

Smoothing Splines

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Here I document the math used in the Julia package *SmoothSpline* that performs regression with B-splines using a Tikhonov regularisation.

The *SmoothSpline* package is a port of the *smooth.spline* function from R. During the implementation I discovered two special things in *smooth.spline*'s implementation that I have not seen in its documentation:

- Two matrix traces are computed. In the code the first two and last two entries on the diagonal are *not* included in the trace.
- In one computation $\frac{1}{3}$ is hard-coded to be 0.333. This approximation is a bit crude when the word size of the computer is 64 bit.

I will comment more on these points later in this document.

1 B-splines

My source for B-splines is the excellent book [3] with very detailed algorithms. The only downside for a Julia implementation is that all algorithms use 0-based arrays. I do not include further details about evaluation of B-splines here, but note that we have algorithms for computing the values of B-splines and all of their derivatives.

In *SmoothSpline* we use cubic B-splines, so the general degree p from [3] is always $p = 3$. We therefore use a more compact notation here: The i 'th spline of degree p is in [3] denoted $N_{i,p}$, but is here simply denoted N_i . However, to avoid “magic” occurrences of 3, I still use p in the following to denote the degree.

A collection of B-splines are determined solely by their knots. Boundaries are handled by reusing the boundary knots: If we have m distinct breakpoints u_1, \dots, u_m we construct the B-splines from the knots, where we have augmented by p endpoints in each end (u_1 and u_m repeated p times each).

The function *bs* from the {splines} package in R can be used to compute B-splines.

2 Regression with B-splines

We consider observations (x_i, y_i) for $i = 1, \dots, n$. It is allowed to have multiple observations with similar x values (and y values). Observation i has an associated weight w_i , that by default is 1. Observations with similar x values are grouped by summing their weights and taking the average of their y values. In the following we assume that all x values are distinct and that the observations are sorted by their x values.

The choice of B-splines (that is, the choice of their knots) of course influences everything. In *smooth.spline* the breakpoints are evenly distributed over from the smallest to the largest x value. I will update this document at a later point with how the number of breakpoints is chosen from the number of observations.

We want to perform regression with m B-splines on the interval $[x_1, x_n]$. That is, compute an approximation with the function

$$f(x) = \sum_{j=1}^M \beta_j N_j(x).$$

The design matrix of the regression problem is the matrix \mathbf{X} of size $n \times m$ with entries

$$X_{i,j} = N_j(u_i).$$

The weights are collected in a diagonal matrix $\mathbf{W} = \text{diag}(w_i, i = 1, \dots, n)$. To enforce a smoother interpolant we choose the β 's with a least squares criterion and limit the curvature (measured by the second derivative):

$$\min_{\beta} \|\mathbf{y} - \mathbf{X}\sqrt{\mathbf{W}}\beta\|^2 + \lambda \int_{x_1}^{x_n} \{f^{(2)}(t)\}^2 dt.$$

We can also write this as a Tikhonov regularisation

$$\min_{\beta} \|\mathbf{y} - \mathbf{X}\sqrt{\mathbf{W}}\beta\| + \lambda \beta^T \mathbf{\Sigma} \beta,$$

where the regularisation term $\mathbf{\Sigma}$ is the Gram matrix of size $m \times m$ with entries

$$\Sigma_{i,j} = \int_{x_1}^{x_n} N_i^{(2)}(t) N_j^{(2)}(t) dt.$$

For each value of $\lambda > 0$, we have a solution β to the corresponding regression problem, namely the solution to the equation

$$\mathbf{A}\beta = (\mathbf{X}^T \mathbf{W} \mathbf{X} + \lambda \mathbf{\Sigma})\beta = \mathbf{X}^T \mathbf{W} \mathbf{y} = \tilde{\mathbf{y}}. \quad (1)$$

This can be solved fast with a few tricks. Both \mathbf{X} and $\mathbf{\Sigma}$ are *banded* with lower and upper band p . That is, $X_{i,j} = \Sigma_{i,j} = 0$ when $|i - j| > p$. This implies that the Cholesky factorization of \mathbf{A} is also banded with the same band. More specifically, we let \mathbf{C} denote the upper triangular matrix of the Cholesky factorization such that

$$\mathbf{C}^T \mathbf{C} = \mathbf{X}^T \mathbf{W} \mathbf{X} + \lambda \mathbf{\Sigma}.$$

With this convention \mathbf{C}^T is a lower triangular matrix and we can use the classic forward and back substitution to solve eq. (1): First solve $\mathbf{C}^T \mathbf{z} = \tilde{\mathbf{y}}$ and then $\mathbf{C} \boldsymbol{\beta} = \mathbf{z}$.

