Solutions of Equations in One Variable, Interpolation and Polynomial Approximation
Accelerating Convergence; Zeros of Polynomials; Deflation; Müller's Method; Lagrange Polynomials; Neville's Method

Lecture Notes \#4

## Joe Mahaffy

Department of Mathematics and Statistics
San Diego State University
San Diego, CA 92182-7720
mahaffy@math.sdsu.edu
http://www-rohan.sdsu.edu/~jmahaffy
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"It is rare to have the luxury of quadratic convergence."
(Burden-Faires, p.83)
There are a number of methods for squeezing faster convergence out of an already computed sequence of numbers.

We here explore one method which seems the have been around since the beginning of numerical analysis... Aitken's $\Delta^{\mathbf{2}}$ method. It can be used to accelerate convergence of a sequence that is linearly convergent, regardless of its origin or application.

A review of modern extrapolation methods can be found in:
"Practical Extrapolation Methods: Theory and Applications," Avram Sidi, Number 10 in Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, June 2003. ISBN: 0-521-66159-5

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Recall: Convergence of a Sequence
Definition: - Suppose the sequence $\left\{p_{n}\right\}_{n=0}^{\infty}$ converges to $p$, with $p_{n} \neq p$ for all $n$. If positive constants $\lambda$ and $\alpha$ exists with

$$
\lim _{n \rightarrow \infty} \frac{\left|p_{n+1}-p\right|}{\left|p_{n}-p\right|^{\alpha}}=\lambda
$$

then $\left\{p_{n}\right\}_{n=0}^{\infty}$ converges to $p$ of order $\alpha$, with asymptotic error constant $\lambda$.

Linear convergence means that $\alpha=1$, and $|\lambda|<1$.

## Aitken's $\Delta^{2}$ Method

Assume $\left\{p_{n}\right\}_{n=0}^{\infty}$ is a linearly convergent sequence with limit $p$.

Further, assume we are far out into the tail of the sequence ( $n$ large), and the signs of the successive errors agree, i.e.

$$
\operatorname{sign}\left(p_{n}-p\right)=\operatorname{sign}\left(p_{n+1}-p\right)=\operatorname{sign}\left(p_{n+2}-p\right)=\ldots
$$

and that

$$
\frac{p_{n+2}-p}{p_{n+1}-p} \approx \frac{p_{n+1}-p}{p_{n}-p} \approx \lambda \quad(\text { the asymptotic limit })
$$

This would indicate

$$
\begin{aligned}
\left(p_{n+1}-p\right)^{2} & \approx\left(p_{n+2}-p\right)\left(p_{n}-p\right) \\
p_{n+1}^{2}-2 p_{n+1} \mathbf{p}+\mathbf{p}^{2} & \approx p_{n+2} p_{n}-\left(p_{n+2}+p_{n}\right) \mathbf{p}+\mathbf{p}^{2}
\end{aligned}
$$

We solve for $p$ and get...

We solve for $p$ and get...

$$
p \approx \frac{p_{n+2} p_{n}-p_{n+1}^{2}}{p_{n+2}-2 p_{n+1}+p_{n}}
$$

A little bit of algebraic manipulation put this into the classical Aitken form:

$$
\widehat{p}_{n}=p=p_{n}-\frac{\left(p_{n+1}-p_{n}\right)^{2}}{p_{n+2}-2 p_{n+1}+p_{n}}
$$

Aitken's $\Delta^{2}$ Method is based on the assumption that the $\widehat{p}_{n}$ we compute from $p_{n+2}, p_{n+1}$ and $p_{n}$ is a better approximation to the real limit $p$.

The analysis needed to prove this is beyond the scope of this class, see e.g. Sidi's book.

Given a sequence finite $\left\{p_{n}\right\}_{n=0}^{N}$ or infinite $\left\{q_{n}\right\}_{n=0}^{\infty}$ sequence which converges linearly to some limit.

Define the new sequences

$$
\widehat{p}_{n}=p_{n}-\frac{\left(p_{n+1}-p_{n}\right)^{2}}{p_{n+2}-2 p_{n+1}+p_{n}}, \quad n=0,1, \ldots, N-2
$$

or

$$
\widehat{q}_{n}=q_{n}-\frac{\left(q_{n+1}-q_{n}\right)^{2}}{q_{n+2}-2 q_{n+1}+q_{n}}, \quad n=0,1, \ldots, \infty
$$

The numerator is a forward difference squared, while the denominator is a second order central difference.

