

On discrete least squares polynomial fit, linear spaces and data classification

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Abstract : The best discrete least squares polynomial fit to a data set is revisited. We point out some properties related to the best polynomial and precise the dimension of vector spaces encountered to solve the problem. Finally, we suggest a classification of data sets based on their increasing or decreasing trend, and on their convexity or concavity form.

Key Words : Polynomial data fitting, weighted least squares, orthogonal polynomials, linear spaces, data classification.

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1. INTRODUCTION

Let $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ be a set of m data points where the t_i 's represent the distinct values of the independent variable, the f_i 's are the values of the measured function, and each ω_i is the weight associated to the data (t_i, f_i) . The problem we consider is to find a polynomial p_n of degree at most n to fit the data. To measure how well the polynomial fit the data we use the weighted least squares deviation given by

$$(1.1) \quad F(p_n) = \sum_{i=1}^m \omega_i (f_i - p_n(t_i))^2.$$

The best polynomial, called the weighted least squares estimate (WLSE), is given by

$$(1.2) \quad p_n^* = \operatorname{argmin}_{p_n \in \mathcal{P}_n} F(p_n).$$

where \mathcal{P}_n is the set of polynomials of degree at most n .

The goal of this paper is to clarify the dimension of some vector spaces encountered in solving this problem, establish a property useful for proving the existence of a WLSE for exponential models [2], and suggest a way to classify data using the best polynomial fits. For a standard presentation of the theory related to best (polynomial) least squares fit see [1, 3, 6, 7].

The best polynomial fit problem can be solved by considering an orthogonal projection onto \mathcal{P}_n or, equivalently, by considering an orthogonal projection onto a subspace of \mathbb{R}^m . In Section 2 we briefly review the solution of the problem in \mathcal{P}_n and specify the dimension of subspaces of polynomials. In the first part of the

Section 3 we consider the subspaces of \mathbb{R}^m that play a role in solving the problem in \mathbb{R}^m . In the second part of this Section 3 we solve the problem using a projection onto a subspace of \mathbb{R}^m . Finally in Section 4 we suggest a way to classify data which will be useful in the problem of finding existence results for weighted least squares estimator [2].

2. POLYNOMIAL WEIGHTED LEAST SQUARES FITTING IN \mathcal{P}_n

In the first part of this section we present the underlying subspaces of $\mathcal{P} = \text{Lin}\{t^j \mid j = 0, 1, 2, \dots\}$ related to the polynomial weighted least squares problem. In the second part we solve the problem using a projection onto a subspace of \mathcal{P} .

2.1. Vector spaces. Let us recall that $\mathcal{P}_n = \text{Lin}\{t^j \mid j = 0, 1, \dots, n\}$. We consider also the following two other polynomial subspaces

$$(2.1) \quad \mathcal{PV}_k^+ = \text{Lin}\{v_{k,i}^+(t) = (t + t_i)^k \mid i = 1, \dots, m\} \subseteq \mathcal{P}_k,$$

$$(2.2) \quad \mathcal{PV}_k^- = \text{Lin}\{v_{k,i}^-(t) = (t - t_i)^k \mid i = 1, \dots, m\} \subseteq \mathcal{P}_k,$$

for any nonnegative integer $k = 0, 1, 2, \dots$. The next two results specify the dimension of these subspaces.

Theorem 2.1. *Let $\mathcal{P}_n = \text{Lin}\{t^j \mid j = 0, \dots, n\} \subseteq \mathcal{P}$, then $\dim \mathcal{P}_n = n + 1$. \square*

Theorem 2.2. *Let k be any nonnegative integer and let \mathcal{PV}_k^+ and \mathcal{PV}_k^- be defined by (2.1) and (2.2).*

(a) *If $k \leq m - 1$ then $\mathcal{PV}_k^+ = \mathcal{P}_k = \mathcal{PV}_k^-$, and $\dim \mathcal{PV}_k^+ = k + 1 = \dim \mathcal{PV}_k^-$.*

