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Abstract

The problem of fitting surfaces to data is a well studied problem in statistics. However when there is prior information the theory is not developed. It often happens in toxicology and in medicine that the effect of a single drug is well understood. However if a pair of drugs is delivered in tandem or if two toxins are interacting the effect is not understood. In this paper we attack the problem of fitting a surface to a data set contained in a square when two of the boundaries

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are known. Our approach generalizes the concept of control theoretic splines.

1 Introduction

The theory of approximation of functions of one variable is one of the most studied areas in mathematics and statistics. To this end the theory of polynomial splines and, more recently, the theory of control theoretic splines, [7, 5, 8, 2], has been extensively developed and used in applications. In statistics the method of smoothing splines has been developed based on the work of Grace Wahba [6], and her collaborators. Common to all splines is a data set of the form

$$D = \{(t_i, \alpha_i) : \ i = 1, \cdots, N\}$$

and a scheme to construct a function $y(t)$ such that either $y(t_i) = \alpha_i$ or $y(t_i) - \alpha_i$ is small in some precise sense.

Control theoretic splines were developed originally as a tool for control theory to be used in such problems as path planning in robotics and terminal area control of aircraft, [7, 1]. The idea was to use a controlled differential equation to push a curve through a set of desired points. This is not far from the original idea of splines and is very close to the development of smoothing splines developed by Wahba. Here the idea is to use a system of the form

$$\dot{x} = Ax + bu, \quad y = cx$$

and then to choose a cost function that controls the input function u. The original development of splines used the following:

$$\ddot{x}(t) = u(t), \quad y = x$$

with $y(t_i) = \alpha_i$ and $\sup_t |u(t)|$ is minimized. Smoothing splines used a quite different concept of "small". In Wahba's original formulation the idea was to solve the following optimization problem:

$$\min_u \left[\int_0^T u^2(t)dt + \sum_{i=1}^{N} (y(t_i) - \alpha_i)^2 \right]$$

where

$$\ddot{x} = u, \quad y = x.$$

These two problems are quite different but have almost the same solution. In fact both problems are solved in a suitable Hilbert space.

In this paper we use the techniques of optimal splines to develop a method of fitting surfaces to data. We do not consider the classical problem of fitting a surface to data points but consider a problem that arises in testing drugs and also arises in toxicology. We often know the effect of a single drug or toxin on some biomarker, but little may be known about the effect of combining two drugs or what the effect of the two drugs will be on the same biomarker. It is often that we have need to know what mixture of the two drugs will be the most effective. Thus we are presented with a problem of surface fitting in which we know a great deal about the boundary of the surface but know little about the interior. The cost of doing multiple experiments with combinations of drugs is expensive in time and laboratory costs. Thus there may be only a few points known in the interior region. We will use the techniques of control theoretic splines to construct such surfaces.

In Section 2 we recall Wahba's smoothing splines, and see that these can be obtained from a variational approach. In Section 3 we formulate the surface fitting problem as a problem in the control of partial differential equations and show that the problem reduces to finding the Green's function for the bilaplacian with nonstandard boundary conditions.

2 Splines in one dimension

We start with a recollection of Wahba's smoothing splines. The given data is $\{x_i, \alpha_i\}_{i=1}^N$. Let $\lambda > 0$ be a fixed constant. The problem is to minimize the entity

$$\frac{\lambda}{2}\int_0^1 u(x)^2\,dx + \frac{1}{2}\sum_{i=1}^N (w(x_i) - \alpha_i)^2 \tag{1}$$

among the solutions of

$$w^{(2)} = u, \tag{2}$$

where $u \in L^2([0,1])$ is an unknown function. In our two dimensional problem we will have prescribed boundary values on some part of the boundary, and have unprescribed values at some other part. To prepare for this situation, we assume that the boundary at $x = 0$ is fixed. For simplicity we choose $w(0) = 0$. At $x = 1$ we leave w unspecified.

