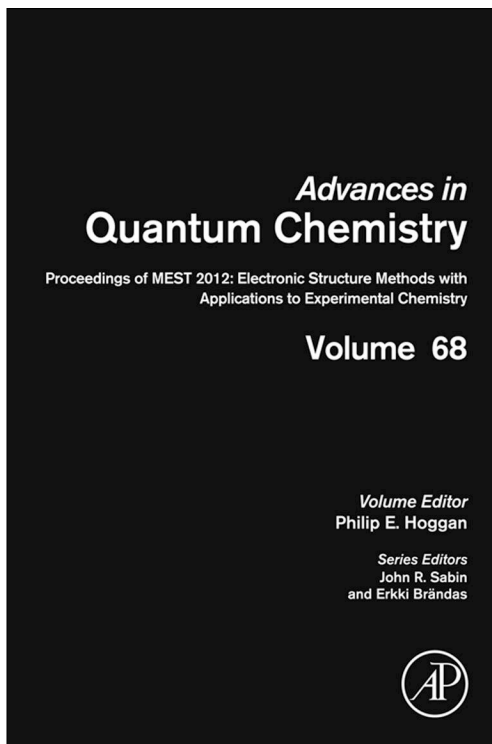


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Behavior Preserving Extension of Univariate and Bivariate Functions

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Abstract

Given function values on a domain D_0 , possibly with noise, we examine the possibility of extending the function to a larger domain $D, D_0 \subset D$. In addition to smoothness at the boundary of D_0 , the extension to $D \setminus D_0$ should also inherit behavioral trends of the function on D_0 , such as growth and decay or even oscillations. The approach chosen here is based upon the framework of linear models, univariate, or bivariate, with constant coefficients or varying coefficients.



1. INTRODUCTION

Prony⁵ has suggested in 1795 to model a data sequence by a linear combination of complex exponentials, and he has shown that such a model is equivalent to finding a linear model, with constant coefficients, for the evolution of the sequence. Shanks⁶ has revived this approach, used it for convergence acceleration, and has shown its relation to Padé approximation. Prony's method for the decomposition of a signal to a series of complex exponentials is a powerful tool for signal analysis. It has been studied by many authors, who made valuable contributions to the practical application of the method, e.g., by Smyth and Osborne.⁴

2-D linear prediction models with constant coefficients have been used in [Ref. 2](#) in the context of double series and bivariate Padé approximation. In the 2-D case the equivalence between linear prediction and exponential fitting is not true anymore, and the class of double sequences satisfying 2-D linear models with constant coefficients is in general richer than just sums of exponentials.

1-D linear models with varying coefficients have been studied in [Ref. 1](#) and in [Ref. 3](#) who introduced new sequence transformations which are efficient for a wide class of sequences, wider than those which are defined by sums of exponentials. For a complete overview see [Ref. 7](#).

Prony's method has a close relationship to the least-squares linear prediction algorithms, and as such it can evidently be used for the extension, or the extrapolation, of sequences. The problem of extending a function is closely related to this, with the extra requirement that the extension should be smooth. In the present paper we begin by showing how univariate linear prediction model, with constant coefficients, may be used for smooth functional extension, *without* the need of solving for the exponents, as required in Prony's method. This new approach allows generalization to higher dimensions, and it is used here for the extension of 2-D data.



2. UNIVARIATE CASE—FROM A LINEAR MODEL TO EXTENSION

Given a function on a domain D_0 , the ideal information for extending the function into a larger domain would be the differential equation which the function satisfies on D_0 . If the differential equation is simple, e.g., with constant coefficients, it can be extended beyond D_0 , and the extension of the function may be defined by solving the differential equation with

proper initial or boundary conditions. If the function is known only on a discrete set of points in D_0 , say on a uniform grid, we may hope to find a difference equation which the data values satisfy on the grid. Knowing the difference equation may serve as a starting point for both approximating the function on D_0 and for extending it beyond D_0 , as explained below. It is important to note that a univariate function is a sum of exponentials if and only if it satisfies a linear differential equation with constant coefficients. Also, the values of a univariate function on a regular grid are a sum of exponentials if and only if they satisfy a linear difference equation with constant coefficients. This equivalence does not hold in 2-D. The case of linear differential or difference equations with varying coefficients is studied in [Ref. 3](#) for the generation of the d -transformation and the D -transformation for efficient extrapolation of infinite series and integrals. It is shown there that the class of functions satisfying such equations covers most of the special functions, and their combinations.

2.1 Extracting linear prediction models

Let $D_0 = [a, b]$ and consider data sets $\{x_i, f_i\}$, where $\{f_i\}$ are function values (possibly with noise) at equidistant points $x_i = a + ih$, $i = 0, \dots, N$, $h = (b - a)/N$. We would like to find a difference equation, or a linear prediction model, by which we can extend the function for $x > b$. Recalling our declared goal, we would like the extension to carry along the characteristic behavior of the function within the interval $[a, b]$. Since h may be very small, difference relation on a sequences of data values at distance h cannot catch the global behavior of f on $[a, b]$. Also, in particular in presence of noise, the problem of finding a difference equation satisfied by the given data may be quite unstable. Let $d = nh$, we quest for a linear prediction model of order m satisfied by all the data sequences of mesh size d , $\{f_{i+(j-1)n}\}_{j=1}^{\lfloor (N+1)/n \rfloor}$, $i = 0, \dots, n - 1$. As we shall see below, the value d determines, by Nyquist sampling theory, the frequencies which can be reconstructed by the prediction model. We consider linear prediction models of the form:

$$[1 + q_{m+1}u(x_i)]f_i = \sum_{k=1}^m [p_k + q_k u(x_i)]f_{i-(m-k+1)n}. \quad (1)$$

Typical choices of the function u would be:

1. $u \equiv 0$ for a model with constant coefficients.
2. $u(x) = x$ for a linearly varying model.

3. $u(x) = \frac{1}{x+\alpha}$ for a model with rational variation.

Now we may use a standard way of defining an approximate prediction model by a least-squares fit, as follows:

We look for model coefficients $P = \{p_k\}_{k=1}^m$ and $Q = \{q_k\}_{k=1}^{m+1}$ such that

$$I_1(P, Q) = \sum_{i=mn}^N \left([1 + q_{m+1}u(x_i)]f_i - \sum_{k=1}^m [p_k + q_k u(x_i)]f_{i-(m-k+1)n} \right)^2 \rightarrow \min. \quad (2)$$

In Section 4 we discuss other options for extracting the model. In particular, we consider improving the numerical stability by minimizing

$$I_1(P, Q) + \nu_1 \sum_{k=1}^m p_k^2 + \nu_2 \sum_{k=1}^{m+1} q_k^2. \quad (3)$$

In Section 5 we use linear models for the bivariate extension problem.



