General properties of staircase and convex dual feasible functions

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Abstract: Dual feasible functions have been used successfully to compute lower bounds and valid inequalities for different combinatorial optimization problems. In this paper, we show that some maximal dual feasible functions proposed in the literature are dominated by others under weak prerequisites. Furthermore, we explore the relation between superadditivity and convexity, and we derive new results for the case where dual feasible functions are convex. Computational results are reported to illustrate the results presented in this paper.

Key-Words: Dual feasible functions; Maximal functions; Extreme functions; Dominance; Convex functions; Lower bounds.

1 Introduction

Dual feasible functions were proposed originally by Johnson in [7]. Since then, different functions were defined and used to compute lower bounds and valid inequalities for general problems including cutting and packing, vehicle routing, and scheduling problems [1, 2, 3, 4, 11].

A function $f:[0,1] \to [0,1]$ is called a *dual feasible function (DFF)*, if for any finite set $\{x_i \in \mathbb{R}_+ : i \in I\}$ of nonnegative real numbers, the following holds

$$\sum_{i\in I} x_i \le 1 \Rightarrow \sum_{i\in I} f(x_i) \le 1.$$

Given a DFF $f:[0,1] \to [0,1]$ and an instance $E := (m; L; \mathfrak{l}; \mathfrak{b})$ of the one-dimensional cutting stock problem (1D-CSP) with $m \in \mathbb{N}$ items of lengths $l_i \in \mathbb{R}_+$ to be cut in the order demands $b_i \in \mathbb{N}$ from initial material of length $L > 0$ ($i = 1, \dots, m$), a valid lower bound for the optimal objective function value of the continuous relaxation (and therefore for the integer problem too) is

$$z[f] := \sum_{i=1}^{m} b_i * f\left(\frac{l_i}{L}\right).$$

A DFF f is a *maximal dual feasible function (MDFF)*, if there is no other DFF $g:[0,1] \to [0,1]$ with $g(x) \ge f(x)$ for all $x \in [0,1]$. A MDFF $f:[0,1] \to [0,1]$ is *extreme* [8], if MDFFs $g,h:[0,1] \to [0,1]$ with $2f(x) = g(x) + h(x)$ for all $x \in [0,1]$ are necessarily identical with f.

To obtain high values for the bound $z[f]$, obviously only MDFFs f should be used. Moreover, if f,g,h are MDFFs with $2f \equiv g + h$ then $2z[f] = z[g] + z[h]$, hence $z[f] \le \max\{z[g], z[h]\}$. Therefore extreme MDFFs should be preferred.

A first characterization of MDFFs was given in [4]. A function $f:[0,1] \to [0,1]$ is a MDFF, if and only if

$$f(0) = 0, \tag{1}$$

f is symmetric, *i.e.*

$$f(x) + f(1-x) = 1 \text{ for all } x \in \left[0, {}^1\!/_2\right], \tag{2}$$

and the following superadditivity condition holds:

$f(x_1 + x_2) \ge f(x_1) + f(x_2)$ for all $x_1, x_2 \in \mathbb{R}_+$ with $x_1 + x_2 \le 1$.

To prove that a function $f:[0,1] \to [0,1]$ is a MDFF, the superadditivity needs to be shown for $0 < x_1 \le x_2 < \frac{1}{2}$ and $x_1 + x_2 \le \frac{2}{3}$ only (see [8]).

In [5], the authors surveyed the different DFFs described in the literature. In the sequel, we recall the formal definition of the functions that will be explored in this paper. The parameters will be omitted when it is possible.

- $f_{FS,1}$, proposed by Fekete and Schepers in [6], with $k \in \mathbb{N}\backslash\{0\}$:

$$f_{FS,1}(x;k)=\begin{cases} x, & \text{if } (k+1)*x \in \mathbb{N}, \\ \dfrac{\lfloor (k+1)x \rfloor}{k}, & \text{otherwise.} \end{cases}$$

- $f_{VB,2}$, obtained from a function proposed originally in [11], using a procedure to make it maximal [5], for any $k \in \mathbb{N}\backslash\{0,1\}$:

$$f_{VB,2}(x;k)=\begin{cases} \dfrac{\max\{0,\lceil kx \rceil - 1\}}{k-1}, & \text{if } x<\dfrac{1}{2}, \\ 1/2, & \text{if } x=1/2, \\ 1-f_{VB,2}(1-x), & \text{for } x>1/2. \end{cases}$$

- $f_{CCM,1}$, proposed by Carlier, Clautiaux and Moukrim in [3], for any $C \in \mathbb{R}$ and $C \geq 1$:

$$f_{CCM,1}(x;C)=\begin{cases} \lfloor Cx \rfloor / \lfloor C \rfloor, & \text{if } x<1/2, \\ 1/2, & \text{if } x=1/2, \\ 1-f_{CCM,1}(1-x), & \text{if } x>\frac{1}{2}. \end{cases}$$

- $f_{BJ,1}$, proposed by Burdett and Johnson in [2], with $C \in \mathbb{R}$ and $C \geq 1$:

$$f_{BJ,1}(x;C)=\frac{\lfloor Cx \rfloor + \max\left\{0, \dfrac{\operatorname{frac}(Cx)-\operatorname{frac}(C)}{1-\operatorname{frac}(C)}\right\}}{\lfloor C \rfloor}.$$

This function is continuous on $[0,1]$ and yields for $C \in \mathbb{N} \setminus \{0\}$ the identity function.

Note that the non-integer part of a real value x is denoted by $\operatorname{frac}(x)$, *i.e.* $\operatorname{frac}(x) \equiv x - \lfloor x \rfloor$, for $x \in \mathbb{R}$.

All these functions are maximal, but not always extreme [8], e.g. $f_{FS,1}, f_{VB,2}$ and $f_{CCM,1}$ are extreme for all possible parameters, while $f_{BJ,1}(\cdot;C)$ is extreme if and only if $C=1$ or $C \geq 2$ [9].

Although $f_{FS,1}$ and $f_{VB,2}$ are extreme, we will show in the following section that in the computation of valid lower bounds for the 1D-CSP these functions are dominated by others, *i.e.* they can be replaced by others without getting worse results, if all data in the given instance are integer. That is a very weak prerequiste, because usually all data are rational, hence multiplying them by the smallest common multiple of the denominators yields an equivalent instance with integer data only. In Section 3 we will discuss functions, which are convex on $\left[0,\frac{1}{2}\right]$. It comes out that these functions easily lead to MDFFs. Section 4 contains computational tests. Conclusions and summary are given in Section 5.