## Example

Consider the sequence $\left\{p_{n}\right\}_{n=1}^{\infty}$, where the sequence is generated by the fixed point iteration $p_{n+1}=\cos \left(p_{n}\right), p_{0}=0$

| Iteration | $\mathbf{p}_{\mathbf{n}}$ | $\widehat{\mathbf{p}}_{\mathbf{n}}$ |
| ---: | :--- | :--- |
| 0 | 0.000000000000000 | $\mathbf{0 . 6 8 5 0 7 3 3 5 7 3 2 6 0 4 5}$ |
| 1 | 1.00000000000000 | $\mathbf{0 . 7 2 8 0 1 0 3 6 1 4 6 7 6 1 7}$ |
| 2 | 0.540302305868140 | $\mathbf{0 . 7 3 3 6 6 5 1 6 4 5 8 5 2 3 1}$ |
| 3 | 0.857553215846393 | $\mathbf{0 . 7 3 6 9 0 6 2 9 4 3 4 0 4 7 4}$ |
| 4 | 0.65428979497779 | $\mathbf{0 . 7 3 8 0 5 0 4 2 1 3 7 1 6 6 4}$ |
| 5 | 0.793480358742566 | $\mathbf{0 . 7 3 8 6 3 6 0 9 6 8 8 1 6 5 5}$ |
| 6 | 0.701368773622757 | $\mathbf{0 . 7 3 8 8 7 6 5 8 2 8 1 7 1 3 6}$ |
| 7 | 0.763959682900654 | $\mathbf{0 . 7 3 8 9 9 2 2 4 3 0 2 7 0 3 4}$ |
| 8 | 0.722102425026708 | 0.739042511328159 |
| 9 | 0.75041776163761 | $\mathbf{0 . 7 3 9 0} 65949599941$ |
| 10 | 0.731404042422510 | $\mathbf{0 . 7 3 9 0} 76383318956$ |
| 11 | 0.74423735490557 | $\mathbf{0 . 7 3 9 0 8 1 1 7 7 2 5 9 5 6 3 ^ { * }}$ |
| 12 | 0.735604740436347 | $\mathbf{0 . 7 3 9 0 8 3 3 3 3 9 0 9 6 8 4 ^ { * }}$ |

Note: Bold digits are correct; $\widehat{p}_{11}$ needs $p_{13}$, and $\widehat{p}_{12}$ additionally needs $p_{14}$.

Faster Convergence for "Aitken-Sequences"

## Theorem: Convergence of Aitken- $\Delta^{2}$-Sequences -

Suppose $\left\{p_{n}\right\}_{n=0}^{\infty}$ is a sequence that converges linearly to the limit $p$, and for $n$ large enough we have $\left(p_{n}-p\right)\left(p_{n+1}-p\right)>0$. Then the Aitken-accelerated sequence $\left\{\hat{p}_{n}\right\}_{n=0}^{\infty}$ converges fast to $p$ in the sense that

$$
\lim _{n \rightarrow \infty}\left[\frac{\widehat{p}_{n}-p}{p_{n}-p}\right]=0
$$

We can combine Aitken's method with fixed-point iteration in order to get a "fixed-point iteration on steroids."

Suppose we have a fixed point iteration:

$$
p_{0}, \quad p_{1}=g\left(p_{0}\right), \quad p_{2}=g\left(p_{1}\right), \quad \ldots
$$

Once we have $p_{0}, p_{1}$ and $p_{2}$, we can compute

$$
\widehat{p}_{0}=p_{0}-\frac{\left(p_{1}-p_{0}\right)^{2}}{p_{2}-2 p_{1}+p_{0}}
$$

At this point we "restart" the fixed point iteration with $p_{0}=\widehat{p}_{0}, ~ e . g$.

$$
p_{3}=\widehat{p}_{0}, \quad p_{4}=g\left(p_{3}\right), \quad p_{5}=g\left(p_{4}\right)
$$

And compute

$$
\widehat{p}_{3}=p_{3}-\frac{\left(p_{4}-p_{3}\right)^{2}}{p_{5}-2 p_{4}+p_{3}}
$$

Below we compare a Fixed Point iteration, Newton's Method, and Steffensen's Method for solving:

$$
f(x)=x^{3}+4 x^{2}-10=0
$$

or alternately,

$$
p_{n+1}=g\left(p_{n}\right)=\sqrt{\frac{10}{p_{n}+4}}
$$

This waltz: $g-g-A(i t k e n), g-g-A, \ldots$ converges quadratically!
Input: Initial approximation $p_{0}$; tolerance $T O L$; maximum number of iterations $N_{0}$.
Output: Approximate solution $p$, or failure message.

