Least-squares Fit of a Continuous Piecewise Linear Function

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Abstract

The paper describes an application of the least-squares method to fitting a continuous piecewise linear function. It shows that the solution is unique and the best fit can be found without resorting to iterative optimization techniques.

Problem

Given a set of pairs of data points:

x_i, y_i, $i = 1..n$

x_i	independent variable;
y_i	dependent variable;
i	index;
n	number of points;

and fixed bounds of the segments of the continuous piecewise linear function:

a_j, $j = 1..m$

a_j	x coordinate of a segment end point;
j	end point index;
m	number of segment end points;
$m-1$	number of segments;

find the y coordinates of the segment end points (b_j) of a continuous piecewise linear function, which minimize the sum of squares of the distance between the function and corresponding data points:

$$S = \Sigma(f(x_i) - y_i)^2$$

$f(x_i)$ fitted piecewise linear function.

Note that the term continuous is used in the sense that the adjacent segments of the function share the same end point.

See Figure 1 for a graphical example of the problem.

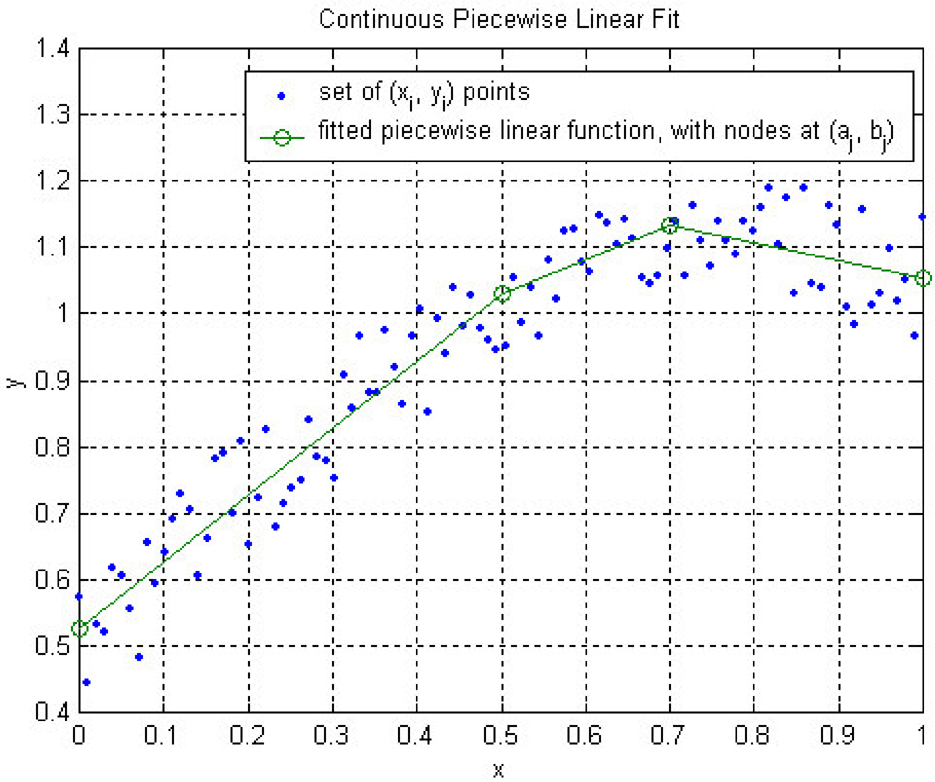

Figure 1. Example of fitting a continuous piecewise linear function.

Solution

General Least-squares Method

First, we will outline some key steps used in the least-squares method. Given a function $f(x, b_1, \ldots b_m)$, where $b_1, \ldots b_m$ are unknown parameters, and a set of data points (x_i, y_i), where i=1..n, we need to minimize the following objective function:

$$s = \sum_{i=1}^{n} \left(f_i - y_i \right)^2 \tag{1.1}$$

$f_i = f(x_i, b_1, \ldots b_m)$ value of the fitted function at x_i;

The minimum of the function can be found by analyzing its partial derivatives in the unknown parameters. The first order derivative would indicate the extremum point(s) when it is equal to zero. The second order derivative would indicate if the extremum point is actually the minimum and if it's a unique minimum. For example, if the second derivative is a positive constant, the first derivative has a unique intersection with zero and it changes sign from negative to positive at the intersection, which corresponds to the function minimum.

The objective function derivatives can be expressed in terms of function f(x, b_1, … b_m) and its derivatives:

$$\frac{ds}{db_t} = 2\sum_{i=1}^{n}(f_i - y_i)\frac{df_i}{db_t} \tag{1.2}$$

$$\frac{d^2 s}{db_t^2} = 2\sum_{i=1}^{n}\left[(f_i - y_i)\frac{d^2 f_i}{db_t^2} + \left(\frac{df_i}{db_t}\right)^2\right] \tag{1.3}$$

t=1..m index of the unknown parameters.

