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CSCD37: Assignment #2

1. Recall the full-Newton algorithm for solving the nonlinear system $F(x) = 0; F, x \in \mathcal{R}^n$:

> Generate an initial approximation $\hat{x}_0$
> for $k = 0, 1 \ldots$ until convergence
>   compute $-F(\hat{x}_k)$
>   compute $\frac{\partial F(\hat{x}_k)}{\partial x}$
>   solve $\frac{\partial F(\hat{x}_k)}{\partial x} \Delta_k = -F(\hat{x}_k)$
>   update $\hat{x}_{k+1} = \hat{x}_k + \Delta_k$
> end for

(a) This algorithm is computationally expensive. Give a detailed analysis of the cost using standard big-oh notation. You may use results from CSCC37; e.e., the cost (measuring flops) of the LU-factorization of an $n \times n$ matrix is $(1/3)n^3 + \mathcal{O}(n^2)$.

The following analysis makes the assumption that each component of F can be evaluated in approx 1 flop, and that taking the derivative also takes around 1 flop. For each iteration of the loop, first evaluating the function F at a point $x \in \mathcal{R}^n$ will take n operations. The evaluation of the n derivatives will also take n, so evaluating n derivatives at n points will take n^2 time. Solving the linear system of the derivative matrix against the original function will take around $(1/3)n^3 + \mathcal{O}(n^2)$ as was seen in CSCC37. Finally updating a vector with an addition of 2 n length vectors will simply be n additions. Overall, the entire loop iteration will take $n^2 + n + (1/3)n^3 + \mathcal{O}(n^2) + n = (1/3)n^3 + \mathcal{O}(n^2) = \mathcal{O}(n^3)$ steps per iteration. This cannot be generalized outside of iterations, as convergence is not always guaranteed and k may run on infinitely.

(b) We briefly discussed in lecture the "quasi-Newton algorithm" for solvling nonlinear systems. Modify the algorithm above to take advantage of the optimizations we discussed. You do not need to implement the modifications ... pseudo-code will suffice. Be careful to discuss both flop optimizations and convergence issues ("X-test" and "F-test" tolerance, maximum number of iterations, condition of Jacobian, how long to hold Jacobian fixed, etc.).

2. In lecture we derived the divided-difference (Newton) form of the interpolating polynomial for the simple interpolation problem. This question will investigate how the Newton polynomial can be used for osculatory interpolation.

(a) Prove that

$$\lim_{\substack{x_{i+j} \to x_i \\ 1 \le j \le k}} y[x_{i+k}, x_{i+k-1}, \ldots, x_i] = \frac{y^{(k)}(x_i)}{k!}$$

Provided $y \in \mathcal{C}^k$.

Proof. Examine first, the error formula given in lecture, $E(x) = y(x) - p(x)$ for any polynomial interpolant, then using the Newton polynomial as $p(x)$, it produces:

$$E(x) = y(x) - y[x_i] + (x - x_i)y[x_{i+1}, x_i] + \cdots + (x - x_i)(x - x_{i+1}) \cdots (x - x_{i+k-1})y[x_{i+k}, \ldots, x_i]$$

Knowing that $E(x)$ has $n+1$ distinct roots (at the interpolation constraints), by Rolle's theorem, gives that the kth derivative of $E(x)$ has at least 1 zero $E(\psi)$ where $\psi \in \text{span}\{x_i, \ldots, x_{i+k}\}$. Looking at the Newton polynomial, the kth derivative will only have the leading coefficient times $k!$ since it is a degree k polynomial. This coefficient, from the definition can be seen as $y[x_{i+k}, \ldots, x_i]$

$$\implies \frac{d^k}{dx^k}E(x) = y^{(k)}(x) - y[x_{i+k}, \ldots, x_i]k!$$
$$\frac{d^k}{dx^k}E(\psi) = y^{(k)}(\psi) - y[x_{i+k}, \ldots, x_i]k!$$
$$0 = y^{(k)}(\psi) - y[x_{i+k}, \ldots, x_i]k!$$
$$y[x_{i+k}, \ldots, x_i]k! = y^{(k)}(\psi)$$
$$y[x_{i+k}, \ldots, x_i] = \frac{y^{(k)}(\psi)}{k!}$$
$$\implies \lim_{\substack{x_{i+j} \to x_i \\ 1 \le j \le k}} y[x_{i+k}, \ldots, x_i] = \lim_{\substack{x_{i+j} \to x_i \\ 1 \le j \le k}} \frac{y^{(k)}(\psi)}{k!}$$
$$\implies \lim_{\substack{x_{i+j} \to x_i \\ 1 \le j \le k}} y[x_{i+k}, \ldots, x_i] = \frac{y^{(k)}(x_i)}{k!}$$

The last line is since if $\forall x_{i+j}, |x_{i+j} - x_i| < \varepsilon \implies \text{span}\{x_i, \ldots, x_{i+k}\} \subset (x_i - \varepsilon, x_i + \varepsilon) \implies \psi \to x_i$.

