Chapter 3

Scattered Data Interpolation with Polynomial Precision and Conditionally Positive Definite Functions

3.1 Scattered Data Interpolation with Polynomial Precision

Sometimes the assumption on the form (1.1) of the solution to the scattered data interpolation Problem 1.2.1 is extended by adding certain polynomials to the expansion, i.e., $\mathcal{P}f$ is now assumed to be of the form

$$\mathcal{P}f(\boldsymbol{x}) = \sum_{k=1}^{N} c_k B_k(\boldsymbol{x}) + \sum_{l=1}^{M} d_l p_l(\boldsymbol{x}), \qquad \boldsymbol{x} \in \mathbb{R}^s, \tag{3.1}$$

where $p_1, \ldots, p_M$ form a basis for the $M = \binom{s+m-1}{m-1}$-dimensional linear space Π_{m-1}^s of polynomials of total degree less than or equal to $m-1$ in s variables.

Since enforcing the interpolation conditions $\mathcal{P}f(\boldsymbol{x}_i) = f(\boldsymbol{x}_i)$, $i = 1, \ldots, N$, leads to a system of N linear equations in the $N+M$ unknowns c_k and d_l one usually adds the M additional conditions

$$\sum_{k=1}^{N} c_k p_l(\boldsymbol{x}_k) = 0, \qquad l = 1, \ldots, M,$$

to ensure a unique solution.

Example: For $m = s = 2$ we add the space of bivariate linear polynomials, i.e., $\Pi_1^2 = \text{span}\{1, x, y\}$. Using the notation $\boldsymbol{x} = (x, y)$ we get the expansion

$$\mathcal{P}f(x, y) = \sum_{k=1}^{N} c_k B_k(x, y) + d_1 + d_2 x + d_3 y, \qquad \boldsymbol{x} = (x, y) \in \mathbb{R}^2,$$

which we use to solve

$$\mathcal{P}f(x_i, y_i) = f(x_i, y_i), \qquad i = 1, \dots, N,$$

together with the three additional conditions

$$\begin{aligned}
\sum_{k=1}^{N} c_k &= 0, \\
\sum_{k=1}^{N} c_k x_k &= 0, \\
\sum_{k=1}^{N} c_k y_k &= 0.
\end{aligned}$$

Remark: While the use of polynomials is somewhat arbitrary (any other set of M linearly independent functions could be used), it is obvious that the addition of polynomials of total degree at most $m-1$ guarantees polynomial precision, i.e., if the data come from a polynomial of total degree less than or equal to $m-1$ they are fitted by that polynomial.

In general, solving the interpolation problem based on the extended expansion (3.1) now amounts to solving a system of linear equations of the form

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{c} \\ \boldsymbol{d} \end{bmatrix} = \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{0} \end{bmatrix}, \tag{3.2}$$

where the pieces are given by $A_{jk} = B_k(\boldsymbol{x}_j)$, $j, k = 1, \dots, N$, $P_{jl} = p_l(\boldsymbol{x}_j)$, $j = 1, \dots, N$, $l = 1, \dots, M$, $\boldsymbol{c} = [c_1, \dots, c_N]^T$, $\boldsymbol{d} = [d_1, \dots, d_M]^T$, $\boldsymbol{y} = [y_1, \dots, y_N]^T$, and $\boldsymbol{0}$ is a zero vector of length M.

It is possible to formulate a theorem concerning the well-posedness of this interpolation problem. As in the previous chapter we begin with an appropriate definition from the linear algebra literature. This, however, covers only the case $m = 1$.

Definition 3.1.1 *A real symmetric matrix A is called* conditionally positive semi-definite of order one *if its associated quadratic form is non-negative, i.e.,*

$$\sum_{j=1}^{N} \sum_{k=1}^{N} c_j c_k A_{jk} \geq 0 \tag{3.3}$$

for all $\boldsymbol{c} = [c_1, \dots, c_N]^T \in \mathbb{R}^N$ which satisfy

$$\sum_{j=1}^{N} c_j = 0.$$

If $\boldsymbol{c} \neq \boldsymbol{0}$ implies strict inequality in (3.3) then A is called conditionally positive definite *of order m.*

Remarks:

1. In the linear algebra literature the definition usually uses "$\leq$", and then A is referred to as (conditionally or almost) *negative* definite.

2. Obviously, conditionally positive definite matrices of order one exist only for $N > 1$.

3. Conditional positive definiteness of order one of a matrix A can also be interpreted as A being positive definite on the space of vectors $\boldsymbol{c}$ such that

$$\sum_{j=1}^{N} c_j = 0.$$

Thus, in this sense, A is positive definite on the space of vectors $\boldsymbol{c}$ "perpendicular" to constant functions.

Since an $N \times N$ matrix which is conditionally positive definite of order one is positive definite on a subspace of dimension $N-1$ it has the interesting property that at least $N-1$ of its eigenvalues are positive. This follows immediately from the Courant-Fischer Theorem of linear algebra (see e.g., [431], Thm. 5.8(a)):

Theorem 3.1.2 *Let A be a symmetric $N \times N$ matrix with eigenvalues*

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N.$$

Let $1 \leq k \leq N$ and for each subspace W with $\dim W = N-k+1$ set

$$c_k(W) = \max_{\boldsymbol{x}\in W, \|\boldsymbol{x}\|=1} \boldsymbol{x}^T A \boldsymbol{x}$$

and

$$d_k(W) = \min_{\boldsymbol{x}\in W, \|\boldsymbol{x}\|=1} \boldsymbol{x}^T A \boldsymbol{x}.$$

Then

$$c_k(W) \geq \lambda_k, \quad d_k(W) \leq \lambda_{N-k+1}, \quad k = 1, \ldots, N.$$

With an additional hypothesis on A we can make an even stronger statement.

