

# Thin-Plate Splines

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## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>The Calculus of Variations</b>	<b>2</b>
2.1	Functionals of $f$ and $f'$ . . . . .	2
2.2	Functionals of $f$ , $f'$ , and $f''$ . . . . .	4
2.3	Cubic Splines and Green's Functions . . . . .	4
2.4	Euler-Lagrange Equations for Multivariate $f$ . . . . .	5
<b>3</b>	<b>Thin-Plate Splines in <math>n</math> Dimensions</b>	<b>5</b>
<b>4</b>	<b>Smoothed Thin-Plate Splines</b>	<b>7</b>

# 1 Introduction

Recall that natural cubic splines are piecewise cubic polynomial and exact interpolating functions for tabulated data  $(x_i, f(x_i))$ . The globally constructed spline has continuous second-order derivatives. The second derivatives at the endpoints are zero (no bending at endpoints). It is also possible to clamp the endpoints by specifying zero first derivatives there. The spline curve represents a thin metal rod that is constrained not to move at the sample points  $x_i$ .

The concept applies equally as well in two dimensions. A *thin-plate spline* is a physically motivated 2D interpolation scheme for arbitrarily spaced tabulated data  $(x_i, y_i, f(x_i, y_i))$ . These splines are the generalization of the natural cubic splines in 1D. The spline surface represents a thin metal sheet that is constrained not to move at the sample points  $(x_i, y_i)$ . The construction is based on choosing a function that minimizes an integral that represents the bending energy of a surface. The origins of thin-plate splines in 2D appears to be [1, 2].

In fact, the concept applies in any dimension for arbitrarily spaced tabulated data  $(\mathbf{x}_i, f(\mathbf{x}_i))$ . The method of construction for all dimensions is presented in [3] and is based on functional analysis.

In  $n$  dimensions, the idea of thin-plate splines is to choose a function  $f(\mathbf{x})$  that exactly interpolates the data points  $(\mathbf{x}_i, y_i)$ , say,  $y_i = f(\mathbf{x}_i)$ , and that minimizes the bending energy,

$$E[f] = \int_{\mathbb{R}^n} |D^2 f|^2 dX \tag{1}$$

where  $D^2 f$  is the matrix of second-order partial derivatives of  $f$  and  $|D^2 f|^2$  is the sum of squares of the matrix entries. The infinitesimal element of hypervolume is  $dX = dx_1 \cdots dx_n$ , where  $x_i$  are the components of  $\mathbf{x}$ .

It is also possible to formulate the problem with a smoothing parameter for regularization [4]. A function  $f$  is chosen that does not necessarily exactly interpolate all the data points but that does minimize

$$E[f] = \sum_{i=1}^m |f(\mathbf{x}_i) - y_i|^2 + \lambda \int_{\mathbb{R}^n} |D^2 f|^2 dX \tag{2}$$

The smoothing parameter is  $\lambda > 0$  and is chosen *a priori*. The summation makes it clear that there are  $m$  data points.

## 2 The Calculus of Variations

The ideas are presented in a mathematically informal manner.

### 2.1 Functionals of $f$ and $f'$

To motivate the minimization, consider a functional that is an integral involving a function  $F$  that depends on an independent variable  $x$ , on a function  $f$  and on the derivative function  $f'$ ,

$$E[f] = \int_a^b F(x, f, f') dx \tag{3}$$

For example,  $F(x, f, f') = f$ , in which case  $E[f] = \int_a^b f(x) dx$  is just the definite integral of  $f$  for the interval  $[a, b]$ . Another example is  $F(x, f, f') = \sqrt{1 + (f')^2}$ , in which case  $E[f] = \int_a^b \sqrt{1 + (f'(x))^2} dx$  is the arclength of the graph of  $f$  for the interval.