Note that the matrix \mathbf{A} may be ill-conditioned even with the Tikhonov term. In fact, I have seen substantial differences between $\boldsymbol{\beta}$'s computed with generic solvers and the special solvers used in *SmoothSpline*.

2.1 Computing matrices

Before solving eq. (1) we must compute the matrices involved.

In the *documentation* for *smooth.spline* (and therefore not under the same license as the *code*) it is noted that the Lagrange multiplier λ is data dependent. That is, an appropriate value for λ depends on the values of the observations. This makes it more delicate to choose λ .

But *smooth.spline* aids the user by offering a data independent parameter “spar”, where $0 < \text{spar} \leq 1$, that is mapped to an appropriate λ . The map is

$$\lambda = r \cdot 256^{3 \cdot \text{spar} - 1}, \quad r = \frac{\text{tr}(\mathbf{X}^T \mathbf{W} \mathbf{X})}{\text{tr}(\boldsymbol{\Sigma})}.$$

In the code, however, it is not the standard traces that are computed – both in *SmoothSpline* and *smooth.spline*. The first two entries and the last two entries of the diagonals are discarded in the sum. I have not found documentation to explain this, but I *suspect* that it is to reduce the impact of the endpoint knots that occur in multiple splines – cf. section 1.

Furthermore, *smooth.spline* rescales the x values to the closed unit interval. This has an impact on $\boldsymbol{\Sigma}$, but the impact on \mathbf{A} is de facto alleviated by the above mapping.

2.1.1 Design matrix

The design matrix to compute is straightforward once we know how to compute the splines.

2.1.2 Gram matrix

We have closed-form expressions for the Tikhonov matrix $\boldsymbol{\Sigma}$. All spline functions are supported on (a subset of) $[u_0, u_m]$ and we first note that

$$\Sigma_{i,j} = \int_{u_0}^{u_m} N_i^{(2)}(t) N_j^{(2)}(t) dt = \sum_{k=0}^{m-1} \int_{u_k}^{u_{k+1}} N_i^{(2)}(t) N_j^{(2)}(t) dt. \quad (2)$$

With partial integration each of the integrals can be computed as

$$\int_{u_k}^{u_{k+1}} N_i^{(2)}(t) N_j^{(2)}(t) dt = \left[N_i'(t) N_j^{(2)}(t) \right]_{u_k}^{u_{k+1}} - \int_{u_k}^{u_{k+1}} N_i'(t) N_j^{(3)}(t) dt.$$

On each interval $[u_k, u_{k+1}]$, every spline is a polynomial of degree at most three. Hence the third derivative is a constant and

$$\int_{u_k}^{u_{k+1}} N_i'(t) N_j^{(3)}(t) dt = N_j^{(3)}(u_k) (N_i(u_{k+1}) - N_i(u_k)).$$

Substituting all this into eq. (2) we note a telescoping sum and arrive at an expression:

$$\Sigma_{i,j} = N_i'(u_m) N_j^{(2)}(u_m) - N_i'(u_0) N_j^{(2)}(u_0) - \sum_{k=0}^{m-1} N_j^{(3)}(u_k) (N_i(u_{k+1}) - N_i(u_k)).$$

In *smooth.spline* the integral in eq. (2) is computed differently: On each interval $[u_k, u_{k+1}]$, the function $N_i^{(2)}$ is a polynomial of degree at most one. In the code, this polynomial is parameterized as

$$N_i^{(2)}(t) = a_{i,k} + b_{i,k}(t - u_k), \quad u_k \leq t \leq u_{k+1}.$$

Expanding parentheses in $N_i^{(2)} N_j^{(2)}$ we see that

$$N_i^{(2)}(t) N_j^{(2)}(t) = a_{i,k} a_{j,k} + (a_{i,k} b_{j,k} + a_{j,k} b_{i,k})(t - u_k) + b_{i,k} b_{j,k} (t - u_k)^2.$$