(b) *If $k \geq m$ then $\mathcal{PV}_k^+ \subsetneq \mathcal{P}_k$, $\mathcal{PV}_k^- \subsetneq \mathcal{P}_k$, and $\dim \mathcal{PV}_k^+ = m = \dim \mathcal{PV}_k^-$.*

Proof. We prove the result for \mathcal{PV}_k^+ only, the proof for \mathcal{PV}_k^- is identical. Since

$$\sum_{i=1}^m \mu_i v_{k,i}^+(t) = \sum_{i=1}^m \mu_i \left(\sum_{j=0}^k \binom{k}{j} t_i^j t^{k-j} \right) = \sum_{j=0}^k \binom{k}{j} \left(\sum_{i=1}^m \mu_i t_i^j \right) t^{k-j},$$

then $\sum_{i=1}^m \mu_i v_{k,i}^+(t) = 0$ if and only if $\sum_{j=0}^k \binom{k}{j} \left(\sum_{i=1}^m \mu_i t_i^j \right) t^{k-j} = 0$. From

Theorem 2.1, the set $\{t^j\}_{j=0}^k$ is linearly independent, it follows that $\sum_{i=1}^m \mu_i t_i^j = 0$ for $j = 0, \dots, k$. The matrix associated to this system is a Vandermonde type matrix. The rank of this matrix in $\min\{k + 1, m\}$ and the result follows. \square

2.2. Polynomial weighted least squares fitting. Under the condition that $n < m$, we introduce the scalar product on \mathcal{P}_n defined by

$$\langle p, q \rangle = \sum_{i=1}^m \omega_i p(t_i) q(t_i)$$

for any pair of polynomials p and q in \mathcal{P}_n . In this case (1.1) becomes

$$F(p_n) = \|f - p_n\|^2$$

where $\|\cdot\|$ is the norm on \mathcal{P}_n induced by the scalar product. For the f_i 's we use the notation $f_i = f(t_i)$ ($i = 1, \dots, m$). It is well known that p_n^* is unique and is characterized by the normal equations

$$\langle f - p_n^*, p_n \rangle = 0$$

for all $p_n \in \mathcal{P}_n$.

In this setting, to simplify the computation of p_n^* , we can find a sequence of orthogonal polynomials by applying the Gram-Schmidt orthogonalization process to the standard basis $\{1, t, t^2, \dots, t^m\}$ of \mathcal{P}_n . These orthogonal polynomials are given by

$$q_0(t) = 1, \quad q_1(t) = t - \alpha_1,$$

and for $j = 2, \dots, n$,

$$q_j(t) = (t - \alpha_j)q_{j-1}(t) - \beta_j q_{j-2}(t)$$

where

$$\alpha_j = \frac{\langle tq_{j-1}, q_{j-1} \rangle}{\langle q_{j-1}, q_{j-1} \rangle} \quad (j = 1, 2, \dots, n),$$

and

$$\beta_j = \frac{\langle tq_{j-1}, q_{j-2} \rangle}{\langle q_{j-2}, q_{j-2} \rangle} \quad (j = 2, 3, \dots, n).$$

Hence the best n -degree least squares polynomial p_n^* can be written as

$$(2.3) \quad p_n^*(t) = \sum_{j=0}^n \gamma_j^* q_j(t)$$

where

$$\gamma_j^* = \frac{\langle f, q_j \rangle}{\langle q_j, q_j \rangle} \quad (j = 0, 1, \dots, n).$$

The next two results will be useful for finding sufficient conditions for the existence of the WLSE for a 3-parametric exponential model [2].

Theorem 2.3. $\langle f - p_{n-1}^*, t^n \rangle = \gamma_n^* \|q_n\|^2$ for $n = 0, \dots, m-1$.