We wish to construct  $f$  for which  $E[f]$  of equation (3) is a minimum. The calculus of variations allows us to do this, a process that is the extension of directional derivatives for multivariate functions to directional derivatives of functions whose independent inputs are themselves functions. Consider the function  $E$  as  $f$  varies in the direction of another function  $g$ ,

$$\phi(t) = E[f + tg] = \int_a^b F(x, f + tg, f' + tg') dx \quad (4)$$

We assume that  $g$  does not change  $f$  at the interval endpoints, so  $g(a) = 0$  and  $g(b) = 0$ . For each scalar  $t$  we obtain the real number  $\phi(t)$  from the integration. If  $f$  is a function that minimizes  $E$ , then we expect  $\phi(t) = E[f + tg] \geq E[f] = \phi(0)$  for  $t$  near zero. From standard calculus, for  $\phi(0)$  to be a minimum we expect that its derivative with respect to  $t$  is zero:  $\phi'(0) = 0$ . If we formally differentiate equation (4) with respect to  $t$ , we obtain

$$\phi'(t) = \int_a^b \frac{\partial F(x, f + tg, f' + tg')}{\partial f} g + \frac{\partial F(x, f + tg, f' + tg')}{\partial f'} g' dx \quad (5)$$

The integrand is an application of the chain rule to differentiate  $F(x, f + tg, f' + tg')$ . Setting  $t$  to zero, we have at a minimum,

$$0 = \phi'(0) = \int_a^b \frac{\partial F(x, f, f')}{\partial f} g + \frac{\partial F(x, f, f')}{\partial f'} g' dx \quad (6)$$

The second term in the integrand involves  $g'(x)$ . We can use integration by parts,  $\int u dv = uv - \int v du$ , with  $u = \partial F/\partial f'$  and  $dv = g' dx$ ,

$$\int_a^b \frac{\partial F}{\partial f'} g' dx = \frac{\partial F}{\partial f'} g \Big|_a^b - \int_a^b \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) g dx = - \int_a^b \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) g dx \quad (7)$$

where the last equality follows from  $g(a) = g(b) = 0$ . Combining this with equation (6), we have

$$0 = \int_a^b \left[ \frac{\partial F}{\partial f} - \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) \right] g dx \quad (8)$$

This equation is true no matter which function direction  $g$  we choose, which forces

$$\frac{\partial F}{\partial f} - \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) = 0 \quad (9)$$

This is referred to as the *Euler-Lagrange differential equation*.

As an example, let us construct the function  $f(x)$  for which the arclength integral is a minimum on the interval  $[x_0, x_1]$ . Let the function values at the endpoints be  $y_0$  and  $y_1$ . The integrand is  $F(x, f, f') = \sqrt{1 + (f')^2}$ . The Euler-Lagrange differential equation is

$$0 = \frac{\partial F}{\partial f} - \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) = 0 - \frac{d}{dx} \left( \frac{f'}{[1 + (f')^2]^{1/2}} \right) = \frac{-f''}{[1 + (f')^2]^{3/2}} \quad (10)$$

The equation is satisfied when  $f''(x) = 0$  for all  $x$ , which means  $f(x) = y_0 + (y_1 - y_0)(x - x_0)/(x_1 - x_0)$ . This is exactly what we expect—the shortest-length curve connecting two points is a line segment.

## 2.2 Functionals of $f$ , $f'$ , and $f''$

The same idea of a directional derivative applies when the integrand depends on the function and its first- and second-order derivatives,  $F(x, f, f', f'')$ . When computing the directional derivative, we use a function  $g(x)$  for which  $g(a) = g(b) = 0$  and  $g'(a) = g'(b) = 0$ . The equivalent of equation (6) is

$$0 = \int_a^b \frac{\partial F}{\partial f} g + \frac{\partial F}{\partial f'} g' + \frac{\partial F}{\partial f''} g'' dx \quad (11)$$

The second term in the integrand is integrated by parts once. The third term is integrated by parts twice, and uses  $g(a) = g(b) = g'(a) = g'(b) = 0$  to eliminate the nonintegral terms that occur. The result is

$$0 = \int_a^b \left[ \frac{\partial F}{\partial f} - \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) + \frac{d^2}{dx^2} \left( \frac{\partial F}{\partial f''} \right) \right] g dx \quad (12)$$

Once again, this equation is true no matter the choice of  $g$  which forces

$$\frac{\partial F}{\partial f} - \frac{d}{dx} \left( \frac{\partial F}{\partial f'} \right) + \frac{d^2}{dx^2} \left( \frac{\partial F}{\partial f''} \right) = 0 \quad (13)$$

The introduction of  $f''$  allows us to handle the bending energy integral.

