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ETH Lecture 401-0674-00L Numerical Methods for Partial Differential Equations

Course Video

Section 9.2.6: Single-Step Methods for Numerical Integration

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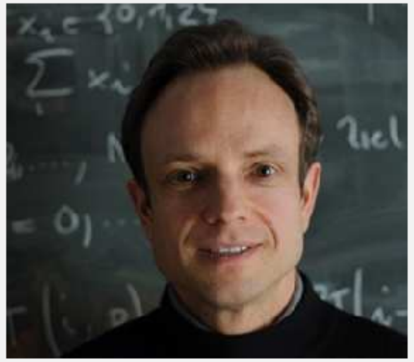


Prerequisites.

- Elementary calculus

Dependency. [Lecture → Section 9.2.5]

Video and accompanying tablet notes may not match completely!

[Corrections and updates may have been made in tablet notes.]

Note the *change in chapter numbers*, which also provide leading digits for labels:
Old Chapter 6 → New Chapter 9 , Old Chapter 8 → New Chapter 11
Trailing digits in labels are not affected.

Duration: 48 minutes

IX. Second-Order Linear Evolution Problems

9.2. Parabolic Initial Boundary Value Problems

9.2.6. Single-Step Methods for Numerical Integration

[Supplementary Section]

ODE $\dot{u} = f(t,u) \Rightarrow$ Evl.-Op $\Phi : I \times I \times \mathbb{R}^N \to \mathbb{R}^N$

Numerical Integr.: Replace $\Phi \longrightarrow \Psi : I \times I \times \mathbb{R}^N \to \mathbb{R}^N$ (discrete evolution)

Definition 9.2.6.2. Discrete evolution operator

A discrete evolution operator belonging to an ODE on $I \times \mathbb{R}^N$ is a mapping $\boldsymbol{\Psi} : I \times I \times \mathbb{R}^N \to \mathbb{R}^N$ such that for all $t \in I$ and $\mathbf{u} \in \mathbb{R}^N$ [$\tau > 0$: timestep]

$$\exists q \in \mathbb{N}_0 ,\ \tau_0 > 0: \quad \underbrace{\left\| \boldsymbol{\Psi}^{t,t+\tau}\mathbf{u} - \boldsymbol{\Phi}^{t,t+\tau}\mathbf{u} \right\|}_{\text{consistency error}} \le C(t,\mathbf{u})\tau^{q+1} \quad \forall |\tau| < \tau_0 , \tag{9.2.6.3}$$

with $C = C(t,\mathbf{u})$ depending on $t, \mathbf{u}$ continuously, and $\boldsymbol{\Phi}$ the evolution operator (→ § 7.1.5.8) associated with the ODE.
Terminology: The largest possible q in (7.1.6.3) is called the order of the discrete evolution.

9.2.6.2 Simple Single-Step Methods

Idea: Difference quotient approximation of $\dot{u}$

- $\dot{\mathbf{u}} = \mathbf{f}(t,\mathbf{u}) \quad\Rightarrow\quad \dfrac{\mathbf{u}(t+\tau)-\mathbf{u}(t)}{\tau} \approx \mathbf{f}(t,\mathbf{u}(t))$.

$$\boxed{\text{explicit (forward) Euler method:}\quad \Psi^{t,t+\tau}\mathbf{u} := \mathbf{u}+\tau\mathbf{f}(t,\mathbf{u})} \;. \tag{9.2.6.5}$$

- $\dot{\mathbf{u}} = \mathbf{f}(t,\mathbf{u}) \quad\Rightarrow\quad \dfrac{\mathbf{u}(t+\tau)-\mathbf{u}(t)}{\tau} \approx \mathbf{f}(t+\tau,\mathbf{u}(t+\tau))$.

$$\boxed{\text{implicit (backward) Euler method:}\quad \Psi^{t,t+\tau}\mathbf{u} := \mathbf{w}:\quad \mathbf{w}=\mathbf{u}+\tau\mathbf{f}(t+\tau,\mathbf{w})} \;. \tag{9.2.6.6}$$

- $\dot{\mathbf{u}} = \mathbf{f}(t,\mathbf{u}) \quad\Rightarrow\quad \dfrac{\mathbf{u}(t+\tau)-\mathbf{u}(t)}{\tau} \approx \mathbf{f}(t+\tfrac{1}{2}\tau,\tfrac{1}{2}(\mathbf{u}(t)+\mathbf{u}(t+\tau)))$.

