The math behind the methods

and some madness...

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PH3105, Autumn Semester 2017

Lagrange interpolation

Given $n+1$ data points $(x_0, y_0), (x_1, y_1), \ldots (x_n, y_n)$, the Lagrange polynomials are defined by

$$L_i(x) = \frac{(x - x_0)\ldots(x - x_{i-1})(x - x_{i+1})\ldots(x - x_n)}{(x_i - x_0)\ldots(x_i - x_{i-1})(x_i - x_{i+1})\ldots(x_i - x_n)}$$

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These satisfy

$$L_i(x_j) = \delta_{ij}$$

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Then, the interpolating polynomial between the data points is

$$p_n(x) \equiv \sum_{i=0}^{n} y_i L_i(x)$$

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Note that we can write $L_i(x)$ in terms of the function $\Psi_n(x) \equiv (x - x_0)\ldots(x - x_n)$ as

$$L_i(x) = \frac{\Psi_n(x)}{(x - x_i)\Psi'_n(x_i)}$$

Lagrange interpolation

Error

Let $f(x)$ be a function with at least $n + 1$ continuous derivatives.

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How good is this approximation?

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How good is this approximation?

Let $t \in \mathbb{R}$. Then $\exists \xi \in I_t \equiv \mathcal{H}\{t, x_0, \ldots x_n\}$:

$$f(t) - p_n(t) = \frac{(t - x_0)\ldots(t - x_n)}{(n+1)!} f^{(n+1)}(\xi)$$

Lagrange interpolation

Error - proof

If $t \in \{x_0, \ldots, x_n\}$ the result is trivial!

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Define

$$\Psi(x) \equiv (x - x_0) \ldots (x - x_n)$$

$$E(x) \equiv f(x) - p_n(x)$$

$$G(x) \equiv E(x) - \frac{\Psi(x)}{\Psi(t)} E(t)$$

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Obviously, $\Psi(x_i) = E(x_i) = 0$ for $i = 0, 1, \ldots n$.

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$$G(x_i) = 0, \qquad i = 0, 1, \ldots, n$$

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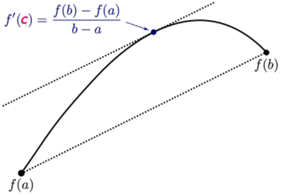
$$G(t) = 0$$

Thus, $G(x)$ has at least $n + 2$ distinct zeros in I_t.

The Mean Value Theorem

If $f(x)$ is defined and continuous on the interval $[a, b]$ and differentiable on (a, b), then there is at least one number c in the interval (a, b) (that is $a < c < b$) such that

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$



The tangent to the curve of $f(x)$ is parallel at at least one point to the chord joining the endpoints $(a, f(a))$ and $(b, f(b))$.

Lagrange interpolation

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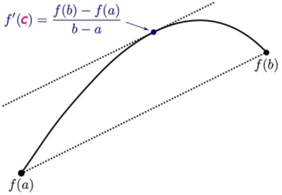

There is at least one zero of $f'(x)$ between two successive zeros of $f(x)$.

Lagrange interpolation

Error - proof

$$\Psi(x) \equiv (x - x_0) \dots (x - x_n)$$

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$G(x)$ has at least $n+2$ distinct zeros in I_t.

$G'(x)$ has at least $n+1$ distinct zeros in this interval!

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$G^{(j)}(x)$ has at least $n+2-j$ distinct zeros in I_t!

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$G^{(n+1)}(x)$ has at least one!

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$G^{(n+1)}(x)$ has at least one!
Let ξ be a zero of $G^{(n+1)}(x)$ in I_t.

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Now, $E^{(n+1)}(x) = f^{(n+1)}(x)$

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Now, $E^{(n+1)}(x) = f^{(n+1)}(x)$and $\Psi^{(n+1)}(x) = (n+1)!$

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$$0 = G^{(n+1)}(\xi) = f^{(n+1)}(\xi) - \frac{(n+1)!}{\Psi(t)} E(t)$$

Lagrange interpolation

Error - estimate

Let us now estimate the error for equally spaced datapoints.