## 2.3 Cubic Splines and Green's Functions

The data points are  $(x_i, y_i)$  for  $1 \leq i \leq m$ . We require that  $f(x_i) = y_i$  for all  $i$ . The bending energy is

$$E[f] = \int_{-\infty}^{\infty} [f''(x)]^2 dx \quad (14)$$

A complicating factor is that the integral is over the entire real line, so the calculus of variations argument must be extended to handle this. Effectively, we need to work with *distributions*. In this case, think of this as introducing *Dirac delta functions* into the problem. Recall that the Dirac delta function has the substitution property  $\phi(a) = \int_{-\infty}^{\infty} \phi(x) \delta(x - a) dx$ .

In the notation for the calculus of variations, the integrand is  $F(x, f, f', f'') = (f'')^2$ ; that is,  $F$  depends only on the second derivative of  $f$ . Equation (13) must be satisfied,  $f^{(4)}(x) = 0$ , where the left-hand side is the fourth-order derivative of  $f$ . If it were the case that  $f$  has a continuous fourth-order derivative, then  $f$  would have to be a cubic polynomial. However, it is then not possible to satisfy all the conditions  $f(x_i) = y_i$  unless the data points do all lie on the same cubic graph. This requires us to treat  $f^{(4)}(x) = 0$  in a distributional sense—the fourth derivative is zero for all  $x$  except at the points  $x_i$  where the fourth derivative is discontinuous.

We can construct a *Green's function*  $G(x, s)$  that is the solution to  $\partial^4 G / \partial x^4 = \delta(x - s)$ , where  $\delta(x)$  is the Dirac delta function. The classical solution is

$$G(x, s) = \frac{1}{12} |x - s|^3 \quad (15)$$

Observe that  $G$  has a derivative discontinuity at  $x = s$ . The function  $f$  that minimizes equation (14) is a linear combination of the  $G(x, s)$  with the  $s$ -values set to the  $x_i$  where the derivative discontinuities must

occur. Also notice that any linear polynomial is in the kernel of  $E[f]$ , the set of functions for which  $E[f] = 0$ ; thus, we need to account for this. The form of  $f$  is

$$f(x) = \sum_{i=1}^m a_i G(x, x_i) + b_0 + b_1 x = \sum_{i=1}^m a_i \frac{|x - x_i|^3}{12} + b_0 + b_1 x \quad (16)$$

This equation has  $m + 2$  unknown values, the  $a_i$  and  $b_j$ , but we have only  $m$  constraints  $f(x_i) = y_i$ . The remaining two come from an orthogonality condition that is mentioned in [3]. Specifically, the linear polynomial  $b_0 + b_1 x$  is in the orthogonal complement of the function space that contains the Green's functions. This manifests itself as  $\sum_{i=1}^m a_i = 0$  and  $\sum_{i=1}^m a_i x_i = 0$ .

