Biostatistics 615 - Statistical Computing

Topic 4 Interpolation and Extrapolation

Hyun Min Kang

Topic Overview

1. Linear interpolation and extrapolation
2. Polynomial interpolation and piecewise interpolation
3. Natural cubic spline

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Interpolation and Extrapolation

Given a set of data points: $\{(x_i, y_i)\}_{i=1}^n$ where $x_i, y_i \in \mathbb{R}$.

- **Interpolation**: find the values of "missing data" in between known values.
- **Extrapolation**: extend the model outside of known data to "predict" new values for which no measure could have been taken.
- **Curve fitting**: find a function $f(x)$ defined on $\mathbb{R}$ such that

$$y_i = \hat{f}(x_i).$$

- It depends on the model assumptions on the association between the outcome variable and predictors
  - Linear function
  - Polynomial function
  - Piecewise linear
  - Smoother curve

Linear Interpolation

- Start with only two observed points: (x_1, y_1) and (x_2, y_2).
- Find a linear function

$$y = mx + b$$

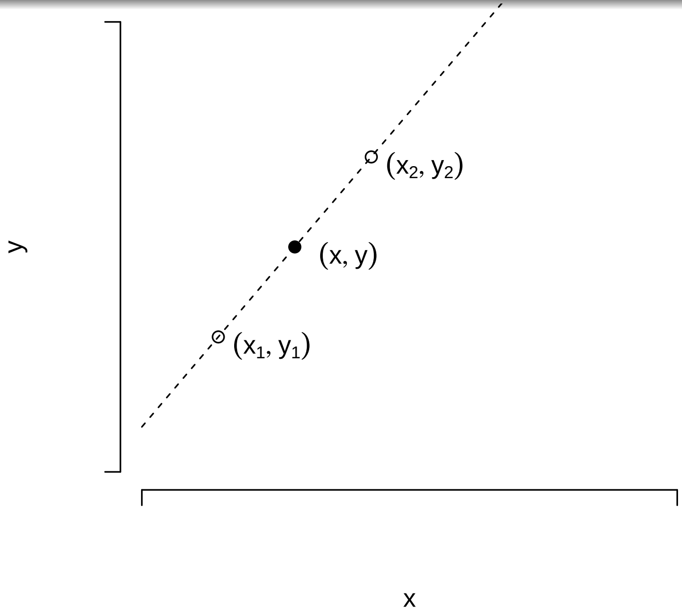
such that it passes the two points, that is,

$$\begin{cases} y_1 & = mx_1 + b \\ y_2 & = mx_2 + b \end{cases}$$

- The solution is

$$\begin{cases} m & = \frac{y_2 - y_1}{x_2 - x_1} \\ b & = y_1 - mx_1 = y_2 - mx_2 \end{cases}$$

Linear Interpolation based on two points



Hands-on Session

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- Implementing linear interpolation

Potential problems with linear interpolation

- True relationship between x and y are not necessarily linear
- More observation points are usually available
- When $x_1 = x_2$ or $|x_1 - x_2|$ is very small. This approach is problematic.

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Higher-Order Polynomial Interpolation

- Given two data points, a line, a polynomial of degree one, will always pass exactly through the two points, provided the two values of x are different.
- For any three points, it is usually that no such line is available, unless those points lie precisely on the same line, but a quadratic function, a polynomial of degree two, will always fit the three data points exactly.
- In general, a polynomial of degree $n-1$ is necessary and sufficient to precisely fit the n data points.

Higher-Order Polynomial Interpolation

- Given a set of ordered pairs, $\{(x_i, y_i)\}_{i=1}^{n}$, the interpolating function $p_{n-1}(x)$ must meet the requirement,

$$p_{n-1}(x_i) = y_i,$$

for all $i = 1, \ldots, n$.

- The interpolating function is a polynomial of order $n-1$:

$$p_{n-1}(x) = \sum_{j=0}^{n-1} \beta_j x^j,$$

where β_j's are the polynomial's coefficients.

$$\sum_{j=0}^{n-1} \beta_j x_i^j = y_i,$$

for each of the i interpolating points.

