Final Review

Igor Yanovsky (Math 151A TA)

1 Root-Finding Methods

Rootfinding methods are designed to find a zero of a function f, that is, to find a value of x such that

$$f(x) = 0.$$

1.1 Bisection Method

To apply Bisection Method, we first choose an interval $[a, b]$ where $f(a)$ and $f(b)$ are of different signs. We define a midpoint

$$p = \frac{a+b}{2}.$$

If $f(p) = 0$, then p is a root and we stop.
Else if $f(a)f(p) < 0$, then a root lies in $[a, p]$, and we assign $b = p$. Otherwise, $a = p$.
We then consider this new interval $[a, b]$, and repeat the procedure.

The formula for midpoint above generates values p_n. We can bound an error of each iterate p_n for the bisection method:

$$|p_n - p| = \frac{b-a}{2^n}.$$

Note, as $n \to \infty$, $p_n \to p$.

Practice Problem: The function $f(x) = \sin x$ satisfies $f(-\pi/2) = -1$ and $f(\pi/2) = 1$. Using bisection method, how many iterations are needed to find an interval of length at most 10^{-4} which contains a root of a function?

Solution: We need to find n such that:

$$\frac{b-a}{2^n} \le 10^{-4}.$$

We have

$$\frac{\pi}{2^n} \le 10^{-4}.$$

$$\begin{aligned} 2^n &\ge \frac{\pi}{10^{-4}}, \\ 2^n &\ge \pi 10^4, \\ n \log 2 &\ge \log(\pi 10^4), \\ n &\ge \frac{\log\left(\pi 10^4\right)}{\log 2} = 14.94. \end{aligned}$$

That is, $n = 15$ iterations are needed to find an interval of length at most 10^{-4} which contains the root.
See Problems 1 and 3 in Homework 1 for other examples of bisection method.

1.2 Newton's Method

The Newton's iteration is defined as:

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}.$$

The iteration converges for smooth functions if $f'(p_0) \neq 0$ and $|p - p_0|$ is small enough.

Practice Problem: Consider the equation $x = x^2 + 5$. Write down an algorithm based on Newton's method to solve this equation.

Solution: We define $f(x) = x^2 - x + 5$, and we want to find x such that $f(x) = 0$. We have

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^2 - x_n + 5}{2x_n - 1}.$$

This equation can be and should be simplified further.

Practice Problem: What is the order of convergence of Newton's method?

Solution: Newton's method is quadratically convergent (second order of convergence), which means that

$$|x^* - x_{n+1}| \leq C|x^* - x_n|^2.$$

Practice Problem: Suppose $g(x)$, a smooth function, has a fixed point x^*; that is $g(x^*) = x^*$. Write a Taylor expansion of $g(x_n)$ around x^*.
Solution:

$$g(x_n) = g(x^*) + (x_n - x^*)g'(x^*) + \frac{(x_n - x^*)^2}{2}g''(\xi_n).$$

We can use the information that is given to us by the problem. A fixed point iteration is defined as $x_{n+1} = g(x_n)$. Also, $g(x^*) = x^*$. Using this, we can rewrite the equation as

$$x_{n+1} = x^* + (x_n - x^*)g'(x^*) + \frac{(x_n - x^*)^2}{2}g''(\xi_n),$$

or

$$x_{n+1} - x^* = (x_n - x^*)g'(x^*) + \frac{(x_n - x^*)^2}{2}g''(\xi_n).$$

Quite a few observations can be made using this equation if additional information is given by a problem.

1.3 Secant Method

The Secant method is derived from Newton's method by replacing $f'(p_{n-1})$ with the following approximation:

$$f'(p_{n-1}) \approx \frac{f(p_{n-2}) - f(p_{n-1})}{p_{n-2} - p_{n-1}}.$$

Then, the Newton's iteration can be rewritten as follows. This iteration is called the Secant method.

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-2} - p_{n-1})}{f(p_{n-2}) - f(p_{n-1})}.$$

2 Computer Arithmetic

Given a *binary number* (also known as a *machine number*), for example

$$\underbrace{0}_{s}\ \underbrace{10000001010}_{c}\ \underbrace{10010011000000\cdots0}_{f}$$

a *decimal number* (also known as a *floating-point decimal number*) is of the form:

$$(-1)^s 2^{c-1023}(1+f). \tag{1}$$

Therefore, in order to find a decimal representation of a binary number, we need to find s, c, and f and plug these into (1).
Problems 3 and 4 in Homework 3 are good applications of this idea. If you understand how to do such problems, consider a similar problem below.

