

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

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(Communicated by Jim Haglund)

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

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

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

Let f be a non-negative function on $[0, \infty)$ and $\omega_N = \{x_1, x_2, \dots, x_N\}$ 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

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

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 a certain class \mathcal{A} of functions f defined on all of \mathbb{R}^d for fixed N (see Theorem 1) as

Received by the editors November 3, 2010 and, in revised form, November 1, 2011 and April 17, 2012.

2010 *Mathematics Subject Classification*. Primary 52C17.

Key words and phrases. Best-packing, optimal configurations, minimal N -point diameter, maximal sphere packing density.

The research of the first author was conducted while visiting the Center for Constructive Approximation in the Department of Mathematics, Vanderbilt University.

The research of all the authors was supported, in part, by the U.S. National Science Foundation under grant DMS-0808093.

well as provide asymptotic results (as $N \rightarrow \infty$) 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,

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

An important role in our investigation is played by the quantity

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

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

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

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 (4), 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 $t > 0$, $\lim_{t \rightarrow \infty} f(t) = 0$, 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

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

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*

$$(6) \quad f(t) = f(\alpha t).$$

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*

$$(7) \quad f(t) = f(D_d(N)t).$$

Then

$$(8) \quad \delta_d(N; f) = f(t_N), \quad N > N_0.$$

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

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

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

$$(10) \quad t_N \leq \|x_i - x_j\| \leq t_N D_d(N) \quad (i \neq j).$$

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

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

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

Let $\tilde{\omega}_N = \{y_k \mid k = 1, \dots, N\}$ 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 $\delta_d^{\tilde{\omega}_N}(f) < f(t_N)$ if $\tilde{t} < t_N$; i.e. the configuration $\tilde{\omega}_N$ is not optimal. On the other hand, if $\tilde{t} \geq t_N$, then $\text{diam}(\tilde{\omega}_N) \geq D_d(N)\tilde{t} \geq D_d(N)t_N$, and so there must be some i, j such that $\|y_i - y_j\| \geq D_d(N)\tilde{t}$. Hence, $\delta_d^{\tilde{\omega}_N}(f) \leq f(D_d(N)t_N) = f(t_N)$ with equality if and only if both $\tilde{t} = t_N$ and $\text{diam} \omega_N^* = D_d(N)t_N$. Therefore, $\delta_d(N; f) = f(t_N)$ and a configuration is optimal if and only if the conditions in (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 $0 \leq t \leq 1$ 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,

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

On letting $p \rightarrow 1$ and $q \rightarrow \infty$, $f_{p,q}$ 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 $\{ck + b \mid k = 0, \dots, N - 1\}$ 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 $\delta_1(N; f) = f(\tau_N)$ and any f -best-packing configuration is of the form $\{t_N k + b \mid k = 0, \dots, N - 1\}$ 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 $D_2(7) = 2$.

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

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

$$(12) \quad N^{1/d} \Delta_d^{-1/d} - 2 \leq D_d(N) \leq N^{1/d} \Delta_d^{-1/d}.$$

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

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

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

For $\rho > 1$, let X_ρ 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 ρ . Then it is known (cf. [6]) that $M(B(0, \rho)) = \rho^d \Delta_d + o(\rho^d)$ as $\rho \rightarrow \infty$. Furthermore, for any fixed $a > 0$ we have $M(B(0, \rho) \setminus B(0, \rho - a)) = O(\rho^{d-1})$ as $\rho \rightarrow \infty$, which implies

$$(13) \quad \#(X_\rho \cap B(0, \rho - a)) = o(\rho^d) \text{ as } \rho \rightarrow \infty,$$

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 $\tilde{K} + t$ is contained in $B(0, \rho)$ and $X'_\rho = (X_\rho \setminus \tilde{K} + t) \cup (Y + t)$ is a 2-separated configuration in $B(0, \rho)$ of $\#X_\rho - \#(X_\rho \cap (\tilde{K} + t)) + M(K)$ points, from which it follows that

$$(14) \quad \#(X_\rho \cap (\tilde{K} + t)) \geq M(K).$$

Let μ_ρ denote the discrete measure $\mu_\rho = \sum_{x \in X_\rho} \delta_x$, where δ_x denotes the unit atomic mass at $x \in \mathbb{R}^d$, and let λ^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 χ_K denote the characteristic function of K . We next consider the following convolution integral which, by Tonelli's theorem, can be written as

$$(15) \quad \begin{aligned} \iint_{B(0,\rho) \times X_\rho} \chi_K(x+t) d\mu_\rho(x) d\lambda^d(t) &= \int_{B(0,\rho)} \#(X_\rho \cap (K-t)) d\mu_\rho(x) d\lambda^d(t) \\ &= \int_{X_\rho} \lambda^d(B(0,\rho) \cap (K-x)) d\mu_\rho(x). \end{aligned}$$

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

$$(16) \quad \begin{aligned} \lambda^d(K) \#(X_\rho \cap B(0,\rho - \text{diam}K)) &\leq \int_{B(0,\rho)} \#(X_\rho \cap (K-t)) d\mu_\rho(x) d\lambda^d(t) \\ &\leq \lambda^d(K) \#(X_\rho). \end{aligned}$$

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 $\rho \rightarrow \infty$

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

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

$$(17) \quad D_d(N) \leq \frac{\text{diam}(B(0, R_N))}{2} = R_N = N^{1/d} \Delta_d^{-1/d}.$$

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 $\text{diam}(K_N) = 2D_d(N)$. Using the second inequality in (16) with $A = \tilde{K}_N$ and the inequality (14), we obtain

$$(18) \quad \begin{aligned} \lambda^d(\tilde{K}_N) \frac{\#X_\rho}{\rho^d} &\geq \frac{1}{\rho^d} \int_{B(0,\rho - \text{diam}(\tilde{K}_N))} \#(X_\rho \cap (\tilde{K}_N - t)) d\lambda^d(t) \\ &\geq M(K_N) \frac{\lambda^d(B(0,\rho - \text{diam}(\tilde{K}_N)))}{\rho^d}. \end{aligned}$$

Recalling the isodiametric inequality ([13]; see also [4]) 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 $\rho \rightarrow \infty$, we have

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

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

$$(19) \quad D_d(N) \geq \Delta_d^{-1/d} N^{1/d} - 2. \quad \square$$

We remark that for the case $d = 2$, Bezdek and Fodor [2] have shown that $D_2(N) \geq \Delta_2^{-1/2} N^{1/2} - 1$, $N \geq 2$. We also note that at the conclusion of their article [1], Bateman and Erdős briefly mention that for $N \rightarrow \infty$ ‘‘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 to be no explicit proof of this fact for arbitrary d in [11] or elsewhere.

Theorem 1 together with equation (4) 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 $f \in \mathcal{A}$. For example, from (11) and (12) we have for $d \geq 1$,

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

We now investigate how well $\delta_d(N; f)$ can be approximated by $f(\tau(N^{1/d} \Delta_d^{-1/d}))$, as $N \rightarrow \infty$, 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:*

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

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

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

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

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

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

and

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

then

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

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 $f(x) = \exp\{-1/x^2\}$ for $x \in (0, 1)$, and $f(x) = \exp\{-x^2\}$ for $x \geq 1$. We have

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

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

and

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

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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