

# Solving Continuous Linear Least-Squares Problems by Iterated Projection

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## Abstract

I present a new divide-and-conquer algorithm for solving continuous linear least-squares problems. The method is applicable when the column space of the linear system relating data to model parameters is “translation invariant”. The central operation is a matrix-vector product, which makes the method very easy to implement. Secondly, the structure of the computation suggests a straightforward parallel implementation.

A complexity analysis for sequential implementation shows that the method has the same asymptotic complexity as well-known algorithms for discrete linear least-squares. For illustration we work out the details for the problem of fitting quadratic bivariate polynomials to a piecewise constant function.

## 1 Introduction

The linear least-squares problem is to determine the parameter values  $\beta^*$  for a function  $f$  that minimizes the sum of squared differences between data values  $\{d_i\}$  and function values  $\{f(x_i; \beta)\}$  for corresponding points  $\{x_i\}$ ,

$$\beta^* = \operatorname{argmin}_{\beta} \sum_{i=1}^m (d_i - f(x_i; \beta))^2. \quad (1)$$

The problem is a *linear least-squares* problem if the model  $f$  is linear in the parameters, that is,

$$f(x; \beta) = \sum_{k=1}^n \beta_k f_k(x).$$

A classical way of determining  $\beta$  goes as follows:

1. Express (1) in matrix form,

$$\beta^* = \min_{\beta} \|d - A\beta\|, \quad (2)$$

where

$$A = \begin{pmatrix} f_1(x_1) & f_2(x_1) & \dots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \dots & f_n(x_2) \\ \vdots & \vdots & \dots & \vdots \\ f_1(x_m) & f_2(x_m) & \dots & f_n(x_m) \end{pmatrix}, \quad (3)$$

and  $d$  is the vector of data values.

2. Construct and solve the so called *normal equations*

$$A^T A \beta = A^T d. \quad (4)$$

Assuming  $m > n$  (more data values than parameters) and that  $A$  has full rank, the solution to (4) may be written in terms of the *pseudoinverse*  $A^+$  of  $A$ ,

$$\beta = (A^T A)^{-1} A^T d = A^+ d. \quad (5)$$

Geometrically speaking,  $\tilde{d} = A\beta$  is the point in the range of  $A$  closest to  $d$  in the Euclidean norm. The pseudoinverse projects  $d$  to the solution  $\beta$ , which may be thought of as the “coordinates” of  $\tilde{d}$  in the column space of  $A$ .

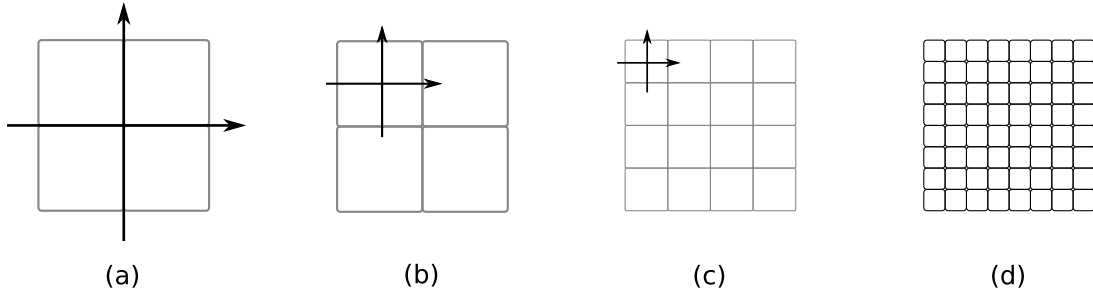
In the following we consider the continuous, linear version of problem (1),

$$\beta^* = \operatorname{argmin}_{\beta} \int_{\Omega} \left( d(x) - \sum_k \beta_k f_k(x) \right)^2 dx. \quad (6)$$

Note that in the continuous setting we assume there is a “data function”  $d(x)$ , defined over some domain  $\Omega$ . An example is single-band image data, which is often interpreted as a piecewise constant function over the image domain [3].

Section 4 introduces the key ideas of the new method and explains its prerequisites. Section 4 gives the algorithm and discusses its computational merits. As an example, in Section 4 I work out the elements of the algorithm for the problem of fitting a bivariate quadratic polynomial. The method for solving (6) that I call *iterated projection* works for any dimension of  $\Omega$ , but for the sake of clear exposition I assume  $\Omega$  has dimension 2 and  $\Omega = \Omega_{2h} = [-h, h] \times [-h, h]$ .

## 2 Linear Least-Squares by Iterated Projection



**Figure 1.** Domain  $\Omega$  with coordinate origin at center (a).  $\Omega$  partitioned into four subdomains  $\Omega_1, \Omega_2, \Omega_3, \Omega_4$  in clockwise order (b), next finer partition (c), finest partition at which the data function  $d$  may be accurately represented over the subdomains (d). A local coordinate system is centered on each subdomain (only shown for upper left subdomains in (b) and (c)).

