COORDINATE PARTITION "PHILOSOPHY"

A DAE system

$$F(x, x', t) = 0 \qquad F: \mathbb{R}^{m+m+1} \to \mathbb{R}^m$$

where $\frac{\partial F}{\partial x'}$ square matrix is SINGULAR FOR DAE

$\Rightarrow$ IT IS NOT POSSIBLE TO SOLVE FOR x' AND TRANSFORM INTO AN ODE $\boxed{x' = \phi(x, t)}$

NOT POSSIBLE

IF $\frac{\partial F}{\partial x'}(x_0, x_0', t_0)$ is NOT singular and $F(x_0, x_0', t_0) = 0$ for the implicit function theorem (+ some regularity conditions) is possible to find a function $\phi(x, t)$ such that $x' = \phi(x, t)$ in a neighbor of (x_0, x_0', t_0)

i.e. $|x - x_0|$, $|x' - x_0'|$, $|t - t_0|$ are small

THE IMPLICIT FUNCTION THEOREM

$F : \mathbb{R}^{m+1} \to \mathbb{R}^n$ with $m > n$ and F regular enough (C^2)

TIME

$F(x_0, t_0) = 0$ and $\frac{\partial F}{\partial x}(x_0, t_0)$ is of maximum RANK

then x can be partitioned in 2 set DEPENDENT and INDEPENDENT coordinates

$y = (x_{i_1}\ x_{i_2} \cdots x_{i_{m-n}})$ $\quad$ $m-n$ independent

$z = (x_{j_1}\ x_{j_2} \quad x_{j_n})$ $\quad$ n dependent

and $\exists$ a map $\phi(y, t)$ and $\delta > 0$ such that

$F(x,t) = F(y, z, t)$ ← AFTER REORDERING OF X

$$F(y, \phi(y,t), t) = 0 \qquad \text{FOR} \quad \begin{array}{l} |y - y_0| < \delta \\ |t - t_0| < \delta \end{array}$$

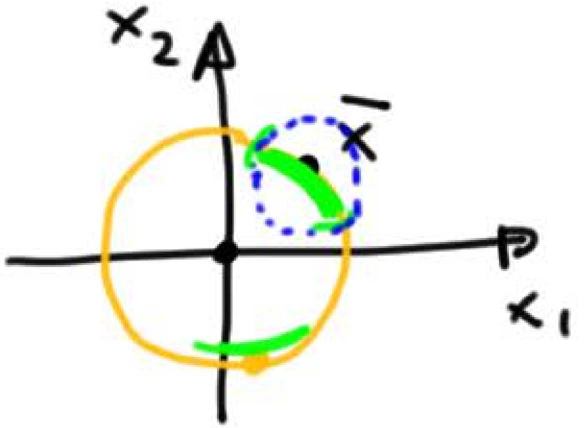
EXAMPLE

$\bar{x}_1 > 0, \ \bar{x}_2 > 0$

$$\boxed{x_2 = \phi(x_1, t) = \sqrt{1 - x_1^2}}$$

$F : \mathbb{R}^2 \to \mathbb{R}$

$n = 2$
$m = 1$



$F(x, t) = x_1^2 + x_2^2 - 1$

$F(x) = 0$

$$\frac{\partial F}{\partial x} = \left[\frac{\partial F}{\partial x_1} \ \ \frac{\partial F}{\partial x_2} \right] = \left[2x_1 \ \ 2x_2 \right]$$

If x_1 and x_2 are not both 0 the rank of $\frac{\partial F}{\partial x} = 1$

so $\frac{\partial F}{\partial x}$ is of maximum RANK.

Let be $\bar{x} = (\bar{x}_1, \bar{x}_2)$ such that $F(\bar{x}, t) = 0$ and $\bar{x}_1 \neq 0$

for the implicit function theorem we can write

$$x_2 = \phi(x_1, t)$$

such that $F([x_1, \phi(x_1, t)], t) = 0$

Example

$F : \mathbb{R}^{3+1} \to \mathbb{R}^1$

$$F(x,t) = F(x_1 x_2 x_3, t) = x_1^2 + x_2^2 - x_3 + 1 + t$$

$$x_3 = x_1^2 + x_2^2 + 1 + t = \phi([x_1 x_2], t)$$

An implicit map exist

$$F(\underbrace{\phi_1([x_1 x_2], t), \phi_2([x_1, x_2], t)}, t) = 0$$

$$F(\phi(x_1 x_2 t), t) = 0$$

$$\frac{\partial F}{\partial x} = [2x_1, 2x_2, -1] \leftarrow \text{Always FULL RANK}$$