$\square$

(b) The result in (a) tells us that divided differences can be replaced with derivatives as data points coincide. Using this result, construct a divided difference table to find the coefficients of the Newton polynomial of degree 6 or less that satisfies the following interpolation conditions:

$$\begin{array}{llll} p(-1) = 4 & p(0) = 7 & p(1) = 28 & p(2) = 247 \\ & p'(0) = 6 & p'(1) = 56 & \\ & & p''(1) = 140 & \end{array}$$

$$
\begin{array}{ll}
x_0 & y(x_0) \\
& \qquad y[x_1, x_0] \\
x_1 & y(x_1) \qquad\qquad\qquad\quad y[x_1, x_1, x_0] \\
& \qquad y[x_1, x_1] \qquad\qquad\qquad y[x_2, x_1, x_1, x_0] \\
x_1 & y(x_1) \qquad\quad y[x_2, x_1, x_1] \qquad\qquad\qquad\quad y[x_2, x_2, x_1, x_1, x_0] \\
& \qquad y[x_2, x_1] \qquad\qquad\qquad y[x_2, x_2, x_1, x_1] \qquad\qquad\qquad\quad y[x_2, x_2, x_2, x_1, x_1, x_0] \\
x_2 & y(x_2) \qquad\quad y[x_2, x_2, x_1] \qquad\qquad\qquad\quad y[x_2, x_2, x_2, x_1, x_1] \qquad\qquad\qquad y[x_3, \ldots x_0] \\
& \qquad y[x_2, x_2] \qquad\qquad\qquad y[x_2, x_2, x_2, x_1] \qquad\qquad\qquad\quad y[x_3, x_2, x_2, x_2, x_1, x_1] \\
x_2 & y(x_2) \qquad\quad y[x_2, x_2, x_2] \qquad\qquad\qquad\quad y[x_3, x_2, x_2, x_2, x_1] \\
& \qquad y[x_2, x_2] \qquad\qquad\qquad y[x_3, x_2, x_2, x_2] \\
x_2 & y(x_2) \qquad\quad y[x_3, x_2, x_2] \\
& \qquad y[x_3, x_2] \\
x_3 & y(x_3)
\end{array}
$$

$$
\begin{array}{ll}
-1 & 4 \\
& \qquad 3 \\
0 & 7 \qquad\qquad\quad 3 \\
& \qquad 6 \qquad\qquad\qquad 6 \\
0 & 7 \qquad\qquad 15 \qquad\qquad\quad 7 \\
& \qquad 21 \qquad\qquad 20 \qquad\quad 4 \\
1 & 28 \qquad\qquad 35 \qquad\qquad 15 \qquad 1 \\
& \qquad 56 \qquad\qquad 35 \qquad\quad 7 \\
1 & 28 \qquad\qquad 70 \qquad\qquad 29 \\
& \qquad 56 \qquad\qquad 93 \\
1 & 28 \qquad\qquad 163 \\
& \qquad 219 \\
2 & 247
\end{array}
$$

$$\implies p(x) = 4+3(x+1)+3(x+1)x+6(x+1)x^2+7(x+1)x^2(x-1)+4(x+1)x^2(x-1)^2+(x+1)x^2(x-1)^3$$

$$\iff p(x) = x^6 + 2x^5 + 3x^4 + 4x^3 + 5x^2 + 6x + 7$$

(c) Use the Method of Undetermined Coefficients (i.e., as discussed in lecture, construct and solve an appropriate Vandermonde system) to find the coefficients of the monomial-basis polynomial of degree 6 or less that satisfies the interpolation conditions specified in (b). You may use *MatLab* for this question if you wish. Verify that you have obtained the same polynomial as in (b).

```matlab
1    size = 7;
2    vandermonde = zeros(size);
3    coeff1 = 0:(size-1);
4    coeff2 = [0,0,2,3*2,4*3,5*4,6*5];
5    powers0 = 0:(size-1);
6    powers1 = [0,0:(size-2)];
7    powers2 = [0,0,0:(size-3)];
8    x = [-1,0,1,2];
9    vandermonde(1,:) = x(1).^powers0;
10   vandermonde(2,:) = x(2).^powers0;
11   vandermonde(3,:) = (x(2).^(powers1)).*coeff1;
12   vandermonde(4,:) = x(3).^powers0;
13   vandermonde(5,:) = (x(3).^(powers1)).*coeff1;
14   vandermonde(6,:) = (x(3).^(powers2)).*coeff2;
15   vandermonde(7,:) = x(4).^powers0;
16   y = [4 7 6 28 56 140 247];
17   soln = vandermonde\y';
```

