Applied Mathematics and Computation 258 (2015) 220–226

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Direct meshless kernel techniques for time-dependent equations

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ARTICLE INFO

Keywords:
Partial differential equation
Expansion kernels
Heat kernel
Trefftz methods

ABSTRACT

We provide a class of positive definite kernels that allow to solve certain evolution equations of parabolic type for scattered initial data by kernel-based interpolation or approximation, avoiding time intergation completely. Some numerical illustrations are given.

1. Introduction

There are plenty of application papers in which kernels or radial basis functions are successfully used for solving partial differential equations by meshless methods. The usage of kernels is typically based on spatial interpolation at scattered locations, writing the trial functions "*entirely in terms of nodes*"[2]. For *stationary* partial differential equations, the discretization can take pointwise analytic derivatives of the trial functions to end up with a linear system of equations. This started in [6] and was pursued in the following years, including a convergence theory in [8]. There are also variations that use weak data, like the Meshless Local Petrov–Galerkin method [1] with a convergence theory in [10]. For the potential equation, there are special kernels that allow the use of trial functions that satisfy the differential equation exactly [9,5]. This is a variation of the general idea of Trefftz [13] to use trial functions that satisfy the PDE exactly.

For *time-dependent* partial differential equations, meshless kernel-based methods were similarly based on a fixed spatial interpolation, but now the coefficients are time-dependent, and one obtains a system of ordinary differential equations for these. This is the well-known *Method of Lines*, sometimes also called *differential quadrature*, and it turned to be experimentally useful in various cases (see e.g. [14,7,4,12]). But we follow the Trefftz philosophy here and use special kernels that satisfy a linear evolution-type PDE

$$u_t(x,t) = Lu(x,t) \tag{1.1}$$

with a purely spatial and elliptic operator L *exactly*. This will eliminate time integration, but at the expense of using time-dependent kernels that consists expansions into eigenfunctions of the spatial differential operator L with time-dependent coefficients. Of course, this is a special case of a *spectral* method, conveniently stated in terms of a time-dependent positive definite kernel.

We give a rigid error analysis of this technique and provide a few numerical examples.

Instead of using trial functions that satisfy the boundary conditions but violate the differential equation, we approximate the solution by selecting functions that violate the boundary conditions but satisfy the differential equation.

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http://dx.doi.org/10.1016/j.amc.2014.12.140

2. Linear elliptic equations

We take a spatial domain $\Omega \subset \mathbb{R}^d$ and some kind of homogeneous boundary condition on $\partial\Omega$. Then, for a linear self-adjoint elliptic differential operator L, we assume to have eigenfunctions u_n on Ω for the associated boundary value problem, i.e.

$$Lu_n = \lambda_n u_n \text{ in } \Omega, \quad n \in N \tag{2.1}$$

with a countable index set N. Our running example will be $L = \Delta$ on $\Omega = [0, \pi]^d$ with homogeneous Dirichlet boundary conditions, leading to

$$u_k(x) = \prod_{i=1}^{d} \sin(k_i x_i), \quad \lambda_k = -\|k\|_2^2, \quad k \in N := \mathbb{N}_0^d \setminus \{0\} \tag{2.2}$$

in standard multi-index notation.

A solution of the problem

$$Lu = f$$

with homogeneous boundary conditions can then be written formally by expanding f into the eigenfunctions as

$$f = \sum_{n\in N} \alpha_n u_n$$

and then writing the solution u as

$$u = \sum_{n\in N} \frac{\alpha_n}{\lambda_n} u_n.$$

This needs a discussion of convergence of the series. We shall do this in a way that is closely linked to reproducing kernel Hilbert spaces.

