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 $D_d(N)$ 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 show that

$$N^{1/d} \Delta_{-1/d} - 2 \leq D_d(N) \leq N^{1/d} \Delta_{-1/d}, \quad N \geq 2,$$

where $\Delta_d$ is the maximal sphere packing density in $\mathbb{R}^d$. Further, we provide asymptotic estimates for the $f$-best-packing constants as $N \to \infty$.

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

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

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

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

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 $\Delta_d$; 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 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 1 and 2. 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,

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

An important role in our investigation is played by the quantity $D_d(N)$, which is called the \textit{minimal $N$-point diameter} for $\mathbb{R}^d$. That the minimum of the ratio in (2) 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. Erdős.

In comparison with [1], whose proof relies on results of [9] that are special for the plane, we show in Theorem 2 that for all $d \geq 1$ we have

$$N^{1/d} \Delta_d^{-1/d} - 2 \leq D_d(N) \leq N^{1/d} \Delta_d^{-1/d} \quad (N \geq 2).$$

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 $\varepsilon$, $M$ ($\varepsilon \leq M$) 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 $\varepsilon$ and $M$ in the above definition further satisfy

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

\textbf{Lemma 1.} Suppose $f \in \mathcal{A}$ with parameters $\varepsilon$ 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, $\tau(\alpha) \in (M/\alpha, \varepsilon)$.

\textit{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

$$g(M/\alpha) = f(M) - f(M/\alpha) = f(\varepsilon) - f(M/\alpha) > 0.$$
Our first main result is the following:

**Theorem 1.** Let $f \in A$ with parameters $\varepsilon$ 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

$$f(t) = f(D_d(N)t).$$

Then

$$\delta_d(N; f) = f(t_N), \quad N > N_0.$$  

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

$$\min_{x, y \in \omega_N \atop x \neq y} \|x - y\| = t_N \text{ and } \operatorname{diam}(\omega_N) = t_N D_d(N).$$

**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 $\operatorname{diam}(\omega_N) = t_N D_d(N)$. Then

$$t_N \leq \|x_i - x_j\| \leq t_N D_d(N) \quad (i \neq j).$$

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

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

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

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

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 $\tilde{t} := \min_{i \neq j} \|y_i - y_j\|$. Since $f$ is increasing on $[0, \varepsilon]$ and $t_N \leq \varepsilon$, we have

$$\delta_d^{\tilde{\omega}_N}(f) < f(t_N) \text{ if } \tilde{t} < t_N; \text{ i.e. the configuration } \tilde{\omega}_N \text{ is not optimal. On the other hand, if } \tilde{t} \geq t_N, \text{ then } \operatorname{diam}(\tilde{\omega}_N) \geq D_d(N)\tilde{t} \geq D_d(N)t_N, \text{ and so there must be some } i, j \text{ such that } \|y_i - y_j\| \geq D_d(N)\tilde{t}. \text{ Hence, } \delta_d^{\tilde{\omega}_N}(f) \leq f(D_d(N)t_N) = f(t_N) \text{ with equality if and only if both } \tilde{t} = t_N \text{ and } \operatorname{diam}(\tilde{\omega}_N) = D_d(N)t_N. \text{ Therefore, } \delta_d(N; f) = f(t_N) \text{ and a configuration is optimal if and only if the conditions in (9) hold.} \quad \square$$

For the sake of illustration, consider the function $f_{p,q} \in A$ defined by $f_{p,q}(t) = t^p$ if $0 \leq t \leq 1$ 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

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

On letting $p \to 1$ and $q \to \infty$, $f_{p,q}$ tends to $f_{1, \infty}$ where $f_{1, \infty}(t) = t$ for $0 \leq t \leq 1$ 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 $N \geq 2$ must be of the form $\{ck + b \mid k = 0, \ldots, N - 1\}$ for any fixed constants $b$ and $c \neq 0$. We thus obtain the following.

**Corollary 1.** Let $f \in A$ and $d = 1$. Let $\tau_N = \tau(N - 1)$ be the unique solution of equation (3) with $\alpha = N - 1 > M/\varepsilon$. Then $\delta_1(N; f) = f(\tau_N)$ and any $f$-best-packing configuration is of the form $\{t_Nk + b \mid k = 0, \ldots, N - 1\}$ 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 $\omega_N = \{t_Nk\}_{k=0}^{N-1}$. (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 $D_2(7) = 2$.

Next we present estimates for the minimal $N$-point diameter.

