$3 n-6$ constraint equations. We should not forget that we additionally want to interpolate all $n$ data points, i.e.:

$$
S\left(x_{i}\right)=y_{i} \text { for } i=1,2, \ldots, n \quad(n \text { equations })
$$

In total, we have $(3 n-6)+n=4 n-6$ equations to satisfy, and $4 n-4$ unknowns; consequently, we will need 2 more equations to ensure that the unknown coefficients will be uniquely determined. Several plausible options exist on how to do that:

1. The "not-a-knot" approach: We stipulate that at the locations of the first ( $x_{2}$ ) and last knot $\left(x_{n-1}\right)$ the third derivative of $S(x)$ should also be continuous, e.g. $S_{1}^{\prime \prime \prime}\left(x_{2}\right)=S_{2}^{\prime \prime \prime}\left(x_{2}\right)$ and $S_{n-2}^{\prime \prime \prime}\left(x_{n-1}\right)=S_{n-1}^{\prime \prime \prime}\left(x_{n-1}\right)$. As we discussed before, these 2 additional constraints will effectively cause $S_{1}(x)$ to be identical with $S_{2}(x)$, and $S_{n-2}(x)$ to coincide with $S_{n-1}(x)$. In this sense, $x_{2}$ and $x_{n-1}$ are no longer "knots" in the sense that the formula for $S(x)$ "changes" at these points (which explains the name for this approach).
2. The Complete spline method: If we have access to the derivative $f^{\prime}$ of the function being sampled by the $y_{i}$ 's (i.e. $y_{i}=f\left(x_{i}\right)$ ), we can formulate the 2 additional constraints as:

$$
\begin{align*}
S^{\prime}\left(x_{1}\right) & =f^{\prime}\left(x_{1}\right) \\
S^{\prime}\left(x_{n}\right) & =f^{\prime}\left(x_{n}\right) \\
\text { or } &  \tag{10}\\
S_{1}^{\prime}\left(x_{1}\right) & =f^{\prime}\left(x_{1}\right) \\
S_{n-1}^{\prime}\left(x_{n}\right) & =f^{\prime}\left(x_{n}\right)
\end{align*}
$$

Note that, qualitatively, using the complete spline approach is a better utilization of the flexibility of the spline curve in matching yet one move property of $f$; in contrast, the not-a-knot makes the spline "less flexible" by two degrees of freedom in order to obtain a unique solution. However, we cannot always assume knowledge of $f^{\prime}$.
Two additional methodologies are:
3. The natural cubic spline: We use the following 2 constraints:

$$
\begin{aligned}
& S^{\prime \prime}\left(x_{1}\right)=0 \\
& S^{\prime \prime}\left(x_{n}\right)=0
\end{aligned}
$$

Thus, $S(x)$ reaches the endpoints looking like a straight line (instead of a curved one).
4. Periodic spline:

$$
\begin{aligned}
S^{\prime}\left(x_{1}\right) & =S^{\prime}\left(x_{n}\right) \\
S^{\prime \prime}\left(x_{1}\right) & =S^{\prime \prime}\left(x_{n}\right)
\end{aligned}
$$

This is useful when the underlying function $f$ is also known to be periodical over $[a, b]$.

We will not discuss the analytic derivation of the cubic spline coefficients; instead, we describe how to access this functionality within MATLAB through the built-in functions spline and ppval.

- The function spline is called as:
$S=\operatorname{spline}(x, y)$
$x$ : The vector containing the $x_{i}$ values $x=\left(x_{1}, x_{2}, \ldots, x_{n}\right)$
$y$ : A corresponding vector of $y_{i}$ values
$S$ : A specially encoded result containing the necessary information for the generalized spline. This is only used indirectly by other MATLAB functions.

The spline function can be used to implement either the not-a-knot or the complete spline method.

- If length $(x)=$ length $(y)$, then $y$ is assumed to contain the values $y=$ $\left(y_{1}, y_{2}, \ldots, y_{n}\right)$ and the spline is generated using the not-a-knot approach.
- To implement the complete spline approach, we provide 2 additional values in the vector $y$, starting with $y_{1}^{\prime}=f^{\prime}\left(x_{1}\right)$ and ending with $y_{n}^{\prime}=f^{\prime}\left(x_{n}\right)$, i.e.

$$
y=\left(y_{1}^{\prime}, y_{1}, y_{2}, \ldots, y_{n-2}, y_{n-1}, y_{n}, y_{n}^{\prime}\right)
$$

In this case, we obviously have length $(y)=$ length $(x)+2$. This triggers MATLAB to implement the complete spline approach.