1. $\quad$ Set $i=1$
2. While $i \leq N_{0}$ do 3-6

3* $^{*} \quad$ Set $p_{1}=g\left(p_{0}\right), p_{2}=g\left(p_{1}\right)$,

$$
p=p_{0}-\left(p_{1}-p_{0}\right)^{2} /\left(p_{2}-2 p_{1}+p_{0}\right)
$$

4. If $\left|p-p_{0}\right|<T O L$ then

4a. output $p$
4b . stop program
5. Set $i=i+1$
6. Set $p_{0}=p$
7. Output: "Failure after $N_{0}$ iterations."

## Fixed Point Iteration

| $i$ | $p_{n}$ | $g\left(p_{n}\right)$ |
| :---: | :---: | :---: |
| 0 | 1.50000 | 1.34840 |
| 1 | 1.34840 | 1.36738 |
| 2 | 1.36738 | 1.36496 |
| 3 | 1.36496 | 1.3652 |
| 4 | 1.36526 | 1.36523 |
| 5 | 1.36523 | 1.36523 |

## Newton's Method

| $i$ | $x_{n}$ | $f\left(x_{n}\right)$ |
| :---: | :---: | :---: |
| 0 | 1.50000 | $1.51600 \mathrm{e}-01$ |
| 1 | 1.36495 | $-3.11226 \mathrm{e}-04$ |
| 2 | 1.36523 | $-1.35587 \mathrm{e}-09$ |

## Steffensen's Method

| $i$ | $p_{n}$ | $p_{1}$ | $p_{2}$ | $p$ | $\left\|p-p_{2}\right\|$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1.50000 | 1.34840 | 1.36738 | 1.36527 | $3.96903 e^{2}$ |

3* If at some point $p_{2}-2 p_{1}+p_{0}=0$ (which appears in the denominator), then we stop and select the current value of $p_{2}$ as our approximate answer.

Notes: Both Newton's and Steffensen's methods give quadratic convergence. In Newton's method we compute one function value and one derivative in each iteration. In Steffensen's method we have two function evaluations and a more complicated algebraic expression in each iteration, but no derivative. It looks like we got something for (almost) nothing. However, in order the guarantee quadratic convergence for Steffensen's method, the fixed point function $g$ must be 3 times continuously differentiable, e.g. $f \in C^{3}[a, b]$, (see theorem-2.14 in Burden-Faires). Newton's method "only" requires $f \in C^{2}[a, b]$ (BF Theorem-2.5).

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## Definition: Degree of a Polynomial -

A polynomial of degree $n$ has the form

$$
P(x)=a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0}, \quad a_{n} \neq 0
$$

where the $a_{i}$ 's are constants (either real, or complex) called the coefficients of $P$.

Why look at polynomials? - We'll be looking at the problem $P(x)=0$ (i.e. $f(x)=0$ for a special class of functions.)

Polynomials are the basis for many approximation methods, hence being able to solve polynomial equations fast is valuable.

We'd like to use Newton's method, so we need to compute $P(x)$ and $P^{\prime}(x)$ as efficiently as possible.

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Key Consequences of the Fundamental Theorem of Algebra, 1 of 2

## Corollary: -

If $P(x)$ is a polynomial of degree $n \geq 1$ with real or complex coefficients then there exists unique constants $x_{1}, x_{2}, \ldots, x_{k}$ (possibly complex) and unique positive integers $m_{1}, m_{2}, \ldots, m_{k}$ such that $\sum_{i=1}^{k} m_{i}=n$ and

$$
P(x)=a_{n}\left(x-x_{1}\right)^{m_{1}}\left(x-x_{2}\right)^{m_{2}} \cdots\left(x-x_{k}\right)^{m_{k}}
$$

- The collection of zeros is unique.
- $m_{i}$ are the multiplicities of the individual zeros.
- A polynomial of degree $n$ has exactly $n$ zeros, counting multiplicity.