Theorem 3.1.3 *An $N \times N$ matrix A which is conditionally positive definite of order one and has a non-positive trace has 1 negative and $N-1$ positive eigenvalues.*

Proof: From the Courant-Fischer Theorem we get that A has at least $N-1$ positive eigenvalues. But since $\mathrm{tr}(A) = \sum_{i=1}^{N} \lambda_i \leq 0$, where the λ_i denote the eigenvalues of A, A also must have at least one negative eigenvalue. $\square$

3.2 Conditionally Positive Definite Functions

In analogy to the earlier discussion of interpolation with positive definite functions we will now introduce conditionally positive definite and strictly conditionally positive definite functions of order m.

Definition 3.2.1 *A complex-valued continuous function* Φ *is called* conditionally positive definite of order m on $\mathbb{R}^s$ *if*

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j \overline{c_k} \Phi(\boldsymbol{x}_j - \boldsymbol{x}_k) \geq 0 \tag{3.4}$$

for any N *points* $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$, *and* $\mathbf{c} = [c_1, \ldots, c_N]^T \in \mathbb{C}^N$ *satisfying*

$$\sum_{j=1}^{N} c_j p(\boldsymbol{x}_j) = 0,$$

for any complex-valued polynomial p *of degree at most* $m-1$. *The function* Φ *is called* strictly conditionally positive definite of order m on $\mathbb{R}^s$ *if the points* $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$ *are distinct, and* $\mathbf{c} \neq \mathbf{0}$ *implies strict inequality in (3.4).*

An immediate observation is that a function which is conditionally positive definite of order m on $\mathbb{R}^s$ also is conditionally positive definite of any higher order. In particular, this definition is more general than that for positive definite functions since the case $m = 0$ yields that class of functions, i.e., (strictly) conditionally positive definite functions of order zero are (strictly) positive definite, and therefore a (strictly) positive definite function is always (strictly) conditionally positive definite of any order.

As for positive definite functions earlier, we can restrict ourselves to real-valued, even functions Φ and real coefficients. A detailed discussion is presented in [634].

Theorem 3.2.2 *A real-valued continuous even function* Φ *is called* conditionally positive definite of order m on $\mathbb{R}^s$ *if*

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k \Phi(\boldsymbol{x}_j - \boldsymbol{x}_k) \geq 0 \tag{3.5}$$

for any N *points* $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$, *and* $\mathbf{c} = [c_1, \ldots, c_N]^T \in \mathbb{R}^N$ *satisfying*

$$\sum_{j=1}^{N} c_j \boldsymbol{x}_j^{\boldsymbol{\alpha}} = 0, \qquad |\boldsymbol{\alpha}| < m, \quad \boldsymbol{\alpha} \in \mathbb{N}_0^s.$$

The function Φ *is called* strictly conditionally positive definite of order m on $\mathbb{R}^s$ *if the points* $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$ *are distinct, and* $\mathbf{c} \neq \mathbf{0}$ *implies strict inequality in (3.5).*

Here we have used the usual *multi-integer notation*, i.e.,

$$\boldsymbol{\alpha} \in \mathbb{N}_0^s, \quad |\boldsymbol{\alpha}| = \sum_{i=1}^{s} \alpha_i, \quad \text{and} \quad \boldsymbol{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_s^{\alpha_s}.$$

Remarks:

1. The matrix A with entries $A_{jk} = \Phi(\boldsymbol{x}_j - \boldsymbol{x}_k)$ corresponding to a real and even strictly conditionally positive definite function of order m can also be interpreted as being positive definite on the space of vectors $\boldsymbol{c}$ such that

$$\sum_{j=1}^{N} c_j \boldsymbol{x}^{\boldsymbol{\alpha}} = 0, \qquad |\boldsymbol{\alpha}| < m.$$

   Thus, in this sense, A is positive definite on the space of vectors $\boldsymbol{c}$ "perpendicular" to polynomials of degree at most $m-1$.

2. The Courant-Fischer Theorem now implies that A has at least $N-m$ positive eigenvalues.

Using Theorem 3.1.3 we can see that interpolation with strictly conditionally positive definite functions of order one is possible even without adding a polynomial term. This was first observed by Micchelli [456].

Theorem 3.2.3 *Suppose Φ is strictly conditionally positive definite of order one and that $\Phi(\mathbf{0}) \le 0$. Then for any distinct points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$ the matrix A with entries $A_{jk} = \Phi(\boldsymbol{x}_j - \boldsymbol{x}_k)$ has $N-1$ positive and 1 negative eigenvalue, and is therefore non-singular.*

Proof: Clearly, the matrix A is conditionally positive definite. Moreover, the trace of A is given by $\operatorname{tr}(A) = N\Phi(0) \le 0$. Therefore, Theorem 3.1.3 applies. □

As we will see below, this theorem covers the *multiquadrics* $\Phi(x) = -(\|\boldsymbol{x}\|^2 + \alpha^2)^\beta$, $\alpha \ge 0$, $0 < \beta < 1$.