$\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3)$ such that $F(\bar{x}, \bar{t}) = 0$

x_1 and x_2 are independent coordinates

x_3 is the dependent coordinate

$\phi(x_1 x_2 t)$ and that

$$F(x_1 x_2\, \phi(x_1 x_2, t), t) = 0$$

$|x_1 - \bar{x}_1| < \delta$

$|x_2 - \bar{x}_2| < \delta$

$|t - \bar{t}| < \delta$

EXAMPLE $F : \mathbb{R}^{3+1} \to \mathbb{R}^1$

$$F(x,t) = F(x_1 x_2 x_3, t) = x_1^2 + e^{x_2} - \frac{x_3}{1+x_3^2} + 1 + t$$

$x_3 = \phi(x_1 x_2, t)$? NOT EASY TO FIND THE MAP EXPLICITLY

$$\frac{\partial F}{\partial x} = \left[2x_1 \quad e^{x_2} \quad \frac{1-x_3^2}{(1+x_3^2)^2} \right]$$

FOR $x_3 \in (-1,1)$ RANK IS maximum

$\frac{\partial F}{\partial x_3}$ is non singular for $x_3 \in (-1,1)$

$\Rightarrow$ using implicit function theorem if

$\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3)$ $\bar{t}$ is such that $F(\bar{x}, \bar{t}) = 0$

($\bar{x}_3 \in (-1,1)$ FOR maximum rank) THEN THERE EXIST $\delta > 0$

$\phi(x_1 x_2, t)$ such that

$|x_1 - \bar{x}_1| < \delta$

$F(x_1 x_2 \, \phi(x_1 x_2 t), t) = 0$

$|x_2 - \bar{x}_2| < \delta$

$|t - \bar{t}| < \delta$

EXAMPLE

$F: \mathbb{R}^{3+1} \to \mathbb{R}^2 \qquad \bar{x} = (0,0,1) \qquad \bar{t} = 0$

$$F(x_1 x_2 x_3\, t) = \begin{pmatrix} x_1 + x_2 + x_3 + t - 1 \\ x_1^2 + x_2^2 - x_3 + 1 \end{pmatrix}$$

$$\frac{\partial F}{\partial x} = \begin{pmatrix} 1 & 1 & 1 \\ 2x_1 & 2x_2 & -1 \end{pmatrix} \qquad \frac{\partial F}{\partial x}(\bar{x}, \bar{t}) = \begin{array}{c} \begin{array}{ccc} \times & \times & \bullet \end{array} \\ \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \end{pmatrix} \end{array}$$

2 choice for the dependent coordinates (x_1, x_3) or (x_2, x_3)

INDEPENDENT $\quad x_1$

DEPENDENT $\quad x_2 \; x_3$

$\Rightarrow$ FOR THE IMPLICIT FUNCTION THEOREM THERE EXISTS MAP $\phi(x_1, t)$ such that

$$x_2 = \phi_1(x_1, t)$$
$$x_3 = \phi_2(x_1, t)$$

$$F(x_1, \phi(x_1, t), t) = 0$$

IMPLICIT FUNCTION THEOREM "USAGE"

$F : \mathbb{R}^{m+1} \to \mathbb{R}^n$

① FIND $(x_0, t_0) \in \mathbb{R}^{m+1}$ such that $F(x_0, t_0) = 0$

② IF rank $\frac{\partial F}{\partial x}(x_0, t_0)$ is maximum

select n-colums $(j_1\ j_2\ \ j_n)$ such that the resulting square matrix is NON SINGULAR

The coordinates $z = (x_{j_1}\ x_{j_2}\ \ x_{j_n})$ are the DEPENDENT coordinates. The other $y = (x_{k_1}\ x_{k_2} \cdots\ x_{k_{m-n}})$ are the INDEPENDENT coordinates.

③ Using implicit function theorem EXIST MAP $\phi(y,t)$ such that $F(\underbrace{y, \phi(y,t)}_{\text{AFTER REORDERING}}, t) = 0$

FOR $|y - y_0| < \delta$

$|t - t_0| < \delta$

COORDINATE PARTITION "PHILOSOPHY"

A DAE system

$$F(x,x',t)=0 \qquad F:\mathbb{R}^{m+m+1}\longrightarrow\mathbb{R}^{m}$$

where $\frac{\partial F}{\partial x'}$ square matrix is SINGULAR FOR DAE

A PARTICULAR CASE is when $Ex' = G(x,t)$

where if E is NOT singular $\Rightarrow$ ODE

if E is singular is possible to find two not singular matrix U, V such that

$$E = U\begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} V$$

$$\begin{cases} z' = H_1(z,w,t) \\ 0 = H_2(z,w,t) \end{cases}$$

so $y = Vx$

$$\begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} y' = U^{-1}G(V^{-1}y,t) = H(y,t)$$

