Spline Fit

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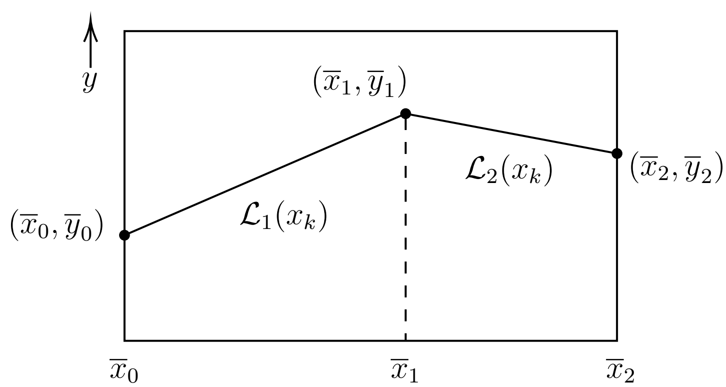
Without loss of generality, consider the points (x_k, y_k) be ordered according to their x values. This is just to make the derivation simpler – the corresponding MATLAB script works whether or not the points are sorted.

Also, for the simplicity of derivation, consider the case of 3 knot points. The design vector in this case will be

$$\bar{\mathbf{y}} = \begin{bmatrix} \bar{y}_0 \\ \bar{y}_1 \\ \bar{y}_2 \end{bmatrix}.$$



We have to solve the least squares problem

$$\min_{\bar{\mathbf{y}}} \sum_{k=1}^{N} (y_k - \hat{y}_k)^2,$$

where y_k is the value of y corresponding to x_k, and $\hat{y}_k$ is the value predicted from the spline fit. Let us call the objective function $f(\bar{\mathbf{y}})$. That is

$$f(\bar{\mathbf{y}}) \triangleq \sum_{k=1}^{N} (y_k - \hat{y}_k)^2.$$

Consider the vector

$$\mathbf{z} = \begin{bmatrix} y_1 - \hat{y}_1 \\ \vdots \\ y_N - \hat{y}_N \end{bmatrix}.$$

Notice that $f(\bar{\mathbf{y}})$ is just the squared norm of $\mathbf{z}$. That is,

$$f(\bar{\mathbf{y}}) = \sum_{k=1}^{N} (y_k - \hat{y}_k)^2 = \|\mathbf{z}\|^2.$$

Therefore, we can reformulate the optimization problem to be the minimization of the squared norm of the vector $\mathbf{z}$, where

$$\|\mathbf{z}\|^2 = \left\| \begin{bmatrix} y_1 - \hat{y}_1 \\ \vdots \\ y_N - \hat{y}_N \end{bmatrix} \right\|^2$$

Let $\mathcal{L}_1(x)$ be the best fit line on the interval $[\bar{x}_0, \bar{x}_1)$, and $\mathcal{L}_2(x)$ be the best fit line on the interval $[\bar{x}_1, \bar{x}_2]$. Then,

$$\hat{y}_i = \begin{cases} \mathcal{L}_1(x_i) & x_i \in [\bar{x}_0, \bar{x}_1) \\ \mathcal{L}_2(x_i) & x_i \in [\bar{x}_1, \bar{x}_2] \end{cases}$$

Since the points are sorted, we will have all points $x_1, \cdots, x_k$ correspond to $\mathcal{L}_1$, and all points $x_{k+1}, \cdots, x_N$ correspond to $\mathcal{L}_2$, for a given k. Therefore, we can write

$$\|\mathbf{z}\|^2 = \left\| \begin{bmatrix} y_1 - \mathcal{L}_1(x_1) \\ \vdots \\ y_k - \mathcal{L}_1(x_k) \\ y_{k+1} - \mathcal{L}_2(x_{k+1}) \\ \vdots \\ y_N - \mathcal{L}_2(x_N) \end{bmatrix} \right\|^2.$$