Another special property of a conditionally positive definite function of order one is

Lemma 3.2.4 *If C is an arbitrary real constant and the real even function Φ is (strictly) conditionally positive definite of order one, then $\Phi + C$ is also (strictly) conditionally positive definite of order one.*

Proof: Simply consider

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k [\Phi(\boldsymbol{x}_j - \boldsymbol{x}_k) + C] = \sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k \Phi(\boldsymbol{x}_j - \boldsymbol{x}_k) + \sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k C.$$

The second term on the right is zero since Φ is conditionally positive definite of order one, i.e., $\sum_{j=1}^{N} c_j = 0$, and thus the statement follows. □

Before we formulate the theorem about the uniqueness of the solution to the interpolation problem based on expansion (3.1), we define a property which forms a very mild restriction on the location of the data sites.

Definition 3.2.5 *We call a set of points* $\mathcal{X} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \mathbb{R}^s$ m-unisolvent *if the only polynomial of total degree at most* m *interpolating zero data on* $\mathcal{X}$ *is the zero polynomial.*

This definition comes from polynomial interpolation, in which case it guarantees a unique solution for interpolation to given data at a subset of the points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$ by a polynomial of degree m. A sufficient condition (to be found in [140], Ch. 9) on the points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$ to form an m-unisolvent set in $\mathbb{R}^2$ is

Theorem 3.2.6 *Suppose* $\{L_0, \dots, L_m\}$ *is a set of* $m+1$ *distinct lines in* $\mathbb{R}^2$, *and that* $\mathcal{U} = \{\boldsymbol{u}_1, \dots, \boldsymbol{u}_M\}$ *is a set of* $M = (m+1)(m+2)/2$ *distinct points such that the first point lies on* L_0, *the next two points lie on* L_1 *but not on* L_0, *and so on, so that the last* $m+1$ *points lie on* L_m *but not on any of the previous lines* $L_0, \dots, L_{m-1}$. *Then there exists a unique interpolation polynomial of total degree at most* m *to arbitrary data given at the points in* $\mathcal{U}$. *Furthermore, if the data sites* $\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ *contain* $\mathcal{U}$ *as a subset then they form an* m*-unisolvent set on* $\mathbb{R}^2$.

Proof: We use induction on m. For $m = 0$ the result is trivial. Take R to be the matrix arising from polynomial interpolation at the points in $\mathcal{U}$, i.e.,

$$R_{jk} = p_k(\boldsymbol{u}_j), \quad j, k = 1, \dots, M,$$

where the p_k form a basis of Π_m^2. We want to show that the only possible solution to $R\boldsymbol{c} = \boldsymbol{0}$ is $\boldsymbol{c} = \boldsymbol{0}$. This is equivalent to showing that if $p \in \Pi_m^2$ satisfies

$$p(\boldsymbol{u}_i) = 0, \quad i = 1, \dots, M,$$

then p is the zero polynomial.

For each $i = 1, \dots, m$, let the equation of the line L_i be given by

$$\alpha_i x_1 + \beta_i x_2 = \gamma_i.$$

Suppose now that p interpolates zero data at all the points $\boldsymbol{u}_i$ as stated above. Since p reduces to a univariate polynomial of degree m on L_m which vanishes at $m+1$ distinct points on L_m, it follows that p vanishes identically on L_m, and so

$$p(x_1, x_2) = (\alpha_m x_1 + \beta_m x_2 - \gamma_m) q(x_1, x_2),$$

where q is a polynomial of degree $m-1$. But now q satisfies the hypothesis of the theorem with m replaced by $m-1$ and $\mathcal{U}$ replaced by $\widetilde{\mathcal{U}}$ consisting of the first $\binom{m+1}{2}$ points of U. By induction, therefore $q \equiv 0$, and thus $p \equiv 0$. This establishes the uniqueness of the interpolation polynomial. The last statement of the theorem is obvious. $\square$

Remarks:

1. This theorem can be generalized to $\mathbb{R}^s$ by using hyperplanes in $\mathbb{R}^s$, and induction on s. Chui also gives an explicit expression for the determinant of the interpolation matrix associated with polynomial interpolation at the set of points $\mathcal{U}$.

2. A theorem similar to Theorem 3.2.6 is already proved by Chung and Yao [143].

3. $(m-1)$-unisolvency of the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ is equivalent to the fact that the matrix P with

$$P_{jl} = p_l(\boldsymbol{x}_j), \quad j = 1, \ldots, N, \ l = 1, \ldots, M,$$

where M and N are chosen as in (3.1), has full (column-)rank.

Example: As can easily be verified, three collinear points in $\mathbb{R}^2$ are not 1-unisolvent, since a linear interpolant, i.e., a plane through three arbitrary heights at these 3 collinear points is not uniquely determined. On the other hand, if a set of points in $\mathbb{R}^2$ contains 3 non-collinear points, then it is 1-unisolvent.

