# Simulation Methods

## Numerical Methods for Ordinary Differential Equations

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# Multistep Formulas

For the Cauchy problem

$$y' = f(t, x), \qquad x(t_0) = x_0, \tag{1}$$

we compute an approximate value $\tilde{x}_{i+k}$ of $x(t_{i+k})$, $k \geq 2$, using the approximate values $\tilde{x}_j$ of $x(t_j)$, $j = i, i+1, \ldots, i+k-1$, at the points $t_j = t_0 + jh$ :

$$\text{for } i = 0, 1, 2, \ldots :$$

$$\tilde{x}_i, \tilde{x}_{i+1}, \ldots, \tilde{x}_{i+k-1} \Rightarrow \tilde{x}_{i+k}. \tag{2}$$

To begin the method we need initial values $\tilde{x}_0$, $\tilde{x}_1, \ldots, \tilde{x}_{k-1}$. For instance, we can use a one-step method to get these values.

# Explicit formula I

- From (1), we get:

$$x(t_{n+1}) = x(t_n) + \int_{t_n}^{t_{n+1}} f(s, x(s))\, ds.$$

- Interpolate $t \mapsto g(t) = f(t, x(t))$ at $t_{n-k+1}, \ldots, t_n$ :
  Define $f_i = f(t_i, x_i)$, for $t_i = t_0 + ih$, $x_i = x(t_i)$. The interpolating polynomial has the form

$$p(t) = p(t_n + sh) = \sum_{j=0}^{k-1} (-1)^j \binom{-s}{j} \nabla^j f_n,$$

where $\nabla^0 f_n = f_n$, $\nabla^{j+1} f_n = \nabla^j f_n - \nabla^j f_{n-1}$ are the **backward differences**.

# Explicit formula II

**Proof.**

We know that

$$p(t) = f_n + g[t_n, t_{n-1}](t - t_n) + g[t_n, t_{n-1}, t_{n-2}](t - t_n)(t - t_{n-1}) +$$

$$\cdots + g[t_n, t_{n-1}, \ldots, t_{n-k+1}](t - t_n)(t - t_{n-1}) \cdots (t - t_{n-k+2}).$$

We prove by induction

$$g[t_n, t_{n-1}, \ldots, t_{n-j}] = \frac{\nabla^j f_n}{h^j \cdot j!},$$

$$(t - t_n)(t - t_{n-1}) \cdots (t - t_{n-j+1}) = (-1)^j (-s)(-s-1) \cdots (-s-j+1) h^j.$$

$\square$

# Explicit formula III

- Integrate the interpolating polynomial.

$$x_{n+1} = x_n + \int_{t_n}^{t_{n+1}} p(t)\,dt = x_n + h\int_0^1 p(t_n+sh)\,ds = x_n + h\sum_{j=0}^{k-1}\gamma_j \nabla^j f_n,$$

$$\gamma_j = (-1)^j \int_0^1 \binom{-s}{j}\,ds.$$

## Explicit Adams Methods

$k=1:\quad x_{n+1} = x_n + hf_n$ (explicit Euler method)

$k=2:\quad x_{n+1} = x_n + h(\frac{3}{2}f_n - \frac{1}{2}f_{n-1})$

$k=3:\quad x_{n+1} = x_n + h(\frac{23}{12}f_n - \frac{16}{12}f_{n-1} + \frac{5}{12}f_{n-2})$

$k=4:\quad x_{n+1} = x_n + h(\frac{55}{24}f_n - \frac{59}{24}f_{n-1} + \frac{37}{24}f_{n-2} - \frac{9}{24}f_{n-3}).$

