Please print your name:

Bonus challenge. Let me know about any typos you spot in the posted solutions (or lecture sketches). Any mathematical typo, that is not yet fixed by the time you send it to me, is worth a bonus point.

Reminder. No notes, calculators (with the exception of one that can only do basic arithmetic—no graphing or additional algebraic capabilities) or tools of any kind will be permitted on the midterm exam.

Problem 1. Determine the minimal polynomial P(x) interpolating (-2,1), (0,1), (1,1), (3,2).

- (a) Write down the polynomial in Lagrange form.
- (b) Write down the polynomial in Newton form.
- (c) Suppose the above points lie on the graph of a smooth function f(x). Write down an "explicit" formula for f(x) P(x), the error when using the interpolating polynomial to approximate f(x).

Solution.

(a) The interpolating polynomial in Lagrange form is

$$P(x) = 1 \frac{x(x-1)(x-3)}{(-2)(-2-1)(-2-3)} + 1 \frac{(x+2)(x-1)(x-3)}{(2)(-1)(-3)} + 1 \frac{(x+2)x(x-3)}{(1+2)1(1-3)} + 2 \frac{(x+2)x(x-1)}{(3+2)3(3-1)}.$$

(If we had a reason to do so (we don't!), we could expand that expression to find $P(x) = 1 - \frac{x}{15} + \frac{x^2}{30} + \frac{x^3}{30}$.)

(b) Newton's divided differences for the four points are:

Accordingly, reading the coefficients from the top edge of the triangle (as shaded above), the Newton form is

$$P(x) = 1 + 0(x+2) + 0(x+2)x + \frac{1}{30}(x+2)x(x-1) = 1 + \frac{1}{30}(x+2)x(x-1).$$

(Since the interpolating polynomial is unique, this polynomial must be the same as the one in the first part.)

Comment. Note that the y-coordinate of the first three points is 1. Therefore, the interpolating polynomial for these three points is simply Q(x) = 1. The Newton form of P(x) is $P(x) = Q(x) + c_3(x+2)x(x-1)$ (we discussed how, in general, the Newton form makes it convenient to add additional point) and we could alternatively find $c_3 = 1/30$ by plugging in the fourth point.

(c) $f(x) - P(x) = \frac{f^{(4)}(\xi)}{4!}(x+2)x(x-1)(x-3)$ for some $\xi \in [-2,3]$ (assuming that $x \in [-2,3]$ as well).

Comment. You don't need to "memorize" the general result we proved in class to write down this error formula. Instead, note that the term (x+2)x(x-1)(x-3) on the right-hand side is natural because we know that the error is 0 at x = -2, 0, 1, 3. On the other hand, (x+2)x(x-1)(x-3) has degree 4 and, therefore, just like for Taylor expansion, it should go with $f^{(4)}(\xi)/4!$ (indeed, as we noted in class, Taylor expansion around $x = x_0$ can be considered as the limiting case where the interpolation nodes all become equal to a single x_0).

Problem 2. Suppose we approximate $f(x) = \cos(\frac{x}{2})$ by the polynomial P(x) interpolating it at x = 1, 2, 3.

- (a) Without computing P(x), give an upper bound for the error when x=0 and when $x=\frac{\pi}{2}$.
- (b) For which x in $[0, \pi]$ is our bound for the error maximal? What is the bound in that case?

Solution.

(a) The error is

$$f(x) - P(x) = \frac{f^{(3)}(\xi)}{3!}(x-1)(x-2)(x-3),$$

where ξ is between 1, 3 and x. Note that $f^{(3)}(x) = \frac{1}{8}\sin(\frac{x}{2})$ so that $|f^{(3)}(\xi)| \leq \frac{1}{8}$. Hence, the error is bounded by

$$|f(x) - P(x)| \le \frac{1}{6} \cdot \frac{1}{8} |(x-1)(x-2)(x-3)|.$$

In particular, in the case x = 0,

$$|f(0) - P(0)| \le \frac{1}{48}|(-1)(-2)(-3)| = \frac{1}{8} = 0.125,$$

while, in the case $x = \frac{\pi}{2}$,

$$\left|f\left(\frac{\pi}{2}\right) - P\left(\frac{\pi}{2}\right)\right| \leqslant \frac{1}{48} \left|\left(\frac{\pi}{2} - 1\right)\left(\frac{\pi}{2} - 2\right)\left(\frac{\pi}{2} - 3\right)\right| \approx 0.00729.$$

Comment. Why is it not surprising that the error bound for x = 0 is considerably larger?

