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ERROR ESTIMATES AND POISEDNESS IN MULTIVARIATE POLYNOMIAL INTERPOLATION

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Abstract: We show how to derive error estimates between a function and its interpolating polynomial and between their corresponding derivatives. The derivation is based on a new definition of well-poisedness for the interpolation set, directly connecting the accuracy of the error estimates with the geometry of the points in the set. This definition is equivalent to the boundedness of Lagrange polynomials, but it provides new geometric intuition. Our approach extracts the error bounds for all of the derivatives using the same analysis; the error bound for the function values is then derived *a posteriori*.

We also develop an algorithm to build a set of well-poised interpolation points or to modify an existing set to ensure its well-poisedness. We comment on the optimal geometries corresponding to the best possible well-poised sets in the case of linear interpolation.

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1. Introduction

Let f be a function defined from $\mathbb{R}^n$ to $\mathbb{R}$ and suppose that its values are known for a given set of points. One way of building an approximate model of f is by interpolating the function values at given points by a polynomial. In this paper we focus on the quality of multivariate polynomial interpolation depending on the geometric properties of the interpolation points.

Our work is motivated by the recent increase in interest in multivariate polynomial interpolation in nonlinear optimization (see Conn, Scheinberg, and Toint [3], [4] and Powell [6], [8]). Typically, in unconstrained nonlinear optimization, when the gradient (and, possibly, the Hessian) of the objective function f is available, a Taylor expansion is used to model the objective function. The iterates are then drawn from the optimal points of the successive Taylor models. However, when gradient information is not available,

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a polynomial interpolation model may replace the Taylor model. To be able to use the standard unconstrained optimization convergence theory in this case, the multivariate interpolation models need to have similar approximation properties to those of the Taylor models.

It has been shown by Powell [7], Sauer and Xu [9], and Waldron [11], that a multivariate polynomial interpolation approximates f locally — in terms of function values — with the same order of accuracy as the Taylor expansion under certain conditions on the interpolation set. In the previous work these conditions are typically tied to some specific bases of polynomials (Lagrange or Newton). The appropriate error bounds are not easy to understand intuitively, one reason being that an upper bound on the absolute value of the polynomials of the basis in the region of interest is one of the components of the overall bound in the error estimates.

In this paper we consider yet another condition on the interpolation set, which we call Λ-poisedness. This condition was developed independently from the previous well-poisedness conditions, it is geometric and, in our opinion, is more "natural". However, it turns out to be equivalent to Λ being the upper bound on the absolute values of the Lagrange polynomials.

The bound on Lagrange polynomials is used in [11] to derive the error estimates for multivariate interpolation. However, that paper is difficult to follow for a reader with mainly an optimization background. It is even difficult to extract the error bound in a simple form. By contrast Powell [7] provides a simple and elegant error bound and derivation, but only for the error in the function value, not for the derivatives.

In this paper we provide a simple and intuitive derivation of the error bounds (including those for the derivatives). The quality of our error estimates for function values is as good as the quality of the previously mentioned estimates.

We will use Λ-poisedness and the associated constant Λ in bounding the approximation errors. We also show that this condition is related to another algebraic condition, which in turn can be used to design an algorithm for generating a set of points with "good" geometry. Such an algorithm is a necessary ingredient for an optimization method based on a combination of a trust-region method and multivariate polynomial interpolation. To ensure the quality of the model one has to guarantee the well-poisedness of the interpolation set before seeking further accuracy by shrinking the size of the trust region (see, e.g., [3], [4]).

We will restrict our attention to linear interpolation (Section 2) and quadratic interpolation (Section 3) for most of the paper. Linear interpolation is simple and is considered separately to introduce the basic steps of the analysis. The quadratic case captures most of the properties of multivariate polynomial interpolation while remaining tractable. After fully considering the quadratic case we will point out how it can be extended to the general case by means of the cubic case (Section 4). Section 5 addresses the connection to the other error estimates and well-poisedness conditions and Section 6 describes the algorithmic framework to ensure good geometry in the interpolation set. We end the paper in Section 7 with our conclusions.

1.1. Basic assumptions. Consider a set of interpolation points given by

$$Y \;=\; \left\{y^0, \ldots, y^{p-1}\right\},$$

where $p = |Y|$ is a positive integer defining the number of points in the interpolation set. Let $m(x)$ denote an interpolating polynomial of degree d satisfying the interpolation conditions

$$m(y^i) \;=\; f(y^i),\; i = 0, \ldots, p-1. \tag{1}$$

Typically, p is the dimension of the space of polynomials of degree less than or equal to d.

Henceforth we make two assumptions about our interpolation set. We consider a closed ball $B(\Delta)$ of radius Δ centered at the origin and we assume that $Y \subseteq B(\Delta)$. This assumption is made without loss of generality. In fact, if the center of the ball is a point $v \neq 0$, we can define the function $f_v(z) = f(z+v)$ and the interpolation set:

$$W \;=\; \left\{w^0, \ldots, w^{p-1}\right\} \;=\; \left\{y^0 - v, \ldots, y^{p-1} - v\right\},$$

for which we can build an interpolating polynomial $m_v(z)$ of degree d based on the interpolating conditions $m_v(w^i) = f_v(w^i),\; i = 0, \ldots, p-1$. We then study the set W and derive estimates for the error between $f_v(z)$ and $m_v(z)$ and its corresponding first d derivatives. Finally, we define the interpolating polynomial for the set Y as $m(x) = m_v(x - v)$. It is straightforward to see that m interpolates f at the points in Y. The error estimates for m can be directly obtained from the corresponding error estimates obtained for m_v.

We now assume that the origin is *one of the interpolation points.* This assumption can always be satisfied by, again, shifting the set Y so that one of the interpolation points, say y^0, is located at the origin and then considering a closed ball $B(2\Delta)$. Clearly, the new shifted set $\{0, y^1 - y^0, \ldots, y^{p-1} - y^0\} \subseteq B(2\Delta)$. The fact that the radius of the ball is doubled does not affect the nature of the results in this paper. However, it will affect some constants by multiplying them by 2, 4, or 8, depending on whether the bound is of the order of Δ, Δ^2, or Δ^3, hence this assumption cannot be made, strictly speaking, without loss of generality. In practice, when polynomial interpolation is used within a trust-region optimization framework [3], [4], the center of the ball is naturally set to be the point with the best function value found so far, which is always included in the interpolation set. Hence in the applications that are of interest to us this assumption always holds.

1.2. Basic facts and notation. Here we introduce some further notation and also state some facts from linear algebra that will be used in the paper.

By $\|\cdot\|_k$, with $k \geq 1$, we denote the standard ℓ_k vector norm or the corresponding matrix norm. By $\|\cdot\|$ (without the subscript) we denote the ℓ_2 norm. We use $B(\Delta) = \{x \in \mathbb{R}^m : \|x\| \leq \Delta\}$ to denote the closed ball in $\mathbb{R}^m$ of radius $\Delta > 0$ centered at the origin (where m is inferred from the particular context). We use several properties of norms. In particular, given a $m \times n$ matrix A, we use the facts

$$\|A\|_2 \leq m^{\frac{1}{2}} \|A\|_\infty, \quad \|A\|_2 \leq \|A\|_F = (\operatorname{tr}(A^\top A))^{\frac{1}{2}}, \quad \|A\|_2 = \|A^\top\|_2.$$

We will use the standard "big-O" notation written as $\mathcal{O}(\cdot)$ to say, for instance, that if for two scalar or vector functions $\beta(x)$ and $\alpha(x)$ one has $\beta(x) = \mathcal{O}(\alpha(x))$ then there exists a constant $C > 0$ such that $\|\beta(x)\| \leq C\|\alpha(x)\|$ for all x in its domain.

We state here a useful lemma whose importance will be evident shortly.

Lemma 1.1. *Let $\mathcal{P}$ be the space of all polynomials in $\mathbb{R}$ of degree at most d (for some fixed $d > 0$). Let Φ be a collection of mappings $\phi(x)$ from $\mathbb{R}^n$ to $\mathbb{R}^p$ such that $\phi(x) = [\phi_0(x), \phi_1(x) \ldots, \phi_{p-1}(x)]^\top$, where $\{\phi_i(x),\ i = 0, \ldots, p-1\}$ are polynomials that form a basis in $\mathcal{P}$. Then if for some given set $Y = \{0, y^1, \ldots, y^{p-1}\} \subset \mathbb{R}^n$, for some given $x \in \mathbb{R}^n$, $\lambda \in \mathbb{R}^{p-1}$, and for some $\bar{\phi}(\cdot) \in \Phi$ it holds that*

$$\sum_{1 \leq i \leq p-1} \lambda_i (\bar{\phi}(y^i) - \bar{\phi}(0)) \ = \ \bar{\phi}(x) - \bar{\phi}(0),$$

then the same holds for any $\phi(\cdot) \in \Phi$, i.e.,

$$\sum_{1 \leq i \leq p-1} \lambda_i (\phi(y^i) - \phi(0) \ = \ \phi(x) - \phi(0),$$

for the same Y, x, and λ.

Proof: Trivial after applying a basis transformation. ■

2. Well-poisedness and error estimates in the linear case

Let us assume that we have $p = n + 1$ interpolation points $\{0, y^1, \ldots, y^n\}$ in a (closed) ball $B(\Delta)$ of radius $\Delta > 0$ centered at 0. We will assume that f is continuously differentiable in an open domain Ω containing this ball and that ∇f is Lipschitz continuous on Ω with constant $\gamma_L > 0$.

Given these $p = n + 1$ points we can aim to build the fully linear interpolation model, written in the form

$$m(x) \ = \ c + g^\top x \ = \ c + \sum_{1 \le k \le n} g_k x_k. \tag{2}$$

The unknown coefficients c, $g_1, \ldots, g_n$ are defined by the linear system arising from the interpolating conditions (1). The coefficient matrix of this linear system is

$$M_L = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 1 & y^1_1 & \cdots & y^1_n \\ \vdots & \vdots & \vdots & \vdots \\ 1 & y^n_1 & \cdots & y^n_n \end{bmatrix}. \tag{3}$$

If this matrix is nonsingular then the set of points $Y = \{0, y^1, \ldots, y^n\}$ is said to be poised, and the polynomial coefficients are well defined. Otherwise we say that the set Y is non-poised. In practice it is desirable for the set Y to be sufficiently well poised in the sense that it is not close to a non-poised set. Hence we need additional conditions on Y.