With this expression and $\Delta_k = u_{k+1} - u_k$,

$$\begin{aligned} \int_{u_k}^{u_{k+1}} N_i^{(2)}(t) N_j^{(2)}(t) dt &= \int_0^{\Delta_k} a_{i,k} a_{j,k} + (a_{i,k} b_{j,k} + a_{j,k} b_{i,k})s + b_{i,k} b_{j,k} s^2 ds \\ &= a_{i,k} a_{j,k} \Delta_k + (a_{i,k} b_{j,k} + a_{j,k} b_{i,k}) \frac{1}{2} \Delta_k^2 + b_{i,k} b_{j,k} \frac{1}{3} \Delta_k^3. \end{aligned} \quad (3)$$

The slope $b_{i,k} = N_i^{(3)}(t)$, but *smooth.spline* only use the second order derivatives. We see readily that $a_{i,k} = N_i^{(2)}(u_k)$. Let $\Delta y_{i,k} = N_i^{(2)}(u_{k+1}) - N_i^{(2)}(u_k)$. Then $b_{i,k} = \Delta y_{i,k} / \Delta_k$. With these expressions, many of the Δ_k 's can be removed from eq. (3):

$$\begin{aligned} \int_{u_k}^{u_{k+1}} N_i^{(2)}(t) N_j^{(2)}(t) dt &= a_{i,k} a_{j,k} \Delta_k + \left(a_{i,k} \frac{\Delta y_{j,k}}{\Delta_k} + a_{j,k} \frac{\Delta y_{i,k}}{\Delta_k} \right) \frac{1}{2} \Delta_k^2 + \frac{\Delta y_{i,k}}{\Delta_k} \frac{\Delta y_{j,k}}{\Delta_k} \frac{1}{3} \Delta_k^3 \\ &= a_{i,k} a_{j,k} \Delta_k + (a_{i,k} \Delta y_{j,k} + a_{j,k} \Delta y_{i,k}) \frac{1}{2} \Delta_k + \Delta y_{i,k} \Delta y_{j,k} \frac{1}{3} \Delta_k. \end{aligned}$$

In *smooth.spline* the value of $\frac{1}{3}$ is hard-coded to be 0.333. Even in small examples this can result in entry-wise deviations of about 1%.

Speed-ups From the definition we readily see that Σ is symmetric. We know from [3, P2.1] that the support of N_i is $[u_i, u_{i+p+1}]$ and therefore

$$\text{supp } N_i \cap \text{supp } N_j = \emptyset \quad \text{if } |i - j| > p.$$

This implies that $\Sigma_{i,j} = 0$ if $|i - j| > p$ and that the sum in eq. (2) goes from $\min\{i, j\}$ to $\min\{\max\{i, j\} + p + 1, m\}$.

2.2 Banded matrices

A banded matrix can be represented and stored efficiently [2, Section 1.2.5]. Furthermore, there are efficient algorithms for computing the Cholesky factorization of a banded matrix [2, Section 4.3].

In R, *smooth.spline* rely on the Fortran routines *dpbfa* and *dpbsl* from Linpack [1] to compute the Cholesky factorization and solving eq. (1), respectively.

References

- [1] J. J. Dongarra et al. *LINPACK Users' Guide*. SIAM, 1979. DOI: [10.1137/1.9781611971811](https://doi.org/10.1137/1.9781611971811).
- [2] Gene H. Golub and Charles F. van Loan. *Matrix Computations*. 4th ed. Johns Hopkins University Press, 2013.
- [3] Les Piegl and Wayne Tiller. *The NURBS Book*. 2nd ed. Springer-Verlag Berlin Heidelberg, 1997. DOI: [10.1007/978-3-642-59223-2](https://doi.org/10.1007/978-3-642-59223-2).