(b) Recall that our bound for the error is $\frac{1}{48}|(x-1)(x-2)(x-3)|$.

We need to determine the maximal absolute value of the cubic polynomial e(x) = (x-1)(x-2)(x-3) on the interval $[0,\pi]$.

We compute $e'(x) = 3x^2 - 12x + 11$ and find that e'(x) = 0 for $x = 2 \pm \frac{1}{\sqrt{3}}$. At these values, $e\left(2 \pm \frac{1}{\sqrt{3}}\right) = \pm \frac{2}{3\sqrt{3}} \approx \pm 0.385$. At the endpoints of the interval $[0, \pi]$, e(0) = -6 and $e(\pi) \approx 0.346$.

Hence, |e(x)| is maximal on $[0, \pi]$ for x = 0. We already computed that, in this case, the error bound is $|f(0) - P(0)| \leq \frac{1}{8}$.

Problem 3. Suppose we approximate a function f(x) by the polynomial P(x) interpolating it at $x = -1, -\frac{2}{3}, \frac{2}{3}, 1$. Suppose that we know that $|f^{(n)}(x)| \le n$ for all $x \in [-1, 1]$.

- (a) Give an upper bound for the error when $x = -\frac{1}{6}$ and when x = 0.
- (b) Give an upper bound for the error for all $x \in [-1, 1]$.
- (c) Suppose we replace the nodes $-1, -\frac{2}{3}, \frac{2}{3}, 1$ with four other values. For which choice of these four interpolation nodes is this upper bound for the error minimal?
- (d) For this optimal choice, what is the upper bound for the error for all $x \in [-1,1]$?

Solution.

(a) The error is

$$f(x) - P(x) = \frac{f^{(4)}(\xi)}{4!}(x+1)\left(x+\frac{2}{3}\right)\left(x-\frac{2}{3}\right)(x-1) = \frac{f^{(4)}(\xi)}{4!}(x^2-1)\left(x^2-\frac{4}{9}\right),$$

where ξ is between -1 and 1 (provided that $x \in [-1, 1]$). Since $\frac{1}{4!} |f^{(4)}(\xi)| \leqslant \frac{4}{4!} = \frac{1}{6}$, the error is bounded by

$$|f(x) - P(x)| \le \frac{1}{6} |(x^2 - 1)(x^2 - \frac{4}{9})|.$$

If $x = -\frac{1}{6}$, then this bound becomes $|f(x) - P(x)| \le \frac{1}{6} \left| \left(\frac{1}{36} - 1 \right) \left(\frac{1}{36} - \frac{4}{9} \right) \right| = \frac{1}{6} \cdot \frac{175}{432} \approx 0.0675$.

If x=0, then this bound becomes $|f(x)-P(x)| \leq \frac{1}{6} |(-1)(-\frac{4}{9})| = \frac{2}{27} \approx 0.0741$.

(b) Consider $g(x) = (x^2 - 1)(x^2 - \frac{4}{9}) = x^4 - \frac{13}{9}x^2 + \frac{4}{9}$. We need to compute $\max_{x \in \lceil -1, 1 \rceil} |g(x)|$.

Since $g(\pm 1) = 0$, the maximum value of |g(x)| must be attained at a point where g'(x) = 0.

We compute $g'(x) = 4x^3 - \frac{26}{9}x$. Hence g'(x) = 0 if x = 0 or $x = \pm \frac{1}{3}\sqrt{\frac{13}{2}}$.