## Corollary: -

Let $P(x)$ and $Q(x)$ be polynomials of degree at most $n$. If $x_{1}, x_{2}$, $\ldots, x_{k}$, with $k>n$ are distinct numbers with $P\left(x_{i}\right)=Q\left(x_{i}\right)$ for $i=1,2, \ldots, k$, then $P(x)=Q(x)$ for all values of $x$.

- If two polynomials of degree $n$ agree at at least $(n+1)$ points, then they must be the same.

Let

$$
P(x)=a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0}
$$

We want an efficient method to solve

$$
P(x)=0 .
$$

In 1819, William Horner developed an efficient algorithm with $n$ multiplications and $n$ additions to evaluate $P\left(x_{0}\right)$.

Technique is called Horner's Method or Synthetic Division.

Huh?!? Where did the expression come from? - Consider

$$
\begin{aligned}
P(x) & =a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0} \\
& =\left(a_{n} x^{n-1}+a_{n-1} x^{n-2}+\cdots+a_{1}\right) x+a_{0} \\
& =\left(\left(a_{n} x^{n-2}+a_{n-1} x^{n-3}+\cdots\right) x+a_{1}\right) x+a_{0} \\
& =\underbrace{(\ldots((\underbrace{a_{n} x+a_{n-1}}_{b_{n-1}}) x+\cdots) x+a_{1}) x+a_{0}}_{n-1}
\end{aligned}
$$

Horner's method is "simply" the computation of this parenthesized expression from the inside-out...

Now, if we need to compute $P^{\prime}\left(x_{0}\right)$ we have

$$
\left.P^{\prime}(x)\right|_{x=x_{0}}=\left(x-x_{0}\right) Q^{\prime}(x)+\left.Q(x)\right|_{x=x_{0}}=Q\left(x_{0}\right)
$$

Which we can compute (again using Horner's method) in $(n-1)$ multiplications and ( $n-1$ ) additions.

Proof? We really ought to prove that Horner's method works. It basically boils down to lots of algebra which shows that the coefficients of $P(x)$ and $\left(x-x_{0}\right) Q(x)+b_{0}$ are the same...

A couple of examples may be more instructive...

Input: Degree $n$; coefficients $a_{0}, a_{1}, \ldots, a_{n} ; x_{0}$
Output: $\quad y=P\left(x_{0}\right), z=P^{\prime}\left(x_{0}\right)$.

1. $\quad$ Set $y=a_{n}, z=a_{n}$
2. For $j=(n-1),(n-2), \ldots, 1$

Set $y=x_{0} y+a_{j}, z=x_{0} z+y$
3. Set $y=x_{0} y+a_{0}$
4. Output $(y, z)$

## 5. End program

For $P(x)=x^{4}-x^{3}+x^{2}+x-1$, compute $P(5)$ :

| $x_{0}=5$ | $a_{4}=1$ | $a_{3}=-1$ | $a_{2}=1$ | $a_{1}=1$ | $a_{0}=-1$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $b_{4} x_{0}=5$ | $b_{3} x_{0}=20$ | $b_{2} x_{0}=105$ | $\mathrm{~b}_{1} \mathrm{x}_{0}=530$ |
|  | $b_{4}=1$ | $b_{3}=4$ | $b_{2}=21$ | $b_{1}=106$ | $\mathrm{~b}_{0}=\mathbf{5 2 9}$ |

Hence, $\mathrm{P}(5)=529$, and

$$
P(x)=(x-5)\left(x^{3}+4 x^{2}+21 x+106\right)+529
$$

Similarly we get $P^{\prime}(5)=Q(5)=436$

| $x_{0}=5$ | $a_{3}=1$ | $a_{2}=4$ | $a_{1}=21$ | $a_{0}=106$ |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $b_{3} x_{0}=5$ | $b_{2} x_{0}=45$ | $b_{1} x_{0}=330$ |
|  | $b_{3}=1$ | $b_{2}=9$ | $b_{1}=66$ | $b_{0}=\mathbf{4 3 6}$ |

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Deflation - Finding All the Zeros of a Polynomial
If we are solving our current favorite problem

$$
P(x)=0, \quad P(x) \text { a polynomial of degree } n
$$

and we are using Horner's method of computing $P\left(x_{i}\right)$ and $P^{\prime}\left(x_{i}\right)$, then after $N$ iterations, $x_{N}$ is an approximation to one of the roots of $P(x)=0$.