2 Dominance between MDFFs

The characteristic mark of a MDFF $f:[0,1] \rightarrow [0,1]$ is by definition, that there is no other DFF $g:[0,1] \rightarrow [0,1]$ with $g(x) \geq f(x)$ for all $x \in [0,1]$, *i.e.* there is no dominance relation on the entire interval between both functions. Nevertheless, sometimes one MDFF f (even if it is extreme) can be replaced by another MDFF g in the calculation of the lower bound $z[f]$ for the optimal objective function value of an instance of the 1D-CSP, such that $z[g] \geq z[f]$ is obtained. This is possible, because the arguments for the functions belong only to a discrete set.

2.1 $f_{FS,1}$ versus $f_{BJ,1}$

The following proposition shows a dominance between the Fekete and Schepers function and the one by Burdett and Johnson [2]. On the contrary, there is no such relation with respect to the function by Carlier, Clautiaux and Moukrim [3]. Moreover, we will present an example, where $z\left[f_{BJ,1}\right]$ (with a certain parameter choice) cannot be achieved by $z\left[f_{FS,1}\right]$ for any possible parameter.

Proposition 1. *For any* $k, L, n \in \mathbb{N}\backslash\{0\}, n \leq L$, *the choice* $C := \frac{(k+1)*kL}{kL+1}$ *leads to* $f_{BJ,1}\left(\frac{n}{L};C\right) = f_{FS,1}\left(\frac{n}{L};k\right)$. *A similar relation does not exist between* $f_{FS,1}(\cdot;2)$ *and* $f_{CCM,1}(\cdot;C)$ *for any* $C \geq 1$.

Proof. Both functions $f_{FS,1}$ and $f_{BJ,1}$ are MDFFs, hence the assertion needs to be verified for $0<\frac{n}{L}<\frac{1}{2}$ only. Since $L, n \in \mathbb{N}\backslash\{0\}$ that allows the assumption $L \geq 3$.

Let $p \in \mathbb{N}$ with $p \leq k$ and $\frac{n}{L} \approx \frac{p}{k+1}$. Since $C = k + \frac{kL-k}{kL+1} \in (k, k+1)$ one obtains

$$f_{BJ,1}\left(\frac{n}{L}\right) = \frac{\left\lfloor\frac{(k+1)*kn}{kL+1}\right\rfloor + \max\left\{0, \frac{(kL+1)*\mathrm{frac}\left(\frac{(k+1)*kn}{kL+1}\right)-kL+k}{1+k}\right\}}{k}.$$

Three cases have now to be distinguished:

1. $n = \frac{Lp}{k+1} > 0$ yields $\frac{(k+1)*kn}{kL+1} = \frac{kLp}{kL+1} = p - 1 + \frac{kL+1-p}{kL+1} \in (p-1, p)$, hence $f_{BJ,1}\left(\frac{n}{L}\right) = \left(p - 1 + \max\left\{0, \frac{kL+1-p-kL+k}{k+1}\right\}\right)/k = \left(p - 1 + \frac{k+1-p}{k+1}\right)/k = \frac{kp+p-p}{(k+1)*k} = \frac{p}{k+1} = f_{FS,1}\left(\frac{p}{k+1}\right) = f_{FS,1}\left(\frac{n}{L}\right)$.

2. $n < \frac{Lp}{k+1}$: since k, L, n, p are integers, it follows that $n \le \frac{Lp-1}{k+1}$. We get $C * \frac{Lp-1}{(k+1)*L} = \frac{k*(Lp-1)}{kL+1} = p - 1 + \frac{kL+1-k-p}{kL+1} \in (p-1, p)$, because the nominator of the last fraction equals $k*(L-1)+1-p \ge 2k+1-p > 0$. Therefore, $f_{BJ,1}\left(\frac{n}{L}\right) \le f_{BJ,1}\left(\frac{Lp-1}{(k+1)*L}\right) = \left(p - 1 + \max\left\{0, \frac{kL+1-k-p-kL+k}{k+1}\right\}\right)/k = \left(p - 1 + \max\left\{0, \frac{1-p}{k+1}\right\}\right)/k = \frac{p-1}{k} = \left\lfloor p - \frac{1}{L}\right\rfloor/k = f_{FS,1}\left(\frac{Lp-1}{(k+1)*L}\right)$.

3. $n > \frac{Lp}{k+1}$: we get $n \ge \frac{Lp+1}{k+1}$ and $C * \frac{Lp+1}{(k+1)*L} = \frac{k*(Lp+1)}{kL+1} = p + \frac{k-p}{kL+1} \in [p, p+1[$, and hence $f_{BJ,1}\left(\frac{n}{L}\right) \ge f_{BJ,1}\left(\frac{Lp+1}{(k+1)*L}\right) = \left(p + \max\left\{0, \frac{k-p-kL+k}{k+1}\right\}\right)/k = \left(p + \max\left\{0, \frac{k*(2-L)-p}{k+1}\right\}\right)/k = \frac{p}{k} = \left\lfloor p + \frac{1}{L}\right\rfloor/k = f_{FS,1}\left(\frac{Lp+1}{(k+1)*L}\right)$.

We get for $\frac{Lp}{k+1} < n < \frac{L*(p+1)}{k+1}$ from the combination of the second and third case $\frac{p}{k} \le f_{BJ,1}\left(\frac{n}{L}\right) \le \frac{p+1-1}{k}$, hence $f_{BJ,1}\left(\frac{n}{L}\right) = \frac{p}{k}$ and analogously $\frac{p}{k} = f_{FS,1}\left(\frac{n}{L}\right)$ because of the monotony.