Since $|g(0)| = \frac{4}{9}$ and $\left|g\left(\pm\frac{1}{3}\sqrt{\frac{13}{2}}\right)\right| = \frac{25}{324} < \frac{4}{9}$, we conclude that $\max_{x \in [-1,1]} |g(x)| = \frac{4}{9}$.

Therefore, our bound for the error is $\max_{x \in [-1,1]} |f(x) - P(x)| \le \frac{1}{6} \max_{x \in [-1,1]} \left| (x^2 - 1) \left(x^2 - \frac{4}{9} \right) \right| = \frac{1}{6} \cdot \frac{4}{9} = \frac{2}{27} \approx 0.0741$.

(c) We have shown in class that $\max_{x \in [-1,1]} |(x-x_1) \cdots (x-x_n)|$ is minimal for the Chebyshev nodes

$$x_j = \cos\left(\frac{(2j-1)}{2n}\pi\right), \quad j = 1, \dots, n.$$

In our case, n=4, and the four Chebyshev nodes are $\cos\left(\frac{\pi}{8}\right), \cos\left(\frac{3\pi}{8}\right), \cos\left(\frac{5\pi}{8}\right), \cos\left(\frac{7\pi}{8}\right)$.

(d) For the Chebyshev nodes, we have $\max_{x \in [-1,1]} |(x-x_1)\cdots(x-x_n)| = \frac{1}{2^{n-1}}$.

In our case, the bound for the error is $\max_{x \in [-1,1]} |f(x) - P(x)| \leqslant \frac{1}{6} \max_{x \in [-1,1]} |(x-x_1) \cdots (x-x_4)| = \frac{1}{6} \cdot \frac{1}{2^3} = \frac{1}{48} \approx 0.0208.$

Problem 4. Suppose that f(x) is a smooth function such that $|f^{(n)}(x)| \le n!$ for all $x \in [-1, 1]$ and all $n \ge 0$. Suppose we approximate f(x) on the interval [-1, 1] by a polynomial interpolation P(x). How many Chebyshev nodes do we need to use in order to guarantee that the maximal error is at most 10^{-6} ?

Solution. We know that, using n Chebyshev nodes, the error is bounded as

$$\max_{x \in [-,1,1]} |f(x) - P_{n-1}(x)| \leq \frac{1}{2^{n-1} n!} \max_{\xi \in [-,1,1]} |f^{(n)}(\xi)| \leq \frac{1}{2^{n-1}}.$$

We need to choose n so that $2^{n-1} \ge 10^6$. Knowing that $2^{10} = 1024 > 10^3$, we see that $2^{20} > 10^6$.

Thus, for n=21 Chebyshev nodes the maximal error is guaranteed to be less than 10^{-6} .

Problem 5. Determine the natural cubic spline through (-3,1), (0,3), (2,1).

Solution. Let us write the spline as $S(x) = \begin{cases} S_1(x), & \text{if } x \in [-3, 0], \\ S_2(x), & \text{if } x \in [0, 2]. \end{cases}$

To simplify our life, we expand both S_i around x = 0 (the middle knot).

$$S_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i.$$

- Note that $d_i = S_i(0)$, $c_i = S_i'(0)$ and $b_i = \frac{1}{2}S_i''(0)$. Because S(x) is C^2 smooth, we have $b_1 = b_2$, $c_1 = c_2$ and $d_1 = d_2$. We simply write b, c and d for these values in the sequel.
- d=3 because $S_1(0)=S_2(0)=3$.
- S(x) further interpolates the other two points, (-3,1) and (2,1), resulting in the following two equations:

$$S_1(-3) = \frac{-27a_1 + 9b - 3c + 3}{S_2(2)} = \frac{8a_2 + 4b + 2c + 3}{S_2(2)} = 1$$

• The natural boundary conditions provide two more equations:

(Note that $S_i^{\prime\prime}(x) = 6a_ix + 2b_i$.)

$$S_1''(-3) = -18a_1 + 2b = 0$$

 $S_2''(2) = 12a_2 + 2b = 0$

We use these last two equations to replace $a_1 = \frac{1}{9}b$ and $a_2 = -\frac{1}{6}b$ in the other two equations in terms of b:

$$\begin{array}{rcl}
-27 \cdot \frac{1}{9}b + 9b - 3c + 3 & = 6b - 3c + 3 = 1 \\
8\left(-\frac{1}{6}b\right) + 4b + 2c + 3 & = \frac{8}{3}b + 2c + 3 = 1
\end{array}$$

Solving these two equations in two unknowns, we find $b = -\frac{1}{2}$ and $c = -\frac{1}{3}$.