The ppval function takes in the information encoded in $S$ (the output of spline) and evaluates the spline curve at a number of different locations.

- Syntax:
$v=\operatorname{ppval}(S, u)$
$u$ : A vector of $m$ new $x$-locations where we want the spline to be interpolated/evaluated $u=\left(u_{1}, u_{2}, \ldots, u_{m}\right)$.
$v$ : The corresponding $y$-values of these $u_{i}$ locations $v=\left(v_{1}, v_{2}, \ldots, v_{m}\right)$

Example:

```
x = 0:pi/5:2*pi;
y = sin(x);
S = spline(x,y);
u = l:pi/100:2*pi;
v = ppval(S,u);
plot(u,v);
plot(x,y,u,v);
w = sin(u)
plot(u,v,u,w);
```

Error analysis: For simplicity, we will again assume that $h_{1}=h_{2}=\cdots=$ $h_{n-1}=h\left(h_{k}=x_{k+1}-x_{k}\right)$. For the not-a-knot method, we have:

$$
|f(x)-S(x)| \leq \frac{5}{384}\left\|f^{\prime \prime \prime \prime}\right\|_{\infty} h^{4}
$$

This is an approximate inequality because the interpolation error can be slightly larger near the endpoints of the interval $[a, b]$.

This a very comparable result with the (non-smooth) piecewise cubic polynomial method:

$$
|f(x)-S(x)| \leq \frac{9}{384}\left\|f^{\prime \prime \prime \prime}\right\|_{\infty} h^{4}
$$

Note, though, that the computation of the piecewise cubic method was very local and simple (Every interval could be independently evaluated.) while the computation of the coefficients of the cubic spline is more elaborate.

## Cubic Hermite Splines

We will now consider a different approach to piecewise cubic polynomial interpolation. In particular, given $n x$-values (in ascending order)

$$
x_{1}<x_{2}<\cdots<x_{n-1}<x_{n}
$$

and $n$ associated $y$-values (sampled from a function $f(x)$ )

$$
y_{1}, y_{2}, \ldots, y_{n-1}, y_{n}, \text { where } y_{k}=f\left(x_{k}\right)
$$

and assume we also know the derivative $f^{\prime}(x)$ at the same locations, denoted by:

$$
y_{1}^{\prime}, y_{2}^{\prime}, \ldots, y_{n-1}^{\prime}, y_{n}^{\prime} \text {, where } y_{k}^{\prime}=f^{\prime}\left(x_{k}\right)
$$

As with other methods based on piecewise polynomials, we construct the interpolant as

$$
S(x)=\left\{\begin{array}{cl}
S_{1}(x), & x \in I_{1} \\
S_{2}(x), & x \in I_{2} \\
\vdots & \\
S_{k}(x), & x \in I_{k} \\
\vdots & \\
S_{n-1}(x), & x \in I_{n-1}
\end{array} \quad \text { where } I_{k}=\left[x_{k}, x_{k+1}\right]\right.
$$

In this case, each individual $S_{k}(x)$ is constructed to match both the function values $y_{k}, y_{k+1}$ as well as the derivatives $y_{k}^{\prime}, y_{k+1}^{\prime}$ at the endpoints of $I_{k}$. In detail:

$$
\left.\begin{array}{rl}
S_{k}\left(x_{k}\right) & =y_{k}  \tag{*}\\
S_{k}\left(x_{k+1}\right) & =y_{k+1} \\
S_{k}^{\prime}\left(x_{k}\right) & =y_{k}^{\prime} \\
S_{k}^{\prime}\left(x_{k+1}\right) & =y_{k+1}^{\prime}
\end{array}\right\}
$$

Since $S_{k}(x)=a_{3} x^{3}+a_{2} x^{2}+a_{1} x+a_{0}$ has 4 unknown coefficients, the 4 equations

Lecture of: 14 Mar 2013 $(*)$ uniquely define the appropriate values of $a_{0}, \ldots, a_{3}$. Also note that:

$$
\begin{aligned}
S_{k}\left(x_{k+1}\right) & =y_{k+1}=S_{k+1}\left(x_{k+1}\right) \\
\text { and } S_{k}^{\prime}\left(x_{k+1}\right) & =y_{k+1}^{\prime}=S_{k+1}^{\prime}\left(x_{k+1}\right)
\end{aligned}
$$

Thus, the resulting interpolant $S(x)$ is continuous with continuous derivatives (e.g. a $C^{1}$ function). However, we do not strictly enforce that the 2nd derivative should be continuous, and in fact, it generally will not be:


In this case $S_{1}^{\prime \prime}(0)=2$, while $S_{2}^{\prime \prime}(0)=0$.