Recall that the pseudoinverse in (5) projects the data directly onto a solution vector. With iterated projection we also obtain the solution by projection. However, instead of directly projecting the data we project solutions of intermediate least-squares problems. Imagine we partition  $\Omega$  into four equally sized subdomains  $\Omega_1, \dots, \Omega_4$  as shown in Figure 1(b), and that we are able to solve (6) for each subdomain, with solutions  $\beta_1^*, \dots, \beta_4^*$ . Can we compute the solution  $\beta^*$  for  $\Omega$  from the four solutions  $\beta_1^*, \dots, \beta_4^*$  for  $\Omega_1, \dots, \Omega_4$ ? As we will see below, the answer is yes, under certain circumstances.

With “problem (6) for subdomain  $\Omega_i$ ” we mean that the integral in (6) is over  $\Omega_i$  instead of  $\Omega$ , and that the coordinates are with respect to a coordinate system centered on  $\Omega_i$  (cf. Figure 1(b)). But centering the coordinate systems with respect to each  $\Omega_i$  means the four integrals are over the same set of points  $\Omega_h = [-h/2, h/2] \times [-h/2, h/2]$ . These are important aspects of iterated projection: the problems corresponding to the four subdomains are four instances of the same problem (only the data term in (6) is different), as well as similar to the original problem ( $\Omega = \Omega_h$  instead of  $\Omega = \Omega_{2h}$ ).

A few more bits of notation are necessary to define the intermediate problems more precisely. We denote the coordinates (with respect to  $\Omega_{2h}$ ) of the four subdomain’s coordinate origins by  $x_1^0, \dots, x_4^0$  and the solutions corresponding to the four subdomain problems by  $\beta_1^*, \dots, \beta_4^*$ , respectively. In the continuous setting  $\beta^*$  are the coordinates of a function closest to  $d$  in the space  $F_{2h}$  of functions over  $\Omega_{2h}$  that is spanned by  $\{f_k|_{\Omega_{2h}}\}_{k=1\dots n}$ . Likewise, the solution  $\beta_i^*$  for subdomain  $\Omega_i$  are the coordinates of a function closest to  $x \mapsto d(x + x_i^0)$ , in the space  $F_h$  of functions over  $\Omega_h$  spanned by  $\{f_k|_{\Omega_h}\}_{k=1\dots n}$ . We can use the space  $F_h$  to construct another space of functions over  $\Omega_{2h}$ ,

$$\tilde{F}_{2h} = \{f: \Omega_{2h} \rightarrow \mathbb{R} \mid x \mapsto f(x + x_i^0) \in F_h \text{ for all } x \in \Omega_h \text{ and } i = 1\dots 4\}.$$

Note that  $F_{2h}$  has dimension  $n$ , whereas  $\tilde{F}_{2h}$  has dimension  $4 \times n$ . The answer to our question is that we can construct a solution  $\beta^*$  for (6) from the solutions  $\beta_i^*$  for the subdomains if  $F_{2h}$  is a subspace of  $\tilde{F}_{2h}$ ,

$$F_{2h} \subset \tilde{F}_{2h}. \quad (7)$$

## 2.1 The Subspace Property

When does the “subspace property” (7) hold for a set of functions  $\{f_k\}$ ? What we must verify is that for any set of parameters  $\beta$  there are parameters  $\beta_1, \dots, \beta_4$  such that

$$\sum_k \beta_k f_k(x - x_i^0) = \sum_k \beta_{i,k} f_k(x), \forall x \in \Omega_h, i = 1, \dots, 4. \quad (8)$$

In other words, relation (7) holds when the space of functions (over  $\mathbb{R}^2$ ) spanned by  $\{f_k\}$  is *translation-invariant*. Examples are the spaces of polynomials of any finite order, or the space of functions spanned by sine-cosine pairs with same wave number.

## 2.2 Solving the Linear Least-Squares Problem

We want to obtain the linear least-squares solution  $\beta^*$  on  $\Omega = \Omega_{2h}$  from the solutions  $\beta_1^*, \dots, \beta_4^*$  for  $\Omega$ 's subdomains  $\Omega_1, \dots, \Omega_4$ , respectively. As we said above, we obtain  $\beta^*$  by projecting the solutions  $\beta_1^*, \dots, \beta_4^*$ . Let a function  $\tilde{f} \in \tilde{F}_{2h}$  be parameterized by  $\tilde{\beta} \in \mathbb{R}^{4 \times n}$ ,  $\tilde{\beta}^T = (\beta_1^T \beta_2^T \beta_3^T \beta_4^T)$ , where  $\beta_i$  corresponds to the part of  $\tilde{f}$  covering subdomain  $\Omega_i$ , and let  $f \in F_{2h}$  be parameterized by  $\gamma \in \mathbb{R}^n$ . The projector from  $\tilde{F}_{2h}$  onto  $F_{2h}$  we seek maps  $\tilde{\beta}$  to the vector

$$\beta^* = \operatorname{argmin}_\gamma \sum_i \int_{\Omega_h} \left( \sum_l \beta_{i,l} f_l(x) - \sum_k \gamma_k f_k(x - x_i^0) \right)^2 dx. \quad (9)$$