Consequently, $a_1 = \frac{1}{9}b = -\frac{1}{18}$ and $a_2 = -\frac{1}{6}b = \frac{1}{12}$.

Hence, the desired natural cubic spline is

$$S(x) = 3 - \frac{1}{3}x - \frac{1}{2}x^2 + x^3 \begin{cases} -\frac{1}{18}, & \text{if } x \in [-3, 0], \\ \frac{1}{12}, & \text{if } x \in [0, 2]. \end{cases}$$

Problem 6. Recall that a cubic spline S(x) through $(x_0, y_0), \ldots, (x_n, y_n)$ with $x_0 < x_1 < \ldots < x_n$ is piecewise defined by n cubic polynomials $S_1(x), \ldots, S_n(x)$ such that $S(x) = S_i(x)$ for $x \in [x_{i-1}, x_i]$. Name three common boundary conditions of cubic splines and state their mathematical definition.

Solution. The following are common choices for the boundary conditions of cubic splines:

- $natural: S''_1(x_0) = S''_n(x_n) = 0$
 - The resulting splines are simply called natural cubic splines.
- not-a-knot: $S_1'''(x_1) = S_2'''(x_1)$ and $S_n'''(x_{n-1}) = S_{n-1}'''(x_{n-1})$
- $periodic: S'_1(x_0) = S'_n(x_n) \text{ and } S''_1(x_0) = S''_n(x_n)$ (only makes sense if $y_0 = y_n$)

There are other common choices such *clamped cubic splines* for which the first derivatives at the endpoints are being set ("clamped") to user-specified values.

Problem 7. Obtain approximations for f'(x) and f''(x) using the values f(x-2h), f(x), f(x+3h) as follows: determine the polynomial interpolation corresponding to these values and then use its derivatives to approximate those of f. In each case, determine the order of the approximation and the leading term of the error.

Solution. We first compute the polynomial p(t) that interpolates the three points (x-2h, f(x-2h)), (x, f(x)), (x+3h, f(x+3h)) using Newton's divided differences:

Hence, reading the coefficients from the top edge of the triangle, the interpolating polynomial is

$$p(t) = f(x) + c_1(t - x + 2h) + c_2(t - x + 2h)(t - x).$$

• (approximating f'(x)) Since $p'(t) = c_1 + c_2(2t - 2x + 2h)$, we have

$$p'(x) = c_1 + 2hc_2 = \frac{f(x) - f(x - 2h)}{2h} + \frac{2f(x + 3h) - 5f(x) + 3f(x - 2h)}{15h}$$
$$= \frac{4f(x + 3h) + 5f(x) - 9f(x - 2h)}{30h}.$$

This is our approximation for f'(x). To determine the order and the error (we expect the error to be of the form $Ch^2 + O(h^3)$ and, since we divide by h, so we expand up to h^3 in the following), we combine

$$\begin{split} f(x+h) &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{f'''(x)}{6}h^3 + O(h^4), \\ f(x-2h) &= f(x) - 2f'(x)h + 2f''(x)h^2 - \frac{4f'''(x)}{3}h^3 + O(h^4), \\ f(x+3h) &= f(x) + 3f'(x)h + \frac{9}{2}f''(x)h^2 + \frac{9f'''(x)}{2}h^3 + O(h^4) \end{split}$$

to find

$$4f(x+3h)+5f(x)-9f(x-2h)=30f'(x)h+30f'''(x)h^3+O(h^4).$$

Hence, dividing by 30h, we conclude that

$$\frac{4f(x+3h)+5f(x)-9f(x-2h)}{30h} = f'(x)+f'''(x)h^2+O(h^3).$$

Consequently, the approximation is of order 2.

