Modeling Physics with Differential-Algebraic Equations

Lecture 3

Numerical Integration of DAEs

Master Cyber-Physical Systems (M2)

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Index Reduction

- Given a DAE $F(x, \dot{x}, t)$, we have seen how to perform a structural analysis to numerically compute $\dot{x}$ function of x. The structural nonsingularity ensures that, generically, one can perform the computation following the block order suggested by the BLT decomposition. Thus, one is able to compute the numerical values of the derivatives given a consistent state of the system and carry on with a **standard numerical integration**.
- Note: the **structural index** is not always equal to the **differentiation index**.

Index reduction transforms a fully implicit DAE to a **semi-explicit DAE**

$$\begin{aligned} \dot{x} &= f(x, y, t) \\ 0 &= g(x, y, t) \end{aligned}$$

Integration Schemes

- Backward Differentiation Formula (BDF)
- Orthogonal Collocation

Outline

1. BDF Method

2. Collocation (Overview)

- **Implicit**: next value not explicitly given.
- **Linear multistep**: the next value is linearly related to the immediate previous (backward) values (eventually more than one).
- For a fixed step size $\delta > 0$, let $t_n = t_0 + n\delta$, and x_s the approximate of the exact $x(t_s)$.
- The general Backward Differentiation Formula:

$$\dot{x}_n = \text{linear combination of } x_n, x_{n-1}, \ldots, x_0$$

- For a Cauchy problem $\dot{x} = f(x, t), x(t_0) = x_0$, one obtains an implicit equation for x_n:

$$x_n = \sum_{n=1}^{q} a_n \; x_{1-n} + \delta \; b_q \; f(x_n, t_n)$$

  where the a_n and b_q depends only on the order q.
- E.g., $q = 1$ (BDF1): $x_n = x_{n-1} + \delta \; f(x_n, t_n)$ (a.k.a. Backward Euler)

$$\begin{aligned}
\mathcal{I}x_n &= x_n && \text{(Identity)}\\
\mathcal{N}x_n &= x_{n+1} && \text{(Forward Shift)}\\
\mathcal{N}^{-1}x_n &= x_{n-1} && \text{(Backward Shift)}\\
\mathcal{D}x_n &= \dot{x}_n && \text{(Differential)}\\
\Delta &= \mathcal{I} - \mathcal{N}^{-1} && \text{(Backward Operator)}
\end{aligned}$$

Observe that $\mathcal{N} = (\mathcal{I} - \Delta)^{-1}$ (Operator Algebra)

$$\begin{aligned}
\mathcal{N}x_n = x_{n+1} &= x_n + \delta\mathcal{D}x_n + \frac{\delta^2}{2!}\mathcal{D}^2x_n + \frac{\delta^3}{3!}\mathcal{D}^3x_n + \cdots\\
&= (\mathcal{I} + \delta\mathcal{D} + \frac{\delta^2}{2!}\mathcal{D}^2 + \frac{\delta^3}{3!}\mathcal{D}^3x_n + \cdots)x_n\\
&= e^{\delta\mathcal{D}}x_n
\end{aligned}$$

Thus: $\mathcal{N} = e^{\delta\mathcal{D}}$

$$\delta\mathcal{D} = \ln(\mathcal{N}) = \ln\left((\mathcal{I} - \Delta)^{-1}\right) = \Delta + \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \cdots$$

$$\delta\dot{x}_n = \delta\mathcal{D}x_n = \Delta x_n + \frac{1}{2}\Delta^2 x_n + \frac{1}{3}\Delta^3 x_n + \cdots$$

BDFq: truncate at order q, for instance for $q = 2$

$$\delta\dot{x}_n = \Delta x_n + \frac{1}{2}\Delta^2 x_n = (x_n - x_{n-1}) + \frac{1}{2}(x_n - 2x_{n-1} + x_{n-2})$$

Thus

$$\delta\dot{x}_n = \frac{3}{2}x_n - 2x_{n-1} + \frac{1}{2}x_{n-2}$$

$$x_n = \frac{4}{3}x_{n-1} - \frac{1}{3}x_{n-2} + \frac{2}{3}\delta f(x_n, t_n)$$

BDF for Semi-Explicit DAE of index 1

$$\dot{x} = f(x, y, t)$$
$$0 = g(x, y)$$

Numerical integration using the BDF2 Scheme

Suppose x_{n-1} and x_{n-2} are known, x_n and y_n are computed by numerically solving the following system (e.g. Newton's methods) at each iteration:

$$x_n = \frac{4}{3}x_{n-1} - \frac{1}{3}x_{n-2} + \frac{2}{3}\delta f(x_n, y_n, t_n)$$
$$0 = g(x_n, y_n)$$

- BDF converges if $m \leq 6$: $x_i - x(t_i) = y_i - y_i(t_i) = o(\delta^m)$
- BDF requires a consistent initial condition

Newton's Methods: Generalization

Could be used to numerically approximate the roots of $F : \mathbb{R}^k \to \mathbb{R}^k$ (F_i continuously differentiable functions):

- Multiply by the inverse of the Jacobian

$$x_{n+1} = x_n - J_F^{-1}(x_n)F(x_n)$$

- Or solve the system of linear equations

$$J_F(x_n)(x_{n+1} - x_n) = -F(x_n)$$

Under some assumptions, the method converges quadratically towards a root of F.

