Supplementary Notes: B-Splines Advanced Topics in Statistical Learning, Spring 2023 Ryan Tibshirani

Note: this is pretty much taken shamelessly from Appendix C of Tibshirani (2022).

To parametrize the space of k^{th} degree splines with knots at t_1, \ldots, t_r , a simple choice is the *truncated* power basis, g_1, \ldots, g_{r+k+1} , which recall is defined as

$$g_j(x) = \frac{1}{(j-1)!} x^{j-1}, \quad j = 1, \dots, k+1,$$

$$g_{j+k+1}(x) = \frac{1}{k!} (x-t_j)_+^k, \quad j = 1, \dots, r,$$
(1)

Here $x_{+} = \max\{x, 0\}$ denotes the positive part of x.

Though the truncated power basis (1) is the simplest basis for splines, the B-spline basis is just as fundamental, and it was "there at the very beginning", appearing in Schoenberg's original paper on splines (Schoenberg, 1946). Here we are quoting de Boor (1976), who gives a masterful survey of the history and properties of B-splines (and points out that the name "B-spline" is derived from Schoenberg's use of the term "basic spline", to further advocate for the idea that B-splines can be seen as *the* basis for splines).

Peano representation. There are different ways to construct B-splines; here we cover a construction based on what is called the *Peano representation* for B-splines. If f is a k + 1 times differentiable function f on an interval [a, b] (and its $(k + 1)^{st}$ derivative is integrable), then by Taylor expansion

$$f(z) = \sum_{i=0}^{k} \frac{1}{i!} (D^{i}f)(a)(z-a)^{i} + \int_{a}^{z} \frac{1}{k!} (D^{k+1}f)(x)(z-x)^{k} dx.$$

Note that we can rewrite this as

$$f(z) = \sum_{i=0}^{k} \frac{1}{i!} (D^{i}f)(a)(z-a)^{i} + \int_{a}^{b} \frac{1}{k!} (D^{k+1}f)(x)(z-x)_{+}^{k} dx.$$
(2)

Next we will take a particular divided difference on both sides of the above display. First we recall the definition of a divided difference: with respect to two centers z_1, z_2 , it is defined by

$$f[z_1, z_2] = \frac{f(z_2) - f(z_1)}{z_2 - z_1},$$

and more generally, with respect to k+1 centers z_1, \ldots, z_{k+1} , for an integer $k \ge 1$, it is defined by

$$f[z_1,\ldots,z_{k+1}] = \frac{f[z_2,\ldots,z_{k+1}] - f[z_1,\ldots,z_k]}{z_{k+1} - z_1}.$$

(For this to reduce to the definition with two centers, when k = 1, we take by convention f[z] = f(z).)

Returning back to our main thread, we take a divided difference in the Taylor expansion (2) with respect to arbitrary centers $z_1, \ldots, z_{k+2} \in [a, b]$, where we assume without a loss of generality that $z_1 < \cdots < z_{k+2}$, and then we use linearity to exchange divided differencing with integration, yielding

$$k! \cdot f[z_1, \dots, z_{k+2}] = \int_a^b (D^{k+1}f)(x) \underbrace{(\cdot - x)_+^k[z_1, \dots, z_{k+2}]}_{P^k(x; z_{1:(k+2)})} dx, \tag{3}$$

where we have also used the fact that a $(k + 1)^{\text{st}}$ order divided difference (with respect to any k + 2 centers) of a k^{th} degree polynomial is zero, and we multiplied both sides by k!. To be clear, the notation $(\cdot - x)_+^k[z_1, \ldots, z_{k+2}]$ means that we are taking the divided difference of the function $z \mapsto (z - x)_+^k$ with respect to centers z_1, \ldots, z_{k+2} .