• (approximating f''(x)) Since $p''(t) = 2c_2$, we have $p''(x) = 2c_2 = \frac{2f(x+3h) - 5f(x) + 3f(x-2h)}{15h^2}$.

This is our approximation for f''(x). To determine the order and the error, we proceed as before to find

$$2f(x+3h) - 5f(x) + 3f(x-2h) = 15f''(x)h^2 + 5f'''(x)h^3 + O(h^4).$$

Hence, dividing by $15h^2$, we conclude that

$$\frac{2f(x+3h)-5f(x)+3f(x-2h)}{15h^2}=f''(x)+\frac{1}{3}f'''(x)h+O(h^2).$$

Consequently, the approximation is of order 1.

Problem 8. Suppose that $A(\frac{1}{4}) = a$ and $A(\frac{1}{10}) = b$ are approximations of order 4 of some quantity A^* . What is the approximation we obtain from using Richardson extrapolation?

Solution. Since A(h) is an approximation of order 4, we expect $A(h) \approx A^* + Ch^4$ for some constant C.

Correspondingly, $A\left(\frac{1}{4}\right) \approx A^* + \frac{1}{4^4}C$ and $A\left(\frac{1}{10}\right) \approx A^* + \frac{1}{10^4}C$.

Hence,
$$10^4 A(\frac{1}{10}) - 4^4 A(\frac{1}{4}) \approx (10^4 - 4^4) A^*$$
.

The Richardson extrapolation is $\frac{10^4 A \left(\frac{1}{10}\right) - 4^4 A \left(\frac{1}{4}\right)}{10^4 - 4^4} = \frac{10000}{9744} b - \frac{256}{9744} a$.

Problem 9. We have shown that $A(h) = \frac{1}{h^2} [f(x+h) - 2f(x) + f(x-h)]$ is an approximation of f''(x) of order 2.

- (a) Determine the leading term of the error.
- (b) Apply Richardson extrapolation to A(h) and A(3h) to obtain an approximation of f''(x) of higher order.
- (c) Explain in a sentence why the resulting approximation is of order 4 (rather than 3).

Solution.

(a) Our goal is to compute C such that $A(h) = f''(x) + Ch^2 + O(h^3)$. By Taylor's theorem, we have (note that, because we will divide by h^2 , we know from the beginning that we need to compute up to h^4 in the following)

$$\begin{split} f(x+h) &= f(x) + h \, f'(x) + \frac{h^2}{2} \, f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{(4)}(x) + O(h^5), \\ f(x-h) &= f(x) - h \, f'(x) + \frac{h^2}{2} \, f''(x) - \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{(4)}(x) + O(h^5). \end{split}$$

Adding these and subtracting 2f(x), we find

$$f(x+h) - 2f(x) + f(x-h) = h^2 f''(x) + \frac{h^4}{12} f^{(4)}(x) + O(h^5).$$

Hence,
$$A(h) = f''(x) + \frac{h^2}{12}f^{(4)}(x) + O(h^3)$$
.

Comment. By computing one more term, we see that we even have $A(h) = f''(x) + \frac{h^2}{12}f^{(4)}(x) + O(h^4)$.

(b) We just showed that $A(h) = f''(x) + Ch^2 + O(h^3)$ for some constant C (we even determined C but it doesn't matter here). Correspondingly, $A(3h) = f''(x) + 9Ch^2 + O(h^3)$. Hence, $9A(h) - A(3h) = (9-1)f''(x) + O(h^3)$. The Richardson extrapolation of A(h) and A(3h) therefore is:

$$\frac{9A(h) - A(3h)}{8} = \frac{9}{8h^2} [f(x+h) - 2f(x) + f(x-h)] - \frac{1}{8(3h)^2} [f(x+3h) - 2f(x) + f(x-3h)]$$
$$= \frac{1}{72h^2} [-f(x+3h) + 81f(x+h) - 160f(x) + 81f(x-h) - f(x-3h)]$$

This is an approximation of f''(x) of higher order.

