(f) = \sup_{\substack{\omega_N\subset\mathbb{R}^d \\ \#\omega_N=N}} \min_{\substack{x,y\in\omega_N \\ x\neq y}} f(\|x-y\|), \tag{1}$$

where $\#A$ denotes the cardinality of a set A. A collection of N points $\omega_N^* \subset \mathbb{R}^d$ is said to be an *N-point f-best-packing configuration* if $\delta_d^{\omega_N^*}(f) = \delta_d(N;f)$.

The classical best-packing problem is the problem of finding a configuration of N points on a given compact set A with the largest minimal pairwise distance. Formulated for the Euclidean space $\mathbb{R}^d$ this becomes the asymptotic problem of finding the largest density of an infinite collection of non-overlapping equal balls in $\mathbb{R}^d$ (see e.g. [3], [7]). We denote this *maximal sphere packing density in* $\mathbb{R}^d$ by Δ_d; e.g. $\Delta_1 = 1$, $\Delta_2 = \pi/\sqrt{12}$ (cf. [9]) and $\Delta_3 = \pi/\sqrt{18}$ (cf. [10]).

As a natural extension, the asymptotics of certain *weighted* best-packing problems on compact sets are investigated in [5]. Here we consider such problems for

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a certain class $\mathcal{A}$ of functions f defined on all of $\mathbb{R}^d$ for fixed N (see Theorem 1) as well as provide asymptotic results (as $N \to \infty$) in Corollaries 2 and 3. For example, for Gaussian weighted best-packing on $\mathbb{R}^2$, i.e, $f(t) = t\exp(-t^2)$, our results yield in particular for $N = 7$ that $\delta_2(7; f) = 2^{-1/3}((1/3)\log 2)^{1/2}$ and, furthermore,

$$\delta_2(N; f) \sim \left(\frac{\Delta_2}{N}\right)^{(\frac{N}{\Delta_2}-1)/2} \left(\frac{N}{\Delta_2} - 1\right)^{1/2} \left(\frac{1}{2}\log\frac{N}{\Delta_2}\right)^{1/2}, \quad N \to \infty. \tag{2}$$

An important role in our investigation is played by the quantity

$$D_d(N) := \min_{x_1,\ldots,x_N \in \mathbb{R}^d} \left\{ \frac{\max_{i\neq j} \|x_i - x_j\|}{\min_{k\neq \ell} \|x_k - x_\ell\|} \right\}, \tag{3}$$

which is called the *minimal N-point diameter for* $\mathbb{R}^d$. That the minimum of the ratio in (3) is attained may be seen using a scaling argument. Clearly, $D_1(N) = N-1$ for each $N \geq 2$. For $d = 2$, the exact values of $D_2(N)$ are known (cf. [1],[2]) for N up to 8, and asymptotically there holds

$$D_2(N) = (N/\Delta_2)^{1/2} + O(1) \quad \text{as } N \to \infty. \tag{4}$$

Furthermore, it is shown by A. Schürmann in [12] that for N sufficiently large, optimal configurations for $D_2(N)$ are (somewhat surprisingly) always non-lattice packings, as conjectured by P. Erdös.

In comparison with (4) whose proof relies on results of [9] that are special for the plane, we show in Theorem 2 that for all $d > 2$ we have $D_d(N) \sim (N/\Delta_d)^{1/d}$ as $N \to \infty$.

Our first theorem applies to the class $\mathcal{A}$ of functions $f \in C([0,\infty))$ such that $f(0) = 0$, $f(t) > 0$ for $t > 0$, $\lim_{t\to\infty} f(t) = 0$, and such that there exist positive numbers ε, M ($\varepsilon \leq M$) with the properties that f is strictly increasing on $[0,\varepsilon]$ and is strictly decreasing on $[M,\infty)$. We may assume, without loss of generality, that, for $f \in \mathcal{A}$, the parameters ε and M in the above definition further satisfy

$$f(\varepsilon) = f(M) = \min_{t\in[\varepsilon,M]} f(t). \tag{5}$$

Lemma 1. *Suppose $f \in \mathcal{A}$ with parameters ε and M that satisfy* (5). *If $\alpha > M/\varepsilon$, then there is a unique positive solution $t = \tau(\alpha)$ to the equation*

$$f(t) = f(\alpha t). \tag{6}$$

Furthermore, $\tau(\alpha) \in (M/\alpha, \varepsilon)$.

