SIAM J. OPTIM.
Vol. 30, No. 1, pp. 853–884

CALCULUS IDENTITIES FOR GENERALIZED SIMPLEX GRADIENTS: RULES AND APPLICATIONS*

WARREN HARE† AND GABRIEL JARRY-BOLDUC†

Abstract. Simplex gradients, essentially the gradient of a linear approximation, are a popular tool in derivative-free optimization (DFO). In 2015, a product rule, a quotient rule, and a sum rule for simplex gradients were introduced by Regis [*Optim. Lett.*, 9 (2015), pp. 845–865]. Unfortunately, those calculus rules only work under a restrictive set of assumptions. The purpose of this paper is to provide new calculus rules that work in a wider setting. The rules place minimal assumptions on the functions involved and the interpolation sets. The rules further lead to an alternative approach to gradient approximation in situations where the rules could be applied. We analyze the new approach, provide error bounds, and include some preliminary testing on numerical stability and accuracy.

Key words. simplex gradient, gradient approximation, calculus identities

AMS subject classifications. 49M25, 90C56, 65K15

DOI. 10.1137/18M1215864

1. Introduction.

Derivative-free optimization (DFO) is defined as the mathematical study of algorithms for continuous optimization that do not employ first-order information (derivatives, gradients, directional derivatives, subgradients, etc.). Derivative-free methods are valuable when derivatives are unavailable, for instance, when the objective function is computed using a blackbox simulation process [5, section 1.1]. We can classify derivative-free methods into two main categories: model-based methods and direct search methods. In both categories, simplex gradients can play an important role.

In DFO, a model-based method approximates the objective function with a model function and then utilizes the model function to command the optimization. The beginning of model-based methods occurred in 1969 when Winfield presented his Ph.D. thesis *Function and Functional Optimization by Interpolation in Data Tables* [19]. However, model-based DFO methods were generally considered too computationally expensive until the mid 1990's, when Powell developed rigorous analysis for a method based on linear interpolation [14]. This led to the development of simplex gradients, essentially the gradient of a linear approximation. Simplex gradients are now frequently used in DFO. More recently, a meticulous theory on building models was developed by Conn, Scheinberg, and Vicente [3, 4]. The main value of simplex gradients in model-based methods is to determine a descent direction of the true function [1, Chapter 10]. Even when the objective function is nonsmooth, simplex gradients can be defined and can help solve the optimization problem [6].

A direct search method (DSM) is a directional type of method that works from an incumbent solution and analyzes a collection of trial points to find improvement in the objective function. If no improvement is found, then a step size parameter is decreased. Initial works on DSM include Hooke and Jeeves [10] and Nelder and

*Received by the editors September 21, 2018; accepted for publication (in revised form) January 7, 2020; published electronically March 10, 2020.
https://doi.org/10.1137/18M1215864
Funding: This work was partially supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada, Discover grant 2018-03865.
†Department of Mathematics, University of British Columbia, Kelowna, BC, V1V 1V7, Canada (warren.hare@ubc.ca, gabjarry@alumni.ubc.ca).

Mead [13], published in the 1960's. In 2007, Custódio and Vicente suggested various strategies to improve the performance of DSMs using the simplex gradient [7]. A year after, Custódio, Dennis, and Vicente [6] demonstrated that the efficiency of DSM can be improved by reordering the poll directions according to descent indicators built from simplex gradients. Moreover, they defined a new stopping criterion for DSMs involving the simplex gradient [6]. Several properties of simplex gradients were analyzed in *Iterative Methods for Optimization* [11]. Error bounds for the simplex gradient were provided, and the notion of centered simplex gradient was introduced. Thereafter, the importance of the sample set geometry (*poisedness*), which is used to build the simplex gradient, was deeply investigated [3, 4]. In 2010, the strong dependence between the geometry of the sample set and global convergence of a model-based algorithm was revealed [17]. The utility of simplex gradients in nonsmooth optimization is an active area of research. On that topic, Bortz and Kelley presented some benefits of using simplex gradients to solve noisy optimization problems [2]. In 2015, Regis proposed some calculus rules for the simplex gradient: a product rule, a quotient rule, and a sum rule [16]. Unfortunately, those rules only work under a restrictive set of assumptions. In 2017, Hare began investigating compositions of functions [9].

To inspire the value of calculus rules for approximate gradients, let us consider a recent publication by Rashki [15]. In [15], Rashki presents a problem in optimization of structural reliability where the objective function takes the form of a probability of failure generated through a blackbox integration. Using Bayes's theorem, Rashki rewrites the problem as the product of conditional probabilities, each of which is given by a blackbox. Rashki demonstrates that the restructured problem provides the objective function value at reduced computational cost. In relevance to this work, we point out that the result is a function that is the product of two blackbox simulations. More generally, suppose the functions $f_i(x)$ for all $i \in \{1, 2, \ldots, n\}$ are blackboxes returning the probability of an event taking place depending on a variable $x \in \mathbb{R}^d$. Assume we are interested in minimizing the probability of these n events happening simultaneously. In other words, we want to minimize $F(x) = f_1(x)f_2(x)\cdots f_n(x)$. If we are to approach this via model-based DFO, then a product rule for approximate gradients becomes immediately valuable.

The goal of this paper is to present a rigorous repertoire of calculus rules for the generalized simplex gradient that works in a wider setting than the one introduced previously. Indeed, the following calculus rules can be used regardless of the number of points in the sample set and place minimal assumptions on the sample set. It also places minimal assumptions on the functions involved. It turns out that the calculus rules for simplex gradients introduced in this paper have the same structure as the classical calculus rules for gradients plus a term E that can be viewed as an error term. Removing the term E from the formula leads to new techniques to approximate gradients named *generalized simplex calculus gradients*. This new approach has some interesting benefits. For instance, in the quotient rule it allows us to remove some assumptions on the functions involved. Also, under a certain assumption on the interpolation set, this new approach suits linear functions perfectly.

Most of the time in DFO, extremely limited information about the functions involved is available to the optimizer. To decide on which gradient approximation technique to use on a specific problem, information about the Lipschitz constants may be useful. In that sense, we propose an algorithm to make this decision based on an approximation of the Lipschitz constants in section 7.

This paper is structured as follows. In section 2, we define the generalized simplex gradient and introduce some basic definitions. In section 3, we provide a product rule, a quotient rule, and a power rule. In section 4, we introduce a general chain rule for the generalized simplex gradient. In section 5, we explore the potential of the calculus rules. The role of the term E in the formulas is examined. We demonstrate that novel gradient approximation techniques can be achieved by removing this term E. The behavior of linear functions when used in the generalized simplex calculus gradient formulas is analyzed. Error bounds for the generalized simplex calculus gradients are also developed. In section 6, we briefly compare the numerical stability of the generalized simplex gradient, the generalized simplex gradient using the quotient rule, and the generalized simplex quotient gradient. Moreover, numerical experiments are conducted using Moré, Garbow, and Hillstrom's Test Set [12]. Last, section 7 summarizes the work we have accomplished, proposes an algorithm to approximate Lipschitz constants, and suggests some topics to explore in future research.

2. Generalized simplex gradient. Throughout this paper, we assume f is a real-valued function, $f : \mathbb{R}^d \to \mathbb{R}$. Consider a finite ordered set of sampling points $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$.[1] Define the *difference matrix*

$$S = S(\mathcal{X}) := \begin{bmatrix} x_1 - x_0 & x_2 - x_0 & \ldots & x_k - x_0 \end{bmatrix} \in \mathbb{R}^{d\times k}.$$

Define the *difference function matrix*[2]

$$\delta_f = \delta_f(\mathcal{X}) := \begin{bmatrix} \big(f(x_1) - f(x_0)\big)^T \\ \vdots \\ \big(f(x_k) - f(x_0)\big)^T \end{bmatrix}.$$

To make notation tighter, we use the notation S and δ_f without specifying the sampling set when there is only one set involved. If more than one set of points are involved (sections 4, 5, and 6), we use the entire notation and specify the sampling set of points to avoid any confusion.

If S is a $d \times d$ invertible matrix, then the simplex gradient of f with respect to $\mathcal{X}$ is

$$\nabla_s f(\mathcal{X}) = S^{-T}\delta_f. \tag{1}$$

We refer to this situation as the determined case. When the number of points $k+1$ is not equal to $d+1$ or S is not invertible, then the simplex gradient can be viewed as a solution of the system

$$S^T\nabla_s f(\mathcal{X}) = \delta_f. \tag{2}$$

If $k + 1 < d + 1$ affinely independent points are available, then we are in the underdetermined case and the simplex gradient can be calculated as the minimum Frobenius norm solution of (2): $\nabla_s f(\mathcal{X}) = \operatorname{argmin}\{\|g\|^2 : S^T g = \delta_f\}$.

If $k+1 > d+1$ distinct points are available and $d+1$ of those points are affinely independent, then we are in the overdetermined case and the simplex gradient is the least squares solution of (2): $\nabla_s f(\mathcal{X}) = \operatorname{argmin}\{\|S^T g - \delta_f\|^2\}$.

[1]It has been proved that the order of the set $\mathcal{X}$ affects our calculation of the generalized simplex gradient [16, Proposition 3]. In particular, the position of x_0 must be fixed. For this reason, we consider an ordered set $\mathcal{X}$.

[2]The usual definition of δ_f does not contain a transpose operator in every row. But for functions where the codomain is not $\mathbb{R}$, it is important to write $(f(x_i) - f(x_0))^T$ so that δ_f is well-defined.

Using the *Moore–Penrose pseudoinverse* of S^T, we can develop an equation to calculate the simplex gradient of f with respect to $\mathcal{X}$ that works for the three cases.

DEFINITION 1 (Moore–Penrose pseudoinverse). *Let $A \in \mathbb{R}^{k\times d}$. A matrix, denoted by $A^\dagger$, is called the Moore–Penrose pseudoinverse of A and satisfies the following four equations:*

1. $AA^\dagger A = A$
2. $A^\dagger AA^\dagger = A^\dagger$
3. $(AA^\dagger)^T = AA^\dagger$
4. $(A^\dagger A)^T = A^\dagger A$.

Note that every matrix $A \in \mathbb{R}^{k\times d}$ has a unique Moore–Penrose pseudoinverse $A^\dagger$.

DEFINITION 2 (generalized simplex gradient). *Let $\mathcal{X} = \langle x_0, x_1, \dots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. The generalized simplex gradient of f with respect to $\mathcal{X}$ is*

$$\nabla_s f(\mathcal{X}) = \left(S^T\right)^\dagger \delta_f. \tag{3}$$

In the determined and overdetermined cases, when f is smooth, an error bound between the generalized simplex gradient and the true gradient can be defined [16]. The accuracy of this bound is measured in terms of $\Delta := \max_{1\le i\le k} \|x_i - x_0\|$. We assume that the gradient of f is Lipschitz continuous on a domain containing the closed ball $B(x_0,\Delta) := \{x \in \mathbb{R}^d : \|x - x_0\| \le \Delta\}$ of the sample set $\mathcal{X}$ centered at x_0.

PROPOSITION 3 (error bound [16, Proposition 7]). *Let $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ where $k \ge d$, and let S have full rank. Assume that ∇f is Lipschitz continuous with Lipschitz constant $L_{\nabla f} \ge 0$ in an open domain Ω containing $B(x_0,\Delta)$. Define*

$$\varepsilon_s f(\mathcal{X}) := \frac{\sqrt{k}}{2} L_{\nabla f} \left\| \left(\widehat{S}^T\right)^\dagger \right\| \Delta,$$

where $\widehat{S} := S/\Delta$. Then

$$\|\nabla_s f(\mathcal{X}) - \nabla f(x_0)\| \le \varepsilon_s f(\mathcal{X}).$$

Now that we have an equation to calculate the generalized simplex gradient and presented the significant definitions, we are ready to discuss calculus rules for the generalized simplex gradient.

2.1. Review of Regis's results. Before presenting our calculus rules for generalized simplex gradient computation, we take a brief detour to examine the rules developed in [16]. We begin with the product rule presented in [16, Proposition 10].

Let f and g be functions from $\mathbb{R}^d$ to $\mathbb{R}$ and $\mathcal{X} = \langle x_0, x_1, \dots, x_k\rangle$ be an ordered set of $k+1$ points. The product rule presented in [16, Proposition 10] states that, under some conditions to be discussed momentarily,

$$\nabla_s(fg)(\mathcal{X}) = f(x_0)\nabla_s g(\mathcal{X}) + \mathrm{diag}[g(x_1)\ g(x_2)\ \dots\ g(x_k)]\nabla_s f(\mathcal{X}), \tag{4}$$

where $\mathrm{diag}[g(x_1)\ \dots\ g(x_k)]$ represents the diagonal matrix that is generated by $[g(x_1)\ \dots\ g(x_k)]$. Proposition 10 of [16] states only that S forms a matrix with full rank. This makes the rule look very flexible in application. However, a quick examination of the rule makes it clear that the square matrix $\mathrm{diag}[g(x_1)\ \dots\ g(x_k)]$ must be $d\times d$, or its multiplication with the $d\times 1$ vector $\nabla_s f(\mathcal{X})$ is nonsense. As such, the rule can only be considered in the determined case.

Unfortunately, the proof of [16, Proposition 10] contains a second error. On page 862, line 1, the proof claims that "a diagonal matrix commutes with any other matrix (assuming the products are defined)." This is easily proven false, as

$$\begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} = \begin{bmatrix} 4 & -3 \\ -2 & 3 \end{bmatrix} \neq \begin{bmatrix} 4 & -2 \\ -3 & 3 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix}\begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}.$$

In the proof, this false statement is applied to the matrices $\operatorname{diag}[g(x_1)\ \dots\ g(x_k)]$ and $\left(S^T\right)^\dagger$ to allow the manipulation required to complete the proof. The example above is a perfectly reasonable situation that, for example, can be generated by setting

$$\mathcal{X} = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \quad \text{and} \quad g(x) = [1\ 1]x.$$

As a result, the correct conditions required for [16, Proposition 10] to hold are that the matrices $\operatorname{diag}[g(x_1)\ \dots\ g(x_k)]$ and $\left(S^T\right)^\dagger$ commute. This appears to be a highly restrictive assumption that is not easily checked.

Continuing to the quotient rule presented in [16, Proposition 11], the proof applies the product rule in [16, Proposition 10]. So again, the conditions required for [16, Proposition 11] to hold are that the matrices $\operatorname{diag}[g(x_1)\ \dots\ g(x_k)]$ and $\left(S^T\right)^\dagger$ commute. Similar statements can be made for Corollary 2, Proposition 12, and Corollary 3 in [16].

3. Product, quotient, and power rules. Throughout this section, let f and g be functions from $\mathbb{R}^d$ to $\mathbb{R}$.

We begin by providing a product rule that can be used regardless of the number of points in the sample set $\mathcal{X}$. First, we define the *product difference vector*.

DEFINITION 4 (product difference vector). *Let $\mathcal{X} = \langle x_0, x_1, \dots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. The product difference vector of f and g with respect to $\mathcal{X}$ is*

$$\delta_{f|g} = \delta_{f|g}(\mathcal{X}) := \begin{bmatrix} (f(x_1) - f(x_0))(g(x_1) - g(x_0)) \\ (f(x_2) - f(x_0))(g(x_2) - g(x_0)) \\ \vdots \\ (f(x_k) - f(x_0))(g(x_k) - g(x_0)) \end{bmatrix}.$$

Note that the product difference vector is the componentwise multiplication $\delta_f \odot \delta_g = \delta_{f|g}$. The product difference vector allows us to create a product rule for the generalized simplex gradient of fg with respect to $\mathcal{X}$. The resulting rule is structurally similar to the true gradient plus a term E_{fg}. Without further ado, let us introduce the product rule.