# Explicit formula IV

## Recurrence relation for the coefficients

Denote by $G(t)$ the series (**generating function**)

$$G(t) = \sum_{j=0}^{\infty} \gamma_j t^j = \sum_{j=0}^{\infty} (-t)^j \int_0^1 \binom{-s}{j} ds = \int_0^1 \sum_{j=0}^{\infty} (-t)^j \binom{-s}{j} ds =$$

$$= \int_0^1 (1-t)^{-s} ds = -\frac{-(1-t)^{-s}}{\log(1-t)}\Bigg|_{s=0}^{1} = -\frac{t}{(1-t)\log(1-t)}.$$

Then

$$-\frac{\log(1-t)}{t} G(t) = \frac{1}{1-t},$$

or, comparing the coefficients of $t^m$, we get the recurrence relation:

$$\gamma_m + \frac{1}{2}\gamma_{m-1} + \frac{1}{3}\gamma_{m-2} + \cdots + \frac{1}{m+1}\gamma_0 = 1.$$

# Implicit formula I

We interpolate also at the point $(t_{n+1}, f_{n+1})$ :

$$p^*(t) = p^*(t_n + sh) = \sum_{j=0}^{k} (-1)^j \binom{-s+1}{j} \nabla^j f_{n+1}.$$

Then

$$x_{n+1} = x_n + h \sum_{j=0}^{k} \gamma_j^* \nabla^j f_{n+1},$$

$$\gamma_j^* = (-1)^j \int_0^1 \binom{-s+1}{j} ds.$$

The formulas are of the form

$$x_{n+1} = x_n + h(\beta_k f_{n+1} + \cdots + \beta_0 f_{n-k+1}).$$

# Implicit formula II

## Implicit Adams methods

$$k = 0: \quad x_{n+1} = x_n + hf_{n+1} = x_n + hf(t_{n+1}, x_{n+1})$$

$$k = 1: \quad x_{n+1} = x_n + h(\tfrac{1}{2} f_{n+1} + \tfrac{1}{2} f_n)$$

$$k = 2: \quad x_{n+1} = x_n + h(\tfrac{5}{12} f_{n+1} + \tfrac{8}{12} f_n - \tfrac{1}{12} f_{n-1})$$

$$k = 3: \quad x_{n+1} = x_n + h(\tfrac{9}{24} f_{n+1} + \tfrac{19}{24} f_n - \tfrac{5}{24} f_{n-1} + \tfrac{1}{24} f_{n-2}).$$

$$\gamma_0^* = 1 \text{ and } \gamma_m^* + \frac{1}{2}\gamma_{m-1}^* + \frac{1}{3}\gamma_{m-2}^* + \cdots + \frac{1}{m+1}\gamma_0^* = 0.$$

# Predictor-corrector methods

To solve the nonlinear equation of the implicit methods we can proceed as follows (PECE):

P: Compute the predictor (explicit Adams or Adams-Bashforth)

$$\hat{x}_{n+1} = x_n + h \sum_{j=0}^{k-1} \gamma_j \nabla^j f_n.$$

E: Evaluate $\hat{f}_{n+1} = f(t_{n+1}, \hat{x}_{n+1})$.

C: Apply the corrector formula (implicit Adams or Adams-Moulton)

$$x_{n+1} = x_n + h(\beta_k \hat{f}_{n+1} + \beta_{k-1} f_n + \cdots + \beta_0 f_{n-k+1}).$$

to obtain $x_{n+1}$.

E: Evaluate the function again: $f_{n+1} = f(t_{n+1}, x_{n+1})$.

Other possibilities: PECECE, PEC.

# Explicit Nyström Methods

Consider the identity

$$x(t_{n+1}) = x(t_{n-1}) + \int_{t_{n-1}}^{t_{n+1}} f(t, x(s))\, ds.$$

We replace the unknown function $f(s, x(s))$ by the polynomial $p(s)$, as in th explicit Adams method:

$$x_{n+1} = x_{n-1} + h \sum_{j=0}^{k-1} \kappa_j \nabla^j f_n,$$

$$\kappa_j = (-1)^j \int_{-1}^{1} \binom{-s}{j} ds.$$

$$k = 1: \quad x_{n+1} = x_{n-1} + 2hf_n \text{ mid-point rule}$$

$$k = 3: \quad x_{n+1} = x_{n-1} + h(\tfrac{7}{3} f_n - \tfrac{2}{3} f_{n-1} + \tfrac{1}{3} f_{n-2})$$

