Penalized Natural Cubic Spline Regression

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We model f(x) as a **linear combination** of basis functions:

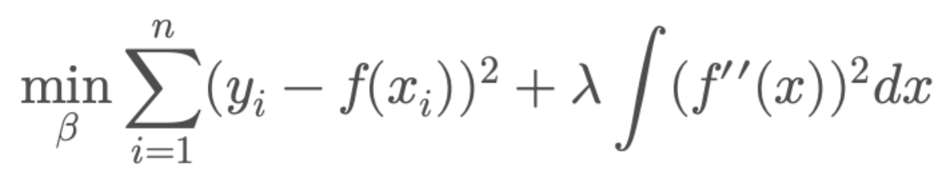
$$f(x) = \sum_{j=1}^{K} \beta_j B_j(x)$$

where:

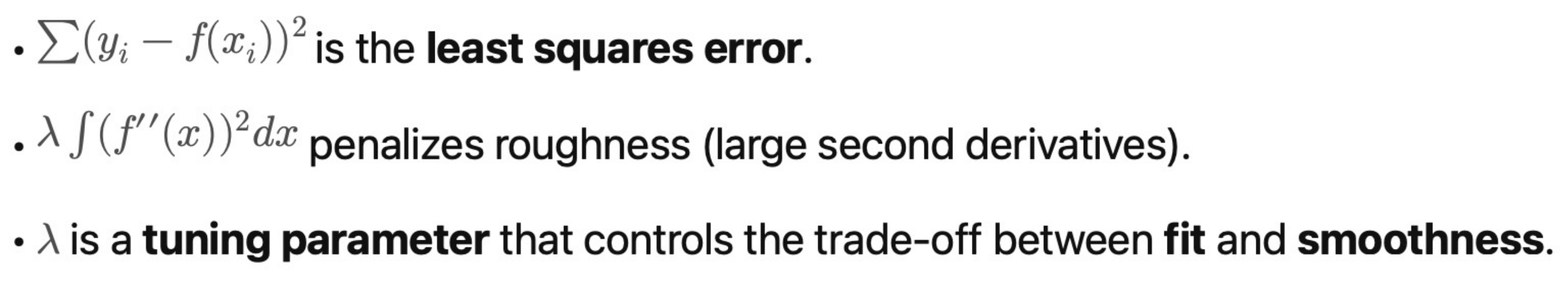
- $B_j(x)$ are cubic **B-spline basis functions**.
- β_j are the coefficients to estimate.
- K is the number of basis functions (determined by knot selection).

Penalized Regression Formulation

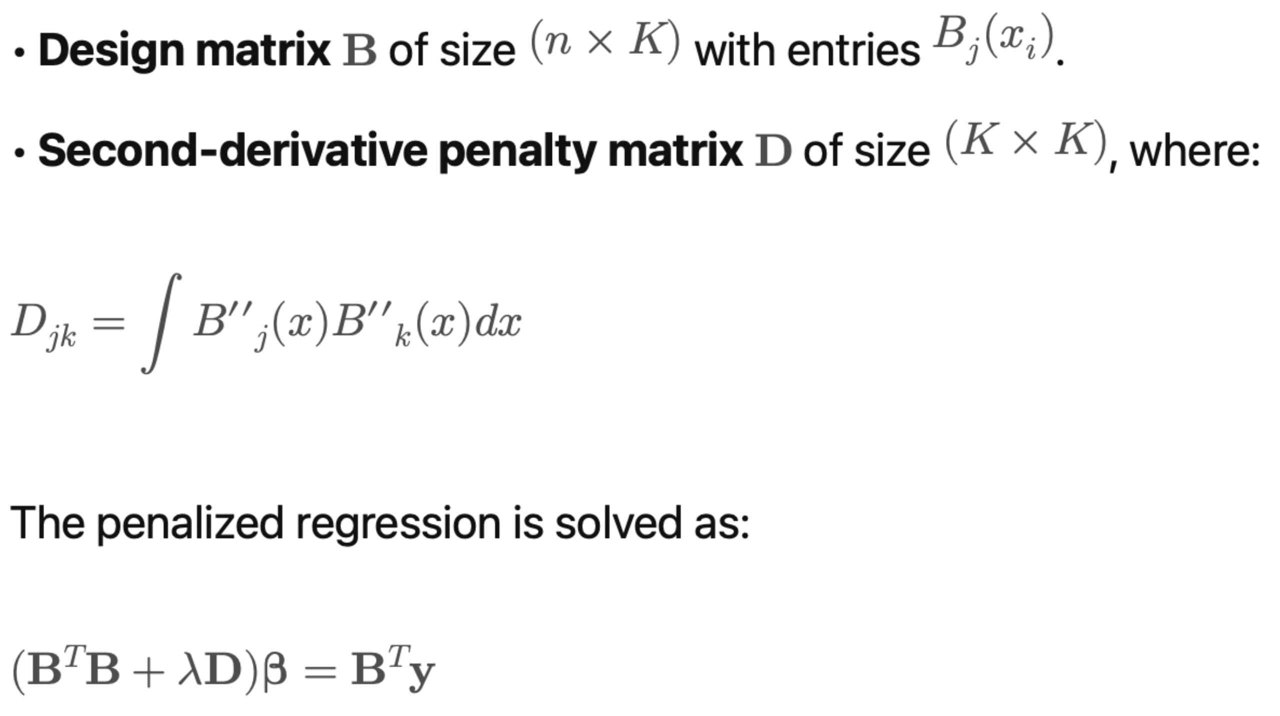
A penalty term is introduced to control overfitting. The objective function is:



$$\min_{\beta} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \int (f''(x))^2 dx$$



- $\sum (y_i - f(x_i))^2$ is the **least squares error**.
- $\lambda \int (f''(x))^2 dx$ penalizes roughness (large second derivatives).
- λ is a **tuning parameter** that controls the trade-off between **fit** and **smoothness**.



- **Design matrix** $\mathbf{B}$ of size $(n \times K)$ with entries $B_j(x_i)$.
- **Second-derivative penalty matrix** $\mathbf{D}$ of size $(K \times K)$, where:

$$D_{jk} = \int {B''}_j(x) {B''}_k(x) dx$$

The penalized regression is solved as:

$$(\mathbf{B}^T\mathbf{B} + \lambda\mathbf{D})\boldsymbol{\beta} = \mathbf{B}^T\mathbf{y}$$

Controlling smoothness by penalizing wiggliness

To control the model's smoothness, we could add a 'wiggliness' penalty to the least squares fitting objective.

For example, rather than fitting the model by minimizing

$$\|y - X\beta\|^2 ,$$

it could be fitted by minimizing

$$\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \sum_{j=2}^{k-1} \{f(x^*_{j-1}) - 2f(x^*_j) + f(x^*_{j+1})\}^2,$$

where the summation term measures wiggliness as a sum of squared second differences of the function at the knots (which crudely approximates the integrated squared second derivative penalty used in cubic spline smoothing).

When f is very wiggly the penalty will take high values and when f is ‘smooth’ the penalty will be low.

If f is a straight line, then the penalty is actually zero.

So the penalty has a null space of functions that are un-penalized: the straight lines in this case.

The dimension of the penalty null space is 2, since the basis for straight lines is 2-dimensional.

The smoothing parameter, λ, controls the trade-off between smoothness of the estimated f and fidelity to the data.

λ →∞ leads to a straight line estimate for f, while λ= 0 results in an un-penalized piecewise linear regression estimate.

For the basis of tent functions, it is easy to see that the coefficients of fare simply the function values at the knots, i.e., $\beta_j = f(x_j^*)$.

This makes it particularly straight-forward to express the penalty as a quadratic form, $\beta^T S \beta$, in the basis coefficients (although in fact linearity of f in the basis coefficients is all that is required for this).

Firstly note that

$$\begin{bmatrix} \beta_1 - 2\beta_2 + \beta_3 \\ \beta_2 - 2\beta_3 + \beta_4 \\ \beta_3 - 2\beta_4 + \beta_5 \\ . \\ . \end{bmatrix} = \begin{bmatrix} 1 & -2 & 1 & 0 & . & . & . \\ 0 & 1 & -2 & 1 & 0 & . & . \\ 0 & 0 & 1 & -2 & 1 & 0 & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ . \\ . \end{bmatrix}$$

so that writing the right-hand side as $D\beta$, by definition of $(k-2) \times k$ matrix D, the penalty becomes

$$\sum_{j=2}^{k-1} (\beta_{j-1} - 2\beta_j + \beta_{j+1})^2 = \boldsymbol{\beta}^{\mathsf{T}} \mathbf{D}^{\mathsf{T}} \mathbf{D} \boldsymbol{\beta} = \boldsymbol{\beta}^{\mathsf{T}} \mathbf{S} \boldsymbol{\beta} \qquad (4.5)$$

where $S = D^T D$ (S is obviously rank deficient by the dimension of the penalty null space).