THEOREM 5 (product rule). *Let $\mathcal{X} = \langle x_0, x_1, \dots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Then*

$$\nabla_s(fg)(\mathcal{X}) = f(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f(\mathcal{X}) + E_{fg},$$

where $E_{fg} = \left(S^T\right)^\dagger \delta_{f|g}$.

Proof. We have

$$\begin{aligned}
\nabla_s(fg)(\mathcal{X}) &= \left(S^T\right)^\dagger \delta_{fg}\\
&= \left(S^T\right)^\dagger \begin{bmatrix} f(x_1)g(x_1) - f(x_0)g(x_0)\\ \vdots \\ f(x_k)g(x_k) - f(x_0)g(x_0)\end{bmatrix}\\
&= \left(S^T\right)^\dagger \left(\begin{bmatrix} f(x_0)g(x_1) - f(x_0)g(x_0)\\ \vdots \\ f(x_0)g(x_k) - f(x_0)g(x_0)\end{bmatrix} + \begin{bmatrix} f(x_1)g(x_0) - f(x_0)g(x_0)\\ \vdots \\ f(x_k)g(x_0) - f(x_0)g(x_0)\end{bmatrix} + \begin{bmatrix} f(x_1)g(x_1) + f(x_0)g(x_0) - f(x_0)g(x_1) - f(x_1)g(x_0)\\ \vdots \\ f(x_k)g(x_k) + f(x_0)g(x_0) - f(x_0)g(x_k) - f(x_k)g(x_0)\end{bmatrix}\right)\\
&= f(x_0)\left(S^T\right)^\dagger \begin{bmatrix} g(x_1) - g(x_0)\\ \vdots \\ g(x_k) - g(x_0)\end{bmatrix} + g(x_0)\left(S^T\right)^\dagger \begin{bmatrix} f(x_1) - f(x_0)\\ \vdots \\ f(x_k) - f(x_0)\end{bmatrix} + \left(S^T\right)^\dagger \begin{bmatrix} (f(x_1) - f(x_0))(g(x_1) - g(x_0))\\ \vdots \\ (f(x_k) - f(x_0))(g(x_k) - g(x_0))\end{bmatrix}\\
&= f(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f(\mathcal{X}) + \left(S^T\right)^\dagger \delta_{f|g}. \qquad \square
\end{aligned}$$

Notice that the product rule is *symmetric*, in the sense that the formula for $\nabla_s(fg)(\mathcal{X})$ is identical to the formula created from $\nabla_s(gf)(\mathcal{X})$.[3] The product rule immediately produces the following corollary for the simplex gradient of f^n with respect to $\mathcal{X}$ where n is a positive integer.

COROLLARY 6 (power rule for a positive integer exponent). *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ and n be a positive integer. Then*

$$\nabla_s f^n(\mathcal{X}) = n[f(x_0)]^{n-1}\nabla_s f(\mathcal{X}) + E_{f^n},$$

where

$$E_{f^n} = \left(S^T\right)^\dagger \left(\sum_{i=1}^{n-1}[f(x_0)]^{n-1-i}\delta_{f|f^i}\right).$$

Proof. We prove this by induction on n. When $n = 1$, we have

$$\begin{aligned}
\nabla_s f(\mathcal{X}) &= 1\nabla_s f(\mathcal{X}) + 0\\
&= 1[f(x_0)]^0\nabla_s f(\mathcal{X}) + \left(S^T\right)^\dagger \left(\sum_{i=1}^{0}[f(x_0)]^{-1}\delta_{f|f^1}\right)
\end{aligned}$$

since an empty sum is equal to zero. Next, assume the equation is true for $n = \ell$ for some integer $\ell \geq 1$. Considering $\nabla_s f^{\ell+1}(\mathcal{X})$, we see that

$$\begin{aligned}
\nabla_s f^{\ell+1}(\mathcal{X}) &= \nabla_s\left(f^\ell(\mathcal{X})f(\mathcal{X})\right)\\
&= [f(x_0)]^\ell\nabla_s f(\mathcal{X}) + f(x_0)\nabla_s f^\ell(\mathcal{X}) + \left(S^T\right)^\dagger \delta_{f|f^\ell}\\
&= [f(x_0)]^\ell\nabla_s f(\mathcal{X}) + f(x_0)\left(\ell[f(x_0)]^{\ell-1}\nabla_s f(\mathcal{X}) + \left(S^T\right)^\dagger \sum_{i=1}^{\ell-1}[f(x_0)]^{\ell-1-i}\delta_{f|f^i}\right) + \left(S^T\right)^\dagger \delta_{f|f^\ell}\\
&= [f(x_0)]^\ell\nabla_s f(\mathcal{X}) + \ell[f(x_0)]^\ell\nabla_s f(\mathcal{X}) + \left(S^T\right)^\dagger f(x_0)\sum_{i=1}^{\ell-1}[f(x_0)]^{\ell-1-i}\delta_{f|f^i} + \left(S^T\right)^\dagger \delta_{f|f^\ell}\\
&= (\ell+1)[f(x_0)]^\ell\nabla_s f(\mathcal{X}) + \left(S^T\right)^\dagger \left(\sum_{i=1}^{\ell-1}[f(x_0)]^{\ell-i}\delta_{f|f^i} + \delta_{f|f^\ell}\right)\\
&= (\ell+1)[f(x_0)]^\ell\nabla_s f(\mathcal{X}) + \left(S^T\right)^\dagger \left(\sum_{i=1}^{\ell}[f(x_0)]^{\ell-i}\delta_{f|f^i}\right).
\end{aligned}$$

Hence, the equation is also true for $n = \ell + 1$. The induction is complete. $\square$

[3] We mention this since the product rule presented in [16, Proposition 10], equation (4) herein, does not share this property.

Next, we extend the product rule for the general case of n functions. We require the following lemma.

LEMMA 7. *Let $f_i : \mathbb{R}^d \to \mathbb{R}$ for all $i \in \{1, 2\}$. Then*

$$\delta_{f_1 f_2} = f_1(x_0)\delta_{f_2} + f_2(x_0)\delta_{f_1} + \delta_{f_1|f_2}.$$

Proof. We have

$$\begin{aligned}
\delta_{f_1 f_2} &= \begin{bmatrix} (f_1 f_2)(x_1) - (f_1 f_2)(x_0) \\ \vdots \\ (f_1 f_2)(x_k) - (f_1 f_2)(x_0) \end{bmatrix} \\
&= \begin{bmatrix} (f_1 f_2)(x_1) - (f_1 f_2)(x_0) + f_1(x_0)f_2(x_1) - f_1(x_0)f_2(x_1) + f_1(x_1)f_2(x_0) - f_1(x_1)f_2(x_0) \\ \vdots \\ (f_1 f_2)(x_k) - (f_1 f_2)(x_0) + f_1(x_0)f_2(x_k) - f_1(x_0)f_2(x_k) + f_1(x_k)f_2(x_0) - f_1(x_k)f_2(x_0) \end{bmatrix} \\
&= f_1(x_0) \begin{bmatrix} f_2(x_1) - f_2(x_0) \\ \vdots \\ f_2(x_k) - f_2(x_0) \end{bmatrix} + f_2(x_0) \begin{bmatrix} f_1(x_1) - f_1(x_0) \\ \vdots \\ f_1(x_k) - f_1(x_0) \end{bmatrix} + \begin{bmatrix} (f_1(x_1) - f_1(x_0))\,(f_2(x_1) - f_2(x_0)) \\ \vdots \\ (f_1(x_k) - f_1(x_0))\,(f_2(x_k) - f_2(x_0)) \end{bmatrix} \\
&= f_1(x_0)\delta_{f_2} + f_2(x_0)\delta_{f_1} + \delta_{f_1|f_2}. \qquad \square
\end{aligned}$$

PROPOSITION 8 (product rule for n functions). *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$, and let $f_i : \mathbb{R}^d \to \mathbb{R}$ for all $i \in \{1, 2, \ldots, n\}$, where $n \geq 2$. Then*

$$\nabla_s \left(f_1 f_2 \cdots f_n \right)(\mathcal{X}) = \sum_{i=1}^{n} \left(\prod_{j \neq i} f_j(x_0) \right) \nabla_s f_i(\mathcal{X}) + E_{f_1 f_2 \cdots f_n},$$

where

$$E_{f_1 f_2 \cdots f_n} = \left(S^T \right)^{\dagger} \left(\delta_{f_1 f_2 \cdots f_n} - \sum_{i=1}^{n} \left(\prod_{j \neq i} f_j(x_0) \right) \delta_{f_i} \right).$$

Proof. We prove this by induction on n. When $n = 2$, using Lemma 7, we have

$$\begin{aligned}
\nabla_s \left(f_1 f_2 \right)(\mathcal{X}) &= f_2(x_0)\nabla_s f_1(\mathcal{X}) + f_1(x_0)\nabla_s f_2(\mathcal{X}) + \left(S^T \right)^{\dagger} \delta_{f_1|f_2} \\
&= f_2(x_0)\nabla_s f_1(\mathcal{X}) + f_1(x_0)\nabla_s f_2(\mathcal{X}) + \left(S^T \right)^{\dagger} \left(\delta_{f_1 f_2} - f_1(x_0)\delta_{f_2} - f_2(x_0)\delta_{f_1} \right) \\
&= \sum_{i=1}^{2} \left(\prod_{j \neq i} f_j(x_0) \right) \nabla_s f_i(\mathcal{X}) + \left(S^T \right)^{\dagger} \left(\delta_{f_1 f_2} - \sum_{i=1}^{2} \left(\prod_{j \neq i} f_j(x_0) \right) \delta_{f_i} \right).
\end{aligned}$$

Next, suppose the equation is true for $n = \ell$ for some integer $\ell \geq 2$.

Define $g := f_1 f_2 \cdots f_n$. Considering $\nabla_s \left(f_1 f_2 \cdots f_n f_{n+1} \right)(\mathcal{X})$, we see that

$$\begin{aligned}
\nabla_s \left(f_1 f_2 \cdots f_{n+1} \right)(\mathcal{X}) &= \nabla_s \left(g f_{n+1} \right)(\mathcal{X}) \\
&= f_{n+1}(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f_{n+1}(\mathcal{X}) + \left(S^T \right)^{\dagger} \delta_{g|f_{n+1}} \\
&= f_{n+1}(x_0) \left(\sum_{i=1}^{n} \left(\prod_{j \neq i} f_j(x_0) \right) \nabla_s f_i(\mathcal{X}) + E_{f_1 f_2 \cdots f_n} \right) + g(x_0)\nabla_s f_{n+1}(\mathcal{X}) + \left(S^T \right)^{\dagger} \delta_{g|f_{n+1}} \\
&= \left(\sum_{i=1}^{n+1} \left(\prod_{j \neq i} f_j(x_0) \right) \nabla_s f_i(\mathcal{X}) \right) + f_{n+1}(x_0) E_{f_1 f_2 \cdots f_n} + \left(S^T \right)^{\dagger} \delta_{g|f_{n+1}}.
\end{aligned}$$

To complete the proof, we must show that

$$f_{n+1}(x_0) E_{f_1 f_2 \cdots f_n} + \left(S^T \right)^{\dagger} \delta_{g|f_{n+1}} = E_{f_1 f_2 \cdots f_n f_{n+1}}.$$

Indeed, we have

$$\begin{aligned}
&f_{n+1}(x_0)E_{f_1f_2\cdots f_n} + \left(S^T\right)^\dagger \delta_{g|f_{n+1}} \\
&\quad= f_{n+1}(x_0)\left(S^T\right)^\dagger \left(\delta_g - \sum_{i=1}^{n}\left(\prod_{j\neq i} f_j(x_0)\right)\delta_{f_i}\right) + \left(S^T\right)^\dagger \delta_{g|f_{n+1}} \\
&\quad= \left(S^T\right)^\dagger \left[f_{n+1}(x_0)\delta_g - f_{n+1}(x_0)\left(\sum_{i=1}^{n}\left(\prod_{j\neq i} f_j(x_0)\right)\delta_{f_i}\right) + \delta_{g|f_{n+1}}\right] \\
&\quad= \left(S^T\right)^\dagger \left[f_{n+1}(x_0)\delta_g + g(x_0)\delta_{f_{n+1}} + \delta_{g|f_{n+1}} - \left(\sum_{i=1}^{n+1}\left(\prod_{j\neq i} f_j(x_0)\right)\delta_{f_i}\right)\right] \\
&\quad= \left(S^T\right)^\dagger \left(\delta_{f_1\cdots f_n f_{n+1}} - \left(\sum_{i=1}^{n+1}\left(\prod_{j\neq i} f_j(x_0)\right)\delta_{f_i}\right)\right) \quad \text{(by Lemma 7)} \\
&\quad= E_{f_1f_2\cdots f_n f_{n+1}}.
\end{aligned}$$

Therefore, the equation is true for $n = \ell + 1$ and the induction is complete. ∎

The following corollary presents an alternative formula whenever all f_i, $i \in \{1, 2, \ldots, n\}$, are equal.

Corollary 9. *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Also, let $f : \mathbb{R}^d \to \mathbb{R}$, and let n be a positive integer. Then*

$$\nabla_s f^n(\mathcal{X}) = n[f(x_0)]^{n-1}\nabla_s f(\mathcal{X}) + E_{f^n},$$

where $E_{f^n} = \left(S^T\right)^\dagger \left(\delta_{f^n} - n[f(x_0)]^{n-1}\delta_f\right)$.

Proof. The result is obtained easily by letting $f_i = f$ for all $i \in \{1, 2, \ldots, n\}$ in Proposition 8. ∎

Note that Corollaries 6 and 9 provide two different formulas to calculate $\nabla_s f^n(\mathcal{X})$. Let us show that they are equivalent.

Lemma 10. *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ and n be a positive integer. Then*

$$\sum_{i=1}^{n-1}[f(x_0)]^{n-1-i}\delta_{f|f^i} = \delta_{f^n} - n[f(x_0)]^{n-1}\delta_f.$$

Proof. We have

$$\begin{aligned}
\sum_{i=1}^{n-1}[f(x_0)]^{n-1-i}\delta_{f|f^i} &= [f(x_0)]^{n-2}\delta_{f|f} + [f(x_0)]^{n-3}\delta_{f|f^2} + \cdots + f(x_0)\delta_{f|f^{n-2}} + \delta_{f|f^{n-1}} \\
&= [f(x_0)]^{n-2}\left(\delta_{f^2} - f(x_0)\delta_f - f(x_0)\delta_f\right) + [f(x_0)]^{n-3}\left(\delta_{f^3} - f(x_0)\delta_{f^2} - [f(x_0)]^2\delta_f\right) \\
&\quad + \cdots + f(x_0)\left(\delta_{f^{n-1}} - f(x_0)\delta_{f^{n-2}} - [f(x_0)]^{n-2}\delta_f\right) + \delta_{f^n} - f(x_0)\delta_{f^{n-1}} - [f(x_0)]^{n-1}\delta_f
\end{aligned}$$

by Lemma 7. After cancelations, we get

$$\begin{aligned}
\sum_{i=1}^{n-1}[f(x_0)]^{n-1-i}\delta_{f|f^i} &= \underbrace{-[f(x_0)]^{n-1}\delta_f - [f(x_0)]^{n-1}\delta_f - \cdots - [f(x_0)]^{n-1}\delta_f}_{n \text{ times}} + \delta_{f^n} \\
&= -n[f(x_0)]^{n-1}\delta_f + \delta_{f^n}.
\end{aligned}$$

∎

Aware of the product rule, we can develop a quotient rule for generalized simplex gradients.