Now we are ready to formulate and prove

Theorem 3.2.7 *If the real-valued even function Φ is strictly conditionally positive definite of order m on $\mathbb{R}^s$ and the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ form an $(m-1)$-unisolvent set, then the system of linear equations (3.2) is uniquely solvable.*

Proof: Assume $[\boldsymbol{c}, \boldsymbol{d}]^T$ is a solution of the homogeneous linear system, i.e., $\boldsymbol{y} = \boldsymbol{0}$. We show that $[\boldsymbol{c}, \boldsymbol{d}]^T = \boldsymbol{0}$ is the only possible solution.

Multiplication of the top block by $\boldsymbol{c}^T$ yields

$$\boldsymbol{c}^T A\boldsymbol{c} + \boldsymbol{c}^T P\boldsymbol{d} = 0.$$

From the bottom block of (3.2) we know $\boldsymbol{c}^T P = \boldsymbol{0}$, and therefore

$$\boldsymbol{c}^T A\boldsymbol{c} = 0.$$

Since the matrix A is conditionally positive definite by assumption we get that $\boldsymbol{c} = \boldsymbol{0}$. The unisolvency of the data sites, i.e., the linear independence of the columns of P, and the fact that $\boldsymbol{c} = \boldsymbol{0}$ guarantee $\boldsymbol{d} = \boldsymbol{0}$ from the top block

$$A\boldsymbol{c} + P\boldsymbol{d} = \boldsymbol{0}$$

of (3.2). $\square$

3.3 An Analog of Bochner's Theorem

In order to give an analog of Bochner's theorem for conditionally positive definite functions we have to introduce a few concepts from distribution theory. The approach described in this section is essentially due to Madych and Nelson [417].

For the definition of generalized Fourier transforms required below we have to define the *Schwartz space* of rapidly decreasing test functions

$$\mathcal{S} = \{\gamma \in C^\infty(\mathbb{R}^s) : \lim_{\|\boldsymbol{x}\| \to \infty} \boldsymbol{x}^{\boldsymbol{\alpha}} (D^{\boldsymbol{\beta}}\gamma)(\boldsymbol{x}) = 0, \ \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^s\},$$

where

$$D^{\boldsymbol{\beta}} = \frac{\partial^{|\boldsymbol{\beta}|}}{\partial x_1^{\beta_1} \cdots \partial x_s^{\beta_s}}, \qquad |\boldsymbol{\beta}| = \sum_{i=1}^s \beta_i.$$

Remarks:

1. The space $\mathcal{S}$ consists of all those functions $\gamma \in C^\infty(\mathbb{R}^s)$ which, together with all their derivatives, decay faster than any power of $1/\|\boldsymbol{x}\|$.

2. The space $\mathcal{S}$ contains the space $C_0^\infty(\mathbb{R}^s)$, the space of all infinitely differentiable functions on $\mathbb{R}^s$ with compact support. We also note that $C_0^\infty(\mathbb{R}^s)$ is a true subspace of $\mathcal{S}$ since, e.g., the function $\gamma(\boldsymbol{x}) = e^{-\|\boldsymbol{x}\|^2}$ belongs to $\mathcal{S}$ but not to $C_0^\infty(\mathbb{R}^s)$.

3. A remarkable fact about the Schwartz space is that $\gamma \in \mathcal{S}$ has a classical Fourier transform $\hat{\gamma}$ which is also in $\mathcal{S}$.

Of particular importance will be the following subspace $\mathcal{S}_m$ of $\mathcal{S}$

$$\mathcal{S}_m = \{\gamma \in \mathcal{S} : \ \gamma(\boldsymbol{x}) = \mathcal{O}(\|\boldsymbol{x}\|^m) \text{ for } \|\boldsymbol{x}\| \to 0, \ m \in \mathbb{N}_0\}.$$

Furthermore, the set $\mathcal{B}$ of slowly increasing functions is given by

$$\mathcal{B} = \{f \in C(\mathbb{R}^s) : \ |f(\boldsymbol{x})| \leq |p(\boldsymbol{x})| \text{ for some polynomial } p \in \Pi^s\}.$$

The generalized Fourier transform is now given by

Definition 3.3.1 *Let $\Phi \in \mathcal{B}$ be complex-valued. A continuous function $\hat{\Phi} : \mathbb{R}^s \setminus \{0\} \to \mathbb{C}$ is called the* generalized Fourier transform *of Φ if there exists an integer $m \in \mathbb{N}_0$ such that*

$$\int_{\mathbb{R}^s} \Phi(\boldsymbol{x})\hat{\gamma}(\boldsymbol{x})d\boldsymbol{x} = \int_{\mathbb{R}^s} \hat{\Phi}(\boldsymbol{x})\gamma(\boldsymbol{x})d\boldsymbol{x}$$

is satisfied for all $\gamma \in \mathcal{S}_{2m}$. The smallest such integer m is called the order *of $\hat{\Phi}$.*

Remarks:

1. Since one can show that the generalized Fourier transform of an s-variate polynomial of degree at most $2m$ is zero, it follows that the inverse generalized Fourier transform is only unique up to addition of such a polynomial.

2. Various definitions of the generalized Fourier transform exist in the literature. A classical reference is the book by Gelfand and Vilenkin [250].

3. The order of the generalized Fourier transform is nothing but the order of the singularity at the origin of the generalized Fourier transform.