For the second assertion let $L := 9$ and $n \in \{2, 3, 4\}$. That yields the function values 0, $\frac{1}{3}$ and $\frac{1}{2}$ for $f_{FS,1}\left(\frac{n}{L}; 2\right)$. Suppose there is a $C \ge 1$ with $f_{CCM,1}\left(\frac{2}{9}; C\right) = 0$ and $f_{CCM,1}\left(\frac{1}{3}; C\right) = \frac{1}{3}$. The first equation implies $\frac{2}{9}C < 1$, hence $C < \frac{9}{2}$. The second demand yields $C \ge 3$ and $C < 4$ due to $C < \frac{9}{2}$, leading to the contradiction $f_{CCM,1}\left(\frac{4}{9}; C\right) = \frac{1}{3} < \frac{1}{2} = f_{FS,1}\left(\frac{4}{9}; 2\right)$. ■

This proposition states mainly that results, which were calculated with $f_{FS,1}$, can also be obtained with $f_{BJ,1}$. On the contrary, it will be shown in the following that sometimes $f_{BJ,1}$ yields better bounds than $f_{FS,1}$ for any possible parameter k.

For any instance $(m; L; \mathfrak{l}; \mathfrak{b})$ of the 1D-CSP with integer data only, a valid lower bound for the optimal objective function value of the integer problem arising from the Fekete and Schepers-function $f_{FS,1}$ can be achieved also with a Burdett and Johnson-function $f_{BJ,1}$. Since the latter function may give better results, $f_{FS,1}$ becomes superfluous for this purpose. To calculate the maximal possible value for $z[f_{BJ,1}(\cdot; C)]$, according to [10], only parameters need to be tested, which belong to the set $P := \left(\left\{\frac{p*L}{l_i}, \frac{p*L}{L-l_i} : i \in \{1, \dots, m\}, 0 < l_i < L, p \in \mathbb{N}\right\} \setminus \mathbb{N}\right) \cup \{1\}$. Nevertheless, trying all these possibilities is impossible, because there are still infinite many elements in this set, and in spite of restricting C by a certain constant from above, the complexity would be too high. On the other hand, we can try to approximate $\hat{C} := \frac{(k+1)*kL}{kL+1}$ by an element of P using continued fractions, *i.e.* we are looking for numbers $p, q \in \mathbb{N}$ with $0 < q < L$ and $\frac{p}{q} \approx \frac{\hat{C}}{L}$. The fraction $\hat{C}$ is never integer, because kL divides the nominator, but not the denominator, hence the greatest common divider (gcd) of nominator and denominator equals $\gcd(k+1, kL+1) \le k+1 < kL+1$, since $L > 1$. Therefore, the calculation can be done with the following simple algorithm:

1. Initialize the numbers $n := 0$, $p_0 := 0$, $p_1 := 1$, $p_2 := k*(k+1)$, $q_0 := 1$, $q_1 := 0$, $q_2 := kL+1$ and $r := p_2/q_2$. Obtain the material bound $z_M := z[f_{BJ,1}(\cdot; 1)] \equiv \mathfrak{l}^T\mathfrak{b}/L$.

2. If $L * p_{n+2}/q_{n+2} \notin \mathbb{N}$ then calculate $z[f_{BJ,1}(\cdot; L * p_{n+2}/q_{n+2})]$ and update the best known lower bound if this bound is better than the current one.

3. Let $n := n+1$, $p_{n+2} := p_{n+1} := p_n * \lfloor r \rfloor + p_{n-1}$, $q_{n+2} := q_{n+1} := q_n * \lfloor r \rfloor + q_{n-1}$ and $r := 1/\mathrm{frac}(r)$.

4. If $q_{n+1} < L \land r \notin \mathbb{N}$ then go to the step 2.

The numbers q_n increase exponentially, such that the loop is left after at most $\log_{\frac{1+\sqrt{5}}{2}} L + \mathcal{O}(1)$ repetitions. In this way, good results can be achieved with small complexity, as illustrated in Section 4.

2.2 $\mathbf{f_{VB,2}}$, $\mathbf{f_{CCM,1}}$ and the identity function

Similarly to the previous subsection, the improved Vanderbeck function $f_{VB,2}$ is dominated by $f_{CCM,1}$, but there is no such dominance relation to $f_{BJ,1}$. Moreover, $f_{VB,2}$ dominates the identity function.

Proposition 2. *For any $k \in \mathbb{N}$ with $k \geq 2$ and any $L \in \mathbb{N}\backslash\{0\}$, the use of $C := k - \frac{1}{L}$ leads to $f_{VB,2}\left(\frac{n}{L}; k\right) = f_{CCM,1}\left(\frac{n}{L}; C\right)$ for all $n \in \mathbb{N}$ with $n \leq L$. Additionally, $f_{VB,2}\left(\frac{n}{L}; L+1\right) = \frac{n}{L}$ holds for all these n. On the other hand, $f_{VB,2}$ cannot always be replaced in the same way by $f_{BJ,1}$.*

Proof. Since $f_{VB,2}$ and $f_{CCM,1}$ are MDFFs, it is enough for the first and second part to verify the proposition for $0 < n < \frac{L}{2}$. Then, it follows that $f_{VB,2}\left(\frac{n}{L}\right) = \left\lceil \frac{kn}{L} - 1 \right\rceil / (k-1)$ and $f_{CCM,1}\left(\frac{n}{L}\right) = \left\lfloor \frac{Cn}{L} \right\rfloor / (k-1)$. For any $x \in \mathbb{R}\backslash\mathbb{Z}$, it holds that $\lceil x - 1 \rceil = \lfloor x \rfloor$. One has $\frac{Cn}{L} = \frac{kn}{L} - \frac{n}{L^2} \in \left(\frac{kn-1}{L}, \frac{kn}{L}\right)$, because $0 < n < \frac{L}{2}$.

If $L|kn$ then $f_{VB,2}\left(\frac{n}{L}\right) = \left(\frac{kn}{L} - 1\right)/(k-1)$ and $\left\lfloor \frac{Cn}{L} \right\rfloor = \frac{kn}{L} - 1$ and therefore $f_{CCM,1}\left(\frac{n}{L}\right) = \left(\frac{kn}{L} - 1\right)/(k-1) = f_{VB,2}\left(\frac{n}{L}\right)$.

If $L \nmid kn$ then $f_{VB,2}\left(\frac{n}{L}\right) = \left\lfloor \frac{kn}{L} \right\rfloor / (k-1) = \left\lfloor \frac{kn-1}{L} \right\rfloor / (k-1) = f_{CCM,1}\left(\frac{n}{L}\right)$.

The choice $k := L+1$ yields $f_{VB,2}\left(\frac{n}{L}\right) = \left\lceil n + \frac{n}{L} - 1 \right\rceil / L = \frac{n}{L}$, because $0 < n < L$.