B-spline definition. The result in (3) shows that the $(k+1)^{\text{st}}$ divided difference of any (smooth enough) function f can be written as a weighted average of its $(k+1)^{\text{st}}$ derivative, in a local neighborhood around the corresponding centers, where the weighting is given by a universal kernel $P^k(\cdot; z_{1:(k+2)})$ (that does not depend on f), which is called the *Peano kernel* formulation for the B-spline; to be explicit, this is

$$P^{k}(x; z_{1:(k+2)}) = (\cdot - x)^{k}_{+}[z_{1}, \dots, z_{k+2}].$$

Since

$$(z-x)_{+}^{k} - (-1)^{k+1}(x-z)_{+}^{k} = (z-x)^{k},$$

and any $(k+1)^{st}$ order divided difference of the k^{th} degree polynomial $z \mapsto (z-x)^k$ is zero, we can rewrite the second-to-last display as

$$P^{k}(x; z_{1:(k+2)}) = (-1)^{k+1}(x - \cdot)^{k}_{+}[z_{1}, \dots, z_{k+2}].$$

The function $P^k(\cdot; z_{1:(k+2)})$ is called a k^{th} degree *B-spline* with knots $z_{1:(k+2)}$. It is a linear combination of k^{th} degree truncated power functions and is hence indeed a k^{th} degree spline.

It is often more convenient to deal with the normalized B-spline:

$$M^{k}(x; z_{1:(k+2)}) = (-1)^{k+1}(z_{k+2} - z_{1})(x - \cdot)^{k}_{+}[z_{1}, \dots, z_{k+2}].$$

It is easy to show that

 $M^{k}(\cdot; z_{1:(k+2)})$ is supported on $[z_{1}, z_{k+2}]$, and $M^{k}(x; z_{1:(k+2)}) > 0$ for $x \in (z_{1}, z_{k+2})$.

To see the support result, note that for $x > z_{k+2}$, we are taking a divided difference of all zeros, which of course zero, and for $x < z_1$, we are taking a $(k + 1)^{\text{st}}$ order divided difference of a polynomial of degree k, which is again zero. To see the positivity result, we can, for example, appeal to induction on k and the recursion to come later.

B-spline basis. To build a local basis the space of k^{th} degree splines with knots t_1, \ldots, t_r , which we assume lie in the interior of [a, b], we first define boundary knots

$$t_{-k} < \cdots < t_{-1} < t_0 = a$$
, and $b = t_{r+1} < t_{r+2} < \cdots < t_{r+k+1}$.

(Any such values for t_{-k}, \ldots, t_0 and $t_{r+1}, \ldots, t_{r+k+1}$ will suffice to produce a basis; in fact, setting $t_{-k} = \cdots = t_0$ and $t_{r+1} = \cdots = t_{r+k+1}$ would suffice, though this would require us to understand how to properly interpret divided differences with repeated centers; as in Definition 2.49 of Schumaker (2007).) We then define the normalized B-spline basis M_j^k , $j = 1, \ldots, r+k+1$

$$M_j^k = M^k(\cdot; t_{(j-k-1):j})\Big|_{[a,b]}, \quad j = 1, \dots, r+k+1.$$

It is clear that each M_j^k , j = 1, ..., r + k + 1 is a k^{th} degree spline with knots in $t_1, ..., t_r$; hence to verify that they are a basis for this space we only need to show their linear independence, which is straightforward using the structure of their supports.

For concreteness, we note that the 0th degree normalized B-splines basis are simply indicator functions,

$$M_j^0 = 1_{I_j}, \quad j = 1, \dots, r+1$$

Here $I_0 = [t_0, t_1]$ and $I_i = (t_i, t_{i+1}]$, i = 1, ..., r, and we use $t_{r+1} = b$ for notational convenience. We note that this particular choice for the half-open intervals (left- versus right-side open) is arbitrary, but consistent with our definition of the truncated power basis (1) when k = 0.

Figure 1 shows example normalized B-splines of degrees 0 through 3.

