The Error in Multivariate Linear Extrapolation with Applications to Derivative-Free Optimization

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Abstract

We study in this paper the function approximation error of multivariate linear extrapolation. The sharp error bound of linear interpolation already exists in the literature. However, linear extrapolation is used far more often in applications such as derivative-free optimization, while its error is not well-studied. We introduce in this paper a method to numerically compute the sharp bound on the error, and then present several analytical bounds along with the conditions under which they are sharp. We analyze in depth the approximation error achievable by quadratic functions and the error bound for the bivariate case. All results are under the assumptions that the function being interpolated has Lipschitz continuous gradient and is interpolated on an affinely independent sample set.

1 Introduction

Polynomial interpolation is one of the most basic techniques for approximating functions and plays an essential role in applications such as finite element methods and derivative-free optimization. This led to a large amount of literature concerning its approximation error. This paper contributes to this area of study by analyzing the function approximation error of linear interpolation and extrapolation. Specifically, given a function $f : \mathbb{R}^n \to \mathbb{R}$ and an affinely independent sample set $\Theta := \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n+1}\} \subset \mathbb{R}^n$, one can find a unique affine function $\hat{f} : \mathbb{R}^n \to \mathbb{R}$ such that $\hat{f}(\mathbf{x}_i) = f(\mathbf{x}_i)$ for all $i \in \{1, \dots, n+1\}$. We investigate in this paper the (sharp) upper bound on the approximation error $|\hat{f}(\mathbf{x}) - f(\mathbf{x})|$ when the sample set Θ and the point where the error is measured $\mathbf{x}$ are given, and f is assumed to belong to $C^{1,1}_\nu(\mathbb{R}^n)$. The class $C^{1,1}_\nu(\mathbb{R}^n)$ represents the differentiable functions defined on $\mathbb{R}^n$ with their first derivative Df being ν-Lipschitz continuous, i.e.,

$$\|Df(\mathbf{u}) - Df(\mathbf{v})\| \leq \nu \|\mathbf{u} - \mathbf{v}\| \quad \text{for all } \mathbf{u}, \mathbf{v} \in \mathbb{R}^n, \tag{1}$$

where $\nu > 0$ is the Lipschitz constant, and the norms are Euclidean. The sharp bound on $|\hat{f}(\mathbf{x}) - f(\mathbf{x})|$ is already discovered and proved in [14] for linear interpolation, but only for the case when the word "interpolation" is used in its narrow sense, i.e., when $\mathbf{x} \in \operatorname{conv}(\Theta)$, the convex hull of Θ. In this paper, we make no assumption on the location of $\mathbf{x}$ relative to Θ, and the word "interpolation" is typically used to refer to this general case.

The function approximation error of univariate ($n = 1$) interpolation using polynomials of any degree is already well-studied, and the results can be found in classical literature such as [3]. If a $(d+1)$-times differentiable function f defined on $\mathbb{R}$ is interpolated by a polynomial of degree d on $d+1$ unique points $\{x_1, x_2, \dots, x_{d+1}\} \subset \mathbb{R}$, then the resulting polynomial has the approximation error

$$\frac{(x - x_1)(x - x_2) \cdots (x - x_{d+1})}{(d+1)!} D^{n+1} f(\xi) \quad \text{for all } x \in \mathbb{R} \tag{2}$$

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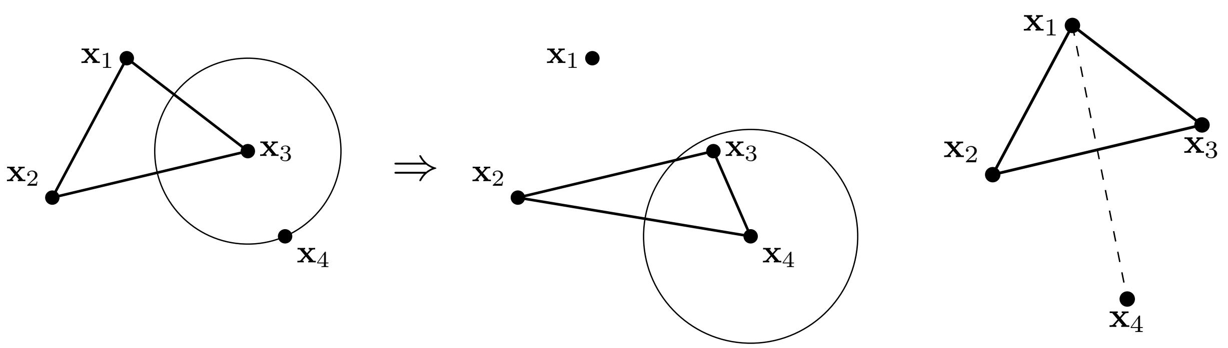
for some ξ with $\min(x, x_1, , \ldots, x_{d+1}) < \xi < \max(x, x_1, \ldots, x_{d+1})$. Unfortunately this result cannot be extended to the multivariate ($n > 1$) case directly, even if the polynomial is linear ($d = 1$).

The function approximation error of multivariate polynomial interpolation has been studied by researchers from multiple research fields. Motivated by their application in finite element methods, formulae for the errors in both Lagrange and Hermite interpolation with polynomials of any degree were derived in [1]. As a part of an effort to develop derivative-free optimization algorithms, a bound on the error of quadratic interpolation was provided in [9]. The sharp error bound for linear interpolation was found by researchers of approximation theory for the case when $\mathbf{x} \in \mathrm{conv}(\Theta)$ using the unique Euclidean sphere that contains Θ in [14]. Following [14], a number of sharp error bounds were derived in [10] for linear interpolation under several different smoothness or continuity assumptions in addition to (1).

While the sharp error bound for the $\mathbf{x} \in \mathrm{conv}(\Theta)$ case is already established, in applications like model-based derivative-free optimization (DFO), where linear interpolation is employed to approximate the black-box objective function [8, 2], the approximation model $\hat{f}$ is used more often than not to estimate the function value at a point outside $\mathrm{conv}(\Theta)$. As illustrated in Figure 1a, these optimization algorithms attempt to minimize the objective function by alternately constructing a linear interpolation model and minimizing the model inside a trust region, where the trust region is typically a ball around the point with the lowest known function value. The minimizer of the model inside the trust region would then have its function value evaluated and become part of the sample set for constructing the linear interpolation model in the next iteration. In practice, this minimizer rarely locates inside $\mathrm{conv}(\Theta)$.

There is also another class of DFO methods known as the simplex methods. One example is the famous Nelder-Mead method [6]. As illustrated in Figure 1b, the main routine of these algorithms involves taking a set of $n + 1$ affinely independent points Θ (the vertices of a simplex) and reflecting the one with the largest function value through the hyperplane defined by the rest. While linear interpolation is not used in these algorithms, the range of the function value at this reflection point ($\mathbf{x}_4$ in Figure 1b and is always outside $\mathrm{conv}(\Theta)$) can be determined by the sum of the value estimated by interpolation model and the error of the estimation.



(a) Two consecutive iterations of a DFO algorithm based on linear interpolation and trust region method. The circle represents the trust region, which changes center and expands after finding the minimizer $\mathbf{x}_4$ that has a lower function value than the current center $\mathbf{x}_3$.

(b) One iteration of the Nelder-Mead method. The next simplex will be formed by $\{\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$.

Figure 1: An illustration of two DFO algorithm when minimizing a bivariate function, where $f(\mathbf{x}_1) > f(\mathbf{x}_2) > f(\mathbf{x}_3)$. The vertices of the triangles represents Θ. This figure only illustrates the algorithms' behavior when the trial point $\mathbf{x}_4$ satisfies $f(\mathbf{x}_4) < f(\mathbf{x}_3)$.

To further the design and analysis of these DFO algorithms, we use both numerical and analytical approaches to investigate the sharp upper bound on the function evaluation error of linear interpolation. The results of this investigation provides a theoretical basis to the analysis of numerical methods that use linear interpolation including the DFO methods mentioned above. Furthermore, it can also be directly applied to improve certain DFO algorithms. For example, the model-based algorithms, which are usually designed to optimize functions that are computationally expensive to evaluate, typically request a function evaluation for one of two purposes: to check a point predicted by the model to have an improvement in function value (as shown in Figure 1a) or to explore a point that can contribute to the construction of a more accurate approximation model. Being able to estimate the magnitude of the approximation error at a given point in the former case allows the algorithm to compare it to the predicted improvement in function value and make an informed decision on whether the point is worth evaluating. By prioritizing spending the function evaluation to improve the model rather than check the point when the error is relatively large, the algorithm's overall efficiency can be improved.

The applications of this paper's results in DFO will be further discussed later, but please keep in mind that our analysis is for linear interpolation in general and can be applied wherever this approximation technique is used. Our main contributions are as follows.

1. We formulate the problem of finding the sharp error bound as a nonlinear programming problem and show that it can be solved numerically to obtain the desired bound.

2. An analytical bound on the function approximation error is derived and proved to be sharp for interpolation and, under certain conditions, for extrapolation.

3. The largest function approximation error that is achievable by quadratic functions in $C^{1,1}_\nu(\mathbb{R}^n)$ is derived, and the condition under which it is an upper bound on the error achievable by all functions in $C^{1,1}_\nu(\mathbb{R}^n)$ is determined.

4. For bivariate ($n = 2$) linear extrapolation, we analyze the case when neither of the two previous results equals to the sharp bound on the function approximation error and provide the formula for the actual sharp bound. We also show piecewise quadratic functions can achieve the approximation error indicated by the sharp bound.

The paper is organized as follows. Our notation and the preliminary knowledge are introduced in Section 2. The nonlinear programming problem is present in Section 3. In Section 4, we generalize an existing analytical bound and then improve it. In Section 5, we study the error in approximating quadratic functions. In Section 6, we show how to calculate the sharp bound on function approximation error of bivariate linear interpolation. We conclude the paper in Section 7 by discussing our findings and some open questions.

2 Notation and Preliminaries

Since the research in this paper involves approximation theory and optimization, to appeal to audiences from both research fields, we provide a detailed introduction to our notation and the preliminary knowledge.

Throughout the paper, vectors are denoted by boldface letters and matrices by capital letters. We denote by $\|\cdot\|$ the Euclidean norm. The dot product between vectors or matrices of the same size, $\mathbf{u}\cdot\mathbf{v}$ or $U\cdot V$, is the summation of the entry-wise product, which are customarily denoted by $\mathbf{u}^T\mathbf{v}$ and $\mathrm{Tr}(U^TV)$ in optimization literature.

Let $\mathbf{e}_i$ be the vector that is all 0 but have 1 as its ith entry. Let $Y \in \mathbb{R}^{(n+1)\times n}$ be the matrix such that its ith row $Y^T\mathbf{e}_i = \mathbf{x}_i - \mathbf{x}$ for all $i = 1, 2, \dots, n+1$. We define $\phi : \mathbb{R}^n \to \mathbb{R}^{n+1}$ as the *basis function* such that $\phi(\mathbf{u}) = \begin{bmatrix} 1 & \mathbf{u}^T \end{bmatrix}^T$ for all $\mathbf{u} \in \mathbb{R}^n$, and Φ as the $(n+1)$-by-$(n+1)$ matrix $\begin{bmatrix} \mathbf{1} & Y \end{bmatrix}$, where $\mathbf{1}$ is the all one vector. Notice the affine independence of Θ implies the nonsingularity of Φ.

Let $\ell_1, \dots, \ell_{n+1}$ be the *Lagrange polynomials*, i.e. the unique set of polynomials such that $\ell_i(\mathbf{x}_j) = 1$ if $i = j$, and $\ell_i(\mathbf{x}_j) = 0$ if $i \neq j$. The values of these polynomials at $\mathbf{x}$ coincides with the set of barycentric coordinates of $\mathbf{x}$ with respect to Θ and have the following properties:

$$\sum_{i=1}^{n+1} \ell_i(\mathbf{x}) f(\mathbf{x}_i) = \hat{f}(\mathbf{x}), \tag{3}$$

$$\sum_{i=1}^{n+1} \ell_i(\mathbf{x}) = 1, \tag{4}$$

$$\text{and } \sum_{i=0}^{n+1} \ell_i(\mathbf{x}) \mathbf{x}_i = \mathbf{0}, . \tag{5}$$

The concepts of basis functions and Lagrange polynomials are fundamental to approximation theory. The book [2] offers a comprehensive introduction to them in the context of derivative-free optimization.

For the ease of exposition, we abbreviate $\ell_i(\mathbf{x})$ to ℓ_i and define $\mathbf{x}_0 = \mathbf{x}$ and $\ell_0 = -1$. Another reason for the artificially defined $\mathbf{x}_0$ and ℓ_0 will be made clear in Section 3. Without loss of generality, we assume the set $\Theta = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{n+1}\}$ is ordered in a way such that $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_{n+1}$. We define the following two sets of indices:

$$\mathcal{I}_+ = \{i \in \{0, 1, \ldots, n+1\} : \ \ell_i > 0\} = \{1, 2, \ldots, |\mathcal{I}_+|\}, \tag{6a}$$
$$\mathcal{I}_- = \{i \in \{0, 1, \ldots, n+1\} : \ \ell_i < 0\} = \{0, n+3-|\mathcal{I}_-|, \ldots, n+1\}. \tag{6b}$$

Notice (4) implies $\mathcal{I}_+ \neq \emptyset$, and $\ell_0 = -1$ implies $\mathcal{I}_- \neq \emptyset$. It is possible for $n+3-|\mathcal{I}_-| > n+1$, in which case $\mathcal{I}_- = \{0\}$.