Substituting in the equations of the lines $\mathcal{L}_1$ and $\mathcal{L}_2$ gives

$$\|\mathbf{z}\|^2 = \left\| \begin{bmatrix} y_1 - \bar{y}_0 - \dfrac{\bar{y}_1 - \bar{y}_0}{\bar{x}_1 - \bar{x}_0}(x_1 - \bar{x}_0) \\ \vdots \\ y_k - \bar{y}_0 - \dfrac{\bar{y}_1 - \bar{y}_0}{\bar{x}_1 - \bar{x}_0}(x_k - \bar{x}_0) \\ y_{k+1} - \bar{y}_1 - \dfrac{\bar{y}_2 - \bar{y}_1}{\bar{x}_2 - \bar{x}_1}(x_{k+1} - \bar{x}_1) \\ \vdots \\ y_N - \bar{y}_1 - \dfrac{\bar{y}_2 - \bar{y}_1}{\bar{x}_2 - \bar{x}_1}(x_N - \bar{x}_1) \end{bmatrix} \right\|^2$$

$$
= \left\| \begin{bmatrix} \bar{y}_0 \left(\dfrac{x_1 - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} - 1 \right) + \bar{y}_1 \left(-\dfrac{x_1 - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} \right) + y_1 \\ \vdots \\ \bar{y}_0 \left(\dfrac{x_k - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} - 1 \right) + \bar{y}_1 \left(-\dfrac{x_k - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} \right) + y_k \\ \bar{y}_1 \left(\dfrac{x_{k+1} - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} - 1 \right) + \bar{y}_2 \left(-\dfrac{x_{k+1} - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} \right) + y_{k+1} \\ \vdots \\ \bar{y}_1 \left(\dfrac{x_N - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} - 1 \right) + \bar{y}_2 \left(-\dfrac{x_N - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} \right) + y_N \end{bmatrix} \right\|^2
$$

$$
= \left\| A\bar{\mathbf{y}} + \mathbf{c} \right\|^2
$$

Here,

$$
A \triangleq \begin{bmatrix} \dfrac{x_1 - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} - 1 & -\dfrac{x_1 - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} & 0 \\ \vdots & \vdots & \vdots \\ \dfrac{x_k - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} - 1 & -\dfrac{x_k - \bar{x}_0}{\bar{x}_1 - \bar{x}_0} & 0 \\ 0 & \dfrac{x_{k+1} - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} - 1 & -\dfrac{x_{k+1} - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} \\ \vdots & \vdots & \vdots \\ 0 & \dfrac{x_N - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} - 1 & -\dfrac{x_N - \bar{x}_1}{\bar{x}_2 - \bar{x}_1} \end{bmatrix}, \quad \bar{\mathbf{y}} \triangleq \begin{bmatrix} \bar{y}_0 \\ \bar{y}_1 \\ \bar{y}_2 \end{bmatrix}, \quad \mathbf{c} \triangleq \begin{bmatrix} y_1 \\ \vdots \\ y_k \\ y_{k+1} \\ \vdots \\ y_N \end{bmatrix}
$$

Note that A is a tridiagonal matrix, and it will remain so for any number of knot points. Also note that we can express $\left\| A\bar{\mathbf{y}} + \mathbf{c} \right\|^2$ as

$$
\begin{aligned}
\left\| A\bar{\mathbf{y}} + \mathbf{c} \right\|^2 &= \left(A\bar{\mathbf{y}} + \mathbf{c} \right)^T \left(A\bar{\mathbf{y}} + \mathbf{c} \right) \\
&= \left(\bar{\mathbf{y}}^T A^T + \mathbf{c}^T \right) \left(A\bar{\mathbf{y}} + \mathbf{c} \right) \\
&= \bar{\mathbf{y}}^T A^T A\bar{\mathbf{y}} + \bar{\mathbf{y}}^T A^T \mathbf{c} + \mathbf{c}^T A\bar{\mathbf{y}} + \mathbf{c}^T \mathbf{c} \\
&= \bar{\mathbf{y}}^T A^T A\bar{\mathbf{y}} + \left(\mathbf{c}^T A\bar{\mathbf{y}} \right)^T + \mathbf{c}^T A\bar{\mathbf{y}} + \mathbf{c}^T \mathbf{c} \\
&= \bar{\mathbf{y}}^T A^T A\bar{\mathbf{y}} + 2\mathbf{c}^T A\bar{\mathbf{y}} + \left\| \mathbf{c} \right\|^2 .
\end{aligned}
$$