For the last assertion, choose any $p \in \mathbb{N}$ with $p \geq 3$. Let $k := 3$ and $L := 3p$. Suppose, there is a $C \in \mathbb{R}$ with $C \geq 1$ and $f_{VB,2}\left(\frac{p+1}{3p}; 3\right) = f_{BJ,1}\left(\frac{p+1}{3p}; C\right)$ and $f_{VB,2}\left(\frac{p}{3p}; 3\right) = f_{BJ,1}\left(\frac{1}{3}; C\right)$. The latter case yields $f_{VB,2}\left(\frac{1}{3}; 3\right) = 0 = \left\lfloor \frac{C}{3} \right\rfloor$, *i.e.* $1 \leq C < 3$, and $\frac{C}{3} \leq \mathrm{frac}(C)$. The case $2 \leq C < 3$ leads to $\mathrm{frac}(C) = C - 2 \geq \frac{C}{3}$, hence $\frac{2}{3}C \geq 2$, implying the contradiction $C \geq 3$. Therefore, we get $1 \leq C < 2$ and $\mathrm{frac}(C) = C - 1 \geq \frac{C}{3}$, hence $\frac{3}{2} \leq C < 2$. One has $f_{BJ,1}\left(\frac{p+1}{3p}; C\right) = \left\lfloor \frac{p+1}{3p} * C \right\rfloor + \max\left\{0, \frac{\mathrm{frac}\left(\frac{p+1}{3p} * C\right) - C + 1}{2 - C}\right\} = 0 + \max\left\{0, \frac{\frac{p+1}{3p} * C - C + 1}{2 - C}\right\}$. Since $p \geq 3$ and $\frac{3}{2} \leq C < 2$, one gets $(p-2) * (3 - 2C) \leq 0$, hence $p * (3 - 2C) \leq 6 - 4C$, therefore $C * (1 - 2p) + 3p \leq 6 - 3C$ and $\frac{\frac{p+1}{3p} * C - C + 1}{2 - C} = \frac{C * (p+1) - 3Cp + 3p}{3p * (2 - C)} = \frac{C * (1 - 2p) + 3p}{p * (6 - 3C)} \leq \frac{1}{p}$ in contradiction to $f_{VB,2}\left(\frac{p+1}{3p}; 3\right) = \frac{1}{2}$. ∎

Here the same discussion as after Proposition 1 applies. Moreover, the structure of $f_{CCM,1}$ is less complex than the one of $f_{VB,2}$. Computational tests to compare both functions are presented in Section 4. The following example illustrates that $z[f_{CCM,1}]$ can be above every possible value of $z[f_{VB,2}]$.

Example. One piece of length 7 and one of length 15 have to be cut from initial material of length 21. That yields $z[f_{CCM,1}(\cdot; 3)] = f_{CCM,1}\left(\frac{1}{3}; 3\right) + 1 - f_{CCM,1}\left(\frac{2}{7}; 3\right) = \frac{1}{3} + 1 - 0 = \frac{4}{3}$. This value cannot be reached by $f_{VB,2}$ for any feasible parameter k, because $k \leq 3$ yields $f_{VB,2}\left(\frac{1}{3}; k\right) = 0$ and of course $f_{VB,2}\left(\frac{5}{7}\right) \leq 1$, while the choice $k \geq 4$ leads to $f_{VB,2}\left(\frac{1}{3}\right) \leq \frac{1}{3}$ and $f_{VB,2}\left(\frac{5}{7}; k\right) \leq 1 - \frac{1}{k-1} < 1$.

This dominance of $f_{CCM,1}$ over $f_{VB,2}$ can only happen if there are items of sizes in $\left(\frac{L}{2}, L\right)$. If there are only small pieces (shorter than $L/2$) then the highest values of $z[f_{CCM,1}(\cdot; C)]$ are found with a large non-integer part $\mathrm{frac}(C)$. In that case set $k := \lceil C \rceil$. That leads to $\lfloor C \rfloor = k - 1$ and $\lfloor Cx \rfloor \leq \lfloor kx \rfloor$ for $x \in \left(0, \frac{1}{2}\right)$ and finally $f_{CCM,1}(x; C) = f_{VB,2}(x; k)$, because if $kx \in \mathbb{N}$ then $\lfloor Cx \rfloor = kx - 1$ due to $C < k$.

Because of the negative assertions in the propositions 1 and 2, there is no dominance relation between $f_{BJ,1}$ and $f_{CCM,1}$, hence both functions should be used to calculate valid bounds.

3 Convex functions

In this section, a connection between superadditivity and convexity is developed and the resulting MDFFs are analyzed. If a real function f is continuous and obeys the equation $f(x+y) = f(x) + f(y)$ for all $x, y \in \mathbb{R}$, then f is necessarily linear. Since superadditivity allows also "greater than", convex functions could be very useful for generating MDFFs under the prerequisite (1).

Let $D \neq \emptyset$ be a convex set. A function $f: D \to \mathbb{R}$ is *convex* if for all $x_1, x_2 \in D$ and $\lambda \in (0,1)$ it holds that $f(\lambda * x_1 + (1-\lambda) * x_2) \leq \lambda * f(x_1) + (1-\lambda) * f(x_2)$.

Theorem 1. *Let $d > 0$ be a constant. Any convex function $f: [0,d] \to \mathbb{R}_+$ fulfilling the condition (1) is superadditive in the entire domain $[0,d]$. Moreover, if $f: [0,1] \to \mathbb{R}_+$ fulfills the conditions (1) and (2) and is convex on $\left[0, \frac{1}{2}\right]$ then f is a MDFF.*

Proof. Let $x_0, x_1, x_2, x_3 \in \mathbb{R}$ be given with $0 \leq x_0 < x_1 < x_2 < x_3 \leq d$. First it is shown, that $f(x_3) \geq s(x_3)$, where s describes the straight line through the points $(x_1; f(x_1))$ and $(x_2; f(x_2))$, *i.e.*

$$s(x) = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1} * (x - x_1).$$

Since f is convex in the interval $[x_1, x_3]$, one has $f(x_2) \leq f(x_1) + \frac{f(x_3)-f(x_1)}{x_3 - x_1} * (x_2 - x_1)$, hence

$$\begin{aligned} &f(x_3) - s(x_3) \\ &= f(x_3) - f(x_1) - \frac{f(x_2) - f(x_1)}{x_2 - x_1} * (x_3 - x_1) \\ &\geq f(x_3) - f(x_1) \\ &- \frac{f(x_1) + \frac{f(x_3) - f(x_1)}{x_3 - x_1} * (x_2 - x_1) - f(x_1)}{x_2 - x_1} \\ &* (x_3 - x_1) = f(x_3) - f(x_1) - \big(f(x_3) - f(x_1)\big) \\ &= 0. \end{aligned}$$