## 2.4 Euler-Lagrange Equations for Multivariate $f$

Consider functions of the form  $f(x_1, \dots, x_n)$ . The function  $F$  is of the form  $F(x_1, \dots, x_n, f, f_{x_1}, \dots, f_{x_n})$ , where  $f_{x_i} = \partial f / \partial x_i$ . The equivalent of equation (9) is

$$\frac{\partial F}{\partial f} - \sum_{i=1}^n \frac{d}{dx_i} \left( \frac{\partial F}{\partial f_{x_i}} \right) = 0 \quad (17)$$

Second-order derivatives  $f_{x_i x_j} = \partial^2 f / \partial x_i \partial x_j$  may also be included in  $F$ . The equivalent of equation (13) is

$$\frac{\partial F}{\partial f} - \sum_{i=1}^n \frac{d}{dx_i} \left( \frac{\partial F}{\partial f_{x_i}} \right) + \sum_{i=1}^n \sum_{j=1}^n \frac{d}{dx_i} \frac{d}{dx_j} \left( \frac{\partial F}{\partial f_{x_i x_j}} \right) = 0 \quad (18)$$

## 3 Thin-Plate Splines in $n$ Dimensions

In 2D, the motivation for thin-plate splines is to exactly interpolate the sample points and to minimize the bending energy of the surface that does so. The presentation here is for  $n$  dimensions, although for  $n \geq 3$ , the physical motivation does not apply. The bending energy is

$$E[f] = \int_{\mathbb{R}^n} \sum_{i=1}^n \sum_{j=1}^n f_{x_i x_j}^2 \quad (19)$$

where  $f_{x_i x_j}$  are the second-order derivatives of  $f$  and where the integration is over the entire set of real-valued  $n$ -tuples. Equation (18) becomes the *biharmonic equation*

$$0 = \Delta^2 f = \sum_{i=1}^n \sum_{j=1}^n f_{x_i x_i x_j x_j} \quad (20)$$

where  $f_{x_i x_j x_k x_\ell}$  are the fourth-order derivatives of  $f$ . The constant factor 2 obtained from differentiation is discarded. The biharmonic equation involves two applications to  $f$  of the Laplacian operator  $\Delta = \sum_{k=1}^n \partial^2 / \partial x_k^2$ .

Just as for the cubic spline,  $f$  need only have fourth-order partial derivatives that are continuous almost everywhere (except at the data points). We need a Green's function  $G(\mathbf{x}, \mathbf{s})$  that is a solution to the nonhomogeneous biharmonic equation,

$$\Delta^2 G(\mathbf{x}, \mathbf{s}) = \delta(\mathbf{x} - \mathbf{s}); \quad \mathbf{x} \in \mathbb{R}^n, \quad \mathbf{s} \in \mathbb{R}^n \quad (21)$$

where  $\delta(\mathbf{z})$  is the Dirac delta function with singularity at  $\mathbf{z} = \mathbf{0}$ . The biharmonic operator has derivatives with respect to the  $\mathbf{x}$  variable. The Green's function is chosen to be of the form  $G(\mathbf{x}, \mathbf{s}) = u(|\mathbf{x} - \mathbf{s}|)$ . The function  $u(r)$  is a solution to the nonhomogeneous biharmonic equation

$$\delta(r) = \Delta^2 u(r) = u^{(4)}(r) + \frac{2(n-1)}{r} u^{(3)}(r) + \frac{(n-1)(n-3)}{r^2} u^{(2)}(r) - \frac{(n-1)(n-3)}{r^3} u^{(1)}(r) \quad (22)$$

for  $r \in [0, \infty)$ , where  $u^{(k)}(r)$  is the  $k$ -th order derivative of  $u(r)$ . The general solution is

$$u(r) = \begin{cases} c_0 + c_1 r^2 + c_2 \ln r + c_3 r^2 \ln r, & n = 2 \\ c_0 + c_1 r^2 + c_2 \ln r + c_3 r^{-2}, & n = 4 \\ c_0 + c_1 r^2 + c_2 r^{2-n} + c_3 r^{4-n}, & \text{all other } n \end{cases} \quad (23)$$