Practice Problem: Consider a *binary number* (also known as a *machine number*)

$$0\ 10000001010\ 10010011000000\cdots00$$

Find the floating point decimal number it represents as well as the next largest floating point decimal number.

Solution: A *decimal number* (also known as a *floating-point decimal number*) is of the form:

$$(-1)^s 2^{c-1023}(1+f).$$

Therefore, in order to find a decimal representation of a binary number, we need to find s, c, and f.
The leftmost bit is zero, i.e. $s = 0$, which indicates that the number is positive.
The next 11 bits, 10000001010, giving the characteristic, are equivalent to the decimal number:

$$\begin{aligned} c &= 1\cdot 2^{10} + 0\cdot 2^9 + \cdots + 0\cdot 2^4 + 1\cdot 2^3 + 0\cdot 2^2 + 1\cdot 2^1 + 0\cdot 2^0 \\ &= 1024 + 8 + 2 \ = \ 1034. \end{aligned}$$

The exponent part of the number is therefore $2^{1034-1023} = 2^{11}$.
The final 52 bits specify that the mantissa is

$$f = 1\cdot\left(\frac{1}{2}\right)^1 + 1\cdot\left(\frac{1}{2}\right)^4 + 1\cdot\left(\frac{1}{2}\right)^7 + 1\cdot\left(\frac{1}{2}\right)^8.$$

Therefore, this binary number represents the decimal number

$$\begin{aligned} (-1)^s 2^{c-1023}(1+f) &= (-1)^0\cdot 2^{1034-1023}\cdot\left(1+\left(\frac{1}{2}\right)^1+\left(\frac{1}{2}\right)^4+\left(\frac{1}{2}\right)^7+\left(\frac{1}{2}\right)^8\right) \\ &= 2^{11}\cdot\left(1+\left(\frac{1}{2}\right)^1+\left(\frac{1}{2}\right)^4+\left(\frac{1}{2}\right)^7+\left(\frac{1}{2}\right)^8\right) \\ &= 2^{11}+2^{10}+2^7+2^4+2^3. \end{aligned}$$

It won't be necessary to further simplify this number on the test.

The next largest machine number is

$$0\ 10000001010\ 10010011000000\cdots01\ .$$

We already know that $s = 0$ and $c = 1034$ for this number. We find f:

$$f = 1\cdot\left(\frac{1}{2}\right)^1 + 1\cdot\left(\frac{1}{2}\right)^4 + 1\cdot\left(\frac{1}{2}\right)^7 + 1\cdot\left(\frac{1}{2}\right)^8 + 1\cdot\left(\frac{1}{2}\right)^{52}.$$

Therefore, this binary number represents the decimal number

$$\begin{aligned} (-1)^s 2^{c-1023}(1+f) &= 2^{11}\left(1+\left(\frac{1}{2}\right)^1+\left(\frac{1}{2}\right)^4+\left(\frac{1}{2}\right)^7+\left(\frac{1}{2}\right)^8+\left(\frac{1}{2}\right)^{52}\right) \\ &= 2^{11}+2^{10}+2^7+2^4+2^3+\left(\frac{1}{2}\right)^{41}. \end{aligned}$$

It won't be necessary to further simplify this number on the test.
Note how these two numbers differ.

3 Interpolation

3.1 Lagrange Polynomials

We can construct a polynomial of degree at most n that passes through $n+1$ points:

$$(x_0, f(x_0)),\ (x_1, f(x_1)),\ \ldots,\ (x_n, f(x_n)).$$

Such polynomial is unique.