Comment. With some more work, we find that the error is $-\frac{1}{40}f^{(6)}(x)h^4 + O(h^6)$ so that this is an approximation of order 4.

(c) In short, this is because our approximation is an even function of h.

Because we started with an approximation of order 2, the Richardson extrapolation of A(h) and A(3h) has at least order 3. However, A(h) is an even function of h (because A(-h) = A(h)). Consequently, A(3h) as well as the extrapolation are even functions of h as well. Therefore, the error, which we know is of the form $Ch^3 + Dh^4 + O(h^5)$, can only feature even powers of h. Thus C = 0 and the error must be of order at least 4.

Problem 10. Use the trapezoidal rule to approximate $\int_0^1 \frac{1}{x^2+1} dx = \frac{\pi}{4}$.

- (a) Use $h = \frac{1}{3}$ and $h = \frac{1}{6}$.
- (b) Using Richardson extrapolation, combine the previous two approximations to obtain an approximation of higher order. What are absolute and relative error?
- (c) The extrapolated approximation is equivalent to the outcome of which method applied with $h = \frac{1}{6}$?

Solution. Let us write $f(x) = \frac{1}{x^2 + 1}$.

(a)
$$h = \frac{1}{3}$$
: $\int_0^1 \frac{1}{x^2 + 1} dx \approx \frac{h}{2} \left[f(0) + 2f\left(\frac{1}{3}\right) + 2f\left(\frac{2}{3}\right) + f(1) \right] = \frac{1}{6} \left[1 + 2 \cdot \frac{9}{10} + 2 \cdot \frac{9}{13} + \frac{1}{2} \right] = \frac{203}{260} \approx 0.7808$

$$h = \frac{1}{6}$$
: $\int_0^1 \frac{1}{x^2 + 1} dx \approx \frac{h}{2} \left[f(0) + 2f\left(\frac{1}{6}\right) + 2f\left(\frac{1}{3}\right) + 2f\left(\frac{1}{2}\right) + 2f\left(\frac{2}{3}\right) + 2f\left(\frac{5}{6}\right) + f(1) \right]$

$$= \frac{1}{12} \left[1 + 2 \cdot \frac{36}{37} + 2 \cdot \frac{9}{10} + 2 \cdot \frac{4}{5} + 2 \cdot \frac{9}{13} + 2 \cdot \frac{36}{61} + \frac{1}{2} \right] = \frac{2,761,249}{3,520,920} \approx 0.7842$$

(b) Let us write $A(h) = \frac{203}{260}$ and $A\left(\frac{h}{2}\right) = \frac{2,761,249}{3,520,920}$ with $h = \frac{1}{3}$ for our two approximations, and A^* for the true value of the integral.

Since A(h) is an approximation of order 2, we expect $A(h) \approx A^* + Ch^2$ for some constant C.

Correspondingly,
$$A\left(\frac{h}{2}\right) \approx A^* + \frac{1}{4}Ch^2$$
. Hence, $4A\left(\frac{h}{2}\right) - A(h) \approx (4-1)A^* = 3A^*$.

Hence, the Richardson extrapolation is
$$R := \frac{1}{3} \left[4A \left(\frac{h}{2} \right) - A(h) \right] = \frac{1}{3} \left[4 \cdot \frac{2,761,249}{3,520,920} - \frac{203}{260} \right] = \frac{829,597}{1,056,276} \approx 0.78539795.$$

Since the exact value is $\frac{\pi}{4} \approx 0.78539816$, the absolute error is $\left|R - \frac{\pi}{4}\right| \approx 2.18 \cdot 10^{-7}$ while the relative error is $\left|\left(R - \frac{\pi}{4}\right) / \left(\frac{\pi}{4}\right)\right| \approx 2.78 \cdot 10^{-7}$.

(Of course, you will not have to calculate with numbers like the above by hand on the exam.)

(c) Simpson's rule