Numerical Integration

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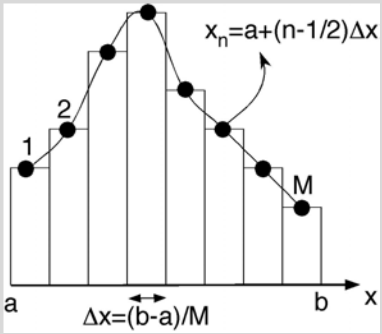
New toolbox (use it! it's user friendly):

1. **Gaussian quadratures (orthogonal functions)**
2. **Newton's method**

Numerical Integration

- **Numerical integration = weighted sum of function values**

$$S = \int_a^b f(x)dx \cong \sum_{k=0}^{n-1} w_k f(x_k)$$

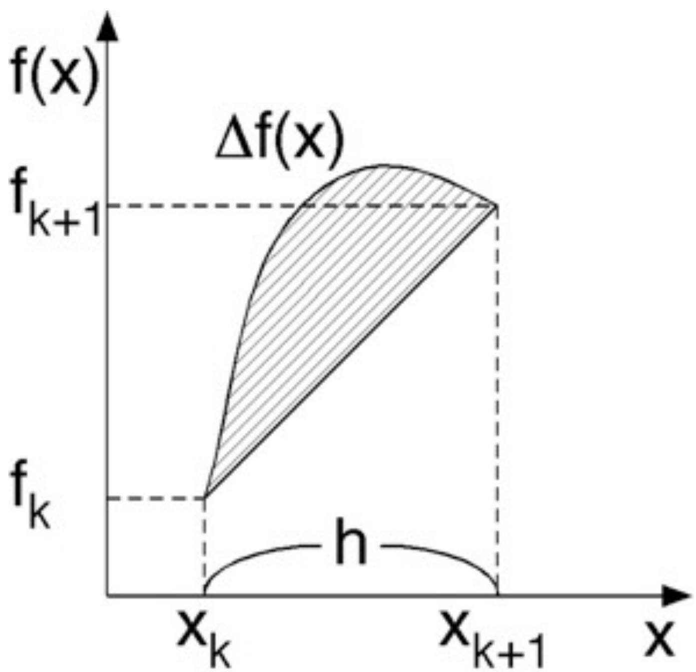


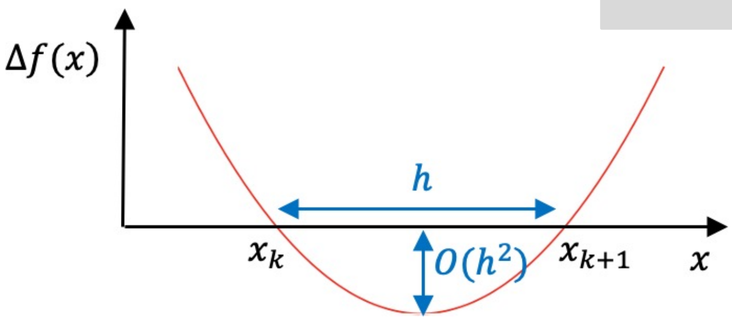
Piecewise constant
$O(h)$ approximation

$$\begin{cases} x_k = kh = (b-a)k/n \\ w_k = h \end{cases}$$

- **Trapezoid quadrature: Piecewise linear approximation**