3. Expansion kernels

We now fix positive real numbers μ_n for all $n \in N$ to let an *expansion kernel*

$$K_\mu(x, y) := \sum_{n\in N} \mu_n u_n(x) u_n(y) \tag{3.1}$$

satisfy the summability condition

$$K_\mu(x, x) = \sum_{n\in N} \mu_n u_n(x)^2 \leqslant C^2 < \infty \text{ for all } \quad x \in \Omega.$$

This kernel is *positive semidefinite* on Ω, i.e. for all selections of finite point sets $X = \{x_1, \ldots, x_M\} \subset \Omega$, the $M \times M$ *kernel matrices* $A = A(X)$ with entries $K_\mu(x_j, x_k),\ 1 \leqslant j, k \leqslant M$ are symmetric and positive semidefinite.

By well-known results [3], such a kernel is reproducing in the Hilbert space H_μ of all functions of the form

$$f_c(x) := \sum_{n\in N} c_n u_n(x), \quad x \in \Omega$$

under the condition

$$\|f_c\|_\mu^2 := \sum_{n\in N} \frac{c_n^2}{\mu_n} < \infty$$

related to the inner product

$$(f_c, f_d)_\mu := \sum_{n\in N} \frac{c_n d_n}{\mu_n}$$

letting the reproduction follow the formula

$$f_c(x) = (f_c, K_\mu(x, \cdot))_\mu \text{ for all } \quad x \in \Omega, \quad f_c \in H_\mu.$$

Note that this gives us a variety of Hilbert spaces that are isomorphic to weight ℓ_2 spaces [3], and we shall check now how L maps functions between these spaces. Taking $u \in H_\mu$ with coefficients c_n, we get that Lu has coefficients $\lambda_n c_n$, and thus

$$L:\ H_\mu \to H_{\mu/\lambda^2}$$

allows to look at solutions of $Lu = f$ for various regularity assumptions. Here, we denote the sequence with values $\frac{\mu_n}{\lambda_n^2}$ by μ/λ^2 for short.

We require the initial function u_0 to be in H so that, by definition of the Hilbert space H, it necessarily has an expansion

$$u_0(x) = \sum_{n\in N}\gamma_n u_n(x)$$

with

$$\|u_0\|_H^2 = \sum_{n\in N}\frac{\gamma_n^2}{\mu_n} < \infty.$$

The basic idea now is to construct a time-dependent kernel K satisfying the differential equation exactly. We do this by defining

$$K(x,y,t) := \sum_{n\in N}\mu_n(t)u_n(x)u_n(y), \quad x,\ y\in\Omega, \quad t \geqslant 0$$

with initial conditions

$$\mu_n(0) = \mu_n, \quad n\in N$$

leading to

$$K(x,y,0) = K_0(x,y) \text{ for all } \quad x,y\in\Omega.$$

To let the differential equation be satisfied in the sense

$$K_t(x,y,t) = L^x K(x,y,t) \text{ for all } \quad x,\ y\in\Omega, \quad t\geqslant 0$$

where the superscript x indicates that L acts on the variable x, we have to satisfy

$$\sum_{n\in N}\mu_n'(t)u_n(x)u_n(y) = \sum_{n\in N}\mu_n(t)L^x u_n(x)u_n(y) = \sum_{n\in N}\mu_n(t)\lambda_n u_n(x)u_n(y)$$

and this leads to the ordinary differential equations

$$\mu_n{}'(t) = \mu_n(t)\lambda_n$$

with the solution

$$\mu_n(t) = \mu_n\exp(\lambda_n t), \quad t\geqslant 0, \quad n\in N.$$

Thus our kernel is

$$K(x,y,t) = \sum_{n\in N}\mu_n\exp(\lambda_n t)u_n(x)u_n(y), \quad x,\ y\in\Omega, \quad t\geqslant 0$$

and in case of positive eigenvalues we need the condition

$$\sum_{n\in N}\mu_n\exp(\lambda_n T)u_n(x)^2 < \infty \text{ for all } \quad x\in\Omega$$

to be able to work in $[0,T]$. This approach generalizes the standard *heat kernel*. Note that elliptic operators will have negative eigenvalues in (2.1), and then the coefficients $\mu_n(t)$ will decay with increasing time.