It is natural to base such conditions on, say, an upper bound on the condition number of M_L. However, rewriting the interpolating conditions (1) as a linear system to determine the coefficients of the interpolating polynomial can be done in various ways, depending on the choice of the basis in the space of linear polynomials. Such bases generate different matrices M and hence the same set of interpolation points can produce different condition numbers for M.

In particular, if the elements in $\phi(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_n(x)]^\top$ form a basis of linear polynomials in $\mathbb{R}$ then the interpolating polynomial can be written as

$$m(x) \ = \sum_{0 \le k \le n} \alpha_k \phi_k(x).$$

Then the interpolation conditions (1) produce a linear system of equations with the matrix

$$M_{\phi(x)} = \begin{bmatrix} \phi_0(0) & \phi_1(0) & \cdots & \phi_n(0) \\ \phi_0(y^1) & \phi_1(y^1) & \cdots & \phi_n(y^1) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_0(y^n) & \phi_1(y^n) & \cdots & \phi_n(y^n) \end{bmatrix}. \tag{4}$$

It is easy to show that if M_L is nonsingular, then $M_{\phi(x)}$ is also nonsingular for any basis $\phi(x)$. Hence, the definition of poisedness is independent of the choice of the basis $\phi(x)$. On the other hand, the condition number of $M_{\phi(x)}$ for the same interpolation set Y can range anywhere from 1 to infinity for particular choices of $\phi(x)$. Hence such a measure of well-poisedness is not only basis dependent but can also be misleading. In the next subsection we will introduce a well-poisedness condition which is independent of the choice of the basis.

One measure of well-poisedness, which was introduced earlier, is the maximum absolute value of Lagrange polynomials on $B(\Delta)$ containing Y (see, e.g., [7], [11] and references therein). Lagrange polynomials are uniquely defined for any poised set Y by their property that $M_{\phi(x)} = I$, where $M_{\phi(x)}$ is defined by (4). An upper bound on the absolute value of Lagrange polynomials does not appear intuitive as a measure of the geometry of Y. The definition of well-poisedness that we propose turns out to be basically equivalent to the boundedness of the Lagrange polynomials, but provides better geometric intuition.

We note here that the discussion above applies equally to the case of quadratic polynomials, cubic polynomials, etc.. Thus, we will not repeat it when introducing the well-poisedness conditions for polynomials of degree higher than one.

2.1. Well-poisedness in the linear case. We begin with our definition of well-poisedness, called Λ_L–poisedness.

Definition 2.1. *Let $\Delta > 0$ and $\Lambda_L > 0$ be given. Let $\phi(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_n(x)]^\top$ be a mapping from $\mathbb{R}^n$ to $\mathbb{R}^{n+1}$ whose elements form a basis of linear polynomials in $\mathbb{R}$.*

A set $Y = \{0, y^1, \ldots, y^n\} \subset B(\Delta)$ is said to be Λ_L–poised in $B(\Delta)$ if and only if for any $x \in B(\Delta)$:

$$\sum_{1\le i\le n} \lambda_i(\phi(y^i) - \phi(0)) \;=\; \phi(x) - \phi(0) \quad \textit{with} \quad \|\lambda\| \le \Lambda_L.$$

In the case of linear interpolation, the definition of Λ_L–poisedness is independent of the scaling, in the sense that if Y is Λ_L–poised in a ball $B(\Delta)$ then for any constant $\kappa > 0$ the set $\kappa Y = \{0, \kappa y^1, \ldots, \kappa y^n\}$ is also Λ_L–poised in the ball $B(\kappa\Delta)$. As we will see, this no longer holds when we consider polynomial interpolations of degrees higher than 1.

From Lemma 1.1 it is clear that this definition is *independent* of the choice of the basis $\phi(x)$. We can rewrite the Λ_L–poisedness definition for the particular choice $\phi(x) = [1, x_1, \ldots, x_n]^\top$, hence the definition simplifies to

$$\sum_{1\le i\le n} \lambda_i y^i \;=\; x \quad \text{with} \quad \|\lambda\| \le \Lambda_L. \tag{5}$$

The concept of Λ_L–poisedness, if viewed from a geometric perspective, is basically saying that the points in Y cannot lie too close to a subspace of dimension less than n (or, equivalently, that the points in Y form a sufficiently "fat" simplex), and to fit Y in such a subspace we would have to move at least one of the points by a distance proportional to Δ/Λ_L. See Section 6.2 for a description of the optimal geometries corresponding to the smallest possible values for Λ_L.

We would like to point out now that we do not abandon the condition number of M_L as an important measure related to well-poisedness. In particular this measure plays a crucial role in constructing the Taylor-like bound for the error in the function and derivative approximations. We will show that our definition of Λ-poisedness implies a bound on the condition number of M_L which in turn implies the Taylor-like error bounds. This is addressed in the next subsection.

2.2. Error estimates in the linear case. Now, we consider a point x in the ball $B(\Delta)$ centered at 0, for which there is some error in the function value,

$$m(x) \;=\; f(x) + e^f(x), \tag{6}$$

and in its gradient

$$g \;=\; \nabla f(x) + e^g(x).$$

The error in the gradient has n components:

$$\begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} = \begin{bmatrix} \frac{\delta f}{\delta x_1}(x) \\ \vdots \\ \frac{\delta f}{\delta x_n}(x) \end{bmatrix} + \begin{bmatrix} e_1^g(x) \\ \vdots \\ e_n^g(x) \end{bmatrix}. \tag{7}$$

Subtracting (6) from each of the $n+1$ equalities in (1) using (2) yields

$$\begin{aligned} (-x)^\top g &= f(0) - f(x) - e^f(x), \\ (y^i - x)^\top g &= f(y^i) - f(x) - e^f(x), \quad i = 1, \ldots, n. \end{aligned}$$

Expanding f by a Taylor's formula of order one around x for all the interpolation points and using the notation for the error in the gradient given by (7), we obtain

$$\begin{aligned} &(-x)^\top e^g(x) \\ &= \int_0^1 (\nabla f(x - tx) - \nabla f(x))^\top (-x) dt - e^f(x) \\ &= \mathcal{O}(\Delta^2) - e^f(x), \end{aligned} \tag{8}$$

$$\begin{aligned} &(y^i - x)^\top e^g(x) \\ &= \int_0^1 \left(\nabla f(x + t(y^i - x)) - \nabla f(x)\right)^\top (y^i - x) dt - e^f(x) \\ &= \mathcal{O}(\Delta^2) - e^f(x), \quad i = 1, \ldots, n, \end{aligned} \tag{9}$$

Now we subtract the first equation from the rest, canceling $e^f(x)$ and obtaining

$$(y^i)^\top e^g(x) \; = \; \mathcal{O}(\Delta^2), \quad 1 \le i \le n,$$

or, using matrix notation,

$$L_{n\times n}\, e^g(x) \; = \; \mathcal{O}(\Delta^2), \tag{10}$$

where

$$L_{n\times n} \; = \; \begin{bmatrix} (y^1)^\top \\ \vdots \\ (y^n)^\top \end{bmatrix} \; = \; \begin{bmatrix} y_1^1 & \cdots & y_n^1 \\ \vdots & \vdots & \vdots \\ y_1^n & \cdots & y_n^n \end{bmatrix}.$$

Note that the coefficient matrix in this linear system does not depend on the point x. Notice also that the matrix $L_{n\times n}$ is obtained from the matrix M_L given in (3) by subtracting the first row from the other n rows. The matrix in positions $(2 : n+1 \times 2 : n+1)$ is exactly $L_{n\times n}$.

Before we proceed with analyzing properties of $L_{n\times n}$, let us estimate an upper bound on the right hand side vector in (10). Each element of this vector is the difference of two quantities of the form $\int_0^1(\nabla f(x+t(y^i-x)) - \nabla f(x))^\top(y^i-x)dt$ and $\int_0^1(\nabla f(x-tx)) - \nabla f(x))^\top(-x)dt$. Because $x \in B(\Delta)$ and $y^i \in B(\Delta)$, these quantities can be bounded above by $2\gamma_L\Delta^2$ and $\gamma_L\Delta^2/2$, respectively, where γ_L is the Lipschitz constant of ∇f in Ω (see [5, Lemma 4.1.12]). Hence the ℓ_∞ norm of the right hand side can be bounded by $(5/2)\gamma_L\Delta^2$, and the bound on the ℓ_2 norm is

$$\|L_{n\times n}\, e^g(x)\| \;\leq\; \frac{5}{2}n^{1/2}\gamma_L\Delta^2. \tag{11}$$

We will use this bound in the proof of the error estimate.

We will further assume in the following lemma that the radius of the ball is one ($\Delta = 1$). We will return to the generalization afterwards. This lemma, which plays an important role in our analysis, introduces a connection between Λ_L–poisedness and the bound on the norm of the inverse of $L_{n\times n}$ (and, hence, the bound on its condition number, since it can be easily seen that $\|L_{n\times n}\|$ is bounded by $\sqrt{n}$ when $\Delta = 1$).

Lemma 2.2. *The set Y is Λ_L–poised in the unit ball $B(1)$ centered at 0 if and only if*

$$\|L_{n\times n}^{-1}\| \;\leq\; \Lambda.$$

Proof: The proof relies on the fact that the matrix that appears in the left-hand side of the definition (5) of Λ_L–poisedness is exactly the matrix $L_{n\times n}^\top$.

Let us assume first that Y is Λ_L–poised in the unit ball. Recall that

$$\|L_{n\times n}^{-\top}\| \;=\; \max_{x\in B(1)} \|L_{n\times n}^{-\top}x\|$$

and let $\hat{x} \in B(1)$ be a maximizer of $\|L_{n\times n}^{-\top}x\|$ in $B(1)$. Then, we have from the definition of Λ_L–poisedness that there exists a $\hat{\lambda}$ satisfying

$$\|L_{n\times n}^{-\top}\| \;=\; \|L_{n\times n}^{-\top}\hat{x}\| = \|\hat{\lambda}\| \;\leq\; \Lambda_L.$$

The reverse implication is proved similarly. ■

This lemma shows that Λ_L–poisedness implies poisedness (since the nonsingularity of M_L is a consequence of the nonsingularity of $L_{n\times n}$).