Assume, for the moment, we know the projector, a  $n \times (4n)$ -matrix, and call it  $R_h$ . Using  $R_h$ , the solution to problem (6) is

$$\beta^* = R_h \tilde{\beta}^* = \begin{pmatrix} R_{h,1} & R_{h,2} & R_{h,3} & R_{h,4} \end{pmatrix} \begin{pmatrix} \beta_1^* \\ \beta_2^* \\ \beta_3^* \\ \beta_4^* \end{pmatrix} \quad (10)$$

( $R_{h,i}$  denotes the obvious  $n \times n$  submatrix of  $R_h$ ). Equation (10) expresses the central idea and operation of the iterated projection algorithm: obtain solutions to smaller versions of the linear least-squares problem first, then derive the solution to the original problem by a simple matrix-vector product. The solutions to the smaller problems are obtained in the same way, by projecting solutions for sub-subdomains, using a similar projection operator  $R_{h/2}$ . The resulting algorithm is recursive. The recursion ends at subdomains over which the data function  $d$  is an element of the space spanned by  $\{f_k\}$  over that domain, or when  $d$  may be approximated in that space with negligible error (Figure 1(d)).

## 2.3 The Projection Operator

We now turn to the problem of determining the projection matrix  $R_h$  used in (10). There are different ways of deriving  $R_h$ . In this section I describe one way, and in Section 4 I demonstrate another way by example.

To begin note that when subspace property (7) holds, for every element  $\beta$  in the range of  $R_h$  there is one vector  $\tilde{\beta}$  for which (9) is exactly zero. If this is the case, then  $\tilde{\beta}$  and  $\beta = R_h \tilde{\beta}$  represent the same function over  $\Omega_{2h}$ . We denote  $P_h$  the  $(4n) \times n$ -matrix that maps  $\beta$  (representing a function in  $F_{2h}$ ) to the vector  $\tilde{\beta}$  representing the same function in  $\tilde{F}_{2h}$ ,

$$\tilde{\beta} = P_h \beta = \begin{pmatrix} P_{h,1} \\ P_{h,2} \\ P_{h,3} \\ P_{h,4} \end{pmatrix} \beta. \quad (11)$$

Determining  $P_h$  for a particular set of functions  $\{f_k\}$  is just another way of confirming that the subspace property (7) holds.  $P_h$  is relevant here because concrete expressions for it are easy to derive, and we can express  $R_h$  in terms of  $P_h$  (below).

The second ingredient we need is the inner product on the parameter space of  $F_{2h}$  that corresponds to the “least-squares” (Euclidean) norm,

$$\begin{aligned}
\langle f, g \rangle_{2h} &= \int_{\Omega_{2h}} f(x) g(x) dx \\
&= \int_{\Omega_{2h}} \left( \sum_k \beta_k f_k(x) \right) \left( \sum_l \gamma_l f_l(x) \right) dx \\
&= \beta^T \begin{pmatrix} \int_{\Omega_{2h}} f_1 f_1 & \int_{\Omega_{2h}} f_1 f_2 & \cdots & \int_{\Omega_{2h}} f_1 f_n \\ \int_{\Omega_{2h}} f_2 f_1 & \int_{\Omega_{2h}} f_2 f_2 & & \vdots \\ \vdots & \vdots & & \int_{\Omega_{2h}} f_{n-1} f_n \\ \int_{\Omega_{2h}} f_n f_1 & \int_{\Omega_{2h}} f_n f_2 & \cdots & \int_{\Omega_{2h}} f_n f_n \end{pmatrix} \gamma \\
&= \beta^T Q_{2h} \gamma.
\end{aligned} \tag{12}$$

$Q_{2h}$  is the Gram matrix of the functions  $\{f_k\}$ . Inner products corresponding to the subdomain-function spaces are defined in the same way,

$$\langle f|_{\Omega_h}, g|_{\Omega_h} \rangle_h = \beta_i^T \begin{pmatrix} \int_{\Omega_h} f_1 f_1 & \int_{\Omega_h} f_1 f_2 & \cdots & \int_{\Omega_h} f_1 f_n \\ \int_{\Omega_h} f_2 f_1 & \int_{\Omega_h} f_2 f_2 & & \vdots \\ \vdots & \vdots & & \int_{\Omega_h} f_{n-1} f_n \\ \int_{\Omega_h} f_n f_1 & \int_{\Omega_h} f_n f_2 & \cdots & \int_{\Omega_h} f_n f_n \end{pmatrix} \gamma_i = \beta_i^T Q_h \gamma_i. \tag{13}$$

With  $P_h$  and  $Q_h$  we can express the least-squares property (9), which is the defining property of  $R_h$ , without using integrals

$$\begin{aligned}
R_h \tilde{\beta} &= \operatorname{argmin}_{\gamma} \sum_i \int_{\Omega_h} \left( \sum_l \beta_{i,l} f_l(x) - \sum_k \gamma_k f_k(x - x_i^0) \right)^2 dx \\
&= \operatorname{argmin}_{\gamma} \sum_i \int_{\Omega_h} \left( \sum_l \beta_{i,l} f_l(x) - \sum_k (P_h \gamma)_{i,k} f_k(x) \right)^2 dx \\
&= \operatorname{argmin}_{\gamma} \sum_i (\beta_i - (P_h \gamma)_i)^T Q_h (\beta_i - (P_h \gamma)_i)
\end{aligned} \tag{14}$$

