Mathematical modelling

Lecture 5, March 19, 2021

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2020/2021

Newton optimization method:

We would like to find the extrema of the function $F : \mathbb{R}^n \to \mathbb{R}$.

Since the extrema are *critical (or stationary) points*, the candidates are zeroes of the gradient, i.e.,

$$G(x) := \text{grad } F(x) = \begin{bmatrix} F_{x_1}(x) & \cdots & F_{x_n}(x) \end{bmatrix} = 0. \tag{1}$$

(1) is a system of n equations for n variables, the Jacobian of the vector function G is the so called *Hessian of F*:

$$DG(x) = H(x) = \begin{bmatrix} F_{x_1 x_1} & \dots & F_{x_1 x_n} \\ \vdots & \ddots & \vdots \\ F_{x_n x_1} & \dots & F_{x_n x_n} \end{bmatrix}.$$

If the sequence of iterates

$$x_0, \quad x_{k+1} = x_k - H^{-1}(x_k) G(x_k)$$

converges, the limit is a critical point of F, i.e., a candidate for the minimum (or maximum).

Newton's method for $m > n > 0$

We have an overdetermined system

$$f : \mathbb{R}^n \to \mathbb{R}^m, \quad f(x) = (0, \ldots, 0) \tag{2}$$

of m nonlinear equations for n unknowns, where $m > n$.

The system (2) generally does not have a solution, so we are looking for a solution of (2) by the least squares method, i.e., $\alpha \in \mathbb{R}^n$ such that the distance of $f(\alpha)$ from the origin is the smallest possible:

$$\|f(\alpha)\|^2 = \min\{\|f(x)\|^2\}.$$

The *Gauss-Newton method* is a generalization of the Newton's method, where instead of the inverse of the Jacobian its MP inverse is used at each step:

- x_0 is initial approximation,
- $x_{k+1} = x_k - Df(x_k)^+ f(x_k)$,

where $Df(x_k)^+$ is the MP inverse of $Df(x_k)$. If the matrix

$(Df(x_k)^T Df(x_k))$ is nonsingular at each step k, then

$$x_{k+1} = x_k - (Df(x_k)^T Df(x_k))^{-1} Df(x_k)^T f(x_k).$$

At each step x_{k+1} is the least squares approximation to the solution of the overdetermined linear system $L_{x_k}(x) = 0$, that is,

$$\|L_{x_k}(x_{k+1})\|^2 = \min\{\|L_{x_k}(x)\|^2, x \in \mathbb{R}^n\}.$$

Convergence is not guaranteed, but:

- if the sequence x_k converges, the limit $x = \lim_k x_k$ is a local (but not necessarily global) minimum of $\|f(x)\|^2$.

It follows that the Gauss-Newton method is an algorithm for the local minimum of $\|f(x)\|^2$.

Example

We are given point $(x_i, y_i) \in \mathbb{R}^2$ for $i = 1, \dots, m$ and are searching for the function

$$f(x, a, b) = ae^{bx}$$

which fits this data best by the method of least squares.

So we have the overdetermined system $F(a, b) = 0$, where

$$F : \mathbb{R}^2 \to \mathbb{R}^m, \quad F(a, b) = (y_1 - ae^{bx_1}, \dots, y_m - ae^{bx_m}).$$

The Jacobian of F is

$$DF(a, b) = \begin{bmatrix} -e^{bx_1} & ax_1 e^{bx_1} \\ \vdots & \\ -e^{bx_m} & ax_m e^{bx_m} \end{bmatrix}.$$

Using the Gauss-Newton method:

- We choose initianl approximation (a_0, b_0),
- Calculate iterates

$$\begin{bmatrix} a_{r+1} \\ b_{r+1} \end{bmatrix} = \begin{bmatrix} a_r \\ b_r \end{bmatrix} - DF(a_r, b_r)^+ F(a_r, b_r)^T.$$

3.2. Parametric curves

Basic definitions, examples

A *parametric curve* (or parametrized curve) in $\mathbb{R}^m$ is a vector function

$$f : I \to \mathbb{R}^m, \qquad f(t) = \begin{bmatrix} f_1(t) \\ \vdots \\ f_m(t) \end{bmatrix},$$

where $I \subset \mathbb{R}$ is a bounded or unbounded interval.

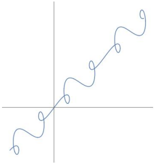
The independent variable (in this case t) is the *parameter* of the curve.

For every value $t \in I$, $f(t)$ represents a point in $\mathbb{R}^m$.

As t runs through I, $f(t)$ traces a path, or a curve, in $\mathbb{R}^m$.

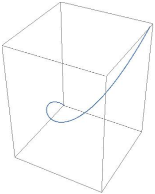
$m = 2$: for every $t \in I$ we get a point in the plane

$$f(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}$$



$m = 3$: for every $t \in I$ we get a point in $\mathbb{R}^3$

$$f(t) = \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix}$$

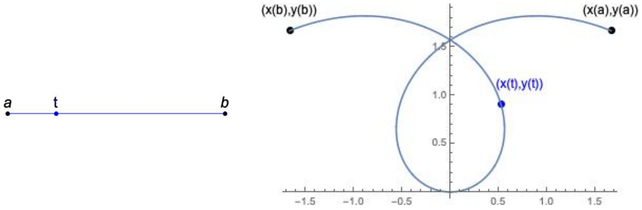


If $m = 2$, then for every $t \in I$,

$$f(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \mathbf{r}(t)$$

is the position vector of a point in the plane $\mathbb{R}^2$.