Higher Order Polynomial Interpolation

In matrix form

$$\begin{pmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ 1 & x_2 & \dots & x_2^{n-1} \\ \dots & \dots & \dots & \dots \\ 1 & x_n & \dots & x_n^{n-1} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_{n-1} \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{pmatrix},$$

In the matrix form, we have

$$\boldsymbol{V}(\boldsymbol{x})\boldsymbol{\beta} = \boldsymbol{y}$$

where

- The matrix $\boldsymbol{V}(\boldsymbol{x})$ is called the Vandermonde matrix and it contains successive columns of $\boldsymbol{x}$ to the ith power, where $i = 0, \dots, n-1$.
- We can solve the above linear system to obtain $\boldsymbol{\beta}$ for the polynomial interpolation.

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- Higher-order Polynomial Interpolation

Approximation Errors

- Similar to the linear interpolation, the higher-order polynomial interpolation may have large numerical errors when x_i and $x_{i'}$ are too close for any $i \neq i' \in \{1, \ldots, n\}$. Or the Vandermonde matrix $\boldsymbol{V}(\boldsymbol{x})$ is close to a singular matrix.
- In addition to numerical errors, the higher-order polynomial interpolation also has the approximation errors. Suppose the true relationship between y and x is $y = f(x)$, where $f(x)$ is a smooth function whose the nth derivative exists. Then the approximation error is

$$p_{n-1}(x) - f(x) = \frac{\prod_{i=1}^{n}(x - x_i)}{n!} f^{(n)}(x)$$

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- Approximation errors in polynomial interpolation

Limitations of higher-order polynomial interpolation

- The computational complexity is $O(n^3)$. It is computationally challenging when n is large.
- Diverge from true values at the endpoints in many cases, especially when n is large.
- While the higher-degreed polynomial pass through all observed points, it may fluctuate wildly between two points, a pattern known as Runge's phenomenon.

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- Runge's phenomenon

Piecewise Interpolation

- The true function may be complex and better approximated using two or more interpolations.
- Piecewise interpolation offers a solution: to use lower degreed polynomials for each part of a curve because we are able to efficiently fit those polynomials to approximately analyze the underlying data.

Piecewise Linear Interpolation

- A linear approach to interpolating between points: draw lines between points.
- The process for piecewise linear interpolation uses the same process as our linear interpolation model, except it repeats it for each consecutive pair of data points along the x-axis.
- Computational complexity is $O(n)$.

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- Piecewise linear interpolation
- Revisiting Runge's phenomenon

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Cubic Spline Interpolation

Revisiting Piecewise Linear Interpolation

- If using a first-degree polynomial, a line over multiple intervals is an improvement over a single interpolating line.
- However, piecewise linear interpolation does not produce differentiable (or smooth) function at the joins.
- What if we use a higher-degree polynomial?

Cubic Spline Interpolation : A potential solution

- It constructs a differentiable, integrable and smooth curve, despite the joins.
- As each individual section is represented by a cubic curve, i.e. **polynomial of degree three**.

Cubic Spline Setup

- Denote by $\{(x_i, y_i)\}_{i=1}^{n}$ the data points to interpolate, where we assume that $x_i \leq x_{i+1}$ for $i = 1, \ldots, n-1$.
- For n data points, we construct $n-1$ interpolating cubic polynomials on $[x_1, x_2], \ldots, [x_{n-1}, x_n]$.
- Let $S_i(x)$ be a cubic polynomial function representing the curve over the domain $[x_i, x_{i+1}]$.
- We assume that

$$
\begin{aligned}
S_i(x) &= \sum_{j=0}^{3} a_{j,i}(x - x_i)^j \\
&= a_{0,i} + a_{1,i}(x - x_i) + a_{2,i}(x - x_i)^2 + a_{3,i}(x - x_i)^3
\end{aligned}
$$

- Then we have

$$
\begin{aligned}
S_i'(x) &= a_{1,i} + 2a_{2,i}(x - x_i) + 3a_{3,i}(x - x_i)^2 \\
S_i''(x) &= 2a_{2,i} + 6a_{3,i}(x - x_i)
\end{aligned}
$$