3. APPROXIMATION AND EXTENSION ALGORITHMS

3.1 Univariate models with constant coefficients

Let us first discuss a linear model with constant coefficients. i.e., we would like to approximate the data on $[a, b]$, and extend it beyond b , using the linear model

$$g_i = \sum_{k=1}^m p_k g_{i-(m-k+1)n}. \quad (4)$$

Such a model takes us back to Prony's method, i.e., approximation by a sum of exponentials. Let $\{\lambda_j\}_{j=1}^m$ be the roots of the characteristic polynomial

$$p(\lambda) = \sum_{k=1}^m p_k \lambda^{k-1} - \lambda^m. \quad (5)$$

For simplicity, let us assume that all the roots of p are simple. Then, all sequences satisfying (4) are of the form

$$g_{m+i} = \sum_{j=1}^m c_j^{(i)} \lambda_j^r, \quad r \in \mathbb{Z} \quad (6)$$

with coefficients $\{c_j^{(i)}\}$ depending on i . We recall that the value g_{m+i} is attached to the point $x = a + (m + i)h = a + rd + ih$, and we would like to define a smooth function g such that $g(a + rd + ih) = g_{m+i}$. W.l.o.g., we may assume that $d = 1$, and obtain the relation

$$g(a + r + ih) = \sum_{j=1}^m c_j^{(i)} \lambda_j^r = \sum_{j=1}^m \tilde{c}_j^{(i)} \lambda_j^{a+r+ih}, \quad r \in \mathbb{Z}. \quad (7)$$

The evident way of defining a smooth g on \mathbb{R} is to make the coefficients independent of i , i.e., $\tilde{c}_j^{(i)} = \tilde{c}_j$ for any i . Then, g is simply

$$g(x) = \sum_{j=1}^m \tilde{c}_j \lambda_j^x, \quad x \in \mathbb{R}. \quad (8)$$

Other ways for constructing a smooth g satisfying the model will be presented in the following sections.

3.1.1 The approximation-extension algorithm for linear model with constant coefficients

1. Find the model coefficients by (2) with $u \equiv 0$.
2. Find the exponents $\{\lambda_j\}_{j=1}^m$ as the roots of the characteristic polynomial (5).
3. Define the approximation on $[a, b]$ and the extension by (8) where the coefficients $\{\tilde{c}_j\}$ are obtained by least-squares approximation to the given data on $[a, b]$.

There are some technical issues to deal with in the above algorithm. One is the case of multiple roots in step 2, and another is the problem of complex approximation to a real function in step 3. The last issue can be resolved by replacing the basis functions in step 3 above by an independent subset of $\{Re(\lambda_j^x), Im(\lambda_j^x)\}_{j=1}^m$. More problematic is the issue of choosing the right order m for the model. If m is too small the model cannot approximate the data, and if m is too large some of the extra resulting exponents may introduce highly oscillatory behavior or another type of instability. Altogether, as shown in examples 1 and 2 below, the above algorithm works quite nicely for noisy data of functions which can be well approximated by sums of exponentials. However, the above approach cannot be applied to models with varying coefficients, and in the bivariate case it is not suitable even for models with constant coefficients. Therefore, the main purpose of this paper would be to suggest more general approximation-extension algorithms which are applicable to those cases as well.

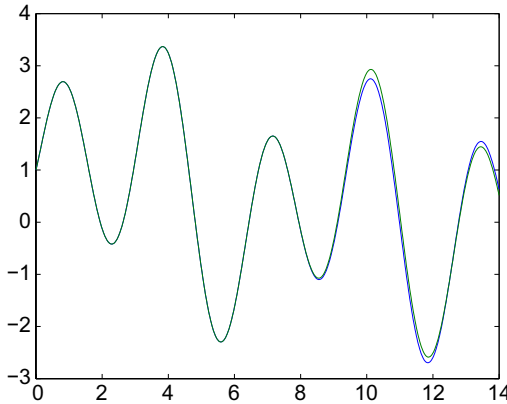


Figure 2.1 Approximation to non-noisy data on $[0, 7]$ and extension on $[0, 14]$. For color version of this figure, the reader is referred to the online version of this chapter.

3.1.2 Examples of approximation extension using exponential's fitting

As an example we consider extension of the function:

$$f_1(x) = .8^x - \cos(x) + 2\sin(2x) + \frac{1}{x+1}, \quad x \in [0, 7] \quad (9)$$

to $[0, 14]$. We first demonstrate the results for non-noisy data. The parameters used are $n = 50$, $h = 0.02$, and a model of the form (4) with $m = 6$. The resulting exponents are:

$$\{\lambda_j\} = \{0.061818, 0.772124, -0.416977 \pm 0.908787i, 0.520298 \pm 0.852041i\}.$$

Note that 0.8 , $e^i = 0.540302 \pm 0.841471i$ and $e^{2i} = -0.416149 \pm 0.909297i$ are the exact exponentials constituting f_1 . However, since f_1 is not a “pure” sum of exponentials, we do not get them exactly. In Figure 2.1 we plot the function f_1 together with the reconstructed approximation-extension g on $[0, 14]$ (defined by (8)), using function values only on $[0, 7]$.

Next we consider the same test function f_1 , measured at the same points in $[0, 7]$, but with an added noise, randomly distributed in $[-0.2, 0.2]$. Here the resulting exponents of a model of the same size, $m = 6$, turn to be

$$\{\lambda_j\} = \{0.273076, -0.864675, -0.414134 \pm 0.908059i, 0.542686 \pm 0.562524i\}.$$

In Figure 2.2 we plot the reconstructed approximation-extension g on $[0, 14]$ together with the data on $[0, 7]$ used in the algorithm, and the exact function f_1 on $(7, 14]$. We note that the complex exponents are not

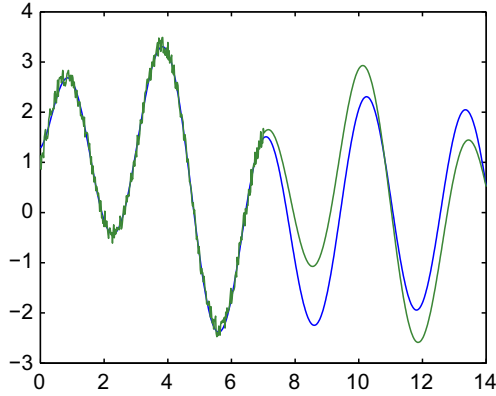


Figure 2.2 Approximation to noisy data on $[0, 7]$ and extension on $[0, 14]$. For color version of this figure, the reader is referred to the online version of this chapter.

so sensitive to the noise, but the real frequencies are quite different. Yet, the approximation in $[0, 7]$ is good, and the extension is also reasonable.

3.2 Univariate models with varying coefficients

Unlike the above Prony's type method, the algorithm presented below does not rely on finding the general solution of sequences satisfying the model. Hence, in principle, it is applicable even for non-linear models with varying coefficients. The method is based upon joining together all the required elements into one objective functional, and minimizing this functional within the space of all sequences satisfying the model. We demonstrate the approach via linear models with constant or varying coefficients.