**Theorem 2.** For all $d \geq 1$ and $N \geq 2$,

$$N^{1/d} \Delta_d^{-1/d} - 2 \leq D_d(N) \leq N^{1/d} \Delta_d^{-1/d}.$$  

*Proof.* We say that a set of points in $\mathbb{R}^d$ is $2$-separated if the distance between any two points in the set is greater than or equal to 2. For a bounded set $K \subset \mathbb{R}^d$, let $M(K)$ denote the maximum number of points that can be placed in $K$ under the constraint that the distance between any two points is greater than or equal to 2; i.e., $M(K)$ is the maximum cardinality of any 2-separated subset of $K$.

For a compact set $K$ in $\mathbb{R}^d$, we let $\tilde{K}$ denote the $2$-neighborhood of $K$ defined by

$$\tilde{K} := \{y \in K \mid \text{dist}(y, K) \leq 2\},$$

and, for $t \in \mathbb{R}^d$, we let $K + t$ denote the translate of $K$ by $t$.

For $\rho > 1$, let $X_\rho$ denote a 2-separated collection of $M(B(0, \rho))$ points in $B(0, \rho)$, where $B(0, \rho)$ denotes the open ball centered at 0 with radius $\rho$. Then it is known (cf. [9]) that $M(B(0, \rho)) = \rho^d \Delta_d + o(\rho^d)$ as $\rho \to \infty$. Furthermore, for any fixed $a > 0$ we have $M(B(0, \rho) \setminus B(0, \rho - a)) = O(\rho^{d-1})$ as $\rho \to \infty$, which implies

$$\#(X_\rho \cap B(0, \rho - a)) = \rho^d \Delta_d + o(\rho^d) \quad \text{as} \quad \rho \to \infty,$$

where $\#A$ denotes the cardinality of a set $A$.

Let $K$ be a compact convex set in $\mathbb{R}^d$ that contains the origin 0 and let $Y$ denote a 2-separated collection of $M(K)$ points in $K$. If $t \in \mathbb{R}^d$ is such that $|t| \leq \rho - \text{diam} \tilde{K}$, then $K + t$ is contained in $B(0, \rho)$ and $X_\rho = (X_\rho \setminus (K + t)) \cup (Y + t)$ is a 2-separated configuration in $B(0, \rho)$ of $\#X_\rho - \#(X_\rho \cap (K + t)) + M(K)$ points, from which it follows that

$$\#(X_\rho \cap (K + t)) \geq M(K).$$
Let $\mu_\rho$ denote the discrete measure $\mu_\rho = \sum_{x \in X_\rho} \delta_x$, where $\delta_x$ denotes the unit atomic mass at $x \in \mathbb{R}^d$, and let $\lambda^d$ denote Lebesgue measure on $\mathbb{R}^d$. As before, suppose $K$ is a compact convex set in $\mathbb{R}^d$ that contains 0 and let $\chi_K$ denote the characteristic function of $K$. We next consider the following convolution integral which, by Tonelli’s theorem, can be written as

$$
\int \int_{B(0,\rho) \times X_\rho} \chi_K(x + t)d\mu_\rho(x)d\lambda^d(t) = \int_{B(0,\rho)} \#(X_\rho \cap (K - t))d\mu_\rho(x)d\lambda^d(t) = \int_{X_\rho} \lambda^d(B(0,\rho) \cap (K - x))d\mu_\rho(x).
$$

(15)

If $|x| + \text{diam}(K) \leq \rho$, then $K - x \subset B(0, \rho)$, and so we have

$$
\lambda^d(K)\#(X_\rho \cap B(0, \rho - \text{diam}K)) \leq \int_{B(0,\rho)} \#(X_\rho \cap (K - t))d\mu_\rho(x)d\lambda^d(t) \leq \lambda^d(K)\#(X_\rho).
$$

(16)

For $N \geq 1$, letting $R_N := N^{1/d} \Delta_d^{-1/d}$ and choosing $K = B(0, R_N)$, the first inequality in (16) shows that

$$
\#(X_\rho \cap B(0, \rho - 2R_N))\lambda^d(B(0, R_N)) \leq \lambda^d(B(0, \rho)) \max_t \#(B(-t, R_N) \cap X_\rho),
$$

and so, using (13), we obtain as $\rho \to \infty$

$$
\max_t \#(B(-t, R_N) \cap X_\rho) \geq \frac{\#(X_\rho \cap B(0, \rho - 2R_N))\lambda^d(B(0, R_N))}{\lambda^d(B(0, \rho))} = R_N \Delta_d + o(1).
$$

Taking $\rho \to \infty$ it then follows that $M(B(0, R_N)) \geq N$, and thus we have

$$
D_d(N) \leq \frac{\text{diam}(B(0, R_N))}{2} = R_N = N^{1/d} \Delta_d^{-1/d}.
$$

(17)

