* Secant method — when the Jacobian DF is not available (or difficult to evaluate), it can be approximated with a matrix D_k satisfying the secant condition:

$$D_k(\bar{x}_k - \bar{x}_{k-1}) = \bar{F}(x_k) - \bar{F}(\bar{x}_{k-1})$$

The choice of D_k is nonunique (unlike in 1D...)

Broyden's method

Specify an "initial guess" D_0 (e.g. $D_0 = I$)

Then iterate

$$D_k(\bar{x}_{k+1} - \bar{x}_k) = -\bar{F}(\bar{x}_k) \qquad \text{(Newton step)}$$

$$D_{k+1} = D_k + \frac{\bar{F}(x_k)(\bar{x}_{k+1} - \bar{x}_k)}{\|\bar{x}_{k+1} - \bar{x}_k\|^2} \qquad \text{(update)}$$

for $k = 0, 1, \ldots$

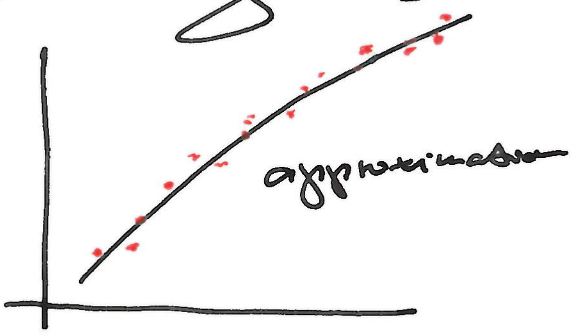
Remarks

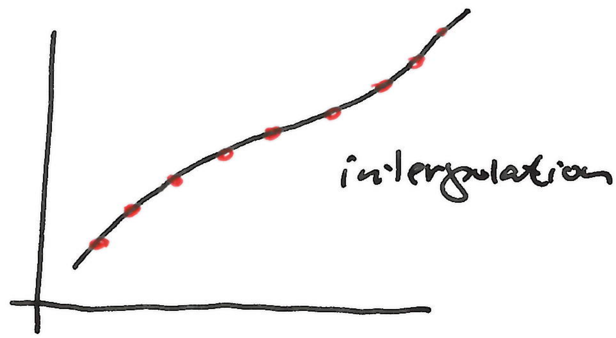
* superlinear convergence
* implemented in MATLAB function "fsolve"

2) INTERPOLATION & APPROXIMATION

(Grasselli & Pelinovsky – chapter 5, Trefethen)

Basic definitions





Given a set of data points $\{x_i, y_i\}_{i=1}^{N}$ and a function $f(x) = \sum_{i=1}^{M} a_i \phi_i(x)$, where $\{\phi_i\}_{i=1}^{M}$ are suitably chosen <u>basis functions</u>

* the <u>interpolation problem</u> is:

find $\{a_i\}_{i=1}^{M}$ ST $f(x_i) = y_i$, $i=1,\dots,M$

* the <u>approximation problem</u> is

find $\{a_i\}_{i=1}^{M}$ ST $\sum_{k=1}^{N} [y_k - f(x_k)]^2 = \min$

Note that usually $N \gg M$.

<u>Questions:</u>

* What are good choices of the basis functions ϕ_i?
  - easy to compute
  - fast decrease of errors with $M \to \infty$

* How to determine the expansion coefficients $a_1, \dots, a_M$?

* Estimates of interpolation/approximation errors
* computational cost

POLYNOMIALS – a first natural choice of basis functions

* MATLAB convention for indexing coefficients

$$P_n(x) = c_1 x^n + c_2 x^{n-1} + \dots + c_n x_1 + c_{n+1}$$

* P_n is determined by a coefficient vector $c \in \mathbb{R}^{n+1}$

Hence, polynomials P_n can be identified with a finite-dimensional vector space

$$P_n \in V = \mathbb{R}^{n+1}$$

* trigonometric functions can also be interpreted as (complex) polynomials

set $z = e^{i\varphi} = \cos\varphi + i\sin\varphi$

then, $z^k = \cos(k\varphi) + i\sin(k\varphi)$

* Roots of polynomials

Fundamental theorem of Algebra – a polynomial of degree n has exactly n possibly multiple complex roots

$$P_n(x) = c_1 (x-x_1)^{m_1}(x-x_2)^{m_2} \cdot \ldots \cdot (x-x_k)^{m_k}$$

$x_1, \dots, x_k$ – distinct roots with multiplicities $m_1, \dots, m_k$

* $m_1 + m_2 + \dots + m_k = n$

Remark

Given the numbers $c_1, c_2, \dots, c_{n+1} \in \mathbb{R}$, consider an $(n \times n)$ companion matrix

$$A = \frac{1}{c_1} \begin{bmatrix} 0 & 0 & \cdots & 0 & -c_{n+1} \\ c_1 & 0 & \cdots & 0 & -c_n \\ 0 & c_1 & & 0 & -c_{n-1} \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_1 & c_2 \end{bmatrix}$$

It can be shown that

$$p_n(\lambda) = \det(A - \lambda I)$$

and the roots of $p_n(\lambda)$ are given by the eigenvalues of the companion matrix A. Solving the eigenvalue problem for the companion matrix A the preferred way of finding the roots of a polynomial (MATLAB's function roots), because

- all roots are found in one computation (both real and complex)

- it is a numerically stable and efficient procedure (no issue of the initial guess, etc.)