We define the following matrix $G \in \mathbb{R}^{n \times n}$:

$$G = \sum_{i=0}^{n+1} \ell_i \mathbf{x}_i \mathbf{x}_i^T, \tag{7}$$

which will be used frequently in our analysis. The notation $\mathbf{x}_i \mathbf{x}_i^T$ is the outer product of $\mathbf{x}_i$ and is sometimes denoted by $\mathbf{x}_i^2$ or $\mathbf{x}_i \otimes \mathbf{x}_i$ otherwise. The matrix G has the property that for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$,

$$\begin{aligned} \sum_{i=0}^{n+1} \ell_i [\mathbf{x}_i - \mathbf{u}][\mathbf{x}_i - \mathbf{v}]^T &= \sum_{i=0}^{n+1} \ell_i \left[\mathbf{x}_i \mathbf{x}_i^T - \mathbf{u}\mathbf{x}_i^T - \mathbf{x}_i \mathbf{v}^T + \mathbf{u}\mathbf{v}^T\right] \\ &\overset{(5)}{=} \sum_{i=0}^{n+1} \ell_i \left[\mathbf{x}_i \mathbf{x}_i^T + \mathbf{u}\mathbf{v}^T\right] \overset{(4)}{=} \sum_{i=0}^{n+1} \ell_i \mathbf{x}_i \mathbf{x}_i^T = G. \end{aligned} \tag{8}$$

The class of functions $C_\nu^{1,1}(\mathbb{R}^n)$ is ubiquitous in the research of nonlinear optimization. It is well-known (see, e.g., section 1.2.2 of the textbook [7]) that the inclusion $f \in C_\nu^{1,1}(\mathbb{R}^n)$ implies

$$|f(\mathbf{v}) - f(\mathbf{u}) - Df(\mathbf{u}) \cdot (\mathbf{v} - \mathbf{u})| \leq \frac{\nu}{2} \|\mathbf{v} - \mathbf{u}\|^2 \text{ for all } \mathbf{u}, \mathbf{v} \in \mathbb{R}^n, \tag{9}$$

and that if f is twice differentiable on $\mathbb{R}^n$, (1) and (9) are equivalent to

$$-\nu I \preceq D^2 f(\mathbf{u}) \preceq \nu I \text{ for all } \mathbf{u} \in \mathbb{R}^n, \tag{10}$$

where the condition (10) is often written as $\| \, |D^2 f| \, \|_{L_\infty(\mathbb{R}^n)} \leq \nu$ in approximation theory literature. What is less well-known about the class $C_\nu^{1,1}(\mathbb{R}^n)$ is that $f \in C_\nu^{1,1}(\mathbb{R}^n)$ also implies

$$\begin{aligned} f(\mathbf{v}) \leq & f(\mathbf{u}) + \frac{1}{2}(Df(\mathbf{u}) + Df(\mathbf{v})) \cdot (\mathbf{v} - \mathbf{u}) \\ & + \frac{\nu}{4} \|\mathbf{v} - \mathbf{u}\|^2 - \frac{1}{4\nu} \|Df(\mathbf{v}) - Df(\mathbf{u})\|^2 \text{ for all } \mathbf{u}, \mathbf{v} \in \mathbb{R}^n. \end{aligned} \tag{11}$$

For differentiable functions, (1), (9), and (11) are equivalent.

3 Error Estimation Problem

In this section, we formulate the problem of finding the sharp error bound as a numerically solvable nonlinear optimization problem. We first make the important observation that the problem of finding the sharp upper bound on the error is the same as asking for the largest error that a function from $C_\nu^{1,1}(\mathbb{R}^n)$ can achieve. Thus, it can be formulated as the following problem of maximizing the approximation error over the functions in $C_\nu^{1,1}(\mathbb{R}^n)$:

$$\begin{aligned} \max_f \quad & |\hat{f}(\mathbf{x}) - f(\mathbf{x})| \\ \text{s.t.} \quad & f \in C_\nu^{1,1}(\mathbb{R}^n), \end{aligned} \tag{EEP}$$

where $\hat{f}$ is the affine function that interpolates f on a given set of $n+1$ affinely independent points $\Theta = \{\mathbf{x}_1, \ldots, \mathbf{x}_{n+1}\}$. We call this problem the *error estimation problem* (EEP), a name inspired by the *performance estimation problem* (PEP).

First proposed in [4], a PEP is a nonlinear programming formulation of the problem of finding an optimization algorithm's worst-case performance over a set of possible objective functions. It involves maximizing a performance measure of the given algorithm (the larger the measure, the worse the performance) over the objective functions and, similar to (EEP), is an infinite-dimensional problem. However, with some algorithms and functions, particularly first-order nonlinear optimization methods and convex functions, the PEP is shown to have finite-dimensional equivalents that can be solved numerically [13, 12], thus providing a computer-aided analysis tool for estimating an algorithm's worst-case performance. Using these theories developed for PEP, we can process the functional constraint $f \in C_\nu^{1,1}(\mathbb{R}^n)$ and turn (EEP) into a finite-dimensional problem. Particularly, we use the following theorem from [12], which states $f \in C_\nu^{1,1}(\mathbb{R}^n)$ can be replaced by (11) for every pair of points in $\Theta \cup \{\mathbf{x}\}$.

Proposition 3.1 (Theorem 3.10 [12])**.** *Let $\nu > 0$ and $\mathcal{I}$ be an index set, and consider a set of triples $\{(\mathbf{x}_i, \mathbf{g}_i, y_i)\}_{i\in\mathcal{I}}$ where $\mathbf{x}_i \in \mathbb{R}^n$, $\mathbf{g} \in \mathbb{R}^n$, and $y_i \in \mathbb{R}$ for all $i \in \mathcal{I}$. There exists a function $f \in C_\nu^{1,1}(\mathbb{R}^n)$ such that both $\mathbf{g}_i = Df(\mathbf{x}_i)$ and $y_i = f(\mathbf{x}_i)$ hold for all $i \in \mathcal{I}$ if and only if the following inequality holds for all $i, j \in \mathcal{I}$:*

$$y_j \le y_i + \frac{1}{2}(\mathbf{g}_i + \mathbf{g}_j) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j - \mathbf{g}_i\|^2. \tag{12}$$

The above proposition allows us to replace the functional variable f with the function values $\{y_i\}$ and gradients $\{\mathbf{g}_i\}$ at Θ and $\mathbf{x}$. Before applying this proposition, we first substitute the approximated function value $\hat{f}(\mathbf{x})$ in (EEP) with $\sum_{i=1}^{n+1} \ell_i f(\mathbf{x}_i)$ using (3) and drop the absolute sign in the objective function. The absolute sign can be dropped thanks to the symmetry of (1), that is, $-f \in C_\nu^{1,1}(\mathbb{R}^n)$ for any $f \in C_\nu^{1,1}(\mathbb{R}^n)$, and the approximation error on the two functions f and $-f$ are negatives of each other. Finally, by applying Proposition 3.1, we arrive at (f-EEP), a finite-dimensional equivalent to (EEP):

$$\begin{aligned} \max_{y_i, \mathbf{g}_i} \quad & \sum_{i=0}^{n+1} \ell_i y_i \\ \text{s.t.} \quad & y_j \le y_i + \frac{1}{2}(\mathbf{g}_i + \mathbf{g}_j) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 \\ & \qquad - \frac{1}{4\nu}\|\mathbf{g}_j - \mathbf{g}_i\|^2 \quad \forall i, j \in \{0, \ldots, n+1\}. \end{aligned} \tag{f-EEP}$$

The optimization problem (f-EEP) is a convex quadratically constrained quadratic program (QCQP). This type of problem can be solved by standard nonlinear optimization solvers. However, (f-EEP) contains $n+1$ redundant degrees of freedom, which means it has infinitely many optimal solutions, and the solvers can sometimes have difficulty solving it. It is best to eliminate these degrees of freedom first. The elimination can be done in many ways. For example, one can fix $\{y_i\}_{i=1}^{n+1}$ in (f-EEP) to their observed values. Indeed, these function values are needed for constructing the affine approximation $\hat{f}$, so it is natural to assume they are known. However, we note that the optimal value of (EEP) and (f-EEP) is affected by the locations of the sample points Θ in the input space but is invariant to the observed function values at these points. Thus, for the purpose of solving (f-EEP), it is also justified to simply set $y_i = 0$ for all $i = 1, \ldots, n+1$. Alternatively, one can also fix $(\mathbf{g}_i, y_i)$ to $(\mathbf{0}, 0)$ for any $i \in \{0, 1, \ldots, n+1\}$. We formally prove in the following proposition the $n+1$ degrees of freedom can be removed in these two ways.

Proposition 3.2. *The following statements are true.*

1. *If any function f is optimal to* (EEP)*, then the function $f'(\mathbf{u}) = f(\mathbf{u}) + c + \mathbf{g} \cdot \mathbf{u}$ is also optimal with any $c \in \mathbb{R}$ and $\mathbf{g} \in \mathbb{R}^n$.*
2. *The optimal value of* (f-EEP) *does not change if $\{y_i\}_{i=1}^{n+1}$ are fixed to any arbitrary values.*
3. *The optimal value of* (f-EEP) *does not change if $\mathbf{g}_k$ and y_k are fixed to any arbitrary values for some $k \in \{0, 1, \ldots, n+1\}$.*

Proof. By the definition (1), it is easy to see $f' \in C_\nu^{1,1}(\mathbb{R}^n)$ whenever $f \in C_\nu^{1,1}(\mathbb{R}^n)$. The two objective values can also be shown to be the same using (3), (4), and (5):

$$\sum_{i=0}^{n+1} \ell_i f'(\mathbf{x}_i) = \sum_{i=0}^{n+1} \ell_i [f(\mathbf{x}_i) + c + \mathbf{g} \cdot \mathbf{x}_i] = \sum_{i=0}^{n+1} \ell_i f(\mathbf{x}_i).$$

The first statement is thus true.

To prove the second statement, we first assume (f-EEP) has an optimal solution $\{y_i^\star, \mathbf{g}_i^\star\}_{i=0}^{n+1}$. Now suppose the problem has an additional set of constraints that fixes the function values of the points in Θ to some arbitrary values $\{y_i\}_{i=1}^{n+1}$. Then, this new problem has the exact same optimal value as the original (f-EEP), and an optimal solution satisfies $\mathbf{g}_i = \mathbf{g}_i^\star + \mathbf{g}$ for all $i = 0, 1, \ldots, n+1$ and $y_0 = y_0^\star + c + \mathbf{g} \cdot \mathbf{x}_0$, where $(\mathbf{g}, c)$ is the unique solution to the linear system $c + \mathbf{g} \cdot \mathbf{x}_i = y_i - y_i^\star, i = 1, \ldots, n+1$. Indeed, the constraints of this new problem are satisfied as

$$\begin{aligned}
&- y_j + y_i + \frac{1}{2}(\mathbf{g}_i + \mathbf{g}_j) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j - \mathbf{g}_i\|^2 \\
&= -y_j + y_i + \frac{1}{2}(\mathbf{g}_i^\star + \mathbf{g}_j^\star + 2\mathbf{g}) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j^\star - \mathbf{g}_i^\star\|^2 \\
&= -y_j^\star + y_i^\star + \frac{1}{2}(\mathbf{g}_i^\star + \mathbf{g}_j^\star) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j^\star - \mathbf{g}_i^\star\|^2 \geq 0
\end{aligned}$$

for all $i, j = 0, 1, \ldots, n+1$, where the second equality is true because $\mathbf{g} \cdot (x_j - x_i) = (y_j - y_j^\star - c) - (y_i - y_i^\star - c)$, and the objective function

$$\sum_{i=0}^{n+1} \ell_i y_i = y_0^\star + c + \mathbf{g} \cdot \mathbf{x}_0 + \sum_{i=1}^{n+1} \ell_i y_i \overset{(4)(5)}{=} y_0^\star + \sum_{i=0}^{n+1} \ell_i [y_i + c + \mathbf{g} \cdot \mathbf{x}_i] = \sum_{i=0}^{n+1} \ell_i y_i^\star.$$