Since $u \in L^2$, it will be convenient to work in the Sobolev space $H^2(0,1) = W^{2,2}(0,1)$, which is the closure of $C^\infty(0,1)$ in the norm

$$\|w\|_{H^2} = \left(\int_0^1 \left(w(x)^2 + w^{(1)}(x)^2 + w^{(2)}(x)^2 \right) dx \right)^{1/2}.$$

We will refer to $H^2(0,1)$ simply as H. As is customary, we identify $w \in H^2(0,1)$ which are equal almost everywhere. Moreover, our boundary condition requires that we look for solutions w in the space H which is the closure of

$$\{w \in C^\infty(0,1);\ w \equiv 0 \text{ in some interval } (0,\delta)\}$$

in the H^2-norm.

By substituting 2 into 1, we see that the problem is equivalent to that of minimizing

$$J(w) = \frac{\lambda}{2} \int_0^1 w^{(2)}(x)^2\, dx + \frac{1}{2} \sum_{i=1}^N \left(w(x_i) - \alpha_i\right)^2$$

among all functions in H.

Let $v \in C^\infty(0,1)$ be a fixed function such that $v \equiv 0$ on some interval $(0,\delta)$. Then for each $\epsilon > 0$, the functions $w + \epsilon v \in H$. Moreover,

$$\frac{d}{d\epsilon} J(w+\epsilon v)|_{\epsilon=0} = \lambda \int_0^1 w^{(2)}(x) v^{(2)}(x)\, dx + \sum_{i=1}^N \left(w(x_i) - \alpha_i\right) v(x_i).$$

If $J(w)$ is minimal, the derivative has to vanish. After two integrations by part we then have

$$\lambda \left(w^{(2)}(1) v^{(1)}(1) - w^{(3)}(1) v(1) + \int_0^1 w^{(4)}(x) v(x)\, dx \right) + \sum_{i=1}^N \left(w(x_i) - \alpha_i\right) v(x_i) = 0$$

Since v is arbitrary, we see that w has to satisfy the equation

$$w^{(4)} = 0 \qquad \text{in } (0,1) \setminus \cup_{i=1}^N \{x_i\}, \tag{3}$$

and the boundary conditions

$$\begin{aligned} w(0) &= w^{(1)}(0) = 0 \\ w^{(2)}(1) &= w^{(3)}(1) = 0. \end{aligned}$$

At the points x_i, we have the conditions

$$\lambda\left(w^{(3)}(x_i+) - w^{(3)}(x_i-)\right) = -(w(x_i) - \alpha_i). \tag{4}$$

Thus, we see that the problem reduces to finding solutions to 3 in each subinterval $(0, x_1)$, (x_i, x_{i+1}) and $(x_N, 1)$. These solutions are third degree polynomials, which at the points x_i are fit together so that w is a C^2 function with jumps in the third derivative given by 4.

3 Surface fitting in two dimensions

Given two real functions f and g, defined on the interval $[0, 1]$ and data points $\{x_i, y_i, \alpha_i\}$, where $(x_i, y_i) \in S = (0, 1) \times (0, 1)$, $i = 1 \ldots N$, we would like to find a function $w(x, y) \in C^2([0, 1] \times [0, 1])$ such that

$$\Delta w = u,$$

which satisfies the boundary values $w(x, 0) = f(x)$ and $w(0, y) = g(y)$. Moreover, we would like to pick the one solution such that, for a fixed number $\lambda > 0$, the entity

$$\lambda \int_0^1 \int_0^1 u(x, y)^2 \, dx \, dy + \sum_{i=1}^{N} (w(x_i, y_i) - \alpha_i)^2$$

is minimal.