Hence the penalized regression fitting problem is to minimize

$$\|\mathbf{y}-\mathbf{X}\beta\|2 + \lambda\beta^{\mathrm{T}}\mathbf{S}\beta \quad (4.6)$$

w.r.t. β.

The problem of estimating the degree of smoothness for the model is now the problem of estimating the smoothing parameter λ.

But before addressing λ estimation, consider β estimation given λ.

It is fairly straightforward to show that the formal expression for the minimizer of (4.6), the penalized least squares estimator of β, is

$$\hat{\beta}= (\mathbf{X}^{\mathrm{T}}\mathbf{X} + \boldsymbol{\lambda}\mathbf{S})^{-1}\ \mathbf{X}^{\mathrm{T}}\mathbf{y}. \quad (4.7)$$

Additive models

Now suppose that two explanatory variables, x and v, are available for a response variable, y, and that a simple additive model structure,

$$y_i = \alpha + f_1(x_i) + f_2(v_i) + \varepsilon_i, \quad (4.8)$$

is appropriate. α is an intercept parameter, the f_j are smooth functions, and the ε_i are independent $N(0,\sigma^2)$ random variables.

There are two points to note about this model.

Firstly, the assumption of additive effects is a fairly strong one: $f_1(x) + f_2(v)$ is a quite restrictive special case of the general smooth function of two variables $f(x,v)$.

Secondly, the fact that the model now contains more than one function introduces an identifiability problem: f_1 and f_2 are each only estimable to within an additive constant.

To see this, note that any constant could be simultaneously added to f_1 and subtracted from f_2, without changing the model predictions.

Hence identifiability constraints have to be imposed on the model before fitting.

Provided that the identifiability issue is addressed, the additive model can be represented using penalized regression splines, estimated by penalized least squares and the degree of smoothing selected by cross validation or (RE)ML, in the same way as for the simple univariate model.

1. *Penalized piecewise regression representation of an additive model*

Each smooth function in (4.8) can be represented using a penalized piecewise linear basis. Specifically, let

$$f_1(x) = \sum_{j=1}^{k_1} b_j(x)\delta_j$$

where the δ_j are unknown coefficients, while the $b_j(x)$ are basis functions of the

form (4.4), defined using a sequence of k_1 knots, x^*_j, evenly spaced over the range of x. Similarly

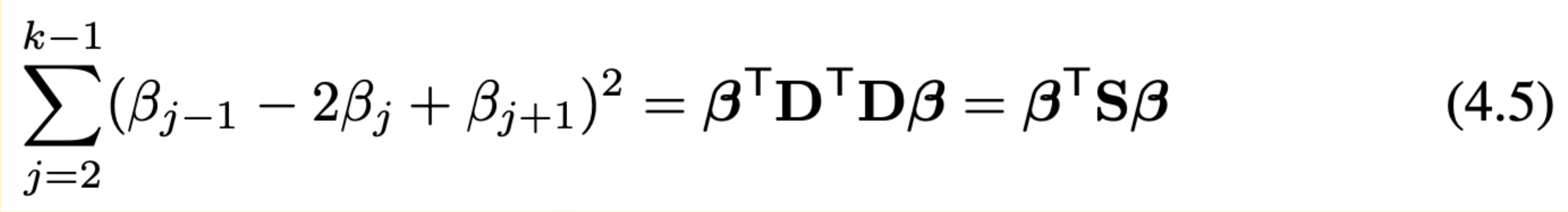
$$f_2(v) = \sum_{j=1}^{k_2} \mathcal{B}_j(v)\gamma_j$$

where the γ_j are the unknown coefficients and the $B_j(v)$ are basis functions of the form (4.4), defined using a sequence of k_2 knots, v^*_j, evenly spaced over the range of v.