Similarly, (f-EEP) with $(\mathbf{g}_k, y_k)$ fixed for some $k \in \{0, 1, \ldots, n+1\}$ also has the same optimal value as (f-EEP), and its optimal solution satisfies $\mathbf{g}_i = \mathbf{g}_i^\star - \mathbf{g}_k^\star + \mathbf{g}_k$ and $y_i = y_i^\star - y_k^\star + y_k + (\mathbf{g}_k - \mathbf{g}_k^\star) \cdot (\mathbf{x}_i - \mathbf{x}_k)$ for all $i = 0, 1, \ldots, n+1$. The constraints are satisfied as

$$\begin{aligned}
&- y_j + y_i + \frac{1}{2}(\mathbf{g}_i + \mathbf{g}_j) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j - \mathbf{g}_i\|^2 \\
&= -[y_j^\star - y_k^\star + y_k + (\mathbf{g}_k - \mathbf{g}_k^\star) \cdot (\mathbf{x}_j - \mathbf{x}_k)] + [y_i^\star - y_k^\star + y_k + (\mathbf{g}_k - \mathbf{g}_k^\star) \cdot (\mathbf{x}_i - \mathbf{x}_k)] \\
&\quad + \frac{1}{2}(\mathbf{g}_i^\star + \mathbf{g}_j^\star + 2\mathbf{g}_k - 2\mathbf{g}_k^\star) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j^\star - \mathbf{g}_i^\star\|^2 \\
&= -y_j^\star + y_i^\star + \frac{1}{2}(\mathbf{g}_i^\star + \mathbf{g}_j^\star) \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{\nu}{4}\|\mathbf{x}_j - \mathbf{x}_i\|^2 - \frac{1}{4\nu}\|\mathbf{g}_j^\star - \mathbf{g}_i^\star\|^2 \geq 0
\end{aligned}$$

for all $i, j = 0, 1, \ldots, n+1$, and the objective function

$$\sum_{i=0}^{n+1} \ell_i y_i = \sum_{i=0}^{n+1} \ell_i [y_i^\star - y_k^\star + y_k + (\mathbf{g}_k - \mathbf{g}_k^\star) \cdot (\mathbf{x}_i - \mathbf{x}_k)] \overset{(4)(5)}{=} \sum_{i=0}^{n+1} \ell_i y_i^\star.$$

$\square$

Apart from its application in model-based derivative-free optimization as introduced in Section 1, (f-EEP) also offers us insight into the approximation error and guidance in seeking the analytical form of the sharp bound. Particularly, it can be used to visualize the sharp error bound for bivariate linear interpolation. We do this by first selecting a fixed set of three affinely independent sample points $\Theta \subset \mathbb{R}^2$ and a 100×100 grid. Then, (f-EEP) is solved repeatedly while $\mathbf{x}$ is set to each point on the grid. The result of one instance of this numerical experiment is shown in Figure 2. It can be observed that this bound is a piecewise smooth function of $\mathbf{x}$, and the boundaries between the smooth pieces align with the edges of the triangle defined by Θ. It will be shown in Section 5 that this piecewise smooth function, at least in the case shown in Figure 2 where $\mathrm{conv}(\Theta)$ is an acute triangle, can the represented by a single formula.

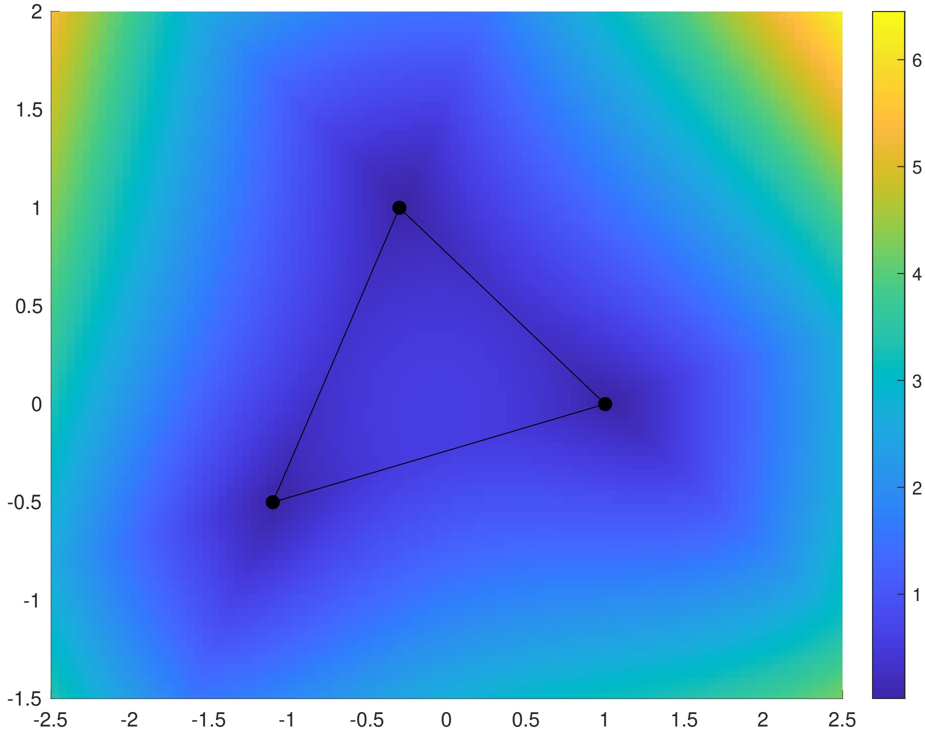


Figure 2: The sharp error bound on $|\hat{f}(\mathbf{x}) - f(\mathbf{x})|$ for each $\mathbf{x}$ on the 100×100 grid that covers the area $[-2.5, 2.5] \times [-1.5, 2.5]$ evenly. The sample set and the Lipschitz constant are chosen as $\Theta = \{(-0.3, 1), (-1.1, -0.5), (1, 0)\}$ and $\nu = 1$.

In (f-EEP), the point $\mathbf{x}$ and its derivative and function value are represented by $(\mathbf{x}_0, \mathbf{g}_0, y_0)$, whereas $(\mathbf{x}_i, \mathbf{g}_i, y_i)$ are used for the points $\mathbf{x}_i \in \Theta$ with $i = 1, \ldots, n+1$. If we ignore what these points represent in linear interpolation and look at the optimization problem (f-EEP) as it is, we can see that, in (f-EEP), the point $\mathbf{x}$ is not special comparing to the points in Θ, with the only difference being the coefficient of y_0 in the objective is fixed to $\ell_0 = -1$. Therefore, to symbolize the point's ordinary status and simplify the expressions, we index $\mathbf{x}$ the zeroth point and sometimes use $\mathbf{x}_0$ in place of the customary $\mathbf{x}$. This observation also leads us to the following proposition, which shows how the sharp error bound changes when $\mathbf{x}$ is swapped with a point in Θ and will be used to greatly simplify the analysis in Section 6.

Proposition 3.3. *Assume there is an affinely independent sample set $\Theta = \{\mathbf{x}_1, \ldots, \mathbf{x}_{n+1}\}$ and a point $\mathbf{x} \in \mathbb{R}^n$ such that $\Theta \setminus \{\mathbf{x}_k\} \cup \{\mathbf{x}\}$ is also affinely independent for a given $k \in \{1, \ldots, n+1\}$. Let ℓ_k be the Lagrange polynomial (with respect to Θ not $\Theta \setminus \{\mathbf{x}_k\} \cup \{\mathbf{x}\}$) corresponding to $\mathbf{x}_k$. Let $\hat{f}$ and $\hat{f}'$ be the affine functions that interpolates some $f : \mathbb{R}^n \to \mathbb{R}$ on Θ and $\Theta \setminus \{\mathbf{x}_k\} \cup \{\mathbf{x}\}$, respectively. The following two statements hold.*

1. *The function approximation error of $\hat{f}'$ at $\mathbf{x}_k$ is the error of $\hat{f}$ at $\mathbf{x}$ divided by $-\ell_k(\mathbf{x})$, i.e., $\hat{f}'(\mathbf{x}_k) - f(\mathbf{x}_k) = (\hat{f}(\mathbf{x}) - f(\mathbf{x}))/(-\ell_k(\mathbf{x}))$.*
2. *If $f \in C_\nu^{1,1}(\mathbb{R}^n)$ and $|\hat{f}(\mathbf{x}) - f(\mathbf{x})|$ is the largest error achievable by any function in $C_\nu^{1,1}(\mathbb{R}^n)$, then f also achieves the largest $|\hat{f}'(\mathbf{x}_k) - f(\mathbf{x}_k)|$.*

Proof. If we divide $\hat{f}(\mathbf{x}) - f(\mathbf{x}) = \sum_{i=0}^{n+1} \ell_i(\mathbf{x}) y_i$ by $-\ell_k(\mathbf{x})$, the coefficient before y_i becomes $\alpha_i = -\ell_i(\mathbf{x})/\ell_k(\mathbf{x})$ for all $i = 0, 1, \ldots, n+1$. Since $\alpha_k = -1$, $\sum_{i=0}^{n+1} \alpha_i = 0$, and $\sum_{i=0}^{n+1} \alpha_i \mathbf{x}_i = 0$, the coefficients $\{\alpha_i\}_{i=0, i\neq k}^{n+1}$ are the values of the Lagrange polynomials with respect to $\Theta \setminus \{\mathbf{x}_k\} \cup \{\mathbf{x}\}$ at $\mathbf{x}_k$. Thus, the quotient is exactly $\hat{f}'(\mathbf{x}_k) - f(\mathbf{x}_k)$.

The premise of the second statement assumes f is an optimal solution to (EEP). The same f must also be an optimal solution to the problem of finding the largest $|\hat{f}'(\mathbf{x}_k) - f(\mathbf{x}_k)|$, since this optimization problem is simply (EEP) with its objective function divided by the constant $-\ell_k(\mathbf{x}_k)$, and, as discussed before, the absolute sign can be ignored due to symmetry. □

4 An Improved Upper Bound

We now begin our attempt at finding the analytical form of the bound. The theoretical results in [1] and [9] are obtained by comparing f against its Taylor expansion at $\mathbf{x}$. We generalize their approach in Theorem 4.1 by using the Taylor expansion of f at an arbitrary $\mathbf{u} \in \mathbb{R}^n$.

Theorem 4.1. *Assume $f \in C_\nu^{1,1}(\mathbb{R}^n)$. Let $\hat{f}$ be the linear function that interpolates f at any set of $n+1$ affinely independent vectors $\Theta = \{\mathbf{x}_1, \ldots, \mathbf{x}_{n+1}\} \subset \mathbb{R}^n$. The function approximation error of $\hat{f}$ at any $\mathbf{x} \in \mathbb{R}^n$ is bounded as*

$$|\hat{f}(\mathbf{x}) - f(\mathbf{x})| \leq \frac{\nu}{2} \left(\|\mathbf{x} - \mathbf{u}\|^2 + \sum_{i=1}^{n+1} |\ell_i(\mathbf{x})| \|\mathbf{x}_i - \mathbf{u}\|^2 \right), \tag{13}$$

where $\mathbf{u}$ can be any vector in $\mathbb{R}^n$.

Proof. By (9), we have for any $\mathbf{u} \in \mathbb{R}^n$

$$\ell_i[f(\mathbf{x}_i) - f(\mathbf{u}) - Df(\mathbf{u}) \cdot (\mathbf{x}_i - \mathbf{u})] \leq \ell_i \frac{\nu}{2} \|\mathbf{x}_i - \mathbf{u}\|^2 \text{ for all } i \in \mathcal{I}_+, \tag{14a}$$

$$-\ell_i[-f(\mathbf{x}_i) + f(\mathbf{u}) + Df(\mathbf{u}) \cdot (\mathbf{x}_i - \mathbf{u})] \leq -\ell_i \frac{\nu}{2} \|\mathbf{x}_i - \mathbf{u}\|^2 \text{ for all } i \in \mathcal{I}_-. \tag{14b}$$

Now add all inequalities above together. The sum of the left-hand sides is

$$\begin{aligned} &\sum_{i=0}^{n+1} \ell_i [f(\mathbf{x}_i) - f(\mathbf{u})] + Df(\mathbf{u}) \cdot \sum_{i=0}^{n+1} \ell_i [\mathbf{u} - \mathbf{x}_i] \\ &\overset{(4)}{=} \sum_{i=0}^{n+1} \ell_i f(\mathbf{x}_i) + Df(\mathbf{u}) \cdot \sum_{i=1}^{n+1} \ell_i \mathbf{x}_i \overset{(3)(5)}{=} \hat{f}(\mathbf{x}) - f(\mathbf{x}), \end{aligned}$$

while the sum of the right-hand sides is $\nu/2 \sum_{i=0}^{n+1} |\ell_i| \|\mathbf{x}_i - \mathbf{u}\|^2$. Thus the sum of the inequalities in (14) is (13) when $\hat{f}(\mathbf{x}) - f(\mathbf{x}) \geq 0$. If the inequalities in (14) have their left-hand sides multiplied by -1, they would still hold according to (9), and their summation would be (13) for the $\hat{f}(\mathbf{x}) - f(\mathbf{x}) < 0$ case. □

The existing bounds from [1] is similar to (13) but has $\mathbf{u}$ fixed to $\mathbf{x}$. In comparison, the new bound provides more convenience in analyzing DFO algorithms that use trusting region methods, since the free point $\mathbf{u}$ can be set to the center of the trust region. Another advantage of the new bound is that it can be minimized with respect of $\mathbf{u}$, especially considering the right-hand side of (13) is a convex function of $\mathbf{u}$ defined on $\mathbb{R}^n$. This results in the improved bound (15).