We would like to relax the assumption that $\Delta = 1$ to allow regions of any radius $\Delta > 0$.

Lemma 2.3. *The set Y is Λ_L–poised in the ball $B(\Delta)$ centered at 0 if and only if*

$$\|L_{n\times n}^{-1}\| \;\le\; \frac{\Lambda}{\Delta}.$$

Proof: If we have a Λ_L–poised set Y in a ball of radius Δ, then, we can scale the points in the set by $\frac{1}{\Delta}$ and apply Lemma 2.2 to the scaled set. If $L_{n\times n}$ is the matrix corresponding to Y, then $L_{n\times n}D_\Delta^{-1}$, where D_Δ is the diagonal matrix with Δ on the diagonal, is the matrix corresponding to the scaled set. Then from applying Lemma 2.2 to $L_{n\times n}D_\Delta^{-1}$ it follows that $\|L_{n\times n}^{-1}\| \le \Lambda_L/\Delta$. ■

Finally, we address the bounds on the approximation errors for linear interpolation. The following theorem establishes error estimates involving constants that depend on the constant $\Lambda_L > 0$ of Λ_L–poisedness: the smaller Λ_L is the better the error estimates are. The error bound between the function and the fully linear interpolating polynomial is of the order of Δ^2 in the case of function values and of the order of Δ in the case of gradient values.

Theorem 2.4. *Let $Y = \{0, y^1, \ldots, y^n\}$ be a Λ_L–poised set of interpolation points contained in a (closed) ball $B(\Delta)$ centered at 0. Assume that f is continuously differentiable in an open domain Ω containing $B(\Delta)$ and that ∇f is Lipschitz continuous in Ω with constant $\gamma_L > 0$.*

Then, for all points x in $B(\Delta)$, we have that

- *the error between the gradient of the fully linear interpolation model and the gradient of the function satisfies*
$$\|e^g(x)\| \;\le\; (5n^{\frac{1}{2}}\gamma_L\Lambda_L/2)\,\Delta, \tag{12}$$
- *the error between the fully linear interpolation model and the function satisfies*
$$|e^f(x)| \;\le\; (5n^{\frac{1}{2}}\gamma_L\Lambda_L/2 + \gamma_L/2)\,\Delta^2.$$

Proof: From Λ_L–poisedness of $Y \subset B(\Delta)$ we have $\|L_{n\times n}^{-1}\| \le \Lambda/\Delta$ and hence, from (11), we have that

$$\|e^g(x)\| \;\le\; \|L_{n\times n}^{-1}\|(5/2)n^{\frac{1}{2}}\gamma_L\Delta^2 \;\le\; \Lambda_L(5/2)n^{\frac{1}{2}}\gamma_L\Delta,$$

From this and the detailed (8), we obtain

$$|e^f(x)| \;\le\; (5n^{\frac{1}{2}}\gamma_L\Lambda_L/2 + \gamma_L/2)\Delta^2.$$

■

2.3. Extensions. One might find it surprising that our bound on e^f does not vanish if x is replaced by one of the interpolation points. This is due to the fact that the bound on the function error is dependent upon the bound on the derivative error, which does not necessarily vanish at the interpolation points. Our goal was to derive general bounds that hold at any point in $B(\Delta)$. However, if we use (9) together with the derivative bound (12), we can derive an error bound for e^f of the form $\mathcal{O}(\Delta\|y^i - x\|)$, for all i, which converges to zero linearly when x converges to y^i.

Our derivation for the bounds in Theorem 2.4 is based on the linear system (10). It is possible that an alternative derivation of the error estimates may produce a different matrix L for which $\|L^{-1}\|$ is smaller. An obvious example of this can be generated by subtracting equations (8)-(9) in pairs (instead of subtracting the first equation from the other $p-1=n$ of them) and then selecting n of the resulting equalities which produce the best conditioned matrix L. One could also work with all of these $q=(p-1)p/2=n(n+1)/2$ equalities, replacing (10) by

$$L_{q\times n}e^g(x) \;=\; \mathcal{O}(\Delta^2).$$

Using the SVD decomposition of $L_{q\times n}$ and following a derivation similar to the one of the proof of Theorem 2.4, we would obtain

$$\|e^g(x)\| \;\leq\; (4q^{\frac{1}{2}}\gamma_L\Upsilon_L)\,\Delta, \tag{13}$$

where Υ_L is an upper bound on the inverse of the smallest nonzero singular value of $L_{q\times n}$. Although $\Upsilon_L=\sigma_{\min}(L_{q\times n})^{-1}<\Lambda_L=\|L_{n\times n}^{-1}\|$ (see Section 6.2) we have that $q>n$ and it is unclear which error bound, (12) or (13), is preferable. We choose to work with $L_{n\times n}$ and (10) not only because of its simplicity and its easy generalization to interpolations of higher degree, but also because of its practical implications in terms of deriving algorithms that are capable of improving the geometry of the interpolation set (see Section 6).

3. Well-poisedness and error estimates in the quadratic case

In the fully quadratic case we must assume that we have $p=(n+1)(n+2)/2$ interpolation points in a (closed) ball $B(\Delta)$ of radius $\Delta>0$. In addition we will assume that f is twice continuously differentiable in an open domain Ω

containing this ball and that $\nabla^2 f$ is Lipschitz continuous in Ω with constant $\gamma_Q > 0$.

Given these p points, if they are poised (defined below), it is possible to build the fully quadratic interpolation model with $p = (n+1)(n+2)/2$. We will write the model in the form

$$m(x) \;=\; c + g^\top x + \frac{1}{2} x^\top H x \;=\; c + \sum_{1 \le k \le n} g_k x_k + \frac{1}{2} \sum_{1 \le k, \ell \le n} h_{k\ell} x_k x_\ell, \qquad (14)$$

where H is a symmetric matrix of order n. The unknown coefficients c, $g_1, \ldots, g_n$, and $h_{k\ell}, 1 \le \ell \le k \le n$, are defined by the interpolating conditions (1). If the coefficient matrix in this linear system,

$$M_Q \;=\; \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 1 & y_1^1 & \cdots & y_n^1 & \frac{1}{2}(y_1^1)^2 & y_1^1 y_2^1 & \cdots & \frac{1}{2}(y_n^1)^2 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ 1 & y_1^{p-1} & \cdots & y_n^{p-1} & \frac{1}{2}(y_1^{p-1})^2 & y_1^{p-1} y_2^{p-1} & \cdots & \frac{1}{2}(y_n^{p-1})^2 \end{bmatrix}, \qquad (15)$$

is nonsingular then the polynomial coefficients are well defined (the set of points Y is poised). As in the linear case, any basis of quadratic polynomials $\phi(x)$ defines a matrix $M_{\phi(x)}$ which is nonsingular if and only if M_Q is nonsingular. However, the condition numbers of these matrices might be very different for the same interpolation set Y. Thus, as before, we would like a well-poisedness condition that does not depend on the choice of polynomial basis that defines $M_{\phi(x)}$. In the following subsection, we extend our definition of Λ_L–poisedness to the quadratic case. Then, as before, we will show how this condition implies the well-conditioning of M_Q defined in (15).

3.1. Well-poisedness in the quadratic case. The extension of the definition of Λ_L–poisedness to the quadratic case makes use of a mapping from $\mathbb{R}^n$ to $\mathbb{R}^p$ whose image elements form a basis of quadratic polynomials in $\mathbb{R}$.

Definition 3.1. *Let $\Delta > 0$ and $\Lambda_Q > 0$ be given. Let $\phi(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_{p-1}(x)]^\top$ be a mapping from $\mathbb{R}^n$ to $\mathbb{R}^p$ whose elements form a basis of quadratic polynomials in $\mathbb{R}$.*

A set $Y = \{0, y^1, \ldots, y^{p-1}\}$ is said to be Λ_Q–poised in $B(\Delta)$ if and only if for any $x \in B(\Delta)$:

$$\sum_{1 \le i \le p-1} \lambda_i (\phi(y^i) - \phi(0)) \;=\; \phi(x) - \phi(0) \quad \textit{with} \quad \|\lambda\| \le \Lambda_Q.$$

By Lemma 1.1 the above definition does not depend on the particular choice of the mapping $\phi(x)$. If we consider the particular choice

$$\phi(x) \;=\; [1, x_1, \ldots, x_n, x_1^2/2, \ldots, x_n^2/2, x_1x_2, \ldots, x_1x_n, \ldots, \ldots, x_{n-1}x_n]^\top,$$

and define $\bar{\phi}(x)$ as

$$\bar{\phi}(x) \;=\; [x_1, \ldots, x_n, x_1^2/2, \ldots, x_n^2/2, x_1x_2, \ldots, x_1x_n, \ldots, \ldots, x_{n-1}x_n]^\top, \quad (16)$$

then the definition simplifies to

$$\sum_{1 \le i \le p-1} \lambda_i \bar{\phi}(y^i) \;=\; \bar{\phi}(x) \quad \text{with} \quad \|\lambda\| \le \Lambda_Q. \quad (17)$$

Here we chose $\phi(x)$ generated by the basis of monomials because it naturally arises in the error estimates through the bound on the condition number of M_Q. As in the linear case, we will show that Λ_Q–poisedness implies a bound on the norm of the inverse (and hence on the condition number) of M_Q.

