Homotopy continuation

1 revision 1D case

$$f(x) = x^d + a_1 x^{d-1} + \cdots + a_d$$

aim: compute all zeros of $f(x)$

introduce homotopy: $H(x,t) = t(x^d - 1) + (1-t) f(x)$

thus $H(x,1) = x^d - 1$ and $H(x,0) = f(x)$

inserting $f(x)$ one gets

$$\boxed{H(x,t) = x^d + (1-t)\sum_{k=1}^{d} a_k x^{d-k} - t}$$

- $H(x,t) = 0$ defines d algebraic curves in $[0,1] \times \mathbb{C}$ with $x = \hat{x}_j(t)$ where

$$\hat{x}_j(1) = e^{2\pi i j/d}, \quad j = 0, \dots, d-1 \quad \text{and}$$

$$f(\hat{x}_j(0)) = 0$$

> **Definition.** The homotopy continuation method is a numerical method to compute the zeros $\hat{x}_j(0)$ using the starting "approximation" $\hat{x}_j(1)$ and a numerical algorithm to get close to $\hat{x}_j(0)$.

the partial derivatives of H are

$$\frac{\partial H}{\partial t} = -\sum_{k=1}^{d} a_k x^{d-k} - 1 \quad \text{and} \quad \frac{\partial H}{\partial x} = d x^{d-1} + (1-t)\sum_{k=1}^{d-1} (d-k) a_k x^{d-k-1}$$

where a path $x(t)$ is differentiable one has

$$\frac{d H(x(t),t)}{dt} = \frac{\partial H}{\partial t}(x(t),t) + \frac{\partial H}{\partial x}\frac{dx(t)}{dt} = 0$$

$\hookrightarrow$

and thus $\frac{dx(t)}{dt} = - \frac{\frac{\partial H}{\partial t}(x(t),t)}{\frac{\partial H}{\partial x}(x(t),t)}$

i.e.

$$\boxed{\frac{dx}{dt} = \frac{\sum_{k=1}^{d} a_k x^{d-k} - 1}{d\cdot x^{d-1} + (1-t)\sum_{k=1}^{d-1}(d-k)a_k x^{d-k-1}}} \quad (*)$$

$x(t)$ then admits the integral eqn

$$\boxed{x(t) = x(1) - \int_t^1 r(x(t),t)\,dt}$$

where $r(x,t)$ is the r.h.s. of $(*)$

- discretise parameter t : $t_\ell = (M-\ell)h$
  $t_\ell = t_{\ell-1} - h$, $t_0 = 1$, $t_M = 0$ $\quad h = \frac{1}{M}$
  $\ell = 0, \dots, M$ $\quad$ - we get from $(*)$:

$$\boxed{\tilde{x}^{(j)}(t_\ell) = \tilde{x}^{(j)}(t_{\ell-1}) + \int_{t_\ell}^{t_{\ell-1}} r(\tilde{x}^{(j)}(t),t)\,dt}$$

- we now approximate $\tilde{x}^{j}(t_\ell) \approx w_\ell^{(j)}$ using a predictor-corrector approach:

(1) <u>predictor</u> gives $\hat{w}_\ell^{(j)}$ using numerical integration

(2) use Newton's method with start $\hat{w}_\ell^{(j)}$ to get $w_\ell^{(j)}$ (<u>corrector</u>)

- approximate $\tilde{x}^{(j)}(t_k) \approx \hat{\omega}_\ell^{(j)}$ by one-step method

$$\boxed{\begin{aligned} \hat{\omega}_\ell^{(j)} &= \text{approx. of } \tilde{x}^{(j)}(t_\ell), \quad \ell = 0, \dots, M \\ \hat{\omega}_\ell^{(j)} &= \omega_{\ell-1}^{j} + h\,\Phi(\omega_{\ell-1}^{j}, t_{\ell-1}; h) \end{aligned}}$$

- Euler method $\Phi(\omega_{\ell-1}^{j}, t_{\ell-1}; h) = r(\omega_{\ell-1}^{j}, t_{\ell-1})$
- aim of this method:
  find $\hat{\omega}_\ell^{(j)}$ such that Newton's method is convergent when starting with $\hat{\omega}_\ell^{(j)}$
- theory & numerics of ODE solving relies on Lipschitz continuity (in x) of rhs of ODE

$$\frac{dx}{dt} = r(x,t) \qquad \text{see } (*)$$

here $r(x,t) = -\dfrac{\partial H/\partial t}{\partial H/\partial x}$ is rational fct

- problems occur when

$$\frac{\partial H}{\partial x} = d \cdot x^{d-1} + (1-t)\sum_{k=1}^{d-1}(d-k)\,a_k x^{d-k-1} = 0$$

$\rightarrow$ later

Solving $H(x,t)=0$ with Newton's method

$$v_{k+1} = v_k - \frac{H(v_k,t)}{\frac{\partial H}{\partial x}(v_k,t)}$$

- Lipschitz constant: $L = \dfrac{H(v_k,t)}{\frac{\partial H}{\partial x}(v_k,t) \cdot \frac{\partial^2 H}{\partial x^2}(v_k,t)}$

L is small if v_k close to zero of $H(x,t)$ and $\frac{\partial H}{\partial x} \cdot \frac{\partial^2 H}{\partial x^2}$ bounded away from zero

e.g. if zero is simple

- this defines the corrector, typically a handfull of iterations suffice to get accurate results
- start at $\hat{w}_e^{(j)}$ and the final v_k we use as
  $w_e^{(j)} = v_k$
- floating point errors do slow down convergence and lead to an error at the end for ill-conditioned problems.
- ill-conditioning in f occurs for t close to 0
  → maybe stop at an earlier t to get some idea of the solution
  (t acts a bit like a regularisation parameter)