THEOREM 11 (quotient rule). *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ for which $g(x_0)$, $g(x_1)$, $\ldots$, $g(x_k)$ are all nonzero. Then*

$$\nabla_s \left(\frac{f}{g}\right)(\mathcal{X}) = \frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2} - E_{\frac{f}{g}},$$

where

$$E_{\frac{f}{g}} = \frac{\left(S^T\right)^\dagger}{g(x_0)}\delta_{\frac{f}{g}|g}.$$

Proof. By the product rule, we have

$$\begin{aligned}\nabla_s f(\mathcal{X}) &= \nabla_s \left(\frac{f}{g}\cdot g\right)(\mathcal{X})\\ &= \left(\frac{f}{g}\right)(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s\left(\frac{f}{g}\right)(\mathcal{X}) + \left(S^T\right)^\dagger \delta_{\frac{f}{g}|g}.\end{aligned}$$

Solving for $\nabla_s\left(\frac{f}{g}\right)(\mathcal{X})$ gives

$$\nabla_s \left(\frac{f}{g}\right)(\mathcal{X}) = \frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2} - \frac{\left(S^T\right)^\dagger}{g(x_0)}\delta_{\frac{f}{g}|g}. \qquad \square$$

Note that Theorem 11 requires $g(x_0) \neq 0$, $g(x_1) \neq 0, \ldots, g(x_k) \neq 0$. This is needed to ensure $\delta_{\frac{f}{g}|g}$ does not include any division by zero.

The following corollary is used to prove the power rule for a negative integer exponent.

COROLLARY 12. *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ for which $f(x_0)$, $f(x_1)$, $\ldots$, $f(x_k)$ are all nonzero. Then*

$$\nabla_s \left(\frac{1}{f}\right)(\mathcal{X}) = -\frac{\nabla_s f(\mathcal{X})}{[f(x_0)]^2} - \frac{\left(S^T\right)^\dagger}{f(x_0)}\delta_{\frac{1}{f}|f}.$$

Finally, we conclude this section by presenting the power rule for a negative integer exponent.

PROPOSITION 13 (power rule for a negative integer exponent). *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ for which $f(x_0)$, $f(x_1)$, $\ldots$, $f(x_k)$ are all nonzero, and let n be any positive integer. Then*

$$\nabla_s f^{-n}(\mathcal{X}) = n[f(x_0)]^{-n+1}\nabla_s\left(\frac{1}{f}\right)(\mathcal{X}) + \left(S^T\right)^\dagger\left(\sum_{i=1}^{n-1}[f(x_0)]^{-n+1+i}\delta_{f^{-1}|f^{-i}}\right).$$

It follows that

$$\nabla_s f^{-n}(\mathcal{X}) = -n[f(x_0)]^{-n-1}\nabla_s f(\mathcal{X}) - E_{f^{-n}},$$

where

$$E_{f^{-n}} = \frac{\left(S^T\right)^\dagger}{[f(x_0)]^n}\left(n\delta_{\frac{1}{f}|f} - \sum_{i=1}^{n-1}[f(x_0)]^{1+i}\delta_{f^{-1}|f^{-i}}\right).$$

Proof. By the power rule for a positive exponent,

$$\begin{aligned}\nabla_s \left(\frac{1}{f}\right)^n (\mathcal{X}) &= n\left(\left(\frac{1}{f}\right)(x_0)\right)^{n-1} \nabla_s \left(\frac{1}{f}\right)(\mathcal{X}) + \left(S^T\right)^\dagger \left(\sum_{i=1}^{n-1}\left(\left(\frac{1}{f}\right)(x_0)\right)^{n-1-i} \delta_{f^{-1}|f^{-i}}\right)\\ &= n[f(x_0)]^{-n+1}\nabla_s \left(\frac{1}{f}\right)(\mathcal{X}) + \left(S^T\right)^\dagger \left(\sum_{i=1}^{n-1}[f(x_0)]^{-n+1+i}\delta_{f^{-1}|f^{-i}}\right),\end{aligned}$$

which proves our first claim.

By Corollary 12,

$$\begin{aligned}\nabla_s f^{-n}(\mathcal{X}) &= n[f(x_0)]^{-n+1}\left(\frac{-\nabla_s f(\mathcal{X})}{[f(x_0)]^2} - \frac{\left(S^T\right)^\dagger}{f(x_0)}\delta_{\frac{1}{f}|f}\right) + \left(S^T\right)^\dagger \left(\sum_{i=1}^{n-1}[f(x_0)]^{-n+1+i}\delta_{f^{-1}|f^{-i}}\right)\\ &= -n[f(x_0)]^{-n-1}\nabla_s f(\mathcal{X}) - \frac{n\left(S^T\right)^\dagger \delta_{\frac{1}{f}|f}}{[f(x_0)]^n} + \left(S^T\right)^\dagger \left(\sum_{i=1}^{n-1}[f(x_0)]^{-n+1+i}\delta_{f^{-1}|f^{-i}}\right)\\ &= -n[f(x_0)]^{-n-1}\nabla_s f(\mathcal{X}) - \frac{\left(S^T\right)^\dagger}{[f(x_0)]^n}\left(n\delta_{\frac{1}{f}|f} - \sum_{i=1}^{n-1}[f(x_0)]^{1+i}\delta_{f^{-1}|f^{-i}}\right). \qquad \square\end{aligned}$$

We now turn our attention to a more advanced calculus rule, the chain rule.

4. Chain rule.

Throughout this section, let $f : \mathbb{R}^p \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}^p$, where

$$g(x) := \begin{bmatrix} g_1(x) \\ g_2(x) \\ \vdots \\ g_p(x) \end{bmatrix} \in \mathbb{R}^p.$$

Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$, and define

$$g(\mathcal{X}) := \langle g(x_0), g(x_1), \ldots, g(x_k)\rangle$$

to be an ordered set of $k+1$ points in $\mathbb{R}^p$. Let I_k denote the identity matrix $\in \mathbb{R}^{k\times k}$. Before inaugurating the chain rule, let us present some matrices involved in the formula. Note that

$$S(g(\mathcal{X})) = \begin{bmatrix} g(x_1) - g(x_0) & \ldots & g(x_k) - g(x_0)\end{bmatrix} \in \mathbb{R}^{p\times k}$$

and

$$\begin{aligned}\delta_f(g(\mathcal{X})) &= \begin{bmatrix} f\left(g(x_1)\right) - f\left(g(x_0)\right) \\ \vdots \\ f\left(g(x_k)\right) - f\left(g(x_0)\right)\end{bmatrix}\\ &= \begin{bmatrix} (f\circ g)(x_1) - (f\circ g)(x_0) \\ \vdots \\ (f\circ g)(x_k) - (f\circ g)(x_0)\end{bmatrix} = \delta_{f\circ g}(\mathcal{X}) \in \mathbb{R}^k.\end{aligned}$$

In the next definition, we define the *generalized simplex Jacobian of* g *with respect to* $\mathcal{X}$ in order to make the notation tighter.

DEFINITION 14 (generalized simplex Jacobian matrix). *Let $g : \mathbb{R}^d \to \mathbb{R}^p : x \mapsto \begin{bmatrix} g_1(x) & g_2(x) & \dots & g_p(x) \end{bmatrix}^T$. Then the generalized simplex Jacobian $\mathbf{J_s}$ of g with respect to $\mathcal{X}$ is an $p \times d$ real matrix defined as*

$$\mathbf{J_s} g(\mathcal{X}) := \begin{bmatrix} \nabla_s g_1(\mathcal{X})^T \\ \nabla_s g_2(\mathcal{X})^T \\ \vdots \\ \nabla_s g_p(\mathcal{X})^T \end{bmatrix}.$$

THEOREM 15 (chain rule). *Let $f : \mathbb{R}^p \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}^p$. Let $\mathcal{X} = \langle x_0, x_1, \dots, x_k \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ and $g(\mathcal{X}) = \langle g(x_0), g(x_1), \dots, g(x_k) \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^p$. Then*

$$\nabla_s (f \circ g)(\mathcal{X}) = (\mathbf{J_s} g(\mathcal{X}))^T \nabla_s f(g(\mathcal{X})) - E_{f \circ g},$$

where

$$E_{f \circ g} = \left(S(\mathcal{X})^T\right)^\dagger \left(S\left(g(\mathcal{X})\right)^T \left(S(g(\mathcal{X}))^T\right)^\dagger - I_k\right) \delta_f(g(\mathcal{X})).$$

Proof. We have

$$\begin{aligned} \nabla_s (f \circ g)(\mathcal{X}) &= \left(S(\mathcal{X})^T\right)^\dagger \delta_{f \circ g}(\mathcal{X}) \\ &= \left(S(\mathcal{X})^T\right)^\dagger \left(S(g(\mathcal{X}))^T \left(S(g(\mathcal{X}))^T\right)^\dagger - \widehat{E}\right) \delta_{f \circ g}(\mathcal{X}), \end{aligned}$$

where

$$\widehat{E} = S(g(\mathcal{X}))^T \left(S(g(\mathcal{X}))^T\right)^\dagger - I_k.$$

In order to make the notation tighter, let $\mathcal{Y} := g(\mathcal{X})$.

Now, using $\delta_{f \circ g}(\mathcal{X}) = \delta_f\left(g(\mathcal{X})\right) = \delta_f(\mathcal{Y})$, we find

$$\begin{aligned} \nabla_s (f \circ g)(\mathcal{X}) &= \left(\left(S(\mathcal{X})^T\right)^\dagger S(\mathcal{Y})^T \left(S(\mathcal{Y})^T\right)^\dagger - \left(S(\mathcal{X})^T\right)^\dagger \widehat{E}\right) \delta_f(\mathcal{Y}) \\ &= \left(S(\mathcal{X})^T\right)^\dagger S(\mathcal{Y})^T \left(S(\mathcal{Y})^T\right)^\dagger \delta_f(\mathcal{Y}) - \left(S(\mathcal{X})^T\right)^\dagger \widehat{E}\, \delta_f(\mathcal{Y}). \end{aligned}$$

Notice that

$$S(\mathcal{Y})^T = \begin{bmatrix} (g(x_1) - g(x_0))^T \\ \vdots \\ (g(x_k) - g(x_0))^T \end{bmatrix} = \delta_g(\mathcal{X}).$$

Hence,

$$\begin{aligned} \nabla_s (f \circ g)(\mathcal{X}) &= \begin{bmatrix} \nabla_s g_1(\mathcal{X}) & \nabla_s g_2(\mathcal{X}) & \dots & \nabla_s g_p(\mathcal{X}) \end{bmatrix} \nabla_s f(\mathcal{Y}) - \left(S(\mathcal{X})^T\right)^\dagger \widehat{E}\, \delta_f(\mathcal{Y}) \\ &= \begin{bmatrix} (\nabla_s g_1(\mathcal{X}))^T \\ (\nabla_s g_2(\mathcal{X}))^T \\ \dots \\ (\nabla_s g_p(\mathcal{X}))^T \end{bmatrix}^T \nabla_s f(\mathcal{Y}) - \left(S(\mathcal{X})^T\right)^\dagger \left(S(\mathcal{Y})^T \left(S(\mathcal{Y})^T\right)^\dagger - I_k\right) \delta_f(\mathcal{Y}) \\ &= (\mathbf{J_s} g(\mathcal{X}))^T \nabla_s f(g(\mathcal{X})) - E_{f \circ g}. \end{aligned}$$ ∎

The next corollary demonstrates that the term E vanishes when $k \leq p$ and $S(g(\mathcal{X}))$ has full rank.

COROLLARY 16. *Let $f : \mathbb{R}^p \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}^p$. Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ and $g(\mathcal{X}) = \langle g(x_0),\, g(x_1),\, \ldots,\, g(x_k) \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^p$. Suppose $S(g(\mathcal{X}))$ has full rank and $k \leq p$. Then*

$$\nabla_s (f \circ g)(\mathcal{X}) = \left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla_s f(g(\mathcal{X})).$$

Proof. Since $S(g(\mathcal{X}))$ has full column rank, $S(g(\mathcal{X}))^T$ has full row rank. This implies that $S(g(\mathcal{X}))^T$ has right inverse $\left(S(g(\mathcal{X}))^T\right)^\dagger \in \mathbb{R}^{p \times k}$. Thus,

$$\begin{aligned} E &= \left(S(\mathcal{X})^T\right)^\dagger \left(S(g(\mathcal{X}))^T \left(S(g(\mathcal{X}))^T\right)^\dagger - I_k\right) \delta_f(g(\mathcal{X})) \\ &= \left(S(\mathcal{X})^T\right)^\dagger (I_k - I_k)\, \delta_f(g(\mathcal{X})) \\ &= 0. \end{aligned}$$

Therefore, $\nabla_s (f \circ g)(\mathcal{X}) = \left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla_s f(g(\mathcal{X}))$. ∎

We now have presented all our calculus rules. We see that all of them have the same structure as the calculus rules for the true gradient plus a term E that can be viewed as an error term. Indeed, E can be viewed as an error term in the sense that, when all the functions involved are linear, removing the term E from the formulas presented in sections 3 and 4 can provide an exact approximation of the true gradient. However, in general, removing the term E from the calculus rules does not imply we get the value of the true gradient. The next section investigates the effects of removing the term E in the formula. This leads to a new approach to approximating the gradient which is less restrictive in certain cases than the calculus rules for generalized simplex gradients.

5. Generalized simplex calculus gradient. Table 1 summarizes the calculus rules from sections 3 and 4.

We now introduce new notation. We use ∇_{sp}, ∇_{sq}, and ∇_{sc} to denote the product rule, quotient rule, and chain rule, respectively, that do not include the term E. We refer to ∇_{sp}, ∇_{sq}, and ∇_{sc} as the generalized simplex calculus gradients. We formally define these in (5), (6), and (7) and present an overview of these rules in Table 2.

Note that if the term E is not equal to 0 in the calculus rules presented in the previous sections, then the generalized simplex calculus gradient returns a value different from the generalized simplex gradient. Hence, the purpose of this section is to compare both approaches. We provide error bounds for generalized simplex calculus gradients and examples where ∇_{sp}, ∇_{sq}, and ∇_{sc} are more accurate than the generalized simplex gradient ∇_s and vice versa.

Throughout this section, let $\widehat{S}(\mathcal{X}) := S(\mathcal{X})/\Delta$. We begin by presenting Lemma 17, which tells us when the generalized simplex gradient is equal to the true gradient.

LEMMA 17. *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Let $f : \mathbb{R}^d \to \mathbb{R} : x \mapsto a^T x + c$, where $a \in \mathbb{R}^d$ and $c \in \mathbb{R}$. Suppose $S(\mathcal{X})$ has full row rank. Then*

$$\nabla_s f(\mathcal{X}) = \nabla f(x_0).$$

Proof. This follows from Definition 2. ∎

We point out that it is not possible for $S(\mathcal{X})$ to have full row rank in the underdetermined case ($k < d$). This makes sense since underdetermined simplex gradients

TABLE 1
The calculus rules for generalized simplex gradients (see Theorem 5, Proposition 8, Corollary 6, Proposition 13, Theorem 11, and Theorem 15, respectively).