Let us denote by $g \in M$ a sequence $g = \{g_i\}_{n_0 \leq i \leq n_1}$, $n_0 \leq 0$ and $n_1 \geq N$, satisfying a model M . We would like to find a sequence $g \in M$ such that:

- A.** $\{g_i\}_{i=0}^N$ approximates the given data sequence $\{f_i\}_{i=0}^N$.
- B.** g is smooth.

Requirement **A** is reflected in the functional.

$$E(g) = \sum_{i=0}^N [f_i - g_i]^2 \quad (10)$$

while the smoothness requirement **B** is characterized by

$$S_p(g) = \sum_{n_0 \leq i \leq n_1 - p} [\Delta^p g_i]^2, \quad (11)$$

where Δ is the ordinary difference operator and p is a parameter representing the smoothness degree.

3.2.1 The approximation-extension algorithm for general models

1. Find an appropriate model M for the data $\{f_i\}_{i=0}^N$.
2. Define the approximation on $\{x_i\}_{i=0}^N$ and its extension as the sequence $g = \{g_i\}_{n_0 \leq i \leq n_1}$ minimizing the functional

$$F_p(g) = S_p(g) + \mu E(g), \quad g \in M. \quad (12)$$

3.2.2 Discussion

The new element here is the inclusion of the smoothing functional S_p . Such a functional is a very common tool in Computer-Aided Geometric Design, where it is used for smooth filling of holes in a surface. In approximation theory S_p is viewed as a regularization functional. Let us explain its special role in our context; In the case of a model with varying coefficients, if the coefficients vary smoothly, each sequence obeying the model may be smooth, in some sense. However, let us recall that the model connects points which are d distance apart, or, equivalently, n indices apart, from each other (see (4)). Therefore, within $g \in M$ there may be n smooth independent subsequences satisfying the model. The first role of the functional S_p is to force those n subsequences of g to unite into one smooth sequence. Furthermore, even in the case of models with constant coefficients, the space of sequences satisfying the model may include parasitic highly oscillatory sequences. The second role of smoothing functional S_p is to invalidate these parasite components in M . The parameter μ determines a balance between the functionals S_p and E . In the examples below we discuss the effects of the parameter μ and the order p of the difference operator in S_p .

One may also argue that it is enough to take care of the smoothness of $\{g_i\}_{i=0}^N$, and to continue the sequence by the model. However, this approach has been found to be unstable, and moreover, as explained in [Section 5](#), this approach cannot work in 2-D.

As an example we have repeated the example with f_1 defined in (9), measured at the same points in $[0, 7]$, with an added noise randomly distributed in $[-0.2, 0.2]$. The model is also of the same size, $m = 6$, with constant coefficients, but the reconstruction is computed by minimization of F_2 defined in (12) with $\mu = 0.001$. The numerical results of the reconstruction and the extension are very similar to those presented in [Figure 2.2](#).

3.3 The scope of linear models with varying coefficients

Shanks⁶ investigated the use of exponentials fitting to a sequence as a tool for convergence acceleration. It is also shown there that fitting a linear model with constant coefficients to the terms of a power series leads to

Padé approximations. The use of linear models with varying coefficients has been studied in [Ref. 1](#) and in [Ref. 3](#) who introduced new sequence transformations which are efficient for a wide class of sequences, wider than those which are defined by sums of exponentials. In [Ref. 3](#) we can find examples of classes of sequences $\{a_k\}$ which satisfy a linear model with coefficients which has asymptotic expansion in inverse powers of k , as $n \rightarrow \infty$. We refer to models of a general order m of the form:

$$a_{k+m+1} = \sum_{i=1}^m p_i(k) a_{k+i}, \quad (13)$$

where

$$p_i(k) \sim k^{r_i} \sum_{j=0}^{\infty} p_{i,j} k^{-j} \quad \text{as } k \rightarrow \infty, \quad r_i \in \mathbb{Z}. \quad (14)$$

As a simple example consider the sequence $a_k = k^\alpha e^{ck}$. Obviously,

$$a_{k+1} = e^c \left(1 - \frac{1}{k+1}\right)^\alpha a_k, \quad (15)$$

which is a linear model, with coefficients that vary with k . For any c and α , the coefficients have asymptotic expansion in inverse powers of k , as $k \rightarrow \infty$. Following [Ref. 3](#) we denote by $B^{(m)}$ the class of sequences satisfying a model of order m of the form (13) with coefficients which has asymptotic expansions of the form (14).

Similar to the case of exponentials, the following algebraic rules hold³:

Let $\{a_k\} \in B^{(m_1)}$ and $\{b_k\} \in B^{(m_2)}$ then

$$\{a_k + b_k\} \in B^{(m_1+m_2)}, \quad \{a_k b_k\} \in B^{(m_1 m_2)}. \quad (16)$$

For example, by the above properties we can analyze sequences of equidistant evaluations of Bessel functions, concluding that $\{a_k\} = \{J_\nu(ks)\} \in B^{(2)}$ for any order ν and for any s . Altogether, we recall here the rich family of sequences satisfying linear models of type $B^{(m)}$. In this paper we report the use of a restricted subclass of $B^{(m)}$, namely models of the form (1) with $u(x) = x$ or $u(x) = 1/x + \alpha$.

3.3.1 Examples of approximation-extension using a model with rational coefficients

As an example we considered extension of the function:

$$f_2(x) = \frac{5 \cos(2x)}{x^2 + 1} + x^{1.5} \sin(x), \quad x \in [0, 7] \tag{17}$$

to $[0, 14]$. Here again f_2 is measured with a noise, randomly distributed in $[-0.2, 0.2]$. The parameters used are $n = 100$, $h = 0.01$, and a model of the form (1) with $u(x) = \frac{1}{x+1}$ and $m = 6$. The reconstruction is computed by minimization of F_2 defined in (12) with $\mu = 0.0001$ ($\mu \sim h^2$) (see Figs. 13.3 and 13.4).

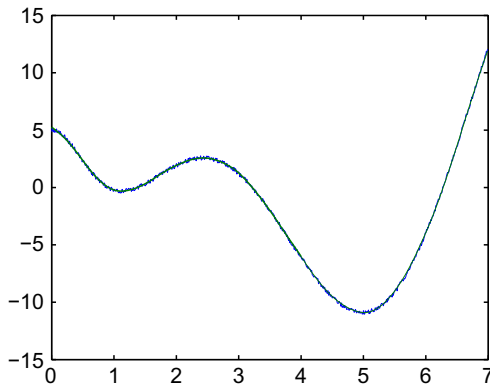


Figure 2.3 Rational coefficients model: approximation to the noisy data on $[0, 7]$. For color version of this figure, the reader is referred to the online version of this chapter.

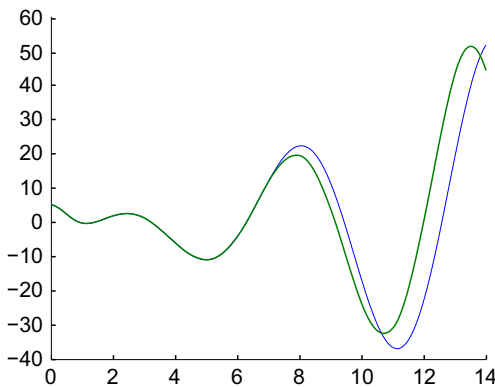


Figure 2.4 Rational coefficients model: approximation-extension on $[0, 14]$. For color version of this figure, the reader is referred to the online version of this chapter.