Command Window

```
Trial>> soln

soln =

    7.0000
    6.0000
    5.0000
    4.0000
    3.0000
    2.0000
    1.0000

fx Trial>> |
```

3. Consider the function $y \in \mathcal{C}^{n+1}$ and the polynomial $p \in \mathcal{P}_n$ which satisfies

$$p^{(j)}(x_i) = y^{(j)}(x_i); \ j = 0, \ldots, j_i; \ i = 0, \ldots, k; \ \sum_{i=0}^{k}(j_i + 1) = n + 1;$$

with all of the x_i distinct. The error in this polynomial interpolant is given by

$$E(x) = y(x) - p(x) = \frac{y^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{j_0+1}(x - x_1)^{j_1+1}\cdots(x - x_k)^{j_k+1} \qquad (1)$$

where $\xi \in \text{span}\{x_0, \ldots, x_k, x\} = [\min\{x_0, \ldots, x_k, x\}, \max\{x_0, \ldots, x_k, x\}]$ provided $y \in \mathcal{C}^{n+1}$ on $\text{span}\{x_0, \ldots, x_k, x\}$.

This is a fundamental formula in Numerical Aprroximation. The following is an outline of a possible derivation of (1). In this question you will expand this outline by proving certain key statements.

If $x = x_i$, $i = 0, \ldots, k$, then $y(x) - p(x) = 0$ since p interpolates y at these $k+1$ points. Also, $E(x_i) = 0$ in (1) since $(x_i - x_i)^{j_1+1} = 0$. Therefore, (1) holds when $x = x_i$.

Now assume $x \neq x_i$ for any $i = 0, \ldots, k$ and consider x *fixed*. Let $F(t) = y(t) - p(t) - CW(t)$ where $C = [y(x) - p(x)]/W(x)$ is a constant and

$$W(t) = (t - x_0)^{j_0+1}(t - x_1)^{j_1+1}\cdots(t - x_k)^{j_k+1} \qquad (2)$$

is a polynomial of degree $n + 1$. Clearly $F(x) = 0$, and also

$$F^{(j)}(x_i) = 0; \ j = 0, \ldots, j_i; \ i = 0, \ldots, k. \qquad (3)$$

Therefore, counting multiplicities, $F(t)$ has at least $n + 2$ zeros in $\text{span}\{x_0, \ldots, x_k, x\}$, which implies $F^{(n+1)}(t)$ has at least 1 zero in $\text{span}\{x_0, \ldots, x_k, x\}$, or, in other words,

$$F^{(n+1)}(\xi) = 0, \xi \in \text{span}\{x_0, \ldots, x_k, x\}. \qquad (4)$$

But

$$F^{(n+1)}(t) = \frac{d^{n+1}}{dt^{n+1}}[y(t) - p(t) - CW(t)] = y^{(n+1)}(t) - (n+1)!C. \qquad (5)$$

Therefore,

$$F^{(n+1)}(\xi) = 0 \implies y^{(n+1)}(\xi) - (n+1)!C = 0 \implies C = \frac{y^{(n+1)}(\xi)}{(n+1)!}.$$

But

$$C = \frac{y(x) - p(x)}{W(x)} \implies y(x) - p(x) = \frac{y^{(n+1)}(\xi)}{(n+1)!}W(x).$$

Now for the statements you must prove:

(a) Prove that $W(t)$ in (2) is a polynomial of degree $n + 1$.

Proof. Polynomials are closed under exponentiation and basic operations, so it is sufficient to show the highest power to be $n + 1$. For each term $(t - x_i)^{j_i+1}$, the highest power of t is $j_i + 1$ respectively using the Binomial Theorem. This means that the final product will highest power of all of these terms together, so the power will be $\sum_{i=0}^{k} j_i + 1 = n + 1$ by definition. $\qquad \square$

(b) Prove (3)

Proof. We know that p must approximate y exactly at the interpolation points, so evidently for a point on the jth derivative, $y^{(j)}(x_i) - p^{(j)}(x_i)$ will be 0. For the other term $CW(t)$, taking the derivative only j times will result in the term $(x - x_i)$ to show up in every term generated by the product rule since it has power of $(j_i + 1)$, hence $W(t)$ will also be 0 making $F^{(j)}(x_i) = 0$ at all interpolation points. $\qquad \square$

(c) Explain how (4) follows from $F(t)$ having at least $n+2$ zeros in $\text{span}\{x_0,\ldots,x_k\}$.