Rule	Formula	E
Product of 2	$f(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f(\mathcal{X}) + E_{fg}$	$E_{fg} = \left(S^T\right)^{\dagger} \delta_{f\|g}$
Product of n	$\sum_{i=1}^n \left(\prod_{j\neq i} f_j(x_0)\right) \nabla_s f_i(\mathcal{X}) + E_{f_1\cdots f_n}$	$E_{f_1\cdots f_n} = \left(S^T\right)^{\dagger} \left(\delta_{f_1\cdots f_n} - \sum_{i=1}^n \left(\prod_{j\neq i} f_j(x_0)\right) \delta_{f_i}\right)$
Positive power	$n[f(x_0)]^{n-1}\nabla_s f(\mathcal{X}) + E_{f^n}$	$E_{f^n} = \left(S^T\right)^{\dagger} \left(\sum_{i=1}^{n-1} [f(x_0)]^{n-1-i} \delta_{f\|f^i}\right)$
Negative power	$-n[f(x_0)]^{-n-1}\nabla_s f(\mathcal{X}) - E_{f^{-n}}$	$E_{f^{-n}} = \frac{\left(S^T\right)^{\dagger}}{[f(x_0)]^n} \left(n\delta_{\frac{1}{f}\|f} - \sum_{i=1}^{n-1} [f(x_0)]^{1+i} \delta_{f^{-1}\|f^{-i}}\right)$
Quotient	$\frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2} - E_{\frac{f}{g}}$	$E_{\frac{f}{g}} = \frac{\left(S^T\right)^{\dagger}}{g(x_0)} \delta_{\frac{f}{g}\|g}$
Chain	$\left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla_s f(g(\mathcal{X})) - E_{f\circ g}$	$E_{f\circ g} = \left(S(\mathcal{X})^T\right)^{\dagger} \left(S\left(g(\mathcal{X})\right)^T \left(S(g(\mathcal{X}))^T\right)^{\dagger} - I_k\right) \delta_{f(g(\mathcal{X}))}$

TABLE 2
Generalized simplex calculus gradients.

Gradient approximation	Relation to ∇_s
$\nabla_{sp}(fg)(\mathcal{X}) := f(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f(\mathcal{X})$	$\nabla_s(fg)(\mathcal{X}) = \nabla_{sp}(fg)(\mathcal{X}) + E_{fg}$
$\nabla_{sq}(f/g)(\mathcal{X}) := \frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2}$	$\nabla_s(f/g)(\mathcal{X}) = \nabla_{sq}(f/g)(\mathcal{X}) - E_{\frac{f}{g}}$
$\nabla_{sc}(f \circ g)(\mathcal{X}) := (\mathbf{J_s} g(\mathcal{X}))^T \nabla_s f(g(\mathcal{X}))$	$\nabla_s(f \circ g)(\mathcal{X}) = \nabla_{sc}(f \circ g)(\mathcal{X}) - E_{f \circ g}$

do not capture enough information to guarantee a perfect approximation of $\nabla f(x_0)$. Example 18 illustrates this fact.

Example 18. Let $f : \mathbb{R}^2 \to \mathbb{R} : (x, y) \mapsto x + \alpha y$, where $\alpha \in \mathbb{R} \setminus \{0\}$. Consider the ordered set $\mathcal{X} = \langle \begin{bmatrix} 0 & 0 \end{bmatrix}^T, \begin{bmatrix} 1 & 0 \end{bmatrix}^T \rangle$. Then $S(\mathcal{X})$ has full (column) rank but $\nabla_s f(\mathcal{X}) \neq \nabla f(x_0)$.

Proof. We have

$$\begin{aligned} \nabla_s f(\mathcal{X}) &= \begin{bmatrix} 1 & 0 \end{bmatrix}^\dagger \begin{bmatrix} 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \end{aligned}$$

But the true gradient

$$\nabla f(x_0) = \begin{bmatrix} 1 \\ \alpha \end{bmatrix}.$$

This completes the proof. ∎

5.1. Product rule. Let us define the *generalized simplex product gradient of fg with respect to $\mathcal{X}$*:

$$\nabla_{sp}(fg)(\mathcal{X}) := f(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f(\mathcal{X}). \tag{5}$$

The next corollary shows us that $\nabla_{sp}(fg)(\mathcal{X})$ is perfectly accurate when f and g are linear functions.

COROLLARY 19. *Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k \rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Let f and g be linear functions from $\mathbb{R}^d$ to $\mathbb{R}$. Suppose $S(\mathcal{X})$ has full row rank. Then*

$$\nabla_{sp}(fg)(\mathcal{X}) = \nabla(fg)(x_0).$$

Proof. This follows from Lemma 17. ∎

Since the product of linear functions is not a linear function, it is clear that $\nabla_{sp}(fg)(\mathcal{X})$ is always as good or better than $\nabla_s(fg)(\mathcal{X})$ whenever f and g are linear functions and $S(\mathcal{X})$ has full row rank.

We can extend $\nabla_{sp}(fg)(\mathcal{X})$ to the case of n functions. We get

$$\begin{aligned} \nabla_{sp}(f_1 f_2 \cdots f_{n-1} f_n)(\mathcal{X}) &= (f_1 f_2 \cdots f_{n-1})(x_0)\nabla_s f_n(\mathcal{X}) + (f_1 f_2 \cdots f_{n-2} f_n)(x_0)\nabla_s f_{n-1}(\mathcal{X}) \\ &\quad + \cdots + (f_1 f_3 f_4 \cdots f_n)(x_0)\nabla_s f_2(\mathcal{X}) + (f_2 f_3 \cdots f_n)(x_0)\nabla_s f_1(\mathcal{X}). \end{aligned}$$

Recall that by the fundamental theorem of algebra, every single-variable degree $n \in \mathbb{N}$ polynomial with complex coefficients has, counted with multiplicity, exactly n complex roots [18, Theorem 2.4]. Hence, $\nabla_{sp}(f_1 f_2 \ldots f_n)(\mathcal{X})$ is an exact approximation whenever $f = f_1 f_2 \cdots f_n$ (where $f_i : \mathbb{R} \to \mathbb{C}$ for all $i \in \{1, 2, \ldots, n\}$ are linear functions) is a real polynomial of degree n and $\mathcal{X}$ has full row rank.

Now, let us present an error bound for the generalized simplex product gradient $\nabla_{sp}(fg)(\mathcal{X})$.

THEOREM 20 (error bound for $\nabla_{sp}(fg)(\mathcal{X})$). *Let $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Assume that $S(\mathcal{X})$ has full row rank and that ∇f and ∇g are Lipschitz continuous with Lipschitz constants $L_{\nabla f} \geq 0$ and $L_{\nabla g} \geq 0$ in an open domain Ω containing $B(x_0, \Delta)$. Define*

$$\varepsilon_{sp}(fg)(\mathcal{X}) := \frac{\sqrt{k}}{2}\left(|f(x_0)|L_{\nabla g} + |g(x_0)|L_{\nabla f}\right)\left\|\left(\widehat{S}\left(\mathcal{X}\right)^T\right)^{\dagger}\right\|\Delta.$$

Then

$$\|\nabla_{sp}(fg)(\mathcal{X}) - \nabla(fg)(x_0)\| \leq \varepsilon_{sp}(fg)(\mathcal{X}).$$

Proof. We have

$$\begin{aligned}\|\nabla_{sp}(fg)(\mathcal{X}) - \nabla(fg)(x_0)\| &= \|f(x_0)\nabla_s g(\mathcal{X}) + g(x_0)\nabla_s f(\mathcal{X}) - (f(x_0)\nabla g(x_0) + g(x_0)\nabla f(x_0))\| \\ &\leq |f(x_0)|\,\|\nabla_s g(\mathcal{X}) - \nabla g(x_0)\| + |g(x_0)|\,\|\nabla_s f(\mathcal{X}) - \nabla f(x_0)\| \\ &\leq \frac{\sqrt{k}}{2}\left(|f(x_0)|L_{\nabla g} + |g(x_0)|L_{\nabla f}\right)\left\|\left(\widehat{S}\left(\mathcal{X}\right)^T\right)^{\dagger}\right\|\Delta\end{aligned}$$

by Proposition 3. ∎

Note that the error bound $\varepsilon_{sp}(fg)(\mathcal{X})$ involves function values at x_0 but the error bound $\varepsilon_s(fg)(\mathcal{X})$ does not. The reason for this can be seen in the proof: by applying a product rule, the product rule gets applied to the error bound, generating function values within the error bound.

Analyzing this error bound, we get the following corollary, which tells us when $\nabla_{sp}(fg)(\mathcal{X})$ is an exact approximation of $\nabla(fg)(x_0)$.

COROLLARY 21. *Let the assumptions of Theorem 20 hold. If any of the following cases hold, then*

$$\nabla_{sp}(fg)(\mathcal{X}) = \nabla(fg)(x_0).$$

(i) *The function values of f and g evaluated at x_0 are $f(x_0) = g(x_0) = 0$.*
(ii) *The functions f and g are linear.*

Obviously, these two cases are highly restrictive. Nevertheless, it provides two cases where the generalized simplex product gradient is a better or as good approximation as the generalized simplex gradient $\nabla_s(fg)(\mathcal{X})$.

We would like to answer the following question: when is the generalized simplex product gradient $\nabla_{sp}(fg)(\mathcal{X})$ more accurate than the generalized simplex gradient $\nabla_s(fg)(\mathcal{X})$? Comparing their respective error bounds gives us a good indicator of how to answer this question. Note that the product of Lipschitz continuous functions on a bounded interval Ω is Lipschitz continuous on that interval Ω [8, section 12.7].

COROLLARY 22. *Let the assumptions of Theorem 20 hold, and hence let $\nabla(fg)$ be Lipschitz continuous on Ω with Lipschitz constant $L_{\nabla(fg)} \geq 0$. If*

$$|f(x_0)|L_{\nabla g} + |g(x_0)|L_{\nabla f} < L_{\nabla(fg)},$$

then the error bound $\varepsilon_{sp}(fg)(\mathcal{X})$ is smaller than the error bound $\varepsilon_s(fg)(\mathcal{X})$.

In practice, we do not know the value of the Lipschitz constants $L_{\nabla f}, L_{\nabla g}$, and $L_{\nabla(fg)}$. For this reason, it is unlikely that we know which gradient approximation has a smaller error bound. A technique to approximate the Lipschitz constants is discussed in section 7. Based on the approximation of the Lipschitz constants, a decision can be made.

Example 23 provides an example where the true absolute error for the generalized simplex product gradient $\nabla_{sp}(fg)(\mathcal{X})$ is smaller than $\nabla_s(fg)(\mathcal{X})$, and Example 24 provides an example where the true absolute error for the generalized simplex product gradient $\nabla_{sp}(fg)(\mathcal{X})$ is greater than $\nabla_s(fg)(\mathcal{X})$.

Example 23. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto e^x$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto 2e^x$. Consider the ordered set $\mathcal{X} = \langle 0, 1\rangle$. First, let us find the error bounds for $\nabla_{sp}(fg)(\mathcal{X})$ and $\nabla_s(fg)(\mathcal{X})$. Note that $L_{\nabla f} = e, L_{\nabla g} = 2e$, and $L_{\nabla(fg)} = 4e^2$ on [0,1]. It follows that

$$|f(x_0)|L_{\nabla g} + |g(x_0)|L_{\nabla f} = 4e \approx 10.87.$$

The error bounds are $\varepsilon_{sp}(fg)(\mathcal{X}) = 2e \approx 5.44$ and $\varepsilon_s(fg)(\mathcal{X}) = 2e^2 \approx 14.78$. The true absolute errors are

$$\|\nabla_{sp}(fg)(\mathcal{X}) - \nabla(fg)(x_0)\| \approx 2.87 \le \varepsilon_{sp}(fg)(\mathcal{X})$$

and

$$\|\nabla_s(fg)(\mathcal{X}) - \nabla(fg)(x_0)\| \approx 8.78 \le \varepsilon_s(fg)(\mathcal{X}).$$

Example 24. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto e^{-x^2}$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto e^{-x^3}$. Consider the ordered set $\mathcal{X} = \langle 0, 1\rangle$. We have $L_{\nabla f} = 2$, $L_{\nabla g} = 3/e$, and $L_{\nabla(fg)} \approx 2.81$ on [0,1]. It follows that

$$|f(x_0)|L_{\nabla g} + |g(x_0)|L_{\nabla f} = \frac{3}{e} + 2 \approx 3.10.$$

The error bounds are $\varepsilon_{sp}(fg)(\mathcal{X}) = \frac{3}{2e} + 1 \approx 1.55$ and $\varepsilon_s(fg)(\mathcal{X}) \approx 1.40$. The true absolute errors are

$$\|\nabla_{sp}(fg)(\mathcal{X}) - \nabla(fg)(x_0)\| \approx 1.26 \le \varepsilon_{sp}(fg)(\mathcal{X})$$

and

$$\|\nabla_s(fg)(\mathcal{X}) - \nabla(fg)(x_0)\| \approx 0.86 \le \varepsilon_s(fg)(\mathcal{X}).$$

Note that all the results obtained for $\nabla_{sp}(fg)(\mathcal{X})$ (Corollary 19, Theorem 20, and Corollaries 21 and 22) can be extended to the case of the product of n functions. Let us present an error bound for the generalized simplex product gradient $\nabla_{sp}(f_1 f_2 \cdots f_{n-1} f_n)(\mathcal{X})$.

PROPOSITION 25 (error bound for $\nabla_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X})$). *Let $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Assume that $S(\mathcal{X})$ has full row rank and that ∇f_i are Lipschitz continuous with Lipschitz constant $L_{\nabla f_i} \ge 0$ for all $i \in \{1, 2, \ldots, n\}$ in an open domain Ω containing $B(x_0, \Delta)$. Define*

$$\varepsilon_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X}) := \frac{\sqrt{k}}{2} \left(\sum_{i=1}^{n} \left(\prod_{j \ne i} |f_j(x_0)| \right) L_{\nabla f_i} \right) \left\| \left(\widehat{S}\,(\mathcal{X})^T \right)^\dagger \right\| \Delta.$$

Then

$$\|\nabla_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X}) - \nabla(f_1 f_2 \cdots f_n)(x_0)\| \le \varepsilon_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X}).$$

Proof. We have

$$
\begin{aligned}
&\|\nabla_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X}) - \nabla(f_1 f_2 \cdots f_n)(x_0)\| \\
&= \big\|(f_1 f_2 \cdots f_{n-1})(x_0)\nabla_s f_n(\mathcal{X}) - (f_1 f_2 \cdots f_{n-1})(x_0)\nabla f_n(\mathcal{X}) + \cdots \\
&\quad + (f_2 f_3 \cdots f_n)(x_0)\nabla_s f_1(x_0) - (f_2 f_3 \cdots f_n)(x_0)\nabla f_1(x_0)\big\| \\
&\le |(f_1 f_2 \cdots f_{n-1})(x_0)|\, \|\nabla_s f_n(\mathcal{X}) - \nabla f_n(x_0)\| + \cdots + |(f_2 f_3 \cdots f_n)(x_0)|\, \|\nabla_s f_1(\mathcal{X}) - \nabla f_1(x_0)\| \\
&\le |(f_1 f_2 \cdots f_{n-1})(x_0)| \frac{\sqrt{k}}{2} L_{\nabla f_n} \left\| \left(\widehat{S}(\mathcal{X})^T\right)^\dagger \right\| \Delta + \cdots + |(f_2 f_3 \cdots f_n)(x_0)| \frac{\sqrt{k}}{2} L_{\nabla f_1} \left\| \left(\widehat{S}(\mathcal{X})^T\right)^\dagger \right\| \Delta \\
&= \frac{\sqrt{k}}{2} \left(\sum_{i=1}^{n} \left(\prod_{j \neq i} |f_j(x_0)| \right) L_{\nabla f_i} \right) \left\| \left(\widehat{S}(\mathcal{X})^T\right)^\dagger \right\| \Delta. \qquad \square
\end{aligned}
$$

Once again, analyzing the previous error bound, we get Corollary 26, which tells us when $\nabla_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X})$ is an exact approximation of $\nabla(f_1 f_2 \cdots f_n)(x_0)$.