4. For functions in $L_1(\mathbb{R}^s)$ the generalized Fourier transform coincides with the classical Fourier transform, and for functions in $L_2(\mathbb{R}^s)$ it coincides with the distributional Fourier transform.

We now immediately give a characterization of strictly conditionally positive definite functions on $\mathbb{R}^s$ due to Iske (see [314] or [634] for details).

Theorem 3.3.2 *Suppose the complex-valued function $\Phi \in \mathcal{B}$ possesses a generalized Fourier transform $\hat{\Phi}$ of order m which is continuous on $\mathbb{R}^s \setminus \{0\}$. Then Φ is strictly conditionally positive definite of order m if and only if $\hat{\Phi}$ is non-negative and non-vanishing.*

Remarks:

1. Theorem 3.3.2 states that strictly conditionally positive definite functions on $\mathbb{R}^s$ are characterized by the order of the singularity of their generalized Fourier transform at the origin, provided that this generalized Fourier transform is non-negative and non-zero.

2. An integral characterization of conditionally positive definite functions of order m also exists. It can be found in a paper by Sun [597] (see also [634]).

Examples: Wendland [634] explicitly computes the generalized Fourier transforms for various popular basis functions.

1. The *multiquadrics*

$$\Phi(\boldsymbol{x}) = (\|\boldsymbol{x}\|^2 + \alpha^2)^\beta, \qquad \boldsymbol{x} \in \mathbb{R}^s,\ \alpha > 0,\ \beta \in \mathbb{R} \setminus \mathbb{N}_0,$$

have generalized Fourier transforms

$$\hat{\Phi}(\boldsymbol{\omega}) = \frac{2^{1+\beta}}{\Gamma(-\beta)} \left(\frac{\|\boldsymbol{\omega}\|}{\alpha} \right)^{-\beta - s/2} K_{\beta+s/2}(\alpha\|\boldsymbol{\omega}\|), \qquad \boldsymbol{\omega} \neq \boldsymbol{0},$$

of order $m = \max(0, \lceil \beta \rceil)$. Here K_ν is the *modified Bessel function of the second kind* (sometimes also called modified Bessel function of the third kind, or MacDonald's function) *of order* ν. Therefore, the functions

$$\Phi(\boldsymbol{x}) = (-1)^{\lceil \beta \rceil} (\|\boldsymbol{x}\|^2 + \alpha^2)^\beta, \qquad \beta > 0,\ \beta \notin \mathbb{N},$$

are strictly conditionally positive definite of order $m = \lceil \beta \rceil$ (and higher). In particular, we can use

$$\mathcal{P}f(\boldsymbol{x}) = \sum_{k=1}^{N} c_k \sqrt{\|\boldsymbol{x} - \boldsymbol{x}_k\|^2 + \alpha^2} + d, \qquad \boldsymbol{x} \in \mathbb{R}^s, \alpha > 0,$$

together will the constraint

$$\sum_{k=1}^{N} c_k = 0$$

to solve the scattered data interpolation problem. The resulting interpolant will be exact for constant data. By Theorem 3.2.3 we can also use

$$\mathcal{P}f(\boldsymbol{x}) = \sum_{k=1}^{N} c_k \sqrt{\|\boldsymbol{x} - \boldsymbol{x}_k\|^2 + \alpha^2}, \qquad \boldsymbol{x} \in \mathbb{R}^s, \alpha > 0.$$

Also, the inverse multiquadrics

$$\Phi(\boldsymbol{x}) = (\|\boldsymbol{x}\|^2 + \alpha^2)^{\beta}, \beta < 0,$$

are again shown to be strictly conditionally positive definite of order $m = 0$, i.e., strictly positive definite.

2. The *powers*

$$\Phi(\boldsymbol{x}) = \|\boldsymbol{x}\|^{\beta}, \qquad \boldsymbol{x} \in \mathbb{R}^s,\ \beta > 0,\ \beta \notin 2\,\mathbb{N},$$

have generalized Fourier transforms

$$\hat{\Phi}(\boldsymbol{\omega}) = \frac{2^{\beta+s/2}\Gamma(\frac{s+\beta}{2})}{\Gamma(-\beta/2)}\|\boldsymbol{\omega}\|^{-\beta-s}, \qquad \boldsymbol{\omega} \neq \mathbf{0},$$

of order $m = \lceil \beta/2 \rceil$. Therefore, the functions

$$\Phi(\boldsymbol{x}) = (-1)^{\lceil \beta/2 \rceil}\|\boldsymbol{x}\|^{\beta}, \qquad \beta > 0,\ \beta \notin 2\,\mathbb{N},$$

are strictly conditionally positive definite of order $m = \lceil \beta/2 \rceil$ (and higher).