* Representation of polynomials: power series (coefficients) vs. factorized (roots + c_1)

* Differentiation and integration of polynomials is trivial

$$p_n'(x) = n c_1 x^{n-1} + (n-1) c_2 x^{n-2} + \dots + c_n$$

$$\int p_n(x)\,dx = \frac{c_1}{n+1} x^{n+1} + \frac{c_2}{n} x^n + \dots + \frac{c_n}{2} x^2 + c_{n+1} x + c_{n+2}$$

* Multiplication of polynomials $P_n(x) \cdot P_m(x) = P_{n+m}(x)$

$$\left(\sum_{i=1}^{n+1} a_i x^{n+1-i}\right)\left(\sum_{j=1}^{m+1} b_j x^{m+1-j}\right) = \sum_{l=1}^{n+m+1} c_l x^{n+m+1-l}$$

c_l - complicated functions of $\{a_i\}$ and $\{b_j\}$

* Division of polynomials leads to <u>rational functions</u> (not polynomials anymore)

$$R(x) = \frac{P_n(x)}{P_m(x)}$$

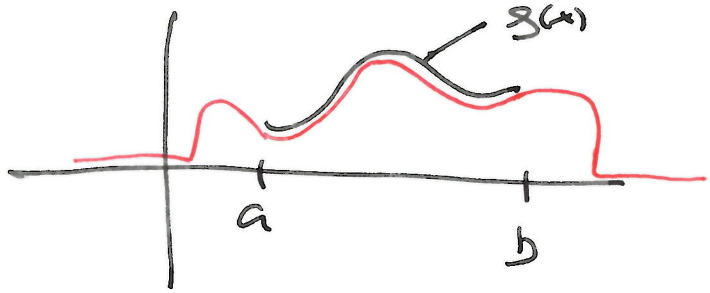
* <u>Weierstrass Approximation Theorem (1885)</u>

Let f be ~~an~~ a continuous function on $[a,b]$ and let $\varepsilon > 0$ be arbitrary. Then, there exists a polynomial p_n such that

$$\max_{a \le x \le b} |p_n(x) - f(x)| < \varepsilon$$

Proof (outline) (original proof given by Weierstrass)

- extend f to a continuous function $\tilde{f}$ with compact support defined on the real line



- consider an initial-value problem for the diffusion equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ on the real line $x \in \mathbb{R}$; as the initial data at $t=0$ take $\tilde{f}$, i.e., $u(0,x) = \tilde{f}(x)$, $x \in \mathbb{R}$

- the solution is given by computing the convolution of $\tilde{f}$ with the gaussian (heat) kernel $G(t,x) = \frac{1}{\sqrt{4\pi t}} e^{-\frac{x^2}{4t}}$

$$u(t,x) = \int_{-\infty}^{\infty} \tilde{f}(x') \, G(t, x-x') \, dx'$$

Note that $u(t,x) \to \tilde{f}(x)$ uniformly in x as $t \to 0$

Thus, $u(t,x)$ can be arbitrarily close to $f(x)$ for $x \in [a,b]$. Due to smoothness of the kernel $G(t,x)$, $\forall t>0$ $u(t,x)$ is analytic in x. Thus, $u(t,x)$ has a uniformly convergent Taylor series which can be truncated at a suitable order to give a polynomial such that

$$\max_{a \le x \le b} |p_n(x) - f(x)| < \varepsilon$$

∎

Remarks

* central result of approximation theory
* the theorem <u>is not</u> constructive; it's not even known what the degree of the polynomial should be

2.1 Interpolating Polynomials

Given $(N+1)$ points $\{(x_i, y_i)\}_{i=0}^{N}$, find a degree N polynomial passing through all these points.

$y(x) = \sum_{k=0}^{N} a_k x^k$ has $(N+1)$ unknown coefficients which can be determined using the following conditions

$$\begin{cases} \sum_{k=0}^{N} a_k x_0^k = y_0 \\ \sum_{k=0}^{N} a_k x_1^k = y_1 \\ \vdots \\ \sum_{k=0}^{N} a_k x_N^k = y_N \end{cases}$$