Let  $B(\mathbf{s}, \varepsilon)$  be the  $n$ -dimensional ball with center  $\mathbf{s}$  and radius  $\varepsilon$ . Let  $S(\mathbf{s}, \varepsilon)$  be the surface of the ball. Integrate equation (21) over the ball region, where  $dV$  is an infinitesimal volume element.  $dS$  is an infinitesimal surface element and  $\mathbf{N}$  are unit-length outer-pointing surface normals,

$$\begin{aligned} 1 &= \int_{B(\mathbf{s}, \varepsilon)} \delta(\mathbf{x} - \mathbf{s}) dV && \text{property of the Dirac delta function} \\ &= \int_{B(\mathbf{s}, \varepsilon)} \Delta^2 G(\mathbf{x}, \mathbf{s}) dV && \text{equation (21)} \\ &= \int_{S(\mathbf{s}, \varepsilon)} \nabla (\Delta G(\mathbf{x}, \mathbf{s})) \cdot \mathbf{N} dS && \text{a surface integral using the divergence theorem} \\ &= \int_{S(0, \varepsilon)} \nabla (\Delta u(r)) \cdot \mathbf{N} dS && \text{setting } r = |\mathbf{x} - \mathbf{s}| \end{aligned} \quad (24)$$

The Laplacian of  $u(r)$  is

$$\Delta u(r) = \begin{cases} 4c_1 + 4c_3(1 + \ln r), & n = 2 \\ 8c_1 + 2c_2 r^{-2}, & n = 4 \\ 2nc_1 + 2c_3(4 - n)r^{2-n}, & \text{all other } n \end{cases} \quad (25)$$

and the gradient of the Laplacian of  $u(r)$  is

$$\nabla (\Delta u(r)) = \begin{cases} 4c_3 r^{-2} \mathbf{x}, & n = 2 \\ -4c_2 r^{-4} \mathbf{x}, & n = 4 \\ 2c_3(4 - n)(2 - n)r^{-n} \mathbf{x}, & \text{all other } n \end{cases} \quad (26)$$

The term  $\mathbf{x}$  occurs in the surface integral of equation (24) and the surface is a ball of radius  $\varepsilon$ , so  $\mathbf{x} = \varepsilon \mathbf{N}$  and  $r = \varepsilon$ . Thus,

$$1 = \int_{S(0, \varepsilon)} \nabla (\Delta u(r)) \cdot \mathbf{N} dS = \text{SurfaceArea}(S(\mathbf{0}, \varepsilon)) \begin{cases} 4c_3 \varepsilon^{-1}, & n = 2 \\ -4c_2 \varepsilon^{-3}, & n = 4 \\ 2c_3(4 - n)(2 - n)\varepsilon^{1-n}, & \text{all other } n \end{cases} \quad (27)$$

The surface area of the ball in  $n$  dimensions is  $2\pi^{n/2}\varepsilon^{n-1}/\Gamma(n/2)$ . The surface integral equation has all  $\varepsilon$  terms cancel, so the  $c$ -constants are determined by the equation. For  $n = 2$ , we have  $c_3 = 1/(8\pi)$ . For

$n = 4$ , we have  $c_2 = -1/(8\pi^2)$ . For all other  $n$ , we have  $c_3 = \Gamma(n/2)/(4\pi^{n/2}(4-n)(2-n))$ . The terms of  $u(r)$  whose constants are not determined by the construction are discarded because they have no effect (in the distributional sense) in determining solutions to the minimization problem. In summary, the Green's functions are

$$G(r) = \alpha \begin{cases} r^{4-n} \ln r, & n = 2 \text{ or } n = 4 \\ r^{4-n}, & \text{otherwise} \end{cases} \quad (28)$$

where  $\alpha = 1/(8\pi)$  for  $n = 2$ ,  $\alpha = -1/(8\pi^2)$  for  $n = 4$  and  $\alpha = \Gamma(n/2 - 2)/(16\pi^{n/2})$  for all other  $n$ . Observe that when  $n = 1$ ,  $\alpha = 1/12$  as shown in equation (15).