3. The *thin plate splines* (or surface splines)

$$\Phi(\boldsymbol{x}) = \|\boldsymbol{x}\|^{2k}\log\|\boldsymbol{x}\|, \qquad \boldsymbol{x} \in \mathbb{R}^s,\ k \in \mathbb{N},$$

have generalized Fourier transforms

$$\hat{\Phi}(\boldsymbol{\omega}) = (-1)^{k+1}2^{2k-1+s/2}\Gamma(k+s/2)k!\|\boldsymbol{\omega}\|^{-s-2k}$$

of order $m = k+1$. Therefore, the functions

$$\Phi(\boldsymbol{x}) = (-1)^{k+1}\|\boldsymbol{x}\|^{2k}\log\|\boldsymbol{x}\|, \qquad k \in \mathbb{N},$$

are strictly conditionally positive definite of order $m = k+1$. In particular, we can use

$$\mathcal{P}f(\boldsymbol{x}) = \sum_{k=1}^{N} c_k\|\boldsymbol{x}-\boldsymbol{x}_k\|^2\log\|\boldsymbol{x}-\boldsymbol{x}_k\| + d_1 + d_2x + d_3y, \qquad \boldsymbol{x} = (x,y) \in \mathbb{R}^2,$$

together will the constraints

$$\begin{aligned} \sum_{k=1}^{N} c_k &= 0, \\ \sum_{k=1}^{N} c_k x_k &= 0, \\ \sum_{k=1}^{N} c_k y_k &= 0, \end{aligned}$$

to solve the scattered data interpolation problem provided the data sites are not all collinear. The resulting interpolant will be exact for data coming from a linear function.

Remark: As for strictly positive definite radial functions, we will be able to connect strictly conditionally positive definite radial functions to completely monotone functions, and thus be able to obtain a simpler criterion for checking conditional positive definiteness.

3.4 Conditionally Positive Definite Radial Functions

In analogy to the discussion in Chapter 2 we now focus on conditionally positive definite functions which are radial on $\mathbb{R}^s$ for all s. The paper [273] by Guo, Hu and Sun contains an integral characterization for such functions. This characterization is too technical to be included here.

The main result in [273] is a characterization of conditionally positive definite radial functions on $\mathbb{R}^s$ for all s in terms of completely monotone functions.

Theorem 3.4.1 *Let $\varphi \in C[0,\infty) \cap C^\infty(0,\infty)$. Then the function $\Phi = \varphi(\|\cdot\|^2)$ is conditionally positive definite of order m and radial on $\mathbb{R}^s$ for all s if and only if $(-1)^m\varphi^{(m)}$ is completely monotone on $(0,\infty)$.*

Proof: Micchelli [456] proved that complete monotonicity implies conditional positive definiteness. He also conjectured that the converse holds, and gave a simple proof for this in the case $m = 1$. For $m = 0$ this is Schoenberg's characterization of positive definite radial functions on $\mathbb{R}^s$ for all s in terms of completely monotone functions (Theorem 2.5.3). The remaining part of the theorem is shown in [273]. $\square$

In order to get strict conditional positive definiteness we need to generalize Theorem 2.5.4, i.e., the fact that φ not be constant.

Theorem 3.4.2 *If φ is as in Theorem 3.4.1 and not a polynomial of degree at most m, then Φ is strictly conditionally positive definite of order m and radial on $\mathbb{R}^s$ for all s.*

Examples: We can now more easily verify the conditional positive definiteness of the functions listed in the previous example.

1. The functions

$$\varphi(r) = (-1)^{\lceil\beta\rceil}(r+\alpha^2)^\beta, \qquad \alpha > 0,\ \beta > 0, \beta \notin \mathbb{N}$$

imply

$$\varphi^{(k)}(r) = (-1)^{\lceil\beta\rceil}\beta(\beta-1)\cdots(\beta-k+1)(r+\alpha^2)^{\beta-k}$$

so that

$$(-1)^{\lceil\beta\rceil}\varphi^{(\lceil\beta\rceil)}(r) = \beta(\beta-1)\cdots(\beta-\lceil\beta\rceil+1)(r+\alpha^2)^{\beta-\lceil\beta\rceil}$$

is completely monotone. Moreover, $m = \lceil\beta\rceil$ is the smallest possible m such that $(-1)^m\varphi^{(m)}$ is completely monotone. Therefore, the multiquadrics

$$\Phi(r) = (-1)^{\lceil\beta\rceil}(r^2+\alpha^2)^\beta, \qquad \alpha > 0,\ \beta > 0,$$

are strictly conditionally positive definite of order $m \geq \lceil\beta\rceil$ and radial on $\mathbb{R}^s$ for all s.

2. The functions
$$\varphi(r) = (-1)^{\lceil \beta/2 \rceil} r^{\beta/2}, \qquad \beta > 0,\ \beta \notin 2\,\mathbb{N},$$
imply
$$\varphi^{(k)}(r) = (-1)^{\lceil \beta/2 \rceil} \frac{\beta}{2} \left(\frac{\beta}{2} - 1\right) \cdots \left(\frac{\beta}{2} - k + 1\right) r^{\beta/2-k}$$
so that $(-1)^{\lceil \beta/2 \rceil} \varphi^{(\lceil \beta/2 \rceil)}$ is completely monotone and $m = \lceil \beta/2 \rceil$ is the smallest possible m such that $(-1)^m \varphi^{(m)}$ is completely monotone. Therefore, the powers
$$\Phi(r) = (-1)^{\lceil \beta/2 \rceil} r^{\beta}, \qquad \beta > 0,\ \beta \notin 2\,\mathbb{N},$$
are strictly conditionally positive definite of order $m \geq \lceil \beta/2 \rceil$ and radial on $\mathbb{R}^s$ for all s.