$$f(x) \cong f_k + (x - x_k)(f_{k+1} - f_k)/h \quad x \in [x_k, x_{k+1}]$$





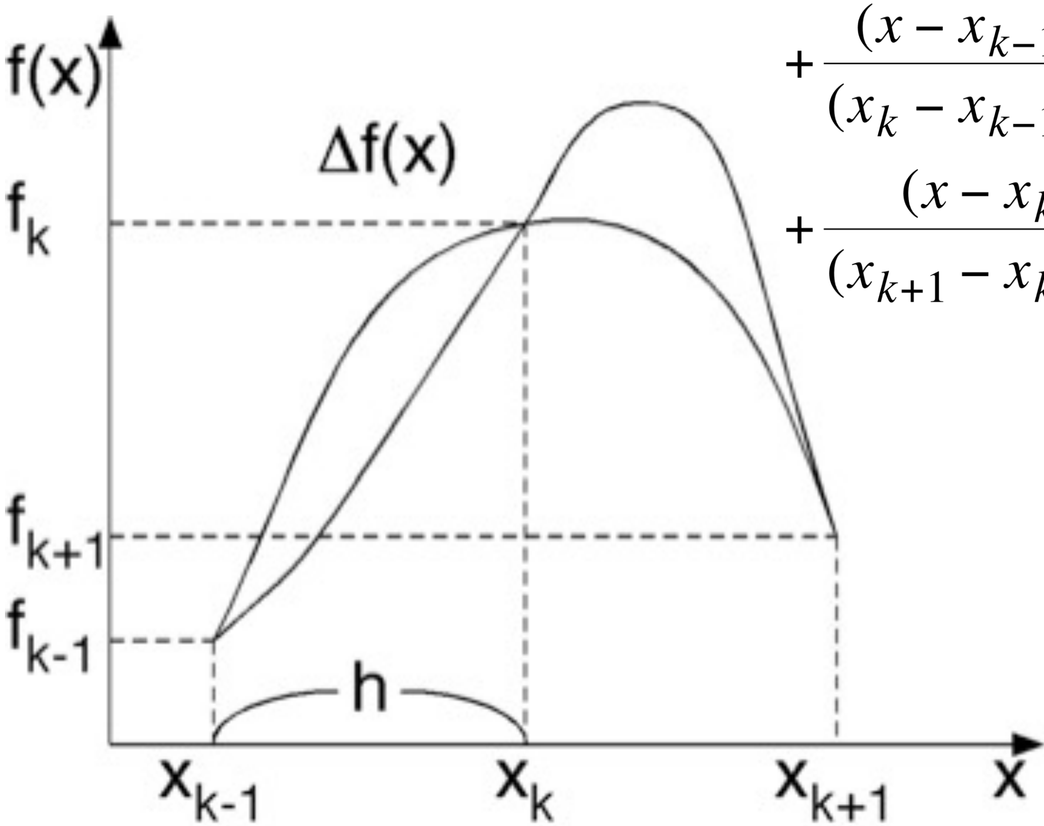
$$error = height\left(O(h^2)\right) \times base(h) \times \#\ of\ bins\left(\frac{b-a}{h}\right) = O(h^2)$$

Resulting area: $\int_a^b f(x)dx \cong \frac{h}{2}\sum_{k=0}^{n-1}(f_k + f_{k+1}) + O(h^2)$

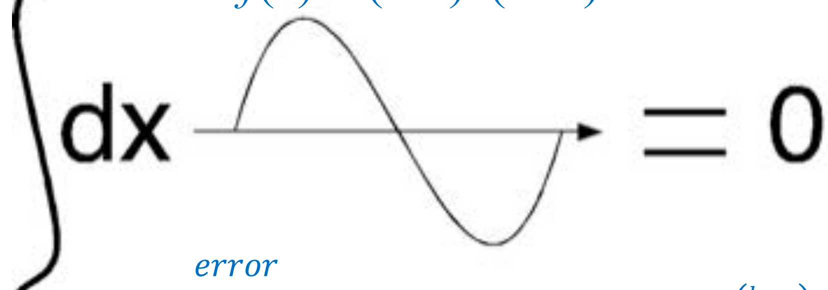
Simpson Rule

- **Simpson quadrature: Piecewise quadratic approximation**
- **Lagrange interpolation:**

$$f(x) \cong \frac{(x-x_k)(x-x_{k+1})}{(x_{k-1}-x_k)(x_{k-1}-x_{k+1})} f_{k-1} + \frac{(x-x_{k-1})(x-x_{k+1})}{(x_k-x_{k-1})(x_k-x_{k+1})} f_k + \frac{(x-x_{k-1})(x-x_k)}{(x_{k+1}-x_{k-1})(x_{k+1}-x_k)} f_{k+1}$$

