Applications of Polynomial Interpolation

- Extrapolation

- Splines

Contents

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- Splines

Problem Formulation

We have a function $f : \mathbb{R} \to \mathbb{R}$ that can be evaluated for all $h > 0$, but f cannot be evaluated easily at $h = 0$. We are interested in computing

$$\lim_{h \to 0} \ f(h) \ .$$

Example: We want to evaluate the expression

$$\lim_{h \to 0} \ \frac{\exp(h) - 1}{\sin(h)} \ .$$

Here, we cannot simply substitute $h = 0$, as we would have to divide by $\sin(0) = 0$.

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There are several solution strategies for computing limites whose applicability depends on the situation. For example L'Hospital's rule gives

$$\lim_{h \to 0} \frac{\exp(h) - 1}{\sin(h)} = \frac{\exp(0)}{\cos(0)} = 1 \; .$$

Thus, if we use algorithmic differentiation, we may be able to implement L'Hospital's rule for expressions of the form

$$\lim_{h \to 0} \frac{f_1(h)}{f_2(h)} = \lim_{h \to 0} \frac{f_1'(h)}{f_2'(h)} \; ,$$

assuming $f_1(0) = f_2(0) = 0$ and that the derivatives of f_1 and f_2 can be computed easily. However, in general L'Hospital's rule may not be applicable.

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Extrapolation

An alternative to L'Hospital's rule is to use extrapolation. For this aim, we evaluate f at a decreasing sequence of points $h_i > 0$, e.g., $h_1 = \frac{1}{4}$, $h_2 = \frac{1}{8}$, and $h_3 = \frac{1}{16}$.

Next, we compute a polynomial $p(x)$ interpolating the evaluation points

$$(h_1, f(h_1)), \quad (h_2, f(h_2)), \quad (h_3, f(h_3)), \quad \ldots$$

and use the approximation $\lim_{h \to 0} \frac{f_1(h)}{f_2(h)} \approx p(0)$.

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Extrapolation Error

If the function f is $(n+1)$-times continuously differentiable in a small neighborhood of 0 and $p(x)$ a polynomial of degree $\leq n$ which interpolates the points

$$(h_1, f(h)), \ (h_2, f(h_2)), \ \ldots, (h_n, f(h_n))$$

for small $h \geq h_1 > h_2 > \ldots > h_n > 0$, then we have

$$|p(0) - f(0)| \leq \mathbf{O}(h^{n+1}) \, .$$

(the proof follows from Taylor's theorem)

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Extrapolation

Splines

Limitations of Polynomial Interpolation

We have learned in the previous lecture that the interpolation
polynomial may not converge uniformly for $n \to \infty$.

Example: [Runge's phenomenon] Interpolation of

$$f(x) = \frac{1}{x^2 + 1}$$

on equidistant grid on the interval $[-5, 5]$ with high order polynomials
leads to (unwanted) highly oscillatory interpolation.

Splines

One strategy to overcome this problem is to use splines. Here, we break up the whole interval $[x_{\min}, x_{\max}]$ into sub-intervals and interpolate the function f on each of these sub-intervals with a polynomial of moderate degree (often $n = 3$).

The most common splines are "piecewise linear interpolation" and "cubic splines".

In this lecture we have a closer look at cubic splines.

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In this lecture we have a closer look at cubic splines.

Cubic Splines using Hermite Interpolation

Let f be continuously differentiable. We divide the whole interval $[x_{\min}, x_{\max}]$ into n sub-intervals

$$x_{\min} = x_0 < x_1 < \ldots < x_n = x_{\max} .$$

Now, we search for a piecewise cubic approximation of the form

$$p(x) = \left\{ \begin{array}{ll} x_{\min} + f'(x_{\min})(x - x_{\min}) & \text{if } x < x_{\min} \\ p_i(x) & \text{if } x \in [x_i, x_{i+1}] \\ x_{\max} + f'(x_{\max})(x - x_{\max}) & \text{if } x > x_{\max} \end{array} \right\}$$

with $i \in \{0, \ldots, n-1\})$, where the cubic polynomials p_i satisfy

$p_i(x_i) = f(x_i)$ and $p_i'(x_i) = f'(x_i)$

$p_i(x_{i+1}) = f(x_{i+1})$ and $p_i'(x_{i+1}) = f'(x_{i+1})$ (Hermite interpolation!)

for all $i \in \{0, \ldots, n\}$. The function p is called a cubic spline.

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$$p_i(x_{i+1}) = f(x_{i+1}) \quad \text{and} \quad p_i'(x_{i+1}) = f'(x_{i+1}) \qquad \text{(Hermite interpolation!)}$$

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Natural Cubic Splines

Another way to construct cubic splines is by imposing the following
conditions on the piecewise cubic function p:

1. The function p satisfies $p(x_i) = f(x_i)$, $i \in \{0, \ldots, n\}$, ($2n$ conditions)

2. The function p is twice continuously differentiable, ($2(n-1)$ conditions)

3. We have $p''(x_{\min}) = p''(x_{\max}) = 0$, ($2$ conditions)

In total, we have $4n$ conditions determining the coefficients of the n cubic polynomials.

Natural Cubic Splines

Notation: $p_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$, assume $x_{i+1} - x_i = h$.