COROLLARY 26. *Let the assumptions of Proposition* 25 *hold. If any of the following cases hold, then*

$$\nabla_{sp}(f_1 f_2 \cdots f_n)(\mathcal{X}) = \nabla(f_1 f_2 \cdots f_n)(x_0).$$

(i) *The function values of $f_i(x_0) = 0$ and $f_j(x_0) = 0$ for some $i, j \in \{1, 2, \ldots, n\}$, $i \neq j$.*
(ii) *The function f_i is linear and $f_i(x_0) = 0$ for some $i \in \{1, 2, \ldots, n\}$.*
(iii) *The function f_i is linear for all $i \in \{1, 2, \ldots, n\}$.*

Next, we analyze the particular case where all functions f_i, $i \in \{1, 2, \ldots, n\}$, are equal.

5.2. Power rule. Let us define the *generalized simplex product gradient of f^n with respect to $\mathcal{X}$*:

$$\nabla_{sp} f^n(\mathcal{X}) := n[f(x_0)]^{n-1} \nabla_s f(\mathcal{X}),$$

where $f(x_0)$ is nonzero whenever n is negative.

Note that $\nabla_{sp} f^n(\mathcal{X})$ only requires $f(x_0)$ to be nonzero when n is a negative integer which is not sufficient in Proposition 13. Therefore, the generalized simplex product gradient is less restrictive than the generalized simplex gradient. First, let us introduce an error bound for $\nabla_{sp} f^n(\mathcal{X})$.

PROPOSITION 27 (error bound for $\nabla_{sp} f^n(\mathcal{X})$). *Let n be a nonzero integer and $f : \mathbb{R}^d \to \mathbb{R}$ and $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ for which $f(x_0)$ is nonzero whenever n is a negative integer. Assume that $S(\mathcal{X})$ has full row rank and that ∇f is Lipschitz continuous with Lipschitz constant $L_{\nabla f} \geq 0$ in an open domain Ω containing $B(x_0, \Delta)$. Define*

$$\varepsilon_{sp} f^n(\mathcal{X}) := \frac{\sqrt{k}}{2} \left(|n| |f(x_0)|^{n-1} L_{\nabla f} \right) \left\| \left(\widehat{S}(\mathcal{X})^T\right)^\dagger \right\| \Delta.$$

Then

$$\|\nabla_{sp} f^n(\mathcal{X}) - \nabla f^n(x_0)\| \leq \varepsilon_{sp} f^n(\mathcal{X}).$$

Proof. We have

$$\begin{aligned}\|\nabla_{sp} f^n(\mathcal{X}) - \nabla f^n(x_0)\| &= \left\|nf(x_0)^{n-1}\nabla_s f(\mathcal{X}) - nf(x_0)^{n-1}\nabla f(x_0)\right\| \\ &\le |n||f(x_0)|^{n-1}\left\|\nabla_s f(\mathcal{X}) - \nabla f(x_0)\right\| \\ &\le \frac{\sqrt{k}}{2}\left(|n||f(x_0)|^{n-1}L_{\nabla f}\right)\left\|\left(\widehat{S}(\mathcal{X})^T\right)^\dagger\right\|\Delta\end{aligned}$$

by Proposition 3. ∎

Corollary 28. *Let the assumptions of Proposition* 27 *hold. If any of the following cases hold, then*

$$\nabla_{sp} f^n(\mathcal{X}) = \nabla f^n(x_0).$$

(i) *The function f is linear.*

(ii) *The function value of f at x_0 is equal to zero and $n \in \mathbb{N}$.*

Next, we provide an example where the error bound $\varepsilon_{sp} f^n(\mathcal{X})$ is smaller than $\varepsilon_s f^n(\mathcal{X})$ independent of the ordered set $\mathcal{X}$ and an example where $\nabla_{sp} f^n(\mathcal{X})$ is less accurate than $\nabla_s f^n(\mathcal{X})$.

Example 29. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto x^2 + 1$, $n = 2$, and hence let $f^2 : \mathbb{R} \to \mathbb{R} : x \mapsto x^4 + 2x^2 + 1$. Let $\mathcal{X} = \langle x_0, x_1\rangle$. Without loss of generality, assume that $x_0 < x_1$. Note that the Lipschitz constants are $L_{\nabla f} = 2$ and $L_{\nabla f^2} = \max|4(3x^2+1)|$ on $[x_0, x_1]$. It follows that

$$n[f(x_0)]^{n-1}L_{\nabla f} = 4(x_0^2 + 1).$$

Since

$$\begin{aligned}4(x_0^2+1) &\le L_{\nabla f^2} \\ &= \max 4(3x^2+1) \quad \text{for any } x \in [x_0, x_1],\end{aligned}$$

the error bound $\varepsilon_{sp} f^2(\mathcal{X})$ is smaller than the error bound $\varepsilon_s f^2(\mathcal{X})$. Notice that if $\mathcal{X} = \langle 1, 2\rangle$, the error bounds are $\varepsilon_{sp} f^2(\mathcal{X}) = 4$ and $\varepsilon_s f^2(\mathcal{X}) = 26$. The true absolute errors are

$$\left\|\nabla_{sp} f^2(\mathcal{X}) - \nabla f^2(x_0)\right\| = 4 \le \varepsilon_{sp} f^2(\mathcal{X})$$

and

$$\left\|\nabla_s f^2(\mathcal{X}) - \nabla f^2(x_0)\right\| = 13 \le \varepsilon_s f^2(\mathcal{X}).$$

Example 30. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto -x^2 + 10$, $n = 2$, and hence let $f^2 : \mathbb{R} \to \mathbb{R} : x \mapsto x^4 - 20x^2 + 100$. Let $\mathcal{X} = \langle 1, 2\rangle$. Note that the Lipschitz constants are $L_{\nabla f} = 2$ and $L_{\nabla f^2} = 28$ on $[1, 2]$. It follows that

$$n[f(x_0)]^{n-1}L_{\nabla f} = 36.$$

The error bounds are $\varepsilon_{sp} f^2(\mathcal{X}) = 18$ and $\varepsilon_s f^2(\mathcal{X}) = 14$. The true absolute errors are

$$\left\|\nabla_{sp} f^2(\mathcal{X}) - \nabla f^2(x_0)\right\| = 18 \le \varepsilon_{sp} f^2(\mathcal{X})$$

and

$$\left\|\nabla_s f^2(\mathcal{X}) - \nabla f^2(x_0)\right\| = 9 \le \varepsilon_s f^2(\mathcal{X}).$$

We continue our investigation by looking at the *generalized simplex quotient gradient of $\left(\frac{f}{g}\right)$ with respect to $\mathcal{X}$ $\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$.*

5.3. Quotient rule. Let $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}$. Let $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ for which $g(x_0)$ is nonzero. Define the *generalized simplex quotient gradient of* $\left(\frac{f}{g}\right)$ *with respect to* $\mathcal{X}$:

$$\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) := \frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2}. \tag{6}$$

Notice that $\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$ does not require $g(x_1), g(x_2), \ldots, g(x_k)$ to be all nonzero, which is the case for $\nabla_s\left(\frac{f}{g}\right)(\mathcal{X})$ in Theorem 11. This provides a good motive to use the generalized simplex quotient gradient over the generalized simplex gradient in certain situations.

THEOREM 31 (error bound for $\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$). *Let $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}$. Let $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ for which $g(x_0)$ is nonzero. Assume that $S(\mathcal{X})$ has full row rank and that ∇f and ∇g are Lipschitz continuous with Lipschitz constants $L_{\nabla f} \geq 0$ and $L_{\nabla g} \geq 0$ in an open domain Ω containing $B(x_0, \Delta)$. Define*

$$\varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) := \frac{\sqrt{k}}{2}\left(\left|\frac{1}{g(x_0)}\right| L_{\nabla f} + \left|\frac{f(x_0)}{[g(x_0)]^2}\right| L_{\nabla g}\right)\left\|\left(\widehat{S}(\mathcal{X})^T\right)^\dagger\right\|\Delta.$$

Then

$$\left\|\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| \leq \varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}).$$

Proof. We have

$$\begin{aligned}\left\|\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| &= \left\|\frac{g(x_0)\nabla_s f(x_0) - f(x_0)\nabla_s g(\mathcal{X}) - (g(x_0)\nabla f(x_0) - f(x_0)\nabla g(x_0))}{[g(x_0)]^2}\right\| \\ &\leq \left|\frac{1}{g(x_0)}\right| \|\nabla_s f(\mathcal{X}) - \nabla f(x_0)\| + \left|\frac{f(x_0)}{[g(x_0)]^2}\right| \|\nabla_s g(\mathcal{X}) - \nabla g(x_0)\| \\ &\leq \frac{\sqrt{k}}{2}\left(\left|\frac{1}{g(x_0)}\right| L_{\nabla f} + \left|\frac{f(x_0)}{[g(x_0)]^2}\right| L_{\nabla g}\right)\left\|\left(\widehat{S}(\mathcal{X})^T\right)^\dagger\right\|\Delta\end{aligned}$$

by Proposition 3. ∎

COROLLARY 32. *Let the assumptions of Theorem 31 hold. If f and g are linear functions, then*

$$\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) = \nabla\left(\frac{f}{g}\right)(x_0).$$

Now, let us compare the error bounds $\varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$ and $\varepsilon_s\left(\frac{f}{g}\right)(\mathcal{X})$. Assume that $\frac{f}{g}$ is Lipschitz continuous with Lipschitz constant $L_{\nabla \frac{f}{g}}$ on Ω. We see that $\varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$ is smaller than $\varepsilon_s\left(\frac{f}{g}\right)(\mathcal{X})$ whenever

$$\left|\frac{1}{g(x_0)}\right| L_{\nabla f} + \left|\frac{f(x_0)}{[g(x_0)]^2}\right| L_{\nabla g} < L_{\nabla \frac{f}{g}}.$$

Next, we provide one example where $\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$ is more accurate than $\nabla_s\left(\frac{f}{g}\right)(\mathcal{X})$ and one example where $\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$ is less accurate than $\nabla_s\left(\frac{f}{g}\right)(\mathcal{X})$.

Example 33. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto 1$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto x$.

First, let us consider the ordered set $\mathcal{X}_1 = \langle 10^{-6}, 0\rangle$. The Lipschitz constants are $L_{\nabla f} = 0$ and $L_{\nabla g} = 0$. Note that the Lipschitz constant $L_{\nabla \frac{f}{g}}$ is not defined on

$[0, 10^{-6}]$. Also, $\nabla_s\left(\frac{f}{g}\right)(\mathcal{X}_1)$ is not defined since there is a division by zero in the vector $\delta_{\frac{f}{g}}$. On the other hand, the error bound is $\varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}_1) = 0$, and so the true absolute error is

$$\left\|\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}_1) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| = 0 \leq \varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}_1).$$

Second, consider the ordered set $\mathcal{X}_2 = \langle 10^{-6}, 1 + 10^{-6}\rangle$. Note that the Lipschitz constant $L_{\nabla\frac{f}{g}}$ is now defined on $[10^{-6}, 1 + 10^{-6}] : L_{\nabla\frac{f}{g}} = 2 \times 10^{18}$. It follows that the error bounds are $\varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}_2) = 0$ and $\varepsilon_s\left(\frac{f}{g}\right)(\mathcal{X}_2) = 10^{18}$. The true absolute errors are

$$\left\|\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}_2) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| = 0 \leq \varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}_2)$$

and

$$\left\|\nabla_{s}\left(\frac{f}{g}\right)(\mathcal{X}_2) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| = 10^{12} \leq \varepsilon_{s}\left(\frac{f}{g}\right)(\mathcal{X}_2).$$

Example 34. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto x^3$, $g : \mathbb{R} \to \mathbb{R} : x \mapsto x^2$ and $\mathcal{X} = \langle 1, 2\rangle$. The Lipschitz constants are $L_{\nabla f} = 12$, $L_{\nabla g} = 2$, and $L_{\nabla\frac{f}{g}} = 0$ on [1,2]. It follows that the error bounds are $\varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) = 7$ and $\varepsilon_s\left(\frac{f}{g}\right)(\mathcal{X}) = 0$. The true absolute errors are

$$\left\|\nabla_{sq}\left(\frac{f}{g}\right)(\mathcal{X}) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| = 3 \leq \varepsilon_{sq}\left(\frac{f}{g}\right)(\mathcal{X})$$

and

$$\left\|\nabla_{s}\left(\frac{f}{g}\right)(\mathcal{X}) - \nabla\left(\frac{f}{g}\right)(x_0)\right\| = 0 \leq \varepsilon_{s}\left(\frac{f}{g}\right)(\mathcal{X}).$$

5.4. Chain rule. We now turn attention to the chain rule. Let us begin by focusing on composition of linear functions. The next proposition shows that the term $E_{f\circ g}$ vanishes in $\nabla_s(f \circ g)(\mathcal{X})$.

PROPOSITION 35 (chain rule for linear functions). *Let $f : \mathbb{R}^p \to \mathbb{R} : x \mapsto a^T x + c_1$ and $g : \mathbb{R}^d \to \mathbb{R}^p : x \mapsto Bx + c_2$, where $a \in \mathbb{R}^p$, $B \in \mathbb{R}^{p\times d}$, and $c_1, c_2 \in \mathbb{R}$. Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ and $g(\mathcal{X}) = \langle g(x_0), g(x_1), \ldots, g(x_k)\rangle$ be an ordered set of $k + 1$ points in $\mathbb{R}^p$. Suppose $S(g(\mathcal{X}))$ has full rank. Then*

$$\nabla_s(f \circ g)(\mathcal{X}) = (\mathbf{J_s} g(\mathcal{X}))^T\, \nabla_s f(g(\mathcal{X})).$$

Proof. If $k \leq p$, then the result follows from Corollary 16. Now, suppose $k > p$. We have

$$\begin{aligned}
E_{f\circ g} &= \left(S(\mathcal{X})^T\right)^\dagger \left(S\left(g(\mathcal{X})\right)^T \left(S(g(\mathcal{X}))^T\right)^\dagger - I_k\right) \delta_f(g(\mathcal{X}))\\
&= \left(S(\mathcal{X})^T\right)^\dagger S(g(\mathcal{X}))^T \nabla_s f(g(\mathcal{X})) - \left(S(\mathcal{X})^T\right)^\dagger \delta_f(g(\mathcal{X}))\\
&= \left(S(\mathcal{X})^T\right)^\dagger S(g(\mathcal{X}))^T \nabla f(g(x_0)) - \left(S(\mathcal{X})^T\right)^\dagger \delta_f(g(\mathcal{X})),
\end{aligned}$$

as $\nabla_s f(g(\mathcal{X})) = \nabla f(g(x_0))$ whenever f is a linear function and $S(g(\mathcal{X}))$ has full row rank (Lemma 17).