The last step utilized the fact that $\mathbf{c}^T A\bar{\mathbf{y}}$ is a scalar, and therefore, $\left(\mathbf{c}^T A\bar{\mathbf{y}} \right)^T = \mathbf{c}^T A\bar{\mathbf{y}}$.

Let

$$
H = 2A^T A, \quad \mathbf{f} = (2\mathbf{c}^T A)^T,
$$

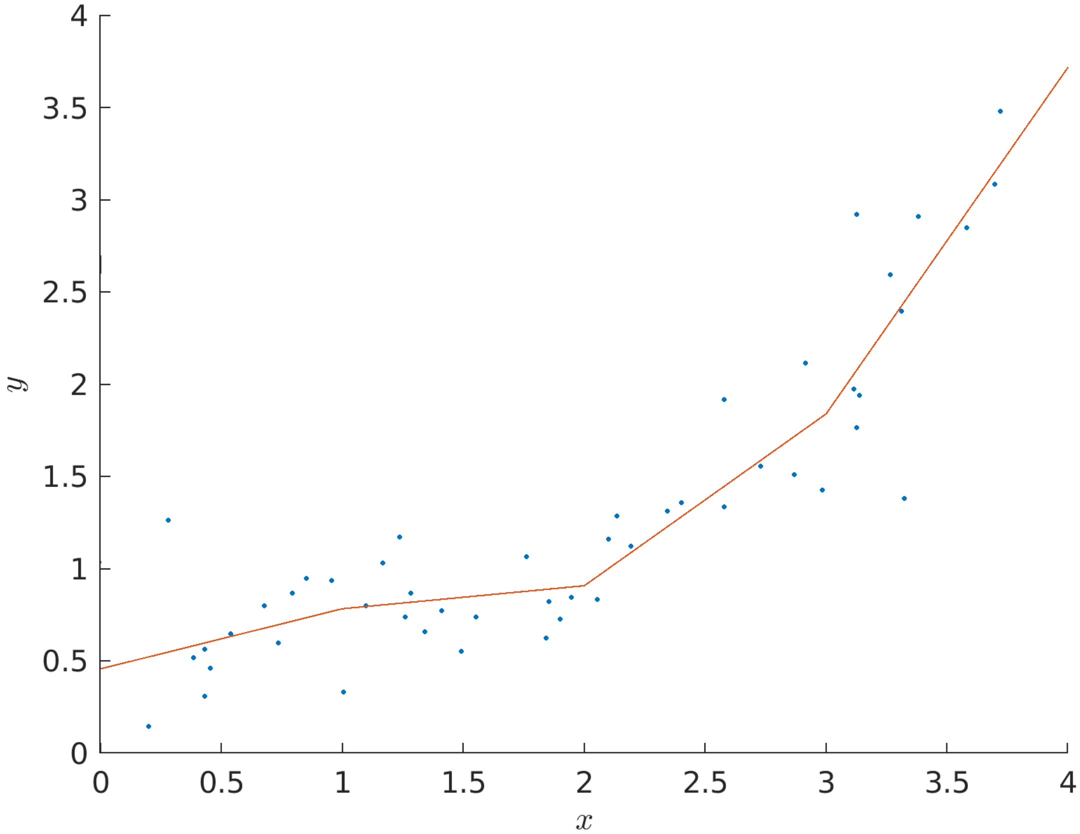
Then,

$$\|A\bar{\mathbf{y}} + \mathbf{c}\|^2 = \frac{1}{2}\,\bar{\mathbf{y}}^T H \bar{\mathbf{y}} + \mathbf{f}^{\,T}\bar{\mathbf{y}} + \|\mathbf{c}\|^2 \,.$$

