Least Squares Fitting of Segments by Line or Plane

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1 Introduction

This document describes algorithms for least-squares fitting of n-dimensional segments by a line (1-dimensional) or by a hyperplane ($(n-1)$-dimensional). The algorithms are usually required in 3D applications where $n = 3$. The fitting uses an extension of orthogonal regression described in Sections 2 and 4 of Least Squares Fitting of Data.

A segment has endpoints $\mathbf{B}$ (the beginning point) and $\mathbf{E}$ (the ending point) and is parameterized by

$$\mathbf{X}(s) = (1-s)\mathbf{B} + s\mathbf{E} = \mathbf{B} + s(\mathbf{E} - \mathbf{B}) = \mathbf{B} + s\mathbf{U} \tag{1}$$

where $\mathbf{U} = \mathbf{E} - \mathbf{B}$ and for $s \in [0,1]$. The input to the fitting algorithm is a set of m segments, $\{\mathbf{X}_i(s)\}_{i=1}^m$.

2 Fitting Segments by a Line

The fitting line parameterized by $\mathbf{A} + t\mathbf{D}$, where $\mathbf{D}$ is unit length and $\mathbf{A}$ is a point on the line. The points on a segment are of the form $\mathbf{X}_i(s) = \mathbf{A} + d_i(s)\mathbf{D} + \mathbf{P}_i(s)$, where $\mathbf{P}_i(s)$ is a vector that is perpendicular to $\mathbf{D}$ or zero; that is, $\mathbf{D} \cdot \mathbf{P}_i(s) = 0$ for all $s \in [0,1]$. Define $\mathbf{Y}_i(s) = \mathbf{X}_i(s) - \mathbf{A}$ and observe that $d_i(s) = \mathbf{D} \cdot \mathbf{Y}_i(s)$. The vector from $\mathbf{X}_i(s)$ to its projection onto the line is $\mathbf{P}_i(s) = \mathbf{Y}_i(s) - d_i(s)\mathbf{D}$ and has squared length

$$\begin{aligned} |\mathbf{P}_i(s)|^2 &= |\mathbf{Y}_i(s) - d_i(s)\mathbf{D}|^2 \\ &= \mathbf{Y}_i(s)^\mathsf{T} \left(I - \mathbf{D}\mathbf{D}^\mathsf{T}\right) \mathbf{Y}_i(s) \\ &= \mathbf{D}^\mathsf{T} \left(\mathbf{Y}_i(s)^\mathsf{T}\mathbf{Y}_i(s) I - \mathbf{Y}_i(s)\mathbf{Y}_i(s)^\mathsf{T}\right) \mathbf{D} \end{aligned} \tag{2}$$

where I is the $n \times n$ identity matrix. The least-squares error function is

$$E(\mathbf{A}, \mathbf{D}) = \sum_{i=1}^m \int_0^1 |\mathbf{P}_i(s)|^2 \, ds \tag{3}$$

The summation is discrete because the number of line segments is finite. The integral is effectively the continuous summation of the squared projection lengths over the points of the segments.

The error function can be written using the second equality of equation (2),

$$E(\mathbf{A}, \mathbf{D}) = \sum_{i=1}^m \int_0^1 \mathbf{Y}_i(s)^\mathsf{T} \left(I - \mathbf{D}\mathbf{D}^\mathsf{T}\right) \mathbf{Y}_i(s) \, ds \tag{4}$$

The partial derivative of E with respect to the components of $\mathbf{A}$ is

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{A}} &= -2\left(I - \mathbf{D}\mathbf{D}^\mathsf{T}\right) \textstyle\sum_{i=1}^m \int_0^1 \mathbf{Y}_i(s) \, ds \\ &= -2\left(I - \mathbf{D}\mathbf{D}^\mathsf{T}\right) \textstyle\sum_{i=1}^m \int_0^1 \left(\mathbf{B}_i - \mathbf{A} + s\mathbf{U}_i\right) \, ds \\ &= -2\left(I - \mathbf{D}\mathbf{D}^\mathsf{T}\right) \textstyle\sum_{i=1}^m \left(\mathbf{B}_i - \mathbf{A} + \mathbf{U}_i/2\right) \\ &= -2\left(I - \mathbf{D}\mathbf{D}^\mathsf{T}\right) \textstyle\sum_{i=1}^m \left(\left(\mathbf{B}_i + \mathbf{E}_i\right)/2 - \mathbf{A}\right) \end{aligned} \tag{5}$$

A necessary condition for the minimum to occur is $\partial E/\partial \mathbf{A} = \mathbf{0}$. We can make this happen by choosing

$$\mathbf{A} = \frac{1}{m}\sum_{i=1}^{m} \frac{\mathbf{B}_i + \mathbf{E}_i}{2} \tag{6}$$

Therefore, the line point $\mathbf{A}$ is chosen to be the average of the midpoints of the segments.