Proof. For $n = 0$ it is obvious because $p_{n-1}^* = 0$. For $n > 0$, since $q_n(t) = t^n + p_{n-1}(t)$ where $p_{n-1}(t)$ is a polynomial of degree $\leq n-1$, and

$$p_n^*(t) = \gamma_n^* q_n(t) + p_{n-1}^*(t),$$

we have

$$\begin{aligned} \gamma_n^* \|q_n\|^2 &= \langle \gamma_n^* q_n, q_n \rangle \\ &= \langle p_n^* - p_{n-1}^*, q_n \rangle \\ &= \langle p_n^* - f, q_n \rangle + \langle f - p_{n-1}^*, q_n \rangle \\ &= \langle f - p_{n-1}^*, t^n + p_{n-1} \rangle \\ &= \langle f - p_{n-1}^*, t^n \rangle. \quad \square \end{aligned}$$

Theorem 2.4. If the q_j 's are the orthogonal polynomials associated to $\{(\omega_i, t_i)\}_{i=1}^m$, the orthogonal polynomials \tilde{q}_j 's associated to $\{(\omega_i, \tilde{t}_i = -t_i)\}_{i=1}^m$ are given by

$$\tilde{q}_j(t) = (-1)^j q_j(-t). \quad \square$$

3. POLYNOMIAL WEIGHTED LEAST SQUARES FITTING IN \mathbb{R}^m

In the first part of this section we present the underlying subspaces of \mathbb{R}^m related to the polynomial weighted least squares problem. In the second part we solve the problem using a projection onto a subspace of \mathbb{R}^m .

3.1. Vector spaces. Let $\{t_i\}_{i=1}^m$ be a set of m distinct real numbers. For any positive integer j let us define the vectors $\vec{t}^j \in \mathbb{R}^m$ by

$$\vec{t}^j = \begin{pmatrix} t_1^j \\ t_2^j \\ \vdots \\ t_m^j \end{pmatrix} \in \mathbb{R}^m.$$

For any positive integer k , we also define the vectors

$$\vec{v}_{k,i}^+ = (\vec{t} + t_i \vec{1})^k = \sum_{j=0}^k \binom{k}{j} t_i^j \vec{t}^{k-j} \quad \text{for } i = 1, \dots, m,$$

and

$$\vec{v}_{k,i}^- = (\vec{t} - t_i \vec{1})^k = \sum_{j=0}^k (-1)^j \binom{k}{j} t_i^j \vec{t}^{k-j} \quad \text{for } i = 1, \dots, m.$$

In this section we clarify the properties of the following vector spaces, in particular the dimension of the vector spaces,

$$(3.1) \quad \mathcal{T}^n = \text{Lin}\{ \vec{t}^j \mid j = 0, \dots, n \},$$

$$(3.2) \quad \mathcal{V}_k^+ = \text{Lin}\{ \vec{v}_{k,i}^+ \mid i = 1, \dots, m \},$$

$$(3.3) \quad \mathcal{V}_k^- = \text{Lin}\{ \vec{v}_{k,i}^- \mid i = 1, \dots, m \},$$

for any integers n and k such that $n \geq 0$ and $0 \leq k \leq m-1$.

Theorem 3.1. Let $\mathcal{T}^n = \text{Lin}\{ \vec{t}^j \mid j = 0, \dots, n \} \subseteq \mathbb{R}^m$.

(a) If $n < m$, the set $\{ \vec{t}^j \}_{j=0}^n$ is linearly independent and $\dim \mathcal{T}^n = n + 1$.

(b) If $n \geq m$, the set $\{ \vec{t}^j \}_{j=0}^n$ is linearly dependent and $\dim \mathcal{T}^n = m$.

Proof. We consider $\sum_{j=0}^n \lambda_j \vec{t}^j = 0$. But the Vandermonde matrix

$$A_{m,n+1} = \begin{pmatrix} \vec{t}^0 & \vec{t}^1 & \dots & \vec{t}^n \end{pmatrix}$$

is of rank $n+1$ as long as $n < m$, and hence $\lambda_j = 0$ for $j = 0, \dots, n$. If $n \geq m$ its rank is m and there exists non zero solutions to the system. Hence the result follows because $\mathcal{T}^n \subseteq \mathbb{R}^m$. \square