Equations to construct cubic splines

- The set of $\{S_i(x)\}$ has a total of $4(n-1)$ parameters.
- Continuity $(2n-2)$: for $i = 1, \ldots, n-1$,

$$S_i(x_i) = y_i, \quad (1)$$
$$S_i(x_{i+1}) = y_{i+1}. \quad (2)$$

- Smoothness $(2n-4)$: for $i = 1, \ldots, n-2$,

$$S_i'(x_{i+1}) = S_{i+1}'(x_{i+1}), \quad (3)$$
$$S_i''(x_{i+1}) = S_{i+1}''(x_{i+1}). \quad (4)$$

- So far we establish $4n-6$ equations, we need to two more constraints to solve all the parameters.
- Boundary conditions: $S_1''(x_1) = 0$ and $S_{n-1}''(x_n) = 0$. We refer to this type of spline as the **Natural Cubic Spline**.

Summary - equations to construct cubic splines

$$
\begin{aligned}
S_i(x) &= a_{0,i} + a_{1,i}(x - x_i) + a_{2,i}(x - x_i)^2 + a_{3,i}(x - x_i)^3 \\
S_i'(x) &= a_{1,i} + 2a_{2,i}(x - x_i) + 3a_{3,i}(x - x_i)^2 \\
S_i''(x) &= 2a_{2,i} + 6a_{3,i}(x - x_i)
\end{aligned}
$$

Equations for natural cubic spline

$$
\begin{aligned}
S_i(x_i) &= y_i & i &= 1, \ldots, n-1 \\
S_i(x_{i+1}) &= y_{i+1} & i &= 1, \ldots, n-1 \\
S_i'(x_{i+1}) &= S_{i+1}'(x_{i+1}) & i &= 1, \ldots, n-2 \\
S_i''(x_{i+1}) &= S_{i+1}''(x_{i+1}) & i &= 1, \ldots, n-2 \\
S_1''(x_1) &= 0 \\
S_{n-1}''(x_n) &= 0
\end{aligned}
$$

Solve the natural cubic spline - Definitions

- For $i = 2, \ldots, n$, let

$$h_i = x_i - x_{i-1}, \quad \delta_i = \frac{y_i - y_{i-1}}{h_i}.$$

- For $i = 2, \ldots, n-1$, let

$$g_i = h_{i+1} + h_i, \quad v_i = \delta_{i+1} - \delta_i.$$

Solve the natural cubic spline - Continuity

- From $S_i(x_i) = y_i, i = 1, \ldots, n-1$,

$$a_{0,i} = y_i$$

- From $S_i(x_{i+1}) = y_{i+1}, i = 1, \ldots, n-1$,

$$a_{0,i} + a_{1,i}h_{i+1} + a_{2,i}h_{i+1}^2 + a_{3,i}h_{i+1}^3 = y_{i+1}$$

- Then for $i = 1, \ldots, n-1$,

$$a_{1,i} + a_{2,i}h_{i+1} + a_{3,i}h_{i+1}^2 = \frac{y_{i+1} - y_i}{h_{i+1}} = \delta_{i+1}. \tag{5}$$

Solve the natural cubic spline - Smoothness

- From $S_i'(x_{i+1}) = S_{i+1}'(x_{i+1}), i = 1, \ldots, n-2$,

$$a_{1,i+1} = a_{1,i} + 2a_{2,i}h_{i+1} + 3a_{3,i}h_{i+1}^2. \quad (6)$$

- From $S_i''(x_{i+1}) = S_{i+1}''(x_{i+1}), i = 1, \ldots, n-2$,

$$a_{2,i+1} = a_{2,i} + 3a_{3,i}h_{i+1}. \quad (7)$$

- From (7), for $i = 1, \ldots, n-2$,

$$a_{3,i} = \frac{a_{2,i+1} - a_{2,i}}{3h_{i+1}}. \quad (8)$$

- From (6), for $i = 1, \ldots, n-2$,

$$a_{1,i+1} - a_{1,i} = (a_{2,i} + a_{2,i+1})h_{i+1}$$

Solve the natural cubic spline - Putting Together

- From (5), for $i = 1, \ldots, n-2$,

$$3a_{1,i} + (2a_{2,i} + a_{2,i+1})h_{i+1} = 3\delta_{i+1} \tag{9}$$

- Then for $i = 2, \ldots, n-1$

$$3a_{1,i-1} + (2a_{2,i-1} + a_{2,i})h_i = 3\delta_i \tag{10}$$

- For $i = 2, \ldots, n-2$, we get this key equation from (9)-(10):

$$h_i a_{2,i-1} + 2g_i a_{2,i} + h_{i+1} a_{2,i+1} = 3v_i \tag{11}$$

Remember:
$a_{1,i+1} - a_{1,i} = (a_{2,i} + a_{2,i+1})h_{i+1}$, $g_i = h_{i+1} + h_i$, $v_i = \delta_{i+1} - \delta_i$.