We have

$$
P(x)=\left(x-x_{N}\right) Q(x)+b_{0}, \quad b_{0} \approx 0
$$

Let $\widehat{r}_{1}=x_{N}$ be the first root, and $Q_{1}(x)=Q(x)$.

We can now find a second root by applying Newton's method to $Q_{1}(x)$.

After some number of iterations of Newton's method we have

$$
Q_{1}(x)=\left(x-\widehat{r}_{2}\right) Q_{2}(x)+b_{0}^{(2)}, \quad b_{0}^{(2)} \approx 0
$$

If $P(x)$ is an $n^{\text {th }}$-degree polynomial with $n$ real roots, we can apply this procedure $(n-2)$ times to find $(n-2)$ approximate zeros of $P(x): \widehat{r}_{1}, \widehat{r}_{2}, \ldots, \widehat{r}_{n-2}$, and a quadratic factor $Q_{n-2}(x)$.

At this point we can solve $Q_{n-2}(x)=0$ using the quadratic formula, and we have $n$ roots of $P(x)=0$.

This procedure is called Deflation.

Now, the big question is "are the approximate roots $\widehat{r}_{1}, \widehat{r}_{2}, \ldots, \widehat{r}_{n}$ good approximations of the roots of $P(x)$ ???"

Unfortunately, sometimes, no.

In each step we solve the equation to some tolerance, i.e.

$$
\left|b_{0}^{(k)}\right|<t o l
$$

Even though we may solve to a tight tolerance $\left(10^{-8}\right)$, the errors accumulate and the inaccuracies increase iteration-by-iteration...

Question: Is deflation therefore useless???

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Improving the Accuracy of Deflation
The problem with deflation is that the zeros of $Q_{k}(x)$ are not good representatives of the zeros of $P(x)$, especially for high $k$ 's.

As $k$ increases, the quality of the root $\widehat{r}_{k}$ decreases.
Maybe there is a way to get all the zeros with the same quality?
The idea is quite simple... in each step of deflation, instead of just accepting $\widehat{r}_{k}$ as a root of $P(x)$, we re-run Newton's method on the full polynomial $P(x)$, with $\widehat{r}_{k}$ as the starting point - a couple of Newton iterations should quickly converge to the root of the full polynomial.

Improved Deflation - Algorithm Outline

1. Apply Newton's method to $P(x) \rightarrow \widehat{\mathbf{r}}_{1}, \mathbf{Q}_{\mathbf{1}}(\mathbf{x})$.
2. For $k=2,3, \ldots,(n-2)$ do 3-4
3. Apply Newton's method to $\mathbf{Q}_{\mathbf{k}-\mathbf{1}} \rightarrow \widehat{\mathbf{r}}_{\mathbf{k}}^{*}, \mathbf{Q}_{\mathbf{k}}^{*}(\mathbf{x})$.
4. Apply Newton's method to $\mathbf{P}(\mathbf{x})$ with $\widehat{\mathbf{r}}_{\mathrm{k}}^{*}$ as the initial point $\rightarrow \widehat{\mathbf{r}}_{\mathrm{k}}$
Apply Horner's method to $\mathrm{Q}_{\mathrm{k}-\mathbf{1}}(\mathrm{x})$ with $\mathrm{x}=\widehat{\mathbf{r}}_{\mathbf{k}}$ $\rightarrow \mathrm{Q}_{\mathrm{k}}(\mathrm{x})$
5. Use the quadratic formula on $\mathbf{Q}_{\mathrm{n}-2}(\mathrm{x})$ to get the two remaining roots.

Note: "Inside" Newton's method, the evaluations of polynomials and their derivatives are also performed using Horner's method.

The Wilkinson Polynomials

$$
P_{n}^{\mathrm{W}}(x)=\prod_{k=1}^{n}(x-k)
$$

have the roots $\{1,2, \ldots, n\}$, but provide surprisingly tough numerical root-finding problems. (Additional details in Math 543.)

In the next few slides we show the results of Deflation and Improved Deflation applied to Wilkinson polynomials of degree $9,10,12$, and 13.