Remark 3.2. For any positive integer l , since $\vec{t}^{m+l} \in \mathcal{T}^{m-1} = \mathbb{R}^m$, we have

$$\vec{t}^{m+l} = \sum_{j=0}^{m-1} \lambda_j(l) \vec{t}^j,$$

where

$$\vec{\lambda}(l) = \begin{pmatrix} \lambda_0(l) \\ \lambda_1(l) \\ \vdots \\ \lambda_{m-1}(l) \end{pmatrix} = A_{m,m}^{-1} \vec{t}^{m+l} = A_{m,m}^{-1} \text{diag}(\vec{t}^m) \vec{t}^l,$$

and

$$\text{diag}(\vec{t}^m) = \begin{pmatrix} t_1^m & 0 & \cdots & 0 \\ 0 & t_2^m & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & t_m^m \end{pmatrix}. \quad \square$$

Theorem 3.3. *Let k be any integer such that $0 \leq k \leq m - 1$, and let \mathcal{V}_k^+ and \mathcal{V}_k^- be defined by (3.2) and (3.3), then*

$$\mathcal{V}_k^+ = \mathcal{T}^k = \mathcal{V}_k^-$$

and

$$\dim \mathcal{V}_k^+ = k + 1 = \dim \mathcal{V}_k^-.$$

Proof. We prove the result for \mathcal{V}_k^+ only, the proof for \mathcal{V}_k^- is identical. Since

$$\begin{aligned} \sum_{i=1}^m \mu_i \vec{v}_{k,i}^+ &= \sum_{i=1}^m \mu_i \left(\sum_{j=0}^k \binom{k}{j} t_i^j \vec{t}^{k-j} \right) \\ &= \sum_{j=0}^k \binom{k}{j} \left(\sum_{i=1}^m \mu_i t_i^j \right) \vec{t}^{k-j}, \end{aligned}$$

then $\sum_{i=1}^m \mu_i \vec{v}_{k,i}^+ = 0$ if and only if $\sum_{j=0}^k \binom{k}{j} \left(\sum_{i=1}^m \mu_i t_i^j \right) \vec{t}^{k-j} = 0$. From

Theorem 3.1, the set $\{\vec{t}^{k-j}\}_{j=0}^k$ is linearly independent for $k < m$, it follows that $\sum_{i=1}^m \mu_i t_i^j = 0$ for $j = 0, \dots, k$. But this system of $k + 1$ equations and m unknowns has a unique solution only for $k = m - 1$. Moreover the matrix associated to this system is $A_{m,k+1}^T$ is of rank $k + 1$ for $k < m$. Hence

$$\dim \mathcal{V}_k^+ = k + 1. \quad \square$$

For $k \geq m$ we have no clear result about the dimension of \mathcal{V}_k^- and \mathcal{V}_k^+ as illustrated by the following example for $m = 3$.

Example 3.4. *Let $m = 3$.*

(a) For \mathcal{V}_k^- , since we have

$$\begin{aligned} \text{Det}(\vec{v}_{k,1}^-, \vec{v}_{k,2}^-, \vec{v}_{k,3}^-) &= \begin{vmatrix} 0 & (t_1 - t_2)^k & (t_1 - t_3)^k \\ (t_2 - t_1)^k & 0 & (t_2 - t_3)^k \\ (t_3 - t_1)^k & (t_3 - t_2)^k & 0 \end{vmatrix} \\ &= [1 + (-1)^k](t_1 - t_2)^k (t_2 - t_3)^k (t_3 - t_1)^k \\ &= \begin{cases} 0 & \text{if } k \text{ is odd,} \\ 2(t_1 - t_2)^k (t_2 - t_3)^k (t_3 - t_1)^k & \text{if } k \text{ is even,} \end{cases} \end{aligned}$$

it follows that

$$\dim \mathcal{V}_k^- = \begin{cases} 2 & \text{if } k \text{ is odd,} \\ 3 & \text{if } k \text{ is even.} \end{cases}$$