In the same way, $f(x_0) \geq s(x_0)$ can be shown. Taking $x_0 := 0$ yields $s(0) \leq f(0) = 0$. The straight line s can be written generally in the form $s(x) = mx + n$ with certain $m, n \in \mathbb{R}$. For $x_1 + x_2 \leq d$ this yields $f(x_1 + x_2) - f(x_1) - f(x_2) \geq s(x_1 + x_2) - s(x_1) - s(x_2) = -n = -s(0) \geq 0$, hence f is superadditive in the interval $[0, d]$.

To prove the second assertion, the superadditivity on the entire interval $\left]0, \frac{2}{3}\right]$ must be shown. For that purpose assume now $0 < x_1, x_2 < \frac{1}{2} < x_1 + x_2 =: x_3$. Since f is symmetric, one has $f\left(\frac{1}{2}\right) = \frac{1}{2}$. Because f is convex on $\left[0, \frac{1}{2}\right]$, it holds that $f\left(\lambda * \frac{1}{2} + (1-\lambda) * 0\right) \leq \lambda * f\left(\frac{1}{2}\right) + (1-\lambda) * f(0)$ for all $\lambda \in (0,1)$, hence $f(\lambda/2) \leq \lambda/2$ for all $\lambda \in (0,1)$. Therefore, $f(x_1) \leq x_1$, $f(x_2) \leq x_2$ and $f(x_3) = 1 - f(1 - x_3) \geq 1 - (1 - x_3) = x_3$, implying $f(x_1) + f(x_2) \leq f(x_1 + x_2)$. ■

Any convex function is continuous in the inner of its domain, but not necessarily differentiable, for instance $e^{|x|}$. Therefore, the prerequisite, that f should be convex on $\left[0, \frac{1}{2}\right]$, is strong, but not too strong. This leads to a wide range of MDFFs. However, many of these functions will not be extreme as shown at the end of this section.

Example. *The following function $f_1: [0,1] \to [0,1]$ is a MDFF:*

$$f_1(x) := \begin{cases} 0, & \text{for } x = 0; \\ e^{2-\frac{1}{x}}/2, & \text{for } 0 < x \leq {}^1\!/_2; \\ 1 - f_1(1-x), & \text{otherwise} \end{cases} \tag{3}$$

Proof. f_1 fulfills the conditions (1) and (2) obviously. For $0 < x < \frac{1}{2}$ one obtains $f_1'(x) = f_1(x) * x^{-2}$ and $f_1''(x) = f_1(x) * (x^{-4} - 2x^{-3}) > 0$, hence f_1 is strictly convex in $\left(0, \frac{1}{2}\right)$. Since f_1 is continuous, Theorem 1 can be applied. ■

The following assertion will be used at the end of this section to simplify the proof of Proposition 4, where we show that there are only two extreme piecwise linear MDFFs, which are convex on $\left[0, \frac{1}{2}\right]$.

Proposition 3. *If an extreme MDFF $f: [0,1] \to [0,1]$, different from the Fekete and Schepers-function with $k = 1$, is convex in $\left(0, \frac{1}{2}\right)$, then f is continuous on $[0,1]$.*

Proof. Due to the convexity in $\left(0, \frac{1}{2}\right)$ it follows immediately that f is continuous in $\left(0, \frac{1}{2}\right)$. Since

$0 \le f(x) \le \frac{1}{\lfloor 1/x \rfloor}$ for $0 < x \le 1$, the continuity holds also at the spot 0. Let $a := \lim_{x \uparrow 1/2} f(x)$. Clearly, $0 < a \le \frac{1}{2}$ due to the restriction on f. If $a < \frac{1}{2}$ would hold, then let $b := \min\left\{2, \frac{1}{2a}\right\} > 1$ and define functions $g, h: [0,1] \to [0,1]$ as

$$g(x) := \begin{cases} b * f(x), \text{ if } 0 \le x < 1/2\,, \\ 1/2\,, \quad \text{ for } x = 1/2\,, \\ 1 - g(x), \quad \text{otherwise;} \end{cases}$$

$$h(x) := 2f(x) - g(x) \text{ for } 0 \le x \le 1.$$

For $0 \le x < \frac{1}{2}$ one has $h(x) = (2 - b) * f(x)$. The convexity of f in $\left(0, \frac{1}{2}\right)$ implies in conjuction with $1 < b \le 2$ that g, h are convex in $\left(0, \frac{1}{2}\right)$ too. Moreover $g \not\equiv f$ and g, h are MDFFs due to Theorem 1. Therefore, f would not be extreme. This contradiction proves $a = 1/2$, hence f is continuous at $\frac{1}{2}$ too. ■

A clue to disprove that a given differentiable function f like (3), which is constructed from a convex function according to Theorem 1, is extreme, is the following. Draw the tangents to the graph of f in the points $(0; 0)$ and $\left(\frac{1}{2}; \frac{1}{2}\right)$. If f isn't the identity function, then both tangents have a unique common point $(a; b)$ with $0 < a < \frac{1}{2}$ because of the convexity of f in $\left[0, \frac{1}{2}\right]$. Let

$$g(x) := \begin{cases} x * f'(0), \text{ if } 0 \le x \le a; \\ \frac{1}{2} + \left(x - \frac{1}{2}\right) * f'\left(\frac{1}{2}\right), \text{ if } x \in [a, 1-a]\,; \\ 1 - g(1 - x), \text{ if } 1 - a \le x \le 1. \end{cases} \qquad (4)$$

Then $g: [0,1] \to [0,1]$ is obviously a MDFF. If the function $h: [0,1] \to [0,1]$ with $h(x) = 2 * f(x) - g(x)$ for all $x \in [0,1]$ is superadditive, then f is not extreme. In the case of the function (3) one has $f'(0) = 0$ and $f'\left(\frac{1}{2}\right) = 2$, hence $a = \frac{1}{4}$.