Finally,

$$\begin{aligned}
E_{f\circ g} &= \left(S(\mathcal{X})^T\right)^\dagger S(g(\mathcal{X}))^T a - \left(S(\mathcal{X})^T\right)^\dagger \delta_f(g(\mathcal{X})) \qquad (\text{since } \nabla f(g(x_0)) = a)\\
&= \left(S(\mathcal{X})^T\right)^\dagger S(g(\mathcal{X}))^T a - \left(S(\mathcal{X})^T\right)^\dagger S(g(\mathcal{X}))^T\\
&= 0,
\end{aligned}$$

as $\delta_f(g(\mathcal{X})) = S(g(\mathcal{X}))^T a$ for linear functions. ∎

In the previous proposition, note that even though the term $E_{f\circ g}$ is equal to 0 does not necessarily mean that $\nabla_s(f\circ g)(\mathcal{X}) = \nabla(f\circ g)(x_0)$. The following example illustrates this situation.

Example 36. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto x$ and $g : \mathbb{R}^2 \to \mathbb{R} : (x, y) \mapsto x + y$. Let

$$\mathcal{X} = \langle \begin{bmatrix}0 & 0\end{bmatrix}^T, \begin{bmatrix}1 & 0\end{bmatrix}^T, \begin{bmatrix}2 & 0\end{bmatrix}^T \rangle.$$

Then $S\left(g(\mathcal{X})\right)$ has full rank and $\nabla(f\circ g) \neq \nabla_s(f\circ g)$.

Proof. We have $g(\mathcal{X}) = \langle 0, 1, 2\rangle$. It follows that $S\left(g(\mathcal{X})\right) = \begin{bmatrix}1 & 2\end{bmatrix}$ has full rank. The gradient of $(f\circ g)$ at x_0 is

$$\begin{aligned}
\nabla(f\circ g)(x_0) &= \left(\mathbf{J}g(x_0)\right)^T \nabla f\left(g(x_0)\right)\\
&= \begin{bmatrix}1\\1\end{bmatrix}.
\end{aligned}$$

But the simplex gradient of $(f\circ g)$ with respect to $\mathcal{X}$ is

$$\begin{aligned}
\nabla_s(f\circ g)(\mathcal{X}) &= \left(\mathbf{J_s}g(\mathcal{X})\right)^T \nabla_s f\left(g(\mathcal{X})\right)\\
&= \begin{bmatrix}1\\0\end{bmatrix}.
\end{aligned}$$ ∎

In the previous example, note that

$$S(\mathcal{X}) = \begin{bmatrix}1 & 2\\0 & 0\end{bmatrix}$$

does not have full row rank. By adding the assumption that both $S(\mathcal{X})$ and $S\left(g(\mathcal{X})\right)$ have full row rank, we get the following result.

PROPOSITION 37 ($\nabla_s(f\circ g)(\mathcal{X}) = \nabla(f\circ g)(x_0)$). *Let $f : \mathbb{R}^p \to \mathbb{R} : x \mapsto a^T x + c_1$ and $g : \mathbb{R}^d \to \mathbb{R}^p : x \mapsto Bx + c_2$, where $a \in \mathbb{R}^p$, $B \in \mathbb{R}^{p\times d}$, and $c_1, c_2 \in \mathbb{R}$. Let $\mathcal{X} = \langle x_0, x_1, \ldots, x_k\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^d$ and $g(\mathcal{X}) = \langle g(x_0), g(x_1), \ldots, g(x_k)\rangle$ be an ordered set of $k+1$ points in $\mathbb{R}^p$. Suppose $S(\mathcal{X})$ and $S(g(\mathcal{X}))$ have full row rank. Then*

$$\nabla_s(f\circ g)(\mathcal{X}) = \nabla(f\circ g)(x_0).$$

Proof. We have

$$
\begin{aligned}
\nabla_s(f\circ g)(\mathcal{X}) &= (\mathbf{J_s} g(\mathcal{X}))^T \nabla_s f(g(\mathcal{X})) && \text{(by Proposition 35)}\\
&= \begin{bmatrix} \nabla_s g_1(\mathcal{X})^T \\ \nabla_s g_2(\mathcal{X})^T \\ \vdots \\ \nabla_s g_p(\mathcal{X})^T \end{bmatrix}^T \nabla_s f(g(\mathcal{X}))\\
&= \begin{bmatrix} \nabla_s g_1(\mathcal{X})^T \\ \nabla_s g_2(\mathcal{X})^T \\ \vdots \\ \nabla_s g_p(\mathcal{X})^T \end{bmatrix}^T \nabla f\left(g(x_0)\right) && \text{(since } S\left(g(\mathcal{X})\right) \text{ has full row rank and } f \text{ is linear)}\\
&= \begin{bmatrix} \nabla g_1(x_0)^T \\ \nabla g_2(x_0)^T \\ \vdots \\ \nabla g_p(x_0)^T \end{bmatrix}^T \nabla f\left(g(x_0)\right) && \text{(since } S(\mathcal{X}) \text{ has full row rank and } g \text{ is linear)}\\
&= \nabla(f\circ g)(x_0). && \square
\end{aligned}
$$

Now, let us define the *generalized simplex chain gradient of* $(f\circ g)$ *with respect to* $\mathcal{X}$:

$$
\nabla_{sc}(f\circ g)(\mathcal{X}) := (\mathbf{J_s} g(\mathcal{X}))^T \nabla_s f(g(\mathcal{X})). \tag{7}
$$

The next theorem provides an error bound for $\nabla_{sc}(f\circ g)(\mathcal{X})$.

THEOREM 38 (error bound for $\nabla_{sc}(f\circ g)$). *Let $g:\mathbb{R}^d\to\mathbb{R}^p$ and $f:\mathbb{R}^p\to\mathbb{R}$, and let $\mathcal{X}$ be an ordered set of $k+1$ points in $\mathbb{R}^d$. Assume that $S(\mathcal{X})$, $S(g(\mathcal{X}))$ have full row rank. Also, assume ∇g is Lipschitz continuous with Lipschitz constant $L_{\nabla g}\geq 0$ in an open domain Ω_1 containing $B_1(x_0,\Delta_{\mathcal{X}})$ and that ∇f is Lipschitz continuous with Lipschitz constant $L_{\nabla f}\geq 0$ in an open domain Ω_2 containing $B_2\left(g(x_0),\Delta_{g(\mathcal{X})}\right)$. Denote $L_{g_i}\geq 0$ to be the Lipschitz constant for g_i in Ω_1 for all $i\in\{1,2,\dots,p\}$. Define*

$$
\varepsilon_{sc}(f\circ g)(\mathcal{X}) := \frac{\sqrt{k}\,p}{2}\left(\sqrt{k}\,L_{g_*}\,L_{\nabla f}\left\|\left(\widehat{S}\left(g(\mathcal{X})\right)^T\right)^{\dagger}\right\| + \|\nabla f(g(x_0))\| L_{\nabla g_*}\right)\left\|\left(\widehat{S}\left(\mathcal{X}\right)^T\right)^{\dagger}\right\|\Delta_*,
$$

where

$$
\begin{aligned}
\Delta_* &= \max\left\{\Delta_{\mathcal{X}},\Delta_{g(\mathcal{X})}\right\},\\
L_{g_*} &= \max\{L_{g_i}: i=1,\dots,p\},\\
L_{\nabla g_*} &= \max\{L_{\nabla g_i}: i=1,\dots,p\},\\
\widehat{S}(\mathcal{X}) &= S(\mathcal{X})/\Delta_{\mathcal{X}},\\
\widehat{S}(g(\mathcal{X})) &= S(g(\mathcal{X}))/\Delta_{g(\mathcal{X})}.
\end{aligned}
$$

Then

$$
\|\nabla_{sc}(f\circ g)(\mathcal{X}) - \nabla(f\circ g)(x_0)\| \leq \varepsilon_{sc}(f\circ g)(\mathcal{X}).
$$

Proof. We have

$$
\begin{aligned}
&\|\nabla_{sc}(f\circ g)(\mathcal{X}) - \nabla(f\circ g)(x_0)\|\\
&= \|\left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla_s f\left(g(\mathcal{X})\right) - \left(\mathbf{J} g(x_0)\right)^T \nabla f\left(g\left(x_0\right)\right)\|\\
&= \|\left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla_s f\left(g(\mathcal{X})\right) - \left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla f\left(g\left(x_0\right)\right) + \left(\mathbf{J_s} g(\mathcal{X})\right)^T \nabla f\left(g\left(x_0\right)\right) - \left(\mathbf{J} g(x_0)\right)^T \nabla f\left(g\left(x_0\right)\right)\|\\
&\leq \|\left(\mathbf{J_s} g(\mathcal{X})\right)^T\|\|\nabla_s f\left(g(\mathcal{X})\right) - \nabla f\left(g\left(x_0\right)\right)\| + \|\nabla f\left(g\left(x_0\right)\right)\|\|\left(\mathbf{J_s} g(\mathcal{X}) - \mathbf{J} g(x_0)\right)^T\|.
\end{aligned}
$$

Note that

$$\|\nabla_s f\left(g(\mathcal{X})\right) - \nabla f\left(g\left(x_0\right)\right)\| \leq \frac{\sqrt{k}}{2} L_{\nabla f} \left\| \left(\widehat{S}\left(g(\mathcal{X})\right)^T\right)^\dagger \right\| \Delta_{g(\mathcal{X})} \qquad \text{(by Proposition 3)}$$

and

$$\begin{aligned}
\|\left(\mathbf{J_s} g(\mathcal{X}) - \mathbf{J} g(x_0)\right)^T\| &= \left\| \begin{bmatrix} (\nabla_s g_1(\mathcal{X}) - \nabla g_1(x_0))^T \\ \vdots \\ (\nabla_s g_p(\mathcal{X}) - \nabla g_p(x_0))^T \end{bmatrix}^T \right\| \\
&\leq \|\nabla_s g_1(\mathcal{X}) - \nabla g_1(x_0)\| + \cdots + \|\nabla_s g_p(\mathcal{X}) - \nabla g_p(x_0)\| \\
&\leq \frac{\sqrt{k}}{2} \Delta_{\mathcal{X}} \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \left(L_{\nabla g_1} + \cdots + L_{\nabla g_p}\right) \\
&\leq \frac{\sqrt{k}\, p}{2} L_{\nabla g_*} \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \Delta_{\mathcal{X}}.
\end{aligned}$$

Also,

$$\begin{aligned}
\|\left(\mathbf{J_s} g(\mathcal{X})\right)^T\| &= \left\| \begin{bmatrix} \nabla_s g_1(\mathcal{X})^T \\ \vdots \\ \nabla_s g_p(\mathcal{X})^T \end{bmatrix}^T \right\| \\
&\leq \|\nabla_s g_1(\mathcal{X})\| + \cdots + \|\nabla_s g_p(\mathcal{X})\| \\
&\leq \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \left\| \frac{\delta_{g_1}}{\Delta_{\mathcal{X}}} \right\| + \cdots + \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \left\| \frac{\delta_{g_p}}{\Delta_{\mathcal{X}}} \right\| \\
&\leq \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \sqrt{k}\, L_{g_1} + \cdots + \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \sqrt{k}\, L_{g_p} \\
&\leq \sqrt{k}\, p\, L_{g_*} \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\|.
\end{aligned}$$

All together,

$$\begin{aligned}
&\|\nabla_{sc}(f \circ g)(\mathcal{X}) - \nabla(f \circ g)(x_0)\| \\
&\leq \sqrt{k}\, p\, L_{g_*} \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \frac{\sqrt{k}}{2} L_{\nabla f} \left\| \left(\widehat{S}\left(g(\mathcal{X})\right)^T\right)^\dagger \right\| \Delta_{g(\mathcal{X})} + \|\nabla f(g(x_0))\| \frac{\sqrt{k}\, p}{2} L_{\nabla g_*} \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \Delta_{\mathcal{X}} \\
&\leq \frac{\sqrt{k}\, p}{2} \left(\sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\left(g(\mathcal{X})\right)^T\right)^\dagger \right\| + \|\nabla f(g(x_0))\| L_{\nabla g_*} \right) \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \Delta_*. \qquad \square
\end{aligned}$$

The following corollary provides an alternative error bound for $\nabla_{sc}(f \circ g)(\mathcal{X})$.

COROLLARY 39. *Let the assumptions of Theorem* 38 *hold. Let* $L_f \geq 0$ *denote the Lipschitz constant of* f *on* Ω_2. *Then*

$$\begin{aligned}
&\|\nabla_{sc}(f \circ g)(\mathcal{X}) - \nabla(f \circ g)(x_0)\| \\
&\leq \frac{kp}{2} \left(L_{g_*}\, L_{\nabla f} + L_f\, L_{\nabla g_*} + L_{\nabla f}\, L_{\nabla g_*} \frac{\Delta_*}{2} \right) \left\| \left(\widehat{S}\left(g(\mathcal{X})\right)^T\right)^\dagger \right\| \left\| \left(\widehat{S}\left(\mathcal{X}\right)^T\right)^\dagger \right\| \Delta_*.
\end{aligned}$$

Proof. Let us consider the term

$$\left(\sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \|\nabla f(g(x_0))\| L_{\nabla g_*}\right)$$

in the error bound presented in Theorem 38. By adding and subtracting $\|\nabla_s f(g(\mathcal{X}))\|\, L_{\nabla g_*}$,

$$\begin{aligned}
&\sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \|\nabla f(g(x_0))\| L_{\nabla g_*} \\
&= \sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \|\nabla_s f(g(\mathcal{X}))\|\, L_{\nabla g_*} - \|\nabla_s f(g(\mathcal{X}))\|\, L_{\nabla g_*} + \|\nabla f(g(x_0))\| L_{\nabla g_*} \\
&\leq \sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \|\nabla_s f(g(\mathcal{X}))\|\, L_{\nabla g_*} + \|\nabla f(g(x_0)) - \nabla_s f(g(\mathcal{X}))\|\, L_{\nabla g_*} \\
&\leq \sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \|\nabla_s f(g(\mathcal{X}))\|\, L_{\nabla g_*} + \frac{\sqrt{k}}{2} L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| \Delta_{g(\mathcal{X})} L_{\nabla g_*} \\
&\leq \sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| \left\| \frac{\delta_{f\circ g}}{\Delta_{g(\mathcal{X})}} \right\| L_{\nabla g_*} + \frac{\sqrt{k}}{2} L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\|\ \Delta_{g(\mathcal{X})} L_{\nabla g_*} \\
&\leq \sqrt{k}\, L_{g_*}\, L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| + \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| \sqrt{k}\, L_f\, L_{\nabla g_*} + \frac{\sqrt{k}}{2} L_{\nabla f} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\|\ \Delta_{g(\mathcal{X})} L_{\nabla g_*} \\
&= \sqrt{k} \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| \left(L_{g_*}\, L_{\nabla f} + L_f\, L_{\nabla g_*} + L_{\nabla f}\, L_{\nabla g_*} \frac{\Delta_{g(\mathcal{X})}}{2} \right).
\end{aligned}$$

It follows that

$$\begin{aligned}
&\|\nabla_{sc}(f\circ g)(\mathcal{X}) - \nabla(f\circ g)(x_0)\| \\
&\leq \frac{kp}{2} \left(L_{g_*}\, L_{\nabla f} + L_f\, L_{\nabla g_*} + L_{\nabla f}\, L_{\nabla g_*} \frac{\Delta_*}{2} \right) \left\| \left(\widehat{S}\,(g(\mathcal{X}))^T\right)^{\dagger} \right\| \left\| \left(\widehat{S}\,(\mathcal{X})^T\right)^{\dagger} \right\| \Delta_*. \quad \square
\end{aligned}$$

Analyzing the previous error bounds, we find when $\nabla_{sc}(f\circ g)(\mathcal{X})$ is an exact approximation of the true gradient $\nabla(f\circ g)(x_0)$.