Proof. Consider $g(t) := f(\alpha t) - f(t)$ for $t \geq 0$. Since $M/\alpha < \varepsilon$, $f(\alpha t)$ is decreasing for $t \in [M/\alpha, \infty)$. Furthermore, since f is increasing on $[0,\varepsilon]$, it easily follows that g is (strictly) decreasing on $[M/\alpha, \varepsilon]$ and that

$$g(M/\alpha) = f(M) - f(M/\alpha) = f(\varepsilon) - f(M/\alpha) > 0.$$

We also have

$$g(\varepsilon) = f(\alpha\varepsilon) - f(\varepsilon) < f(M) - f(\varepsilon) = 0$$

since f is decreasing on $[M,\infty)$ and $\alpha\varepsilon > M$. Hence, g has exactly one zero in $(M/\alpha,\varepsilon)$, or equivalently, (6) has exactly one solution $t=\tau(\alpha)\in(M/\alpha,\varepsilon)$.

If $t\geq M$, then $f(\alpha t)<f(t)$ since f is increasing on $[M,\infty)$. If $\varepsilon\leq t\leq M$, then $f(t)\geq f(M)>f(\alpha t)$ since $\alpha t\geq\alpha\varepsilon>M$. Therefore, there are no values of $t\geq\varepsilon$ that satisfy (6). A similar analysis shows that (6) has no solutions in $(0,M/\alpha]$ and so $t=\tau(\alpha)$ is the unique solution of (6) for $t>0$. □

Our first main result is the following:

Theorem 1. *Let $f\in\mathcal{A}$ with parameters ε and M that satisfy* (5)*. Let N_0 be such that $D_d(N)>M/\varepsilon$ for $N>N_0$ and $t_N=\tau(D_d(N))$ denote the unique value of $t>0$ such that*

$$f(t)=f(D_d(N)t). \tag{7}$$

Then

$$\delta_d(N;f)=f(t_N),\qquad N>N_0. \tag{8}$$

Moreover, a collection of $N(>N_0)$ distinct points $\omega_N=\{x_k\}_{k=1}^N\subset\mathbb{R}^d$ is an N-point f-best-packing configuration if and only if

$$\min_{\substack{x,y\in\omega_N\\ x\neq y}}\|x-y\|=t_N \text{ and } \operatorname{diam}(\omega_N)=t_ND_d(N). \tag{9}$$

Proof. Let $N>N_0$ and let $\omega_N=\{x_k\}_{k=1}^N$ be a collection of N points in $\mathbb{R}^d$ such that $\min_{i\neq j}\|x_i-x_j\|=t_N$ and $\operatorname{diam}(\omega_N)=t_ND_d(N)$. Then

$$t_N\leq\|x_i-x_j\|\leq t_ND_d(N),\qquad (i\neq j). \tag{10}$$

By Lemma 1, we have $t_N<\varepsilon$ and $t_ND_d(N)>M$. From (5), the definition of t_N and the monotonicity properties of f we have

$$f(t_N)=\min_{t\in[t_N,t_ND_d(N)]}f(t)$$

which, together with (10) implies that $f(\|x_i-x_j\|)\geq f(t_N)$ for all i,j $(i\neq j)$. Since $\|x_i-x_j\|=t_N$ for some pair i,j $(i\neq j)$, we have

$$\delta_d^{\omega_N}(f)=\min_{i\neq j}f(\|x_i-x_j\|)=f(t_N)$$

and so $\delta_d(N;f)\geq f(t_N)$.