Since the sum in (14) is quadratic in  $\gamma$  we can set its gradient w.r.t  $\gamma$  to zero and solve for  $\gamma$  to find the minimizer. The result is the following expression for  $R_h$ ,

$$R_h = \left( \sum_{i=1}^4 P_{h,i}^T Q_h P_{h,i} \right)^{-1} \begin{pmatrix} P_{h,1}^T Q_h & P_{h,2}^T Q_h & P_{h,3}^T Q_h & P_{h,4}^T Q_h \end{pmatrix}. \tag{15}$$

### 3 Computational Characteristics

The following algorithm ITERATED\_PROJECTION\_LSQ is a very simple instance of iterated projection; it requires that the data function is piecewise constant over square regions of a regular partition of  $\Omega$  into  $m \times m = 2^l \times 2^l$  regions. Not included in the algorithm description is the construction of the projection matrices  $R_h$ . These are assumed to have been precomputed for all relevant scales prior to calling ITERATED\_PROJECTION\_LSQ.

ITERATED\_PROJECTION\_LSQ( $D, h$ )

**Input.**  $D$ :  $m \times m$  data matrix,  $h$ : scale of domain

**Output.**  $\beta^*$ : least-squares solution over domain  $\Omega = [-h, h] \times [-h, h]$

**Steps.**

1. If  $m = 1$ :
2.  $\beta^* \leftarrow$  project constant function  $d(x) = D_{1,1}$  (Section 2.2)
3. else:
4. partition  $D$ ,  $D = \begin{pmatrix} D_1 & D_2 \\ D_4 & D_3 \end{pmatrix}$

$$\begin{aligned}
5. \quad & \beta_i^* \leftarrow \text{ITERATED\_PROJECTION\_LSQ}(D_i, h/2), \text{ for } i=1, \dots, 4 \\
6. \quad & \beta^* \leftarrow R_h \begin{pmatrix} \beta_1^* \\ \beta_2^* \\ \beta_3^* \\ \beta_4^* \end{pmatrix} \qquad \qquad \qquad (\text{Equation 10})
\end{aligned}$$

### 3.1 Computational Complexity of Iterated Projection

Algorithm `ITERATED_PROJECTION_LSQ` is formulated for two-dimensional domains. However, adapting the algorithm to domains of different dimensionality is straightforward and we discuss computational complexity for the general case ( $d$  dimensions). In the general case

- $D$  is assumed to have  $m^d$  entries and is partitioned into  $2^d$  parts in Step 4,
- the projection matrix  $R_h$  is of size  $n \times 2^d n$ ,
- the depth of the recursion  $l = \log_2 m$  is independent of  $d$ .

We assume that analytical expressions for  $R_h$  are available, thus, precomputing the projection matrices means evaluating those expressions for all  $l$  scales. Assuming that the amount of computation for evaluating each  $R_h$ -entry is independent of  $h$ , precomputing the projecting matrices requires  $O(\log_2 m \times 2^d \times n^2)$  operations and  $O(\log_2 m \times 2^d \times n^2)$  space.

Computing  $\beta^*$  in Step 2. requires  $O(n)$  operations per entry of  $D$ , or  $O(m^d \times n)$  operations total. Computing  $\beta^*$  in Step 6. requires a matrix-vector product of  $O(2^d \times n^2)$ . Step 6 is carried out  $\sum_{i=0}^{l-1} (2^d)^i = \frac{2^{d \times l} - 1}{2^d - 1}$  times, resulting in a total operation count of  $O(2^{d \times \log_2 m} \times n^2)$  or  $O(m^d \times n^2)$  for Step 6.

Steps 5. and 6. together may be organized in a loop over all  $D_i$ . In that case the amount of space required by iterated projection (in addition to the space required for the projection matrices) is proportional to  $n$  and proportional to the depth of the recursion,  $O(\log_2 m \times n)$ .

### 3.2 Comparison to Classical Linear Least-Squares Algorithms

In discrete linear least-squares problems, the problem domain  $\Omega$  has been abstracted away and its dimension usually plays no part in a complexity analysis. Instead, the complexity of those algorithms are expressed in the size of matrix  $A$  in (4), say  $M \times n$  [4]. Setting  $M = m^d$  for comparison, the cost of iterated projection is  $O(M \times n^2)$  operations, and  $O\left(\frac{2^d}{d} \times \log_2 M \times n^2\right)$  units of space (ignoring space required for entering the problem).