Lemma. *Counting multiplicities, if $F(t)$ is C^1 over $\text{span}\{x_0,\ldots,x_k\}$ has at least k zeros in $\text{span}\{x_0,\ldots,x_k\}$ then $F'(t)$ has at least $k-1$ zeros in $\text{span}\{x_0,\ldots,x_k\}$.*

Proof. Suppose the distinct roots of $F(t)$ are ordered as $a_1 < a_2 < \cdots < a_s$ with multiplicities $m(a_i)$ such that $\sum_{i=0}^{s} m(a_i) = n$. From Rolle's Theorem, we have that there is some $\rho \in (a_i, a_{i+1})$, $1 \le i < s$ where $F'(\rho) = 0$ immediately giving us $s-1$ roots in the derivative. Now counting the multiplicities of the previous roots, we get that there are $\sum_{i=0}^{s}(m(a_i)-1)$ more roots, which summing together gives $\sum_{i=0}^{s} m(a_i) - s + (s-1) = n-1$ roots, which are all in the span. $\qquad\square$

From this, it follows immediately that taking $n+1$ derivatives of a function with $n+2$ roots will have one root in the same span.

(d) Prove (5).

Proof. Since p is a polynomial of degree n, taking $n+1$ derivatives will immediately cause it to vanish. On the otherhand, for $W(t)$, we know it is a polynomial of degree $n+1$ from (a), so taking the $(n+1)$th derivative gives us the leading coefficient times $(n+1)!$. Looking back at how $W(t)$ is setup though, since none of the t in each binomial term have any coefficient the resulting expanded polynomials leading coefficient will be 1. This means the $(n+1)$th derivative of $CW(t)$ is just $C(n+1)!$.

$$\implies F^{(n+1)}(t) = \frac{d^{n+1}}{dt^{n+1}}[y(t) - p(t) - CW(t)]$$
$$= \frac{d^{n+1}}{dt^{n+1}}y(t) - \frac{d^{n+1}}{dt^{n+1}}p(t) - \frac{d^{n+1}}{dt^{n+1}}CW(t)$$
$$= y^{(n+1)}(t) - (n+1)!C.$$

$\qquad\square$

4. In lecture we proved that the roots of the Chebyshev polynomial
$$T_k(x) = \cos(k \cos^{-1}(x)), k = 0, 1, \ldots \tag{6}$$
are the optimal interpolation points on [-1,1].

(a) Prove that (6) is a polynomial of degree k for all $k \geq 0$.

Proof. For the case of $k = 0, 1$, we have that
$$\cos(k \arccos(x))|_{k=0} = \cos(0) = 1$$
$$\cos(k \arccos(x))|_{k=1} = \cos(\arccos x) = x$$

So these cases hold. Using induction, assume that $T_n(x)$ is a polynomial for $n < k$, then there are two inductive cases:

First $k = 2t$ is even
$$\cos(k \arccos(x)) = \cos(2(t \arccos(x)))$$
$$= 2(\cos(t \arccos(x)))^2 - 1 \text{ [Double angle identity]}$$
$$= 2(T_t(x))^2 - 1$$

This is again a polynomial since T_t is one by IH, so this case holds.

Second $k = 2t + 1$ is odd
$$\cos(k \arccos(x)) = \cos(2(t \arccos(x)) + \arccos(x))$$
$$\overset{\text{angle sum}}{=} \cos(2t \arccos(x))(\cos(\arccos(x))) - \sin(2t \arccos(x))(\sin(\arccos(x)))$$
$$= xT_{2t}(x) - \sin(2t \arccos(x))(\sin(\arccos(x)))$$
$$\overset{\text{double angle}}{=} xT_{2k}(x) - 2\cos(t \arccos(x)) \sin(t \arccos(x))(\sin(\arccos(x)))$$
$$= xT_{2t}(x) - 2T_t(x) \sin(t \arccos(x))(\sin(\arccos(x)))$$
$$\overset{\text{angle prod}}{=} xT_{2k}(x) - T_t(x)(\cos((t-1) \arccos(x)) - \cos((t+1) \arccos(x)))$$
$$= xT_{2t}(x) - T_t(x)(T_{t-1} - T_{t+1})$$

Which is again a polynomial all the lower degrees of T are polynomials by IH, so both cases hold. □

(b) Derive the leading coefficient of (6) (i.e., the coefficient of x^k).
The coefficient is 2^{k-1} for $k \geq 1$ and 1 for $k = 0$.