This approach needs not to work always. To show that, a special differentiable convex (but not strict convex) function $f: \left[0, \frac{1}{2}\right] \to \left[0, \frac{1}{2}\right]$ is constructed, which can be used with Theorem 1 as counter example. First choose a very small $c > 0$. Let initially

$$f(x) := \begin{cases} x^2/(8c) \text{ for } 0 \le x \le c; \\ x/4 - c/8 \text{ for } c \le x < 2/5\,; \\ 4x - 3/2 \text{ for } 2/5 \le x \le 1/2\,. \end{cases}$$

Now replace f in an environment of $x = \frac{2}{5}$ by a strict convex function, such that f becomes differentiable in the whole interval $\left(0, \frac{1}{2}\right)$. That yields $f'(0) = 0$ and $f'\left(\frac{1}{2}\right) = 4$, hence $a = \frac{3}{8}$. For some $x \in \left(a, \frac{2}{5}\right)$ it follows that $f'(x) = \frac{1}{4}$, but $g'(x) = 4 > 2 * f'(x)$, where g is the function (4). Hence, $h'(x) < 0$, yielding that the other function h is not monotonous and therefore not a MDFF.

Let X and Y be metrical spaces with metrics ϱ and σ, respectively. A *uniform continuous* function $f: X \to Y$ has the property that for each $\varepsilon > 0$ there is a $\delta > 0$, such that for any $x, y \in X$ with $\varrho(x, y) < \delta$ it holds that $\sigma\big(f(x), f(y)\big) < \varepsilon$. Any continuous function on a compact set is there uniformly continuous. If the domain of f is not compact, then this property of f is more than the point-by-point continuity where δ may depend on the point x or y.

In the following, sometimes a derivative f' of a function f will be discussed on a closed interval $[a, b]$. In that case we mean that f' exists in an open set, which contains $[a, b]$.

Theorem 2. *Let $f: [0,1] \to [0,1]$ be a MDFF, such that f is convex on $\left[0, \frac{1}{2}\right]$. If there is an $\tilde{x} \in \left(0, \frac{1}{2}\right)$, such that f is twice continuously differentiable in an environment of $\tilde{x}$ and if $f''(\tilde{x}) > 0$, then f is not extreme.*

Proof. Due to the continuity of f'' in an environment of $\tilde{x}$ and $f''(\tilde{x}) > 0$ there are numbers a, b, c with $0 < a < b < \frac{1}{2}$ and $c > 0$, such that f has a continuous second derivative on $[a, b]$ and $f''(x) \ge c$ for all $x \in [a, b]$. As a MDFF, f is monotonous, hence $f'(b) \ge 0$. For an enough small $\lambda \in \left]0, \frac{\sqrt{3}(b-a)^2 c}{(b-a)c + 4\sqrt{3} f'(b)}\right]$, let

$$l(x) := \begin{cases} x^4 - 2x^3 + x^2, \quad \text{if } 0 \le x \le 1, \\ 0, \quad \text{otherwise,} \end{cases}$$

and

$$m(x) := x + \lambda * l\left(\frac{x - a}{b - a}\right).$$

The function l is once continuously differentiable, and it holds that $0 \le l(x) \le \frac{1}{16}$ for all x, because $x^4 - 2x^3 + x^2 = (x^2 - x)^2$.

The functions g, h are defined by

$$g(x) := \begin{cases} f(m(x)), & \text{if } 0 \le x \le 1/2, \\ 1 - g(1-x), & \text{otherwise,} \end{cases}$$

and

$$h(x) := 2f(x) - g(x),$$

hence $f(x) = g(x) = h(x)$ for $x \in \left[0, \frac{1}{2}\right] \backslash (a, b)$. Moreover, g, h are continuously differentiable on $[a, b]$, even twice in (a, b). It remains to show that g', h' are monotonously increasing on $[a, b]$ and $f \not\equiv g$.

For $0 < x < 1$ one has $l'(x) = 4x^3 - 6x^2 + 2x$ and $l''(x) = 12x^2 - 12x + 2$, hence l has turning points at $x_{1,2} = \frac{1}{2} \pm \frac{\sqrt{3}}{6}$ with $l(x_{1,2}) = \frac{1}{36}$ and $l'(x_{1,2}) = \mp\frac{\sqrt{3}}{9}$. Therefore, $m'(x) \ge 1 - \frac{\lambda}{b-a} * \frac{\sqrt{3}}{9} \ge 1 - \frac{(b-a)c}{3(b-a)c + 12\sqrt{3}f'(b)} \ge \frac{2}{3}$, *i.e.* m is strictly monotonous, hence $a \le m(x) \le b$ for all $x \in [a, b]$. Since $l'(x) > 0$ for $0 < x < \frac{1}{2}$, one has $g'(x) > f'(x)$ for $a < x < \frac{a+b}{2}$, *i.e.* $g \not\equiv f$. Because of $-1 \le l''(x) \le 2$ for all $x \in (0, 1)$ it follows for $a < x < b$ that $g''(x) = f''(m(x)) * m'(x) + f'(m(x)) * m''(x) \ge c * \left(1 - \frac{\lambda}{b-a} * \frac{\sqrt{3}}{9}\right) - \frac{\lambda}{(b-a)^2} * f'(b) \ge c - \frac{c}{(b-a)c + 4\sqrt{3}f'(b)} * \left(\frac{c}{3}(b-a) + f'(b) * \sqrt{3}\right) \ge \frac{2}{3}c$, hence g' is monotonously increasing on $[a, b]$ due to the mean value theorem of differential calculus.