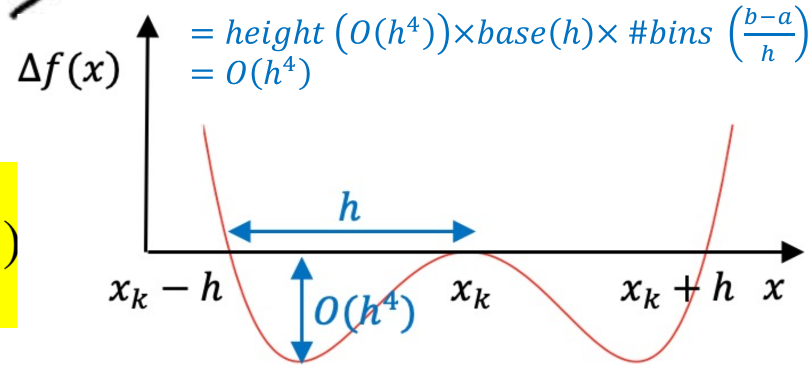


$\Delta f(x) = c(x-h)x(x+h)$



$$\int_a^b f(x)dx \cong \frac{h}{3} \sum_{l=0}^{n/2-1} (f_{2l} + 4f_{2l+1} + f_{2l+2}) + O(h^4)$$

$error$
$= height\ (O(h^4)) \times base(h) \times \#bins\ \left(\frac{b-a}{h}\right)$
$= O(h^4)$



Gaussian Quadratures

- **Idea of Gaussian quadrature: Freedom to choose both weighting coefficients & the location of abscissas to evaluate the function**
- **Gaussian quadrature: Chooses the weight & abscissas to make the integral exact for a class of integrands "polynomials times some known function $W(x)$".**
  - **Gauss-Legendre:** $W(x) = 1; -1 < x < 1$
  - **Gauss-Chebyshev:** $W(x) = (1 - x^2)^{-1/2}; -1 < x < 1$
  - •••

$$\int_a^b W(x) f(x) dx = \sum_{k=1}^{n} w_k f(x_k)$$

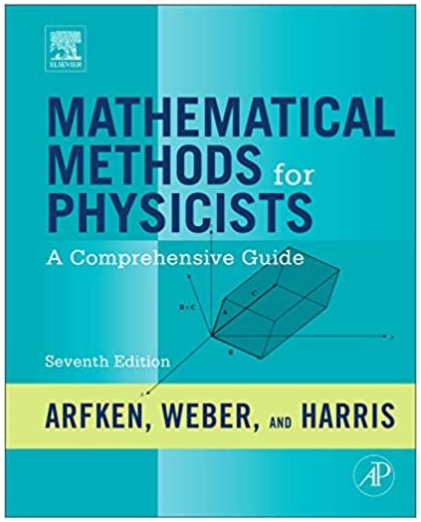
- **New toolbox: (1) orthogonal functions (recursive generation *via* a generating function); (2) Newton method for root finding**

See gauleg-driver.c **&** gauleg.c

W.H. Press, B.P. Flannery, S.A. Teukolsky, & W.T. Vetterling,
Numerical Recipes, 2nd Ed. (Cambridge U Press, '93), Sec. 4.5

Orthogonal Functions

- Gaussian quadratures are defined through orthogonal functions
- Orthogonal functions are often introduced as solutions to differential equations
- Examples: Legendre, Bessel, Laguerre, Hermite, Chebyshev, …
- Operationally well-defined to compute the function values & derivatives
- Efficiently computable through recursive relations (more than elementary functions like sin(x), exp(x), ...)



Orthogonal Functions

- **Scalar product (vector space):**

$$\langle f \mid g \rangle \equiv \int_a^b W(x) f(x) g(x) dx$$

- **Orthonormal set of functions: Mutually orthogonal & normalized**

$$\langle p_m | p_n \rangle = \delta_{m,n} = \begin{cases} 1, & m = n \\ 0, & m \neq n \end{cases}$$

- **Recurrence relation to construct an orthonormal set:**

$$p_{-1}(x) \equiv 0$$
$$p_0(x) \equiv 1$$
$$p_{j+1}(x) = (x - a_j) p_j(x) - b_j p_{j-1}(x) \quad j = 0,1,2,\ldots$$

$$a_j = \frac{\langle x p_j | p_j \rangle}{\langle p_j | p_j \rangle} \quad j = 0,1,\ldots$$

$$b_j = \frac{\langle p_j | p_j \rangle}{\langle p_{j-1} | p_{j-1} \rangle} \quad j = 1,2,\ldots$$