Linear (first order) interpolation is achieved by constructing the Lagrange polynomial P_1 of order 1, connecting the two points. We have:

$$P_1(x) = L_0(x)f(x_0) + L_1(x)f(x_1),$$

where [1]

$$L_0(x) = \frac{x - x_1}{x_0 - x_1},$$
$$L_1(x) = \frac{x - x_0}{x_1 - x_0}.$$

Quadratic (second order) interpolation is achieved by constructing the Lagrange polynomial P_2 of order 2, connecting the three points. We have:

$$P_2(x) = L_0(x)f(x_0) + L_1(x)f(x_1) + L_2(x)f(x_2),$$

where

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)},$$
$$L_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)},$$
$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}.$$

In general, to construct a polynomial of order n, connecting $n+1$ points, we have

$$P_n(x) = L_0(x)f(x_0) + L_1(x)f(x_1) + \ldots + L_n(x)f(x_n),$$

where

$$L_k(x) = \frac{(x - x_0)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_n)}{(x_k - x_0)\cdots(x_k - x_{k-1})(x_k - x_{k+1})\cdots(x_k - x_n)}.$$

L_k are called the $k-$Lagrange basis functions.

[1] Note that in some sources, $L_{n,k}$ notation is used for functions below, where n designates the order of polynomial. To avoid confusion, I omit n-index since it is usually obvious what order of the polynomial we are considering. I write those functions as L_k.

3.2 Newton's Divided Differences

The polynomial of degree n, interpolating $n+1$ points, can be written in terms of Newton's divided differences:

$$\begin{aligned} P_n(x) &= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &+ \ldots + f[x_0, x_1, \ldots, x_n](x - x_0)(x - x_1) \cdots (x - x_{n-1}). \end{aligned}$$

The zeroth divided difference of f with respect to x_i is

$$f[x_i] = f(x_i).$$

The first divided difference of f with respect to x_i and x_{i+1} is

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}.$$

The second divided difference is

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}.$$

3.3 Error Analysis

Rolle's Theorem:
If $f \in C^1[a,b]$ has two roots x_0 and x_1 in $[a,b]$, then there exists $a < \xi < b$ s.t. $f'(\xi) = 0$.
If $f \in C^2[a,b]$ has three roots x_0, x_1, x_2 in $[a,b]$, then there exists $a < \xi < b$ s.t. $f''(\xi) = 0$.
If $f \in C^n[a,b]$ has $n+1$ roots, $x_0, \ldots, x_n$ in $[a,b]$, then there exists $a < \xi < b$ s.t. $f^n(\xi) = 0$.

Theorem: Suppose $x_0, x_1, \ldots, x_n$ be $n+1$ distinct numbers in the interval $[a,b]$ and $f \in C^{n+1}[a,b]$. Then, for each $x \in [a,b]$, there exists ξ such that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n),$$

where $p_n(x)$ is the Lagrange interpolating polynomial.

Proof: We introduce the function $G(x)$ defined as

$$G(t) = \big[f(x) - p_n(x)\big](t-x_0)\cdots(t-x_n) - \big[f(t) - p_n(t)\big](x-x_0)\cdots(x-x_n). \quad \circledast$$

Note that

$$\begin{aligned} G(x_0) &= 0, \\ G(x_1) &= 0, \\ &\cdots \\ G(x_n) &= 0, \end{aligned}$$

and

$$G(x) = 0.$$

Thus, G has $n+2$ distinct zeros. Thus, by Rolle's theorem, there exists $\xi \in [a,b]$ such that $\frac{d^{(n+1)}G}{dt^{(n+1)}}(\xi) = 0$. Differentiating equations $\circledast$ $n+1$ times with respect to t, we therefore obtain

$$G^{(n+1)}(t) = \big[f(x) - p_n(x)\big](n+1)! - \big[f^{(n+1)}(t) - p_n^{(n+1)}(t)\big](x-x_0)\cdots(x-x_n).$$

Since $p_n(x)$ is a polynomial of degree n, we obtain $p_n^{(n+1)} = 0$. Thus,

$$G^{(n+1)}(t) = \big[f(x) - p_n(x)\big](n+1)! - f^{(n+1)}(t)(x-x_0)\cdots(x-x_n).$$

Evaluating this expression at $t = \xi$, we get

$$0 = \big[f(x) - p_n(x)\big](n+1)! - f^{(n+1)}(\xi)(x-x_0)\cdots(x-x_n),$$

or

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)\cdots(x-x_n). \quad \checkmark$$

4 Differentiation

Practice Problem: Show that

$$f''(x_0) = \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi),$$

for some ξ lying in between x_0-h and x_0+h.