Defining n-vector $\boldsymbol{f}_1 = [f_1(x_1), ..., f_1(x_n)]$, we have $\boldsymbol{f}_1 = \mathbf{X}_1\boldsymbol{\delta}$ where $b_j(x_i)$ is element i, j of X_1.

Similarly, $\boldsymbol{f}_2 = \boldsymbol{X}_2\boldsymbol{\gamma}$, where $B_j(v_i)$ is element i, j of $\boldsymbol{X}_2$.

A penalty of the form (4.5)



$$\sum_{j=2}^{k-1}(\beta_{j-1} - 2\beta_j + \beta_{j+1})^2 = \boldsymbol{\beta}^\mathsf{T}\mathbf{D}^\mathsf{T}\mathbf{D}\boldsymbol{\beta} = \boldsymbol{\beta}^\mathsf{T}\mathbf{S}\boldsymbol{\beta} \qquad (4.5)$$

is also associated with each function:

$\boldsymbol{\delta}^T\boldsymbol{D}_1^T\boldsymbol{D}_1\boldsymbol{\delta} = \boldsymbol{\delta}^T\overline{\boldsymbol{S}}_1\boldsymbol{\delta}$ for f_1 and $\boldsymbol{\gamma}^T\boldsymbol{D}_2^T\boldsymbol{D}_2\boldsymbol{\gamma} = \boldsymbol{\gamma}^T\overline{\boldsymbol{S}}_2\boldsymbol{\gamma}$ for f_2.

Now it is necessary to deal with the identifiability problem.

For estimation purposes, almost any linear constraint that removed the problem could be used, but most choices lead to uselessly wide confidence intervals for the constrained functions.

The best constraints from this viewpoint are sum-to-zero constraints, such as

$$\sum_{i=1}^{n} f_1(x_i) = 0$$

or equivalently $\mathbf{1}^{\mathrm{T}}\boldsymbol{f}_1 = 0$, where $\mathbf{1}$ is an n vector of 1's.

Notice how this constraint still allows f_1 to have exactly the same shape as before constraint, with exactly the same penalty value.

The constraint's only effect is to shift f_1, vertically, so that its mean value is zero. To apply the constraint, note that we require $\mathbf{1}^{\mathrm{T}}\mathbf{X}_1\boldsymbol{\delta}= 0$ for all $\boldsymbol{\delta}$, which implies that $\mathbf{1}^{\mathrm{T}}\mathbf{X}_1 = 0$.

To achieve this latter condition the column mean can be subtracted from each column of $\mathbf{X}_1$. That is, we define a column centred matrix

$$\widetilde{\boldsymbol{X}}_1 = \boldsymbol{X}_1 - \mathbf{1}\mathbf{1}^T\boldsymbol{X}_1/n$$

and set $\tilde{\boldsymbol{f}}_1 = \widetilde{\boldsymbol{X}}_1\boldsymbol{\delta}$.

It's easy to check that this constraint imposes no more than a shift in the level of $\boldsymbol{f}_1$:

$$\tilde{\boldsymbol{f}}_1 = \tilde{\boldsymbol{X}}_1\boldsymbol{\delta} = \boldsymbol{X}_1\boldsymbol{\delta} - \frac{\mathbf{1}\mathbf{1}^T\boldsymbol{X}_1\boldsymbol{\delta}}{n} = \boldsymbol{X}_1\boldsymbol{\delta} - \mathbf{1}\mathrm{c} = \boldsymbol{f}_1 - c$$

by definition of the scalar $\mathrm{c} = \frac{\mathbf{1}^T\boldsymbol{X}_1\boldsymbol{\delta}}{n}$.