(Theorem) $p_j(x)$ has exactly j distinct roots in (a,b), & the roots interleave the j–1 roots of $p_{j-1}(x)$

Legendre Polynomial

$$W(x) = 1 \quad -1 < x < 1$$

- **Recursive function evaluation**

$$(j+1)P_{j+1} = (2j+1)xP_j - jP_{j-1} \quad P_0 = 1 \quad P_1 = x$$

- **Generating function: The recurrence may be obtained through the Taylor expansion of the following function with respect to *t***

$$g(t,x) = \frac{1}{\sqrt{1-2xt+t^2}} \equiv \sum_{j=0}^{\infty} P_j(x)t^j$$

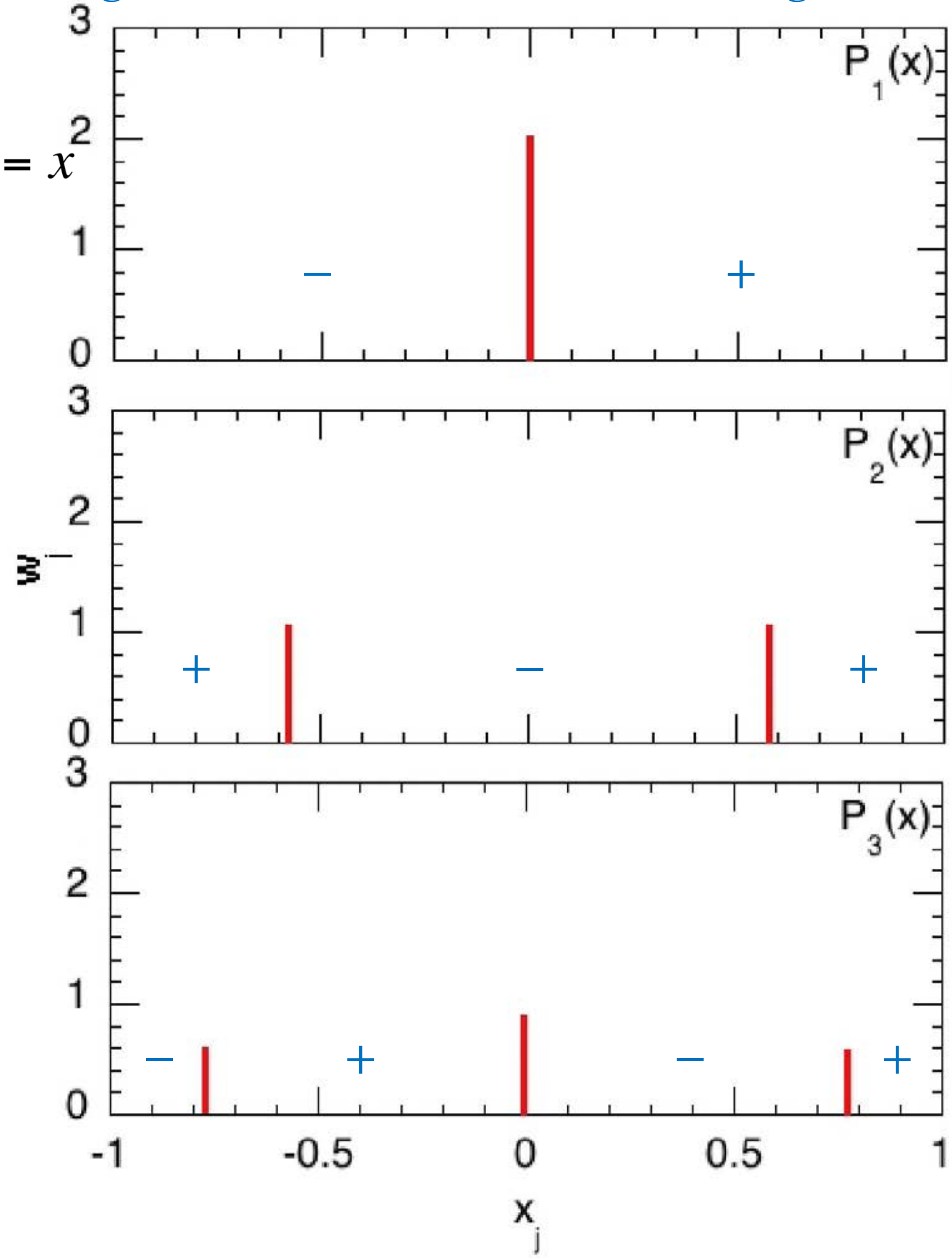
(Hint) Differentiate both sides by *t* & compare the coefficients of t^j