The parameters are found by equating the first derivative equations to zero and solving the resulting system of equations:

$$\sum_{i=1}^{n}(f_i - y_i)\frac{df_i}{db_t} = 0 \tag{1.4}$$

Note that if the fitted function is a polynomial, the second derivative of the objective function is positive (unless x_i are zero) and simplifies to:

$$\frac{d^2 s}{db_t^2} = 2\sum_{i=1}^{n}\left(\frac{df_i}{db_t}\right)^2 \tag{1.5}$$

Therefore, fitting polynomials results in a unique solution.

Fitting Segmented Functions

If the fitted function consists of several consecutive segments, the same least-squares method can be used with some additional constraints. The constraints depend on how the segments are connected, e.g.:

1) the function is continuous at the joint points between segments (the same point is shared by adjacent segments);
2) the function is continuous and smooth at the joint points (the same point is shared by adjacent segments and the first derivative in x is continuous).

The equations 1.1-1.4 can be expressed in a slightly different way for segmented functions:

$$s = \sum_{j=1}^{m-1}\sum_{i=1}^{n_j}\left(f_{j,i} - y_{j,i}\right)^2 \tag{1.6}$$

$$\frac{ds}{db_t} = 2\sum_{j=1}^{m-1}\sum_{i=1}^{n_j}\left(f_{j,i} - y_{j,i}\right)\frac{df_{j,i}}{db_t} \tag{1.7}$$

$$\frac{d^2 s}{db_t^2} = 2\sum_{j=1}^{m-1}\sum_{i=1}^{n_j}\left[\left(f_{j,i} - y_{j,i}\right)\frac{d^2 f_{j,i}}{db_t^2} + \left(\frac{df_{j,i}}{db_t}\right)^2\right] \tag{1.8}$$

$$\sum_{j=1}^{m-1}\sum_{i=1}^{n_j}\left(f_{j,i} - y_{j,i}\right)\frac{df_{j,i}}{db_t} = 0 \tag{1.9}$$

m	number of segment end points;
m-1	number of segments;
j=1..m-1	segment index;
n_j	number of points in j-th segment;
$i=1..n_j$	point index in j-th segment;
$x_{j,i}$	independent variable;
$y_{j,i}$	dependent variable;
$f_{j,i}= f_j(x_{j,i}, b_1, \dots b_k)$	fitted function value;
$f_j(x, b_1, \dots b_k)$	fitted function used in j-th segment;
k	number of unknown variables;
t=1..k	index of an unknown variable (corresponds to an equation for each unknown variable).

In order to solve the system of equations (1.9), the functions f_j must include the constraints for the segment joint points. If the constraints are formulated separately, using additional equations, the system becomes overdetermined and there is no solution.

Fortunately, it is possible to factor the continuity and smoothness constraints in the fitted functions f_j provided they have a polynomial form:

$$f_j(x) = \sum_{q=0}^{p} b_{j,q}\left(x - a_j\right)^q \tag{1.10}$$

p	polynomial order;
q=0..p	polynomial coefficient index;
$b_{j,0}, \dots b_{j,p}$	unknown parameters (polynomial coefficients);
a_j	fixed x coordinate of the first end point of j-th segment.

The *continuity* constraint implies that $f_j(a_{j+1})= f_{j+1}(a_{j+1})$. After substituting this condition in (1.10), we find:

$$\sum_{q=0}^{p} b_{j,q}\left(a_{j+1} - a_j\right)^q = b_{j+1,0} \tag{1.11}$$

In other words, one of the parameters in function f_{j+1} is determined from the previous segment – function f_j.

The *smoothness* constraint can be handled similarly:

$$\frac{df_j\left(a_{j+1}\right)}{dx} = \frac{df_{j+1}\left(a_{j+1}\right)}{dx} \tag{1.12}$$

$$\sum_{q=1}^{p} q \cdot b_{j,q}\left(a_{j+1} - a_j\right)^{q-1} = b_{j+1,1} \tag{1.13}$$

The smoothness constraint determines another parameter in function f_{j+1} from function f_j, $b_{j+1,1}$.

Fitting Continuous Piecewise Linear Function

A continuous piecewise linear function consists of segments defined by first-order polynomials (1.10) with the continuity constraint (1.11):

$$f_j(x) = b_{j,0} + b_{j,1}\left(x - a_j\right) \tag{1.14}$$

After including the continuity constraint in (1.14), all fitted functions can be expressed in the same form:

$$f_j(x) = \frac{(b_{j+1,0} - b_{j,0})x + b_{j,0}a_{j+1} - b_{j+1,0}a_j}{a_{j+1} - a_j} \tag{1.15}$$

j=1..m-1	segment index;
m-1	number of segments;
(a_j, $b_{j,0}$)	x,y coordinates of the first end point of j-th segment;
(a_{j+1}, $b_{j+1,0}$)	x,y coordinates of the second end point of j-th segment.