Let $\tilde{\omega}_N=\{y_k\mid k=1,\ldots,N\}$ denote an arbitrary N-point configuration in $\mathbb{R}^d$ and let $\bar{t}:=\min_{i\neq j}\|y_i-y_j\|$. Since f is increasing on $[0,\varepsilon]$ and $t_N\leq\varepsilon$, we have $\delta_d^{\tilde{\omega}_N}(f)<f(t_N)$ if $\bar{t}<t_N$, i.e. the configuration $\tilde{\omega}_N$ is not optimal. On the other hand, if $\bar{t}\geq t_N$, then diam $(\tilde{\omega}_N)\geq D_d(N)\bar{t}\geq D_d(N)t_N$ and so there must be some i,j such that $\|y_i-y_j\|\geq D_d(N)\bar{t}$. Hence, $\delta_d^{\tilde{\omega}_N}(f)\leq f(D_d(N)t_N)=f(t_N)$ with equality if and only if both $\bar{t}=t_N$ and diam $\omega_N^*=D_d(N)t_N$. Therefore, $\delta_d(N;f)=f(t_N)$ and a configuration is optimal if and only if the conditions (9) hold. □

For the sake of illustration, consider the function $f_{p,q} \in \mathcal{A}$ defined by $f_{p,q}(t) = t^p$ if $0 \le t \le 1$ and $f_{p,q}(t) = t^{-q}$ if $t > 1$ where $p, q > 0$ satisfy $1/p + 1/q = 1$. The unique solution of (6) is $\tau(\alpha) = \alpha^{-q/(p+q)}$ for $\alpha > 1$. Then $f_{p,q}(\tau(\alpha)) = 1/\alpha$ and, by Theorem 1,

$$\delta_d(N; f_{p,q}) = 1/D_d(N) = \max_{x_1,\ldots,x_N \in \mathbb{R}^d} \left\{ \frac{\min_{k\neq\ell} \|x_k - x_\ell\|}{\max_{i\neq j} \|x_i - x_j\|} \right\}. \tag{11}$$

On letting $p \to 1$ and $q \to \infty$, $f_{p,q}$ tends to $f_{1,\infty}$ where $f_{1,\infty}(t) = t$ for $0 \le t \le 1$ and $f_{1,\infty}(t) = 0$ for $t > 1$ for which the equality in (11) is apparent from the definitions of these quantities.

For the case $d = 1$, we have $D_1(N) = N - 1$ and any configuration of N points that attains $D_1(N)$ in (3) for $N \ge 2$ must be of the form $\{ck + b \,|\, k = 0, \ldots, N-1\}$ for any fixed constants b and $c \neq 0$. We thus obtain the following.

Corollary 1. *Let $f \in \mathcal{A}$ and $d = 1$. Let $\tau_N = \tau(N-1)$ be the unique solution of equation (6) with $\alpha = N - 1 > M/\varepsilon$. Then $\delta_1(N; f) = f(t_N)$ and any f-best-packing configuration is of the form $\{t_N k + b \,|\, k = 0, \ldots, N-1\}$ for some constant b.*

For example if $f(t) = t\exp(-t^\beta)$, $\beta > 0$, we can take $\varepsilon = M = \beta^{-1/\beta}$ and we deduce that for $d = 1$ and $N > 2$,

$$t_N = \left[\frac{\log(N-1)}{(N-1)^\beta - 1} \right]^{1/\beta}$$

and

$$\delta_1(N; f) = \left[\frac{\log(N-1)}{(N-1)^\beta - 1} \right]^{1/\beta} (N-1)^{-1/[(N-1)^\beta - 1]}$$

with an optimal configuration $\omega_N = \{t_N k\}_{k=0}^{N-1}$. (For $N = 2$, we find $\delta_1(2; f) = \beta^{-1/\beta}\exp(-1/\beta)$ with an optimal configuration being $\{0, \beta^{1/\beta}\}$.)