A classical algorithm for solving the normal equations (4) is Cholesky factorization,

`CHOLESKY_LSQ`( $A, d$ )

**Input.**  $A$ :  $M \times n$  model matrix,  $d$ :  $M$  data vector

**Output.**  $\beta^*$ : least-squares solution  $\text{argmin}_\beta \|A\beta - d\|_2$

**Steps.**

1. Compute  $B = A^T A$
2. Compute  $y = A^T d$
3. Factorize  $B$ ,  $B = R^T R$  ( $R$  upper triangular)
4. Solve  $R^T x = y$
5. Solve  $R\beta^* = x$

The costs of these steps are, respectively,  $O(M \times n^2)$ ,  $O(M \times n^2)$ ,  $O(n^3)$ ,  $O(n^2)$ , and  $O(n^2)$  operations. In most situations where iterated projection is applicable we could carry out Step 1. and Step 3. of `CHOLESKY_LSQ` in advance, and the asymptotic cost would be dominated by Step 2.,  $O(M \times n^2)$ . Storing the Cholesky factors requires  $O(n^2)$  units of space.

Other classical algorithm's complexity characteristics are essentially the same ([4], Chapter 11), and we conclude that the asymptotic computational cost of iterated projection is the same as the cost of well-known algorithms for discrete linear least-squares.

## 4 Discussion

I have presented a new idea, iterated projection, for computing the solution to continuous linear least-squares problems. The idea is to project the data—which is thought of as a function—into a sequence of function spaces of decreasing dimensionality. The final projection in this sequence is into the space in which the solution is sought.

As discussed in Section 3.2, iterated projection is asymptotically as efficient as other linear least-squares algorithms. However, ITERATED\_PROJECTION\_LSQ is a strikingly simple algorithm, consisting essentially of a single operation (the matrix-vector product in Step 6) and is arguably easier to accelerate by special hardware. Secondly, the way the computation is organized in ITERATED\_PROJECTION\_LSQ makes it easy to distribute the work among multiple processors.

Classical linear least-squares algorithms and iterated projection do not solve exactly the same problem. The former solve the problem

$$\text{Find } \beta^* \text{ such that } \|A\beta - d\|_2 \text{ is minimal for } \beta = \beta^*, \quad (16)$$

iterated projection solves the problem (with  $f$  linear in  $\beta$ )

$$\text{Find } \beta^* \text{ such that } \int_{\Omega} (f(x; \beta) - d(x))^2 dx \text{ is minimal for } \beta = \beta^*. \quad (17)$$

In practice problem (17) is often approximated by a problem of the form (16), obtained through sampling  $d$  and  $f$  at selected points  $\{x_i\}$  (cf. (1) to (3) in Section 1). In such situations, and when the subspace property (7) holds, iterated projection is a compelling alternative to discrete linear least-squares algorithms. It may give exact solutions (except for rounding errors), and it may require less computation when  $d$  is of appropriate form (e.g., functions in finite-element spaces; Step 2 in ITERATED\_PROJECTION\_LSQ needs to be adapted accordingly).

Another interesting aspect of iterated projection is that, since no linear system needs to be solved, the problems of underdetermined or singular systems do not occur. This recommends iterated projection for problems like least-squares based image reconstruction and segmentation [1, 2], where small regions often lead to underdetermined or singular least-squares problems.

## 5 Appendix—Iterated Projection with Quadratic Polynomials

As a concrete example, and to demonstrate an alternative to (15) for deriving the projection matrices, I consider problem (6) with

$$\begin{aligned} f_1(x) &= 1 \\ f_2(x) &= x_1 \\ f_3(x) &= x_2 \\ f_4(x) &= \frac{1}{2} x_1^2 \\ f_5(x) &= x_1 x_2 \\ f_6(x) &= \frac{1}{2} x_2^2. \end{aligned} \quad (18)$$

At first we verify that the space spanned by  $f_1, \dots, f_6$  is translation invariant. Let  $\beta$  represent any such function,  $f(x; \beta) = \sum_{k=1}^6 \beta_k f_k(x)$ ,  $x^0$  be the origin of another coordinate system, and  $f'(x'; \beta')$  denote the representation with respect to the coordinate system centered at  $x^0$ . Function  $f'$  is the same as  $f$  if their values and that of all their derivatives are identical at any point. Choose  $x^0$  as that point and write down the identities to obtain  $\beta'$  in terms of  $\beta$  and  $x^0$ .

$$\begin{aligned} \beta'_1 &= \beta_1 + \beta_2 x_1^0 + \beta_3 x_2^0 + \frac{\beta_4}{2} (x_1^0)^2 + \beta_5 x_1^0 x_2^0 + \frac{\beta_6}{2} (x_2^0)^2 \\ \beta'_2 &= \beta_2 + \beta_4 x_1^0 + \beta_5 x_2^0 \\ &\dots \end{aligned}$$