$$\boxed{\text{implicit midpoint method:}\quad \Psi^{t,t+\tau}\mathbf{u} := \mathbf{w}:\quad \mathbf{w}=\mathbf{u}+\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\tfrac{1}{2}(\mathbf{w}+\mathbf{u}))} \;. \tag{9.2.6.7}$$

Treatment of consistency error $\tau \to \Phi^{t,t+\tau}u - \Psi^{t,t+\tau}u$ by means of Taylor expansion

$$\begin{aligned}\Phi^{t,t+\tau}\mathbf{u}_0 = \mathbf{v}(\tau) &= \mathbf{v}(0)+\tau\frac{d\mathbf{v}}{d\tau}(0)+\tfrac{1}{2}\tau^2\frac{d^2\mathbf{v}}{d\tau^2}(0)+O(\tau^3)\\ &= \mathbf{u}_0+\tau\mathbf{f}(t,\mathbf{u}_0)+\tfrac{1}{2}\tau^2\left(\frac{\partial\mathbf{f}}{\partial t}(t,\mathbf{u}_0)+\frac{\partial\mathbf{f}}{\partial\mathbf{u}}(t,\mathbf{u}_0)\mathbf{f}(t,\mathbf{u}_0)\right)+O(\tau^3)\end{aligned} \tag{9.2.6.10}$$

[$\dot{v}(\tau) = f(t+\tau, v(\tau))$ by ODE]

For explicit Euler:

$\Psi^{t,t+\tau}u_0 = u_0 + \tau f(t,u_0)$

▷ $\Phi^{t,t+\tau}u_0 - \Psi^{t,t+\tau}u_0 = O(\tau^2)$ as $\tau \to 0$

▷ Order 1

Impl. MPR: Trick: recursive insertion

$$\begin{aligned}\mathbf{w}(\tau) &= \mathbf{u}_0+\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\tfrac{1}{2}(\mathbf{u}_0+\mathbf{w}(\tau)))\\ &= \mathbf{u}_0+\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\mathbf{u}_0+\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\tfrac{1}{2}(\mathbf{u}_0+\mathbf{w}(\tau))))\\ &= \mathbf{u}_0+\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\mathbf{u}_0+\tfrac{1}{2}\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\mathbf{u}_0+O(\tau))) \quad\text{for}\quad \tau\to 0\,.\end{aligned}$$

Next: Taylor in higher dimensions

$$\mathbf{f}(t+\delta,\mathbf{u}_0+\mathbf{v}) = \mathbf{f}(t,\mathbf{u}_0)+\delta\frac{\partial\mathbf{f}}{\partial t}(t,\mathbf{u}_0)+\frac{\partial\mathbf{f}}{\partial\mathbf{u}}(t,\mathbf{u}_0)\mathbf{v}+O(\delta^2+\|\mathbf{v}\|^2) \tag{9.2.6.11}$$

③ $\Psi^{t,t+\tau}u_0 = w(\tau) =$

$$\mathbf{w}(\tau) = \mathbf{u}_0 + \tau\left(\mathbf{f}(t,\mathbf{u}_0) + \tfrac{1}{2}\tau\frac{\partial f}{\partial t}(t,\mathbf{u}_0) + \frac{\partial \mathbf{f}}{\partial \mathbf{u}}(t,\mathbf{u}_0)\tfrac{1}{2}\tau\mathbf{f}(t+\tfrac{1}{2}\tau,\mathbf{u}_0+O(\tau))\right) + O(\tau^3)$$

$$= \mathbf{u}_0 + \tau\left(\mathbf{f}(t,\mathbf{u}_0) + \tfrac{1}{2}\tau\frac{\partial f}{\partial t}(t,\mathbf{u}_0) + \frac{\partial \mathbf{f}}{\partial \mathbf{u}}(t,\mathbf{u}_0)\tfrac{1}{2}\tau(\mathbf{f}(t,\mathbf{u}_0)+O(\tau))\right) + O(\tau^3)\,.$$