Corollary 40. *Let the assumptions of Theorem* 38 *hold. If f and g are linear functions, then*

$$\nabla_{sc}(f\circ g)(\mathcal{X}) = \nabla(f\circ g)(x_0).$$

Note that if g is Lipschitz continuous on a set Ω_1 and f is Lipschitz continuous on a set Ω_2 such that $g(\Omega_1) \subseteq \Omega_2$, then $f\circ g$ is Lipschitz continuous on Ω_1. Thus, $L_{(f\circ g)}$ is well-defined on Ω_1.

Let us give one example where $\nabla_{sc}(f\circ g)(\mathcal{X})$ is a better approximation than $\nabla_s(f\circ g)(\mathcal{X})$ and one example where $\nabla_{sc}(f\circ g)(\mathcal{X})$ is not a better approximation.

Example 41. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto 1/(x+1)$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto x^2$. First, consider the ordered set $\mathcal{X}_1 = \langle 0, 0.5, 1\rangle$. Note that $L_{g*} = 2$, $L_{\nabla g*} = 2$, $L_{\nabla f} = 2$, and $L_{\nabla(f\circ g)} = 2$ on $[0,1]$. Using Theorem 38 and Proposition 3, the error bounds are $\varepsilon_{sc}(f\circ g)(\mathcal{X}_1) \approx 3.48$ and $\varepsilon_s(f\circ g)(\mathcal{X}_1) \approx 1.27$. The true absolute errors are

$$\|\nabla_{sc}(f\circ g)(\mathcal{X}_1) - \nabla(f\circ g)(x_0)\| \approx 0.47 \leq \varepsilon_{sc}(f\circ g)(\mathcal{X}_1)$$

and

$$\|\nabla_s(f\circ g)(\mathcal{X}_1) - \nabla(f\circ g)(x_0)\| \approx 0.48 \leq \varepsilon_s(f\circ g)(\mathcal{X}_1).$$

Now let us consider $\mathcal{X}_2 = \langle 0, 0.5, -0.5, 1\rangle$. The Lipschitz constants are now $L_{g*} = 2$, $L_{\nabla f} = 16$, $L_{\nabla g*} = 2$, and $L_{\nabla(f\circ g)} = 2$ on $[-0.5, 1]$. The error bounds are $\varepsilon_{sc}(f\circ g)(\mathcal{X}_2) \approx 36.96$ and $\varepsilon_s(f\circ g)(\mathcal{X}_2) \approx 1.42$.

The true absolute errors are

$$\|\nabla_{sc}(f \circ g)(\mathcal{X}_2) - \nabla(f \circ g)(x_0)\| \approx 0.36 \le \varepsilon_{sc}(f \circ g)(\mathcal{X}_2)$$

and

$$\|\nabla_s(f \circ g(\mathcal{X}_2) - \nabla(f \circ g)(x_0)\| \approx 0.33 \le \varepsilon_s(f \circ g)(\mathcal{X}_2).$$

To conclude this section, it is worth mentioning that all the error bounds defined for generalized simplex calculus gradients remain $\mathcal{O}(\Delta)$.

6. Numerical experiments. In this section, we briefly explore the *numerical stability* of the formulas introduced previously. Second, we investigate the numerical accuracy of generalized simplex calculus gradients on Moré, Garbow, and Hillstrom's Test Set [12]. All numerical calculations are performed using MATLAB 2018a. Note that MATLAB constructs the double-precision data type according to IEEE Standard 754.

6.1. Stability of the calculus rules. Let us denote the generalized simplex gradient that uses the quotient rule by ∇_{sqe}. We now have three approaches to build an approximation of the gradient. For instance, $\nabla\left(\frac{f}{g}\right)(x_0)$ can be approximated with

$$\text{(i)} \quad \nabla_s \left(\frac{f}{g}\right)(\mathcal{X}) = \left(S(\mathcal{X})^T\right)^{\dagger} \delta_{\frac{f}{g}} \qquad \text{(Definition 2)},$$

$$\text{(ii)} \quad \nabla_{sqe} \left(\frac{f}{g}\right)(\mathcal{X}) = \frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2} - E_{\frac{f}{g}} \qquad \text{(Theorem 11)},$$

and

$$\text{(iii)} \quad \nabla_{sq} \left(\frac{f}{g}\right)(\mathcal{X}) = \frac{g(x_0)\nabla_s f(\mathcal{X}) - f(x_0)\nabla_s g(\mathcal{X})}{[g(x_0)]^2} \qquad \text{(equation (6))}.$$

Next, we provide three examples. They cover the cases where
- (i) is more stable that (ii),
- (i) is more stable than (iii),
- (ii) is more stable than (i),
- (ii) is more stable than (iii),
- (iii) is more stable than (i), and
- (iii) is more stable than (ii).

Let us clarify some details about Tables 3, 4, and 5. The parameter β_m is defined as

$$\beta_m = 10^{-m}, \quad m \in \{0, 1, 2, \dots\}. \tag{8}$$

The role of β_m is to shrink $S(\mathcal{X})$. That is ,$S(\mathcal{X})_m = \beta_m S(\mathcal{X})$.

The absolute error for a gradient approximation technique, for instance $\nabla_s(\cdot)(\mathcal{X})$, is denoted by AE $\nabla_s(\cdot)(\mathcal{X})$ and equal to

$$\text{AE}\,\nabla_s(\cdot)(\mathcal{X}) = \|\nabla_s(\cdot)(\mathcal{X}) - \nabla(\cdot)(x_0)\|.$$

The relative error for $\nabla_s(\cdot)(\mathcal{X})$, denoted by RE $\nabla_s(\cdot)(\mathcal{X})$, is

$$\text{RE}\,\nabla_s(\cdot)(\mathcal{X}) = \frac{\text{AE}\,\nabla_s(\cdot)(\mathcal{X})}{\|\nabla(\cdot)(x_0)\|}.$$

Table 3
An example where $\nabla_s(\frac{f}{g})(\mathcal{X})$ is stable and accurate.

β_m	RE $\nabla_s(\frac{f}{g})(\mathcal{X})$	RE $\nabla_{sqe}(\frac{f}{g})(\mathcal{X})$	RE $\nabla_{sq}(\frac{f}{g})(\mathcal{X})$
10^{0}	0.0000e+00	0.0000e+00	2.5000e-01
10^{-1}	0.0000e+00	**3.9968e-15**	2.5000e-02
10^{-2}	0.0000e+00	5.7732e-15	2.5000e-03
10^{-3}	0.0000e+00	2.5691e-13	2.5000e-04
10^{-4}	0.0000e+00	2.0690e-12	2.5000e-05
10^{-5}	0.0000e+00	4.4202e-11	2.5000e-06
10^{-6}	0.0000e+00	4.2186e-10	2.4958e-07
10^{-7}	0.0000e+00	1.6454e-09	2.6645e-08
10^{-8}	0.0000e+00	2.5000e-09	**0.0000e+00**
10^{-9}	0.0000e+00	2.5000e-10	0.0000e+00
10^{-10}	0.0000e+00	2.5000e-11	0.0000e+00
10^{-11}	**1.1102e-16**	2.5001e-12	1.1102e-16

For the purpose of this paper, we say that the formula becomes *unstable* at $m = \ell$ whenever the relative error at ℓ is greater than the relative error at $\ell - 1$, or the relative error at ℓ is equal to zero and all the relative errors are not equal to zero for all $m \in \{1, 2, \ldots, \ell - 1\}$. Essentially, we are looking for points where any pattern in the value of the relative error changes drastically. This concept of stability is an indicator of how small Δ can be before numerical errors occur. Since Δ is intimately linked to the accuracy of our approximation, stability also provides information about the maximal accuracy that an approximation technique can reach on the functions considered.

In the following tables, a boldface number exhibits when a formula becomes unstable.

Example 42. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto x^2$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto x$. Consider $\mathcal{X} = \langle 4, 5 \rangle$. Table 3 shows that (i) is more stable than (ii), (i) is more stable than (iii), and (iii) is more stable than (ii).

Example 43. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto 1$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto \log(x)$. Consider $\mathcal{X} = \langle 2, 3 \rangle$. Table 4 shows that (ii) is more stable than (i), while (ii) is more stable than (iii).

Example 44. Let $f : \mathbb{R} \to \mathbb{R} : x \mapsto 1$ and $g : \mathbb{R} \to \mathbb{R} : x \mapsto x$. Consider $\mathcal{X} = \langle 10^{-8}, 1 + 10^{-8} \rangle$. Table 5 shows that (iii) is more stable than (i). Note that (iii) is much more accurate than (i) and (ii) since f and g are linear functions.

6.2. Numerical accuracy. In this section, we test the chain rule and the product rule using the functions defined in Moré, Garbow, and Hillstrom's Test Set [12]. First, we compare the generalized simplex gradient $\nabla_s(f \circ g)(\mathcal{X})$ with the generalized simplex chain gradient $\nabla_{sc}(f \circ g)(\mathcal{X})$. Second, we compare the generalized simplex gradient $\nabla_s(f_1 \cdots f_p)(\mathcal{X})$ with the generalized simplex product gradient $\nabla_{sp}(f_1 \cdots f_p)(\mathcal{X})$. The sample set of points on every problem is $\mathcal{X} = \langle x_0, x_0 + \beta e_1, \ldots, x_0 + \beta e_d, x_0 - \beta e_1, \ldots, x_0 - \beta e_d \rangle$, where x_0 is the starting point defined in [12] and β is a real number in the interval (0,1]. Once again, the role of β is to shrink the matrix $S(\mathcal{X})$. Our goal is to determine the largest value of β necessary to obtain a relative error less than 10^{-3}. To achieve this goal, we do the following:

1. Compute the approximate gradient using $\beta = 1$ and the resulting relative error. If the relative error is less than 10^{-3}, then stop (return $\beta = 1$).

TABLE 4
An example where $\nabla_{sqe}(\frac{f}{g})(\mathcal{X})$ is the most stable.

β_m	(1) RE $\nabla_s(\frac{f}{g})(\mathcal{X})$	(2) RE $\nabla_{sqe}(\frac{f}{g})(\mathcal{X})$	(3) RE $\nabla_{sq}(\frac{f}{g})(\mathcal{X})$
10^{0}	4.8836e-01	4.8836e-01	1.8907e-01
10^{-1}	8.8366e-02	8.8366e-02	2.4197e-02
10^{-2}	9.6180e-03	9.6180e-03	2.4917e-03
10^{-3}	9.7038e-04	9.7038e-04	2.4992e-04
10^{-4}	9.7125e-05	9.7125e-05	2.4999e-05
10^{-5}	9.7134e-06	9.7134e-06	2.5000e-06
10^{-6}	9.7151e-07	9.7137e-07	2.5002e-07
10^{-7}	9.7287e-08	9.6560e-08	2.4425e-08
10^{-8}	1.1768e-08	7.2135e-09	**0.0000e+00**
10^{-9}	**1.4326e-07**	7.2135e-10	0.0000e+00
10^{-10}	1.4234e-06	7.2135e-11	0.0000e+00
10^{-11}	5.6907e-06	7.2134e-12	0.0000e+00
10^{-12}	5.1831e-05	7.2138e-13	0.0000e+00
10^{-13}	6.5773e-04	7.2117e-14	0.0000e+00
10^{-14}	2.6846e-03	7.4677e-15	0.0000e+00
10^{-15}	3.9094e-02	6.4009e-16	0.0000e+00
10^{-16}	1.0000e+00	**1.0000e+00**	1.0000e+00

TABLE 5
An example where $\nabla_{sq}(\frac{f}{g})(\mathcal{X})$ is stable and accurate.

β_m	(1) RE $\nabla_s(\frac{f}{g})(\mathcal{X})$	(2) RE $\nabla_{sqe}(\frac{f}{g})(\mathcal{X})$	(3) RE $\nabla_{sq}(\frac{f}{g})(\mathcal{X})$
10^{0}	1.0000e+00	1.0000e+00	2.0000e-16
10^{-1}	1.0000e+00	1.0000e+00	2.0000e-16
10^{-2}	1.0000e+00	1.0000e+00	2.0000e-16
10^{-3}	9.9999e-01	9.9999e-01	2.0000e-16
10^{-4}	9.9990e-01	9.9990e-01	2.0000e-16
10^{-5}	9.9900e-01	9.9900e-01	2.0000e-16
10^{-6}	9.9010e-01	9.9010e-01	2.0000e-16
10^{-7}	9.0909e-01	9.0909e-01	2.0000e-16
10^{-8}	5.0000e-01	5.0000e-01	2.0000e-16
10^{-9}	9.0909e-02	9.0909e-02	2.0000e-16
10^{-10}	9.9010e-03	9.9010e-03	2.0000e-16
10^{-11}	9.9900e-04	9.9900e-04	2.0000e-16
10^{-12}	9.9990e-05	9.9990e-05	2.0000e-16
10^{-13}	9.9999e-06	9.9999e-06	2.0000e-16
10^{-14}	1.0000e-06	1.0000e-06	2.0000e-16
10^{-15}	1.0016e-07	1.0000e-07	2.0000e-16
10^{-16}	1.5220e-08	1.0000e-08	2.0000e-16
10^{-17}	**4.3380e-08**	1.0000e-09	2.0000e-16
10^{-18}	3.8723e-07	1.0000e-10	2.0000e-16
10^{-19}	6.8405e-06	1.0000e-11	2.0000e-16
10^{-20}	4.4430e-05	1.0002e-12	2.0000e-16
10^{-21}	6.3422e-04	1.0020e-13	2.0000e-16
10^{-22}	5.8039e-03	1.0200e-14	2.0000e-16
10^{-23}	5.0840e-02	1.2000e-15	2.0000e-16
10^{-24}	9.9280e-02	4.0000e-16	2.0000e-16
10^{-25}	1.0000e+00	**1.0000e+00**	**1.0000e+00**

2. Compute the approximate gradient using $\beta \in \{10^{-1}, 10^{-2}, \ldots, 10^{-8}\}$ and the resulting relative error, until a value is found that gives a relative error less than 10^{-3}. If none of these values provides a relative error less than 10^{-3},

then return "`error`."

3. Apply a bisection method with a tolerance of 10^{-6} to find the highest value of β that returns a relative error less than 10^{-3}.

Our findings are presented in Tables 6 and 7. In the tables, a boldface number is associated with the approach that does better on a certain problem. An underlined boldface number is used when the resulting β is at least one order of magnitude higher for the given method.

Table 6 provides our results regarding the chain rule. The outer function used is $f : \mathbb{R}^p \to \mathbb{R} : x \mapsto \sum_{i=1}^{p} \|x_i\|^2$, and the inner functions are provided from Moré, Garbow, and Hillstrom's Test Set [12]. In the table, the dimension of the domain of the inner function g is given by d and the dimension of the codomain by p. In general, we see that the generalized simplex gradient $\nabla_s(f \circ g)(\mathcal{X})$ performs better on these test problems. However, in most problems the difference is not large, with only three values of β underlined and boldface.

Some precautions are necessary to generalize these results and claim that the generalized simplex gradient is a better approximation than the generalized simplex chain gradient. Indeed, we have only considered one outer function f. Choosing another outer function could affect our conclusion regarding the accuracy of both methods.