We remark that for the Gaussian weighted problem mentioned earlier, the computation of $\delta_2(7; f)$ follows easily from Theorem 1 and the fact that $D_2(7) = 2$.

Theorem 2. *For $d = 1, 2, 3, \ldots,$ we have*

$$\lim_{N\to\infty} \frac{D_d(N)}{N^{1/d}} = \Delta_d^{-1/d},$$

where Δ_d denotes, as before, the maximal sphere packing density in $\mathbb{R}^d$.

Proof. For a compact set $A \subset \mathbb{R}^d$, let $M(A, \rho)$ denote the maximum number of points that can be placed in A under the constraint that the distance between any two points is greater than or equal to ρ. Then it is known (cf. [6, Appendix A]) that for any compact convex set $A \subset \mathbb{R}^d$ of unit volume that

$$\Delta_d = \lim_{\rho\to 0} M(A, 2\rho)\beta_d\rho^d \tag{12}$$

where β_d denotes the volume of the unit ball in $\mathbb{R}^d$.

Now let $N \geq 2$ and $B(a, r)$ denote the closed ball centered at a with radius r. To obtain an upper limit, we make the following observations.
(i) Since D_d is a nondecreasing function, the inequality $D_d(N) < D_d(N')$ implies $N < N'$.
(ii) For $T > 0$, we have $T \geq D_d(M(B(0, T/2), 1))$ since there is a configuration of $M(B(0, T/2), 1)$ points that lie in a set of diameter T.
(iii) For $T > 1$, the strict inequality $M(B(0, (T+1)/2), 1)) > M(B(0, T/2), 1))$ holds since $B(-(1/2)\mathbf{e}_1, T/2) \cup \{(T+1)/2)\mathbf{e}_1\} \subset B(0, (T+1)/2)$.
(iv) For $N > 2$ it follows from (ii) and (iii) that

$$D_d(N) \geq D_d(M(B(0, D_d(N)/2), 1)) > D_d(M(B(0, (D_d(N)-1)/2), 1)).$$

Hence by (i) we have

$$N > M(B(0, (D_d(N)-1)/2), 1) = M(B(0,1), 2/(D_d(N)-1)).$$

Then, using (10) and defining $\rho_N := 1/(D_d(N)-1)$, we have

$$\begin{aligned} \limsup_{N\to\infty} \frac{D_d(N)}{N^{1/d}} &\leq \limsup_{N\to\infty} D_d(N)[M(B(0,1), 2/(D_d(N)-1))]^{-1/d} \\ &= [\lim_{N\to\infty} (1+\rho_N)^{-d} {\rho_N}^d M(B(0,1), 2\rho_N)]^{-1/d} = \Delta_d^{-1/d}, \end{aligned}$$

since $D_d(N) \to \infty$ and hence $\rho_N \to 0$ as $N \to \infty$.

To obtain the lower estimate, let ω_N denote a configuration of $N \geq 2$ points in $\mathbb{R}^d$ such that $\min\limits_{\substack{x,y\in\omega_N \\ x\neq y}} \|x-y\| = 1$ and $\operatorname{diam}(\omega_N) = D_d(N)$. Also, let K_N denote the convex hull of ω_N.

For $\gamma > 1$, let $\mathcal{T}_\gamma := \{\gamma[0,1]^d + \gamma x \mid x \in \mathbb{Z}^d\}$,

$$\tilde{K}_{N,\gamma} := \bigcup_{\substack{V\in\mathcal{T}_\gamma \\ V\cap K_N\neq\emptyset}} V,$$

and $L_{N,\gamma} := \#\{V \in \mathcal{T}_\gamma \,|\, V \cap K_N \neq \emptyset\}$. Note that $\tilde{K}_{N,\gamma} \subset K_N(\gamma\sqrt{d})$ where, for $\rho > 0$, $A(\rho)$ denotes the set of points in $\mathbb{R}^d$ whose distance from A is less than or equal to ρ. Then $\operatorname{diam}(K_N(\gamma\sqrt{d})) = D_d(N) + 2\gamma\sqrt{d}$ and we have, for $\gamma > 1$,