# Milne-Simpson Methods

We proceed as in the case of the Implicit Adams Method:

$$x_{n+1} = x_{n-1} + h \sum_{j=0}^{k} \kappa_j^* \nabla^j f_{n+1},$$

$$\kappa_j^* = (-1)^j \int_{-1}^{1} \binom{-s+1}{j} ds.$$

$$k = 2: \quad x_{n+1} = x_{n-1} + h(\tfrac{1}{3} f_{n+1} + \tfrac{4}{3} f_n + \tfrac{1}{3} f_{n-1}), \ \text{(Milne method)}$$

$$k = 4: \quad x_{n+1} = x_{n-1} + h(\tfrac{29}{90} f_{n+1} + \tfrac{124}{90} f_n + \tfrac{24}{90} f_{n-1} + \tfrac{4}{90} f_{n-2} - \tfrac{1}{90} f_{n-3}).$$

## Comment

*The Milne method is a generalization of the Simpson rule: we approximate the integral $\int_{t_{n-1}}^{t_{n+1}} f(s, x(s))\, ds$ using the Simpson rule.*

# Methods Based on Differentiation (BDF) I

Assume that the approximations $x_{n-k+1}, \ldots, x_n$ are known.

- We consider the polynomial $q(t)$ which interpolates the values $(t_i, x_i)$, $i = n-k+1, \ldots, n+1$ :

$$q(t) = q(t_n + sh) = \sum_{j=0}^{k} (-1)^j \binom{-s+1}{j} \nabla^j x_{n+1}.$$

- We impose that $q(t)$ satisfies the ode at $t = t_{n+1-r}$ ($r = 1$ explicit, $r = 0$ implicit):

$$q'(t_{n+1-r}) = f(t_{n+1-r}, x_{n+1-r}).$$

# Methods Based on Differentiation (BDF) II

## Explicit formulas

$$k = 1: \quad \text{Explicit Euler Method}$$

$$k = 2: \quad \text{Mid-point rule}$$

$$k = 3: \quad \frac{1}{3}x_{n+1} + \frac{1}{2}x_n - x_{n-1} + \frac{1}{6}x_{n-2} = hf_n.$$

# Implicit BDF formulas I

We have

$$\sum_{j=0}^{k} \delta_j^* \nabla^j x_{n+1} = h f_{n+1},$$

$$\delta_j^* = (-1)^j \frac{d}{ds} \binom{-s+1}{j} \bigg|_{s=1}.$$

As

$$(-1)^j \binom{-s+1}{j} = \frac{1}{j!}(s-1)s(s+1)\cdots(s+j-2),$$

$$\delta_0^* = 0, \qquad \delta_j^* = \frac{1}{j} \text{ for } j \geq 1.$$

Then the implict formulas have the form

# Implicit BDF formulas II

## Backward differentiation formulas or BDF methods

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j x_{n+1} = h f_{n+1}.$$

$$k = 1: \quad x_{n+1} - x_n = h f_{n+1}$$

$$k = 2: \quad \tfrac{3}{2} x_{n+1} - 2 x_n + \tfrac{1}{2} x_{n-1} = h f_{n+1}$$

$$k = 3: \quad \tfrac{11}{6} x_{n+1} - 3 x_n + \tfrac{3}{2} x_{n-1} - \tfrac{1}{3} x_{n-2} = h f_{n+1}$$

# Local error of a multistep method I

Consider a linear multistep method:

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = h(\beta_k f_{n+k} + \cdots + \beta_0 f_n), \qquad (3)$$

where

$$f_i = f(t_i, x_i), \qquad t_i = t_0 + ih, \qquad \alpha_k \neq 0, \quad |\alpha_0| + |\beta_0| > 0.$$