Solution: Using Taylor expansion, we obtain

$$\begin{aligned} f(x_0+h) &= f(x_0)+hf'(x_0)+\frac{h^2}{2}f''(x_0)+\frac{h^3}{6}f'''(x_0)+\frac{h^4}{24}f^{(4)}(\xi_1), \\ f(x_0-h) &= f(x_0)-hf'(x_0)+\frac{h^2}{2}f''(x_0)-\frac{h^3}{6}f'''(x_0)+\frac{h^4}{24}f^{(4)}(\xi_{-1}). \end{aligned}$$

Then,

$$f(x_0+h)+f(x_0-h) = 2f(x_0)+h^2f''(x_0)+\frac{h^4}{12}f^{(4)}(\xi),$$

or

$$f(x_0+h)-2f(x_0)+f(x_0-h) = h^2f''(x_0)+\frac{h^4}{12}f^{(4)}(\xi),$$

$$f''(x_0) = \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi). \quad \checkmark$$

Note that we could do this problem differently.
Consider the expression

$$f''(x_0) = af(x_0-h)+bf(x_0)+cf(x_0+h).$$

We will expand the right hand side in a Taylor polynomial. Then, we will equate coefficients to obtain a, b, c.

$$\begin{aligned} f''(x_0) &= a\Big[f(x_0)-hf'(x_0)+\frac{h^2}{2}f''(x_0)-\frac{h^3}{6}f'''(x_0)+\frac{h^4}{24}f^{(4)}(\xi_1)\Big] \\ &+ b\Big[f(x_0)\Big] \\ &+ c\Big[f(x_0)+hf'(x_0)+\frac{h^2}{2}f''(x_0)+\frac{h^3}{6}f'''(x_0)+\frac{h^4}{24}f^{(4)}(\xi_2)\Big] \\ &= (a+b+c)\,f(x_0) \;+\; (-a+c)\,h\,f'(x_0) \;+\; (a+c)\,\frac{h^2}{2}\,f''(x_0) \\ &+ \big(-a+c\big)f'''(x_0)\,\frac{h^3}{6} \;+\; \big(af^{(4)}(\xi_1)+cf^{(4)}(\xi_2)\big)\,\frac{h^4}{24}. \end{aligned}$$

Since we have 3 unknowns, we consider the first 3 equations:

$$\begin{aligned} a+b+c &= 0, \\ -a+c &= 0, \\ a+c &= \frac{2}{h^2}. \end{aligned}$$

Solving this linear system, we obtain coefficients $a=\frac{1}{h^2}$, $b=-\frac{2}{h^2}$, $c=\frac{1}{h^2}$, and thus,

$$f''(x_0) = \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} + O(h),$$

where $O(h) = \big(-a+c\big)f'''(x_0)\,\frac{h^3}{6} \;+\; \big(af^{(4)}(\xi_1)+cf^{(4)}(\xi_2)\big)\,\frac{h^4}{24}$.
However, for such values of a, b, c, we have
$\big(-a+c\big)f'''(x_0)\,\frac{h^3}{6} \;+\; \big(af^{(4)}(\xi_1)+cf^{(4)}(\xi_2)\big)\,\frac{h^4}{24} \;=\; \big(f^{(4)}(\xi_1)+f^{(4)}(\xi_2)\big)\,\frac{h^4}{24} \;=\; f^{(4)}(\xi)\,\frac{h^2}{12}$,
and therefore,

$$f''(x_0) \quad = \quad \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} \;+\; \frac{h^2}{12}f^{(4)}(\xi). \quad \checkmark$$

Note that it is not important which sign we have in front of the error term. The important thing is the order of truncation and truncation constant.

Also, study homework 5 problems.

5 Integration

Practice Problem: Derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$.