$$L_{N,\gamma} \leq \gamma^{-d} \operatorname{Vol}(K_N(\gamma\sqrt{d})) \leq \gamma^{-d} \left(\frac{D_d(N) + 2\gamma\sqrt{d}}{2}\right)^d \beta_d,$$

where we used the isodiametric inequality ([13], see also [4]) that $\operatorname{Vol}(A) \leq \beta_d(\operatorname{diam}(A)/2)^d$ for any bounded measurable set $A \subset \mathbb{R}^d$. Then we obtain

$$\begin{aligned} N \leq M(K_N, 1) \leq M(\tilde{K}_{N,\gamma}, 1) &\leq L_{N,\gamma} M(\gamma[0,1]^d, 1) \\ &\leq (2\gamma)^{-d} \left(D_d(N) + 2\gamma\sqrt{d}\right)^d \beta_d M([0,1]^d, 1/\gamma). \end{aligned}$$

Let $(\gamma_N)_{N=2}^{\infty}$ be such that $\gamma_N > 1$, and $\gamma_N \to \infty$ and $\gamma_N N^{-1/d} \to 0$ as $N \to \infty$. Then

$$\begin{aligned}\liminf_{N\to\infty} \frac{D_d(N)}{N^{1/d}} &\geq \liminf_{N\to\infty} \left(M([0,1]^d, 1/\gamma_N)\beta_d(1/(2\gamma_N))^d\right)^{-1/d} - \frac{\gamma_N\sqrt{d}}{N^{1/d}} \\ &= {\Delta_d}^{-1/d}.\end{aligned}$$

□

It seems plausible (cf. [2]) that the following stronger result holds.

Conjecture. For all $d \geq 3$,

$$D_d(N) = N^{1/d}\Delta_d^{-1/d} + O(1), \quad N \to \infty.$$

We remark that at the conclusion of their article [1], Bateman and Erdös briefly mention that for $N \to \infty$ "there are asymptotic relations of the form $\frac{1}{2}D_d(N) \sim c_d N^{1/d}$," for some unknown constant c_d and refer to a paper of Rankin [11]. However, to the authors' knowledge, there appears no explicit proof of this fact for arbitrary d in [11] or elsewhere.

Theorem 1 together with Equation (4) and Theorem 2 allow us to establish some asymptotic estimates for the N-point f-best-packing constant $\delta_d(N; f)$ of a fixed function $f \in \mathcal{A}$. For example, from (4) and (11) we have

$$\delta_2(N; f_{p,q}) = 1/D_2(N) = \frac{\pi^{1/2}}{12^{1/4}}N^{-1/2} + O(N^{-1}), \quad N \to \infty,$$

and, for $d > 2$,

$$\delta_d(N; f_{p,q}) = 1/D_d(N) = \Delta_d^{1/d}N^{-1/d} + o(N^{-1/d}), \quad N \to \infty.$$

We will now investigate how well $\delta_d(N; f)$ can be approximated by $f(\tau(N^{1/d}\Delta_d^{-1/d}))$, as $N \to \infty$, where $\tau(\alpha)$ is the unique solution of (6). For this purpose the following simple lemma is useful.

Lemma 2. *Let f, M, and ε be as in Lemma 1 and let A and $A+\lambda$ both be greater than M/ε. If $\lambda \leq 0$, we further assume that $A \leq (A+\lambda)^2$. Then the following inequalities hold:*

$$f(A\tau(A)/(A+\lambda)) \leq f(\tau(A+\lambda)) \leq f(\tau(A)), \ \textit{if}\ \lambda \geq 0, \tag{13}$$

$$f((A+\lambda)\tau(A)) \leq f(\tau(A+\lambda)) \leq f(A\tau(A)), \ \textit{if}\ \lambda \geq 0, \tag{14}$$

$$f(\tau(A)) \leq f(\tau(A+\lambda)) \leq f\left(\frac{A\tau(A)}{A+\lambda}\right), \ \textit{if}\ \lambda \leq 0,\ \frac{A\tau(A)}{(A+\lambda)} \leq M, \tag{15}$$

$$f(A\tau(A)) \leq f(\tau(A+\lambda)) \leq f((A+\lambda)\tau(A)), \ \textit{if}\ \lambda \leq 0,\ \varepsilon \leq (A+\lambda)\tau(A). \tag{16}$$