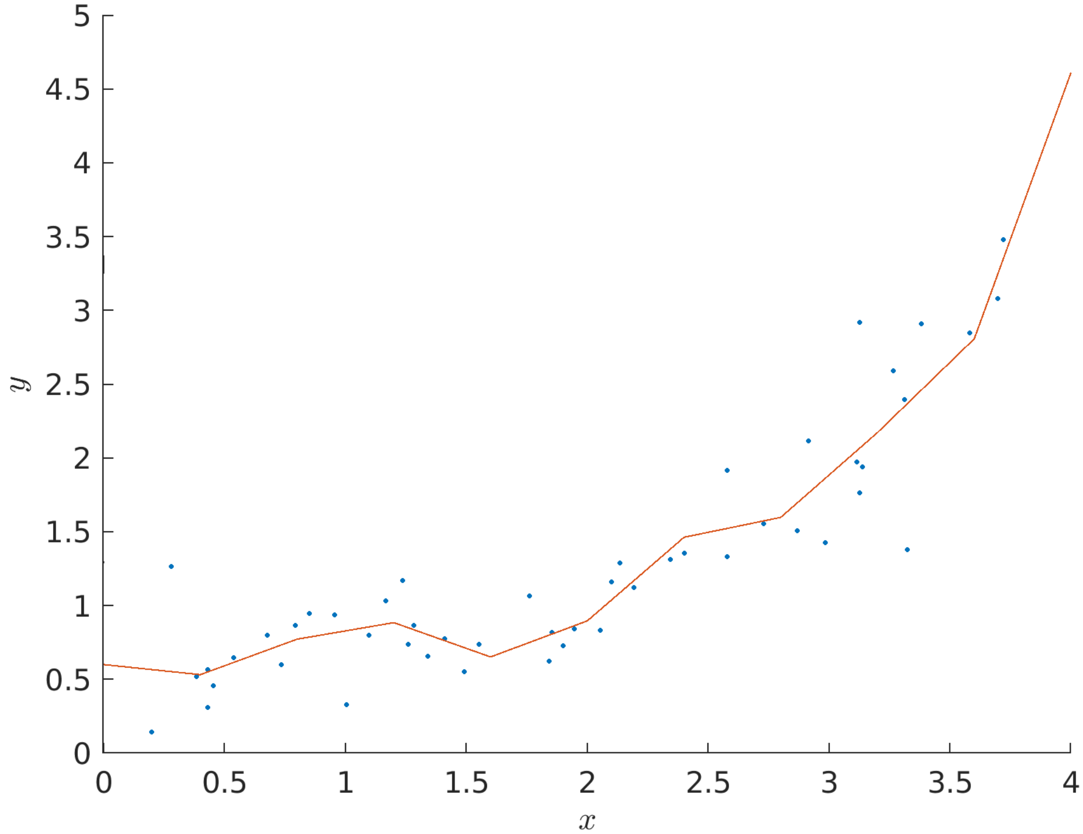
This transformation allows to formulate the given least squares problem as a quadratic program. All in all, we have established the following equivalent formulations

$$\min_{\bar{\mathbf{y}}} \sum_{k=1}^{N} (y_k - \hat{y}_k)^2 \iff \min_{\bar{\mathbf{y}}} \|\mathbf{z}\|^2 \iff \min_{\bar{\mathbf{y}}} \|A\bar{\mathbf{y}} + \mathbf{c}\|^2 \iff \min_{\bar{\mathbf{y}}} \frac{1}{2}\,\bar{\mathbf{y}}^T H \bar{\mathbf{y}} + \mathbf{f}^{\,T}\bar{\mathbf{y}} + \|\mathbf{c}\|^2 \,,$$

where $\mathbf{z}, A, \mathbf{c}, H, \mathbf{f}$ are as defined above in the derivation.



4
3.5
3
2.5
2
1.5
1
0.5
0
y
0
0.5
1
1.5
2
2.5
3
3.5
4
x



5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
y
0
0.5
1
1.5
2
2.5
3
3.5
4
x