Remarks

1. Using the above characterization rules, the function (17) is in $B^{(4)}$, and it cannot satisfy a linear model with constant coefficients. Our model, with rational coefficients of low degree, is also not ideal here, but it performs better than a model with constant coefficients.
2. The right choice of the parameter μ is important. Choosing μ too big results in a bad approximation to the data, while a too small μ yields non-smooth approximation. The rule $\mu \sim h^2$ has been found to work well.



4. THE BIVARIATE CASE—FROM A LINEAR MODEL TO A SMOOTH EXTENSION

W.l.o.g, let $D_0 = [a, b] \times [a, b]$ and consider data sets $\{(x_i, y_j), f_{i,j}\}$, where $\{f_{i,j}\}$ are function values (possibly with noise) on a square mesh $(x_i, y_j) = (a + ih, a + jh)$, $i, j = 0, \dots, N$, $h = (b - a)/N$. We would like to find a difference equation, or a linear prediction model, by which we can extend the function into $D = [c, d] \times [c, d]$, $c < a, d > b$. As in the univariate case, we start by finding a linear model of size $m \times m$ satisfied by all the data sequences of mesh size $d = nh$, $\{f_{i+(k-1)n, j+(\ell-1)n}\}_{k, \ell=1}^{\lfloor (N+1)/n \rfloor}$, $i, j = 0, \dots, n-1$. Denoting $K = \{(k, \ell) : k, \ell = 1, \dots, m\}$, we consider linear models of the form:

$$\sum_{(k, \ell) \in K} p_{k, \ell} f_{i+(k-1)n, j+(\ell-1)n} = 0 \quad (18)$$

with the normalization $p_{m, m} = 1$.

The first step in the extension algorithm is finding an approximate model M for the given data. As in the 1-D case we do it by a least-squares minimization. Defining $K^- = K \setminus \{(m, m)\}$ we look for model coefficients $P = \{p_{(k, \ell)}\}_{(k, \ell) \in K^-}$ such that

$$I_2(P) = \sum_{(i, j)} \left(\left[\sum_{(k, \ell) \in K^-} p_{k, \ell} f_{i+(k-1)n, j+(\ell-1)n} \right] + f_{i+(m-1)n, j+(m-1)n} \right)^2 \rightarrow \min. \quad (19)$$

As remarked in the introduction, 2-D linear prediction models with constant coefficients describe function spaces which are much richer than sums of exponentials. In fact the space of functions satisfying a given 2-D model is usually of infinite dimension. Hence, the method of

fitting exponentials cannot work here, and we use the above approximation + smoothing algorithm, which does not rely on finding the general solution of sequences satisfying the model.

Let us denote by $g \in M$ a sequence $g = \{g_{i,j}\}_{n_0 \leq i,j \leq n_1}$, $n_0 \leq 0$ and $n_1 \geq N$, satisfying a model M . We would like to find a sequence $g \in M$ such that:

A. $\{g_{i,j}\}_{i,j=0}^N$ approximates the given data sequence $\{f_{i,j}\}_{i,j=0}^N$.

B. g is smooth.

Requirement **A** is reflected in the functional

$$E(g) = \sum_{i,j=0}^N [f_{i,j} - g_{i,j}]^2 \quad (20)$$

while the smoothness requirement **B** is characterized by

$$S(g) = \sum_{n_0+1 \leq i,j \leq n_1-1} Qg_{i,j}, \quad (21)$$

where Q is the following quadratic operator:

$$Qg_{i,j} = [\Delta_{xx}g_{i,j}]^2 + [\Delta_{yy}g_{i,j}]^2 + \frac{1}{4} \{ [\Delta_{xy}g_{i,j}]^2 + [\Delta_{xy}g_{i+1,j}]^2 + [\Delta_{xy}g_{i,j+1}]^2 + [\Delta_{xy}g_{i+1,j+1}]^2 \} \quad (22)$$

with $\Delta_{xx}g_{i,j} = g_{i-1,j} - 2g_{i,j} + g_{i+1,j}$, $\Delta_{yy}g_{i,j} = g_{i,j-1} - 2g_{i,j} + g_{i,j+1}$, and $\Delta_{xy}g_{i,j} = g_{i,j} - g_{i-1,j} - g_{i,j-1} + g_{i-1,j-1}$. We note that the functional $S(g)$ is related to the bi-harmonic operator.

4.1 The bivariate approximation-extension algorithm

1. Find the model parameter P for the data by minimizing I_2 .
2. Define the approximation on D_0 , and its extension into D , as the sequence $g = \{g_{i,j}\}_{n_0 \leq i,j \leq n_1}$ satisfying the model M and minimizing the smooth approximation functional

$$F(g) = S(g) + \mu E(g), \quad g \in M. \quad (23)$$

4.2 Examples of bivariate approximation-extension using a model and a smoothing functional

Unlike the method of fitting exponentials, the algorithm based upon the smooth approximation functional is completely linear. It is important to

note that in the bivariate case, even if we knew g on D_0 , a direct extension of g into the larger domain D by the model would be impossible. Hence, we must solve here for g on the entire mesh in the larger domain D . Of course, the size of the linear system gets larger with the size m of the model and the size of the domain D .

In the following we demonstrate the performance of the proposed algorithm for two test functions:

$$f_3(x, y) = 0.4 \cos(4(x + y)) + 0.6y \sin(3(x - y)) - (x - 2)^2, \quad (24)$$

$$f_4(x, y) = x^2 - y^3 + 2 + x - y + 20 \exp(-(x - 2)^2). \quad (25)$$

In both cases the data is given on a square mesh, of mesh size $h = 0.1$, in $D_0 = [0, 4]^2$, with an added random noise in $[-0.2, 0.2]$. The extension is into a square mesh, of the same mesh size, in $D = [-2, 6]^2$. A 4×4 linear model is computed by (19), and the approximation-extension g is computed by minimizing the smooth approximation functional (23) with $\mu = 100$. The linear system involves a sparse matrix of size 8900×8900 , and the solution is done by MINRES iterations.

For the function f_3 the resulting model coefficients are:

$$P = \begin{pmatrix} -0.0539 & 0.1662 & -0.0964 & -0.7606 \\ 0.3700 & -0.0796 & -0.3966 & -0.4032 \\ -0.2253 & 0.0797 & -0.4422 & 0.2967 \\ -0.1989 & 0.1743 & 0.5024 & 1.0000 \end{pmatrix}.$$

The noisy data of f_3 is shown in Figure 2.5 and the resulting extension is shown in Figure 2.6.