The minimizer  $f$  is a linear combination of the Green's function with the argument  $\mathbf{s}$  set to the  $\mathbf{x}_i$  of the data points. There is also a linear polynomial term; this term is in the kernel of  $E[f]$ . The function is

$$f(\mathbf{x}) = \sum_{i=1}^m a_i G(\mathbf{x}, \mathbf{x}_i) + \left( b_0 + \sum_{j=1}^n b_j x_j \right) \quad (29)$$

where  $x_j$  is the  $j$ th component of variable  $\mathbf{x}$ . **NOTE:** This is of practical value for interpolation in dimensions 1, 2, and 3 because  $G(\mathbf{x}, \mathbf{x}_i)$  are bounded functions; however, for dimensions 4 and larger,  $G(\mathbf{x}, \mathbf{x}_i)$  has a singularity at  $\mathbf{x}_i$ , so the interpolating function is not defined at the sample points. This is clearly not desired. In practice,  $u(r)$  is chosen so that  $G(\mathbf{x}, \mathbf{s}) = u(|\mathbf{x} - \mathbf{s}|)$  is bounded and  $\Delta^2 G(\mathbf{x}, \mathbf{s}) = 0$ ; that is,  $G$  is no longer the fundamental solution of the biharmonic equation because the Dirac delta function is omitted. The simplest bounded choice for  $n \geq 4$  is  $u(r) = r^2$ . Sometime the basis function for the 2-dimensional case is chosen,  $u(r) = r^2 \ln r$ , but then  $G$  is no longer a solution to the biharmonic equation. Choosing a different radial basis function for dimensions  $n \geq 4$  produces  $f(\mathbf{x})$  that is not generally the minimizer for  $E[f]$  for the specified sample points.

Define  $\mathbf{y}$  to be the  $m \times 1$  vector whose components are the data point  $y_i$  values. Define  $\mathbf{a}$  to be the  $m \times 1$  vector whose components are the coefficients  $a_i$ . Define  $\mathbf{b}$  to be the  $(n+1) \times 1$  vector whose components are the  $b_j$ . The constraints  $y_i = f(\mathbf{x}_i)$  lead to the system of equations

$$\mathbf{y} = M\mathbf{a} + N\mathbf{b} \quad (30)$$

where  $M$  is the  $m \times m$  matrix whose entries are  $M_{ij} = G(\mathbf{x}_i, \mathbf{x}_j)$  and where  $N$  is the  $m \times (n+1)$  matrix whose rows are  $[1 \ \mathbf{x}_i^T]$ . An orthogonality condition that comes from the functional analysis in [3] is  $N^T \mathbf{a} = \mathbf{0}$ . The equations have solution

$$\mathbf{a} = M^{-1}(\mathbf{y} - N\mathbf{b}), \quad \mathbf{b} = (N^T M^{-1} N)^{-1} N^T M^{-1} \mathbf{y} \quad (31)$$

Of course,  $\mathbf{b}$  is computed first. The minimum bending energy is  $\mathbf{a}^T M \mathbf{a}$ . When  $\mathbf{a}$  is zero, this quadratic form is zero—this is the case when  $f$  is a linear function whose graph is a hyperplane (no bending of the surface).

## 4 Smoothed Thin-Plate Splines

The smoothed functional is mentioned in equation (2), which may be rewritten as

$$E[f] = \int_{\mathbb{R}^n} \left( \sum_{i=1}^m (f(\mathbf{x}) - y_i)^2 \delta(\mathbf{x} - \mathbf{x}_i) + \lambda |D^2 f(\mathbf{x})|^2 \right) dX = \int_{\mathbb{R}^n} F(f(\mathbf{x}), D^2 f(\mathbf{x})) dX \quad (32)$$

where  $\delta(\mathbf{x})$  is the Dirac delta function of a multivariate input. The Euler-Lagrange differential equation for the integrand  $F(f, D^2f)$  is computed using equation (18),

$$\sum_{i=1}^m (f(\mathbf{x}) - y_i) \delta(\mathbf{x} - \mathbf{x}_i) + \lambda \Delta^2 f(\mathbf{x}) = 0 \quad (33)$$

where  $\Delta^2$  is the biharmonic operator. The factor of 2 that occurs during the differentiation has been discarded. Using the Green's functions defined previously, the solution to the differential equation is of the form