Corollary 4.2. *Under the setting of* (4.1)*, the function approximation error of $\hat{f}$ at any $\mathbf{x} \in \mathbb{R}^n$ is bounded as*

$$|\hat{f}(\mathbf{x}) - f(\mathbf{x})| \leq \frac{\nu}{2}\left(\|\mathbf{x}-\mathbf{w}\|^2 + \sum_{i=1}^{n+1} |\ell_i| \|\mathbf{x}_i - \mathbf{w}\|^2\right), \tag{15}$$

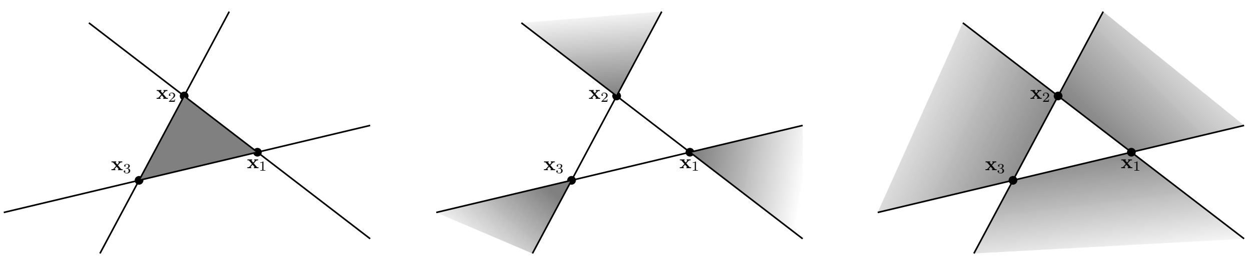
where

$$\mathbf{w} = \frac{\mathbf{x} + \sum_{i=1}^{n+1} |\ell_i| \mathbf{x}_i}{1 + \sum_{i=1}^{n+1} |\ell_i|}.$$

To check the sharpness of the bound (15), we compare it against the optimal value of (f-EEP) numerically. The comparison shows that (15) is sharp if and only if $\mathbf{x}$ is located in $\mathrm{conv}(\Theta)$ or in one of the cones

$$\left\{\mathbf{x}_i + \sum_{j=1}^{n+1} \alpha_j (\mathbf{x}_i - \mathbf{x}_j) : \ \alpha_j \geq 0 \text{ for all } j = 1, 2, \ldots, n+1\right\} \tag{16}$$

for some $i \in \{1, \ldots, n+1\}$. We illustrate the geometric meaning of this observation in Figure 3, which shows the three sets of areas in which $\mathbf{x}$ can locate relative to the sample set Θ from Figure 2. Figure 3a shows the convex hull of Θ, and Figure 3b shows the cones. In all the remaining areas, as shown in Figure 3c, the bound (15) is observed to be smaller than the solution of (f-EEP). Additionally, we want to mention that these areas can also be classified using the signs of the values of the Lagrange functions at $\mathbf{x}$. The point $\mathbf{x} \in \mathrm{conv}(\Theta)$ if and only if $\ell_i \geq 0$ for all $i = 1, \ldots, n+1$; and $\mathbf{x}$ is in the cone (16) if and only if ℓ_i is the only positive one among $\{\ell_i\}_{i=1}^{n+1}$.



(a) The convex hull covered by Theorem 4.3

(b) The cones covered by Theorem 4.4

(c) The areas where (15) holds but is not sharp

Figure 3: A visualization of results in Section 4 for bivariate interpolation. The ordering of the points in $\Theta = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ in this figure and all figures hereafter is arbitrary and not determined by the values of the Lagrange polynomials at $\mathbf{x}$.

When $f \in C_\nu^{1,1}(\mathbb{R}^n)$, the proof of Theorem 3.1 in [14] essentially shows that

$$|\hat{f}(\mathbf{x}) - f(\mathbf{x})| \leq \frac{\nu}{2}\left(\sum_{i=1}^{n+1} \ell_i \|\mathbf{x}_i\|^2 - \|\mathbf{x}\|^2\right), \tag{17}$$

holds for all $\mathbf{x} \in \mathrm{conv}(\Theta)$ and is a sharp upper bound, as linear interpolation makes an error equal to this upper bound when approximating the quadratic function $f(\mathbf{u}) = \nu\|\mathbf{u}\|^2/2$. We show in Theorem 4.3 that (15) is indeed the same as (17) in this case.

Theorem 4.3. *When $\mathbf{x} \in \mathrm{conv}(\Theta)$, the bound* (15) *has $\mathbf{w} = \mathbf{x}$ and is identical to* (17)*.*

Proof. This theorem is a direct result of the properties of the Lagrange functions (4) and (5). □

In Theorem 4.4, we verify mathematically that the improved bound (15) is sharp for linear extrapolation when $\mathbf{x}$ is in one of the cones indicated by (16) and depicted in Figure 3b.

Theorem 4.4. *Assume the sample points are ordered such that $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_{n+1}$ and ℓ_1 is the only positive one, then the bound* (15) *is sharp with* $\mathbf{w} = \mathbf{x}_1$.

Proof. Since $\ell_i \leq 0$ for all $i = 0, 2, 3, \ldots, n+1$,

$$\mathbf{w} = \frac{2\ell_1 \mathbf{x}_1 - \sum_{i=0}^{n+1} \ell_i \mathbf{x}_i}{2\ell_1 - \sum_{i=0}^{n+1} \ell_i} \overset{(4)(5)}{=} \frac{2\ell_1 \mathbf{x}_1}{2\ell_1} = \mathbf{x}_1.$$

The bound (15) equals $\nu/2$ multiplies

$$\sum_{i=0}^{n+1} |\ell_i| \|\mathbf{x}_i - \mathbf{w}\|^2 = -\sum_{i=0}^{n+1} \ell_i \|\mathbf{x}_i - \mathbf{x}_1\|^2 = \mathrm{Tr}\left(-\sum_{i=0}^{n+1} \ell_i [\mathbf{x}_i - \mathbf{x}_1][\mathbf{x}_i - \mathbf{x}_1]^T\right)$$
$$\overset{(8)}{=} \mathrm{Tr}\left(-\sum_{i=0}^{n+1} \ell_i \mathbf{x}_i \mathbf{x}_i^T\right) = -\sum_{i=0}^{n+1} \ell_i \|\mathbf{x}_i\|^2.$$

Consider the function $f(\mathbf{u}) = -\frac{\nu}{2}\|\mathbf{u}\|^2 \overset{(10)}{\in} C_\nu^{1,1}(\mathbb{R}^n)$. We have

$$\hat{f}(\mathbf{x}) - f(\mathbf{x}) \overset{(3)}{=} \sum_{i=0}^{n+1} \ell_i f(\mathbf{x}_i) = -\sum_{i=0}^{n+1} \ell_i \frac{\nu}{2} \|\mathbf{x}_i\|^2,$$

which matches (15). $\square$

5 The Worst Quadratic Function

We have derived an improved error bound in the previous section and showed when it is sharp. In this section, we try to find the mathematical formula for the piecewise smooth function in the remaining areas indicated in Figure 3c. Instead of attempting to improve another existing upper bound, we take the opposite approach by trying to find the function that can achieve the maximum error. Considering quadratic functions are easier to analyze as they share a general closed-form formula and, under the settings of both Theorem 4.3 and Theorem 4.4, the optimal set of (EEP) contains at least one quadratic function, we investigate whether (EEP) has an analytical solution when f is restricted to be quadratic.

Let f be a quadratic function of the form $f(\mathbf{u}) = c + \mathbf{g} \cdot \mathbf{u} + \frac{1}{2} H\mathbf{u} \cdot \mathbf{u}$ with $c \in \mathbb{R}, \mathbf{g} \in \mathbb{R}^n$, and symmetric $H \in \mathbb{R}^{n \times n}$. Because of (10) and

$$\hat{f}(\mathbf{x}) - f(\mathbf{x}) \overset{(3)}{=} \sum_{i=0}^{n+1} \ell_i f(\mathbf{x}_i) = \sum_{i=0}^{n+1} \ell_i \left[c + \mathbf{g} \cdot \mathbf{x}_i + \frac{1}{2} H\mathbf{x}_i \cdot \mathbf{x}_i\right]$$
$$\overset{(5)}{=} \sum_{i=0}^{n+1} \ell_i \left[c + \frac{1}{2} H\mathbf{x}_i \cdot \mathbf{x}_i\right] \overset{(4)}{=} \sum_{i=0}^{n+1} \ell_i \left[\frac{1}{2} H\mathbf{x}_i \cdot \mathbf{x}_i\right]$$
$$= \frac{1}{2} H \cdot \sum_{i=0}^{n+1} \ell_i \mathbf{x}_i \mathbf{x}_i^T \overset{(7)}{=} \frac{1}{2} G \cdot H,$$

the problem of maximizing linear interpolation's approximation error over quadratic functions in $C_\nu^{1,1}(\mathbb{R}^n)$ can be formulated as

$$\begin{array}{ll} \max\limits_{H} & G \cdot H/2 \\ \text{s.t.} & -\nu I \preceq H \preceq \nu I. \end{array} \tag{18}$$

The absolute sign in the objective function is again dropped due to symmetry.

It turns out the problem (18) can be solved analytically. Since G is real and symmetric, it must have eigendecomposition $G = P \Lambda P^T$, where $\Lambda \in \mathbb{R}^{n \times n}$ is the diagonal matrix of the eigenvalues $\lambda_1, \ldots, \lambda_n$, and

$P \in \mathbb{R}^{n\times n}$ is the orthonormal matrix whose columns are the corresponding eigenvectors. The objective function $G \cdot H/2 = (P\Lambda P^T) \cdot H/2 = \Lambda \cdot (P^T HP)/2$. Since P is orthonormal, the constraint in (18) is equivalent to $-\nu I \preceq P^T HP \preceq \nu I$, indicating all diagonal elements of $P^T HP$ are bounded between $-\nu$ and ν. Since Λ is diagonal, only the diagonal elements of $P^T HP$ would affect the objective function value. Therefore, a solution to (18), denoted by $H^\star$, has the property $P^T H^\star P = \nu \text{sign}(\Lambda)$. This optimal solution is

$$H^\star = \nu P \text{sign}(\Lambda) P^T. \tag{19}$$

Solution (19) indicates the maximum approximation error by quadratic functions of

$$G \cdot H^\star/2 = \frac{\nu}{2}\sum_{i=1}^{n} |\lambda_i|. \tag{20}$$

We again compare this new bound to the optimal value of (f-EEP) numerically. Our results show these two are exactly the same in all three cases in Figure 3, and (20) is a formula of the piecewise smooth function in Figure 2. However, this does not mean (20) is a formula to the optimal value of (f-EEP). For example, for bivariate linear interpolation, it is observed that when the triangle conv(Θ) is obtuse and $\mathbf{x}$ locates in one of the four shaded areas indicated in Figure 4, the optimal value of (f-EEP) is larger than (20). These shaded areas are open subsets of $\mathbb{R}^2$ and do not include their boundaries. From left to right, they can be described as

- $\ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_2[\mathbf{x}_3 - \mathbf{x}_2] \cdot [\mathbf{x}_1 - \mathbf{x}_2] > 0$ and $\ell_2 > 0$;
- $\ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_2[\mathbf{x}_3 - \mathbf{x}_2] \cdot [\mathbf{x}_1 - \mathbf{x}_2] < 0$, $\ell_3 > 0$, and $\ell_2 < 0$;
- $\ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3[\mathbf{x}_2 - \mathbf{x}_3] \cdot [\mathbf{x}_1 - \mathbf{x}_3] < 0$, $\ell_2 > 0$, and $\ell_3 < 0$;
- $\ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3[\mathbf{x}_2 - \mathbf{x}_3] \cdot [\mathbf{x}_1 - \mathbf{x}_3] > 0$ and $\ell_3 > 0$.

In the remaining parts of this section, we will investigate analytically when (20) is the sharp error bound.

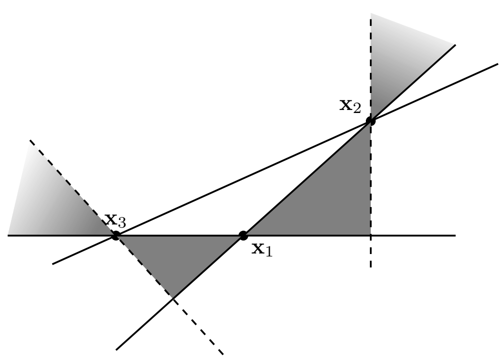


Figure 4: The areas to which if $\mathbf{x}$ belongs, (20) is not an upper bound on the function approximation error for bivariate interpolation. The dashed line on the left is perpendicular to the line going through $\mathbf{x}_1$ and $\mathbf{x}_2$; and the one on the right is perpendicular to the line going through $\mathbf{x}_3$ and $\mathbf{x}_1$.

5.1 Certification of Upper Bound

The maximum error (20) provides a lower bound to the optimal value of (EEP), while (15) provides an upper bound. By evaluating both (15) and (20), one can have a reasonable estimation of sharp error bound without having to solve the QCQP (f-EEP). However, the formula (20) would be a lot more useful if there is an efficient way to check whether $\mathbf{x}$ is in one of those areas where (20) is not an upper bound on the approximation error.