3.2. Error estimates in the quadratic case. Analogous to the linear case, we consider a point x in the ball $B(\Delta)$, for which we will try to estimate the error in the function value

$$m(x) \;=\; f(x) + e^f(x), \quad (18)$$

in the gradient

$$\nabla m(x) \;=\; Hx + g \;=\; \nabla f(x) + e^g(x), \quad (19)$$

and, in this quadratic case, also in the Hessian

$$H \;=\; \nabla^2 f(x) + E^H(x).$$

The error in the gradient has n components $e_k^g(x), k = 1, \ldots, n$, just as in the linear case. Since the Hessians of f and m are symmetric, we only need to consider the error in the second-order derivatives in the diagonal elements and in the elements below the diagonal

$$h_{k\ell} \;=\; \nabla^2_{k\ell} f(x) + E^H_{k\ell}(x), \quad 1 \le \ell \le k \le n.$$

Using (14) and subtracting (18) from all the p equalities in (1), we have that

$$\begin{aligned} -x^\top g + \frac{1}{2}x^\top Hx - x^\top Hx \;&=\; f(0) - f(x) - e^f(x), \\ (y^i - x)^\top g + \frac{1}{2}(y^i - x)^\top H(y^i - x) + (y^i - x)^\top Hx \end{aligned}$$

$$= f(y^i) - f(x) - e^f(x), \quad i = 1, \ldots, p-1.$$

Now we expand f by a Taylor's formula of order two around x for all the p interpolation points and use the notation for the error in the gradient given by (19), to get

$$\begin{aligned} -x^\top e^g(x) + \frac{1}{2}x^\top[H - \nabla^2 f(x)]x & \\ = \mathcal{O}(\Delta^3) - e^f(x), & \quad (20) \\ (y^i - x)^\top e^g(x) + \frac{1}{2}(y^i - x)^\top[H - \nabla^2 f(x)](y^i - x) & \\ = \mathcal{O}(\Delta^3) - e^f(x), \quad i = 1, \ldots, p-1. & \quad (21) \end{aligned}$$

The next step, as in the linear case, is to subtract the first of these equations from the other equations, canceling $e^f(x)$ and obtaining

$$(y^i)^\top(e^g(x) - E^H(x)x) + \frac{1}{2}(y^i)^\top[H - \nabla^2 f(x)](y^i) \;=\; \mathcal{O}(\Delta^3), \quad 1 \le i \le p-1.$$

The linear system that we need to analyze in this quadratic case can be written as

$$\sum_{1\le k\le n} y_k^i t_k(x) + \frac{1}{2}\sum_{1\le k\le n}(y_k^i)^2 E_{kk}^H(x) + \sum_{1\le \ell<k\le n}[y_k^i y_\ell^i]E_{k\ell}^H(x) \\ = \mathcal{O}(\Delta^3), \quad 1 \le i \le p-1,$$

or, in matrix form, as

$$Q_{p-1\times p-1}\begin{bmatrix} t(x) \\ e^H(x) \end{bmatrix} \;=\; \mathcal{O}(\Delta^3), \tag{22}$$

with

$$t(x) \;=\; e^g(x) - E^H(x)x \;=\; e^g(x) - [H - \nabla^2 f(x)]x. \tag{23}$$

Here $e^H(x)$ is a vector of dimension $n + n(n-1)/2$ storing the elements $E_{kk}^H(x)$, $k = 1, \ldots, n$ and $E_{k\ell}^H(x)$, $1 \le \ell < k \le n$.

Once again we remark that the matrix $Q_{p-1\times p-1}$ defining this linear system does not depend on the point x. When $n = 2$ (and $p = 6$) this matrix reduces to

$$Q_{5\times 5} = \begin{bmatrix} y_1^1 & y_2^1 & \frac{1}{2}(y_1^1)^2 & y_1^1 y_2^1 & \frac{1}{2}(y_2^1)^2 \\ y_1^2 & y_2^2 & \frac{1}{2}(y_1^2)^2 & y_1^2 y_2^2 & \frac{1}{2}(y_2^2)^2 \\ y_1^3 & y_2^3 & \frac{1}{2}(y_1^3)^2 & y_1^3 y_2^3 & \frac{1}{2}(y_2^3)^2 \\ y_1^4 & y_2^4 & \frac{1}{2}(y_1^4)^2 & y_1^4 y_2^4 & \frac{1}{2}(y_2^4)^2 \\ y_1^5 & y_2^5 & \frac{1}{2}(y_1^5)^2 & y_1^5 y_2^5 & \frac{1}{2}(y_2^5)^2 \end{bmatrix}.$$

Notice also that the matrix $Q_{p-1\times p-1}$ is obtained from the matrix M_Q by subtracting the first row from the other $p-1$ rows. The matrix in positions $(2:p\times 2:p)$ is exactly $Q_{p-1\times p-1}$.

Before we proceed further in the analysis of $Q_{p-1\times p-1}$, we will estimate an upper bound on the right hand side vector in (22). Each element of this vector is the difference of two terms that can be bounded by $\gamma_Q\|y^i - x\|^3/6$ and $\gamma_Q\|x\|^3/6$, respectively, where γ_Q is the Lipschitz constant of $\nabla^2 f$ in Ω (see [5, Lemma 4.1.14]). Since $\|y^i - x\| \le 2\Delta$ and $\|x\| \le \Delta$, the difference can be bounded by $3\Delta^3/2$. Hence the ℓ_∞ norm of the right hand side can be bounded by that, and a bound on the ℓ_2 norm is

$$\left\| Q_{p-1\times p-1} \begin{bmatrix} t(x) \\ e^H(x) \end{bmatrix} \right\| \le \frac{3}{2}(p-1)^{\frac{1}{2}}\gamma_Q\Delta^3. \tag{24}$$

We will use this bound in the proof of our error estimate.

The lemma below is an extension of Lemma 2.2 to the quadratic case. As before, we will temporarily assume that $\Delta = 1$.

Lemma 3.2. *If the set Y is Λ_Q–poised in the unit ball $B(1)$ centered at 0 then*

$$\|Q_{p-1\times p-1}^{-1}\| \le \theta_Q\Lambda_Q, \tag{25}$$

where $\theta_Q > 0$ is dependent on n and $d = 2$ but independent of Y and Λ_Q. Conversely, if $\|Q_{p-1\times p-1}^{-1}\| \le \Lambda_Q$ then the set Y is Λ_Q–poised in the unit ball $B(1)$ centered at 0.

Proof: The matrix $Q_{p-1\times p-1}^\top$ is exactly the same matrix that appears in the definition of Λ_Q–poisedness (17). Consequently, the second implication is immediate.

Let us prove the first implication. First let us show that the matrix $Q_{p-1\times p-1}^\top$ is nonsingular. Let us assume it is singular. By definition of Λ_Q–poisedness, for any $x \in B(1)$, $\bar\phi(x)$ lies in the range space of $Q_{p-1\times p-1}^\top$. This means that there exists a vector $v \neq 0$ in the image space of $\bar\phi$ such that for any $x \in B(1)$ we get $\bar{\phi}(x)^\top v = 0$. Hence, we have a quadratic polynomial in x which is identically zero on a unit ball, which implies that all coefficients of this polynomial are zero, i.e., $v = 0$. We arrived to a contradiction.

Now we want to show that there exists a constant $\theta_Q > 0$, independent of Y and Λ_Q, such that $\|Q_{p-1\times p-1}^{-\top}\| \leq \theta_Q \Lambda_Q$. From the definition of Λ_Q–poisedness we have that for any $x \in B(1)$, $\|Q_{p-1\times p-1}^{-\top}\bar{\phi}(x)\| \leq \Lambda_Q$. From the definition of the matrix norm

$$\|Q_{p-1\times p-1}^{-\top}\| \;=\; \max_{\|v\|=1} \|Q_{p-1\times p-1}^{-\top} v\|$$

and we can consider a vector $\bar{v}$ such that

$$\|Q_{p-1\times p-1}^{-\top}\| \;=\; \|Q_{p-1\times p-1}^{-\top}\bar{v}\|, \quad \|\bar{v}\| \;=\; 1. \tag{26}$$

Let us assume first that there exists an $x \in B(1)$ such that $\bar{\phi}(x) = \bar{v}$. Then from the fact that Y is Λ_Q-poised we have that

$$\|Q_{p-1\times p-1}^{-\top}\bar{v}\| \;=\; \|Q_{p-1\times p-1}^{-\top}\bar{\phi}(x)\| \;\leq\; \Lambda_Q,$$

and from (26) the statement of the lemma holds with $\theta_Q = 1$.

Notice that $\bar{v}$ does not necessarily belong to the image of $\bar{\phi}$, which means that there might be no $x \in B(1)$ such that $\bar{\phi}(x) = \bar{v}$, and hence we have that $\|Q_{p-1\times p-1}^{-\top}\bar{v}\| \neq \|Q_{p-1\times p-1}^{-\top}\bar{\phi}(x)\|$. However, we will show that there exists a constant $\theta_Q > 0$ independent of $\bar{v}$ such that for any $\bar{v}$ which satisfies (26) there exists an $y \in B(1)$, such that

$$\frac{\|Q_{p-1\times p-1}^{-\top}\bar{v}\|}{\|Q_{p-1\times p-1}^{-\top}\bar{\phi}(y)\|} \;\leq\; \theta_Q. \tag{27}$$

Once we have shown that such constant θ_Q exists the result of the lemma follows trivially from the definition of $\bar{v}$.

To show that (27) holds, we first show that there exists $\sigma_Q > 0$ such that for any $\bar{v}$ with $\|\bar{v}\| = 1$, there exists an $y \in B(1)$ such that $|\bar{v}^\top \bar{\phi}(y)| \geq \sigma_Q$. Consider

$$\psi(v) \;=\; \max_{x \in B(1)} |v^\top \bar{\phi}(x)|.$$

It is easy to show that $\psi(v)$ is a norm in the space of vectors v. Since the ratio of any two norms in finite dimensional spaces can be uniformly bounded by a constant, there exists a (maximal) $\sigma_Q > 0$ such that $\psi(\bar{v}) \geq \sigma_Q \|\bar{v}\| = \sigma_Q$. Hence, there exists a $y \in B(1)$ such that $|\bar{v}^\top \bar{\phi}(y)| \geq \sigma_Q$.

