Theoretical background for cubic B-spline evaluation

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1 Definition of B-spline basis functions

Consider a given dataset of m points $y_0(x_0)\,,\,y_1(x_1)\,,\,\ldots\,,\,y_m(x_m)$ on an interval $[L_1 : L_2]$ (black crosses in fig.1). In order to perform the interpolation, first that interval is split into segments represented by n equidistant knots t_i $(i = 0, 1, \ldots, n-1)$ marked as black circles. As implemented in the GNU Scientific Library for B-spline-interpolation, the $n+2$ basis functions $s_i(x)$ of order k are segmentwise recursively defined following equations 1 and 2. For cubic B-splines, k goes from 1 to 4.

$$s_{i,1}(x) = \begin{cases} 1 & : t_i \leq x < t_{i+1} \\ 0 & : else \end{cases} \tag{1}$$

$$s_{i,k}(x) = \frac{x - t_i}{t_{i+k-1} - t_i} s_{i,k-1}(x) + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} s_{i+1,k-1}(x) \tag{2}$$

2 Interpolation and least squares fitting (LSF) as implemeted in rapi*d*STORM

The interpolation to the dataset is computed as in eq.3 and represents a set of linear equations with $\vec{y} = (y_0(x_0)\,,\,y_1(x_1)\,,\,\ldots\,,\,y_m(x_m))$ and $\vec{c} = (c_0\,,\,c_1\,,\,\ldots\,,\,c_n\,,\,c_{n+1}\,,\,c_{n+2})$. Matrix notation (eq.4) indicates, that S is of diagonal form.

$$\begin{aligned} y_m(x_m) &= \sum_i s_{i,k}(x_m) c_i \\ \vec{y} &= S \cdot \vec{c} \end{aligned} \tag{3}$$

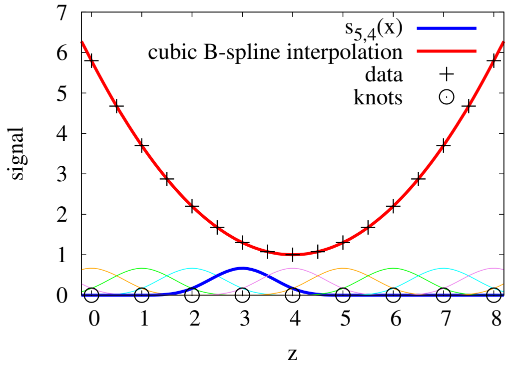

Figure 1: This diagram (arbitrary units) aims to visualise exemplarily how to handle data with cubic B-spline interpolation. The black crosses represent seventeen given data points while the rainbow-colored pseudo-Gaussians at the bottom of the diagram are plots of the B-spline basis functions $s_{i,4}(x)$ $(i = 0, 1, \ldots, 11)$ with the $n = 9$ knots indicated by black circles. Evaluation of eq.5 leads to amplitude factors for each basis function. The superposition with given amplitudes results in the interpolation represented by the red parabola.

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{m-3} \\ y_{m-2} \\ y_{m-1} \\ y_m \end{pmatrix} = \begin{pmatrix} s_0(x_0) & s_1(x_0) & s_2(x_0) & 0 & 0 & \cdots & 0 \\ s_0(x_1) & s_1(x_1) & s_2(x_1) & s_3(x_1) & 0 & \cdots & 0 \\ 0 & s_1(x_2) & s_2(x_2) & s_3(x_2) & 0 & \cdots & 0 \\ 0 & s_1(x_3) & s_2(x_3) & s_3(x_3) & s_4(x_3) & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & s_{n-1}(x_{m-1}) & s_n(x_{m-1}) & s_{n+1}(x_{m-1}) & s_{n+2}(x_{m-1}) \\ 0 & 0 & 0 & 0 & s_n(x_m) & s_{n+1}(x_m) & s_{n+2}(x_m) \end{pmatrix} \cdot \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{n-1} \\ c_n \\ c_{n+1} \\ c_{n+2} \end{pmatrix} \tag{4}$$

In equation 3 the vector $\vec{c}$ is unknown and is object to least squares fitting, which is performed following eq.5.

$$\vec{c} = (S^T \cdot S)^{-1} \cdot S^T \cdot \vec{y} \tag{5}$$

2.1 Derivation of the formula for LSF (eq.5)

The fit residuals are defined as: $\vec{r}(\vec{c}) = \vec{y} - S \cdot \vec{c}$ with the i-th component of r being: $r_i(c_j) = y_i - \sum\limits_j S_{ij} \cdot c_j$. The least squares fitting criteria is fulfilled when

$$\left|\vec{r}(\vec{c})^2\right| = \min \Leftrightarrow \frac{\partial \vec{r}(\vec{c})^2}{\partial \vec{c}} = 0 \qquad . \tag{6}$$

Evaluation of the right side of eq.6 for r_i gives

$$\begin{aligned}
0 &= \sum_i \frac{\partial \left(r_i(c_j)^2\right)}{\partial c_j} = \sum_i \frac{\partial r_i(c_j)}{\partial c_j} \cdot 2r_i(c_j) \\
&= \sum_i -S_{ij} \cdot 2r_i(c_j) = \sum_i S_{ij} \cdot \left[y_i - \sum_k S_{ik} \cdot c_k \right] \\
&= \sum_i S_{ij} \cdot y_i \; - \; \sum_i S_{ij} \cdot \sum_k S_{ik} \cdot c_k
\end{aligned}$$

$$\begin{aligned}
\sum_i S_{ij} \cdot y_j &= \sum_k \left[\sum_i S_{ij} \cdot S_{ik} \right] \cdot c_k \\
\sum_i S^T_{ji} \cdot y_i &= \sum_k \left[\sum_i S^T_{ji} \cdot S_{ik} \right] \cdot c_k \\
&= \sum_k \left(S^T \cdot S\right)_{jk} \cdot c_k \\
\left(S^T \cdot \vec{y}\right)_j &= \left[\left(S^T \cdot S\right) \vec{c}\right]_j
\end{aligned} \tag{7}$$

which, rewritten in vector notation leads to the form of eq.5:

$$\begin{aligned}
S^T \vec{y} &= \left(S^T \cdot S\right) \vec{c} \\
\Leftrightarrow \left(S^T \cdot S\right)^{-1} S^T \vec{y} &= \mathbb{1} \vec{c} \qquad .
\end{aligned} \tag{8}$$