The existence of these areas appears to be influence by the existence of obtuse angles at the vertices of the simplex $\text{conv}(\Theta)$. Unlike triangles, which can only have up to one obtuse angle, simplices in higher dimension can have obtuse angles in many ways. They can have $(\mathbf{x}_j - \mathbf{x}_i) \cdot (\mathbf{x}_k - \mathbf{x}_i) < 0$ at multiple vertices $\mathbf{x}_i$ and at the same time for multiple (j, k) for each $\mathbf{x}_i$. While there can only be up to four disconnected subset of $\mathbb{R}^2$ where (20) is not an upper bound on the approximation error, our numerical experiments show this number can go up to at least twenty for trivariate ($n = 3$) linear interpolation. Considering a precise description of the four shaded areas in Figure 4 already requires four unintuitive inequalities or some wordy explanation, any description of these areas would almost certainly be extremely complicated, especially in higher dimension.

Regardless, we have found an efficient way to check whether $\mathbf{x}$ is in one of these areas without having to describe any of them. The theoretical proof that validates our approach is extremely technical and will be presented later in section 5.2. Our approach relies on a set of parameters $\{\mu_{ij}\}_{(i,j)\in\mathcal{I}_+\times\mathcal{I}_-}$ that can be computed as follows. Remember Θ is assumed to be ordered in a way so that $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_{n+1}$, and let $\text{diag}(\ell) \in \mathbb{R}^{(n+1)\times(n+1)}$ be the diagonal matrix containing $\ell_1, \ldots, \ell_{n+1}$. We now partition $\text{diag}(\ell), G$, and $H^\star$ with respect to $\mathcal{I}_+$ and $\mathcal{I}_-$. Let $\text{diag}(\ell_+) \in \mathbb{R}^{|\mathcal{I}_+|\times|\mathcal{I}_+|}$ be the diagonal matrix containing $\{\ell_i\}_{i\in\mathcal{I}_+}$, and $\text{diag}(\ell_-) \in \mathbb{R}^{(|\mathcal{I}_-|-1)\times(|\mathcal{I}_-|-1)}$ be the diagonal matrix containing $\{\ell_i\}_{i\in\mathcal{I}_-\setminus\{0\}}$. Let $Y_+ \in \mathbb{R}^{|\mathcal{I}_+|\times n}$ and $Y_- \in \mathbb{R}^{(|\mathcal{I}_-|-1)\times n}$ be the first $|\mathcal{I}_+|$ and the last $|\mathcal{I}_-| - 1$ rows of Y, respectively. The matrix G has $|\mathcal{I}_+| - 1$ positive eigenvalues and $|\mathcal{I}_-| - 1$ negative eigenvalues, as will be proved later. Let $\Lambda_+ \in \mathbb{R}^{(|\mathcal{I}_+|-1)\times(|\mathcal{I}_+|-1)}$ and $\Lambda_- \in \mathbb{R}^{(|\mathcal{I}_-|-1)\times(|\mathcal{I}_-|-1)}$ respectively be the the diagonal matrices that contain the positive and negative eigenvalues of G, and $P_+ \in \mathbb{R}^{n\times(|\mathcal{I}_+|-1)}$ and $P_- \in \mathbb{R}^{n\times(|\mathcal{I}_-|-1)}$ their corresponding eigenvector matrices. Then we have

$$\begin{aligned} G &\overset{(8)}{=} Y^T \text{diag}(\ell) Y = Y_+^T \text{diag}(\ell_+) Y_+ + Y_-^T \text{diag}(\ell_-) Y_- \\ &= P\Lambda P^T = P_+\Lambda_+P_+^T + P_-\Lambda_-P_-^T \end{aligned} \tag{21}$$

and

$$H^\star = \nu P \text{sign}(\Lambda) P^T = \nu(P_+P_+^T - P_-P_-^T). \tag{22}$$

We now present the definition of $\{\mu_{ij}\}_{(i,j)\in\mathcal{I}_+\times\mathcal{I}_-}$ and the main theorem of this section.

Theorem 5.1. *Consider the matrix* $M \overset{\text{def}}{=} \text{diag}(\ell_+)Y_+P_-(Y_-P_-)^{-1}$. *Let* $\mu_{ij} = \mathbf{e}_i^T M \mathbf{e}_{j-n-1+|\mathcal{I}_-|}$ *for all* $i \in \mathcal{I}_+$ *and* $j \in \mathcal{I}_- \setminus \{0\}$, *and* $\mu_{i0} = \ell_i - \sum_{j\in\mathcal{I}_-\setminus\{0\}} \mu_{ij}$ *for all* $i \in \mathcal{I}_+$. *Assume* $f \in C_\nu^{1,1}(\mathbb{R}^n)$. *If* $\mu_{ij} \geq 0$ *for all* $(i,j) \in \mathcal{I}_+ \times \mathcal{I}_-$, *then* (20) *is a sharp upper bound on the function approximation error* $|\hat{f}(\mathbf{x}) - f(\mathbf{x})|$ *for linear interpolation.*

Remark 1. *We note that* $\{j - n - 1 + |\mathcal{I}_-|\}_{j\in\mathcal{I}_-\setminus\{0\}} = \{1, 2, \ldots, |\mathcal{I}_-|\}$. *The matrix* M *is of size* $|\mathcal{I}_+| \times (|\mathcal{I}_-| - 1)$. *Each of its row corresponds to a sample point with positive Lagrange polynomial values at* $\mathbf{x}$, *while each of its column corresponds to a sample point with negative Lagrange polynomial values at* $\mathbf{x}$.

5.2 Technical Proofs

In the remaining of this section, we provide the complete proof to Theorem 5.1. We start with the number of positive and negative eigenvalues in the matrix G.

Lemma 5.2. *The numbers of positive and negative eigenvalues in* G *are* $|\mathcal{I}_+| - 1$ *and* $|\mathcal{I}_-| - 1$, *respectively.*

Proof. Let $\text{diag}(\ell)$ be the diagonal matrix containg $\ell_1, \ldots, \ell_{n+1}$. Consider the matrix $\bar{G} = \sum_{i=1}^{n+1} \ell_i \phi(\mathbf{x}_i - \mathbf{x})\phi(\mathbf{x}_i - \mathbf{x})^T = \Phi^T \text{diag}(\ell)\Phi$. The first element of the first column is $\sum_{i=1}^{n+1} \ell_i \overset{(4)}{=} 1$, while the rest of the column is $\sum_{i=1}^{n+1} \ell_i[\mathbf{x}_i - \mathbf{x}] \overset{(5)}{=} \mathbf{x} - \sum_{i=1}^{n+1} \ell_i \mathbf{x} \overset{(4)}{=} \mathbf{0}$. The bottom-right $n \times n$ submatrix of $\bar{G}$ is

$$\sum_{i=1}^{n+1} \ell_i[\mathbf{x}_i - \mathbf{x}][\mathbf{x}_i - \mathbf{x}]^T = \sum_{i=0}^{n+1} \ell_i[\mathbf{x}_i - \mathbf{x}][\mathbf{x}_i - \mathbf{x}]^T \overset{(8)}{=} G.$$

Thus, $\bar{G}$ and its eigendecomposition should be

$$\bar{G} = \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & G \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & P \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \Lambda \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & P^T \end{bmatrix}.$$

Then we have

$$\bar{\Lambda} \overset{\text{def}}{=} \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \Lambda \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & P^T \end{bmatrix} \Phi^T \operatorname{diag}(\ell) \Phi \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & P \end{bmatrix},$$

which shows $\bar{\Lambda}$ is congruent to $\operatorname{diag}(\ell)$. Then by Sylvester's law of inertia [11] (or Theorem 4.5.8 of [5]), the number of positive and negative eigenvalues in $\bar{\Lambda}$ are $|\mathcal{I}_+|$ and $|\mathcal{I}_-|-1$, respectively. Since $\bar{G}$ shares the same eigenvalues as G except an additional one that is 1, the lemma is proven. $\square$

The next lemma shows that $\{\mu_{ij}\}_{(i,j)\in\mathcal{I}_+\times\mathcal{I}_-}$ is well-defined by proving the invertibility of Y_-P_-.

Lemma 5.3. *The matrix Y_-P_- is invertible.*

Proof. For the purpose of contradiction, assume Y_-P_- is singular. That means there is a non-zero vector $\mathbf{u} \in \mathbb{R}^{|\mathcal{I}_-|-1}$ such that $Y_-P_-\mathbf{u} = \mathbf{0}$. Let $\mathbf{v} = P_-\mathbf{u}$. We have $Y_-\mathbf{v} = \mathbf{0}$, $P_+\mathbf{v} = P_+P_-\mathbf{u} = \mathbf{0}$ and $P_-^T\mathbf{v} = P_-^TP_-\mathbf{u} = \mathbf{u}$. Then we have the contradiction

$$\begin{aligned} \mathbf{v}^TG\mathbf{v} &= (Y_+\mathbf{v})^T \operatorname{diag}(\ell_+)Y_+\mathbf{v} + (Y_-\mathbf{v})^T \operatorname{diag}(\ell_-)Y_-\mathbf{v} = (Y_+\mathbf{v})^T \operatorname{diag}(\ell_+)Y_+\mathbf{v} \geq 0 \\ \mathbf{v}^TG\mathbf{v} &= (P_+^T\mathbf{v})^T\Lambda_+P_+^T\mathbf{v} + (P_-^T\mathbf{v})^T\Lambda_-P_-^T\mathbf{v} = (P_-^T\mathbf{v})^T\Lambda_-P_-^T\mathbf{v} = \mathbf{u}^T\Lambda_-\mathbf{u} < 0. \end{aligned}$$

$\square$

We develop in the following lemma the essential properties of $\{\mu_{ij}\}$.

Lemma 5.4. *The following properties hold:*

$$\sum_{j\in\mathcal{I}_-} \mu_{ij} = \ell_i \qquad \textit{for all } i \in \mathcal{I}_+, \tag{23}$$

$$\sum_{i\in\mathcal{I}_+} \mu_{ij} = -\ell_j \qquad \textit{for all } j \in \mathcal{I}_-, \tag{24}$$

$$(\nu I - H^\star) \sum_{j\in\mathcal{I}_-} \mu_{ij}\mathbf{x}_j = (\nu I - H^\star)\ell_i\mathbf{x}_i \qquad \textit{for all } i \in \mathcal{I}_+, \tag{25}$$

$$(\nu I + H^\star) \sum_{i\in\mathcal{I}_+} \mu_{ij}\mathbf{x}_i = -(\nu I + H^\star)\ell_j\mathbf{x}_j \qquad \textit{for all } j \in \mathcal{I}_-. \tag{26}$$

Proof. The equations (23) are true by their definition. Since

$$\begin{aligned} \operatorname{diag}(\ell_-)\mathbf{1} + M^T\mathbf{1} &= \operatorname{diag}(\ell_-)\mathbf{1} + (P_-^TY_-^T)^{-1}P_-^TY_+^T \operatorname{diag}(\ell_+)\mathbf{1} \\ &= (P_-^TY_-^T)^{-1}P_-^T[Y_-^T \operatorname{diag}(\ell_-)\mathbf{1} + Y_+^T \operatorname{diag}(\ell_+)\mathbf{1}] \overset{(5)}{=} \mathbf{0}, \end{aligned}$$

the equations (24) are also true. Notice $P_-^T(Y_-^TM^T - Y_+^T \operatorname{diag}(\ell_+)) = \mathbf{0}$ by the definition of M, and $\nu I - H^\star \overset{(22)}{=} \nu(P_+P_+^T + P_-P_-^T) - \nu(P_+P_+^T - P_-P_-^T) = 2\nu P_-P_-^T$. Following these two equations, we have for all $i \in \mathcal{I}_+$,

$$\begin{aligned} (\nu I - H^\star)\left[\sum_{j\in\mathcal{I}_-} \mu_{ij}\mathbf{x}_j - \ell_i\mathbf{x}_i\right] &\overset{(24)}{=} (\nu I - H^\star)\left[\sum_{j\in\mathcal{I}_-} \mu_{ij}(\mathbf{x}_j - \mathbf{x}) - \ell_i[\mathbf{x}_i - \mathbf{x}]\right] \\ &= (\nu I - H^\star)(Y_-^TM^T - Y_+^T \operatorname{diag}(\ell_+))\mathbf{e}_i \\ &= 2\nu P_-P_-^T(Y_-^TM^T - Y_+^T \operatorname{diag}(\ell_+))\mathbf{e}_i \\ &= 2\nu P_-\mathbf{0}\mathbf{e}_i = \mathbf{0}, \end{aligned}$$

which proves (25). To prove (26), we use G and its eigendecomposition. The diagonal matrix of the eigenvalues Λ is

$$\begin{bmatrix} \Lambda_- & \mathbf{0} \\ \mathbf{0} & \Lambda_+ \end{bmatrix} = \begin{bmatrix} P_-^T Y_-^T & P_-^T Y_+^T \\ P_+^T Y_-^T & P_+^T Y_+^T \end{bmatrix} \begin{bmatrix} \operatorname{diag}(\ell_-) & \\ & \operatorname{diag}(\ell_+) \end{bmatrix} \begin{bmatrix} Y_- P_- & Y_- P_+ \\ Y_+ P_- & Y_+ P_+ \end{bmatrix},$$

which contains two equivalent block equalities with zero left-hand side. They are $P_+^T Y_-^T \operatorname{diag}(\ell_-) Y_- P_- + P_+^T Y_+^T \operatorname{diag}(\ell_+) Y_+ P_- = \mathbf{0}$, so

$$P_+^T Y_-^T \operatorname{diag}(\ell_-) + P_+^T Y_+^T \operatorname{diag}(\ell_+) Y_+ P_- (Y_- P_-)^{-1} = P_+^T Y_-^T \operatorname{diag}(\ell_-) + P_+^T Y_+^T M = \mathbf{0}.$$