Investigating h, one has first $h''(x) \ge 2f''(x) - f''(m(x)) * \left(1 + \frac{\lambda}{b-a} * \frac{\sqrt{3}}{9}\right) - f'(b) * \frac{2\lambda}{(b-a)^2}$. Since f'' is uniformly continuous on $[a, b]$, there is a constant $\delta > 0$, such that $|f''(x) - f''(y)| < \frac{c}{2}$ for all $x, y \in [a, b]$ with $|x - y| \le \delta$. If $\lambda \le 16\delta$ then $|m(x) - x| \le \delta$ and therefore $f''(m(x)) \le f''(x) + \frac{c}{2}$, hence $h''(x) \ge c * \left(1 - \frac{\lambda}{b-a} * \frac{\sqrt{3}}{9}\right) - \frac{c}{2} * \left(1 + \frac{\lambda}{b-a} * \frac{\sqrt{3}}{9}\right) - f'(b) * \frac{2\lambda}{(b-a)^2} \ge \frac{c}{2} - \left((b-a)c * \frac{\sqrt{3}}{6} + 2f'(b)\right) * \frac{\sqrt{3}c}{(b-a)c + 4\sqrt{3}f'(b)} = 0$. The new restriction $0 < \lambda \le \min\left\{16\delta, \frac{\sqrt{3}(b-a)^2 c}{(b-a)c + 4\sqrt{3}f'(b)}\right\}$ guarantees $h''(x) \ge 0$ for all $x \in (a, b)$ and therefore also the monotony of h'. ■

One opportunity to avoid the prerequisites of Theorem 2 is the usage of piecewise linear functions, but that does not guarantee extremality, as the following proposition shows.

Proposition 4. *Let $f: [0, 1] \to [0, 1]$ be a MDFF different from $f_{FS,1}(\cdot; 1)$ and from the identity function, such that f is convex in $\left(0, \frac{1}{2}\right)$ and piecewise linear. Then f is not extreme.*

Proof. Suppose that f is extreme. Then Proposition 3 states that f is continuous on $[0, 1]$. We have to distinguish several cases about the intervals of different slopes.

A. Let us begin with the case of many such intervals, *i.e.* assume that there are $x_0, x_1, x_2, x_3, y_0, y_1, y_2, y_3 \in \mathbb{R}$ with $0 \le x_0 < x_1 < x_2 < x_3 = \frac{1}{2}$ and $m_i := \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$ for $i \in \{0, 1, 2\}$, such that $m_0 < m_1 < m_2$ and $f(x) = y_i + (x - x_i) * m_i$ for all $x \in [x_i, x_{i+1}]$, $i \in \{0, 1, 2\}$. The idea will be to replace f in the interval (x_1, x_3) by two other piecewise linear functions, such that they remain convex in $\left[0, \frac{1}{2}\right]$. Let

$$t := \max\left\{y_1 + m_0 * (x_2 - x_1), 2y_2 - \frac{(x_2 - x_1) * y_3 + (x_3 - x_2) * y_1}{x_3 - x_1}\right\}.$$

Now $t < y_2$ will be shown. Indeed, we have $y_2 - y_1 - m_0 * (x_2 - x_1) = (x_2 - x_1) * (m_1 - m_0) > 0$ and $m_2 > m_1$, hence $(y_3 - y_2) * (x_2 - x_1) + (y_2 - y_1) * (x_2 - x_3) > 0$, implying $(x_2 - x_1) * y_3 + (x_3 - x_2) * y_1 > (x_3 - x_1) * y_2$ and again $t < y_2$. Define the functions $g, h: \left[0, \frac{1}{2}\right] \to \left[0, \frac{1}{2}\right]$ by

$$g(x) := \begin{cases} f(x), \text{ if } x \notin (x_1, x_3), \\ y_1 + (x - x_1) * \frac{t - y_1}{x_2 - x_1}, \text{ if } x \in [x_1, x_2], \\ y_3 + (x - x_3) * \frac{t - y_3}{x_2 - x_3}, \text{ if } x \in [x_2, x_3], \end{cases}$$

and

$$h(x) := \begin{cases} f(x), \text{ if } x \notin (x_1, x_3), \\ y_1 + (x - x_1) * \dfrac{2y_2 - t - y_1}{x_2 - x_1}, \text{ if } x \in [x_1, x_2], \\ y_3 + (x - x_3) * \dfrac{2y_2 - t - y_3}{x_2 - x_3}, \text{ if } x \in [x_2, x_3]. \end{cases}$$

Both functions g, h are convex, as shown next. They are piecewise linear and continuous. It remains to check the slopes: $t < y_2$ implies $\frac{t-y_1}{x_2-x_1} < \frac{y_2-y_1}{x_2-x_1} < \frac{y_3-y_2}{x_3-x_2} < \frac{y_3-t}{x_3-x_2}$ and $m_0 < m_1 < \frac{2y_2-t-y_1}{x_2-x_1}$. The definition of t yields the other two needed inequalities, namely $m_0 \leq \frac{t-y_1}{x_2-x_1}$ since $t \geq y_1 + m_0 * (x_2 - x_1)$, and $t \geq 2y_2 - \frac{(x_2-x_1)*y_3+(x_3-x_2)*y_1}{x_3-x_1}$ implies $\frac{2y_2-t-y_3}{x_2-x_3} - \frac{2y_2-t-y_1}{x_2-x_1} = \frac{(t-2y_2)*(x_3-x_1)+y_1*(x_3-x_2)+y_3*(x_2-x_1)}{(x_2-x_1)*(x_3-x_2)} \geq 0$, as desired. Since $g(0) = h(0) = f(0) = 0$ and g, h are convex on $\left[0, \frac{1}{2}\right]$, both functions can be used according to Theorem 1 to construct MDFFs different from f. Since it holds that $2f(x) = g(x) + h(x)$ for all $x \in \left[0, \frac{1}{2}\right]$ and $f(x_2) = y_2 > t = g(x_2)$, the function f is not extreme. To finish the proof, we need to check the situation of at most two intervals of different slopes in $\left[0, \frac{1}{2}\right]$.

B. If there are $x_1, x_2, x_3, y_1, y_2, y_3 \in \mathbb{R}$ with $0 = x_1 < x_2 < x_3 = \frac{1}{2}$ and $m_i := \frac{y_{i+1}-y_i}{x_{i+1}-x_i}$ for $i \in \{1, 2\}$, such that $0 < m_1 < m_2$ and $f(x) = y_i + (x - x_i) * m_i$ for $x \in [x_i, x_{i+1}]$ and $i \in \{1, 2\}$, then the same proof can be used with $m_0 := 0$.

C. If f has the same behaviour as in case (B.) except $m_1 = 0$ instead of $m_1 > 0$, then we get $y_2 = 0$, such that f becomes the Burdett ad Johnson-function $f_{BJ,1}$ with parameter $C = \frac{1}{1-x_2} \in (1, 2)$. As proved in [9], Proposition 1, $f_{BJ,1}$ is not extreme for $1 < C < 2$, hence f is not extreme in this case too.