Next we derive the lower estimate for $D_d(N)$. For $N \geq 2$, let $K_N$ denote the convex hull of a 2-separated configuration of $N$ points such that diam($K_N$) = $2D_d(N)$. Using the second inequality in (16) with $A = K_N$ and the inequality (14), we obtain

$$
\lambda^d(K_N)\frac{\#X_\rho}{\rho^d} \geq \frac{1}{\rho^d} \int_{B(0, \rho - \text{diam}(K_N))} \#(X_\rho \cap (K_N - t))d\lambda^d(t) \geq M(K_N)\frac{\lambda^d(B(0, \rho - \text{diam}(K_N)))}{\rho^d}.
$$

(18)

Recalling the isodiametric inequality (13); see also [3] that $\lambda^d(A) \leq \beta_d (\text{diam}(A)/2)^d$ for any bounded measurable set $A \subset \mathbb{R}^d$ and using (13) and taking $\rho \to \infty$, we have

$$
\left(\frac{\text{diam}(K_N)}{2}\right)^d \Delta_d \geq M(K_N) \geq N.
$$

Since $\text{diam}(K_N) = 4 + \text{diam}(K_N) = 4 + 2D_d(N)$, it follows that

$$
D_d(N) \geq \Delta_d^{-1/d} N^{1/d} - 2.
$$

(19)

We remark that for the case $d = 2$, Bezdek and Fodor [2] have shown that $D_2(N) \geq \Delta_d^{-1/2} N^{1/2} - 1$, $N \geq 2$. We also note that at the conclusion of their article [1], Bateman and Erdős briefly mention that for $N \to \infty$ “there are asymptotic relations of the form $\frac{1}{2} D_d(N) \sim c_d N^{1/d^d}$ for some unknown constant $c_d$ and refer
The inequalities follow easily from the facts that hold, \( f(22) \) asymptotic estimates for the \( \mathbf{be no explicit proof of this fact for arbitrary d in [11] or elsewhere.} \)

Theorem [11] together with equation (12) and Theorem [2] allows us to establish some asymptotic estimates for the \( N\)-point \( f\)-best-packing constant \( \delta_d(N;f) \) of a fixed function \( f \in A \). For example, from (11) and (12) we have for \( d \geq 1, \)

\[
\delta_d(N; f_{p,q}) = 1/D_d(N) = \Delta_d^{1/d}N^{-1/d} + O(N^{-2/d}), \quad N \to \infty.
\]

We 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 \( \varepsilon \) be as in Lemma [1] and let \( A \) and \( A + \lambda \) both be greater than \( M/\varepsilon \). If \( \lambda \leq 0 \), we further assume that \( A \leq (A + \lambda)^2 \). Then the following inequalities hold:

\[
(20) \quad f(A\tau(A)/(A + \lambda)) \leq f(\tau(A + \lambda)) \leq f(\tau(A)), \quad \text{if } \lambda \geq 0,
\]

\[
(21) \quad f((A + \lambda)\tau(A)) \leq f(\tau(A + \lambda)) \leq f(A\tau(A)), \quad \text{if } \lambda \geq 0,
\]

\[
(22) \quad f(\tau(A)) \leq f(\tau(A + \lambda)) \leq f \left( \frac{A\tau(A)}{A + \lambda} \right), \quad \text{if } \lambda \leq 0, \quad \frac{A\tau(A)}{A + \lambda} \leq M,
\]

\[
(23) \quad f(A\tau(A)) \leq f(\tau(A + \lambda)) \leq f((A + \lambda)\tau(A)), \quad \text{if } \lambda \leq 0, \quad \varepsilon \leq (A + \lambda)\tau(A).
\]

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

This lemma allows us to obtain asymptotic estimates on \( \delta_d(N; f) \), \( d \geq 2 \), for some subclasses of functions \( f \in A \). 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 \( f \in A \). If, for some \( \beta \in (0,1) \), both of the following conditions hold,

\[
(24) \quad \lim_{t \to 0^+} \frac{f(t + g(t))}{f(t)} = 1, \quad \text{for each } g(t) = O(t^{1+1/\beta}), \ t \to 0^+,
\]

and

\[
(25) \quad \lim_{t \to \infty} \frac{f(t + g(t))}{f(t)} = 1, \quad \text{for each } g(t) = O(t^{-\beta/(1-\beta)}), \ t \to \infty,
\]

then

\[
(26) \quad \lim_{N \to \infty} \frac{\delta_d(N; f)}{f(\tau(N^{1/d}/\Delta_d))} = 1.
\]

**Proof.** If \( \tau(D_d(N)) > N^{-\beta/d} \) for some sequence of integers \( N \), then (26) holds by (12), (20), (22), (24), while if \( \tau(D_d(N)) \leq N^{-\beta/d} \) for infinitely many \( N \), then (26) holds by (12), (21), (23), (25). ∎
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).

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

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

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

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 2 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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