Let $\bar{v}^\perp$ be the orthogonal projection of $\bar{\phi}(y)$ onto the subspace orthogonal to $\bar{v}$. Now, notice that from the definition (26) of $\bar{v}$ it follows that $\bar{v}$ is the right singular vector corresponding to the largest singular value of $Q_{p-1\times p-1}^{-\top}$. Then $Q_{p-1\times p-1}^{-\top}\bar{v}$ and $Q_{p-1\times p-1}^{-\top}\bar{v}^\perp$ are orthogonal vectors (since $Q_{p-1\times p-1}^{-\top}\bar{v}$ is a scaled left singular vector corresponding to largest singular value and $Q_{p-1\times p-1}^{-\top}\bar{v}^\perp$ is a vector spanned by the other left singular vectors). Hence $\|Q_{p-1\times p-1}^{-\top}\bar{\phi}(y)\| \geq |\bar{v}^\top\bar{\phi}(y)|\|Q_{p-1\times p-1}^{\top}\bar{v}\|$. It follows from $|\bar{v}^\top\bar{\phi}(y)| \geq \sigma_Q$ that

$$\|Q_{p-1\times p-1}^{-\top}\bar{\phi}(y)\| \;\geq\; \sigma_Q\|Q_{p-1\times p-1}^{-\top}\bar{v}\|,$$

Assigning $\theta_Q = 1/\sigma_Q$ shows (27), concluding the proof of the bound on the norm of $Q_{p-1\times p-1}^{-\top}$. This completes the proof since $\|Q_{p-1\times p-1}^{-1}\| = \|Q_{p-1\times p-1}^{-\top}\|$. ■

The constant θ_Q can be estimated using the following lemma.

Lemma 3.3. *Let $\hat{v}^\top\bar{\phi}(x)$ be a quadratic polynomial with $\bar{\phi}(x)$ given by (16) and $\|\hat{v}\|_\infty = 1$ and let $B(1)$ be a (closed) ball of radius 1 centered at the origin. Then*

$$\max_{x\in B(1)} |\hat{v}^\top\bar{\phi}(x)| \;\geq\; \frac{1}{2}.$$

Proof: Since $\|\hat{v}\|_\infty = 1$ then at least one of the elements of $\hat{v}$ is 1 or -1, and thus one of the coefficients of the polynomial $q(x) = \hat{v}^\top\bar{\phi}(x)$, is equal to 1, -1, $1/2$, or $-1/2$. Let us consider only the cases where one of the coefficients of $q(x)$ is 1 or $1/2$. The cases -1 or $-1/2$ would be analyzed similarly.

The largest coefficient in absolute value in $\hat{v}$ corresponds to a term which is either a linear term x_i or a quadratic term $x_i^2/2$ or x_ix_j. Let us restrict all variables that do not appear in this term to zero. And let us consider only the unrestricted variables. Clearly the maximum of the absolute value of $q(x)$ over the set of unrestricted variables is a lower bound on the maximum over $B(1)$. We can have three cases.

- $q(x) = x_i^2/2 + \alpha x_i$. It is easy to see that

$$\max_{x_i\in[-1,1]} |q(x)| \;=\; \max\{q(1), q(-1)\} \;\geq\; \frac{1}{2}.$$

- $q(x) = \alpha x_i^2/2 + x_i$. In this case we have

$$\max_{x_i\in[-1,1]} |q(x)| \;\geq\; \max\{|q(1)|, |q(-1)|\} \;\geq\; 1.$$

- $q(x) = \alpha x_i^2/2 + \beta x_j^2/2 + x_i x_j + \gamma x_i + \delta x_j$. This time we are considering the quadratic function over a two dimensional ball. By considering four points, $p_1 = (1/\sqrt{2}, 1/\sqrt{2})$, $p_2 = (1/\sqrt{2}, -1/\sqrt{2})$, $p_3 = (-1/\sqrt{2}, 1/\sqrt{2})$ and $p_4 = (-1/\sqrt{2}, -1/\sqrt{2})$, on the boundary of the ball, and looking at all the possible signs of $\alpha + \beta$, $\gamma + \delta$, and $\gamma - \delta$, we get

$$\max\{|q(p_i)|,\ i = 1, 2, 3, 4\} \ \geq \ \frac{1}{2}.$$

■

We can replace the constant θ_Q of Lemma 3.2 by an upper bound, which is easily derived for the quadratic case. Recall that $\theta_Q = 1/\sigma_Q$, where

$$\sigma_Q \ = \ \min_{\|\bar{v}\|=1} \max_{x \in B(1)} |\bar{v}^\top \bar{\phi}(x)|.$$

Given any $\bar{v}$ such that $\|\bar{v}\| = 1$, we can scale $\bar{v}$ by at most $\sqrt{p-1}$ to $\hat{v} = \alpha \bar{v}$, $0 < \alpha \leq \sqrt{p-1}$, such that $\|\hat{v}\|_\infty = 1$. Then

$$\sigma_Q \ = \ \min_{\|\bar{v}\|=1} \max_{x \in B(1)} |\bar{v}^\top \bar{\phi}(x)| \ \geq \ \frac{1}{\sqrt{p-1}} \min_{\|\hat{v}\|_\infty=1} \max_{x \in B(1)} |\hat{v}^\top \bar{\phi}(x)| \ \geq \ \frac{1}{2\sqrt{p-1}}.$$

The last inequality is due to Lemma 3.3 applied to the polynomials of the form $\hat{v}^\top \bar{\phi}(x)$. Hence we have

$$\theta_Q \ \leq \ 2(p-1)^{\frac{1}{2}}. \tag{28}$$

We did not include this argument in the proof of Lemma 3.2 and chose to stay with the argument that σ_Q is the unspecified constant connecting two norms because this latter argument extends easier to the case of polynomials of higher degree and it also provides better intuition for the existence of the constant θ_Q. Specifying the bound on θ_Q for polynomials of higher degree is also possible, but is beyond the scope of this paper.

Remark 3.1. *It is important to note that θ_Q depends on the choice of $\bar{\phi}(\cdot)$. For example, if we scale every element of $\bar{\phi}(\cdot)$ by 2 then the appropriate θ_Q will decrease by 2. Here we are interested in the condition number of a specific matrix $Q_{p-1 \times p-1}$ arising in the error estimates and, hence, in a specific choice of $\bar{\phi}(\cdot)$.*

As in the linear case, we can also say in the quadratic case that Λ_Q–poisedness implies poisedness. In fact, we have just shown that Λ_Q–poisedness implies that $Q_{p-1\times p-1}$ is nonsingular, which in turn implies, as we have already pointed out, that M_Q in (15) is nonsingular.

The next theorem generalizes the error estimates obtained in Theorem 2.4 for the linear case to the quadratic case. The error estimates in the quadratic case are linear in Δ for the second derivatives, quadratic in Δ for the first derivatives, and cubic in Δ for the function values, where Δ is the radius of the ball containing Y.

Theorem 3.4. *Let $Y = \{0, y^1, \ldots, y^{p-1}\}$, with $p = (n+1)(n+2)/2$, be a Λ_Q–poised set of interpolation points contained in a (closed) ball $B(\Delta)$ centered at 0. Assume that f is twice continuously differentiable in an open domain Ω containing $B(\Delta)$ and that $\nabla^2 f$ is Lipschitz continuous in Ω with constant $\gamma_Q > 0$.*

Then, for all points x in $B(\Delta)$, we have that

- *the error between the Hessian of the fully quadratic interpolation model and the Hessian of the function satisfies*

$$\|E^H(x)\| \;\leq\; (\alpha_Q^H (p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q)\, \Delta,$$

- *the error between the gradient of the fully quadratic interpolation model and the gradient of the function satisfies*

$$\|e^g(x)\| \;\leq\; (\alpha_Q^g (p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q)\, \Delta^2,$$

- *the error between the fully quadratic interpolation model and the function satisfies*

$$|e^f(x)| \;\leq\; (\alpha_Q^f (p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q + \beta_Q^f \gamma_Q)\, \Delta^3,$$

where α_Q^H, α_Q^g, α_Q^f, and β_Q^f are small positive constants dependent on $d = 2$ and independent of n, Y, and Λ_Q:

$$\alpha_Q^H = \frac{3\sqrt{2}}{2}, \quad \alpha_Q^g = \frac{3(1+\sqrt{2})}{2}, \quad \alpha_Q^f = \frac{6+9\sqrt{2}}{4}, \quad \beta_Q^f = \frac{1}{6}.$$

Proof: Let us first write the matrix of the system (22) in the form

$$Q_{p-1\times p-1} \begin{bmatrix} D_\Delta^{-1} & 0 \\ 0 & D_{\Delta^2}^{-1} \end{bmatrix} \begin{bmatrix} D_\Delta t(x) \\ D_{\Delta^2} e^H(x) \end{bmatrix},$$

where D_Δ is a diagonal matrix of dimension n with Δ in the diagonal entries and D_{Δ^2} is a diagonal matrix of dimension $p-1-n$ with Δ^2 in the diagonal entries. Then using the bound (24) we obtain

$$\left\| \begin{bmatrix} D_\Delta t(x) \\ D_{\Delta^2} e^H(x) \end{bmatrix} \right\| \;\leq\; \frac{3}{2}(p-1)^{\frac{1}{2}} \gamma_Q \left\| \left(Q_{p-1\times p-1} \begin{bmatrix} D_\Delta^{-1} & 0 \\ 0 & D_{\Delta^2}^{-1} \end{bmatrix} \right)^{-1} \right\| \Delta^3.$$

The matrix in the right hand side of this inequality corresponds to a scaled set of interpolation points in $B(1)$. Thus, from (25), we get

$$\left\| \begin{bmatrix} D_\Delta t(x) \\ D_{\Delta^2} e^H(x) \end{bmatrix} \right\| \;\leq\; \frac{3}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^3. \tag{29}$$

Inequality (29) gives us

$$\|D_{\Delta^2} e^H(x)\| \;\leq\; \frac{3}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^3,$$

yielding the bound $\|e^H(x)\| \leq (3/2)(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta$. The error in the Hessian is therefore given by

$$\|E^H(x)\| \;\leq\; \|E^H(x)\|_F \;\leq\; \sqrt{2}\|e^H(x)\| \;\leq\; \frac{3\sqrt{2}}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta.$$

Now, we would like to derive the bound on $\|e^g(x)\|$. From (29) we also have

$$\|D_\Delta t(x)\| \;\leq\; \frac{3}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^3,$$

and

$$\|t(x)\| \;\leq\; \frac{3}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^2,$$

and therefore, from (23),

$$\begin{aligned} \|e^g(x)\| \;&\leq\; \|t(x)\| + \|E^H(x)\|\|x\| \\ &\leq\; \tfrac{3}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^2 + (\tfrac{3\sqrt{2}}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta)\Delta \\ &=\; \tfrac{3(1+\sqrt{2})}{2}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^2. \end{aligned}$$

Here we have used the fact that x is in the ball $B(\Delta)$ centered at the origin.