(b) For \mathcal{V}_k^+ , we have

$$\begin{aligned}
\text{Det}(\vec{v}_{k,1}^+, \vec{v}_{k,2}^+, \vec{v}_{k,3}^+) &= \begin{vmatrix} (2t_1)^k & (t_1+t_2)^k & (t_1+t_3)^k \\ (t_2+t_1)^k & (2t_2)^k & (t_2+t_3)^k \\ (t_3+t_1)^k & (t_3+t_2)^k & (2t_3)^k \end{vmatrix} \\
&= (8t_1t_2t_3)^k + 2(t_1+t_2)^k(t_2+t_3)^k(t_3+t_1)^k \\
&\quad - 2^k[t_1^k(t_2+t_3)^{2k} + t_2^k(t_3+t_1)^{2k} + t_3^k(t_1+t_2)^{2k}].
\end{aligned}$$

This determinant can be 0. Indeed for $t_1+t_3=0$ and $t_2=0$ the determinant is 0 for odd k . It follows that $\dim \mathcal{V}_k^+$ is 2 or 3 depending on the values of t_1 , t_2 and t_3 . \square

Remark 3.5. In [4] it is asserted that \mathcal{V}_2^- is of dimension m which is clearly false except for $m=3$. As a consequence the proof given in [4] for the existence of a WLSE for a 3-parametric exponential function is not correct. There are also errors in the proof of the existence of a WLSE in [5]. \square

3.2. Polynomial weighted least squares fitting. We introduce the scalar product on \mathbb{R}^m defined by

$$\langle \vec{u}, \vec{v} \rangle = \sum_{i=1}^m \omega_i u_i v_i,$$

for any pair of vectors \vec{u} and \vec{v} in \mathbb{R}^m

$$\vec{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix} \quad \text{and} \quad \vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{pmatrix}.$$

The norm on \mathbb{R}^m induced by the scalar product is $\|\vec{u}\| = \langle \vec{u}, \vec{u} \rangle^{1/2}$. Then (1.1) becomes

$$F(p_n) = \|\vec{f} - \vec{p}_n\|^2,$$

where

$$\vec{p}_n = \sum_{j=0}^n \alpha_j \vec{t}^j, \quad \vec{t}^j = \begin{pmatrix} t_1^j \\ t_2^j \\ \vdots \\ t_m^j \end{pmatrix}, \quad \text{and} \quad \vec{f} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{pmatrix}.$$

The problem is to find the orthogonal projection of \vec{f} on \mathcal{T}^n . This projection is completely characterized by the normal equations

$$\langle \vec{f} - \vec{p}_n^*, \vec{p}_n \rangle = 0$$

for all $\vec{p}_n \in \mathcal{T}^n$.

Again, to simplify the computation of p_n^* , we can determine an orthogonal basis $\{\vec{q}_j\}_{j=0}^n$ for \mathcal{T}^n by applying the Gram-Schmidt process to its basis $\{\vec{t}^j\}_{j=0}^n$. We obtain

$$\vec{q}_0 = \vec{1}, \quad \vec{q}_1 = \vec{t} - \alpha_1 \vec{1},$$

and for $j=2, \dots, n$,

$$\vec{q}_j = (\vec{t} - \alpha_j \vec{1}) \cdot \vec{q}_{j-1} - \beta_j \vec{q}_{j-2}$$

where

$$\alpha_j = \frac{\langle \vec{t} \cdot \vec{q}_{j-1}, \vec{q}_{j-1} \rangle}{\langle \vec{q}_{j-1}, \vec{q}_{j-1} \rangle} \quad (j = 1, 2, 3, \dots),$$

and

$$\beta_j = \frac{\langle \vec{t} \cdot \vec{q}_{j-1}, \vec{q}_{j-2} \rangle}{\langle \vec{q}_{j-2}, \vec{q}_{j-2} \rangle} \quad (j = 2, 3, 4, \dots).$$

In these identities, $\vec{u} \cdot \vec{v}$ is the coordinatewise multiplication of two vectors of \mathbb{R}^m defined by

$$\vec{u} \cdot \vec{v} = \begin{pmatrix} u_1 v_1 \\ u_2 v_2 \\ \vdots \\ u_m v_m \end{pmatrix}.$$

Let us observe that $\vec{q}_j \in \mathcal{T}^j$ for $j = 0, \dots, n$.