Then with $\nu I + H^\star \overset{(22)}{=} \nu(P_+ P_+^T + P_- P_-^T) + \nu(P_+ P_+^T - P_- P_-^T) = 2\nu P_+ P_+^T$, we obtain

$$(\nu I + H^\star)(Y_-^T \operatorname{diag}(\ell_-) + Y_+^T M) = 2\nu P_+ P_+^T (Y_-^T \operatorname{diag}(\ell_-) + Y_+^T M) = 2\nu P_+ \mathbf{0} = \mathbf{0},$$

which proves (26) for all $j \in \mathcal{I}_- \setminus \{0\}$; and

$$\begin{aligned} (\nu I + H^\star)\left(\ell_0 \mathbf{x} + \sum_{i \in \mathcal{I}_+} \mu_{i0} \mathbf{x}_i\right) &\overset{(24)}{=} 2\nu P_+ P_+^T \sum_{i \in \mathcal{I}_+} \mu_{i0}(\mathbf{x}_i - \mathbf{x}) \\ &= 2\nu P_+ P_+^T \sum_{i \in \mathcal{I}_+} \left(\ell_i - \sum_{j \in \mathcal{I}_- \setminus \{0\}} \mu_{ij}\right)(\mathbf{x}_i - \mathbf{x}) \\ &= 2\nu P_+ P_+^T Y_+^T (l_+ - M\mathbf{1}) \\ &= 2\nu P_+ P_+^T (Y_+^T l_+ + Y_-^T \ell_-) \overset{(5)}{=} \mathbf{0}, \end{aligned}$$

which proves (26) for $j = 0$. □

The function ψ is defined and proved non-positive in Lemma 5.5. It will be used to prove Theorem 5.1 in conjunction with the parameters $\{\mu_{ij}\}$.

Lemma 5.5. *Assume $f \in C_\nu^{1,1}(\mathbb{R}^n)$. For any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ and any matrix $H \in \mathbb{R}^{n \times n}$, we have*

$$\begin{aligned} \psi(\mathbf{u}, \mathbf{v}, H) \overset{\text{def}}{=} & f(\mathbf{u}) - f(\mathbf{v}) - \frac{1}{2\nu}[(\nu I - H)(\mathbf{u} - \mathbf{v})] \cdot Df(\mathbf{u}) \\ & - \frac{1}{2\nu}[(\nu I + H)(\mathbf{u} - \mathbf{v})] \cdot Df(\mathbf{v}) - \frac{1}{4\nu}\|H(\mathbf{u} - \mathbf{v})\|^2 - \frac{\nu}{4}\|\mathbf{u} - \mathbf{v}\|^2 \le 0. \end{aligned} \tag{27}$$

Proof. For the purpose of contradiction, assume (27) is false. Then we have

$$\begin{aligned} -f(\mathbf{u}) < & -f(\mathbf{v}) - \frac{1}{2\nu}[(\nu I + H)(\mathbf{u} - \mathbf{v})] \cdot Df(\mathbf{u}) \\ & - \frac{1}{2\nu}[(\nu I - H)(\mathbf{u} - \mathbf{v})] \cdot Df(\mathbf{v}) - \frac{1}{4\nu}\|H(\mathbf{u} - \mathbf{v})\|^2 - \frac{\nu}{4}\|\mathbf{u} - \mathbf{v}\|^2. \end{aligned}$$

Add this inequality to (11) and we arrive at

$$\frac{1}{4\nu}\|H(\mathbf{u} - \mathbf{v}) - (Df(\mathbf{u}) - Df(\mathbf{v}))\|^2 < 0,$$

which leads to contradiction. □

Finally, we prove the main result of this section, Theorem 5.1, which states (20) is a sharp bound when $\{\mu_{ij}\}$ are all non-negative.

proof of Theorem 5.1. We only provide the proof for the case when $\hat{f}(\mathbf{x}) - f(\mathbf{x}) \geq 0$. When $\mu_{ij} \geq 0$ for all $(i,j) \in \mathcal{I}_+ \times \mathcal{I}_-$, the following inequality holds

$$\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}\psi(\mathbf{x}_i, \mathbf{x}_j, H^\star) \overset{(27)}{\leq} 0. \tag{28}$$

The zeroth-order term in the summation (28) is

$$\begin{aligned}
\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}(f(\mathbf{x}_i) - f(\mathbf{x}_j)) &= \left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij} f(\mathbf{x}_i)\right] - \left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij} f(\mathbf{x}_j)\right] \\
&\overset{(23)(24)}{=} \left[\sum_{i\in\mathcal{I}_+} \ell_i f(\mathbf{x}_i)\right] + \left[\sum_{j\in\mathcal{I}_-} \ell_j f(\mathbf{x}_j)\right] \\
&\overset{(3)}{=} \hat{f}(\mathbf{x}) - f(\mathbf{x}).
\end{aligned}$$

The sum of the first-order terms is $-1/(2\nu)$ multiplies

$$\begin{aligned}
&\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}\big([(\nu I - H^\star)(\mathbf{x}_i - \mathbf{x}_j)] \cdot Df(\mathbf{x}_i) + [(\nu I + H^\star)(\mathbf{x}_i - \mathbf{x}_j)] \cdot Df(\mathbf{x}_j)\big) \\
&= \left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}[(\nu I - H^\star)\mathbf{x}_i] \cdot Df(\mathbf{x}_i)\right] - \left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}[(\nu I + H^\star)\mathbf{x}_j] \cdot Df(\mathbf{x}_j)\right] \\
&\quad - \left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}[(\nu I - H^\star)\mathbf{x}_j] \cdot Df(\mathbf{x}_i)\right] + \left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}[(\nu I + H^\star)\mathbf{x}_i] \cdot Df(\mathbf{x}_j)\right] \\
&= \left[\sum_{i\in\mathcal{I}_+} \ell_i[(\nu I - H^\star)\mathbf{x}_i] \cdot Df(\mathbf{x}_i)\right] + \left[\sum_{j\in\mathcal{I}_-} \ell_j[(\nu I + H^\star)\mathbf{x}_j] \cdot Df(\mathbf{x}_j)\right] \\
&\quad - \left[\sum_{i\in\mathcal{I}_+} \ell_i[(\nu I - H^\star)\mathbf{x}_i] \cdot Df(\mathbf{x}_i)\right] - \left[\sum_{j\in\mathcal{I}_-} \ell_j[(\nu I + H^\star)\mathbf{x}_j] \cdot Df(\mathbf{x}_j)\right] = \mathbf{0},
\end{aligned}$$

where the second equality holds because of (23), (24), (25), and (26) respectively for the four terms. Notice $H^{\star T}H^\star = \nu^2 I$. The constant term in the summation (28) is $-1/2$ multiplies

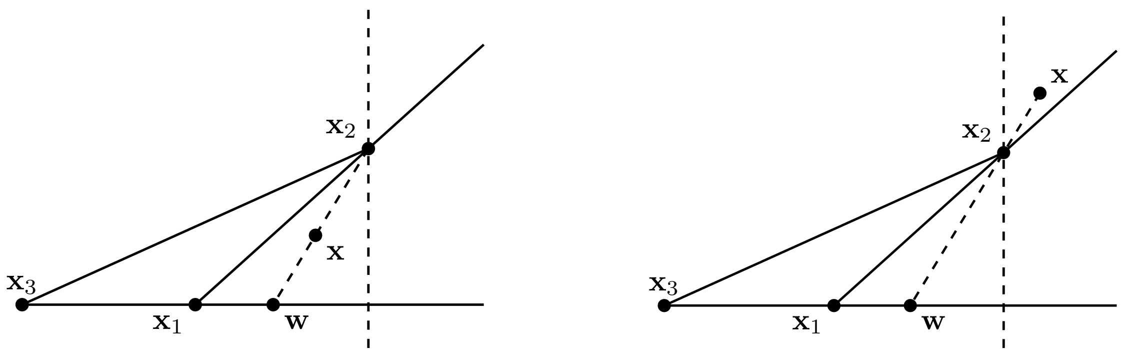
$$\begin{aligned}
&\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}\left(\frac{1}{2\nu}\|H^\star(\mathbf{x}_i - \mathbf{x}_j)\|^2 + \frac{\nu}{2}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right) \\
&= \nu\left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}(\mathbf{x}_i - \mathbf{x}_j) \cdot \mathbf{x}_i\right] - \nu\left[\sum_{i\in\mathcal{I}_+}\sum_{j\in\mathcal{I}_-} \mu_{ij}(\mathbf{x}_i - \mathbf{x}_j) \cdot \mathbf{x}_j\right] \\
&\overset{(23)(24)}{=} \sum_{i\in\mathcal{I}_+} \nu\left(\ell_i\mathbf{x}_i - \sum_{j\in\mathcal{I}_-}\mu_{ij}\mathbf{x}_j\right) \cdot \mathbf{x}_i - \sum_{j\in\mathcal{I}_-} \nu\left(\sum_{i\in\mathcal{I}_+}\mu_{ij}\mathbf{x}_i + \ell_j\mathbf{x}_j\right) \cdot \mathbf{x}_j \\
&\overset{(25)(26)}{=} \sum_{i\in\mathcal{I}_+} \left[H^\star\left(\ell_i\mathbf{x}_i - \sum_{j\in\mathcal{I}_-}\mu_{ij}\mathbf{x}_j\right)\right] \cdot \mathbf{x}_i + \sum_{j\in\mathcal{I}_-} \left[H^\star\left(\sum_{i\in\mathcal{I}_+}\mu_{ij}\mathbf{x}_i + \ell_j\mathbf{x}_j\right)\right] \cdot \mathbf{x}_j \\
&= \left[\sum_{i\in\mathcal{I}_+} \ell_i[H^\star\mathbf{x}_i] \cdot \mathbf{x}_i\right] + \left[\sum_{j\in\mathcal{I}_-} \ell_j[H^\star\mathbf{x}_j] \cdot \mathbf{x}_j\right] = G \cdot H^\star.
\end{aligned}$$

Thus the summation (28) is (20) when $\hat{f}(\mathbf{x}) - f(\mathbf{x}) \geq 0$. $\square$

6 Sharp Error Bounds for Bivariate Extrapolation

We investigate in this section the sharp error bounds when $\mathbf{x}$ is in the four areas shown in Figure 4. This investigation is not just for the completeness of our analysis of the sharp error bound, but also to understand what type of function can be more difficult for linear interpolation to approximate than the quadratics.

We first notice the case where $\mathbf{x}$ is in the shaded triangle on the left in Figure 4 is symmetric to the case where $\mathbf{x}$ is in the triangle on the right, and they are essentially the same. The same argument applies the two shaded cones. This reduces the cases that need to be studied to the two in Figure 5. Furthermore, after we obtain a formula for the sharp error bound for the case in Figure 5a, a formula for the case in Figure 5b can be obtained by switching the roles of $\mathbf{x}$ and $\mathbf{x}_2$ and apply Proposition 3.3. Therefore, the only case that needs to be studied is the one in Figure 5a.



(a) When $\mathbf{x}$ is in the open triangle such that $\ell_1[\mathbf{x}_2-\mathbf{x}_1]\cdot[\mathbf{x}_3-\mathbf{x}_1]-\ell_3[\mathbf{x}_2-\mathbf{x}_3]\cdot[\mathbf{x}_1-\mathbf{x}_3]<0$, $\ell_2>0$, and $\ell_3<0$

(b) When $\mathbf{x}$ is in the open cone such that $\ell_1[\mathbf{x}_2-\mathbf{x}_1]\cdot[\mathbf{x}_3-\mathbf{x}_1]-\ell_3[\mathbf{x}_2-\mathbf{x}_3]\cdot[\mathbf{x}_1-\mathbf{x}_3]>0$ and $\ell_3>0$

Figure 5: Two configurations of Θ and $\mathbf{x}$ where (20) is an invalid error bound for bivariate extrapolation.