4. Interpolatory methods

Since we have a positive semidefinite kernel K_0 on the spatial domain, we can choose a set $X = \{x_1,\ldots,x_M\}\subset\Omega$ of points in Ω and interpolate the initial function u_0 by a linear combination of the functions $K_0(x,x_m),\ 1\leqslant m\leqslant M$ via the linear system

$$u_0(x_i) = \sum_{m=1}^{M}\alpha_m K_0(x_i,x_m) \tag{4.1}$$

for $1\leqslant i\leqslant M$. If the initial function u_0 lies in H, this problem is solvable, though the kernel matrix is only positive semidefinite. We then define

$$\tilde{u}(x,t) := \sum_{m=1}^{M}\alpha_m K(x,x_m,t)$$

to see that the differential equation and the boundary conditions are satisfied.

The error satisfies the differential equation and the boundary conditions. Thus the error is exactly the evolution of the initial error under the differential equation. If the maximum principle holds, the error for all positive times is thus bounded by the L_∞ interpolation error $\|\tilde{u}(\cdot,0) - u_0\|_\infty$ at startup. A theoretical analysis of this error requires an application of kernel interpolation theory to $K(x,y,0)$.

The choice of the weights in the kernel series (3.1) will depend on the smoothness of the starting function u_0, since kernel interpolation theory [15,11] tells us that the smoothness of the kernel $K(x,y,0)$ should be not lower than the smoothness of the function supplying the data. And since, for example, the smoothness of the functions generated by trigonometric series is related to the decay of the coefficients, the smoothness of $K(x,y,0)$ will usually be controlled by decay of the λ_k.

Direct interpolation of initial data by linear combinations of eigenfunctions is not possible in general. The use of kernels always allows interpolation.

5. Examples

We start the simple example from (2.2) here.

The choice $\mu_k = 1/k!$ gives a series which generates an analytic kernel plotted in Fig. 5.1. It has an explicit representation

$$4K(x,y,0) = \exp(\exp(\pi(x+y))) + \exp(\exp(-\pi(x+y))) - \exp(\exp(\pi(x-y))) - \exp(\exp(-\pi(x-y)))$$

which unfortunately suffers from severe cancelation. But the rapid convergence of the series (3.1) allows to sum the series up until the limit of double precision is reached, i.e. at $k = 19$. This will, however, lead to inevitable rank loss in (4.1) for more than $n = 19$ data points. Nonetheless, and in particular if the initial function u_0 is very smooth, there are usually good projections of the right-hand side into the column space of the matrix, leading to pretty good results. Fig. 5.2 shows an example for the starting function $u_0(x) = 1 - 2|x - 0.5|$ using only 12 interior points. The error is bounded by the visible difference of the starting function and its first interpolant.

By simple spectral shifts, this example generalizes to the case $Lu = \Delta u + \kappa u$, and similarly for other spatial operators that have known eigenfunction expansions.

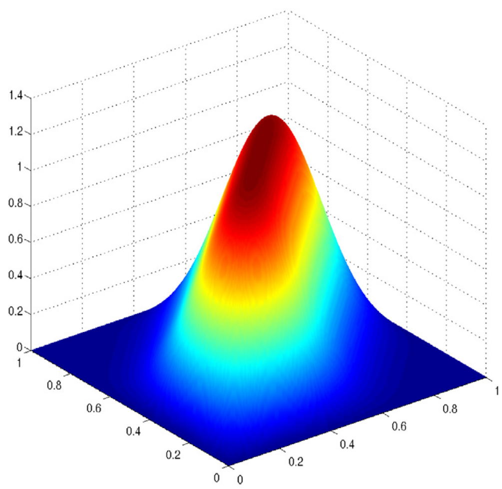
If one tries to solve the heat equation backwards this way, the solution must increase exponentially. Fig. 5.3 shows two examples:

- starting with $u_0(x) = x(1-x)$ up to time $t = -0.005$ in steps of 0.0001,
- starting with $u_0(x) = 1 - 2|x - 0.5|$ up to time $t = -0.001$ in steps of 0.0001.