The results of the second numerical experiment are presented in Table 7. In this case, we compare the generalized simplex gradient $\nabla_s F(\mathcal{X})$, where $F = f_1 \cdot f_2 \cdots f_p$, and the generalized simplex product gradient $\nabla_{sp}(f_1 f_2 \cdots f_p)(\mathcal{X})$, where the f_i functions are provided from the Test Set [12]. In this case, the generalized simplex product gradient appears a clear winner. Except for the problem Box3D, the generalized simplex product gradient does better on every problem. We note that in many of these problems the functions f_i for all $i \in \{1, 2, \ldots, p\}$ are not linear. The excellent performance of the generalized simplex product gradient can be partly explained by looking at the conditions enumerated in Corollary 26. In particular, the following hold:

- Condition (i) is satisfied on problem 7.
- Condition (ii) is satisfied on problems 7, 14, 20, 23, and 35.
- Condition (iii) is satisfied on 32, 33, and 34.

In addition, the following holds:

- Condition (i) is *almost* satisfied on problems 9, 15, 17, 18, 19, 24, 25, 26, 28, and 29, in the sense that at least two function values at (x_0) are $\in [-0.1, 0.1]$.

This explains the excellent performance on those problems; however, we note that there are still many problems with excellent performance that are not explained by Corollary 26.

While we must still be cautious about drawing any universal conclusions, since there is only really one way to create an experiment where the product rule would be applied, this result seems more likely to be generalizable.

7. Conclusions and open directions. The new calculus rules introduced in this paper provide an attractive framework that holds for underdetermined, determined, and overdetermined simplex gradients and under minimal assumptions. The calculus rules for generalized simplex gradients can be written in a way similar to those for the true gradients plus a term E. Removing the term E from the calculus rules leads to several new approaches for approximating gradients. The new approaches, named generalized simplex calculus gradients, have some interesting benefits. In particular, under certain assumptions, they suit linear functions perfectly. In regards to

Table 6
Testing the chain rule on Moré, Garbow, and Hillstrom's Test Set.

Description			β to Attain $RE \le 10^{-3}$	
Function	d	p	$\nabla_s(f \circ g)(\mathcal{X})$	$\nabla_{sc}(f \circ g)(\mathcal{X})$
1. Rosenbrock	2	2	**2.20e-02**	1.76e-02
2. Freudenstein	2	2	**4.15e-02**	1.12e-02
3. PowellBS	2	2	**<u>1</u>**	3.83e-04
4. BrownBS	2	3	1	1
5. Beale	2	3	3.19e-02	3.19e-02
6. Jenrich	2	4	9.56e-03	9.56e-03
7. Helical	3	3	**6.65e-02**	6.55e-02
8. Bard	3	15	4.27e-02	4.27e-02
9. Gaussian	3	15	7.48e-03	7.48e-03
10. Meyer	3	16	1	1
11. Gulf	3	20	7.18e-03	7.18e-03
12. Box3D	3	3	6.41e-01	**7.29e-01**
13. PowellS	4	4	**6.24e-02**	4.58e-02
14. Wood	4	6	1.00e-01	1.00e-01
15. Kowalik	4	11	2.65e-02	2.65e-02
16. Brown	4	4	**8.83e-01**	3.15e-01
17. Osborne1	5	33	2.09e-04	2.09e-04
18. Biggs	6	6	1.30e-01	1.30e-01
19. Osborne2	11	65	1.26e-02	1.26e-02
20. Watson	31	31	**<u>1</u>**	4.47e-02
21. RosenbrockE	4	4	**2.52e-02**	2.02e-02
22. PowellExt	8	8	**6.29e-02**	4.48e-02
23. Penalty1	4	5	1.47e-01	1.47e-01
24. Penalty2	6	12	2.92e-02	2.92e-02
25. VariablyDim	7	9	1.04e-01	1.04e-01
26. Trigonometric	7	7	**6.44e-03**	3.21e-03
27. BrownAlm	9	9	1	1
28. DiscreteBnd	5	5	**<u>1.56e-02</u>**	6.99e-03
29. DiscreteInt	3	3	**2.12e-02**	1.63e-02
30. BroydenTri	5	5	**2.74e-02**	2.02e-02
31. BroydenBan	8	8	**2.05e-02**	1.69e-02
32. LinearFR	10	13	1	1
33. LinearR1	10	10	1	1
34. LinearR1W0	10	10	1	1
35.Chebyquad	4	5	**6.31e-03**	1.98e-03
Average			**3.01e-01**	2.28e-01
Median			**4.27e-02**	3.19e-02

the quotient rule and the power rule for a negative exponent, the new approaches further permit us to remove the assumption that $g(x_i) \neq 0$ for all $i \in \{1, 2, \ldots, k\}$.

Error bounds for generalized simplex calculus gradients were presented (Theorem 20, Propositions 25 and 27, and Theorems 31 and 38). These error bounds are all $\mathcal{O}(\Delta)$. Analyzing those error bounds, we obtained results regarding when generalized simplex calculus gradients are exact approximations of the true gradients (Corollaries 21, 26, 28, 32, and 40).

In regards to the chain rule, it is enchanting to see that, when $k \le p$ and $S(g(\mathcal{X}))$ has full rank, the term $E_{f \circ g}$ vanishes and we get back the chain rule for the true gradient (Corollary 16). In all cases, the term $E_{f \circ g}$ vanishes for linear functions whenever $S(g(\mathcal{X}))$ has full rank (Proposition 35). Furthermore, we showed that the chain rule is perfectly accurate for linear functions whenever $S(\mathcal{X})$ and $S\left(g(\mathcal{X})\right)$ have

TABLE 7
Testing the product rule on Moré, Garbow, and Hillstrom's Test Set.

Description			β to attain $RE \leq 10^{-3}$	
Function	d	p	$\nabla_s(f_1 \ldots f_p)(\mathcal{X})$	$\nabla_{sp}(f_1 \ldots f_p)(\mathcal{X})$
1. Rosenbrock	2	2	7.82e-02	**<u>1</u>**
2. Freudenstein	2	2	1.74e-02	**4.03e-02**
3. PowellBS	2	2	2.71e-02	**<u>1</u>**
4. BrownBS	2	3	1	1
5. Beale	2	3	2.72e-02	**8.41e-02**
6. Jenrich	2	4	1.67e-02	**2.25e-02**
7. Helical	3	3	1	1
8. Bard	3	15	7.65e-03	**<u>8.51e-02</u>**
9. Gaussian	3	15	9.15e-06	**<u>4.60e-02</u>**
10. Meyer	3	16	2.28e-04	**<u>1</u>**
11. Gulf	3	3	1.03e-02	**1.09e-02**
12. Box3D	3	3	**6.91e-01**	5.95e-01
13. PowellS	4	4	3.30e-02	**<u>1</u>**
14. Wood	4	6	1.99e-01	**<u>1</u>**
15. Kowalik	4	11	9.03e-04	**<u>1.68e-02</u>**
16. Brown	4	4	3.43e-01	**<u>1</u>**
17. Osborne1	5	33	1.03e-05	**<u>1</u>**
18. Biggs	6	6	3.39e-03	**<u>1</u>**
19. Osborne2	11	65	3.28e-04	**<u>3.81e-02</u>**
20. Watson	2	31	5.77e-03	**<u>1</u>**
21. RosenbrockE	4	4	7.89e-02	**<u>1</u>**
22. PowellExt	8	8	3.29e-02	**<u>1</u>**
23. Penalty1	4	5	2.34e-01	**<u>1</u>**
24. Penalty2	6	12	5.24e-02	**<u>1</u>**
25. VariablyDim	7	9	1.19e-01	**<u>1</u>**
26. Trigonometric	7	7	1.73e-03	**<u>1</u>**
27. BrownAlm	9	9	8.78e-01	**<u>1</u>**
28. DiscreteBnd	5	5	8.26e-04	**<u>1</u>**
29. DiscreteInt	3	3	3.38e-02	**<u>1</u>**
30. BroydenTri	5	5	3.09e-02	**<u>1</u>**
31. BroydenBan	8	8	2.30e-02	**<u>1</u>**
32. LinearFR	10	13	6.28e-02	**<u>1</u>**
33. LinearR1	10	10	5.90e-02	**<u>1</u>**
34. LinearR1W0	10	10	6.81e-02	**<u>1</u>**
35.Chebyquad	2	2	1.05e-02	**<u>1</u>**
Average			1.47e-01	**7.69e-01**
Median			3.09e-02	**<u>1</u>**

full row rank.

The results allowed us to state three novel approaches to approximate, for instance, the true gradient $\nabla(fg)(x_0)$: the generalized simplex gradient $\nabla_s(fg)(\mathcal{X})$ (Definition 2), the generalized simplex gradient $\nabla_s(fg)(\mathcal{X})$ using the product rule (Theorem 5), and the generalized simplex product gradient $\nabla_{sp}(fg)(\mathcal{X})$ (equation (5)). From a numerical perspective, we showed that, at least in some cases, the generalized simplex gradient that uses the calculus rule and the generalized simplex calculus gradient can improve the stability of our calculations. We have provided three examples for the quotient rule illustrating a situation where each approach is stable. These examples have also showed the important gain in accuracy we can obtain using the quotient rule or the generalized simplex quotient gradient.

Based on the numerical experiments executed on Moré, Garbow, and Hillstrom's

Test Set, the performance of the generalized simplex gradient and the generalized simplex chain gradient is almost similar. In general, the generalized simplex gradient does slightly better than the generalized simplex chain gradient. The results of the second experiment using the generalized simplex product are striking. Even when the p functions involved are not linear, the generalized simplex product performed better except on one problem.

In practice, it can be difficult to say which approach will do better on a certain problem. One strategy to determine the best approach could be to approximate the Lipschitz constants involved. Algorithm 1 proposes a procedure to decide between the generalized simplex gradient $\nabla_s(fg)(\mathcal{X})$ and the generalized simplex product gradient $\nabla_{sp}(fg)(\mathcal{X})$ based on an approximation of the Lipschitz constants.

Algorithm 1: Approximating the Lipschitz constants.

Given an optimization problem involving a function $F = f \cdot g$, where $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^d \to \mathbb{R}$. At iteration $j \in \mathbb{N}$:

0. Input

$\mathcal{X}^j = \langle x_0^j, \ldots, x_k^j \rangle$	sample set of points
x_0^{j-1}	x_0 at iteration $j-1$
$\tilde{\nabla} f^{j-1}, \tilde{\nabla} g^{j-1}, \tilde{\nabla} F^{j-1}$	gradient approximation of f, g, and F at x_0^{j-1}

1. Approximate the Lipschitz constants

Assume $x_0^j \neq x_0^{j-1}$. Then

$$\tilde{L}_{\nabla f} = \frac{\|\nabla_s f(\mathcal{X}^j) - \tilde{\nabla} f^{j-1}\|}{\|x_0^j - x_0^{j-1}\|}$$

$$\tilde{L}_{\nabla g} = \frac{\|\nabla_s g(\mathcal{X}^j) - \tilde{\nabla} g^{j-1}\|}{\|x_0^j - x_0^{j-1}\|}$$

$$\tilde{L}_{\nabla F} = \min\left\{ \frac{\|\nabla_s F(\mathcal{X}^j) - \tilde{\nabla} F^{j-1}\|}{\|x_0^j - x_0^{j-1}\|}, \frac{\|\nabla_{sp} F(\mathcal{X}^j) - \tilde{\nabla} F^{j-1}\|}{\|x_0^j - x_0^{j-1}\|} \right\}$$

2. Update

if $|f(x_0^j)|\tilde{L}_{\nabla g} + |g(x_0^j)|\tilde{L}_{\nabla f} \leq \tilde{L}_{\nabla F}$ **then**
  $\tilde{\nabla} F^j = \nabla_{sp} F(\mathcal{X}^j)$
else
  $\tilde{\nabla} F^j = \nabla_s F(\mathcal{X}^j)$
end

The effectiveness of this algorithm, when embedded within a model-based DFO method, is a clear next step in this research direction.

Acknowledgments. The authors express their gratitude to the anonymous referees and the SIOPT editor, who helped improve this paper through their constructive feedback.

REFERENCES

[1] C. Audet and W. Hare, *Derivative-Free and Blackbox Optimization*, Springer Ser. Oper. Res. Financ. Eng., Springer, Cham, 2017, https://doi.org/10.1007/978-3-319-68913-5.

[2] D.M. Bortz and C.T. Kelley, *The simplex gradient and noisy optimization problems*, in Computational Methods for Optimal Design and Control, Birkhäuser Boston, Boston, MA, 1998, pp. 77–90.

[3] A.R. Conn, K. Scheinberg, and L.N. Vicente, *Geometry of interpolation sets in derivative free optimization*, Math. Program., 111 (2008), pp. 141–172.

[4] A.R. Conn, K. Scheinberg, and L.N. Vicente, *Geometry of sample sets in derivative-free optimization: Polynomial regression and underdetermined interpolation*, IMA J. Numer. Anal., 28 (2008), pp. 721–748.

[5] A.R. Conn, K. Scheinberg, and L.N. Vicente, *Introduction to Derivative-Free Optimization*, MOS-SIAM Ser. Optim. 8, SIAM, Philadelphia, 2009, https://doi.org/10.1137/1.9780898718768.

[6] A.L. Custódio, J.E. Dennis, and L.N. Vicente, *Using simplex gradients of nonsmooth functions in direct search methods*, IMA J. Numer. Anal., 28 (2008), pp. 770–784.

[7] A.L. Custódio and L.N. Vicente, *Using sampling and simplex derivatives in pattern search methods*, SIAM J. Optim., 18 (2007), pp. 537–555, https://doi.org/10.1137/050646706.

[8] K. Eriksson, D. Estep, and C. Johnson, *Applied Mathematics: Body and Soul: Volume* 1: *Derivatives and Geometry in* $\mathbb{R}^3$, Springer-Verlag, Berlin, 2013.

[9] W. Hare, *Compositions of convex functions and fully linear models*, Optim. Lett., 11 (2017), pp. 1217–1227.

[10] R. Hooke and T.A. Jeeves, *"Direct search" solution of numerical and statistical problems*, J. ACM, 8 (1961), pp. 212–229.

[11] C.T. Kelley, *Iterative Methods for Optimization*, Frontiers Appl. Math. 18, SIAM, Philadelphia, 1999, https://doi.org/10.1137/1.9781611970920.

[12] J.J. Moré, B.S. Garbow, and K.E. Hillstrom, *Testing unconstrained optimization software*, ACM Trans. Math. Software, 7 (1981), pp. 17–41.

[13] J.A. Nelder and R. Mead, *A simplex method for function minimization*, Computer J., 7 (1965), pp. 308–313.

[14] M.J. Powell, *A direct search optimization method that models the objective and constraint functions by linear interpolation*, in Advances in Optimization and Numerical Analysis, Kluwer Academic Publishers, Dordrecht, The Netherlands, 1994, pp. 51–67.

[15] M. Rashki, *Hybrid control variates-based simulation method for structural reliability analysis of some problems with low failure probability*, Appl. Math. Model., 60 (2018), pp. 220–234.

[16] R.G. Regis, *The calculus of simplex gradients*, Optim. Lett., 9 (2015), pp. 845–865.

[17] K. Scheinberg and Ph.L. Toint, *Self-correcting geometry in model-based algorithms for derivative-free unconstrained optimization*, SIAM J. Optim., 20 (2010), pp. 3512–3532, https://doi.org/10.1137/090748536.

[18] I.N. Stewart, *Galois Theory*, CRC Press, Boca Raton, FL, 2015.

[19] D.H. Winfield, *Function and Functional Optimization by Interpolation in Data Tables*, Ph.D. thesis, Harvard University, Cambridge, MA, 1970.