Proof. The inequalities follow easily from the facts that $\tau(t)$ is decreasing and $t\tau(t)$ is increasing for $t > M/\varepsilon$. $\square$

This lemma allows us to obtain asymptotic estimates on $\delta_d(N; f)$, $d \geq 2$, for some subclasses of functions $f \in \mathcal{A}$. Set $A := N^{1/d}\Delta_d^{-1/d}$, $\lambda := D_d(N) - A$. Then by applying Theorem 2 and Lemma 2 we immediately obtain the following.

Corollary 2. *Let $f \in \mathcal{A}$, $d \geq 2$. If at least one of the following two conditions holds,*

(i) $\lim_{t\to 0^+} \frac{f(t+g(t))}{f(t)} = 1$, *for any g such that $t + g(t) \geq 0$ for $t > 0$ and $g = o(t)$, $t \to 0^+$, or*

(ii) $\lim_{t\to\infty} \frac{f(t+g(t))}{f(t)} = 1$, *for any $g = o(t)$, $t \to \infty$,*

then

$$\lim_{N\to\infty} \frac{\delta_d(N; f)}{f(\tau(N^{1/d}\Delta_d^{-1/d}))} = 1. \tag{17}$$

For the Gaussian weighted best-packing problem in $\mathbb{R}^2$ mentioned earlier, where $f(t) = t\exp(-t^2)$, the above corollary readily yields the asymptotic result (2).

Similarly, if $d = 2$, then (4) implies the following:

Corollary 3. *Let $f \in \mathcal{A}$. If, for some $\beta \in (0, 1)$, both of the following conditions hold,*

$$\lim_{t\to 0^+} \frac{f(t+g(t))}{f(t)} = 1, \quad \textit{for each } g(t) = O(t^{1+1/\beta}),\ t \to 0^+, \tag{18}$$

and

$$\lim_{t\to\infty} \frac{f(t+g(t))}{f(t)} = 1, \quad \textit{for each } g(t) = O(t^{-\beta/(1-\beta)}),\ t \to \infty, \tag{19}$$

then

$$\lim_{N\to\infty} \frac{\delta_2(N; f)}{f(\tau(\frac{12^{1/4}}{\pi^{1/2}}N^{1/2}))} = 1. \tag{20}$$

Proof. If $\tau(D_2(N)) > N^{-\beta/2}$ for some sequence of integers N, then (20) holds by (4), (13), (15), (18), while if $\tau(D_2(N)) \leq N^{-\beta/2}$ for infinitely many N, then (20) holds by (4), (14), (16), (19). $\square$

The following example illustrates the sharpness of Corollary 3. Let $f(x) = \exp\{-1/x^2\}$ for $x \in (0, 1)$, and $f(x) = \exp\{-x^2\}$ for $x \geq 1$. We have

$$\delta_2(N; f) = \exp\{-D_2(N)\} = O(\exp\{-\frac{12^{1/4}}{\pi^{1/2}}N^{1/2}\}), \quad N \to \infty,$$

$$f(t + g(t)) = O(f(t)), \quad \text{for each } g(t) = O(t^3),\ t \to 0,$$

and

$$f(t+g(t)) = O(f(t)), \quad \text{for each } g(t) = O(1/t),\ t \to \infty.$$

This example shows that Corollary 3 is optimal in the sense that it is not possible to simultaneously increase the constant $1 + 1/\beta$ and reduce the constant $-\beta/(1-\beta)$.

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