Lagrange interpolation

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Let us use the notation $c_{n+1} = \text{Max}_{\, t \in I} \left| f^{(n+1)}(t) \right|$

- $n = 1$: Linear interpolation

$$E(t) = \frac{(t - x_0)(t - x_1)}{2!} f''(\xi) \implies |E(t)| \leq \frac{h^2}{8} c_2$$

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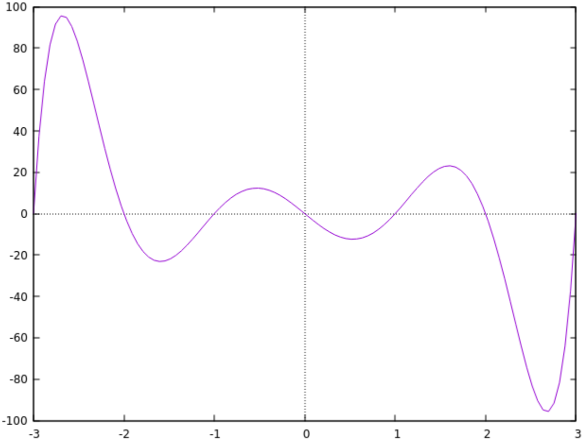
- $n = 2$:

$$E(t) = \frac{(t-x_0)(t-x_1)(t-x_2)}{2!} f'''(\xi) \implies |E(t)| \leq \frac{\sqrt{3}\, h^3}{27} c_3$$

Lagrange interpolation

Error - warning!!

Higher order interpolation is bad near the edges!



$\Psi_6(x)$ for equally spaced points $-3, -2, \ldots, 2, 3$

Newton interpolation

Another look

Let's say we have a $n-1$ th order polynomial $p_{n-1}(x)$ interpolating a function $f(x)$ at the n points $x_0, x_1, \ldots, x_{n-1}$.

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Let's say we have a $n-1$ th order polynomial $p_{n-1}(x)$ interpolating a function $f(x)$ at the n points $x_0, x_1, \ldots, x_{n-1}$. How can we get $p_n(x)$ - the interpolating polynomial if we add one more interpolation point x_n?

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We are seeking a n-th order *correction polynomial* $C(x)$

$$p_n(x) = p_{n-1}(x) + C(x)$$

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$$C(x) = a_n(x - x_0)\ldots(x - x_{n-1})$$

Since $p_n(x_n) = f(x_n)$, we have

$$f(x_n) = p_{n-1}(x_n) + a_n(x_n - x_0)\ldots(x_n - x_{n-1})$$

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$$f(x_n) = p_{n-1}(x_n) + a_n (x_n - x_0) \ldots (x_n - x_{n-1})$$

Which gives us $a_n \equiv f[x_0, x_1, \ldots, x_n]$

Newton interpolation

Another look

$$f\left[x_0, x_1, \ldots, x_n\right] = \frac{f\left(x_n\right) - p_{n-1}\left(x_n\right)}{\left(x_n - x_0\right)\ldots\left(x_n - x_{n-1}\right)}$$

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Alternatively, note that a_n is the coefficient of x^n in $p_n\left(x\right)$.

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We already know that

$$p_n\left(x\right) = \sum_{i=0}^{n} \frac{\Psi_n\left(x\right)}{\left(x - x_i\right)\Psi_n'\left(x_i\right)} f\left(x_i\right)$$

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Thus

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Thus

$$f\left[x_0, x_1, \ldots, x_n\right] = \sum_{i=0}^{n} \frac{f\left(x_i\right)}{\Psi_n'\left(x_i\right)}$$

Which shows that $f\left[x_0, x_1, \ldots, x_n\right]$ is invariant under a permutation of the nodes $x_0, x_1, \ldots, x_n$.

Newton interpolation

Another look

We can use this to derive (HW!!!)

$$f\left[x_0, x_1, \ldots, x_n\right] = \frac{f\left[x_1, \ldots, x_n\right] - f\left[x_0, \ldots, x_{n-1}\right]}{x_n - x_0}$$

which is why this is called the **divided difference**!

Newton interpolation

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Another form (Hermite-Genocchi) - assuming the function f is n times continuously differentiable

$$f[x_0, x_1, \ldots, x_n] = \int \ldots \int f^{(n)}(t_0 x_0 + \ldots + t_n x_n)\, dt_1 \ldots dt_n$$

where $t_0 + \ldots + t_n = 1$ and the integration is over the region $\tau = \{(t_1, \ldots, t_n) \mid t_i \geq 0, \sum_{i=1}^{n} t_i \leq 1\}$

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Consider an interpolating polynomial $p_{n+1}(x)$ that has $x_0, \ldots, x_n, t$ as nodes.