To derive matrix  $P_h$  in (11) we set  $x^0$  to  $\left(\frac{-h}{2}, \frac{-h}{2}\right)$ ,  $\left(\frac{h}{2}, \frac{-h}{2}\right)$ ,  $\left(\frac{h}{2}, \frac{h}{2}\right)$ , and  $\left(\frac{-h}{2}, \frac{h}{2}\right)$ , respectively, and obtain

$$P_{h,1} = \begin{pmatrix} 1 & \frac{-h}{2} & \frac{-h}{2} & \frac{h^2}{8} & \frac{h^2}{4} & \frac{h^2}{8} \\ & 1 & & \frac{-h}{2} & \frac{-h}{2} & \\ & & 1 & \frac{-h}{2} & \frac{-h}{2} & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix} \quad P_{h,2} = \begin{pmatrix} 1 & \frac{h}{2} & \frac{-h}{2} & \frac{h^2}{8} & \frac{-h^2}{4} & \frac{h^2}{8} \\ & 1 & & \frac{h}{2} & \frac{-h}{2} & \\ & & 1 & & \frac{h}{2} & \frac{-h}{2} \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix}$$

$$P_{h,4} = \begin{pmatrix} 1 & \frac{-h}{2} & \frac{h}{2} & \frac{h^2}{8} & \frac{-h^2}{4} & \frac{h^2}{8} \\ & 1 & & \frac{-h}{2} & \frac{h}{2} & \\ & & 1 & \frac{-h}{2} & \frac{h}{2} & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix} \quad P_{h,3} = \begin{pmatrix} 1 & \frac{h}{2} & \frac{h}{2} & \frac{h^2}{8} & \frac{h^2}{4} & \frac{h^2}{8} \\ & 1 & & \frac{h}{2} & \frac{h}{2} & \\ & & 1 & & \frac{h}{2} & \frac{h}{2} \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix}.$$

Matrix  $Q_h$  in (13) can be seen to be

$$Q_h = \begin{pmatrix} h^2 & & & & & \\ & \frac{1}{12}h^4 & & & & \\ & & \frac{1}{3}h^4 & & & \\ \frac{1}{24}h^4 & & & \frac{1}{320}h^6 & & \frac{1}{576}h^6 \\ & & & & \frac{1}{144}h^6 & \\ \frac{1}{24}h^4 & & & \frac{1}{576}h^6 & & \frac{1}{320}h^6 \end{pmatrix} \quad (19)$$

These are the ingredients needed to derive  $R_h$  via (15).

### 5.1 Deriving $R_h$ by QR Factorization

One algorithm for solving least-squares problem is by QR factorization. It consists of computing the (reduced) QR factorization of  $A$  in (4),  $A = QR$ , by which we obtain an orthonormal basis for the column space of  $A$ . Next, the data vector is expanded in that orthonormal basis, and, finally, an expansion in the basis of interest (the columns of  $A$ ) is obtained by solving a triangular system.

I now show how to derive  $R_h$  by applying essentially this algorithm, but in the continuous setting. The polynomials (18) do not form an orthogonal basis with respect to the inner product (12), otherwise  $Q_h$  in (19) were diagonal. An orthonormal basis for the space spanned by (18) are the Legendre polynomials up to order two. Defined over  $\Omega = [-h, h] \times [-h, h]$ , these are

$$\begin{aligned} \phi_1(x) &= \frac{1}{h} \frac{1}{2} \\ \phi_2(x) &= \frac{1}{h^2} \frac{\sqrt{3}}{2} x_1 \\ \phi_3(x) &= \frac{1}{h^2} \frac{\sqrt{3}}{2} x_2 \\ \phi_4(x) &= \frac{1}{h^3} \frac{\sqrt{5}}{4} (3x_1^2 - h^2) \\ \phi_5(x) &= \frac{1}{h^3} \frac{3}{2} x_1 x_2 \\ \phi_6(x) &= \frac{1}{h^3} \frac{\sqrt{5}}{4} (3x_2^2 - h^2). \end{aligned}$$

The “QR factorization” of  $A = (f_1 \ f_2 \ f_3 \ f_4 \ f_5 \ f_6)$  over  $\Omega$  is

$$(f_1 \ f_2 \ f_3 \ f_4 \ f_5 \ f_6) = (\phi_1 \ \phi_2 \ \phi_3 \ \phi_4 \ \phi_5 \ \phi_6) \begin{pmatrix} 2h & & & & & \\ & \frac{2}{\sqrt{3}}h^2 & & & & \\ & & \frac{2}{\sqrt{3}}h^2 & & & \\ & & & \frac{2}{3\sqrt{5}}h^3 & & \\ & & & & \frac{2}{3}h^3 & \\ & & & & & \frac{2}{3\sqrt{5}}h^3 \end{pmatrix} \\ = \Phi C$$