The final example concerns the wave equation. The time-dependent part now is

$$\mu_n(t) = \mu_n(0)\cos(\lambda_n t) = \frac{1}{n!}\cos(n\pi t)$$

in this case, using (2.2) in the spatial variables. The result is in Fig. 5.4 for $u_0(x) = 1 - 2|x - 0.5|$ and times up to $t = 1$ in steps of 0.05. Note that the wave starts with the interpolant and reflects back to it.



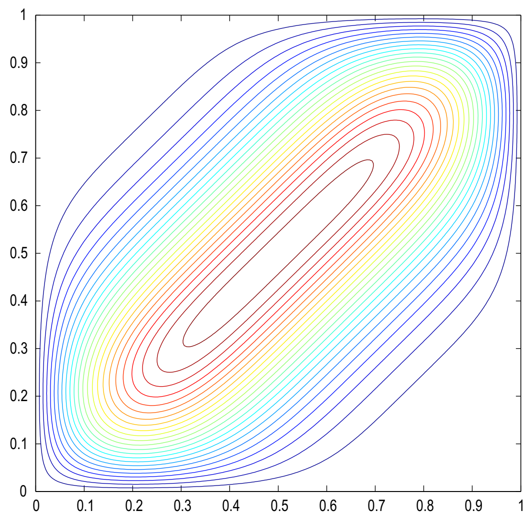


Fig. 5.1. Kernel with weights $1/n!$.

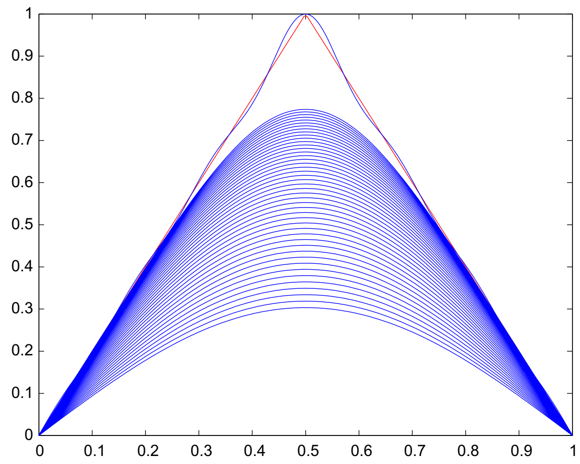


Fig. 5.2. Solution of heat equation.

6. Extensions

This approach generalizes to other cases where separation of variables works, e.g. for the wave equation. If there is a linear differential operator D acting with respect to time, the problem $Du(x,t) = Lu(x,t)$ can be split into eigenvalue problems

$$Dv_n(t) = \lambda_n v_n(t), \quad Lu_n(x) = \lambda_n u_n(x),$$

for appropriate homogeneous boundary conditions, and we can define a kernel

$$K(x,y,t) := \sum_n \mu_n u_n(x) u_n(y) v_n(t)$$

under the summability condition

$$K(x,x,t) = \sum_n \mu_n u_n^2(x) |v_n(t)| < \infty$$

To make interpolation at $t = 0$ work, additional conditions must be satisfied. In case of the wave equation $u_{tt} = \Delta u$, we use trial functions

$$u(x,t) := \sum_{j=1}^N a_j K(x,x_j,t) + \sum_{j=1}^N b_j K_t(x,x_j,t)$$

since for a useful initial-value problem we have to prescribe both $u(x,0)$ and $u_t(x,0)$. On the spatial domain $[0,\pi]$ we can use $u_n(x) = \sin(nx)$ and $v_n(t) = \cos(nt)$ to form kernels. We pose interpolation conditions