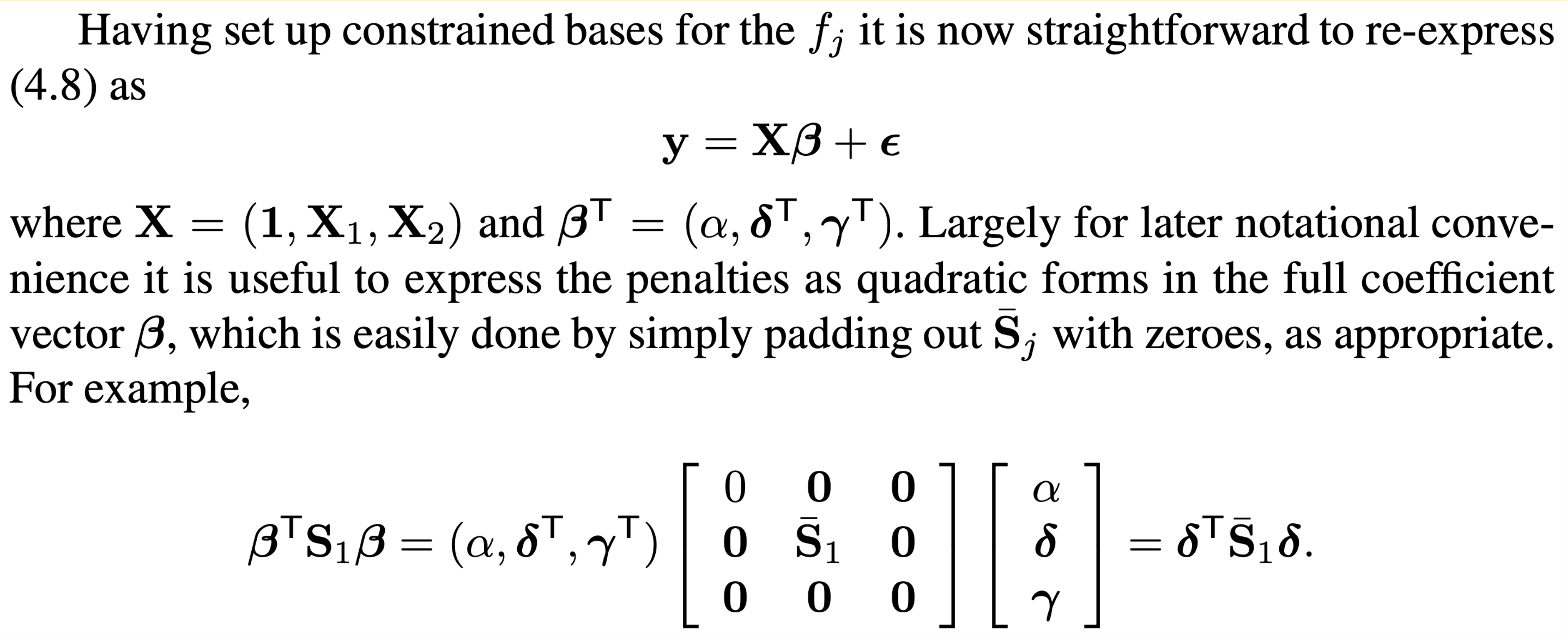
Finally note that the column centring reduces the rank of $\tilde{\boldsymbol{X}}_1$ to $\mathrm{k}_1 - 1$, so that only $\mathrm{k}_1 - 1$ elements of the k_1 vector $\boldsymbol{\delta}$ can be uniquely estimated.

A simple identifiability constraint deals with this problem: a single element of $\boldsymbol{\delta}$ is set to zero, and the corresponding column of $\tilde{\boldsymbol{X}}_1$ and $\mathbf{D}$ is deleted.

The column centred rank reduced basis will automatically satisfy the identifiability constraint.

In what follows the tildes will be dropped, and it is assumed that the $\mathbf{X}_j$, $\mathbf{D}_j$, etc. are the constrained versions.