The error function can also be written using the third equality of equation (2),

$$E(\mathbf{A},\mathbf{D}) = \mathbf{D}^{\mathsf{T}} \left(\sum_{i=1}^{m} \int_0^1 \left(\mathbf{Y}_i(s)^{\mathsf{T}}\mathbf{Y}_i(s) I - \mathbf{Y}_i(s)\mathbf{Y}_i(s)^{\mathsf{T}} \right) \, ds \right) \mathbf{D} = \mathbf{D}^{\mathsf{T}} M(\mathbf{A}) \mathbf{D} \tag{7}$$

where M is a positive definite matrix. The computation of M is straightforward. Define $\mathbf{\Delta}_i = \mathbf{B}_i - \mathbf{A}$; then

$$\mathbf{Y}_i(s)^{\mathsf{T}}\mathbf{Y}_i(s) = s^2|\mathbf{U}_i|^2 + 2s\mathbf{U}_i \cdot \mathbf{\Delta}_i + |\mathbf{\Delta}_i|^2 \tag{8}$$

and

$$\mathbf{Y}_i(s)\mathbf{Y}_i(s)^{\mathsf{T}} = s^2 \mathbf{U}_i\mathbf{U}_i^{\mathsf{T}} + s\left(\mathbf{U}_i\mathbf{\Delta}^{\mathsf{T}} + \mathbf{\Delta}\mathbf{U}_i^{\mathsf{T}}\right) + \mathbf{\Delta}\mathbf{\Delta}^{\mathsf{T}} \tag{9}$$

Integrating these leads to

$$M = \sum_{i=1}^{m} \left[\frac{1}{3}|\mathbf{U}_i|^2 + \mathbf{U}_i \cdot \mathbf{\Delta}_i + |\mathbf{\Delta}_i|^2 - \frac{1}{3}\mathbf{U}_i\mathbf{U}_i^{\mathsf{T}} - \frac{1}{2}\left(\mathbf{U}_i\mathbf{\Delta}^{\mathsf{T}} + \mathbf{\Delta}\mathbf{U}_i^{\mathsf{T}}\right) - \mathbf{\Delta}\mathbf{\Delta}^{\mathsf{T}} \right] \tag{10}$$

The line direction $\mathbf{D}$ is chosen to be a unit-length eigenvector for the minimum eigenvalue of M.

If all segments are degenerate, then $\mathbf{U}_i = \mathbf{0}$, $\mathbf{X}_i = \mathbf{B}_i$ and $\mathbf{\Delta}_i = \mathbf{X}_i - \mathbf{A}$. Equation (10) becomes the equation for M in the least-squares fitting of points by a line.

3 Fitting Segments by a Hyperplane

Let the hyperplane be implicitly defined by $\mathbf{N} \cdot (\mathbf{X} - \mathbf{A})$ where $\mathbf{A}$ is a point on the hyperplane and $\mathbf{N}$ is a unit-length normal to the hyperplane. The input segments can be written as $\mathbf{X}_i(s) = \mathbf{A} + h_i(s)\mathbf{N} + \mathbf{P}_i(s)$, where $\mathbf{P}_i(s)$ is a vector that is perpendicular to $\mathbf{N}$ or zero; that is $\mathbf{N} \cdot \mathbf{P}_i(s) = 0$ for all $s \in [0,1]$. Define $\mathbf{Y}_i(s) = \mathbf{X}_i(s) - \mathbf{A}$ and observe that $h_i(s) = \mathbf{N} \cdot \mathbf{Y}_i(s)$. The projection of $\mathbf{X}_i(s)$ onto the normal line has squared length

$$\begin{aligned} h_i(s)^2 &= (\mathbf{N} \cdot \mathbf{Y}_i(s))^2 \\ &= \mathbf{Y}_i(s)^{\mathsf{T}} \left(\mathbf{N}\mathbf{N}^{\mathsf{T}}\right) \mathbf{Y}_i(s) \\ &= \mathbf{N}^{\mathsf{T}} \left(\mathbf{Y}_i(s)\mathbf{Y}_i(s)^{\mathsf{T}}\right) \mathbf{N} \end{aligned} \tag{11}$$

The least-squares error function is

$$E(\mathbf{A},\mathbf{N}) = \sum_{i=1}^{m} \int_0^1 h_i(s)^2 \, ds \tag{12}$$

The summation is discrete because the number of line segments is finite. The integral is effectively the continuous summation of the squared projection lengths over the points of the segments.