**Definition (local error)**

*The* **local error** *of (3) is defined by*

$$x(t_k) - x_k,$$

*where $x(t)$ is the exact solution of $x' = f(t,x)$, $x(t_0) = x_0$ and $x_k$ is the numerical solution obtained from (3) by using the exact starting values $x_i = x(t_i)$, $(i = 0, 1, \ldots, k-1)$.*

# Local error of a multistep method II

**Comment**

*This definition is a generalization of the definition for one-step methods.*

Let $L$ be defined by

$$L(x,t,h) = \sum_{i=0}^{k} (\alpha_i x(t+ih) - h\beta_i x'(t+ih)).$$

**Lemma**

*Suppose that $f(t,x)$ is $C^1$. Then*

$$x(t_k) - x_k = \left(\alpha_k I - h\beta_k \frac{\partial f}{\partial x}(t_k,\eta)\right)^{-1} L(x,t_0,h).$$

*Here $\eta \in \langle x(t_k), t_k\rangle$ if $f$ is a scalar function, and in general the matrix $\frac{\partial f}{\partial x}(t_k,\eta)$ has rows evaluated at different values in $\overline{x(t_k), x_k}$.*

# Local error of a multistep method III

**Proof.**

By definition 1,

$$\sum_{i=0}^{k-1}(\alpha_i x(t_i) - h\beta_i f(t_i, x(t_i))) + \alpha_k x_k - h\beta_k f(t_k, x_k) = 0.$$

Then

$$L(x, t_0, h) = \alpha_k(x(t_k) - x_k) - h\beta_k(f(t_k, x(t_k)) - f(t_k, x_k)),$$

and we apply the MVT. □

# Local error of a multistep method IV

## Comment

*The lemma shows that* $\alpha_k^{-1} L(x, t_0, h)$ *is essentially equal (or equal if the method is explicit) to the local error. Sometimes this term is also called the local error (Dahlquist).*

# Order of a Multistep Method I

## Definition

*The multistep method*

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = h(\beta_k f_{n+k} + \cdots + \beta_0 f_n),$$

*has* **order** $p$*, if* $L(x, t, h) = O(h^{p+1})$*, for al sufficiently regular functions* $x(t)$.

## Definition

*The* **generating** *or* **characteristic** *polynomials of the multistep method are*

$$\rho(\mu) = \alpha_k \mu^k + \alpha_{k-1} \mu^{k-1} + \cdots + \alpha_0,$$
$$\sigma(\mu) = \beta_k \mu^k + \beta_{k-1} \mu^{k-1} + \cdots + \beta_0,$$

# Order of a Multistep Method II

**Theorem**

*The multistep method is of order p, iff one of the following equivalent conditions is satisfied:*

1. $\rho(1) = 0$ *and* $\sum_{i=0}^{k} \alpha_i i^q = q \sum_{i=0}^{k} \beta_i i^{q-1}$, *for* $q = 1, \ldots, p$,
2. $\rho(e^h) - h\sigma(e^h) = O(h^{p+1})$ *for* $h \to 0$.
3. $\frac{\rho(\mu)}{\log \mu} - \sigma(\mu) = O((\mu - 1)^p)$ *for* $\mu \to 1$.

# Order of a Multistep Method III

## Proof.

- To see the equivalence between $L(x,t,h) = O(h^{p+1})$ and 1), we expand $x(t+ih)$ and $x'(t+ih)$ into a Taylor series.
- To see the equivalence between 1) and 2) we us that

$$L(\exp, 0, h) = \rho(e^h) - h\sigma(e^h)$$

and

$$L(\exp, 0, h) = \sum_{i=0}^{k} \alpha_i + \sum_{q \geq 1} \frac{h^q}{q!} \left( \sum_{i=0}^{k} \alpha_i i^q - q \sum_{i=0}^{k} \beta_i i^{q-1} \right).$$

- To see the equivalence between 2) and 3) we use the transformation $\mu = e^h$ in condition 2). Then

$$\rho(\mu) - (\log \mu)\sigma(\mu) = O((\log \mu)^{p+1}), \quad \text{for } \mu \to 1.$$

The result follows from $\log \mu = (\mu - 1) + O((\mu - 1)^2)$ for $\mu \to 1$.