1. Interpolation ($i \in \{1, \ldots, n\}$):

$$a_i = f(x_i) \quad \text{and} \quad a_i - b_i h + c_i h^2 - d_i h^3 = f(x_{i-1})$$

2. First derivatives ($i \in \{1, \ldots, n-1\}$):

$$b_i = b_{i+1} - 2c_{i+1}h + 3d_{i+1}h^2$$

3. Second derivatives ($i \in \{1, \ldots, n-1\}$):

$$c_i = c_{i+1} - 3d_{i+1}h$$

4. Boundaries: $c_n = 0 \quad c_1 - 3d_1 h = 0.$

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The equation system can be simplified as follows:

1. We know the coefficients $a_i = f(x_i)$.

2. From $c_i = c_{i+1} - 3d_{i+1}h$ we conclude $d_i = \frac{c_i - c_{i-1}}{3h}$ (define $c_0 = 0$).

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$$b_i = \frac{f(x_i) - f(x_{i-1})}{h} + \frac{2c_i + c_{i-1}}{3} h \ .$$

So, in summary, we can express the coefficients a_i, b_i, and d_i in dependence on the sequence $c_0, \ldots, c_n$.

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The next step is a bit cumbersome: we have to substitute our expression for a_i, b_i, and d_i into $b_i = b_{i+1} - 2c_{i+1}h + 3d_{i+1}h^2$. This gives the recursion:

$$\frac{f(x_i) - f(x_{i-1})}{h} + \frac{2c_i + c_{i-1}}{3} h$$

$$= \frac{f(x_{i+1}) - f(x_i)}{h} + \frac{2c_{i+1} + c_i}{3} h - 2c_{i+1}h + (c_{i+1} - c_i)h$$

$$\implies h(c_{i-1} + 4c_i + c_{i+1}) = r_i$$

for $i = 1, \ldots, n-1$ and $c_0 = c_n = 0$ as well as the short-hand

$$r_i = \frac{3}{h} \left(f(x_{i+1}) - 2f(x_i) + f(x_{i-1}) \right) .$$

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$$r_i = \frac{3}{h}\left(f(x_{i+1}) - 2f(x_i) + f(x_{i-1})\right) .$$

Natural Cubic Splines

Thus, the equation system for $c_1, \ldots, c_{n-1}$ can be written in the form

$$
\begin{pmatrix}
4h & h & & \ldots & 0 \\
h & 4h & h & & \\
& \ddots & \ddots & \ddots & \\
\vdots & & h & 4h & h \\
0 & & & h & 4h
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
\vdots \\
c_{n-2} \\
c_{n-1}
\end{pmatrix}
=
\begin{pmatrix}
r_1 \\
r_2 \\
\vdots \\
r_{n-2} \\
r_{n-1}
\end{pmatrix}
$$

This equation system has a unique solution and can be solved using tridiagonal matrix inversion algorithms. (for non-equidistant points x_i a similar result can be obtained)

Properties of Natural Cubic Splines

The natural cubic splines satisfy the inequality

$$\int_{x_{\min}}^{x_{\max}} |p''(x)|^2 \, \mathrm{d}x \leq \int_{x_{\min}}^{x_{\max}} |f''(x)|^2 \, \mathrm{d}x \, .$$

"The natural cubic spline p never oscillates more than the function f."

Proof: Any twice continuously differentiable function w with

$w(x_0) = w(x_1) = \ldots w(x_n) = 0$ satisfies

$$
\begin{aligned}
\int_{x_{\min}}^{x_{\max}} p''(x)w''(x)\mathrm{d}x &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} p''(x)w''(x)\mathrm{d}x \\
&= \sum_{i=0}^{n-1} p''w'\big|_{x_i}^{x_{i+1}} - \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} p'''(x)w'(x)\mathrm{d}x \\
&= \sum_{i=0}^{n-1} \left\{ p''w'\big|_{x_i}^{x_{i+1}} - p'''w\big|_{x_i}^{x_{i+1}} \right\} \\
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Proof (continued)

As p is a cubic polynomial, we have $p'''' = 0$ which implies

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\int_{x_{\min}}^{x_{\max}} p''(x)w''(x)\mathrm{d}x &= \sum_{i=0}^{n-1} p''w'|_{x_i}^{x_{i+1}} \\
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since $p''(x_0) = p''(x_n) = 0$. For $w = f - p$ we find

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\int_{x_{\min}}^{x_{\max}} \left|f''(x)\right|^2 \mathrm{d}x = \int_{x_{\min}}^{x_{\max}} \left|p''(x) + w''(x)\right|^2 \mathrm{d}x \geq \int_{x_{\min}}^{x_{\max}} \left|p''(x)\right|^2 \mathrm{d}x \,.
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Summary

- Extrapolation can be used to compute limit values of functions with high accuracy (only needed if L'Hospital's rule in combination with algorithmic differentiation is not applicable).

- We have discussed two ways to construct cubic splines:
  - Hermite interpolation (continuously differentiable interpolation)
  - Natural Splines (twice continuously differentiable interpolation)

- Natural splines do not require us to evaluate derivatives of f.

- The average of the square of the second derivative of a natural spline p is bounded by the average of the square of the second derivative of the original function f.