Finally, from the detailed version of (20) and the bounds on $\|e^g(x)\|$ and $\|E^H(x)\|$ we have

$$\begin{aligned} |e^f(x)| \;&\leq\; \|e^g(x)\|\Delta + \|E^H(x)\|\Delta^2/2 + \gamma_Q \Delta^3/6 \\ &\leq\; \tfrac{6+9\sqrt{2}}{4}(p-1)^{\frac{1}{2}} \theta_Q \gamma_Q \Lambda_Q \Delta^3 + \tfrac{\gamma_Q}{6}\Delta^3. \end{aligned}$$

■

The remarks made in Section 2.3 for the linear case about alternative derivations of the error bounds are also pertinent in the quadratic case.

4. Extension to higher degree

The error estimates and the definition of Λ–poisedness extend naturally to interpolation polynomials of higher degree than quadratics. We will briefly sketch here the cubic case.

The procedure to derive the error estimates in the cubic case goes one step further than the quadratic case but the arguments used are the same. After subtracting the equation $m(x) - f(x) = e^f(x)$ on the error in the function from all the p interpolating conditions (1) and expanding f by a Taylor's formula of order three around $x \in B(\Delta)$, we get the following analog of (20)–(21):

$$\begin{aligned}
&\sum_{1\le k\le n} -e^g_k(x)x_k + \frac{1}{2}\sum_{1\le k,\ell\le n} E^H_{k\ell}(x)x_kx_\ell \\
&- \frac{1}{6}\sum_{1\le k,\ell,m\le n} E^c_{k\ell m}(x)x_kx_\ell x_m \;=\; \mathcal{O}(\Delta^4) - e^f(x), \\
&\sum_{1\le k\le n} e^g_k(x)(y^i_k - x_k) + \frac{1}{2}\sum_{1\le k,\ell\le n} E^H_{k\ell}(x)(y^i_k - x_k)(y^i_\ell - x_\ell) \\
&+ \frac{1}{6}\sum_{1\le k,\ell,m\le n} E^c_{k\ell m}(x)(y^i_k - x_k)(y^i_\ell - x_\ell)(y^i_m - x_m) \;=\; \mathcal{O}(\Delta^4) - e^f(x),
\end{aligned}$$

for $i = 1,\ldots,p-1$, where p is the number of points in the interpolation set $Y = \{0, y^1, \ldots, y^{p-1}\}$, to be defined later. Here we have $E^c_{k\ell m}(x) = C_{k\ell m} - \frac{\delta^3 f}{\delta x_k \delta x_\ell \delta x_m}(x)$, where $C_{k\ell m}$ is the corresponding coefficient of the cubic interpolating polynomial. Subtracting the first of these equations from the others, yields

$$\begin{aligned}
&\sum_{1\le k\le n} y^i_k \left(e^g_k(x) - \sum_{1\le \ell\le n} E^H_{k\ell}(x)x_\ell - \frac{1}{2}\sum_{1\le \ell,m\le n} E^c_{k\ell m}(x)x_\ell x_m \right) \\
&+ \frac{1}{2}\sum_{1\le k,\ell\le n} y^i_k y^i_\ell \left(E^H_{k\ell}(x) - \sum_{1\le m\le n} E^c_{k\ell m}(x)x_m \right) \\
&+ \frac{1}{6}\sum_{1\le k,\ell,m\le n} y^i_k y^i_\ell y^i_m E^c_{k\ell m}(x) \;=\; \mathcal{O}(\Delta^4), \quad i = 1,\ldots,p-1.
\end{aligned}$$

We denote the matrix of this linear system by $C_{p-1\times p-1}$.

As before the definition of Λ–poisedness involves the mapping $\phi(x)$ formed by the elements of a basis of the space of cubic polynomials. The number of elements in the basis is given by

$$p \;=\; \frac{1}{2}(n+1)(n+2) + n + (n^2 - n) + \frac{1}{6}n(n-1)(n-2). \qquad (30)$$

As usual we assume that the constant $\Lambda_C > 0$ is specified *a priori*.

Definition 4.1. *Let $\Delta > 0$ and $\Lambda_C > 0$ be given. Let $\phi(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_{p-1}(x)]^\top$ be a mapping from $\mathbb{R}^n$ to $\mathbb{R}^p$ whose elements form a basis of cubic polynomials in $\mathbb{R}$.*

A set $Y = \{0, y^1, \ldots, y^{p-1}\}$ is said to be Λ_C–poised in $B(\Delta)$ if and only if for any $x \in B(\Delta)$:

$$\sum_{1 \le i \le p-1} \lambda_i(\phi(y^i) - \phi(0)) \;=\; \phi(x) - \phi(0) \quad \textit{with} \quad \|\lambda\| \le \Lambda_C.$$

Again, from Lemma 1.1 it is clear that the above definition is independent of the choice of ϕ. We choose the basis formed by all the monomials of degree less than or equal to 3:

$$\phi(x) \;=\; [1, x_k, x_k^2/2, x_k x_\ell, x_k^3/6, x_k^2 x_\ell/2, x_k x_\ell x_m/6]^\top,$$

where the indices vary respectively as follows: $1 \le k \le n$, $1 \le k \le n$, $1 \le \ell < k \le n$, $1 \le k \le n$, $1 \le \ell \ne k \le n$, and $1 \le \ell < k < m \le n$. And, as before, our choice of ϕ here is dictated by its relevance to the matrix $C_{p-1\times p-1}$. We now state without proofs the two structural results of our analysis: the algebraic characterization of Λ_C–poisedness in terms of the inverse of the matrix $C_{p-1\times p-1}$ and the error bounds on the difference between the interpolating polynomial and the function being interpolated.

Lemma 4.2. *If the set Y is Λ_C–poised in the unit ball $B(1)$ centered at 0 then*

$$\|C_{p-1\times p-1}^{-1}\| \;\le\; \theta_C \Lambda_C,$$

where $\theta_C > 0$ is dependent on n and $d = 3$ but independent of Y and Λ_C. Conversely, if $\|C_{p-1\times p-1}^{-1}\| \le \Lambda_C$ then the set Y is Λ_C–poised in the unit ball $B(1)$ centered at 0.

In the cubic case the error estimates includes the error in the third derivatives. The result is stated for any $\Delta > 0$.

Theorem 4.3. *Let $Y = \{0, y^1, \ldots, y^{p-1}\}$, with p given by (30), be a Λ_C–poised set of interpolation points contained in a (closed) ball $B(\Delta)$ centered at 0. Assume that f is thrice continuously differentiable in an open domain Ω containing $B(\Delta)$ and that the vector of the third-order derivatives is Lipschitz continuous in Ω with constant $\gamma_C > 0$.*

Then, for all points x in $B(\Delta)$, we have that

- *the error between the vector of the third-order derivatives of the fully cubic interpolation model and the vector of the third-order derivatives of the function satisfies*

$$\|e^c(x)\| \;\le\; (\alpha_C^c (p-1)^{\frac{1}{2}} \theta_C \gamma_C \Lambda_C)\, \Delta,$$

- *the error between the Hessian of the fully cubic interpolation model and the Hessian of the function satisfies*

$$\|E^H(x)\| \;\le\; (\alpha_C^H (p-1)^{\frac{1}{2}} \theta_C \gamma_C \Lambda_C)\, \Delta^2,$$

- *the error between the gradient of the fully cubic interpolation model and the gradient of the function satisfies*

$$\|e^g(x)\| \;\le\; (\alpha_C^g (p-1)^{\frac{1}{2}} \theta_C \gamma_C \Lambda_C)\, \Delta^3,$$

- *the error between the fully cubic interpolation model and the function satisfies*

$$|e^f(x)| \;\le\; (\alpha_C^f (p-1)^{\frac{1}{2}} \theta_C \gamma_C \Lambda_C + \beta_C^f \gamma_C)\, \Delta^4,$$

where α_C^c, α_C^H, α_C^g, α_C^f, and β_C^f are small positive constants dependent on $d = 3$ and independent of n, Y, and Λ_C.

The extension to polynomial interpolation of degree higher than cubic would follow in a similar fashion.

5. Connection to other error estimates

Bounds on the error of approximation by polynomial interpolation have been derived in the literature for bases of Lagrange polynomials and bases of Newton polynomials.

5.1. Lagrange polynomials. Using a basis of Lagrange polynomials, Powell [7] derived the following bound for the error between the quadratic interpolating polynomial and the function being interpolated:

$$|e^f(x)| \;=\; |m(x) - f(x)| \;\leq\; \frac{1}{6} M \sum_{0 \leq j \leq p-1} |\mathcal{L}_j(x)| \|x - y^j\|^3, \tag{31}$$

where M is an upper bound on the size of the third-order derivatives. We point out that our approach uses instead a Lipschitz constant γ_Q for the Hessian of f, but this is a minor difference since in most instances the practical value for γ_Q is given by M.

The reader is also referred to Waldron [11] and the references therein for related material about Lagrange interpolation.

In order to compare our bound for $e^f(x)$ given in Theorem 3.4 to the bound (31), we show here that the definition of Λ-poisedness implies a bound on the elements of the bases of Lagrange polynomials. This result is valid for spaces of polynomials of any degree d. We start by giving the definition of Lagrange polynomials.

Definition 5.1. *Given a set of interpolation points $Y = \{0, y^1, \ldots, y^{p-1}\}$, a basis of p polynomials $\mathcal{L}_j(x)$, $j = 0, \ldots, p-1$, is called a basis of Lagrange polynomials if*

$$\mathcal{L}_j(y^i) \;=\; \delta_{ij} \;=\; \begin{cases} 1 & \text{if} \quad i = j, \\ 0 & \text{if} \quad i \neq j. \end{cases}$$

The constant Λ mentioned in the following result can be interpreted as Λ_L, Λ_Q or Λ_C.