# Orders of classical methods

| | |
|---|---|
| explicit Adams | $k$ |
| implicit Adams | $k+1$ |
| midpoint rule | 2 |
| Nyström, $k>2$ | $k$ |
| Milne, $k=2$ | 4 |
| Milne-Simpson, $k>3$ | $k+1$ |
| BDF | $k$ |

# Zero-stability and the first Dahlquist barrier I

Among all explicit 2-step methods, the formula

$$x_{n+1} + 4x_{n+1} - 5x_n = h(4f_{n+1} + 2f_n)$$

has maximum order equal to 3.
Consider the Cauchy problem $x' = x$, $x(0) = 1$. Then we obtain the linear difference relation

$$x_{n+2} + 4(1-h)x_{n+1} - (5+2h)x_n = 0,$$

with starting values $x_0 = 1$ and $x_1 = \exp(h)$.
The general solution of the relation recurrence is

$$x_n = A\mu_1(h)^n + B\mu_2(h)^n,$$

where $A = 1 + O(h)$ and $B$ depend on $x_0$ and $x_1$ and $\mu_1(h)$ and $\mu_2(h)$ are the roots of the characteristic polynomial

$$\mu^2 + 4(1-h)\mu - (5+2h),$$

# Zero-stability and the first Dahlquist barrier II

$$\mu_1(h) = 1 + h + O(h^2), \qquad \mu_2(h) = -5 + O(h).$$

Since $\mu_1(h)$ aproximates $\exp(h)$, the first term approximates $\exp(t)$ at $t = nh$. The second term (**parasitic solution**) becomes very large!!

### Definition

*A multistep method is called* **zero-stable**, *if the generating polynomial $\rho(\mu)$ satisfies the* **root condition**, *that is*

1. *The root of $\rho(\mu)$ lie on or within the unit circle.*
2. *The roots on the unit circle are simple.*

# Zero-stability and the first Dahlquist barrier III

## Comment

*The relation*

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = 0,$$

*can be interpreted as the numerical solution of the method for the ode* $x' = 0$*. The fact that the general solution of this difference equation is*

$$x_n = p_1(n)\mu_1^n + \cdots + p_\ell(n)\mu_\ell^n,$$

*where* $\mu_i$ *is a root of multiplicity* $i$ *of the characteristic polynomial and* $p_i(n)$ *are polynomials of degree* $m_i - 1$*, justifies the previous definition.*

# Zero-stability and the first Dahlquist barrier IV

**Theorem (The first Dalhquist barrier)**

*The order $p$ of a stable linear $k$-step method satisfies*

- $p \leq k + 2$ *if* $k$ *is even,*
- $p \leq k + 1$ *if* $k$ *is odd,*
- $p \leq k$ *if* $\beta_k / \alpha_k \leq 0$ *(in particular if the method is explicit).*

# Zero-stability of classical methods

- Adams methods: $\rho(\mu) = \mu^k - \mu^{k-1}$ and zero stable.
- Nyström and Milne-Simpson methods: $\rho(\mu) = \mu^k - \mu^{k-2}$ and zero-stable.
- The $k$-step BDF formula is zero-stable for $k \leq 6$ and zero-unstable for $k \geq 7$.

# Convergence of Multistep Methods

Suppose that we consider the CP $x' = f(t,x)$, $x(t_0) = x_0$ s.t.