3. The thin plate splines
$$\Phi(\|\boldsymbol{x}\|) = (-1)^{k+1} \|\boldsymbol{x}\|^{2k} \log \|\boldsymbol{x}\|, \qquad k \in \mathbb{N},$$
are strictly conditionally positive definite of order $m \geq k+1$ and radial on $\mathbb{R}^s$ for all s. To see this we observe that
$$2\Phi(\|\boldsymbol{x}\|) = (-1)^{k+1} \|\boldsymbol{x}\|^{2k} \log(\|\boldsymbol{x}\|^2).$$
Therefore, we let
$$\varphi(r) = (-1)^{k+1} r^k \log r, \qquad k \in \mathbb{N},$$
and get
$$\varphi^{(\ell)}(r) = (-1)^{k+1} k(k-1)\cdots(k-\ell+1) r^{k-\ell} \log r + p_\ell(r), \qquad 1 \leq \ell \leq k,$$
with p_ℓ a polynomial of degree $k - \ell$. Therefore,
$$\varphi^{(k)}(r) = (-1)^{k+1} k! \log r + C$$
and
$$\varphi^{(k+1)}(r) = (-1)^{k+1} \frac{k!}{r},$$
which is completely monotone on $(0, \infty)$.

We can also apply the integral representation of completely monotone functions from the Hausdorff-Bernstein-Widder Theorem to the previous result. Then we get

Theorem 3.4.3 *A necessary and sufficient condition that the function $\Phi = \varphi(\|\cdot\|^2)$ be conditionally positive definite of order m and radial on $\mathbb{R}^s$ for all s is that its $\varphi^{(m)}$ satisfy*
$$(-1)^m \varphi^{(m)}(r) = \int_0^\infty e^{-rt} d\mu(t), \quad r > 0,$$
where μ is a non-negative Borel measure on $(0, \infty)$ such that
$$\int_0^1 d\mu(t) < \infty \quad \textit{and} \quad \int_1^\infty \frac{d\mu(t)}{t^m} < \infty.$$

The following examples of functions which are conditionally positive definite of order $m = 0$ or $m = 1$ and radial on $\mathbb{R}^s$ for all s are taken from [521]. They are listed with the associated measures corresponding to the formulation of Theorem 3.4.3.

Example:

1. $\Phi(r) = -r$: $\quad m = 1, \quad d\mu(t) = -\frac{1}{2\sqrt{\pi t}}dt,$

2. $\Phi(r) = -\sqrt{1+r^2}$: $\quad m = 1, \quad d\mu(t) = -\frac{e^{-t}}{2\sqrt{\pi t}}dt,$

3. $\Phi(r) = \frac{1}{\sqrt{1+r^2}}$: $\quad m = 0, \quad d\mu(t) = \frac{e^{-t}}{\sqrt{\pi t}}dt,$

4. $\Phi(r) = e^{-\alpha r^2}$, $\alpha > 0$: $\quad m = 0, \quad d\mu(t) = \delta(t-\rho)dt$, i.e., point evaluation at ρ.

Finally, Micchelli proved a more general version of Theorem 2.6.3 theorem relating conditionally positive definite radial functions of order m on $\mathbb{R}^s$ and multiply monotone functions. We state a stronger version due to Buhmann [79] which ensures strict conditional positive definiteness.

Theorem 3.4.4 *Let $k = \lfloor s/2 \rfloor - m + 2$ be a positive integer, and suppose $\varphi \in C^{m-1}[0,\infty)$ is not a polynomial of degree at most m. If $(-1)^m \varphi^{(m)}$ is k-times monotone on $(0,\infty)$ but not constant, then $\Phi = \varphi(\|\cdot\|^2)$ is strictly conditionally positive definite of order m and radial on $\mathbb{R}^s$.*

Remark: The converse of the above result is open.

Just as we showed earlier that compactly supported radial function cannot be strictly positive definite on $\mathbb{R}^s$ for all s, it is important to note that there are no truly conditionally positive definite functions with compact support. More precisely,

Theorem 3.4.5 *Assume that the complex-valued function $\Phi \in C(\mathbb{R}^s)$ has compact support. If Φ is strictly conditionally positive definite of (minimal) order m, then m is necessarily zero, i.e., Φ is already strictly positive definite.*

Proof: The hypotheses on Φ ensure that it is integrable, and therefore it possesses a classical Fourier transform $\hat{\Phi}$ which is continuous. For integrable functions the generalized Fourier transform coincides with the classical Fourier transform. Theorem 3.3.2 ensures that $\hat{\Phi}$ is non-negative in $\mathbb{R}^s \setminus \{\mathbf{0}\}$ and not identically equal to zero. By continuity we also get $\hat{\Phi}(\mathbf{0}) \geq 0$, and Theorem 2.3.3 shows that Φ is strictly positive definite. $\square$.

Remark: Theorem 3.4.4 together with Theorem 3.4.5 implies that if we perform m-fold anti-differentiation on a non-constant k-times monotone function, then we obtain a function that is strictly positive definite and radial on $\mathbb{R}^s$ for $s \leq 2(k+m) - 3$.