Boundary conditions for natural cubic splines

- By $S_1''(x_1) = 0$, we have $a_{2,1} = 0$, so from (11),

$$2g_2 a_{2,2} + h_3 a_{2,3} = 3v_2$$

- By $S_{n-1}''(x_n) = 0$, we have $a_{2,n-1} + 3a_{3,n-1}h_n = 0$
- From (5),

$$3a_{1,n-1} + 2a_{2,n-1}h_n = 3\delta_n$$

- Also,

$$3a_{1,n-2} + (2a_{2,n-2} + a_{2,n-1})h_{n-1} = 3\delta_{n-1}$$

$$a_{1,n-1} - a_{1,n-2} = (a_{2,n-2} + a_{2,n-1})h_{n-1}$$

- Therefore, we also have

$$h_{n-1}a_{2,n-2} + 2g_{n-1}a_{2,n-1} = 3v_{n-1}$$

Thus

$$\begin{pmatrix} 2g_2 & h_3 & 0 & \ldots & \ldots & \ldots \\ h_3 & 2g_3 & h_4 & 0 & \ldots & \ldots \\ 0 & h_4 & 2g_4 & h_5 & 0 & \ldots \\ \ldots & 0 & \ldots & \ldots & \ldots & 0 \\ \ldots & \ldots & 0 & h_{n-2} & 2g_{n-2} & h_{n-1} \\ \ldots & \ldots & \ldots & 0 & h_{n-1} & 2g_{n-1} \end{pmatrix} \begin{pmatrix} a_{2,2} \\ a_{2,3} \\ \ldots \\ \ldots \\ a_{2,n-2} \\ a_{2,n-1} \end{pmatrix} = 3 \begin{pmatrix} v_2 \\ v_3 \\ \ldots \\ \ldots \\ v_{n-2} \\ v_{n-1} \end{pmatrix}$$

This implies that we can apply tridiagonal matrix algorithm to obtain $a_{2,i}$ for $i = 2, \ldots, n-1$.

Defining the remaining variables

Recall that $a_{2,1} = 0$, and also $a_{2,n} = 0$ holds.
Then for $i = 1, \ldots, n-1$, from (8) and (9), we have

$$a_{3,i} = \frac{a_{2,i+1} - a_{2,i}}{3h_{i+1}},$$
$$a_{1,i} = \delta_{i+1} - \frac{2a_{2,i} + a_{2,i+1}}{3} h_{i+1},$$

Recall that

$$a_{0,i} = y_i$$

This completes that the natural cubic spline fitting.

Tridiagonal Matrix Algorithm

For linear system $A\mathbf{x} = \mathbf{b}$, A is a general tridiagonal matrix

$$A = \begin{pmatrix} d_1 & u_1 & 0 & ... & ... & \\ l_1 & d_2 & u_2 & 0 & \dots & ... \\ 0 & l_2 & d_3 & u_3 & 0 & \dots \\ \dots & 0 & \dots & \dots & \dots & u_{n-1} \\ \dots & \dots & \dots & 0 & l_{n-1} & d_n \end{pmatrix}$$

which is determined by three vectors $\mathbf{d} = (d_1, \dots, d_n)$, $\mathbf{u} = (u_1, \dots, u_{n-1})$ and $\mathbf{l} = (l_1, \dots, l_{n-1})$.

What would happen if we solve this linear system with typical linear algebraic solution?

Can you think of more efficient way to solve this equation?