DAE IN SEMI-EXPLICIT FORM

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases}$$

The most general form for DAE is $F(z, z', t) = 0$

BUT THIS FORM IS GENERAL ENOUGH FOR OUR PURPOSE

Using semi-explicit form is EASIER TO UNDERSTAND index-1, index-2, .. DAE

INDEX-1 semi-explicit DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases}$$

IF $\frac{\partial G}{\partial y}$ is not singular is AN INDEX-1 DAE (EXERCIZE)

IF is possible to write $y = \phi(x,t)$ such that $G(x,\phi(x,t),t) = 0$ we can eliminate y FROM the DAE

$$x' = F(x,\phi(x,t),t) = \tilde{F}(x,t)$$

$0 = G(x,\phi(x,t),t)$ ← identically satisfied by the map $\phi(x,t)$

INDEX-1 ARE VERY CLOSE TO ODE AND USING IMPLICIT FUNCTIO THEOREM CAN BE MANIPULATED AS ODE

NUMERICALLY SOLVE INDEX-1 DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases}$$

By implicit function theorem we assume to know a map $\phi(x,t)$ such that

$$G(x,\phi(x,t),t) = 0$$

$$\Rightarrow x' = F(x,\phi(x,t),t) = \tilde{F}(x,t)$$ IS AN ODE!

CAN BE APPROXIMATED USING EXPLICIT EULER

x_0 = initial condition

$$x_{k+1} = x_k + h\,\underbrace{\tilde{F}(x_k, t_k)}$$

$t_n = t_0 + hk$

$$\tilde{F}(x_k,t) = F(x_k, \phi(x_k,t), t_n)$$

not explicitly known to be computed numerically

NUMERICALLY SOLVE INDEX-1 DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases} \qquad x' = F(x,\phi(x,t),t) = \tilde{F}(x,t)$$

$$\left.\begin{aligned} &x_0 = \text{initial condition} \\ &x_{k+1} = x_k + h\tilde{F}(x_k,t_k) \end{aligned}\right\} \text{Explicit Euler}$$

$$\tilde{F}(x_k,t_k) = F(x_k,\phi(x_k,t_k),t_k)$$

$$G(x_k,\phi(x_k,t_k),t_k) = 0$$

$\phi(x_k,t_k)$ = solution of $G(x_k,y,t_k) = 0$

$\Rightarrow$ use for example Newton

$$y^{(e+1)} = y^{(e)} - \frac{\partial G}{\partial y}(x_k,y^{(e)},t_k)\,G(x_k,y^{(e)},t_k)$$

NUMERICALLY SOLVE INDEX-1 DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases} \qquad x' = F(x,\phi(x,t),t) = \widetilde{F}(x,t)$$

$$\left.\begin{array}{l} x_0 = \text{initial condition} \\ x_{k+1} = x_k + h\,\widetilde{F}(x_k,t_k) \end{array}\right\} \text{Explicit Euler}$$

$$\widetilde{F}(x_k,t_k) = F(x_k,\phi(x_k,t_k),t_k)$$

$$G(x_k,\phi(x_k,t_k),t_k) = 0$$

$$\phi(x_k,t_k) = \text{solution of } G(x_k,y,t_k) = 0$$

$\Rightarrow$ use for example Newton

$$y^{(e+1)} = y^{(e)} - \frac{\partial G}{\partial y}(x_k,y^{(e)},t_k)\,G(x_k,y^{(e)},t_k)$$

Numerically solve index-1 DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases} \qquad x' = F(x,\psi(x,t),t) = \tilde{F}(x,t)$$

x_0 = initial condition

x_{k+1} is the solution of $x - h\tilde{F}(x, t_{n+1}) - x_n = 0$

Find x using Newton for example

$$x^{(\ell+1)} = x^{(\ell)} - \underbrace{\left(I - h\frac{\partial \tilde{F}}{\partial x}(x, t_{n+1})\right)^{-1}}_{Df^{-1}} \underbrace{\left(x^{(\ell)} - h\tilde{F}(x^{(\ell)}, t_{n+1}) - x_n\right)}_{f}$$

$$\tilde{F}(x, t_{n+1}) = F(x, \phi(x, t_{n+1}), t_{n+1})$$

compute ψ by using Newton iterative

$$\frac{\partial \tilde{F}}{\partial x}(x, t_{n+1}) = \ ?$$

Numerically solve index-1 DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases} \qquad \tilde{F}(x,t) = F(x,\phi(x,t),t)$$

$$\frac{\partial \tilde{F}}{\partial x}(x,t_{n+1}) = \frac{\partial F(x,\phi(x,t_{n+1}),t_{n+1})}{\partial x} + \frac{\partial F}{\partial y}(x,\phi(x,t_{n+1}),t_{n+1}) \boxed{\frac{\partial \phi(x,t_{n+1})}{\partial x}}$$