For the function f_4 the resulting model coefficients are:

$$P = \begin{pmatrix} 0.1505 & 0.0772 & 0.1560 & -0.3483 \\ 0.0480 & 0.2556 & 0.1838 & -0.0669 \\ -0.1204 & -0.0840 & -0.0200 & -0.4786 \\ -0.1863 & -0.2081 & -0.3254 & 1.0000 \end{pmatrix}.$$

The non-noisy data of f_4 is shown in Figure 2.7 and the resulting extension is shown in Figure 2.8.

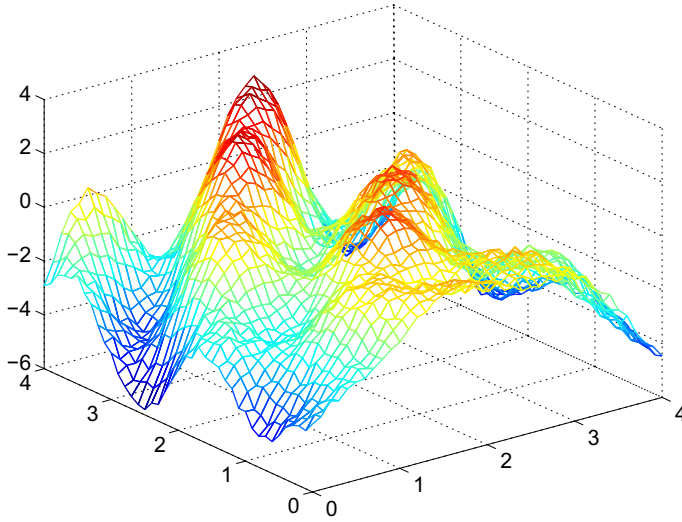


Figure 2.5 The noisy data of f_3 on $D_0 = [0, 4]^2$. For color version of this figure, the reader is referred to the online version of this chapter.

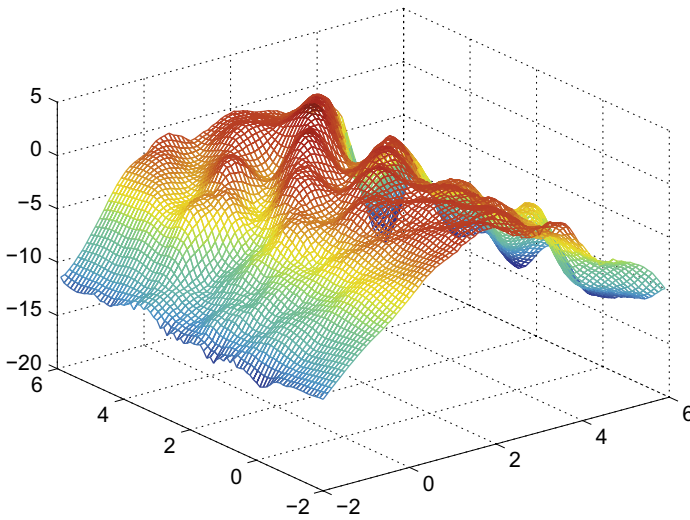


Figure 2.6 Approximation-extension of f_3 on $D = [-2, 6]^2$. For color version of this figure, the reader is referred to the online version of this chapter.

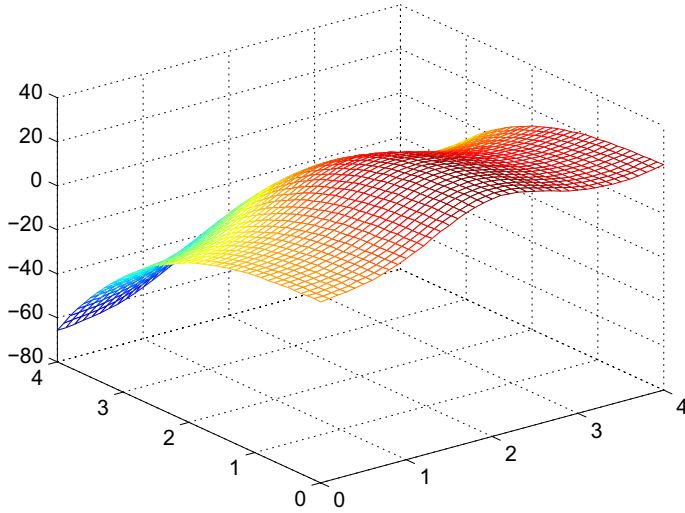


Figure 2.7 The non-noisy data of f_4 on $D_0 = [0, 4]^2$. For color version of this figure, the reader is referred to the online version of this chapter.

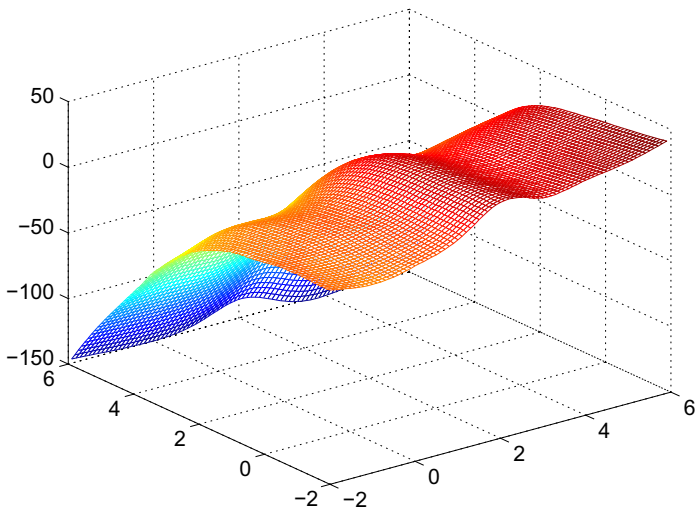


Figure 2.8 Approximation-extension of f_4 on $D = [-2, 6]^2$. For color version of this figure, the reader is referred to the online version of this chapter.



5. EFFICIENT APPROXIMATION-EXTENSION USING MODEL-SPLINE BASIS FUNCTIONS

The two main deficiencies in the above method for smooth approximation-extension are the high complexity in the bivariate case, and the need to find a proper balancing parameter μ between the approximation and the smoothing functionals in (23). In the following we present another method, which is very efficient, and does not involve any balancing parameter. Yet, it is less appropriate for models with varying coefficients, or for more general models. The method is based upon the following simple observation:

Proposition 5.1

Let $P = \{p_{k,\ell}\}_{(k,\ell) \in K}$ represent a linear model with constant coefficients, where K is a finite subset of \mathbb{Z}^2 , and let ϕ be a function of compact support in \mathbb{R}^2 . Consider

$$g(x, y) = \sum_{(i,j) \in \mathbb{Z}^2} c_{i,j} \phi(x - i, y - j), \quad (x, y) \in \mathbb{R}^2, \quad (26)$$

where $\{c_{i,j}\}_{(i,j) \in \mathbb{Z}^2}$ is a bi-infinite sequence satisfying the model, i.e.,

$$\sum_{(k,\ell) \in K} p_{k,\ell} c_{i+k,j+\ell} = 0 \quad \forall (i, j) \in \mathbb{Z}^2. \quad (27)$$

Then, the function g satisfies the model, i.e.,

$$\sum_{(k,\ell) \in K} p_{k,\ell} g(x + k, y + \ell) = 0 \quad \forall (x, y) \in \mathbb{R}^2. \quad (28)$$