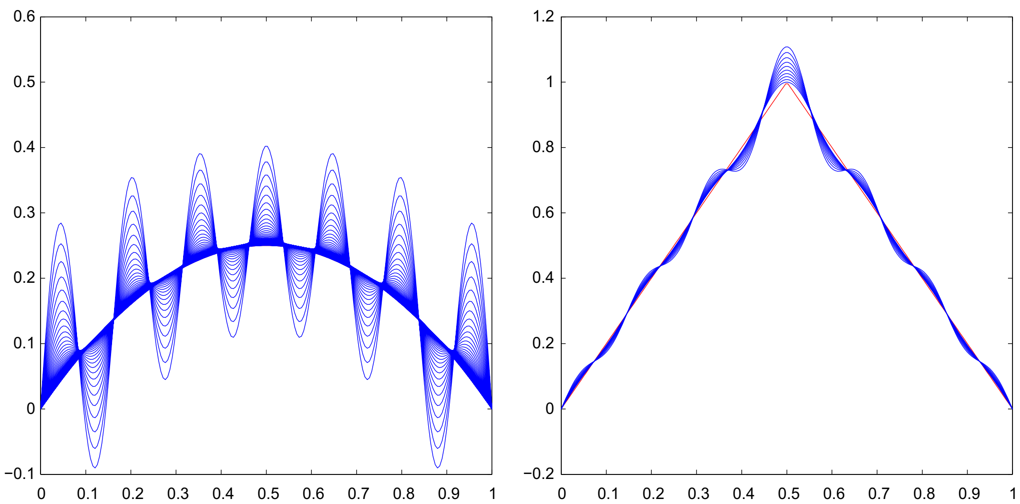


Fig. 5.3. Two backward calculations.

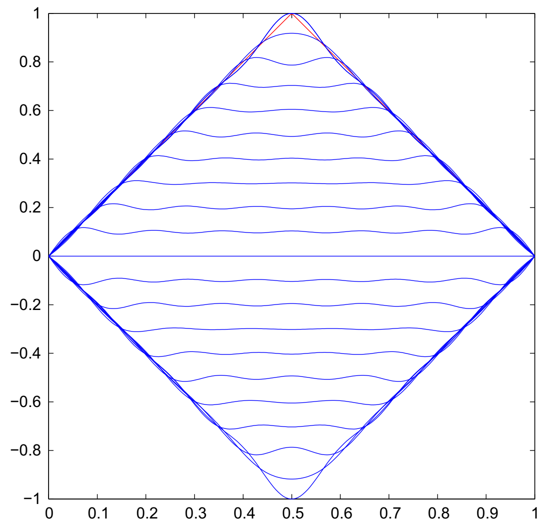


Fig. 5.4. Solution of wave equation.

$$u(x_k,0)=\sum_{j=1}^{N}a_jK(x_k,x_j,0)+\sum_{j=1}^{N}b_jK_t(x_k,x_j,0)=\sum_{j=1}^{N}a_jK(x_k,x_j,0)$$
$$u_t(x_k,0)=\sum_{j=1}^{N}a_jK_t(x_k,x_j,0)+\sum_{j=1}^{N}b_jK_{tt}(x_k,x_j,0)=\sum_{j=1}^{N}b_jK_{tt}(x_k,x_j,0)$$

that simplify because of $v_n')=0$ and thus $K_t(x,y,0)=0$. The kernels K and

$$K_{tt}(x,y,t)=\sum_n \lambda_n\mu_n u_n(x)u_n(y)v_n(t)$$

are both positive definite, and the interpolation problem is solvable.

7. Conclusion

Based on the recent successful development of meshless computational methods using direct kernel-based approximation techniques for solving various kinds of partial differential equations, we give in this paper a class of positive definite kernels that allow the extension of the methods to solve certain kinds of evolution equations of parabolic type. Similar to the theoretical development of finite element method, the future works will be devoted to the extension to solve equations of hyperbolic type.

Acknowledgement

The work described in this paper was supported by a grant from the City University of Hong Kong, Hong Kong (Project No. ARG 9667078).

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.amc.2014.12.140.

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