All points $\{f(t), t \in I\}$ form a *plane curve*:

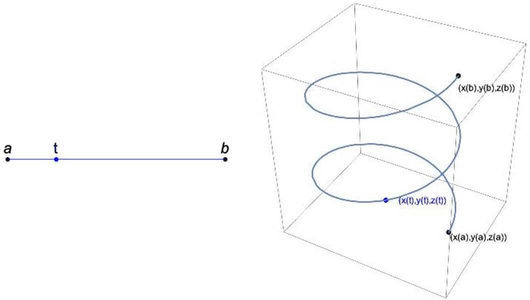


In this example $x(t) = t \cos t, y(t) = t \sin t, t \in [-3\pi/4, 3\pi/4]$

If $m = 3$, then

$$f(t) = \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} = \mathbf{r}(t)$$

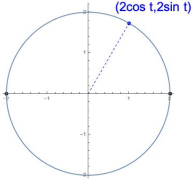
is the position vector of a point in $\mathbb{R}^3$ for every t, and $\{f(t), t \in I\}$ is a *space curve*:



In this example $x(t) = \cos t, y(t) = \sin t, z(t) = t/5, t \in [0, 4\pi]$

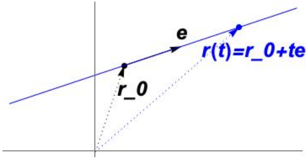
Example

$$f(t) = \begin{bmatrix} 2\cos t \\ 2\sin t \end{bmatrix}, t \in [0, 2\pi]$$



a circle with radius 2 and center $(0, 0)$

$f(t) = \mathbf{r}_0 + t\mathbf{e}, t \in \mathbb{R},$
$\mathbf{r}_0, \mathbf{e} \in \mathbb{R}^m, \mathbf{e} \neq \mathbf{0}$

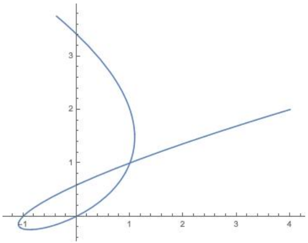


line through $\mathbf{r}_0$ in the direction of $\mathbf{e}$ in $\mathbb{R}^m$

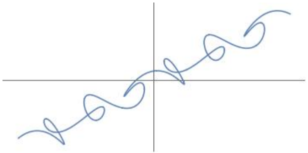
m=2:
slope $k = e_2/e_1$ if $e_1 \neq 0$
vertical if $\mathbf{e} = (0, e_2)$
horizontal if $\mathbf{e} = (e_1, 0)$

Example

$$f(t) = \begin{bmatrix} t^3 - 2t \\ t^2 - t \end{bmatrix}, t \in \mathbb{R}$$



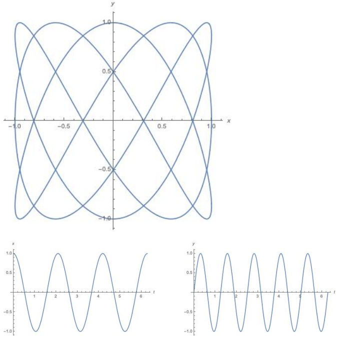
$$f(t) = \begin{bmatrix} t + \sin(3t) \\ t + \cos(5t) \end{bmatrix}, t \in \mathbb{R}$$



A parametric curve $f(t), t \in [a, b]$ is *closed* if $f(a) = f(b)$.

Example

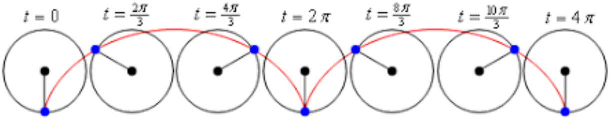
$$f(t) = \begin{bmatrix} \cos 3t \\ \sin 5t \end{bmatrix}, t \in [0, 2\pi]$$



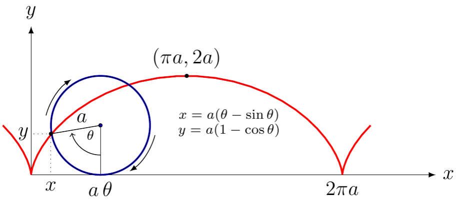
Lissajous curves: $x(t) = \sin(nt + \delta)$, $y(t) = \sin mt$, are closed if the ratio n/m is rational. They describe 2D harmonic motion.

Problem: What path does the valve on your bicycle wheel trace as you bike along a straight road?

Represent the wheel as a circle of radius a rolling along the x-axis, the valve as a fixed point on the circle, the parameter is the angle of rotation:



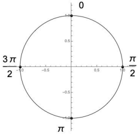
The curve is *a cycloid*: $x(\theta) = a\theta - a\sin\theta, y(\theta) = a - a\cos\theta$.



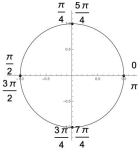
A parametric curve $f(t)$ describes the motion of a point with respect to t. The path that it traces is simply a *curve* C.

The following parametric curves all describe the circle with radius a around the origin (as well as many others):

$$f_1(t) = \begin{bmatrix} a \sin t \\ a \cos t \end{bmatrix},\ t \in [0, 2\pi]$$



$$f_2(t) = \begin{bmatrix} a \cos 2t \\ a \sin 2t \end{bmatrix},\ t \in [0, 2\pi]$$



$$f_3(t) = \begin{bmatrix} a \cos t \\ a \sin t \end{bmatrix},\ t \in \mathbb{R}$$