Proof

Using the compact support of K and of ϕ ,

$$\begin{aligned} \sum_{(k,\ell) \in K} p_{k,\ell} g(x + k, y + \ell) &= \sum_{(k,\ell) \in K} p_{k,\ell} \sum_{(i,j) \in \mathbb{Z}^2} c_{i,j} \phi(x - i + k, y - j + \ell) \\ &= \sum_{(k,\ell) \in K} p_{k,\ell} \sum_{(r,s) \in \mathbb{Z}^2} c_{r+k,s+\ell} \phi(x - r, y - s) \quad (29) \\ &= \sum_{(r,s) \in \mathbb{Z}^2} \phi(x - r, y - s) \sum_{(k,\ell) \in K} p_{k,\ell} c_{r+k,s+\ell} \\ &= 0. \end{aligned} \quad \square$$

Proposition 5.2

Let $P = \{p_{k,\ell}\}_{(k,\ell) \in K}$ represent a linear model with constant coefficients, where K is a finite subset of \mathbb{Z}^2 , and let ϕ be a function of compact support in \mathbb{R}^2 such that its integer shifts are linearly independent. Consider

$$g(x, y) = \sum_{(i,j) \in \mathbb{Z}^2} c_{i,j} \phi(x - i, y - j), \quad (x, y) \in \mathbb{R}^2. \quad (30)$$

If the function g satisfies the model, i.e., (28) holds, then $\{c_{i,j}\}_{(i,j) \in \mathbb{Z}^2}$ satisfies the model, i.e., (27) holds.

Proof

The proof follows directly from (29) using the linear independence of $\{\phi(x - i, y - j)\}$. □

Remark

The propositions are formulated for the bivariate case, but the results hold in any dimension.

In view of [Proposition 5.1](#) we can easily generate many functions which satisfy a given model by sums of integer shifts of any function ϕ . We look for functions which satisfy a given model and are also smooth, and can form a basis for approximating the data. One possible choice for our problem is to define ϕ as a B-spline (e.g., tensor product) with equidistant knots, of mesh size d . The size d should be chosen so that d -shifts of the B-spline can provide good approximation to the function f we would like to extend. Then, a spline approximation to f will approximately satisfy the same model as f does, and, in view of [Proposition 5.2](#), the B-spline coefficients will also approximately satisfy the same model. The choice of B-splines is natural here in view of the smoothness functionals used above, which are related to splines. In our tests we have used cubic B-splines, and their tensor products. Next, we would like to find a convenient way for generating the space of splines satisfying a model.

5.1 M spline basis functions for approximation-extension

Let us begin with the univariate case. Having decided upon the basis function ϕ as a cubic B-spline, and the parameter d , we would like to construct a basis for all the splines with equidistant knots, of mesh size d , which satisfy a given model. Here again we assume, w.l.o.g., that $d = 1$.

We consider coefficients satisfying a univariate model M of order m of the form

$$c_{i+m+1} = \sum_{k=1}^m p_k c_{i+k}, \quad i \in \mathbb{Z}. \quad (31)$$

For convenience we denote by $\{c_i\} \in M$ a sequence satisfying the model. Viewing (31) as a prediction model, any vector of m initial values $\{c_i\}_{i=r}^{r+m-1}$ generates a sequence satisfying (31) for $i \geq r$. A basis for all the sequences $\{c_i\} \in M$ for $i \geq r$ may be obtained by using m independent initial vectors, e.g., the standard basis vectors $e^{(j)} = \{\delta_{i,j}\}_{i=1}^m$, $j = 1, \dots, m$. For an approximation in $[0, N]$, using the standard cubic B-spline representation, we need the coefficients $\{c_i\}_{i=-1}^{N+1}$. We thus generate a basis of m sequences $\{c_i^{(j)}\} \in M$, for $i \geq -1$, by m independent vectors of initial condition $\{c_i^{(j)}\}_{i=-1}^{m-2} = e^{(j)}$, $j = 1, \dots, m$. The m spline functions corresponding to these m sequences are

$$S_j(x) = \sum_{i=-1}^{N+1} c_i^{(j)} B(x-i), \quad j = 1, \dots, m. \quad (32)$$

By Proposition 5.1, any $g \in \text{span}\{S_j\}_{j=1}^m$ satisfies the model M . We call such g an M spline. Therefore, all we need to do for the approximation-extension procedure is to find $g \in \text{span}\{S_j\}_{j=1}^m$ which best approximates the given data. To demonstrate the method we go back to the previous examples, with noisy data for the test functions f_1 and f_2 , with $m = 6$. First, we present plots of the M spline basis functions $\{S_j\}_{j=1}^6$, corresponding to the model found for f_1 in Figure 2.9, and for f_2 in Figure 2.10. One can already see the behavior of f_1 and of f_2 living in their corresponding basis functions. The approximation-extension using these basis functions is depicted in Figure 2.11.

Remark

The above approach is both faster in application and is parameters' free. The smoothness is determined directly by the choice of the basis function ϕ .

5.1.1 M spline basis functions for the bivariate case

The main motivation for using the basis functions' approach is the high complexity involved in the application of the smoothing approach in 2-D. Consider an $m \times m$ order bivariate model of the form (18). W.l.o.g.,

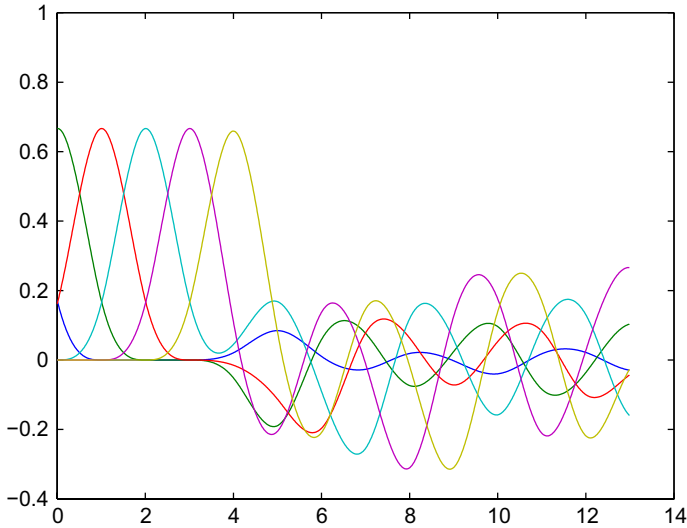


Figure 2.9 $\{S_j\}_{j=1}^6$ for the model found for f_1 . For color version of this figure, the reader is referred to the online version of this chapter.