The product  $R_h \tilde{\beta}$  may now be expressed as

$$\begin{aligned} R_h \tilde{\beta} &= C^{-1} \sum_{i=1}^4 \left( \int_{\Omega_i} \Phi^T ( f_1 \ f_2 \ f_3 \ f_4 \ f_5 \ f_6 ) dx \right) \beta_i \\ &= C^{-1} \sum_{i=1}^4 \begin{pmatrix} \langle \phi_1, f_1 \rangle_{h/2} & \langle \phi_1, f_2 \rangle_{h/2} & \dots & \langle \phi_1, f_6 \rangle_{h/2} \\ \langle \phi_2, f_1 \rangle_{h/2} & \langle \phi_2, f_2 \rangle_{h/2} & & \vdots \\ \vdots & \vdots & & \langle \phi_5, f_6 \rangle_{h/2} \\ \langle \phi_6, f_1 \rangle_{h/2} & \langle \phi_6, f_2 \rangle_{h/2} & \dots & \langle \phi_6, f_6 \rangle_{h/2} \end{pmatrix} \beta_i \\ &= C^{-1} \left( \tilde{R}_{h,1} \ \tilde{R}_{h,2} \ \tilde{R}_{h,3} \ \tilde{R}_{h,4} \right) \tilde{\beta}, \end{aligned}$$

hence  $R_h = ( C^{-1} \tilde{R}_{h,1} \ C^{-1} \tilde{R}_{h,2} \ C^{-1} \tilde{R}_{h,3} \ C^{-1} \tilde{R}_{h,4} )$ . Evaluating the integrals in  $\tilde{R}_{h,i}$  we get

$$\begin{aligned} \tilde{R}_{h,1} &= \begin{pmatrix} \frac{1}{2}h & 0 & 0 & \frac{1}{48}h^3 & 0 & \frac{1}{48}h^3 \\ -\frac{\sqrt{3}}{4}h & \frac{\sqrt{3}}{24}h^2 & 0 & -\frac{\sqrt{3}}{96}h^3 & 0 & -\frac{\sqrt{3}}{96}h^3 \\ -\frac{\sqrt{3}}{4}h & 0 & \frac{\sqrt{3}}{24}h^2 & -\frac{\sqrt{3}}{96}h^3 & 0 & -\frac{\sqrt{3}}{96}h^3 \\ 0 & -\frac{\sqrt{5}}{16}h^2 & 0 & \frac{\sqrt{5}}{480}h^3 & 0 & 0 \\ \frac{3}{8}h & -\frac{1}{16}h^2 & -\frac{1}{16}h^2 & \frac{1}{64}h^3 & \frac{1}{96}h^3 & \frac{1}{64}h^3 \\ 0 & 0 & -\frac{\sqrt{5}}{16}h^2 & 0 & 0 & \frac{\sqrt{5}}{480}h^3 \end{pmatrix} & \tilde{R}_{h,2} &= \begin{pmatrix} \frac{1}{2}h & 0 & 0 & \frac{1}{48}h^3 & 0 & \frac{1}{48}h^3 \\ \frac{\sqrt{3}}{4}h & \frac{\sqrt{3}}{24}h^2 & 0 & \frac{\sqrt{3}}{96}h^3 & 0 & \frac{\sqrt{3}}{96}h^3 \\ -\frac{\sqrt{3}}{4}h & 0 & \frac{\sqrt{3}}{24}h^2 & -\frac{\sqrt{3}}{96}h^3 & 0 & -\frac{\sqrt{3}}{96}h^3 \\ 0 & \frac{\sqrt{5}}{16}h^2 & 0 & \frac{\sqrt{5}}{480}h^3 & 0 & 0 \\ -\frac{3}{8}h & -\frac{1}{16}h^2 & \frac{1}{16}h^2 & -\frac{1}{64}h^3 & \frac{1}{96}h^3 & -\frac{1}{64}h^3 \\ 0 & 0 & -\frac{\sqrt{5}}{16}h^2 & 0 & 0 & \frac{\sqrt{5}}{480}h^3 \end{pmatrix} \\ \tilde{R}_{h,4} &= \begin{pmatrix} \frac{1}{2}h & 0 & 0 & \frac{1}{48}h^3 & 0 & \frac{1}{48}h^3 \\ -\frac{\sqrt{3}}{4}h & \frac{\sqrt{3}}{24}h^2 & 0 & -\frac{\sqrt{3}}{96}h^3 & 0 & -\frac{\sqrt{3}}{96}h^3 \\ \frac{\sqrt{3}}{4}h & 0 & \frac{\sqrt{3}}{24}h^2 & \frac{\sqrt{3}}{96}h^3 & 0 & \frac{\sqrt{3}}{96}h^3 \\ 0 & -\frac{\sqrt{5}}{16}h^2 & 0 & \frac{\sqrt{5}}{480}h^3 & 0 & 0 \\ -\frac{3}{8}h & \frac{1}{16}h^2 & -\frac{1}{16}h^2 & -\frac{1}{64}h^3 & \frac{1}{96}h^3 & -\frac{1}{64}h^3 \\ 0 & 0 & \frac{\sqrt{5}}{16}h^2 & 0 & 0 & \frac{\sqrt{5}}{480}h^3 \end{pmatrix} & \tilde{R}_{h,3} &= \begin{pmatrix} \frac{1}{2}h & 0 & 0 & \frac{1}{48}h^3 & 0 & \frac{1}{48}h^3 \\ \frac{\sqrt{3}}{4}h & \frac{\sqrt{3}}{24}h^2 & 0 & \frac{\sqrt{3}}{96}h^3 & 0 & \frac{\sqrt{3}}{96}h^3 \\ \frac{\sqrt{3}}{4}h & 0 & \frac{\sqrt{3}}{24}h^2 & \frac{\sqrt{3}}{96}h^3 & 0 & \frac{\sqrt{3}}{96}h^3 \\ 0 & \frac{\sqrt{5}}{16}h^2 & 0 & \frac{\sqrt{5}}{480}h^3 & 0 & 0 \\ \frac{3}{8}h & \frac{1}{16}h^2 & \frac{1}{16}h^2 & \frac{1}{64}h^3 & \frac{1}{96}h^3 & \frac{1}{64}h^3 \\ 0 & 0 & \frac{\sqrt{5}}{16}h^2 & 0 & 0 & \frac{\sqrt{5}}{480}h^3 \end{pmatrix}. \end{aligned}$$