Proposition 5.2. *Assume we are given $Y \subset B(\Delta)$ which is Λ-poised for some $\Lambda > 0$. Then the Lagrange polynomials $\mathcal{L}_j(x)$, $j = 0, \ldots, p-1$, for the set Y are bounded in $B(\Delta)$, namely*

$$\max_{x \in B(\Delta)} |\mathcal{L}_j(x)| \;\leq\; \Lambda, \quad j = 1, \ldots, p-1$$

and

$$\max_{x \in B(\Delta)} |\mathcal{L}_0(x)| \;\leq\; 1 + (p-1)\Lambda.$$

On the other hand, if the Lagrange polynomials $\mathcal{L}_j(x)$, $j = 0, \ldots, p-1$, for the set Y are bounded in absolute value in $B(\Delta)$ by Λ, then the set Y is $((p-1)^{1/2}\Lambda)$-poised.

Proof: The Lagrange polynomials $\{\mathcal{L}_j(x),\, j=0,\ldots,p-1\}$ form a basis in the space of polynomials (of appropriate degree). Then by Lemma 1.1 and from the Λ-poisedness of Y we have for any $x \in B(\Delta)$:

$$\mathcal{L}_j(x) = \mathcal{L}_j(0) + \sum_{1\le i\le p-1} \lambda_i(x)(\mathcal{L}_j(y^i) - \mathcal{L}_j(0)) \quad \text{with} \quad |\lambda_i(x)| \le \Lambda,$$

$i=0,\ldots,p-1$. From the fact that $\mathcal{L}_j(y^i) = \delta_{ij}$, it is easy to see that

$$\mathcal{L}_j(x) \;=\; \lambda_j(x), \quad j=1,\ldots,p-1 \tag{32}$$

and, therefore,

$$|\mathcal{L}_j(x)| \;\le\; \Lambda, \quad j=1,\ldots,p-1. \tag{33}$$

From $\mathcal{L}_0(0)=1$ and $\mathcal{L}_0(y^i)=0$ for $1\le i\le p-1$, we obtain

$$\mathcal{L}_0(x) \;=\; 1 - \sum_{1\le i\le p-1} \lambda_i(x),$$

which in turn implies

$$|\mathcal{L}_0(x)| \;\le\; 1 + (p-1)\Lambda.$$

The first part of proof is completed.

Conversely, if $|\mathcal{L}_j(x)| \le \Lambda$, $j=0,\ldots,p-1$, for all $x\in B(\Delta)$ then, from (32), $\|\lambda(x)\| \le (p-1)^{\frac{1}{2}}\Lambda$ for all $x \in B(\Delta)$. ■

Note that by setting x in (33) to y^j, we conclude that

$$\Lambda \;\ge\; 1.$$

By combining the error bound (31) for quadratic interpolation with the result given in Proposition 5.2, we get

$$|e^f(x)| \;\le\; \left(\frac{3}{2}(p-1)M\Lambda_Q + \frac{1}{6}M\right)\Delta^3.$$

This result is comparable to the error bound derived in this paper (see Theorem 3.4 for the error estimate and (28) for a bound on θ_Q):

$$|e^f(x)| \;\le\; \left(\bar{\alpha}_Q^f(p-1)\gamma_Q\Lambda_Q + \beta_Q^f\gamma_Q\right)\Delta^3,$$

where $\bar{\alpha}_Q^f = 3 + 4\sqrt{2}/2$ and $\beta_Q^f = 1/6$. The two bounds are the same in the main components, except for the constants. Our first constant, $\bar{\alpha}_Q^f$, is higher because of the influence of the derivative terms (see Section 2.3).

5.2. Newton polynomials. We briefly comment on the error estimate derived by Sauer and Xu [9] for function values using bases of Newton polynomials. This condition is of interest to us because it has been used in [3] to prove global convergence of a trust-region method based on polynomial interpolation. The analysis in [3] can now be simplified by using the results in this paper. A bound on Newton polynomials can be derived in a similar manner as was done for the Lagrange polynomials. However, the definition of Newton polynomials is significantly more technical than that of Lagrange polynomials and would not add substantial value to the paper. Consequently, we omit the analysis.

5.3. Estimating the error in the derivatives. Our approach provides a relatively straightforward analysis for the bounds on the approximation errors in the derivatives. These bounds are necessary for the proof of convergence of a trust-region interpolation-based optimization method. When using an approach like the one followed in [7] or [9], where the error estimate for function values is derived first, the error estimates for the derivatives would then have to be obtained *a posteriori*. Except for the linear case, there is no alternative simple derivation of the bounds on the error in the derivatives that is known to the authors (see [11] for possible general bounds). In the next paragraph we show why it is difficult to derive bounds on the error in the derivatives directly from the bound on the error in the function.

Let us see first how to derive a bound on $\|e^g(x)\|$ from a bound like $|e^f(x)| \leq c_L^f \Delta^2$, with $c_L^f > 0$, for linear interpolation. Simple manipulation using an expansion of f around $x \in B(\Delta)$ with increment h such that $x + h \in B(\Delta)$, lead us to

$$e^g(x)^\top h \;\leq\; 2c_L^f \Delta^2 + \frac{\gamma_L}{2}\|h\|^2,$$

where γ_L is the Lipschitz constant of ∇f. By setting $h = (\Delta/\|e^g(x)\|)e^g(x)$, we obtain

$$\|e^g(x)\| \;\leq\; \left(2c_L^f + \frac{\gamma_L}{2}\right)\Delta.$$

Now, let us see what is needed to derive bounds on $\|e^g(x)\|$ and $\|E^H(x)\|$ from a bound like $|e^f(x)| \leq c_Q^f \Delta^3$, with $c_Q^f > 0$, for quadratic interpolation. Once again, simple manipulation using an expansion of f around $x \in B(\Delta)$ with increment h such that $x + h \in B(\Delta)$, lead us to

$$e^g(x)^\top h + \frac{1}{2}h^\top E^H(x)h \;\leq\; 2c_Q^f \Delta^3 + \frac{\gamma_Q}{6}\|h\|^3,$$

where γ_Q is the Lipschitz constant of $\nabla^2 f$. To derive a bound on either $e^g(x)$ or $E^H(x)$ from this expression one needs to have the other unknown term bounded. In [3] it was assumed that the Hessians of the quadratic model and of the function are uniformly bounded and, hence, so is $E^H(x)$. This results in the bound $\|e^g(x)\| \leq \mathcal{O}(\Delta)$, which is clearly inferior to our bound and can only provide global convergence to first-order critical points.

6. Ensuring well-poisedness

6.1. Ensuring well-poisedness in the quadratic case. In a typical interpolation-based trust-region optimization method an interpolation set is maintained at each iteration. Based on this set an interpolation model is constructed. To guarantee the quality of the interpolation model, i.e., the appropriate error estimates in the function and in its derivatives, one needs to make sure that the poisedness of the interpolation set does not deteriorate arbitrarily from iteration to iteration. That can be guaranteed in at least two ways. One is to select a "good" interpolation set *a priori* and keep shifting and scaling at each iteration to place it inside the current region of interest. This is somehow related with the use of a finite number of positive bases in pattern search methods (see [2], [10]). An alternative method (used in [3], [4]) is to update the interpolation set by one or two interpolation points per iteration, while ensuring that it satisfies some sufficient well-poisedness condition. If such a condition is not satisfied then at least one "bad" point is replaced by a "good" point.

The algorithm that we describe in this section builds an interpolation set Y, or modifies an already existing one, using Gaussian elimination. The outcome of the algorithm is therefore a matrix $Q_{p-1\times p-1}$ (defining Y) and its LU factors. The Gaussian elimination is performed by rows. Thus, since the points in Y appear by rows in $Q_{p-1\times p-1}$, the algorithm computes a new point y^i — or modifies the already existing one — only when the i-th row is being factorized.

Our algorithm checks if the current set is well-poised, and if not, identifies "bad" points and replace them by "good" points. We will later explain how the criterion of the good geometry used by the algorithm relates to the Λ-poisedness condition.

We will present the algorithm for the case of quadratic interpolation. The extension to higher degree interpolations is straightforward. We describe the algorithm in the situation where the points lie in a ball of radius 1. If the radius is $\Delta \neq 1$ then one can simply scale Y by $1/\Delta$, apply the algorithm and then scale back the (possibly) new interpolation set.

Algorithm 6.1 (Ensuring well-poisedness — fully quadratic model).

Step 0: Let $\bar{\phi}(x)$ denote the mapping defined in (16). Choose some threshold ξ such that $0 < \xi < \frac{1}{2}$,

Step 1: Choose i^* such that $i^* = \operatorname{argmax}\{|\bar{\phi}_1(y^i)| : i = 1, \ldots, p-1\}$. If $|\bar{\phi}_1(y^{i^*})| \geq \xi$, then swap the points y^1 and y^{i^*} in Y and set $U_{1\times 1:p-1} = \bar{\phi}(y^1)^\top$.