$$f(\mathbf{x}) = \sum_{j=1}^m w_j G(\mathbf{x}, \mathbf{x}_j) + \left( b_0 + \sum_{k=1}^n b_k x_k \right) \quad (34)$$

where the  $w_i$  and  $b_i$  are the unknown parameters to be determined. The values  $x_k$  are the components of  $\mathbf{x}$ . For the function  $f(\mathbf{x})$  in equation (34), observe that

$$\Delta^2 f(\mathbf{x}) = \sum_{j=1}^m w_j \Delta^2 G(\mathbf{x}, \mathbf{x}_j) = \sum_{j=1}^m w_j \delta(\mathbf{x} - \mathbf{x}_j) \quad (35)$$

where the second equality is based on  $G$  being the Green's function for the biharmonic equation (21). Substituting this into equation (33) and factoring out the Dirac delta function leads to the distributional equation

$$\sum_{i=1}^m (f(\mathbf{x}) - y_i + \lambda w_i) \delta(\mathbf{x} - \mathbf{x}_i) = 0 \quad (36)$$

Let  $B(\mathbf{s}, \varepsilon)$  be the  $n$ -dimensional ball with center  $\mathbf{s}$  and radius  $\varepsilon < \min_{i_0 \neq i_1} |\mathbf{x}_{i_0} - \mathbf{x}_{i_1}|$ . At a sample point  $\mathbf{x}_j$ , integrate equation (36) over the ball  $B(\mathbf{x}_j, \varepsilon)$ . The only sample point in this ball is  $\mathbf{x}_j$ , so

$$0 = \int_{B(\mathbf{x}_j, \varepsilon)} (f(\mathbf{x}) - y_i + \lambda w_i) \delta(\mathbf{x} - \mathbf{x}_i) dX = \begin{cases} f(\mathbf{x}_j) - y_j + \lambda w_j, & i = j \\ 0 & i \neq j \end{cases} \quad (37)$$

where the substitution property of the Dirac delta function was used. Equation (37) is rewritten as

$$y_j = f(\mathbf{x}_j) + \lambda w_j = \sum_{i=1}^m w_i G(\mathbf{x}_j, \mathbf{x}_i) + \left( b_0 + \sum_{k=1}^n b_k x_k \right), \quad 1 \leq j \leq m \quad (38)$$

where we have computed  $f(\mathbf{x}_j)$  using equation (34) with  $x_k^{(j)}$  the  $k$ th component of  $\mathbf{x}_j$ . Writing this in vector and matrix form, we have the matrix system

$$\mathbf{y} = (M + \lambda I) \mathbf{w} + N \mathbf{b}, \quad N^T \mathbf{w} = \mathbf{0} \quad (39)$$

The matrix  $M$  has size  $m \times m$  with entry  $M_{rc} = G(\mathbf{x}_r, \mathbf{x}_c)$ . The matrix  $I$  is the  $m \times m$  identity matrix. The vector  $\mathbf{w}$  has size  $m \times 1$  and stores the  $w_i$  coefficients. The matrix  $N$  has size  $m \times (n+1)$  with rows  $[1 \ \mathbf{x}_r^T]$ . The vector  $\mathbf{b}$  has size  $(n+1) \times 1$  and stores the  $b_k$  coefficients. The equation  $N^T \mathbf{w} = \mathbf{0}$  is an orthogonality condition similar to what was used for thin-plate splines without smoothing. The solution is

$$\mathbf{w} = (M + \lambda I)^{-1} (\mathbf{y} - N \mathbf{b}), \quad \mathbf{b} = \left( N^T (M + \lambda I)^{-1} N \right)^{-1} N^T (M + \lambda I)^{-1} \mathbf{y} \quad (40)$$

The minimum of the functional is  $\lambda \mathbf{w}^T (M + \lambda I) \mathbf{w}$ . As  $\lambda$  increases, the value is asymptotic to the discrete summation (first term) of the functional.



## References

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