$\phi(x,t_{n+1})$ = computed by solving $G(x,y,t_{k+1}) = 0$

by the implicit function theorem we write

$$G(x,\phi(x,t_{k+1}),t_{n+1}) = 0 \qquad \frac{\partial}{\partial x}\left(G(x,\phi(x,t_{n+1}),t_{n+1}) \right) = 0$$

$$\Rightarrow \frac{\partial G}{\partial x}(x,y,t_{n+1}) + \frac{\partial G}{\partial y}(\ ) \boxed{\frac{\partial \phi}{\partial x}} = 0$$

$y \equiv \phi(x,t_{n+1})$

NUMERICALLY SOLVE INDEX-1 DAE

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases} \qquad \tilde{F}(x,t) = F(x,\phi(x,t),t)$$

$$\frac{\partial \tilde{F}}{\partial x}(x,t_{n+1}) = \frac{\partial F(x,\phi(x,t_{n+1}),t_{n+1})}{\partial x} + \frac{\partial F}{\partial y}(x,\phi(x,t_{n+1}),t_{n+1}) \boxed{\frac{\partial \phi(x,t_{n+1})}{\partial x}}$$

$$\frac{\partial G}{\partial x}(x,y,t_{n+1}) + \underbrace{\frac{\partial G}{\partial y}(x,y,t_{n+1})}_{\text{NOT SINGULAR}} \frac{\partial \phi}{\partial x}(x,t_{n+1}) = 0 \qquad y \equiv \phi(x,t_{n+1})$$

$$\Rightarrow \frac{\partial \phi}{\partial x}(x,t_{n+1}) = -\frac{\partial G}{\partial y}(x,y,t_{n+1})^{-1} \frac{\partial G}{\partial x}(x,y,t_{n+1})$$

WHAT WE HAVE DONE?

$$\begin{cases} x' = F(x,y,t) \\ 0 = G(x,y,t) \end{cases}$$

USING IMPLICIT FUCTION THEOREM

$y = \phi(x,t) \Rightarrow y$ IS FORMALLY ELIMINATED

$$x' = \tilde{F}(x,t) = F(x, \phi(x,t), t)$$

$\Rightarrow$ THE DAE IS TRANSFORMED IN A SMALLER ODE

NOT FREE LUNCH
THE COMPUTATION OF $\tilde{F}$ IS COSTLY

IN PRACTICE YOU NEED TO COMPUTE $\phi(x,t)$ and $\frac{\partial \phi}{\partial x}$ numerically

A STEP FORWARD SEMI-EXPLICIT INDEX-2

$$\begin{cases} x' = F(x, y, t) \\ 0 = G(x, y, t) \end{cases}$$

but $\frac{\partial G}{\partial y}$ NOT FULL RANK

A SIMPLIFIED SITUATION IS when $G(x, t)$

$$\begin{cases} x' = F(x, y, t) \\ 0 = G(x, t) \end{cases}$$

$\frac{\partial G}{\partial x}$ must be Full rank

so that by Applying implicit Function theorem we partition $x = (z, w)$ with

z = independent

w = dependent coordinates

A STEP FORWARD SEMI-EXPLICIT INDEX-2

$$\begin{cases} x' = F(x, y, t) \\ 0 = G(x, t) \end{cases} \qquad x = (z, w) \qquad \begin{cases} z' = F_1(z, w, y, t) \\ w' = F_2(z, w, y, t) \\ 0 = G(z, w, t) \end{cases}$$

$$w = \phi(z, t)$$

$$G(z, \phi(z, t), t) = 0 \quad \Rightarrow \text{ELIMINATED FROM THE DAE}$$

$$\begin{cases} z' = F_1(z, \phi(z, t), y, t) \\ \underbrace{\dfrac{d}{dt}\phi(z(t), t)}_{\dfrac{\partial \phi}{\partial z}(z, t)\, z' + \dfrac{\partial \phi}{\partial t}(z, t)} = F_2(z, \phi(z, t), y, t) \end{cases}$$

$$\boxed{\text{To be continued}}$$