Deflation \& Improvement
$P_{12}^{W}(x)$ and $P_{13}^{W}(x)$


Figure: [LEFT] The result of the two algorithms on the Wilkinson polynomial of degree 12; in this case the roots are computed so that $\left|b_{0}^{(k)}\right|<10^{-4}$. [Right] The result of the two algorithms on the Wilkinson polynomial of degree 13; in this case the roots are computed so that $\left|b_{0}^{(k)}\right|<10^{-3}$. In both cases the lower line corresponds to improved deflation and we see that we get an improvement in the relative error of several orders of magnitude.


Figure: [LEFT] The result of the two algorithms on the Wilkinson polynomial of degree 9 ; in this case the roots are computed so that $\left|b_{0}^{(k)}\right|<10^{-6}$. [Right] The result of the two algorithms on the Wilkinson polynomial of degree 10 ; in this case the roots are computed so that $\left|b_{0}^{(k)}\right|<10^{-6}$. In both cases the lower line corresponds to improved deflation and we see that we get an improvement in the relative error of several orders of magnitude.

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What About Complex Roots???
One interesting / annoying feature of polynomials with real coefficients is that they may have complex roots, e.g. $P(x)=x^{2}+1$ has the roots $\{-i, i\}$. Where by definition $i=\sqrt{-1}$.

If the initial approximation given to Newton's method is real, all the successive iterates will be real... which means we will not find complex roots.

One way to overcome this is to start with a complex initial approximation and do all the computations in complex arithmetic.

Another solution is Müller's Method...

Müller's method is an extension of the Secant method...

Recall that the secant method uses two points $x_{k}$ and $x_{k-1}$ and the function values in those two points $f\left(x_{k}\right)$ and $f\left(x_{k-1}\right)$. The zero-crossing of the linear interpolant (the secant line) is used as the next iterate $x_{k+1}$.

Müller's method takes the next logical step: it uses three points: $x_{k}$, $x_{k-1}$ and $x_{k-2}$, the function values in those points $f\left(x_{k}\right), f\left(x_{k-1}\right)$ and $f\left(x_{k-2}\right)$; a second degree polynomial fitting these three points is found, and its zero-crossing is the next iterate $x_{k+1}$.

Next slide: $f(x)=x^{4}-3 x^{3}-1, x_{k-2}=1.5, x_{k-1}=2.5, x_{k}=3.5$.


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Müller's Method - Identifying the Zero
We now have a quadratic equation for $\left(x-x_{k}\right)$ which gives us two possibilities for $x_{k+1}$ :

$$
x_{k+1}-x_{k}=\frac{-2 c}{b \pm \sqrt{b^{2}-4 a c}}
$$

In Müller's method we select

$$
x_{k+1}=x_{k}-\frac{2 c}{b+\operatorname{sign}(b) \sqrt{b^{2}-4 a c}}
$$

we are maximizing the (absolute) size of the denominator, hence we select the root closest to $x_{k}$.

Note that if $b^{2}-4 a c<0$ then we automatically get complex roots.

Input: $x_{0}, x_{1}, x_{2}$; tolerance tol; max iterations $N_{0}$
Output: Approximate solution $p$, or failure message.

1. Set $h_{1}=\left(x_{1}-x_{0}\right), h_{2}=\left(x_{2}-x_{1}\right), \delta_{1}=\left[f\left(x_{1}\right)-f\left(x_{0}\right)\right] / h_{1}$, $\delta_{2}=\left[f\left(x_{2}\right)-f\left(x_{1}\right)\right] / h_{2}, d=\left(\delta_{2}-\delta_{1}\right) /\left(h_{2}+h_{1}\right), j=3$.
2. While $j \leq N_{0}$ do 3-7
3. $b=\delta_{2}+h_{2} d, D=\sqrt{b^{2}-4 f\left(x_{2}\right) d}$ complex?
4. If $|b-D|<|b+D|$ then set $E=b+D$ else set $E=b-D$
5. Set $h=-2 f\left(x_{2}\right) / E, p=x_{2}+h$
6. If $|h|<t o l$ then output $\mathbf{p}$; stop program
7. Set $x_{0}=x_{1}, x_{1}=x_{2}, x_{2}=p, h_{1}=\left(x_{1}-x_{0}\right), h_{2}=\left(x_{2}-x_{1}\right)$, $\delta_{1}=\left[f\left(x_{1}\right)-f\left(x_{0}\right)\right] / h_{1}, \quad \delta_{2}=\left[f\left(x_{2}\right)-f\left(x_{1}\right)\right] / h_{2}$, $d=\left(\delta_{2}-\delta_{1}\right) /\left(h_{2}+h_{1}\right), j=j+1$
8. output - "Müller's Method failed after $N_{0}$ iterations."