Proof. Again, using induction, the case of 1 and 0 are trivial, as $T_0(x) = 1$ and $T_1(x) = x$. For the inductive case, consider again even and odd, and assume that it holds for $n < k$.
For $k = 2t$ even, the leading coefficient $\mathcal{LC}(T_k)$:
$$\mathcal{LC}(T_k) = 2\mathcal{LC}(T_t)^2 \text{ From the recurrence in (a)}$$
$$= 2(2^{t-1})^2 = 2(2^{2t-2}) = 2^{k-1} \text{ By IH}$$

For $k = 2t + 1$ odd,
$$\mathcal{LC}(T_k) = \mathcal{LC}(T_{k-1}) + \mathcal{LC}(T_t)\mathcal{LC}(T_{t+1}) \text{ From the other recurrence in (a)}$$
$$= 2^{k-2} + (2^{t-1})(2^t) \text{ From IH}$$
$$= 2^{k-2} + 2^{2t-1}$$
$$= 2^{k-2} + 2^{k-2} = 2^{k-1}$$

□

(c) Derive the roots of (6) (i.e., the so-called Chebyshev points).

The roots for a polynomial of degree k are $x_i = \cos(\frac{(2i+1)\pi}{2k})$ where $i = 0, \ldots k - 1$.

Proof. Given the definition for T_k, plugging in x_i gives

$$\cos(k \arccos(x_i)) = \cos(k \arccos(\cos\left(\frac{(2i+1)\pi}{2k}\right)))$$
$$= \cos\left(k \frac{(2i+1)\pi}{2k}\right)$$
$$= \cos\left(\frac{(2i+1)\pi}{2}\right)$$
$$= 0 \text{ When } i \in \mathbb{N}$$

□

(d) Complete the proof showing why the Chebyshev points are optimal.

Since the Chebyshev polynomial is infact a polynomial, with coefficient 2^{k-1}, we can write it out as $2^{k-1}(x - x_1)(x - x_2) \cdots (x - x_k)$, where x_i, $1 \le i \le k$ are the roots of x_i. It can also be converted to a monic polyomial by dividing by 2^{k-1}. Note that it is also bound between -1 and 1 because of the cos definition of T_k To show that they are optimal, we prove the following:

Theorem. *If $W(x)$ is a monic polynomial of degree $\le k$, then $\max_x |W(x)| \ge \max_x \left|\frac{T_k(x)}{2^{k-1}}\right| = \frac{1}{2^{k-1}}$*

Proof. Suppose $\max_x |W(x)| < \max_x \left|\frac{T_k(x)}{2^{k-1}}\right|$, then in particular $|W(y_i)| < \left|\frac{T_k(y_i)}{2^{k-1}}\right| = \frac{1}{2^{k-1}}$ where $y_i = \cos(\frac{i\pi}{k})$ since looking at the definition of T_k these are the absolute maximums, specifically

$$T_k(y_i) = \begin{cases} 1 & i \text{ even} \\ -1 & i \text{ odd} \end{cases}$$

□

Now consider the polynomial $q(x) = \frac{T_k(x)}{2^{k-1}} - W(x)$ which is in $\mathcal{P}_{k-1}$ since both polynomials are monic, hence the highest power will cancel. Now look at what happens in the case of plugging in y_i. So

$$q(y_i) = \frac{T_k(y_i)}{2^{k-1}} - W(y_i) = \begin{cases} > 0 & i \text{ even} \\ < 0 & i \text{ odd} \end{cases}$$

This is the case, since at even points T_k is positive, and the absolute value of W is less then $T_k/2^{k-1}$ so it could not possibly subtract more then 1. Likewise for the i odd case it cannot add enough since the absolute value is less than $T_k/2^{k-1}$. This means that $q(x)$ has a root in each interval $[y_i, y_{i+1}]$ for $i = 0, \ldots, k-1$ so q has k roots, but $q \in \mathcal{P}_{k-1}$ so $q = 0$, so $\frac{T_k(x)}{2^{k-1}} - W(x) = 0$, which is a contradiction to our assumption. Hence, $\frac{T_k(x)}{2^{k-1}}$ is the smallest possible polynomial that W could be, so using the Chebyshev points will make W optimal.