The error function can be written using the second equality of equation (11),

$$E(\mathbf{A},\mathbf{N}) = \sum_{i=1}^{m} \int_0^1 \mathbf{Y}_i(s)^\mathsf{T} \left(\mathbf{N}\mathbf{N}^\mathsf{T}\right) \mathbf{Y}_i(s)\, ds \tag{13}$$

The partial derivative of E with respect to the components of $\mathbf{A}$ is

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{A}} &= 2\left(\mathbf{N}\mathbf{N}^\mathsf{T}\right) \textstyle\sum_{i=1}^{m} \int_0^1 \mathbf{Y}_i(s)\, ds \\ &= 2\left(\mathbf{N}\mathbf{N}^\mathsf{T}\right) \textstyle\sum_{i=1}^{m} \int_0^1 \left(\mathbf{B}_i - \mathbf{A} + s\mathbf{U}_i\right)\, ds \\ &= 2\left(\mathbf{N}\mathbf{N}^\mathsf{T}\right) \textstyle\sum_{i=1}^{m} \left(\mathbf{B}_i - \mathbf{A} + \mathbf{U}_i/2\right) \\ &= 2\left(\mathbf{N}\mathbf{N}^\mathsf{T}\right) \textstyle\sum_{i=1}^{m} \left(\left(\mathbf{B}_i + \mathbf{E}_i\right)/2 - \mathbf{A}\right) \end{aligned} \tag{14}$$

A necessary condition for the minimum to occur is $\partial E/\partial \mathbf{A} = \mathbf{0}$. We can make this happen by choosing

$$\mathbf{A} = \frac{1}{m} \sum_{i=1}^{m} \frac{\mathbf{B}_i + \mathbf{E}_i}{2} \tag{15}$$

Therefore, the plane point $\mathbf{A}$ is chosen to be the average of the midpoints of the segments.

The error function can also be written using the third equality of equation (11),

$$E(\mathbf{A},\mathbf{N}) = \mathbf{N}^\mathsf{T} \left(\sum_{i=1}^{m} \int_0^1 \mathbf{Y}_i(s)\mathbf{Y}_i(s)^\mathsf{T}\, ds \right) \mathbf{N} = \mathbf{N}^\mathsf{T} M(\mathbf{A}) \mathbf{N} \tag{16}$$

where M is a positive definite matrix. The computation of M is straightforward. Define $\mathbf{\Delta}_i = \mathbf{B}_i - \mathbf{A}$; then

$$\mathbf{Y}_i(s)\mathbf{Y}_i(s)^\mathsf{T} = s^2 \mathbf{U}_i \mathbf{U}_i^\mathsf{T} + s\left(\mathbf{U}_i \mathbf{\Delta}^\mathsf{T} + \mathbf{\Delta}\mathbf{U}_i^\mathsf{T}\right) + \mathbf{\Delta}\mathbf{\Delta}^\mathsf{T} \tag{17}$$

Integrating these leads to

$$M = \sum_{i=1}^{m} \left[\frac{1}{3}\mathbf{U}_i\mathbf{U}_i^\mathsf{T} + \frac{1}{2}\left(\mathbf{U}_i \mathbf{\Delta}^\mathsf{T} + \mathbf{\Delta}\mathbf{U}_i^\mathsf{T}\right) + \mathbf{\Delta}\mathbf{\Delta}^\mathsf{T} \right] \tag{18}$$

The plane normal $\mathbf{N}$ is chosen to be a unit-length eigenvector for the minimum eigenvalue of M.

If all segments are degenerate, then $\mathbf{U}_i = \mathbf{0}$, $\mathbf{X}_i = \mathbf{B}_i$ and $\mathbf{\Delta}_i = \mathbf{X}_i - \mathbf{A}$. Equation (18) becomes the equation for M in the least-squares fitting of points by a plane.