Example: The function $\varphi_k(r) = (1-r)_+^k$ is k-times monotone. To avoid the integration constant for the compactly supported truncated power function we compute the anti-derivative via

$$I\varphi_k(r) = \int_r^\infty \varphi_k(s)ds = \int_r^\infty (1-s)_+^k ds = \frac{(-1)^k}{k+1}(1-r)_+^{k+1}.$$

m-fold anti-differentiation yields

$$I^m\varphi_k(r) = II^{m-1}\varphi_k(r) = \frac{(-1)^{mk}}{(k+1)(k+2)\cdots(k+m)}(1-r)_+^{k+m}.$$

Therefore, by the Buhmann-Micchelli Theorem, the function

$$\varphi(r) = (1-r)_+^{k+m}$$

is strictly conditionally positive definite of order m and radial on $\mathbb{R}^s$ for $s \le 2(k+m)-3$, and by Theorem 3.4.5 it is even strictly positive definite and radial on $\mathbb{R}^s$. This was also observed in Example 1 at the end of Section 2.4. In fact, we saw there that φ is strictly positive definite and radial on $\mathbb{R}^s$ for $s \le 2(k+m)-1$.

We see that we can construct strictly positive definite compactly supported radial functions by anti-differentiating the truncated power function. This is essentially the approach taken by Wendland to construct his popular compactly supported radial basis functions. We describe this construction in the next chapter.

3.5 Composition of Conditionally Positive Definite Functions

When Schoenberg first studied conditionally positive definite matrices of order one it was in connection with isometric embeddings. Based on earlier work by Karl Menger [453] he had the following result characterizing a conditionally positive definite matrix as a certain *distance matrix* (see [568]).

Theorem 3.5.1 *Let A be a real symmetric $N \times N$ matrix with all diagonal entries zero and all other elements positive. Then $-A$ is conditionally positive semi-definite if and only if there exist N points $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N \in \mathbb{R}^N$ for which*

$$A_{jk} = \|\boldsymbol{y}_j - \boldsymbol{y}_k\|^2.$$

These points are the vertices of a simplex in $\mathbb{R}^N$.

There is also a close connection between conditionally positive semi-definite matrices and those which are positive semi-definite. This is a classical result from linear algebra called Schur's theorem. We state a stronger version due to Micchelli [456] that also covers the strict case.

Theorem 3.5.2 *A symmetric matrix $-A$ is conditionally positive semi-definite if and only if the Schur exponential $(e^{-\alpha A_{jk}})_{j,k=1}^N$ is positive semi-definite for all $\alpha > 0$. Moreover, it is positive definite if and only if*

$$A_{jk} > \frac{A_{jj} + A_{kk}}{2}, \qquad j \neq k.$$

A proof of the classical (non-strict) Schur Theorem can be found, e.g., in the book by Horn and Johnson [308].

As an immediate corollary we get an earlier result by Schoenberg (see [569], Thm. 5). We have translated Schoenberg's embedding language into that of conditionally positive definite and completely monotone functions.

Corollary 3.5.3 *A function $\varphi(\cdot)$ is conditionally positive definite of order one and radial on $\mathbb{R}^s$ for all s if and only if the functions $e^{-\alpha\varphi(\cdot^2)}$ are positive definite and radial on $\mathbb{R}^s$ for all s and for all $\alpha > 0$, i.e., $e^{-\alpha\varphi(\cdot)}$ is completely monotone for all $\alpha > 0$.*

Example: The matrix B defined by

$$B_{jk} = e^{-\|\boldsymbol{x}_j - \boldsymbol{x}_k\|^\alpha}, \quad 0 < \alpha \le 2, \quad j,k = 1,\ldots,N,$$

is positive semi-definite, and if the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ are distinct B is positive definite. This is true since Schoenberg [569] showed that the matrix A defined by

$$A_{jk} = -\|\boldsymbol{x}_j - \boldsymbol{x}_k\|^\alpha, \quad 0 < \alpha \le 2, \quad j,k = 1,\ldots,n,$$

is conditionally positive semi-definite, and conditionally positive definite for distinct points.

A more general result regarding the composition of conditionally positive definite functions is given by Baxter [26].

Theorem 3.5.4 *Suppose φ and ψ are functions that are conditionally positive definite of order one are radial on $\mathbb{R}^s$ with $\varphi(0) = 0$. Then $\psi \circ \varphi$ is also conditionally positive definite of order one and radial on $\mathbb{R}^s$. Indeed, if ψ is strictly conditionally positive definite of order one and radial and φ vanishes only at zero, then $\psi \circ \varphi$ is strictly conditionally positive definite of order one and radial.*

We close with some remarks.

Remarks:

1. More results with a similar flavor can be found in [26], [456], and [445].

2. Many of the results given in the previous sections can be generalized to vector-valued or even matrix-valued functions. Some work is done in [407, 408], [474], [484], and [548].

3. Another possible generalization is to consider (strictly) (conditionally) positive definite *kernels* on $X \times X$, where X is some abstract point set and $k_1, \ldots, k_m$ are given real-valued functions governing the order m of conditional positive definiteness.

4. We point out that the approach to solving the interpolation problems taken in the previous section always assumes that the *knots*, i.e., the points $\boldsymbol{x}_k$, $k = 1, \ldots, N$, at which the basis functions are centered, coincide with the data sites. This is a fairly severe restriction, and it has been shown in examples in the context of least squares approximation of scattered data (see e.g., [237, 238], or [192]) that better results can be achieved if the knots are chosen different from the data sites. Theoretical results in this direction are very limited, and are reported in [521] and in [596].