D. If f has a constant slope in the entire interval $\left[0, \frac{1}{2}\right]$ and is continuous on $[0, 1]$, then f is the identity function, but this case was disclosed in the prerequisites. Therefore, all cases were checked. ∎

Theorem 2 and Proposition 4 imply that MDFFs, which are convex in $\left(0, \frac{1}{2}\right)$, are generally not extreme.

4 Computational tests

To illustrate the observation that $f_{BJ,1}$ dominates $f_{FS,1}$ in the 1D-CSP with integer data, fast feasible lower bounds for 54000 instances of 1D-BPP (with order demands 1 for all items, which may occur repeatedly) were calculated with very low complexity as described in Subsection 2.1. Each of the following classes contained 1000 instances:

1. Container size $L = 100$

    a) all item sizes between 1 and 100
        A) $m = 100$ items
        B) $m = 500$ items
        C) $m = 1000$ items

    b) like classes 1aA–1aC, but item sizes between 20 and 100
    c) like classes 1aA–1aC, but item sizes between 35 and 100

2. Same instances as in classes 1aA–1cC except the changed container size $L = 125$

3. Same instances as in classes 1aA–1cC except the changed container size $L = 150$

4. Same instances as in classes 1aA–1cC except the changed container size $L = 200$

5. Same instances as in classes 1aA–1cC except the changed container size $L = 250$

6. Same instances as in classes 1aA–1cC except the changed container size $L = 300$

The only change between the classes 1.–6. (for the same subclass) was the container size; the item sizes and their order demands were exactly the same. The idea for this approach was that the instances of the classes 1cA–1cC can be solved easily to optimality. Increasing the container size, such that three small items may fit in one container, makes the instances harder to solve them exactly.

For each instance $E := (m; L; \mathfrak{l}; \mathfrak{b})$, the material bound $z_M = \mathfrak{l}^T\mathfrak{b}/L$ and the bounds $z[f_{FS,1}]$ and $z[f_{BJ,1}]$ were calculated. The parameters for the MDFFs $f_{FS,1}$ and $f_{BJ,1}$ were chosen on the base of continued fractions.

The results presented in Table 1 were obtained in each class for the sum of the material bounds ($\sum z_M$), the sum S_1 and the minimum M_1 of the differences $z[f_{FS,1}] - z_M$, *i.e.* $S_1 := \sum(z[f_{FS,1}] - z_M)$ and $M_1 := \min\{z[f_{FS,1}] - z_M\}$, and the sum S_2 and the minimum M_2 of the differences $z[f_{BJ,1}] - z[f_{FS,1}]$, *i.e.* $S_2 := \sum(z[f_{BJ,1}] - z[f_{FS,1}])$ and $M_2 := \min\{z[f_{BJ,1}] - z[f_{FS,1}]\}$.

Class	$\sum z_M$	S_1	M_1	S_2	M_2
2bB	238086.33	1355.49	0	23.21	0
2bC	476101.21	1107.12	0	30.79	0
3cA	44679.79	365.63	0	80.66	0
3cB	223333.96	308.63	0	413.16	0
3cC	446756.26	265.05	0	725.6	0

Table 1: Computational results (part I)

For the set of instances that are not reported in Table 1, the sum S_2 was less than 20. Clearly, if there are DFFs f and g with $z[f] < z[g]$, then multiplying the order demands by an integer above 1 increases the difference between the found bounds. Therefore, the highest values of S_2 could occur for large numbers m of items only.

The function $f_{BJ,1}$ clearly dominates $f_{FS,1}$, particularly in the classes 3cC and 3cB, while the computational effort remained very small. That confirms the stated opportunity to replace $f_{FS,1}$ by $f_{BJ,1}$.

The comparison between $f_{VB,2}$ and $f_{CCM,1}$ is much more impressive (see Table 2). We used the same instances again. The parameter k was also chosen based on continued fractions. Let S denote the sum of the differences $z[f_{CCM,1}] - z[f_{VB,2}]$, *i.e.* $S := \sum(z[f_{CCM,1}] - z[f_{VB,2}])$. The minimum $\min\{z[f_{CCM,1}] - z[f_{VB,2}]\}$ was always zero. For ease of compactness, only classes with $S > 20$ are shown in Table 2.

Class	$\sum z_M$	$\sum z[f_{VB,2}]$	S
1aA	50005.53	51779.76	491.21
2aA	40004.49	40408.82	266.87
1aB	250165.18	254053.81	1194.78
2aB	200132.25	200223	70.33
1aC	500403.26	505836.81	1734.92
1bA	59451.46	63513.37	671.39
2bA	47561.2	48726.35	490.57
1bB	297608.04	313255.01	1504.97
2bB	238086.33	239440.62	582.77
1bC	595126.43	624250.86	2219.16
2bC	476101.21	477208.24	483.18
1cA	67019.66	77215.5	1175.5
2cA	53615.76	58627.08	1161.81
3cA	44679.79	45049.56	88.45
1cB	335001.04	382188.5	3341.5
2cB	268000.73	288241.83	2669.9
3cB	223333.96	223643.02	45.53
1cC	670134.43	763144	5422
2cC	536107.61	574557	3799.45

Table 2: Computational results (part II)

Of course, the largest difference between the two calculated bounds occurred normally, when the order demands were the highest, namely in class 1cC. On the other hand, the effect of no dominance in the case of small items only (classes 4–6) could also be verified. Then always $z[f_{VB,2}] = z[f_{CCM,1}]$ was found.

5 Conclusion

In this paper, we proved that the MDFFs $f_{FS,1}$ and $f_{VB,2}$ are dominated by other MDFFs under the very weak prerequisite that all data are integer. Therefore, these functions can be replaced by others without getting worse results. On the other hand, none of the MDFFs $f_{BJ,1}$ and $f_{CCM,1}$ is dominated by the other, therefore both functions should be used to calculate valid bounds. Since it is impossible to try all feasible parameters for $f_{BJ,1}$ to replace $f_{FS,1}$, we proposed an algorithm to find useful parameters with very small complexity and tested it with success.

Convex functions can be used to construct MDFFs. In this paper, we have shown that, except the identity function and $f_{FS,1}(\cdot; 1)$, there is no piecewise linear extreme MDFF, which is convex in $\left(0, \frac{1}{2}\right)$.

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