We can drop the second index in the b parameters because it is always zero:

$$f_j(x) = \frac{(b_{j+1} - b_j)x + b_j a_{j+1} - b_{j+1}a_j}{a_{j+1} - a_j} \tag{1.16}$$

j = 1..m-1	segment index;
m-1	number of segments;
(a_j, b_j)	x,y coordinates of the first end point of j-th segment;
(a_{j+1}, b_{j+1})	x,y coordinates of the second end point of j-th segment.

Let’s analyze the derivatives of the function in respect to its parameters. There are only two parameters involved – b_j and b_{j+1}:

$$\frac{df_j}{db_j} = \frac{-x + a_{j+1}}{a_{j+1} - a_j} \tag{1.17}$$

$$\frac{df_j}{db_{j+1}} = \frac{x - a_j}{a_{j+1} - a_j} \tag{1.18}$$

$$\frac{d^2 f_j}{db_j^2} = 0 \tag{1.19}$$

$$\frac{d^2 f_j}{db_{j+1}^2} = 0 \tag{1.20}$$

The second derivatives are equal to zero. Therefore, the second derivatives of the objective function are positive (1.8) and the solution is unique.

The system of equations can be formed by removing the first derivatives in parameters equal to zero from (1.9):

$$\sum_{i=1}^{n_{t-1}} \left(f_{t-1,i} - y_{t-1,i} \right) \frac{df_{t-1,i}}{db_t} + \sum_{i=1}^{n_t} \left(f_{t,i} - y_{t,i} \right) \frac{df_{t,i}}{db_t} = 0 \tag{1.21}$$

t=1..m	parameter index (corresponds to an equation per each value);
m	number of unknown parameters;
m-1	number of segments;
n_j	number of points in j-th segment;
$n_0=n_m=0$	number of points in undefined segments (corresponding sums disappear);
i	point index in a segment;

There are two exceptions in the system when n_{t-1} or n_t are equal to zero (t=1 or t=m). They correspond to undefined functions f_0 and f_m. Since the sum of squares doesn't depend on functions f_0 and f_m, the corresponding sums in (1.21) should be omitted.

The system of equations can be expanded by substituting expressions from (1.16-1.18) into (1.21):

$$\begin{aligned}
&\sum_{i=1}^{n_{t-1}} \left(\frac{(b_t - b_{t-1})x_{t-1,i} + b_{t-1}a_t - b_t a_{t-1}}{a_t - a_{t-1}} - y_{t-1,i} \right) \frac{x_{t-1,i} - a_{t-1}}{a_t - a_{t-1}} + \\
&\sum_{i=1}^{n_t} \left(\frac{(b_{t+1} - b_t)x_{t,i} + b_t a_{t+1} - b_{t+1} a_t}{a_{t+1} - a_t} - y_{t,i} \right) \frac{-x_{t,i} + a_{t+1}}{a_{t+1} - a_t} = 0
\end{aligned} \tag{1.22}$$

The terms can be regrouped in regards to the unknown parameters:

$$\frac{-b_{t-1}\left(\sum_{i=1}^{n_{t-1}}\left(x_{t-1,i}-a_{t-1}\right)\left(x_{t-1,i}-a_{t}\right)\right)+b_{t}\left(\sum_{i=1}^{n_{t-1}}\left(x_{t-1,i}-a_{t-1}\right)^{2}\right)}{\left(a_{t}-a_{t-1}\right)^{2}}+$$
$$\frac{b_{t}\left(\sum_{i=1}^{n_{t}}\left(x_{t,i}-a_{t+1}\right)^{2}\right)-b_{t+1}\left(\sum_{i=1}^{n_{t}}\left(x_{t,i}-a_{t}\right)\left(x_{t,i}-a_{t+1}\right)\right)}{\left(a_{t+1}-a_{t}\right)^{2}}= \tag{1.23}$$
$$\frac{\left(\sum_{i=1}^{n_{t-1}}x_{t-1,i}y_{t-1,i}\right)-a_{t-1}\left(\sum_{i=1}^{n_{t-1}}y_{t-1,i}\right)}{a_{t}-a_{t-1}}+\frac{-\left(\sum_{i=1}^{n_{t}}x_{t,i}y_{t,i}\right)+a_{t+1}\left(\sum_{i=1}^{n_{t}}y_{t,i}\right)}{a_{t+1}-a_{t}};$$

t=1..m	parameter index (corresponds to an equation per each value);
m	number of unknown parameters;
m-1	number of segments;
n_j	number of points in j-th segment;
$n_0=n_m=0$	number of points in undefined segments (corresponding sums disappear);
i	point index in a segment;

Just like in (1.21), the sums over segments 0 and m should be omitted.

Solution of the normal linear system of equation (1.23) produces the answer to the problem of fitting a piecewise linear function.