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$$p_{n+1}(x) = p_n(x) + (x - x_0) \ldots (x - x_n) f[x_0, \ldots, x_n, t]$$

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Since $p_{n+1}(t) = f(t)$, we have

$$f(t) - p_n(t) = (t - x_0) \ldots (t - x_n) f[x_0, \ldots, x_n, t]$$

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$$f(t) - p_n(t) = (t - x_0) \ldots (t - x_n) f[x_0, \ldots, x_n, t]$$

Comparing with $f(t) - p_n(t) = \Psi_n(t) \dfrac{f^{(n+1)}(\xi)}{(n+1)!}$, we get

$$f[x_0, \ldots, x_n, t] = \frac{f^{(n+1)}(\xi)}{(n+1)!}, \qquad \text{for some } \xi \in \mathcal{H}\{x_0, \ldots, x_n, t\}$$

Newton-Cotes integration

To calculate $\int_a^b f(x)\,dx$ numerically, we can approximate the function $f(x)$ in (a, b) by an interpolating polynomial $p_n(x)$ and estimate

$$\int_a^b f(x)\,dx = \int_a^b p_n(x)\,dx + E \approx \int_a^b p_n(x)\,dx$$

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We usually take the nodes to be an evenly spaced set of $n+1$ points

$$x_0 = a, x_1 = a + h, \ldots, x_j = a + jh, \ldots, x_n = b$$

where $h = \dfrac{b-a}{n}$.

Newton-Cotes integration

$n = 1$ - the Trapezoidal rule

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Using $\int_a^b (x-a)\,dx = \dfrac{(b-a)^2}{2} = -\int_a^b (x-b)\,dx$, we get

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\left[f(a) + f(b)\right]$$

Newton-Cotes integration

Trapezoidal rule - Error estimate

$$f(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a} + (x-a)(x-b)\,f[a,b,x]$$

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To evaluate the integral we use the

Integral Mean Value Theorem

Let $w\left(x\right)$ be non-negative and integrable on $\left[a,b\right]$, and let $f\left(x\right)$ be continuous on $\left[a,b\right]$ .Then $\exists\xi\in\left(a,b\right)$:

$$\int_a^b w\left(x\right)f\left(x\right)dx=f\left(\xi\right)\int_a^b w\left(x\right)dx$$

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$$E = f\left[a, b, \xi\right] \int_a^b \left(x - a\right)\left(x - b\right) dx$$

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$$E = f\left[a, b, \xi\right] \int_a^b (x - a)(x - b)\, dx$$

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The error is not very small for large intervals - which is why we use the Composite version!

Newton-Cotes integration

Composite Trapezoidal rule - Error estimate

For the n interval composite trapezoidal rule, the error is

$$E_n = -\frac{h^3}{12}\sum_{i=0}^{n-1} f''(\eta_i) \qquad \eta_i \in (a + ih, a + ih + h)$$

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For large n, we can estimate

$$E_n \approx -\frac{h^2}{12}\left[f'(b) - f'(a)\right]$$

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$$E_2 = -f[a, b, c, \xi, \xi] \int_a^b w(x)\,dx \qquad \text{for some } \xi \in (a, b)$$

leading to

$$E_2 = -\frac{h^5}{90} f^{(4)}(\eta) \qquad \text{for some } \eta \in (a, b)$$

Hermite interpolation

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We need to find $2n$ polynomials $h_1, \ldots h_n, \tilde{h}_1, \ldots \tilde{h}_n$, each of degree $2n-1$ satisfying

$$h_i(x_j) = \delta_{ij}, \qquad h_i'(x_j) = 0$$

and

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Then

$$H_n\left(x\right)=\sum_{i=1}^{n}\left[y_i h_i\left(x\right)+y_i'\tilde{h}_i\left(x\right)\right]$$

is the Hermite interpolating polynomial.

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Similarly

$$h_i(x) = \left(1 - 2L_i'(x_i)(x - x_i)\right)\left[L_i(x)\right]^2$$

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Thus $R(x)$must be identically zero!

The error can be shown to be

$$f(x) - H_n(x) = [\Psi_n(x)]^2 \frac{f^{(2n)}(x)}{(2n)!}$$

Gauss quadrature

Recall that the Gauss quadrature formula is

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where the freedom of choice of the n weights w_i and the n nodes x_i is expolited to get an expression that is correct for all polynomials up to degree $2n-1$.

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As we have already seen, in principle we can find the w_i and x_i from the $2n$ equations

$$\sum_{i=1}^{n} w_i x_i^j = \begin{cases} 0 & \text{for } j = 1, 3, \ldots, 2n-1 \\ \frac{2}{j+1} & \text{for } j = 2, 4, \ldots, 2n-2 \end{cases}$$

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This is a set of non-linear equations - not only are they difficult to solve, the existence of solutions for general n is not even clear *a priori.*

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