- **Function derivative: A recurrence derived by differentiating *g* by *x***

$$(x^2-1)P_j' = jxP_j - jP_{j-1}$$

See lecture on recursive formula for Legendre polynomials

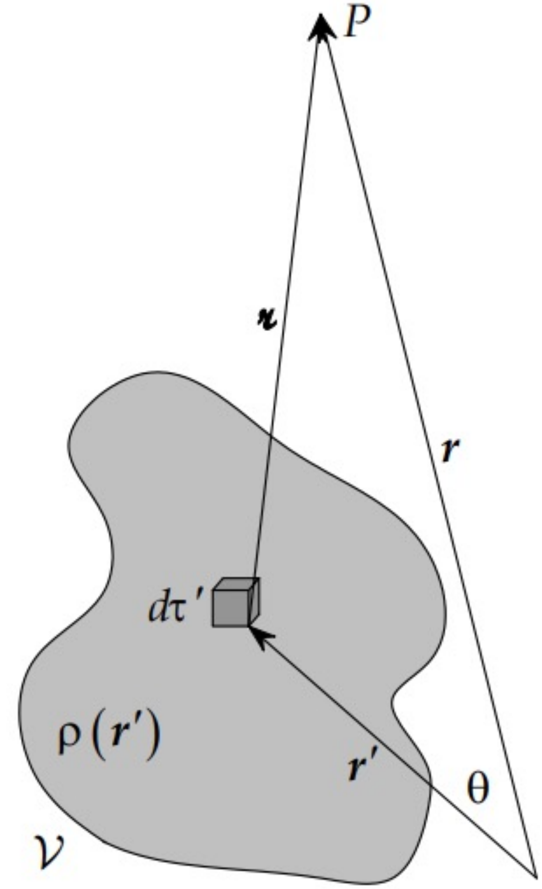
Orthogonalization necessitates interleaving nodes



Origin of Legendre Polynomial

- **Generating function of the Legendre polynomial is used for multipole expansion in electrostatics**

$$
\begin{aligned}
\frac{1}{|\vec{r}-\vec{r}'|} &= \frac{1}{\sqrt{r^2 - 2rr'\cos\theta + r'^2}} \\
&= \frac{1}{r\sqrt{1 - 2\frac{r'}{r}\cos\theta + \left(\frac{r'}{r}\right)^2}} \\
&= \frac{1}{r}\sum_{j=0}^{\infty} P_j(\cos\theta)\left(\frac{r'}{r}\right)^j
\end{aligned}
$$