The case in Figure 5a can be defined mathematically as $\ell_2 > 0, \ell_3 < 0$, and $\ell_1[\mathbf{x}_2-\mathbf{x}_1]\cdot[\mathbf{x}_3-\mathbf{x}_1]-\ell_3[\mathbf{x}_2-\mathbf{x}_3]\cdot[\mathbf{x}_1-\mathbf{x}_3]<0$. The following lemma shows the point $\mathbf{w}$, as defined in (29), is the intersection of the line going through $\mathbf{x}_1$ and $\mathbf{x}_3$ and the line going through $\mathbf{x}$ and $\mathbf{x}_2$.

Lemma 6.1. *Assume* $-\ell_0-\ell_2 \overset{(4)}{=} \ell_1+\ell_3 \neq 0$ *for some affinely independent* $\Theta \subset \mathbb{R}^2$ *and* $\mathbf{x} \in \mathbb{R}^2$. *Let*

$$\mathbf{w} = \frac{-\ell_0\mathbf{x}+\ell_1\mathbf{x}_1-\ell_2\mathbf{x}_2+\ell_3\mathbf{x}_3}{-\ell_0+\ell_1-\ell_2+\ell_3}. \tag{29}$$

Then

$$\mathbf{w} = \frac{\ell_1\mathbf{x}_1+\ell_3\mathbf{x}_3}{\ell_1+\ell_3} = \frac{\ell_0\mathbf{x}+\ell_2\mathbf{x}_2}{\ell_0+\ell_2},$$

and

$$\ell_0[\mathbf{x}-\mathbf{w}]+\ell_2[\mathbf{x}_2-\mathbf{w}] = 0, \tag{30a}$$

$$\ell_1[\mathbf{x}_1-\mathbf{w}]+\ell_3[\mathbf{x}_3-\mathbf{w}] = 0. \tag{30b}$$

Proof. These equalities are direct results of (4) and (5). $\square$

We define in the following lemma an $H^\star$, which is different from the one defined in (19) and is asymmetric.

Lemma 6.2. *Assume for some affinely independent* $\Theta \subset \mathbb{R}^2$ *and* $\mathbf{x} \in \mathbb{R}^2$ *that* $\ell_2 > 0, \ell_3 < 0$*, and* $\ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3[\mathbf{x}_2 - \mathbf{x}_3] \cdot [\mathbf{x}_1 - \mathbf{x}_3] < 0$*. Let*

$$H^\star = P \begin{bmatrix} +\nu & 0 \\ 0 & -\nu \end{bmatrix} P^{-1} \text{ with } P = \begin{bmatrix} \mathbf{x}_2 - \mathbf{x} & \mathbf{x}_1 - \mathbf{x}_3 \end{bmatrix}. \tag{31}$$

Let $\mathbf{w}$ *be defined as* (29)*. Then*

$$\begin{aligned} H^\star(\mathbf{x}_i - \mathbf{w}) &= \nu(\mathbf{x}_i - \mathbf{w}) \text{ for } i \in \{0, 2\}, \\ H^\star(\mathbf{x}_i - \mathbf{w}) &= -\nu(\mathbf{x}_i - \mathbf{w}) \text{ for } i \in \{1, 3\}. \end{aligned} \tag{32}$$

Proof. It is clear from Figure 5a that the assumption guarantees the invertibility of P and $-\ell_0 - \ell_2 = \ell_1 + \ell_3 \neq 0$. Notice by the definition of $H^\star$, we have $H^\star(\mathbf{x}_2 - \mathbf{x}) = \nu(\mathbf{x}_2 - \mathbf{x})$ and $H^\star(\mathbf{x}_1 - \mathbf{x}_3) = -\nu(\mathbf{x}_1 - \mathbf{x}_3)$. The lemma holds true because $\mathbf{x}_i - \mathbf{w}$ is parallel to $\mathbf{x}_2 - \mathbf{x}$ for $i \in \{0, 2\}$ and to $\mathbf{x}_1 - \mathbf{x}_3$ for $i \in \{1, 3\}$. □

Now we are ready to show $G \cdot H^\star/2$, with $H^\star$ defined in (31), is an upper bound on the function approximation error for the case in Figure 5a.

Theorem 6.3. *Assume* $f \in C^{1,1}_\nu(\mathbb{R}^2)$*. Let* $\hat{f}$ *be the affine function that interpolates* f *at any set of three affinely independent vectors* $\Theta = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\} \subset \mathbb{R}^2$ *such that* $(\mathbf{x}_2 - \mathbf{x}_1) \cdot (\mathbf{x}_3 - \mathbf{x}_1) < 0$*. Let* $\mathbf{x}$ *be any vector in* $\mathbb{R}^2$ *such that its barycentric coordinates satisfies* $\ell_2 > 0, \ell_3 < 0$*, and* $\ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3[\mathbf{x}_2 - \mathbf{x}_3] \cdot [\mathbf{x}_1 - \mathbf{x}_3] < 0$*. Let* G *and* $H^\star$ *be the matrices defined in* (7) *and* (31)*. Then the function approximation error of* $\hat{f}$ *at* $\mathbf{x}$ *is bounded as*

$$|\hat{f}(\mathbf{x}) - f(\mathbf{x})| \leq \frac{1}{2} G \cdot H^\star. \tag{33}$$

Proof. We only provide the proof for the case when $\hat{f}(\mathbf{x}) - f(\mathbf{x}) \geq 0$. We use the function ψ defined in (27) again. Since $\ell_3 < 0$, $(\mathbf{x}_2 - \mathbf{x}_1) \cdot (\mathbf{x}_3 - \mathbf{x}_1) < 0$, and

$$\begin{aligned} 0 &> \ell_1[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3[\mathbf{x}_2 - \mathbf{x}_3] \cdot [\mathbf{x}_1 - \mathbf{x}_3] \\ &\overset{(4)}{=} (1 - \ell_2 - \ell_3)[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3[\mathbf{x}_2 - \mathbf{x}_3] \cdot [\mathbf{x}_1 - \mathbf{x}_3] \\ &= (1 - \ell_2)[\mathbf{x}_2 - \mathbf{x}_1] \cdot [\mathbf{x}_3 - \mathbf{x}_1] - \ell_3 \|\mathbf{x}_1 - \mathbf{x}_3\|^2, \end{aligned}$$

we have $1 - \ell_2 > 0$, and thus the following inequalities hold:

$$(1 - \ell_2)\psi(\mathbf{x}_1, \mathbf{x}, H^\star) \leq 0, \tag{34a}$$

$$\ell_2 \psi(\mathbf{x}_2, \mathbf{x}, H^\star) \leq 0, \tag{34b}$$

$$-\ell_3 \psi(\mathbf{x}_1, \mathbf{x}_3, H^\star) \leq 0. \tag{34c}$$

Similar to the previous proofs, we add these inequalities together. The sum of their zeroth-order terms is

$$\begin{aligned} &(1 - \ell_2)[f(\mathbf{x}_1) - f(\mathbf{x})] + \ell_2[f(\mathbf{x}_2) - f(\mathbf{x})] - \ell_3[f(\mathbf{x}_1) - f(\mathbf{x}_3)] \\ &\quad = (1 - \ell_2 - \ell_3) f(\mathbf{x}_1) + \ell_2 f(\mathbf{x}_2) + \ell_3 f(\mathbf{x}_3) - f(\mathbf{x}) \overset{(3)(4)}{=} \hat{f}(\mathbf{x}) - f(\mathbf{x}). \end{aligned}$$

The sum of their first-order terms is $-1/(2\nu)$ multiplies

$$\begin{aligned} &(1 - \ell_2)\left\{[(\nu I - H^\star)(\mathbf{x}_1 - \mathbf{x})] \cdot Df(\mathbf{x}_1) + [(\nu I + H^\star)(\mathbf{x}_1 - \mathbf{x})] \cdot Df(\mathbf{x})\right\} \\ &+ \ell_2 \left\{[(\nu I - H^\star)(\mathbf{x}_2 - \mathbf{x})] \cdot Df(\mathbf{x}_2) + [(\nu I + H^\star)(\mathbf{x}_2 - \mathbf{x})] \cdot Df(\mathbf{x})\right\} \\ &- \ell_3 \left\{[(\nu I - H^\star)(\mathbf{x}_1 - \mathbf{x}_3)] \cdot Df(\mathbf{x}_1) + [(\nu I + H^\star)(\mathbf{x}_1 - \mathbf{x}_3)] \cdot Df(\mathbf{x}_3)\right\} \\ &\quad = \left\{(\nu I - H^\star)[(1 - \ell_2)(\mathbf{x}_1 - \mathbf{x}) - \ell_3(\mathbf{x}_1 - \mathbf{x}_3)]\right\} \cdot Df(\mathbf{x}_1) \\ &\qquad + \ell_2[(\nu I - H^\star)(\mathbf{x}_2 - \mathbf{x})] \cdot Df(\mathbf{x}_2) - \ell_3[(\nu I + H^\star)(\mathbf{x}_1 - \mathbf{x}_3)] \cdot Df(\mathbf{x}_3) \\ &\qquad + \left\{(\nu I + H^\star)[(1 - \ell_2)(\mathbf{x}_1 - \mathbf{x}) + \ell_2(\mathbf{x}_2 - \mathbf{x})]\right\} \cdot Df(\mathbf{x}) \\ &\quad \overset{(4)(5)}{=} \ell_2[(\nu I - H^\star)(\mathbf{x} - \mathbf{x}_2)] \cdot Df(\mathbf{x}_1) + \ell_2[(\nu I - H^\star)(\mathbf{x}_2 - \mathbf{x})] \cdot Df(\mathbf{x}_2) \\ &\qquad - \ell_3[(\nu I + H^\star)(\mathbf{x}_1 - \mathbf{x}_3)] \cdot Df(\mathbf{x}_3) + \ell_3[(\nu I + H^\star)(\mathbf{x}_1 - \mathbf{x}_3)] \cdot Df(\mathbf{x}) \\ &\quad \overset{(32)}{=} \mathbf{0}. \end{aligned}$$

Let $\mathbf{w}$ be defined as (29). The sum of the constant terms is $-1/2$ times

$$\begin{aligned}
&(1-\ell_2)\left[\frac{1}{2\nu}\|H^\star(\mathbf{x}_1-\mathbf{x})\|^2+\frac{\nu}{2}\|\mathbf{x}_1-\mathbf{x}\|^2\right]+\ell_2\left[\frac{1}{2\nu}\|H^\star(\mathbf{x}_2-\mathbf{x})\|^2\right.\\
&\left.+\frac{\nu}{2}\|\mathbf{x}_2-\mathbf{x}\|^2\right]-\ell_3\left[\frac{1}{2\nu}\|H^\star(\mathbf{x}_1-\mathbf{x}_3)\|^2+\frac{\nu}{2}\|\mathbf{x}_1-\mathbf{x}_3\|^2\right]\\
&\overset{(32)}{=}(1-\ell_2)\left\{-H^\star(\mathbf{x}_1-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{w})+H^\star(\mathbf{x}-\mathbf{w})\cdot(\mathbf{x}-\mathbf{w})\right\}\\
&\qquad+\ell_2H^\star(\mathbf{x}_2-\mathbf{x})\cdot(\mathbf{x}_2-\mathbf{x})+\ell_3H^\star(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{x}_1-\mathbf{x}_3)\\
&\overset{(4)}{=}H^\star[\ell_3(\mathbf{x}_1-\mathbf{x}_3)-(\ell_1+\ell_3)(\mathbf{x}_1-\mathbf{w})]\cdot(\mathbf{x}_1-\mathbf{w})-\ell_3H^\star(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{x}_3-\mathbf{w})\\
&\qquad+H^\star[(1-\ell_2)(\mathbf{x}-\mathbf{w})-\ell_2(\mathbf{x}_2-\mathbf{x})]\cdot(\mathbf{x}-\mathbf{w})+\ell_2H^\star(\mathbf{x}_2-\mathbf{x})\cdot(\mathbf{x}_2-\mathbf{w})\\
&\overset{(4)(5)}{=}0-\ell_3[H^\star(\mathbf{x}_1-\mathbf{w})-H^\star(\mathbf{x}_3-\mathbf{w})]\cdot(\mathbf{x}_3-\mathbf{w})\\
&\quad+0+\ell_2[H^\star(\mathbf{x}_2-\mathbf{w})-H^\star(\mathbf{x}-\mathbf{w})]\cdot(\mathbf{x}_2-\mathbf{w})\\
&\overset{(30)}{=}\sum_{i=0}^{3}\ell_iH^\star(\mathbf{x}_i-\mathbf{w})\cdot(\mathbf{x}_i-\mathbf{w})\overset{(8)}{=}G\cdot H^\star.
\end{aligned}$$

Thus, the sum of the inequalities in (34) is (33) when $\hat{f}(\mathbf{x})-f(\mathbf{x})\geq 0$. □

We show in Theorem 6.4 the upper bound (33) can be achieved by a piecewice quadratic, and therefore (33) is sharp.

Theorem 6.4. *Under the setting of Theorem 6.3, the bound* (33) *is sharp and can be achieved by*

$$f(\mathbf{u})=\begin{cases}\dfrac{\nu}{2}\|\mathbf{u}-\mathbf{w}\|^2-\dfrac{\nu[(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{u}-\mathbf{w})]^2}{\|\mathbf{x}_1-\mathbf{x}_3\|^2} & \textit{if } (\mathbf{u}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)\leq 0,\\ \dfrac{\nu}{2}\|\mathbf{u}-\mathbf{w}\|^2 & \textit{if } (\mathbf{u}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)\geq 0.\end{cases},$$

where $\mathbf{w}$ *is defined in* (29).