Multiplying  $\tilde{R}_{h,i}$  by  $C^{-1}$  we finally arrive at the four components of  $R_h$ ,

$$\begin{aligned} R_{h,1} &= \begin{pmatrix} \frac{1}{4} & \frac{5}{64}h & \frac{5}{64}h & \frac{1}{128}h^2 & 0 & \frac{1}{128}h^2 \\ -\frac{3}{8} \frac{1}{h} & \frac{1}{16} & 0 & -\frac{1}{64}h & 0 & -\frac{1}{64}h \\ -\frac{3}{8} \frac{1}{h} & 0 & \frac{1}{16} & -\frac{1}{64}h & 0 & -\frac{1}{64}h \\ 0 & -\frac{15}{32} \frac{1}{h} & 0 & \frac{1}{64} & 0 & 0 \\ \frac{9}{16} \frac{1}{h^2} & -\frac{3}{32} \frac{1}{h} & -\frac{3}{32} \frac{1}{h} & \frac{3}{128} & \frac{1}{64} & \frac{3}{128} \\ 0 & 0 & -\frac{15}{32} \frac{1}{h} & 0 & 0 & \frac{1}{64} \end{pmatrix} & R_{h,2} &= \begin{pmatrix} \frac{1}{4} & -\frac{5}{64}h & \frac{5}{64}h & \frac{1}{128}h^2 & 0 & \frac{1}{128}h^2 \\ \frac{3}{8} \frac{1}{h} & \frac{1}{16} & 0 & \frac{1}{64}h & 0 & \frac{1}{64}h \\ -\frac{3}{8} \frac{1}{h} & 0 & \frac{1}{16} & -\frac{1}{64}h & 0 & -\frac{1}{64}h \\ 0 & \frac{15}{32} \frac{1}{h} & 0 & \frac{1}{64} & 0 & 0 \\ -\frac{9}{16} \frac{1}{h^2} & -\frac{3}{32} \frac{1}{h} & \frac{3}{32} \frac{1}{h} & -\frac{3}{128} & \frac{1}{64} & -\frac{3}{128} \\ 0 & 0 & -\frac{15}{32} \frac{1}{h} & 0 & 0 & \frac{1}{64} \end{pmatrix} \\ R_{h,4} &= \begin{pmatrix} \frac{1}{4} & \frac{5}{64}h & -\frac{5}{64}h & \frac{1}{128}h^2 & 0 & \frac{1}{128}h^2 \\ -\frac{3}{8} \frac{1}{h} & \frac{1}{16} & 0 & -\frac{1}{64}h & 0 & -\frac{1}{64}h \\ \frac{3}{8} \frac{1}{h} & 0 & \frac{1}{16} & \frac{1}{64}h & 0 & \frac{1}{64}h \\ 0 & -\frac{15}{32} \frac{1}{h} & 0 & \frac{1}{64} & 0 & 0 \\ -\frac{9}{16} \frac{1}{h^2} & \frac{3}{32} \frac{1}{h} & -\frac{3}{32} \frac{1}{h} & -\frac{3}{128} & \frac{1}{64} & -\frac{3}{128} \\ 0 & 0 & \frac{15}{32} \frac{1}{h} & 0 & 0 & \frac{1}{64} \end{pmatrix} & R_{h,3} &= \begin{pmatrix} \frac{1}{4} & -\frac{5}{64}h & -\frac{5}{64}h & \frac{1}{128}h^2 & 0 & \frac{1}{128}h^2 \\ \frac{3}{8} \frac{1}{h} & \frac{1}{16} & 0 & \frac{1}{64}h & 0 & \frac{1}{64}h \\ \frac{3}{8} \frac{1}{h} & 0 & \frac{1}{16} & \frac{1}{64}h & 0 & \frac{1}{64}h \\ 0 & \frac{15}{32} \frac{1}{h} & 0 & \frac{1}{64} & 0 & 0 \\ \frac{9}{16} \frac{1}{h^2} & \frac{3}{32} \frac{1}{h} & \frac{3}{32} \frac{1}{h} & \frac{3}{128} & \frac{1}{64} & \frac{3}{128} \\ 0 & 0 & -\frac{15}{32} \frac{1}{h} & 0 & 0 & \frac{1}{64} \end{pmatrix}. \end{aligned}$$

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