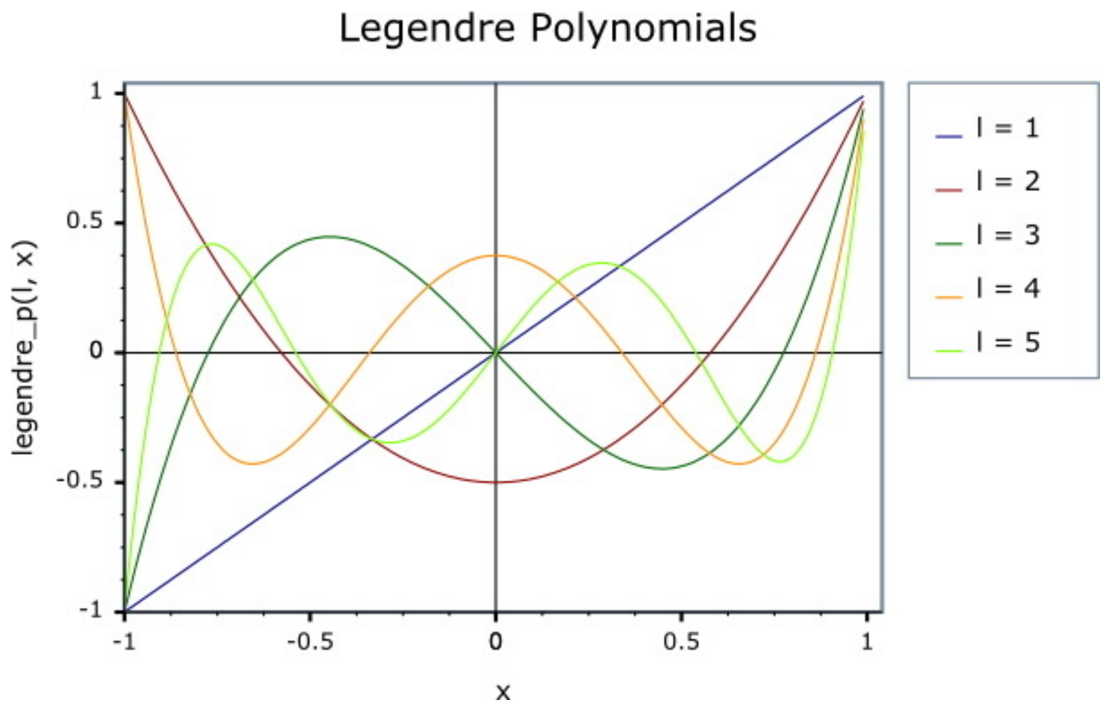


See lecture note on *O*(*N*) fast multipole method

Open-source code: S. Ogata *et al*., *Comput. Phys. Commun* **153**, 445 ('03)

Gauss-Legendre Quadrature

$$\int_{-1}^{1} W(x) f(x) dx = \sum_{k=1}^{n} w_k f(x_k)$$



- **Abscissae from roots, x_k**

$$P_n(x_k) = 0 \quad k = 1, \dots, n$$

- **Weights, w_k: To reproduce some integrals exactly (linear equation)**

$$\int_{-1}^{1} P_0(x) P_n(x) dx = \frac{2}{2n+1} \delta_{0,n} = \sum_{k=1}^{n} w_k P_n(x_k)$$

or

$$w_k = \frac{2}{n P_{n-1}(x_k) P_n'(x_k)} = \frac{2}{(1 - x_k^2)[P_n'(x_k)]^2}$$