1 BDF Method

2 Collocation (Overview)

- Collocate means approximate/study an unknown function by means of other "simpler" functions
- For instance using **polynomial** or trigonometric functions

Weierstrass Theorem (1885)

If $x(t)$ is a continuous function on $[a, b]$, then for any given $\epsilon > 0$, there exists a polynomial $p(t)$ such that

$$\max_{t \in [a,b]} |x(t) - p(t)| < \epsilon$$

The theorem has a constructive proof using **Bernstein polynomials**.

Integration by Collocation

Unlike BDF, Collocation could be used to construct **at once** n points $(t_1, x_1), \ldots, (t_n, x_n)$ such that x_i approximates the function $x(t)$ at t_i for all i. Useful for **Consistent Initialization**.

If $p(t)$ is a polynomial that approximates $x(t)$, solution of our semi-explicit DAE, such that $p(t_i) = x(t_i) = x_i$ for some known t_i, where $i = 1, \dots, n$. Then, for each i, we can compute x_i, y_i by solving

$$\dot{p}(t_i) = f(p(t_i), y_i, t_i)$$
$$0 = g(p(t_i), y_i)$$

- The collocation methods attempts to construct such p as well as finding appropriate t_i.
- Observe that the polynomial p may be dependent on x_i, the unknowns we want to determine.
- Again, Newton's methods could be used to solve iteratively for $p(t_i)$ and hence x_i.

Suppose we have n points $(t_1, x_1), \dots, (t_n, x_n)$, then we construct the polynomial $p(t)$ such that:

$$p(t_i) = x_i,\ \ i = 1, \dots, n$$

- There exists a (unique) polynomial p of degree n **interpolating** the n points

$$p(t) = \sum_{i=1}^{n} x_i L_i(t)$$

- L_i are the **Lagrange polynomials**

$$L_i(t) = \prod_{k=0, k\neq i}^{n} \frac{t - t_k}{t_i - t_k},\ \ i = 1, \dots, n$$

satisfying in particular $L_i(t_j) = \delta_{ij}$ (Kronecker delta)

We want to determine the instants $t_i \in [a, b]$ such that there exists positive weights w_i which make the Gauss quadrature integral *exact* for the polynomial p, that is

$$\mathbf{I}[p] = \int_a^b p(t)dt = \sum_{i=1}^{n} w_i p(t_i) = \mathbf{Q_n}[p]$$

Without loss of generality, we can suppose that $a = -1$ and $b = 1$ since

$$\int_a^b f(t)dt = \frac{b-a}{2} \int_{-1}^{1} f\left(\frac{a+b}{2} + t\frac{b-a}{2}\right) dt \ .$$

Gauss Quadrature Fundamental Theorem $(w(x) = 1)$

If the t_i are the zeros of the Legendre polynomial ℓ_n, then there exist n weights w_i which make the Gauss quadrature integral exact for all polynomials of degree $2n - 1$ or less (in particular for our polynomial p of degree n).

Rodrigues' Formula

$$\ell_n(t) = \frac{1}{2^n n!} \frac{d^n}{dt^n} (t^2 - 1)^n$$

- ℓ_n has degree n
- Legendre polynomials are orthogonal

$$< \ell_i, \ell_j > = \int_{-1}^{1} \ell_i(t)\ \ell_j(t) dt = \frac{2}{2n+1} \delta_{ij}$$

- $\ell_0(t) = 1$, $\ell_1(t) = t$, $\ell_3(t) = \frac{1}{2}(5t^3 - 3t)$
- There are effective methods to compute the zeros of ℓ_n and w_i (Golub-Welsch algorithm)
- Thus we have the t_i **which depend only on** n **and not on our original DAE system !**.

$$\dot{x} = x + y$$
$$0 = x^2 + y^2 - 1$$

- Suppose $[a, b] = [0, 0.1]$, $n = 3$
- The t_i are derived from τ_i the roots of $\ell_3(t)$: $t_i = \frac{a+b}{2} + \tau_i \frac{b-a}{2}$
- $\tau_i \in \left\{ -\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}} \right\}$
- $w_i = \int_a^b L_i(t)dt$ (Lagrange Polynomials)
- $w_i \in \{\frac{1}{36}, \frac{2}{45}, \frac{1}{36}\}$
- $p(t) = x_1 L_1(t) + x_2 L_2(t) + x_3 L_3(t)$
- $\dot{p}(t) = x_1 \dot{L}_1(t) + x_2 \dot{L}_2(t) + x_3 \dot{L}_3(t) \quad (\dot{L}_i(t_j) \neq \delta_{ij})$

System to Solve

$$
\begin{aligned}
\dot{p}(t_1) &= x_1 + y_1 \\
\dot{p}(t_2) &= x_2 + y_2 \\
\dot{p}(t_3) &= x_3 + y_3 \\
0 &= x_1^2 + y_1^2 - 1 \\
0 &= x_2^2 + y_2^2 - 1 \\
0 &= x_3^2 + y_3^2 - 1
\end{aligned}
$$

One solution for $[0, 0.1]$: $x_1 = x_2 = x_3 = \frac{1}{\sqrt{2}} \qquad y_1 = y_2 = y_3 = \frac{-1}{\sqrt{2}}$

Note that in this particular simple example, the system has a singularity at $(x, y) = (1, 0)$, so not all initial conditions and intervals $[a, b]$ work. In general, such problems occur and one wants to find an initial condition that has no singularities at least as long as $t \in [a, b]$.

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