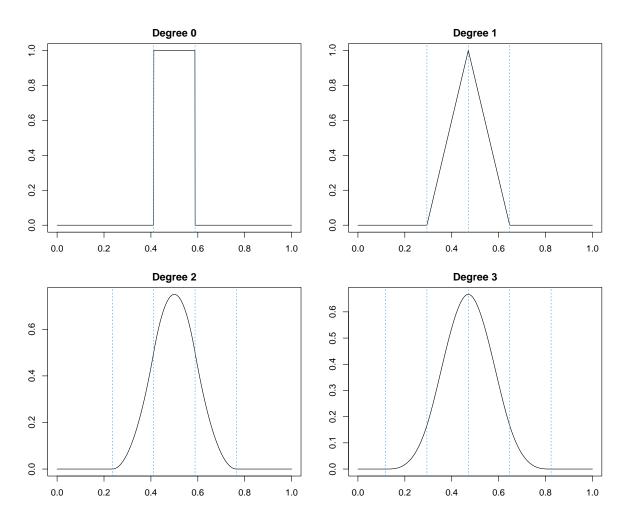


Figure 1: B-splines of degrees 0 through 3. The knot points are marked by dashed blue vertical lines.

Recursive formulation. B-splines satisfy a recursion relation that can be seen directly from the recursive nature of divided differences: for any $k \ge 1$ and centers $z_1 < \cdots < z_{k+2}$,

$$(x-\cdot)_{+}^{k}[z_{1},\ldots,z_{k+2}] = \frac{(x-\cdot)_{+}^{k}[z_{2},\ldots,z_{k+2}] - (x-\cdot)_{+}^{k}[z_{1},\ldots,z_{k+1}]}{z_{k+2}-z_{1}}$$
$$= \frac{(x-z_{k+2})(x-\cdot)_{+}^{k-1}[z_{2},\ldots,z_{k+2}] - (x-z_{1})(x-\cdot)_{+}^{k-1}[z_{1},\ldots,z_{k+1}]}{z_{k+2}-z_{1}},$$

where in the second line we applied the Leibniz rule for divided differences

$$fg[z_1, \dots, z_{k+1}] = \sum_{i=1}^{k+1} f[z_1, \dots, z_i]g[z_i, \dots, z_{k+1}]$$

to conclude that

$$(x - \cdot)_{+}^{k}[z_{1}, \dots, z_{k+1}] = (x - z_{1}) \cdot (x - \cdot)_{+}^{k-1}[z_{1}, \dots, z_{k+1}]$$
$$(x - \cdot)_{+}^{k}[z_{2}, \dots, z_{k+2}] = (x - \cdot)_{+}^{k-1}[z_{2}, \dots, z_{k+2}] \cdot (x - z_{k+2}).$$

Translating the above recursion over to normalized B-splines, we get

$$M^{k}(x; z_{1:(k+2)}) = \frac{x - z_{1}}{z_{k+1} - z_{1}} \cdot M^{k-1}(x; z_{1:(k+1)}) + \frac{z_{k+2} - x}{z_{k+2} - z_{2}} \cdot M^{k-1}(x; z_{2:(k+2)}),$$

which means that for the normalized basis,

$$M_j^k(x) = \frac{x - t_{j-k-1}}{t_{j-1} - t_{j-k-1}} \cdot M_{j-1}^{k-1}(x) + \frac{t_j - x}{t_j - t_{j-k}} \cdot M_j^{k-1}(x), \quad j = 1, \dots, r+k+1.$$

Above, we naturally interpret $M_0^{k-1} = M^{k-1}(\cdot; t_{-k:0})|_{[a,b]}$ and $M_{r+k+1}^{k-1} = M^{k-1}(\cdot; t_{(r+1):(r+k+1)})|_{[a,b]}$.

The above recursions are very important, both for verifying numerous properties of B-splines and for computational purposes. In fact, many authors prefer to use recursion to define a B-spline basis in the first place.

References

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