Note $(x^2 - 1) P_n' = \underbrace{n x P_n}_{0 \text{ at root}} - n P_{n-1}$

Newton's Method for Root Finding

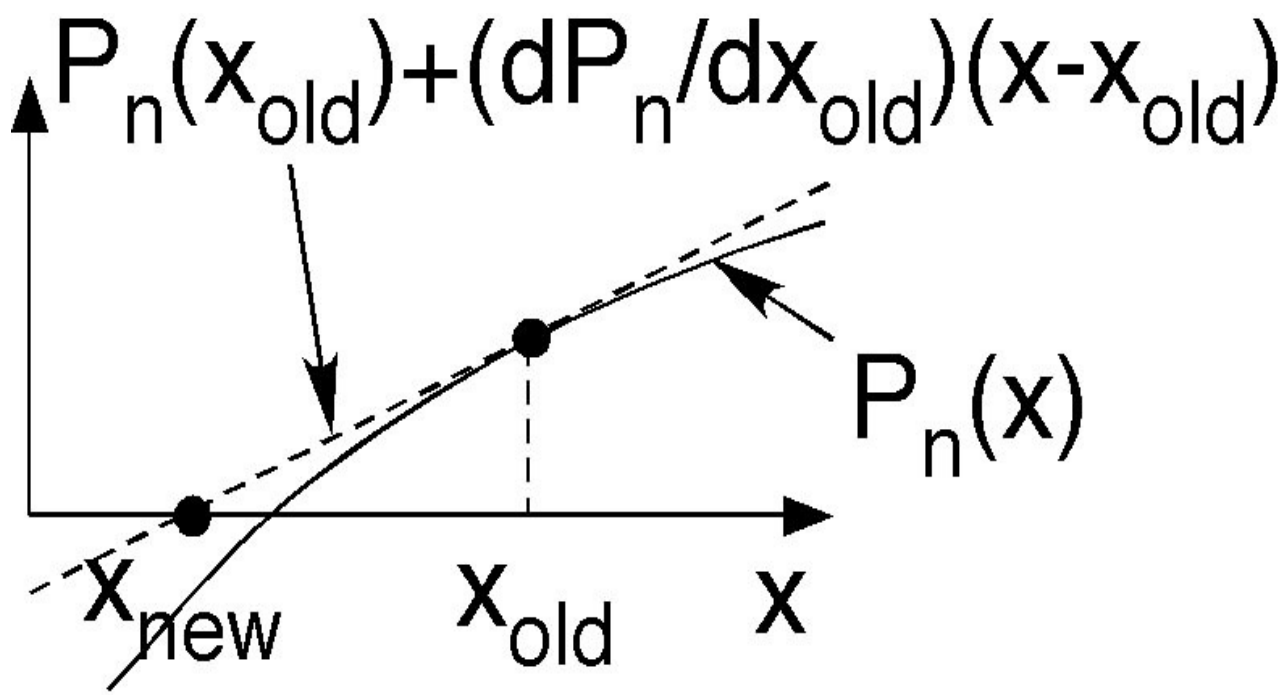
- **Problem:** **Find a root of a function**

$$P_n(x) = 0$$

- **Newton iteration:** **Successive linear approximation of the function**
  1. **Start from an initial guess, x_0, of the root**
  2. **Given the k-th guess, x_k, obtain a refined guess, x_{k+1}, from the linear fit:**

$$P_n(x) \cong P_n'(x_k)(x - x_k) + P_n(x_k) = 0$$

$$\rightarrow \boxed{x_{k+1} = x_k - \frac{P_n(x_k)}{P_n'(x_k)}}$$



Gauss-Legendre Program

- **Given the lower & upper limits (x_1 & x_2) of integration & n, returns the abscissas & weights of the Gauss-Legendre n-point quadrature in $x[1:n]$ & $w[1:n]$.**

```
void gauleg(float x1,float x2,float x[],float w[],int n) {
  int m,j,i;
  double z1,z,xm,xl,pp,p3,p2,p1;
  m=(n+1)/2; // Find only half the roots because of symmetry
  xm=0.5*(x2+x1);
  xl=0.5*(x2-x1);
  for (i=1;i<=m;i++) {
    z=cos(3.141592654*(i-0.25)/(n+0.5));
    do {
      p1=1.0; p2=0.0;
      for (j=1;j<=n;j++) { // Recurrence relation
        p3=p2; p2=p1;
        p1=((2.0*j-1.0)*z*p2-(j-1.0)*p3)/j;
      }
      pp=n*(z*p1-p2)/(z*z-1.0); // Derivative
      z1=z;
      z=z1-p1/pp; // Newton's method
    } while (fabs(z-z1) > EPS); // EPS=3.0e-11
    x[i]=xm-xl*z;
    x[n+1-i]=xm+xl*z;
    w[i]=2.0*xl/((1.0-z*z)*pp*pp);
    w[n+1-i]=w[i]; // Weights
  }
}
```

$$\begin{cases} P_{-1} = 0 \\ P_0 = 1 \\ jP_j = (2j-1)zP_{j-1} - (j-1)P_{j-2} \end{cases}$$