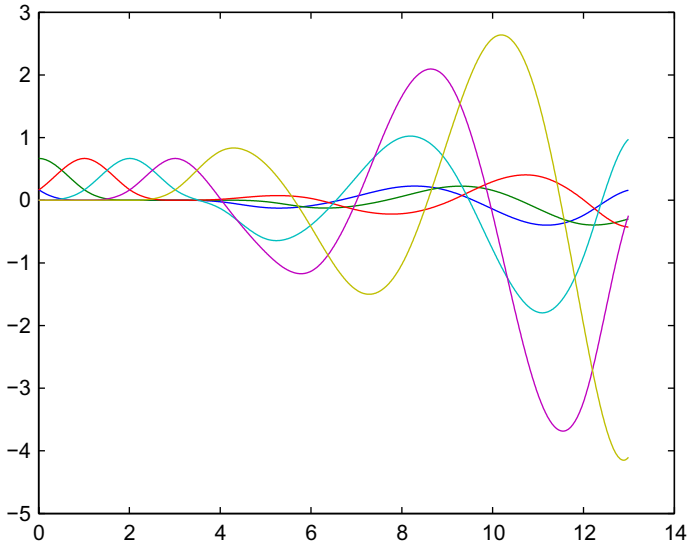


Figure 2.10 $\{S_j\}_{j=1}^6$ for the model found for f_2 . For color version of this figure, the reader is referred to the online version of this chapter.

we would like to form a basis for all the tensor-product bi-cubic splines, with integer knots, which satisfy the model on $[0, N]^2$. Any such bi-cubic spline can be written as

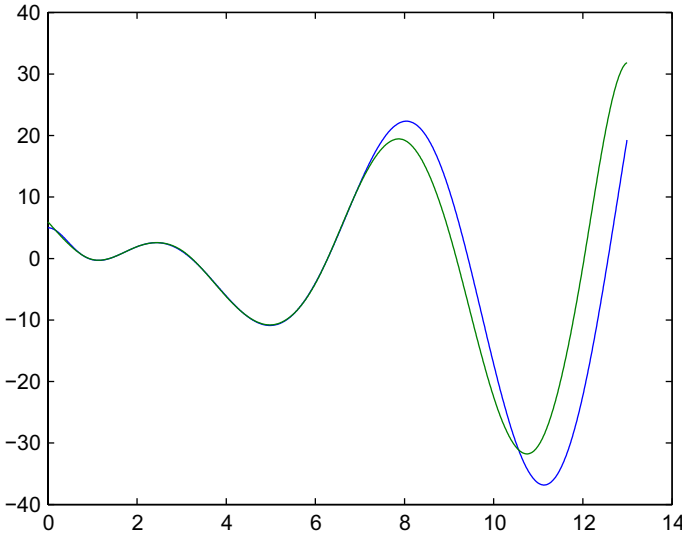


Figure 2.11 Approximation-extension of f_2 using the model-spline basis. For color version of this figure, the reader is referred to the online version of this chapter.

$$S(x, y) = \sum_{i,j=-1}^{N+1} c_{i,j} B(x-i) B(y-j). \quad (33)$$

According to [Propositions 5.1 and 5.2](#), the coefficients $\{c_{i,j}\}$ should satisfy the model. I.e.,

$$\sum_{1 \leq k, \ell \leq m} p_{k, \ell} c_{i+k, j+\ell} = 0 \quad \text{with} \quad p_{m, m} = 1. \quad (34)$$

Let $L = \{(i, j) \mid -1 \leq i \vee j \leq m-1\}$ denote the $m-1$ layers of indices along the bottom and the left boundary of the set of indices $\{(i, j)\}_{i,j=-1}^{N+1}$. Given any boundary values for $\{c_{i,j}\}_{(i,j) \in L}$, we can use the above model to fill out the rest of the coefficients by:

$$c_{i+m, j+m} = - \sum_{1 \leq k, \ell \leq m; (k, \ell) \neq (m, m)} p_{k, \ell} c_{i+k, j+\ell}, \quad i, j = 0, \dots, N-m+1. \quad (35)$$

Hence, the space of all the tensor-product bi-cubic splines, with integer knots, which satisfy the model on $[0, N]^2$ is of dimension $\#(L)$. A basis to this space can be generated, as in the univariate case, by taking a basis for the space $V_L = \{c_{i,j} \mid (i, j) \in L\}$, extending each vector in the basis by (35), and using the resulting coefficients to define a basis function by (33).

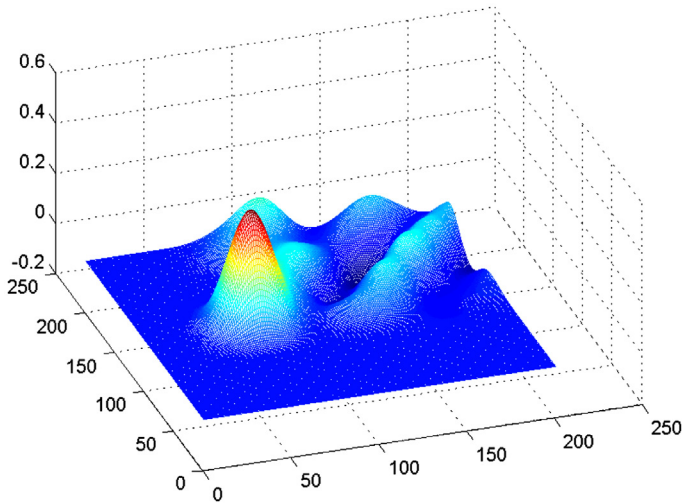


Figure 2.12 One of the model-spline basis functions for reconstructing f_3 . For color version of this figure, the reader is referred to the online version of this chapter.

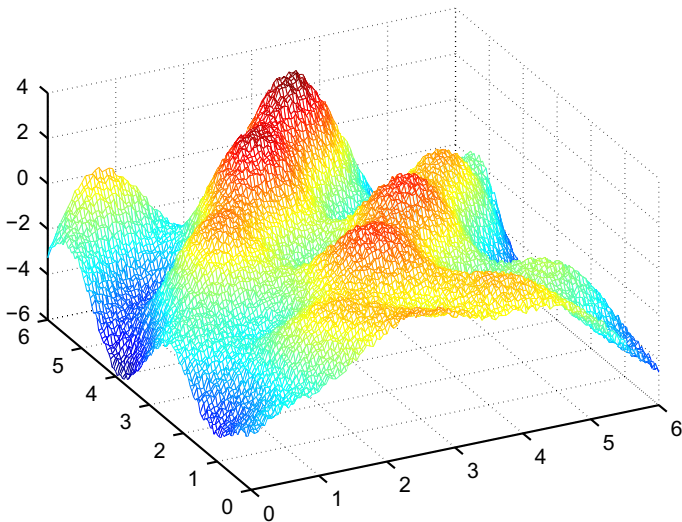


Figure 2.13 The noisy data for f_3 . For color version of this figure, the reader is referred to the online version of this chapter.

In the following we go back to the bivariate example with noisy data for f_3 , now with a 6×6 model. In this case the dimension of the approximating space of spline functions satisfying the model is 85. To get the feeling of the M spline basis functions involved we plot one of them in [Figure 2.12](#). In [Figure 2.13](#) we see the given data, in [Figure 2.14](#) the approximation to the data by the spline basis functions, and in [Figure 2.15](#) the extension into a larger domain.