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Recap, continued...
Basic error analysis: order $\alpha$, asymptotic error constant $\lambda$. - Which one has the most impact on convergence? Convergence rate for general fixed point iterations?

Multiplicity of zeros: What does it mean? How do we use this knowledge to "help" Newton's method when we're looking for a zero of high multiplicity?

Convergence acceleration: Aitken's $\Delta^{2}$-method. Steffensen's Method.

Zeros of polynomials: Horner's method, Deflation (with improvement), Müller's method.

Let's recap... Things to remember...

The relation between root finding $(f(x)=0)$ and fixed point $(g(x)=x)$.

Key algorithms for root finding: Bisection, Secant Method, and Newton's Method. - Know what they are (the updates), how to start (one or two points? bracketing or not bracketing the root?), can the method break, can breakage be fixed? Convergence properties.

Also, know the mechanics of the Regula Falsi method, and understand why it can run into trouble.

Fixed point iteration: Under what conditions do FP-iteration converge for all starting values in the interval?

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## Interpolation and Polynomial Approximation

The following theorem is the basis for polynomial approximation:

```
Theorem: Weierstrass Approximation Theorem -
Suppose f}\inC[a,b]\mathrm{ . Then }\forall\epsilon>0\exists\mathrm{ a polynomial }P(x)\mathrm{ :
|f(x)-P(x)|<\epsilon,\forallx\in[a,b].
```

Note: The bound is uniform, i.e valid for all $x$ in the interval.
Note: The theorem says nothing about how to find the polynomial, or about its order.

## Natural Question:

Are our old friends, the Taylor Polynomials, good candidates for polynomial interpolation?

## Answer:

No. The Taylor expansion works very hard to be accurate in the neighborhood of one point. But we want to fit data at many points (in an extended interval).
[Next slide: The approximation is great near the expansion point $x_{0}=$ 0 , but get progressively worse at we get further away from the point, even for the higher degree approximations.]


Figure: Weierstrass approximation Theorem guarantees that we (maybe with substantial work) can find a polynomial which fits into the "tube" around the function $f$, no matter how thin we make the tube.


Let

$$
f(x)=\frac{1}{x}
$$

The Taylor expansion about $x_{0}=1$ is

$$
P_{n}(x)=\sum_{k=0}^{n}(-1)^{k}(x-1)^{k} .
$$

Note: $f(3)=1 / 3$, but $P_{n}(3)$ satisfies:

| $n$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $P_{n}(3)$ | 1 | -1 | 3 | -5 | 11 | -21 | 43 |

The Taylor's series only converges $|x-1|<1$ by the ratio test (a geometric series). Thus, not valid for $x=3$.

Clearly, Taylor polynomials are not well suited for approximating a function over an extended interval.

We are going to look at the following:

- Lagrange polynomials - Neville's Method. [This Lecture]
- Newton's divided differences.
- Hermite interpolation.
- Cubic splines - Piecewise polynomial approximation.
- (Parametric curves)
- (Bézier curves - used in e.g. computer graphics)

New idea: Instead of working hard at one point, we will prescribe a number of points through which the polynomial must pass.

As warm-up we will define a function that passes through the points $\left(x_{0}, f\left(x_{0}\right)\right)$ and $\left(x_{1}, f\left(x_{1}\right)\right)$. First, lets define

$$
L_{0}(x)=\frac{x-x_{1}}{x_{0}-x_{1}}, \quad L_{1}(x)=\frac{x-x_{0}}{x_{1}-x_{0}}
$$

and then define the interpolating polynomial

$$
P(x)=L_{0}(x) f\left(x_{0}\right)+L_{1}(x) f\left(x_{1}\right)
$$

then $P\left(x_{0}\right)=f\left(x_{0}\right)$, and $P\left(x_{1}\right)=f\left(x_{1}\right)$.