Forward Sweep: Step 1

$$\begin{pmatrix} d_1 & u_1 & 0 & ... & ... & ... \\ l_1 & d_2 & u_2 & 0 & \ldots & ... \\ 0 & l_2 & d_3 & u_3 & 0 & \ldots \\ \ldots & 0 & \ldots & \ldots & \ldots & u_{n-1} \\ \ldots & \ldots & \ldots & 0 & l_{n-1} & d_n \end{pmatrix} \boldsymbol{x} = \begin{pmatrix} b_1 \\ b_2 \\ \ldots \\ b_{n-1} \\ b_n \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} 1 & u_1/d_1 & 0 & ... & ... & ... \\ l_1 & d_2 & u_2 & 0 & \ldots & ... \\ 0 & l_2 & d_3 & u_3 & 0 & \ldots \\ \ldots & 0 & \ldots & \ldots & \ldots & u_{n-1} \\ \ldots & \ldots & \ldots & 0 & l_{n-1} & d_n \end{pmatrix} \boldsymbol{x} = \begin{pmatrix} b_1/d_1 \\ b_2 \\ \ldots \\ b_{n-1} \\ b_n \end{pmatrix}$$

Set $u_1^* = u_1/d_1$ and $b_1^* = b_1/d_1$.

Forward Sweep: Step 2

$$\rightarrow \begin{pmatrix} 1 & u_1^* & 0 & ... & ... & ... \\ 0 & d_2 - u_1^* * l_1 & u_2 & 0 & \dots & ... \\ 0 & l_2 & d_3 & u_3 & 0 & \dots \\ \dots & 0 & \dots & \dots & \dots & u_{n-1} \\ \dots & \dots & \dots & 0 & l_{n-1} & d_n \end{pmatrix} \mathbf{x} = \begin{pmatrix} b_1^* \\ b_2 - b_1^* * l_1 \\ \dots \\ b_{n-1} \\ b_n \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} 1 & u_1^* & 0 & ... & ... & ... \\ 0 & 1 & \frac{u_2}{d_2 - u_1^* * l_1} & 0 & \dots & ... \\ 0 & l_2 & d_3 & u_3 & 0 & \dots \\ \dots & 0 & \dots & \dots & \dots & u_{n-1} \\ \dots & \dots & \dots & 0 & l_{n-1} & d_n \end{pmatrix} \mathbf{x} = \begin{pmatrix} b_1^* \\ \frac{b_2 - b_1^* * l_1}{d_2 - u_1^* * l_1} \\ b_3 \\ \dots \\ b_n \end{pmatrix}$$

Set $u_2^* = \frac{u_2}{d_2 - u_1^* * l_1}$ and $b_2^* = \frac{b_2 - b_1^* * l_1}{d_2 - u_1^* * l_1}$.

Forward Sweep: Step i

For $i = 2, \ldots, n-1$, set

$$u_i^* = \frac{u_i}{d_i - u_{i-1}^* * l_{i-1}},$$
$$b_i^* = \frac{b_i - b_{i-1}^* * l_{i-1}}{d_i - u_{i-1}^* * l_{i-1}}.$$

And

$$b_n^* = \frac{b_n - b_{n-1}^* * l_{n-1}}{d_n - u_{n-1}^* * l_{n-1}}$$

Backward Sweep:

$$\begin{pmatrix} 1 & u_1^* & 0 & \dots & \dots & \dots \\ 0 & 1 & u_2^* & 0 & \dots & \dots \\ 0 & 0 & 1 & u_3^* & 0 & \dots \\ \dots & 0 & \dots & \dots & \dots & u_{n-1}^* \\ \dots & \dots & \dots & 0 & 0 & 1 \end{pmatrix} \boldsymbol{x} = \begin{pmatrix} b_1^* \\ b_2^* \\ \dots \\ b_{n-1}^* \\ b_n^* \end{pmatrix}$$

Then

$$x_n = b_n^*$$

For $i = n-1, n-2, \dots, 1$,

$$x_i = b_i^* - u_i^* * x_{i+1}$$

Hands-on Session

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- Implementing natural cubic spline
- Testing natural cubic spline
- Revisiting Runge's phenomenon

Discussion

- What are the advantages and disadvantages of each interpolation method?
  - Linear interpolation
  - Higher-order polynomial interpolation
  - Piecewise linear interpolation
  - Natural cubic spline
- Can you explain the time complexity of computing natural cubic spline?
- Why is natural cubic spline useful? If we implement similar splines with quadratic (2nd-order) or quartic (4th-order) functions, what are the advantages and disadvantages?