- $f$ is continuous on $D = \{(t,x);\; t \in [t_0, \hat{t}],\, \|x(t) - x\| \leq b\}$
- $\|f(t,x) - f(t,y)\| \leq L\|x - y\|, \qquad (t,x),(t,y) \in D.$

If we apply the multistep method

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = h(\beta_k f_{n+k} + \cdots + \beta_0 f_n),$$

with step size $h$, we obtain a sequence $\{x_i\}$. For given $t$ and $h$ s.t. $(t - t_0)/h = n$ is an integer, we introduce

$$x_h(t) = x_n \qquad \text{if } t - t_0 = nh.$$

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = h(\beta_k f_{n+k} + \cdots + \beta_0 f_n),$$

## Definition (Convergence)

1. *The LMM is called* **convergent**, *if for all initial value problems as defined*
$$x(t) - x_h(t) \to 0 \qquad \text{for } h \to 0,\ t \in [t_0, \hat{t}],$$
*whenever the starting values satisfy*
$$x(t_0 + ih) - x_h(t_0 + ih) \to 0 \qquad \text{for } h \to 0,\ i = 0, 1, \ldots, k-1.$$

2. *The LMM is* **convergent of order p**, *if to any problem as defined with $f$ differentiable enough, $\exists\ h_0 > 0$ s.t.*
$$\|x(t) - x_h(t)\| \leq C h^p \qquad \text{for } h \leq h_0$$
*whenever the starting values satisfy*
$$\|x(t_0 + ih) - x_h(t_0 + ih)\| \leq C_0 h^p \qquad \text{for } h \leq h_0,\ i = 0, 1, \ldots, k-1.$$

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = h(\beta_k f_{n+k} + \cdots + \beta_0 f_n),$$

**Theorem (Convergence)**

1. *The multistep method is convergent iff it is zero-stable and of order 1 (consistent).*
2. *If the method is zero-stable and of order $p$ then it is convergent of order $p$.*

# Linear stability I

Consider

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = h(\beta_k f_{n+k} + \cdots + \beta_0 f_n),$$

with generating polynomials:

$$\rho(\mu) = \alpha_k \mu^k + \alpha_{k-1}\mu^{k-1} + \cdots + \alpha_0,$$

$$\sigma(\mu) = \beta_k \mu^k + \beta_{k-1}\mu^{k-1} + \cdots + \beta_0.$$

We assume that it is convergent. If we apply the method to $x' = \lambda x$ and define $\tilde{h} = \lambda h$,

$$\alpha_k x_{n+k} + \alpha_{k-1} x_{n+k-1} + \cdots + \alpha_0 x_n = \tilde{h}(\beta_k x_{n+k} + \cdots + \beta_0 x_n),$$

or

$$(\alpha_k - \tilde{h}\beta_k)x_{n+k} + (\alpha_{k-1} - \tilde{h}\beta_{k-1})x_{n+k-1} + \cdots + (\alpha_0 - \tilde{h}\beta_0)x_n = 0,$$

# Linear stability II

with characteristic polynomial $\pi(\mu, \tilde{h}) = \rho(\mu) - \tilde{h}\sigma(\mu)$.

## Definition

*We call* $\pi(\mu, \tilde{h})$ *the* **stability polynomial** *of the LMSF. We say that the LMSF is* **stable** *for* $\tilde{h} \in \mathbb{C}$ *iff the roots* $r_s$ *of* $\pi(\cdot, \tilde{h})$ *satisfy* $|r_s| < 1$. *The* **stability domain** *is*

$$D = \{\tilde{h} \in \mathbb{C}; \; \text{the LMSF is stable for } \tilde{h}\}.$$

*The method is* **A-stable** *iff* $\{\tilde{h} \in \mathbb{C}; \; Re\, \tilde{h} < 0\} \subset D$.

# Linear stability III

## Second Dalhquist barrier

An A-stable multistep method must be of order $p \leq 2$. The trapezoidal rule

$$x_{n+1} = x_n + \frac{h}{2}(f_n + f_{n+1})$$

is the only A-stable method of order 2.