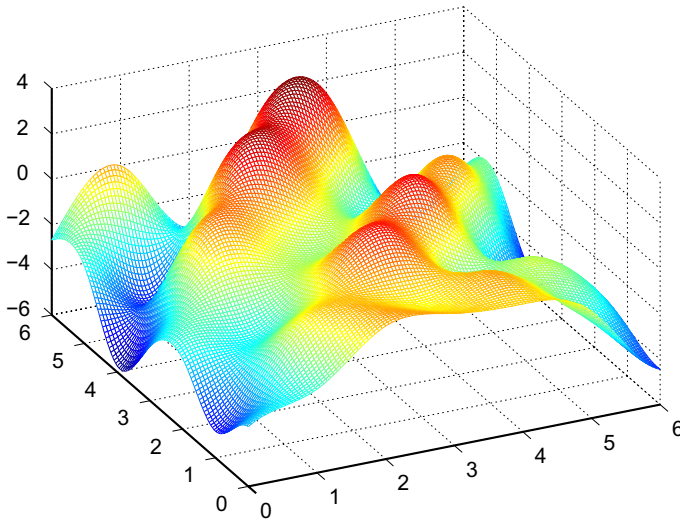


Figure 2.14 The approximation of f_3 by model-splines f_3 . For color version of this figure, the reader is referred to the online version of this chapter.

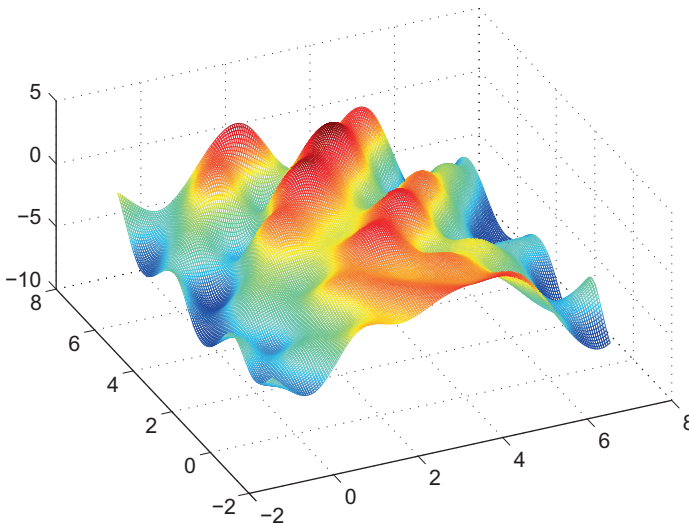


Figure 2.15 The extension of f_3 by model splines. For color version of this figure, the reader is referred to the online version of this chapter.

5.2 Interpolation between models

In all the above examples we have demonstrated methods for functions' extensions which preserve their behavior. Now we consider the possibility of generating a smooth extension of a function which blends its behavior

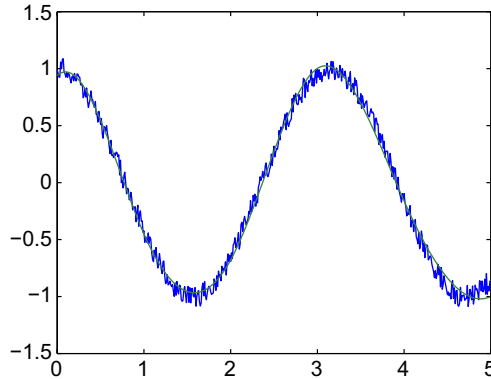


Figure 2.16 The approximation of the data of $\cos(2x)$ by the blended model. For color version of this figure, the reader is referred to the online version of this chapter.

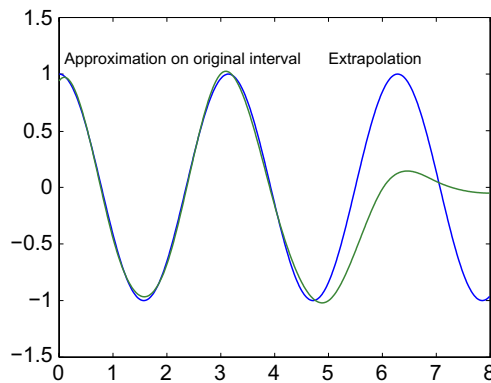


Figure 2.17 The approximation of $\cos(2x)$ extended to decay as e^{-2x} . For color version of this figure, the reader is referred to the online version of this chapter.

into another desired behavior. This seems a whole project by itself, but with the tools presented in this work we can already present a basic method and an example which illustrate the potential of this direction. We consider the univariate case, and start by fitting a model to a given data on $[a, b]$. Denoting this model by M_1 , we would like to approximate the data by a smooth function on $[a, b]$, and extend this approximation into $[b, c]$, so that the behavior model will change smoothly from M_1 on $[a, b]$ to another behavior M_2 on $[b, c]$.

We assume that both models are linear and of the same order m . The simple idea is to define a linear model M on $[a, c]$ that is a blending of the two models. In [Figure 2.16](#) we depict the noisy data

of $f(x) = \cos(2x)$ on $[0, 5]$. Computing a linear model of order 4, with constant coefficients, for this data yields the coefficients of M_1 : $P = \{0.0803, 0.6555, -0.4325, -0.2470, -1.0000\}$. We have chosen M_2 to be the model for the function $f(x) = e^{-2x}$. The corresponding model coefficients are: $P = \{0, 0, 0.0178, 0.0024, -1.0000\}$. We now define a linear model with linear coefficients (as in (1)), by a linear interpolation between the corresponding coefficients of the two models, such that it agrees with M_1 at $x = 0$ and with M_2 at $x = 8$. The resulting model is of the form (1) with $u(x) = x$, and we can use it as in Section 3.3 to define the approximation extension of the data. The result is shown in Figure 2.17.

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REFERENCES

1. Levin, David Development of Non-linear Transformations for Improving Convergence of Sequences. *Int. J. Comput. Math.* **1973**, 3 (1), 371–388.
2. Levin, David On Accelerating the Convergence of Infinite Double Series and Integrals. *Math. Comput.* **1980**, 35 (152), 1331–1345.
3. Levin, David; Sidi, Avram Two New Classes of Nonlinear Transformations for Accelerating the Convergence of Infinite Integrals and Series. *Appl. Math. Comput.* **1981**, 9 (3), 175–215.
4. Smyth, G. K. M. R.; Osborne, M. R. A Modified Prony Algorithm for Exponential Function Fitting. *SIAM J. Sci. Statist. Comput.* **1995**, 16, 119–138.
5. Prony, R. Essai experimental et analytique: sur les lois de la dilatabilite de fluides elastique et sur celles de la force expansive de la vapeur de l'alkool, a differentes temperatures. *J. L'Ecole Polytech. (Paris)* **1795**, 1 (22), 24–76.
6. Shanks, D. Non-linear Transformations of Divergent and Slowly Convergent Sequences. *J. Math. Phys.* **1955**, 34, 1–42.
7. Sidi, A. *Practical Extrapolation Methods*; Cambridge University Press