It follows that the projection is given by

$$(3.4) \quad \vec{p}_n^* = \sum_{j=0}^n \gamma_j^* \vec{q}_j$$

where

$$\gamma_j^* = \frac{\langle \vec{f}, \vec{q}_j \rangle}{\langle \vec{q}_j, \vec{q}_j \rangle} \quad (j = 0, 1, \dots, n).$$

The next theorem is equivalent to Theorem 2.3.

Theorem 3.6. $\langle \vec{f} - \vec{p}_{n-1}^*, \vec{t}^n \rangle = \gamma_n^* \|\vec{q}_n\|^2$ for $n = 0, \dots, m-1$.

Proof. For $n = 0$ we have $\vec{p}_{n-1}^* = \vec{0}$ and the result follows. For $n > 0$, since $\vec{q}_n = \vec{t}^n + \vec{p}_{n-1}$ where \vec{p}_{n-1} is a vector in \mathcal{T}^{n-1} , and

$$\vec{p}_n^* = \gamma_n^* \vec{q}_n + \vec{p}_{n-1}^*,$$

we have

$$\begin{aligned} \gamma_n^* \|\vec{q}_n\|^2 &= \langle \gamma_n^* \vec{q}_n, \vec{q}_n \rangle \\ &= \langle \vec{p}_n^* - \vec{p}_{n-1}^*, \vec{q}_n \rangle \\ &= \langle \vec{p}_n^* - \vec{f}, \vec{q}_n \rangle + \langle \vec{f} - \vec{p}_{n-1}^*, \vec{q}_n \rangle \\ &= \langle \vec{f} - \vec{p}_{n-1}^*, \vec{t}^n + \vec{p}_{n-1} \rangle \\ &= \langle \vec{f} - \vec{p}_{n-1}^*, \vec{t}^n \rangle. \quad \square \end{aligned}$$

4. CLASSIFICATION OF DATA

Let $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ be a set of m data points. If we use a discrete least squares polynomial to fit the data with the orthogonal basis $\{q_j\}_{j=0}^n$, the coefficients of p_n^* with respect to its expansion (2.3) or (3.4) suggest the following classification of the data.

Definition 4.1. The data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ are said to be :

- (i) essentially stationary if $\gamma_1^* = 0$;
- (ii) essentially increasing, respectively decreasing, if $\gamma_1^* > 0$, respectively $\gamma_1^* < 0$;
- (iii) essentially linear if $\gamma_2^* = 0$;
- (iv) essentially convex, respectively concave, if $\gamma_2^* > 0$, respectively $\gamma_2^* < 0$. □

Let us note that we could continue the classification with the higher order coefficients γ_n^* for $n = 3, \dots, m - 1$.

Finally if we apply symmetric transformations to the data we obtain the following result.

Theorem 4.2. *Effect of symmetric transformations on the data.*

- (a) *If the data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ are essentially increasing, resp. decreasing, then the data $\{(\omega_i, -t_i, f_i)\}_{i=1}^m$ are essentially decreasing, resp. increasing. The stationarity, linearity, and concavity or convexity properties are not modified by this transform.*
- (b) *If the data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ are essentially increasing, resp. decreasing, and essentially convex, resp. concave, then the data $\{(\omega_i, t_i, -f_i)\}_{i=1}^m$ are essentially decreasing, resp. increasing, and essentially concave, resp. convex. The stationarity and linearity properties are not modified by this transform. \square*

5. CONCLUSION

We have revisited the polynomial weighted least squares analysis. Doing so we have specified the dimension of three vector subspaces of \mathcal{P} (Theorem 2.1 and Theorem 2.2) and of \mathbb{R}^m (Theorem 3.1 and Theorem 3.3) used for solving this problem. We also have established a property (Theorem 2.3 and Theorem 3.6) and suggested a classification of data (Definition 4.1) which will play a role in finding sufficient conditions for the existence of a WLSE for a 3-parametric exponential model [2].

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