$$y_i = \alpha + f_1(x_i) + f_2(v_i) + \varepsilon_i, \quad (4.8)$$

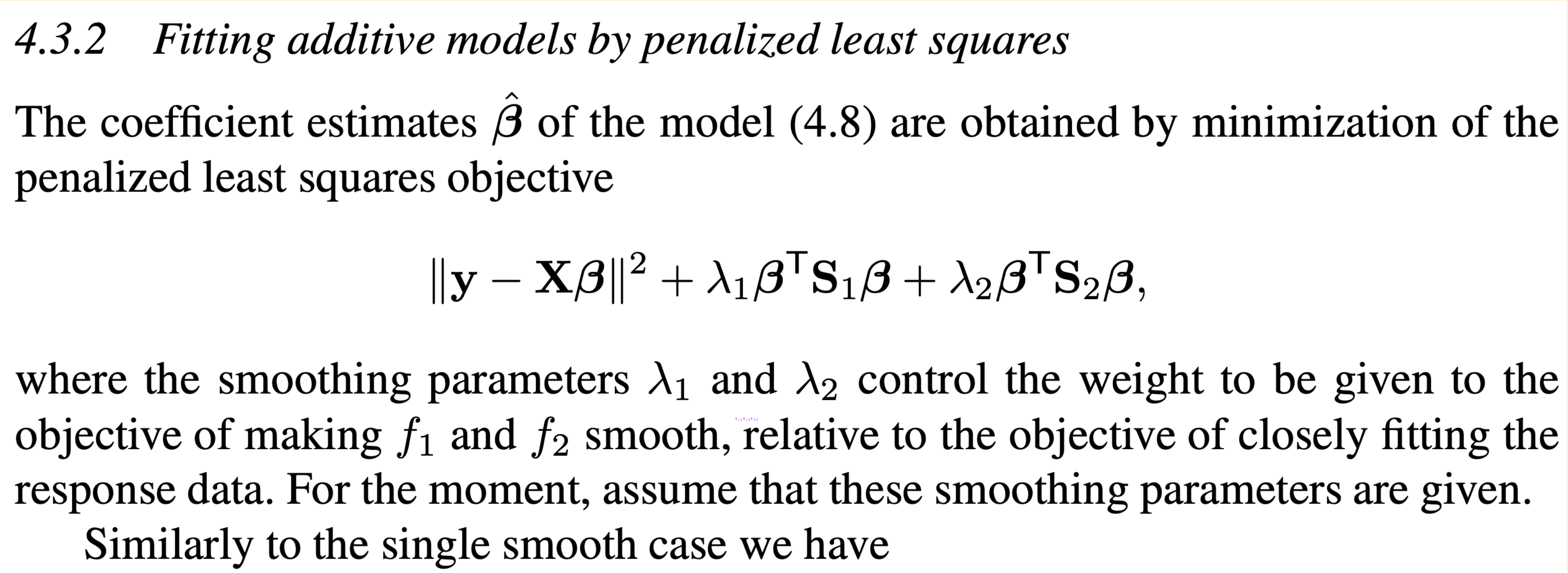


Having set up constrained bases for the f_j it is now straightforward to re-express (4.8) as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where $\mathbf{X} = (\mathbf{1}, \mathbf{X}_1, \mathbf{X}_2)$ and $\boldsymbol{\beta}^{\mathsf{T}} = (\alpha, \boldsymbol{\delta}^{\mathsf{T}}, \boldsymbol{\gamma}^{\mathsf{T}})$. Largely for later notational convenience it is useful to express the penalties as quadratic forms in the full coefficient vector $\boldsymbol{\beta}$, which is easily done by simply padding out $\bar{\mathbf{S}}_j$ with zeroes, as appropriate. For example,

$$\boldsymbol{\beta}^{\mathsf{T}}\mathbf{S}_1\boldsymbol{\beta} = (\alpha, \boldsymbol{\delta}^{\mathsf{T}}, \boldsymbol{\gamma}^{\mathsf{T}}) \begin{bmatrix} 0 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{S}}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \alpha \\ \boldsymbol{\delta} \\ \boldsymbol{\gamma} \end{bmatrix} = \boldsymbol{\delta}^{\mathsf{T}}\bar{\mathbf{S}}_1\boldsymbol{\delta}.$$



4.3.2 *Fitting additive models by penalized least squares*

The coefficient estimates $\hat{\boldsymbol{\beta}}$ of the model (4.8) are obtained by minimization of the penalized least squares objective

$$\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda_1 \boldsymbol{\beta}^{\mathsf{T}} \mathbf{S}_1 \boldsymbol{\beta} + \lambda_2 \boldsymbol{\beta}^{\mathsf{T}} \mathbf{S}_2 \boldsymbol{\beta},$$

where the smoothing parameters λ_1 and λ_2 control the weight to be given to the objective of making f_1 and f_2 smooth, relative to the objective of closely fitting the response data. For the moment, assume that these smoothing parameters are given.

Similarly to the single smooth case we have

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X} + \lambda_1 \mathbf{S}_1 + \lambda_2 \mathbf{S}_2\right)^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{y}$$