The space we work in is the Sobolev space $H^2(S)$, which is the closure of $C^\infty(S)$ in the norm

$$\|w\|_{H^2} = \left(\sum_{|\alpha| \leq 2} \int_0^1 \int_0^1 |D^\alpha w|^2 \, dx \, dy \right)^{1/2}.$$

As before, we identify $w \in H^2(S)$ which are equal almost everywhere. The boundary conditions require that we seek solutions w in the affine subspace M of $H^2(S)$, which is the closure of

$$\{w \in C^\infty(S);\ w \equiv 0 \text{ in a neighborhood of the axes } x = 0 \text{ and } y = 0\}.$$

As in Section 2, we bypass the control u, and minimize the functional

$$J(w) = \frac{\lambda}{2} \int_0^1 \int_0^1 (\Delta w)^2 \, dx \, dy + \frac{1}{2} \sum_{i=1}^{N} (w(x_i, y_i) - \alpha_i)^2$$

among all functions $w \in M$.

Let $v \in C^\infty(S)$ be such that $v \equiv 0$ in a neighborhood of the axes $x = 0$ and $y = 0$. Then the comparison functions $w + \epsilon v$ are also in M, and if $J(w)$ is minimal we must have

$$\frac{d}{d\epsilon} J(w + \epsilon v)|_{\epsilon=0} = 0,$$

i.e.

$$\lambda \int_0^1 \int_0^1 \Delta w \Delta v \, dx \, dy + \sum_{i=1}^N (w(x_i, y_i) - \alpha_i) \, v_i(x) = 0.$$

After two integrations by part, we then have

$$\lambda \left(\int_{\partial S} \Delta w \nabla v \cdot \mathbf{n} \, ds - \int_{\partial S} \nabla(\Delta w) \cdot \mathbf{n} \, v \, ds \right.$$
$$\left. + \int_0^1 \int_0^1 \Delta^2 w \, v \, dx \, dy \right) + \sum_{i=1}^N (w(x_i, y_i) - \alpha_i) \, v(x_i) = 0,$$

where $\mathbf{n}$ is the outward pointing unit normal.

Now, this should hold for all v satisfying the appropriate boundary conditions. Thus, it must in particular hold for all $v \in C^2(S)$ which are zero in a neighborhood of (x_i, y_i), and which satisfy $v(x, 1) = v(1, y) = 0$ and $\nabla v(x, y) = 0$ for $(x, y) \in \partial S$. But then w must be biharmonic, i.e.

$$\Delta^2 w = 0$$

in $S \backslash \cup_{i=1}^N \{(x_i, y_i)\}$. Then, by choosing v appropriately, we obtain the boundary conditions

$$\Delta w(x, 1) = \Delta w(1, y) = \frac{\partial}{\partial x} \Delta w(1, y) = \frac{\partial}{\partial y} \Delta w(x, 1) = 0,$$

together with the imposed boundary condition

$$\begin{aligned} w(x, 0) &= f(x), \\ w(0, y) &= g(y), \\ \frac{\partial}{\partial x} w(0, y) &= \frac{\partial}{\partial y} w(x, 0) = 0. \end{aligned} \tag{5}$$

Moreover, at the points (x_i, y_i), there are singularities in the third derivative:

$$\lambda \left(\lim_{\epsilon \to 0} \iint_{B_\epsilon(x_i, y_i)} \Delta^2 w \, dx \, dy \right) = \alpha_i - w(x_i, y_i).$$

At this point, we substitute the control u back in, and note that since $u = \Delta w$, it must satisfy

$$\Delta u = 0 \quad \text{in } S \setminus \cup_{i=1}^{N} \{(x_i, y_i)\},$$
$$u(x, 1) = u(1, y) = 0,$$
$$\frac{\partial u}{\partial x}(1, y) = \frac{\partial u}{\partial y}(x, 1) = 0,$$
$$\lambda \left(\lim_{\epsilon \to 0} \iint_{B_\epsilon(x_i, y_i)} \Delta u \, dx \, dy \right) = \tau_i,$$

where $\tau_i = \alpha_i - w(x_i, y_i)$ are constants to be determined.

Thus, it seems that the problem reduces to that of finding a Green's function for the Laplacian with these somewhat unusual boundary conditions.

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