$$(z^2 - 1)P'_j = jzP_j - jP_{j-1}$$

$$z \leftarrow z - \frac{P_n(z)}{P'_n(z)}$$

$$w_i = \frac{2}{(1 - x_i^2)[P'_n(x_i)]^2}$$

How to Use the Gauss-Legendre Program

$ cc -o gauleg-driver gauleg-driver.c gauleg.c -lm

```
//gauleg-driver.c
#include <stdio.h>
#include <math.h>

double *dvector(int, int);
void gauleg(double, double, double *, double *, int);

int main() {
  double *x,*w;
  double x1= -1.0,x2=1.0,sum;
  int N,i;
  printf("Input the number of quadrature points\n");
  scanf("%d",&N);
  x = dvector(1,N);  // Allocate & use array elements x[1], ..., x[N]
  w = dvector(1,N);  // It's Numerical Recipe's utility function (in gauleg.c)
  gauleg(x1,x2,x,w,N);
  sum=0.0;
  for (i=1; i<=N; i++)
    sum += w[i]*2.0/(1.0 + x[i]*x[i]);
  printf("Integration = %f\n", sum);
}
```

$$\pi = \int_{-1}^{1} dx \frac{2}{x^2+1} \cong \sum_{k=1}^{N} w_k \frac{1}{x_k^2+1}$$

Recursive Function Evaluation

- **Legendre function**

```
p1=1.0; p2=0.0;
for (j=1;j<=n;j++) { // Recurrence relation
  p3=p2;
  p2=p1;
  p1=((2.0*j-1.0)*z*p2-(j-1.0)*p3)/j;
}
pp=n*(z*p1-p2)/(z*z-1.0); // Derivative
```

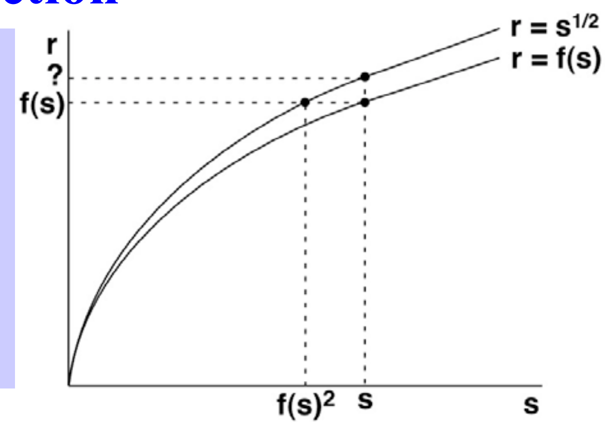
$$\begin{cases} P_{-1} = 0 \\ P_0 = 1 \\ jP_j = (2j-1)zP_{j-1} - (j-1)P_{j-2} \end{cases}$$

$$(z^2-1)P_j' = jzP_j - jP_{j-1}$$

- **Compare it with a (low-accuracy) square-root function**

```
#define C0 0.188030699
#define C1 1.48359853
#define C2 (-1.0979059)
#define C3 0.430357353

fs = C0+x*(C1+x*(C2+x*C3)); // Polynomial approximation
sr = fs+0.5*(x/fs-fs); // Newton correction
```



$$r - f(s) \approx \frac{dr}{ds}(s - f(s)^2)$$

$$\frac{dr}{ds} = \frac{d}{ds}s^{1/2} = \frac{1}{2}s^{-1/2} \approx \frac{1}{2f(s)}$$

$$\therefore r - f(s) = \frac{1}{2f(s)}(s - f(s)^2) = \frac{1}{2}\left(\frac{s}{f(s)} - f(s)^2\right)$$

Where to Go from Here?

- **Gaussian quadrature for multiscale simulations?** *cf*. quasicontinuum method, where each function evaluation is an expensive quantum-mechanical calculation
  cf. Knap & Ortiz, *J. Mech. Phys. Solids* **49**, 1899 (2001)
- **Adaptive Gaussian quadrature?** *cf*. power of Metropolis importance sampling: $2 \times 10^{6} \ll 2^{400} \sim 10^{120}$ configurations
  Lepage, *J. Comput. Phys.* **27**, 192 (1978)
  Evila *et al*., *IEEE T. Signal Process.* **69**, 474 (2021)
- **Related technique: Bayesian optimization (active learning, kriging), using Gaussian process regression with minimal number of function evaluations (trade-off between *exploration* & *exploitation*)**
  Bassman *et al*., *npj Comput. Mater.* **4**, 74 (2018)
  Shields *et al*., *Nature* **590**, 89 (2021)