- $\quad P(x)$ is the unique linear polynomial passing through $\left(x_{0}, f\left(x_{0}\right)\right)$ and $\left(x_{1}, f\left(x_{1}\right)\right)$.


This is $L_{6,3}(x)$, for the points $x_{i}=i, i=0, \ldots, 6$.

We use $L_{n, k}(x), k=0, \ldots, n$ as building blocks for the Lagrange interpolating polynomial:

$$
P(x)=\sum_{k=0}^{n} f\left(x_{k}\right) L_{n, k}(x)
$$

which has the property

$$
P\left(x_{i}\right)=f\left(x_{i}\right), \quad \forall i=0, \ldots, n
$$

This is the unique polynomial passing through the points $\left(x_{i}, f\left(x_{i}\right)\right), i=0, \ldots, n$.

Suppose $x_{i}, i=0, \ldots, n$ are distinct numbers in the interval $[a, b]$, and $f \in C^{n+1}[a, b]$. Then $\forall x \in[a, b] \exists \xi(x) \in(a, b)$ so that:

$$
f(x)=P_{\text {Lagrange }}(x)+\frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n}\left(x-x_{i}\right)
$$

where $P_{\text {Lagrange }}(x)$ is the $n^{\text {th }}$ Lagrange interpolating polynomial.

Compare with the error formula for Taylor polynomials

$$
f(x)=P_{\text {Taylor }}(x)+\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\left(x-x_{0}\right)^{n+1}
$$

Problem: Applying the error term may be difficult...
The error formula is important as Lagrange polynomials are used for numerical differentiation and integration methods.

Applying (estimating) the error term is difficult.
The degree of the polynomial needed for some desired accuracy is not known until after cumbersome calculations - checking the error term.

If we want to increase the degree of the polynomial (to e.g. $n+1$ ) the previous calculations are not of any help...

Building block for a fix: Let $f$ be a function defined at $x_{0}, \ldots, x_{n}$, and suppose that $m_{1}, m_{2}, \ldots, m_{k}$ are $k(<n)$ distinct integers, with $0 \leq m_{i} \leq n \forall i$. The Lagrange polynomial that agrees with $f(x)$ the $k$ points $x_{m_{1}}, x_{m_{2}}, \ldots, x_{m_{k}}$, is denoted $P_{m_{1}, m_{2}, \ldots, m_{k}}(x)$.

Note: $\left\{m_{1}, m_{2}, \ldots, m_{k}\right\} \subset\{1,2, \ldots, n\}$.

Theorem: - Let $f$ be defined at $x_{0}, x_{1}, \ldots, x_{k}$, and $x_{i}$ and $x_{j}$ be two distinct points in this set, then
$P(x)=\frac{\left(x-x_{j}\right) P_{0, \ldots, j-1, j+1, \ldots, k}(x)-\left(x-x_{i}\right) P_{0, \ldots, i-1, i+1, \ldots, k}(x)}{x_{i}-x_{j}}$
is the $k^{\text {th }}$ Lagrange polynomial that interpolates $f$ at the $k+1$ points $x_{0}, \ldots, x_{k}$.

We can generate new polynomials recursively:

| $x_{0}$ | $P_{0}$ |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :--- |
| $x_{1}$ | $P_{1}$ | $P_{0,1}$ |  |  |  |
| $x_{2}$ | $P_{2}$ | $P_{1,2}$ | $P_{0,1,2}$ |  |  |
| $x_{3}$ | $P_{3}$ | $P_{2,3}$ | $P_{1,2,3}$ | $P_{0,1,2,3}$ |  |
| $x_{4}$ | $P_{4}$ | $P_{3,4}$ | $P_{2,3,4}$ | $P_{1,2,3,4}$ | $P_{0,1,2,3,4}$ |

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To evaluate the polynomial that interpolates the $n+1$ points $\left(x_{i}, f\left(x_{i}\right)\right), i=0, \ldots, n$ at the point $x$ :

1. Initialize $Q_{i, 0}=f\left(x_{i}\right)$.
2. 

FOR $i=1: n$
FOR $j=1: i$
$Q_{i, j}=\frac{\left(x-x_{i-j}\right) Q_{i, j-1}-\left(x-x_{i}\right) Q_{i-1, j-1}}{x_{i}-x_{i-j}}$
END
END
3. Output the $Q$-table.