For $k = 2, \ldots, p-1$**:**

Step k**:** Assume that the first $k-1$ steps of Gaussian elimination have been completed, hence, we have the first $k-1$ rows of the upper triangular matrix U: $U_{1:k-1\times 1:p-1}$. If $y^k = x$ then the element $U_{k,k}$, i.e., the k-th pivot element in the Gaussian elimination process, can be expressed as

$$U_{k,k}(x) \;=\; \bar{\phi}_k(x) - \bar{\phi}_1(x)\frac{U_{1,k}}{U_{1,1}} - \cdots - \bar{\phi}_{k-1}(x)\frac{U_{k-1,k}}{U_{k-1,k-1}}.$$

Clearly $U_{k,k}(x)$ is a quadratic polynomial in x, and can be written as $(v^k)^\top \bar{\phi}(x)$ with $v^k \in \mathbb{R}^{p-1}$ and $\|v^k\|_\infty \geq 1$.
Find $i^* = \operatorname{argmax}\{|(v^k)^\top \bar{\phi}(y^i)| : i = k, \ldots, p-1\}$.
If $|(v^k)^\top \bar{\phi}(y^{i^*})| \geq \xi$ then set $x = y^{i^*}$ and swap the points y^k and y^{i^*} in Y.
If $|(v^k)^\top \bar{\phi}(y^{i^*})| < \xi$ then find

$$x = y^k = \operatorname{argmax}_{x\in B(1)} |(v^k)^\top \bar{\phi}(x)|.$$

- Update the factorization

$$U_{k,i} \;=\; \bar{\phi}_i(x) - \bar{\phi}_1(x)\frac{U_{1,i}}{U_{1,1}} - \cdots - \bar{\phi}_{k-1}(x)\frac{U_{k-1,i}}{U_{k-1,k-1}}, \quad k < i \leq p-1.$$

Since $\|v^k\|_\infty \geq 1$ and $\xi < 1/2$ we know from Lemma 3.3 that

$$\max_{x\in B(1)} |(v^k)^\top \bar{\phi}(x)| \;\geq\; \frac{1}{2} \;>\; \xi.$$

Proposition 6.1. *Algorithm 6.1 computes a set Y of $p = (n+1)(n+2)/2$ points in the unit ball $B(1)$ centered at $y^0 = 0$ for which the pivots of the*

Gaussian elimination of $Q_{p-1\times p-1}$ *satisfy*

$$\left|d_{ii}^{Q}\right| \;\geq\; \frac{1}{2} \;>\; \xi,\; i = 1,\ldots,p-1.$$

The effort required by the algorithm for the Gaussian elimination is of the order of $\mathcal{O}(n^6)$ floating point operations. The algorithm requires, moreover, in the worst case, the maximization of $n-1$ linear functions and $p-1-n$ quadratic functions and the minimization of their symmetric counterparts, in a ball of radius 1. Strictly speaking we only need to guarantee the computation of a point with objective function value greater than or equal to 1/2. This can be done by using the same arguments used in Lemma 3.3 to prove that this bound of 1/2 is achievable, which has the advantage of reducing each pair of optimization problems to a trivial enumeration.

The outcome of Algorithm 6.1 can be written in the form $Q_{p-1\times p-1} = LDU$ where $\|D^{-1}\| \leq \xi(p-1)^{\frac{1}{2}}$ and L and U are lower and upper triangular matrices, respectively, with ones in the diagonals. Thus, the constant Λ_Q in the definition of Λ_Q–poisedness can be estimated as

$$\|Q_{p-1\times p-1}^{-1}\| \;\leq\; \xi(p-1)^{\frac{1}{2}}\|L^{-1}\|\|U^{-1}\| \;=\; \Lambda_Q.$$

The sizes of $\|L^{-1}\|$ and $\|U^{-1}\|$ are related with the growth factor of the factorization, and are expected to be of reasonable size for most practical instances.

6.2. Ensuring well-poisedness in the linear case. It is straightforward to adapt Algorithm 6.1 to the linear case for which the threshold ξ for the absolute value of the pivots is required to satisfy $0 < \xi < 1$. Moreover, in the linear case it is possible to identify the geometry in Y that yields the smallest possible bound on the norm of $L_{n\times n}^{-1}$. Let us also assume here that $y^0 = 0$ and that the points lie in a ball of radius 1. The problem we are looking at can be formulated as

$$\min_{L\in\mathbb{R}^{n\times n}} \|L^{-1}\| \quad \text{s.t.} \quad \|e_i^\top L\| = 1,\; i = 1,\ldots,n,$$

reflecting the fact that the points lie on the boundary of the ball $B(1)$. Using the SVD representation $L = UDV$, we can pose the problem as

$$\min_{U,D\in\mathbb{R}^{n\times n}} \|D^{-1}\| \quad \text{s.t.} \quad \|DU^\top e_i\| = 1,\; i = 1,\ldots,n,$$

where D represents a diagonal matrix and U is an orthogonal matrix. Now, squaring the n constraints and summing them up, we obtain (recall that the columns of U have norm 1)

$$\sum_{j=1}^{n} D_{jj}^2 \;=\; n. \tag{34}$$

Our goal is to minimize $\|D^{-1}\|$, in other words, to find the largest smallest value for the diagonal entries of D verifying (34). It is obvious that the best solution is when all the entries of D are equal to 1. Thus, an optimal solution for the problem is given by $D = U = I$. By setting $V = I$, we conclude that

$$L_{n\times n} \;=\; I,$$

i.e., $y^i = e_i$, $i = 1, \ldots, n$, is an optimal geometry, in the sense that it minimizes $\|L^{-1}\|$ and consequently it minimizes the constant Λ_L in the definition of Λ_L–poisedness. In the case where $y^0 = 0$ and $Y \subset B(1)$, the optimal value for Λ_L is 1. The resulting geometry corresponds to a simplex with a vertex y^0 at the origin and with $n-1$ angles of amplitude $\pi/2$ between faces. When $n = 2$ we get one angle of amplitude $\pi/2$ and two angles of amplitude $\pi/4$:

$$y^0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad y^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad y^2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

We point out that the angles between the faces of the simplex corresponding to the optimal geometry described above do not share the same amplitude. The reason lies in the fact that the measure of well-poisedness was related to the matrix $L_{n\times n}$ and the specifically chosen basis of monomials. If, instead, we consider the matrix $L_{q\times n}$ as suggested in Section 2.3 and optimize with respect to the smallest nonzero singular value, the resulting geometry would consist of a simplex with angles of uniform amplitude between the faces. Such a simplex could be computed as follows. First we compute n normalized vectors $w^0, \ldots, w^{n-1}$ such that

$$(w^i)^\top w^j \;=\; -1/n, \qquad i, j \in \{0, \ldots, n-1\},\ i \neq j.$$

By setting $W = [w^0 \cdots w^{n-1}]$, we have that $W^\top W = A$, where A is the matrix given by

$$A = \begin{bmatrix} 1 & -1/n & -1/n & \cdots & -1/n \\ -1/n & 1 & -1/n & \cdots & -1/n \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ -1/n & -1/n & -1/n & \cdots & 1 \end{bmatrix}.$$

The matrix A is symmetric, diagonally dominant with positive diagonal elements, and therefore positive definite. Using the eigenvalue decomposition $A = QDQ^\top$, one obtains $W = QD^{\frac{1}{2}}Q^\top$. The $n+1$-th point is given by $w^n = -\sum_{0 \le i \le n-1} w^i$, yielding $\|w^n\| = 1$ and $(w^i)^\top w^n = -1/n$, $i = 0, \ldots, n-1$. The resulting geometry is a simplex with angles of uniform amplitude between the faces. To obtain the desired simplex we would have to scale the simplex formed by $w^0, \ldots, w^n$ so that its faces have unitary length, shift one of its vertices to the origin, and fix $y^1 = e_1$. When $n = 2$, we have that $q = n(n+1)/2 = 3$ and

$$L_{3\times 2} = \begin{bmatrix} (y^1 - y^0)^\top \\ (y^2 - y^0)^\top \\ (y^2 - y^1)^\top \end{bmatrix} = \begin{bmatrix} (y^1)^\top \\ (y^2)^\top \\ (y^2 - y^1)^\top \end{bmatrix},$$

and we get three angles of amplitude $\pi/3$:

$$y^0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad y^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad y^2 = \begin{bmatrix} 1/2 \\ \sqrt{3}/2 \end{bmatrix}.$$

This uniform simplex is associated with the uniform minimal positive basis [1] used in pattern search methods.

7. Concluding remarks

In this paper we have addressed multivariate polynomial interpolation for interpolation sets in n-dimensional spaces and polynomials spaces of any degree d. Our approach is motivated from numerical considerations in the sense that we are only interested in developing error bounds involving constants coming from identifiable and, if possible, controllable sources of error. Our error estimates identify two main sources for the error: the smoothness of the function being interpolated and the geometric disposition of the interpolating points. In practical situations only the geometry of the interpolation set is controllable.

We have introduced a measure of the quality of the geometry of the interpolating set, called Λ–poisedness. The better the geometry, the better Λ–poised is the set, meaning that the smaller the constant Λ is. The constant Λ appears in all interpolating error bounds, directly linking the quality of the interpolating geometry with the quality of the interpolating estimation. Moreover, we developed algorithms to improve the geometry of the interpolation set.

Our approach is also novel in the way the error estimates are derived. The proofs are simple and follow directly from the interpolating conditions. In just one argument related with a system of linear equations, we show how to derive the bounds in all the derivative errors between the function and its interpolating polynomial. The error in the function values is then derived *a posteriori*.

References

[1] P. Alberto, F. Nogueira, H. Rocha, and L. N. Vicente, *Pattern search methods for user-provided points: Application to molecular geometry problems*, Tech. Rep. 00-20, Departamento de Matemática, Universidade de Coimbra, 2000.

[2] C. Audet and J. E. Dennis, *Analysis of generalized pattern searches*, SIAM J. Optim., 13 (2002), pp. 889–903.

[3] A. R. Conn, K. Scheinberg, and P. L. Toint, *On the convergence of derivative-free methods for unconstrained optimization*, in Approximation Theory and Optimization, Tributes to M. J. D. Powell, edited by M. D. Buhmann and A. Iserles, Cambridge University Press, Cambridge, 1997, pp. 83–108.

[4] ——, *Recent progress in unconstrained nonlinear optimization without derivatives*, Math. Programming, 79 (1997), pp. 397–414.

[5] J. E. Dennis and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice–Hall, Englewood Cliffs, (republished by SIAM, Philadelphia, in 1996, as Classics in Applied Mathematics, 16), 1983.

[6] M. J. D. Powell, *Direct search algorithms for optimization calculations*, Acta Numerica, 7 (1998), pp. 287–336.

[7] ——, *On the Lagrange functions of quadratic models that are defined by interpolation*, Optim. Methods Softw., 16 (2001), pp. 289–309.

[8] ——, *On trust region methods for unconstrained optimization*, Tech. Rep. DAMTP 2002/NA02, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, 2002.

[9] T. Sauer, *On multivariate Lagrange interpolation*, Math. Comp., 64 (1995), pp. 1147–1170.

[10] V. Torczon, *On the convergence of pattern search algorithms*, SIAM J. Optim., 7 (1997), pp. 1–25.

[11] S. Waldron, *Multipoint Taylor formulae*, Numer. Math., 80 (1998), pp. 461–494.

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