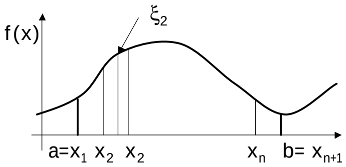
Integration

- One of the motivating problem for the invention of integral calculus was the calculation of areas and volumes of irregularly shaped regions (quadrature).
- By analytical integration of an integrand function f(x) $\int f(x)\,dx = F(x) + C$ must be found so that F(x) is antiderivative of f(x) => $F'(x) = f(x)$.
- Using Fundamental theorem of Calculus definite integral will be calculated as:
  $I(f) = \int_a^b f(x)\,dx = F(b)-F(a)$
- Some integrals can not be calculated in such a closed form (e.g., $f(x) = e^{-x^2}$), other are too complicated. So, we often need numerical methods to evaluate numerical integrals.

Numerical Integration



- $I(f) = \int_a^b f(x)\,dx = F(b)-F(a) \cong \sum_{i=1}^{n} (x_{i+1} - x_i)\, f(\xi_i) = R_n$
  for $a=x_1<x_2<...<x_n<x_{n+1}=b$, $\xi_i \in [x_i, x_{i+1}]$, i=1...n
- If we have $\lim_{n\to\infty} R_n = R$, where R is finite, then f is said to be Riemann Integrable on [a,b], and the value of the integral is R.

Existence, Conditioning

- EXISTENCE:
  The integral exists if the function f(x) is bounded and has finite number of discontinuities.
- CONDITIONING:
  For determination of Conditioning define the infinite norm of f(x) as: $\text{norm}_\infty f(x) = \max_{x\in[a,b]} |f(x)|$.
  Suppose that f^ is a perturbation of the integrand function f, then we have:

  $\Delta(\text{output}) = |I(f\hat{})-I(f)| = |\int_a^b f\hat{}(x)\,dx - \int_a^b f(x)\,dx| = \int_a^b |f\hat{}(x) - f(x)|\,dx = (b-a)\,\text{norm}_\infty(f\hat{}-f) =$
  cond * Δ(input).
  Cond is at most (b-a) -> well conditioned (smoothing).

Quadrature Rule Derived by Polynomials

- For n points the interpolating polynomial of order (n-1) can be derived (e.g., represented in the Lagrange form):
  $p_{n-1}(x) = f(x_1)\, l_1(x) + ... + f(x_n)\, l_n(x)$
- Integral of interpolant is taken as an approximate integral of the original function f(x):
  $\int_a^b p_{n-1}(x)\,dx = f(x_1) \int_a^b l_1(x)dx + ... + f(x_n) \int_a^b l_n(x)dx$
  The above expression is the quadrature rule with weights equal to integrals of Lagrange basis functions.

Accuracy Estimation

- $|I(f)-Q_n(f)| = |I(f)-I(p_{n-1})|$
  (from the previous slide on the quadrature approximation)
  $\le (b-a)\,\text{norm}_\infty(f - p_{n-1})$
  (from the error of interpolation - Chap 5)
  $\le (1/4n)\,(b-a)\,h^n\,\text{norm}_\infty f^{(n)}$
  (because (b-a) = n*h)
  $\le (1/4)\,h^{n+1}\,\text{norm}_\infty f^{(n)}$.
- With larger number of points n or/and smaller h the accuracy can be improved.

Stability of Quadrature Rules

- $|Q_n(f\hat{})-Q_n(f)| = |Q_n(f\hat{}-f)| = |\sum_{i=1}^{n} w_i\,(f\hat{}(x_i) - f(x_i))|$
  $\le \sum_{i=1}^{n} (|w_i|_* |(f\hat{}(x_i) - f(x_i))|)$
  $\le (\sum_{i=1}^{n} |w_i|)\,\text{norm}_\infty(f\hat{}- f)$.
- From the first moment equation we know that $\sum_{i=1}^{n} |w_i| = (b-a)$.
- If all weights are nonnegative then the absolute condition number of the quadrature rule is (b-a) (same as integration) - stable quadrature rule.
- If some weights are negative then the absolute condition number of the quadrature rule can be much larger - unstable quadrature rule.

Change of Interval [α,β]->[a,b]

- $\int_\alpha^\beta f(x)\,dx \;\Rightarrow\; \int_a^b g(t)\,dt = I(g)$
  $t=[(b-a)x+a\beta-b\alpha]/(\beta-\alpha)$ $\quad dt/dx = (b-a)/(\beta-\alpha)$

- $\int_a^b g(t)\,dt = (b-a)/(\beta-\alpha) \int_\alpha^\beta g([(b-a)x+a\beta-b\alpha]/(\beta-\alpha))\,dx$
  $\approx (b-a)/(\beta-\alpha) \sum_{i=1}^n w_i\, g([(b-a)x_i+a\beta-b\alpha]/(\beta-\alpha))$
- Example: Use two-point Gaussian quadrature G_2 on [-1,1] to approximate the integral: $I(g) = \int_0^1 e^{-t^2}\,dt$
- $x_1 = -1/\mathrm{sqrt}(3)$, $x_2 = 1/\mathrm{sqrt}(3)$, $w_1 = w_1 = 1$,
  $t=(x+1)/2$, $(b-a)/(\beta-\alpha) = 1/2$

$G_2(g) = 1/2\,[\,e^{-((x_1+1)/2)^2} + e^{-((x_2+1)/2)^2}\,] \approx 0.746595$

which is more accurate as by Simpson's rule, despite using only two points.

Adaptive quadrature

```
procedure adaptquad(f,a,b,I^)
  I1=Qn1(f,a,b)          //evaluate quadrature rules
  I2=Qn2(f,a,b)
  m=a+(b-a)/2            //compute midpoint of the
  interval
  if (m<=a)or(m>=b)      //if no more machine numbers
     warning             //tolerance may not be met
     return I2           //return best result
  end
  if I^+(I2-I1) = I^ then   //converg.tolerance met
     return I2           //return converged result
  else                   //refine recursively
     return(adaptquad(f,a,m,I^) +
            adaptquad(f,m,b,I^))
  end
end
```


Integral Equation

- Integral equations arise in observational sciences (e.g., astronomy, seismology, spectrometry). A typical representative of integral equations is the Fredholm IE of the first kind
  $\int_a^b K(s,t)u(t)dt=f(s)$
  K and f are known, u must be determined.
- We have to determine a function, which results in known definite integral. It is obvious that this problem could be ill-conditioned, because many different functions can have same integrals.
- Solution procedure:
  - discretize s, and t,
  - Replace the integral by quadrature rule,
  - Solve the resulting linear system.

Integral Equation

- IEs arise in observational sciences (e.g., astronomy, seismology, spectrometry).
  K - response function of an calibrated instrument,
  f – measured data and,
  u - signal to be sought.
- In effect, we try to resolve the measured data as a linear combination of standard signals.
- $\int_{-1}^1 (1-a*s*t)u(t)dt=1$, $\quad K= 1-a*s*t$, $f(s)=1$, $a>0$
  - taking 2 subintervals and using midpoint rule: t1=-1/2, t2=1/2, w1=w2=1. Taking also s1=-1/2, s2=1/2 we get:

    Ax=[1+a/4, 1-a/4; 1-a/4, 1+a/4]*[x1;x2]=[1;1]=y

    with the solution x=[1/2; 1/2], which is independent of a.
- If a is small (insensitive instrument), **A** becomes near singular, ill-conditioned, error can be arbitrary large.