Solution: We derive the Trapezoidal rule using the **Lagrange polynomial** method. We consider the linear Lagrange polynomial.
Let $x_0 = a$, $x_1 = b$, and $h = b - a$.

$$\begin{aligned}
\int_{a=x_0}^{b=x_1} f(x)\,dx &= \int_{x_0}^{x_1} P_1(x)\,dx \;+\; \frac{1}{2}\int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)\,dx \\
&= \int_{x_0}^{x_1} \left[\frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1)\right] dx \;+\; \frac{1}{2}\int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)\,dx \\
&= \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1)\right]_{x_0}^{x_1} + \frac{1}{2} f''(\xi)\int_{x_0}^{x_1} (x-x_0)(x-x_1)\,dx \\
&= -\frac{(x_0-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x_1-x_0)^2}{2(x_1-x_0)} f(x_1) + \frac{1}{2} f''(\xi)\Big(-\frac{h^3}{6}\Big) \\
&= \frac{h}{2}\Big[f(x_0) + f(x_1)\Big] - \frac{h^3}{12} f''(\xi).
\end{aligned}$$

Thus, the Trapezoidal rule is

$$\boxed{\int_a^b f(x)\,dx \;=\; \frac{h}{2}\Big[f(a) + f(b)\Big] - \frac{h^3}{12} f''(\xi) \;\approx\; \frac{b-a}{2}\Big[f(a) + f(b)\Big].}$$

Since the error term for the Trapezoidal rule involves f'', the rule gives the exact result when applied to any function whose second derivative is identically zero. That is, the Trapezoidal rule gives the exact result for polynomials of degree up to or equal to one.

Practice Problem: Let $\theta \in (0,1)$. Determine constants a, b, c so that the quadrature formula

$$\int_0^1 f(x)\,dx \quad \approx \quad af(0) + bf(\theta) + cf(1),$$

is exact for all polynomials of degree at most 2.

Solution: We want the formula

$$\int_0^1 f(x)\,dx \quad = \quad af(0) + bf(\theta) + cf(1),$$

to hold for polynomials $1, x, x^2$. Plugging these into the formula, we obtain:

$$\begin{aligned}
f(x) = x^0 \qquad & \int_0^1 1\,dx = x\big|_0^1 = 1 &&= a\cdot 1 + b\cdot 1 + c\cdot 1,\\
f(x) = x^1 \qquad & \int_0^1 x\,dx = \frac{x^2}{2}\Big|_0^1 = \frac{1}{2} &&= a\cdot 0 + b\cdot\theta + c\cdot 1,\\
f(x) = x^2 \qquad & \int_0^1 x^2\,dx = \frac{x^3}{3}\Big|_0^1 = \frac{1}{3} &&= a\cdot 0^2 + b\cdot\theta^2 + c\cdot 1^2.
\end{aligned}$$

We have 3 equations:

$$\begin{aligned}
a + b + c &= 1,\\
b\theta + c &= \frac{1}{2},\\
b\theta^2 + c &= \frac{1}{3}.
\end{aligned}$$

After some manipulations, we obtain the following expressions for a, b, c in terms of θ:

$$a = \frac{-1+3\theta}{6\theta}, \qquad b = \frac{1}{6\theta(1-\theta)}, \qquad c = \frac{2-3\theta}{6(1-\theta)},$$

and therefore,

$$\int_0^1 f(x)\,dx \quad = \quad \frac{-1+3\theta}{6\theta}\,f(0) + \frac{1}{6\theta(1-\theta)}\,f(\theta) + \frac{2-3\theta}{6(1-\theta)}\,f(1). \qquad \checkmark$$

The formula above holds for all polynomials of degree at most 2, by construction. Note that if we choose $\theta = \frac{1}{2}$, then we would obtain precisely the Simpson's rule:

$$\int_0^1 f(x)\,dx \quad = \quad \frac{1}{6}\,f(0) + \frac{2}{3}\,f\Big(\frac{1}{2}\Big) + \frac{1}{6}\,f(1).$$

Also, study homework 6 problems.

There are a few well-known quadrature rules that have to be remembered:

Left endpoint rule: $$\int_a^b f(x)\,dx = (b-a)\,f(a),$$

Right endpoint rule: $$\int_a^b f(x)\,dx = (b-a)\,f(b),$$

Midpoint rule: $$\int_a^b f(x)\,dx = (b-a)\,f\Big(\frac{a+b}{2}\Big),$$

Trapezoidal rule: $$\int_a^b f(x)\,dx = \frac{b-a}{2}\big[f(a)+f(b)\big],$$

Simpson's rule: $$\int_a^b f(x)\,dx = \frac{b-a}{6}\Big[f(a)+4f\Big(\frac{a+b}{2}\Big)+f(b)\Big].$$