Proof. The function approximation error for this piecewise quadratic function is

$$\begin{aligned}
\hat{f}(\mathbf{x})-f(\mathbf{x})&=\sum_{i=0}^{n+1}\ell_i\mathbf{x}_i\\
&=\frac{\nu}{2}\sum_{i=0}^{3}\ell_i\|\mathbf{x}_i-\mathbf{w}\|^2-\frac{\nu\ell_1[(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{x}_1-\mathbf{w})]^2}{\|\mathbf{x}_1-\mathbf{x}_3\|^2}-\frac{2\nu\ell_3[(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{x}_3-\mathbf{w})]^2}{\|\mathbf{x}_1-\mathbf{x}_3\|^2}\\
&=\frac{\nu}{2}\sum_{i=0}^{3}\ell_i\|\mathbf{x}_i-\mathbf{w}\|^2-\nu\ell_1\|\mathbf{x}_1-\mathbf{w}\|^2-2\nu\ell_3\|\mathbf{x}_3-\mathbf{w}\|^2\\
&=\frac{\nu}{2}\left(\ell_0\|\mathbf{x}-\mathbf{w}\|^2-\ell_1\|\mathbf{x}_1-\mathbf{w}\|^2+\ell_2\|\mathbf{x}_2-\mathbf{w}\|^2-\ell_3\|\mathbf{x}_3-\mathbf{w}\|^2\right)\\
&\overset{(32)}{=}\frac{1}{2}\sum_{i=0}^{3}\ell_i\|\mathbf{x}_i-\mathbf{w}\|_{H^\star}\overset{(8)}{=}\frac{1}{2}G\cdot H^\star.
\end{aligned}$$

Now we prove $f\in C^{1,1}_\nu(\mathbb{R}^n)$. Firstly, it is clear that f is continuous on $\mathbb{R}^2$ and differentiable on the two half spaces $\{\mathbf{u}:\ (\mathbf{u}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)<0\}$ and $\{\mathbf{u}:\ (\mathbf{u}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)>0\}$. Then given any $\mathbf{u}$ such that

$(\mathbf{u}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)=0$, it can be calculated for any $\mathbf{v}\in\mathbb{R}^2$ that

$$
\begin{aligned}
&|f(\mathbf{u}+\mathbf{v})-f(\mathbf{u})-\nu(\mathbf{u}-\mathbf{w})\cdot\mathbf{v}| \\
&\qquad\qquad = \begin{cases} -\dfrac{\nu}{2}\|\mathbf{v}\|^2-\dfrac{\nu[(\mathbf{x}_1-\mathbf{x}_3)\cdot\mathbf{v}]^2}{\|\mathbf{x}_1-\mathbf{x}_3\|^2} & \text{if } (\mathbf{u}+\mathbf{v}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)\le 0, \\ -\dfrac{\nu}{2}\|\mathbf{v}\|^2 & \text{if } (\mathbf{u}+\mathbf{v}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)\ge 0. \end{cases}
\end{aligned}
$$

Thus

$$\lim_{v\to\mathbf{0}}\frac{|f(\mathbf{u}+\mathbf{v})-f(\mathbf{u})-\nu(\mathbf{u}-\mathbf{w})\cdot\mathbf{v}|}{\|\mathbf{v}\|}=0,$$

which shows f is differentiable with gradient $\nu(\mathbf{u}-\mathbf{w})$ on $\{\mathbf{u}:\ (\mathbf{u}-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)=0\}$. The condition (1) is clearly satisfied if $\mathbf{u}_1$ and $\mathbf{u}_2$ are in the same half space. Now assume $(\mathbf{u}_1-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)<0$ and $(\mathbf{u}_2-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)>0$. Then, we have

$$
\begin{aligned}
&\|Df(\mathbf{u}_1)-Df(\mathbf{u}_2)\|^2 \\
&=\|\nu(\mathbf{u}_1-\mathbf{w})-2\nu\left[(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{u}_1-\mathbf{w})/\|\mathbf{x}_1-\mathbf{x}_3\|^2\right](\mathbf{x}_1-\mathbf{x}_3)-\nu(\mathbf{u}_2-\mathbf{w})\|^2 \\
&=\nu^2\|\mathbf{u}_1-\mathbf{u}_2\|^2+4\nu^2[(\mathbf{u}_1-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)][(\mathbf{u}_2-\mathbf{w})\cdot(\mathbf{x}_1-\mathbf{x}_3)]/\|\mathbf{x}_1-\mathbf{x}_3\|^2 \\
&<\nu^2\|\mathbf{u}_1-\mathbf{u}_2\|^2,
\end{aligned}
$$

which shows (1) always holds. Therefore $f\in C^{1,1}_\nu(\mathbb{R}^n)$. □

7 Discussion

We presented a numerical approach to calculate the sharp bound on the function approximation error of linear interpolation and extrapolation and proved several conditionally sharp analytical bound along with their conditions for sharpness. These analytically bounds include one that improves the existing ones to better cover the extrapolation case (15), a sharp bound for quadratic functions (20), and one for bivariate extrapolation (33). The two bounds (20) and (33) together provide the sharp error bound for bivariate linear interpolation under any configuration of $\mathbf{x}$ and an affinely independent Θ. These bounds can provide an important theoretical foundation for the design and analysis of derivative-free optimization methods and any other numerical methods that utilizes linear interpolation.

While our results are developed under the condition that $f\in C^{1,1}_\nu(\mathbb{R}^n)$, they can stand under weaker conditions (but would require more complicated analysis). In existing literature, the condition often used is that $\||D^2f|\|_{L_\infty(Q)}\le\nu$, where Q, for example, is the star-shaped set that connects $\mathbf{x}$ to each point in Θ in [1] and conv(Θ) in [14]. Our results do not necessarily require the twice-differentiability of f and only need $f\in C^{1,1}_\nu(Q)$ for some $Q\subset\mathbb{R}^n$. For (15), Q at least needs to cover (almost everywhere, same hereafter) the star-shaped set $\cup_{i=0}^{n+1}\{\alpha\mathbf{x}_i+(1-\alpha)\mathbf{w}:\ 0\le\alpha\le 1\}$. For (20), we need Q to cover

$$\bigcup_{(i,j)\in\mathcal{I}_+\times\mathcal{I}_-}\begin{pmatrix}\{\alpha\mathbf{x}_i+(1-\alpha)[(\mathbf{u}_i+\mathbf{u}_j)/2+H^\star(\mathbf{u}_i-\mathbf{u}_j)/(2\nu)]:\ 0\le\alpha\le 1\} \\ \cup\{\alpha\mathbf{x}_j+(1-\alpha)[(\mathbf{u}_i+\mathbf{u}_j)/2+H^\star(\mathbf{u}_i-\mathbf{u}_j)/(2\nu)]:\ 0\le\alpha\le 1\}\end{pmatrix},$$

where $H^\star$ is defined as (19). For (33), we need

$$Q\supseteq\{\alpha\mathbf{x}_2+(1-\alpha)\mathbf{w}:\ 0\le\alpha\le 1\}\cup\{\alpha\mathbf{x}_3+(1-\alpha)\mathbf{w}:\ 0\le\alpha\le 1\},$$

where $\mathbf{w}$ is defined as (29).

We proposed to compute $\{\mu_{ij}\}$ and check their signs to determine whether (20) is a sharp bound and proved in Theorem 5.1 that $\{\mu_{ij}\}$ being all non-negative is a sufficient condition. We want to mention that one of our numerical experiments seems to indicate that it is also a necessary condition. This experiment involves generating many different Θ and $\mathbf{x}$ with various n and calculated the corresponding $\{\mu_{ij}\}$. From this experiment, we also observed some geometric pattern of the signs of $\{\mu_{ij}\}$, which we present in the following conjecture.

Conjecture 1. *Assume $f \in C_\nu^{1,1}(\mathbb{R}^n)$. Let $\hat{f}$ be the linear function that interpolates f at any set of $n+1$ affinely independent vectors $\Theta = \{\mathbf{x}_1, \ldots, \mathbf{x}_{n+1}\} \subset \mathbb{R}^n$. Let $\mathbf{x}$ be any vector in $\mathbb{R}^n$. Let $\{\mu_{ij}\}_{i \in \mathcal{I}_+,\ j \in \mathcal{I}_-}$ be the set of parameters defined in Theorem 5.1. Then the following statements are true.*

1. *When there is no obtuse angle at the vertices of the simplex* $\mathrm{conv}(\Theta)$*, that is, when*
$$(\mathbf{x}_j - \mathbf{x}_i) \cdot (\mathbf{x}_k - \mathbf{x}_i) \geq 0 \text{ for all } i, j, k = 1, 2, \ldots, n+1, \tag{35}$$
the parameters $\{\mu_{ij}\}$ are all non-negative for any $\mathbf{x} \in \mathbb{R}^n$.

2. *If there is at least one obtuse angle at the vertices of the simplex* $\mathrm{conv}(\Theta)$*, then there is a non-empty subset of $\mathbb{R}^n$ to which if $\mathbf{x}$ belongs, there is at least one negative element in $\{\mu_{ij}\}$.*

A general formula for the sharp bound on the function approximation error of linear interpolation and extrapolation remains an open question. It would appear $G \cdot H^\star/2$ is a good candidate, since all the bounds developed in this paper can be written in this form, but the matrix $H^\star$ depends on the geometry of Θ and $\mathbf{x}$. Using $G \cdot H^\star/2$ as the general formula, we would need five different definition of $H^\star$ even for the bivariate case ((19) and four variants of (31) that corresponds to the four shaded areas in Figure 4). Note that the matrix $H^\star$ is tied to $\{\mu_{ij}\}$ in (25) and (26), and we believe even when there are negatives in $\{\mu_{ij}\}$, they are still tied in the same manner to a version of $\{\mu_{ij}\}$ that is modified to be all non-negative. In fact, (23) - (26) all hold true under the setting of Theorem 6.3 if $H^\star$ is defined as (31) and $\{\mu_{ij}\}$ is defined as

$$\mu_{10} = 1 - \ell_2, \quad \mu_{13} = -\ell_3, \quad \mu_{20} = \ell_2, \quad \mu_{23} = 0,$$

which are the coefficients in (34). Considering the difficulty in analyzing the signs of $\{\mu_{ij}\}$, it is unlikely for $G \cdot H^\star/2$ to be suitable for this general formula. Whether there even exists a concise analytical form to the sharp error bound that can fit all the geometric configurations of Θ and $\mathbf{x}$ is still unclear to us.

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References

[1] Philippe G Ciarlet and Pierre-Arnaud Raviart. General Lagrange and Hermite interpolation in $\mathbb{R}^n$ with applications to finite element methods. *Archive for Rational Mechanics and Analysis*, 46(3):177–199, 1972.

[2] Andrew R Conn, Katya Scheinberg, and Luis N Vicente. *Introduction to derivative-free optimization*. SIAM, 2009.

[3] Philip J Davis. *Interpolation and Approximation*. Courier Corporation, 1975.

[4] Yoel Drori and Marc Teboulle. Performance of first-order methods for smooth convex minimization: a novel approach. *Mathematical Programming*, 145(1-2):451–482, 2014.

[5] Roger A Horn and Charles R Johnson. *Matrix Analysis*. Cambridge university press, 2012.

[6] John A Nelder and Roger Mead. A simplex method for function minimization. *The computer journal*, 7(4):308–313, 1965.

[7] Y Nesterov. *Introductory Lectures on Convex Optimization: A Basic Course*, volume 87. Springer Science & Business Media, 2013.

[8] Michael JD Powell. A direct search optimization method that models the objective and constraint functions by linear interpolation. In *Advances in optimization and numerical analysis*, pages 51–67. Springer, 1994.

[9] MJD Powell. On the Lagrange functions of quadratic models that are defined by interpolation. *Optimization Methods and Software*, 16(1-4):289–309, 2001.

[10] Martin Stämpfle. Optimal estimates for the linear interpolation error on simplices. *Journal of Approximation Theory*, 103(1):78–90, 2000.

[11] James Joseph Sylvester. Xix. a demonstration of the theorem that every homogeneous quadratic polynomial is reducible by real orthogonal substitutions to the form of a sum of positive and negative squares. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 4(23):138–142, 1852.

[12] Adrien B Taylor, Julien M Hendrickx, and François Glineur. Exact worst-case performance of first-order methods for composite convex optimization. *SIAM Journal on Optimization*, 27(3):1283–1313, 2017.

[13] Adrien B Taylor, Julien M Hendrickx, and François Glineur. Smooth strongly convex interpolation and exact worst-case performance of first-order methods. *Mathematical Programming*, 161:307–345, 2017.

[14] Shayne Waldron. The error in linear interpolation at the vertices of a simplex. *SIAM Journal on Numerical Analysis*, 35(3):1191–1200, 1998.