$\Updownarrow$

$$\Phi^{t,t+\tau}\mathbf{u}_0 = \mathbf{v}(\tau) = \mathbf{v}(0) + \tau\frac{d\mathbf{v}}{d\tau}(0) + \tfrac{1}{2}\tau^2\frac{d^2\mathbf{v}}{d\tau^2}(0) + O(\tau^3)$$

$$= \mathbf{u}_0 + \tau\mathbf{f}(t,\mathbf{u}_0) + \tfrac{1}{2}\tau^2\left(\frac{\partial \mathbf{f}}{\partial t}(t,\mathbf{u}_0) + \frac{\partial \mathbf{f}}{\partial \mathbf{u}}(t,\mathbf{u}_0)\mathbf{f}(t,\mathbf{u}_0)\right) + O(\tau^3) \qquad (9.2.6.10)$$

▷ Cons. error $= O(\tau^3)$ $\Rightarrow$ Order 2

9.2.6.3. Single-Step Methods (SSM) for IVPs

IVP: $\dot{u} = f(t,u)$ & $u(t_0) = u_0$

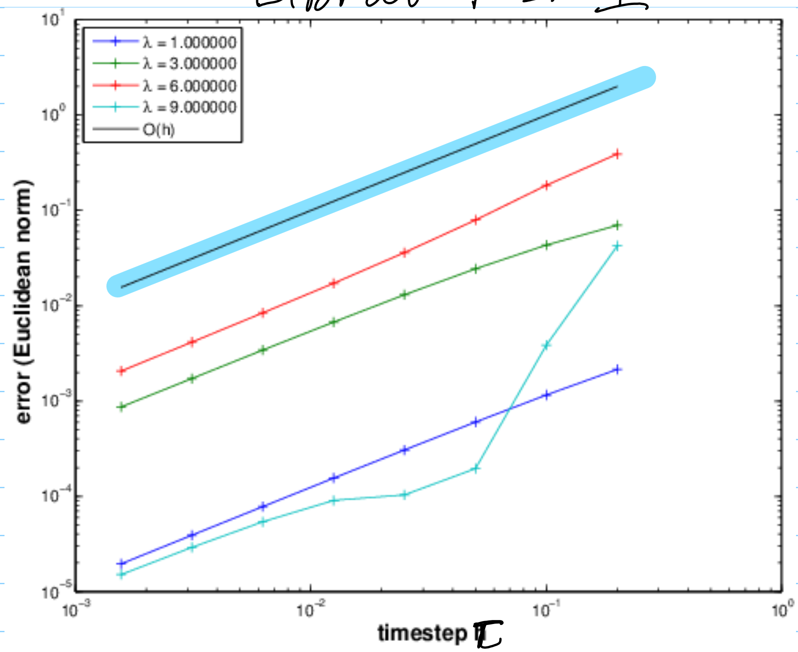
- Temporal mesh: $t_0 < t_1 < t_2 < \dots < t_M = T$
- SSM: $\begin{cases} u^{(0)} = u_0 \\ u^{(j+1)} = \Psi^{t_j,t_{j+1}} u^{(j)} \end{cases}$ $\quad j = 0,\dots,M-1$

Convergence: $-\ \|u^{(M)} - u(T)\| \to 0$? as $\tau \to 0$

$-\ \max_j \|u^{(j)} - u(t_j)\| \to 0$? $\tau := \max_j |t_j - t_{j-1}|$

Experiment: $\dot{u} = \lambda(1-u)u$, $u(0) = 0.01$, $\lambda > 0$ $(N=1)$

Error at $T = 1$

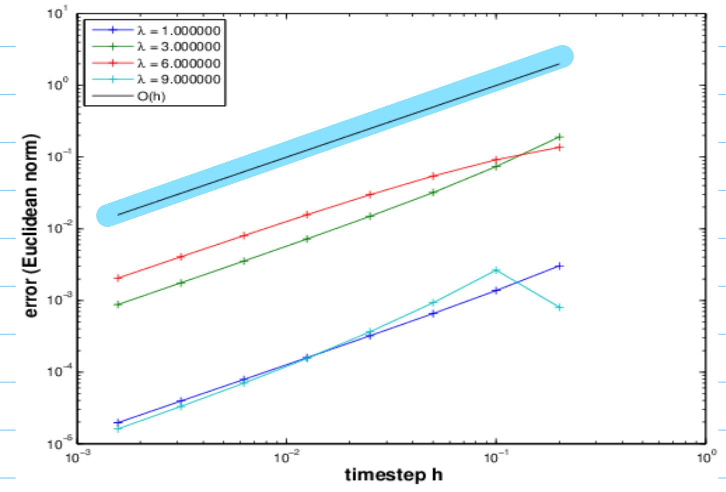


explicit Euler method

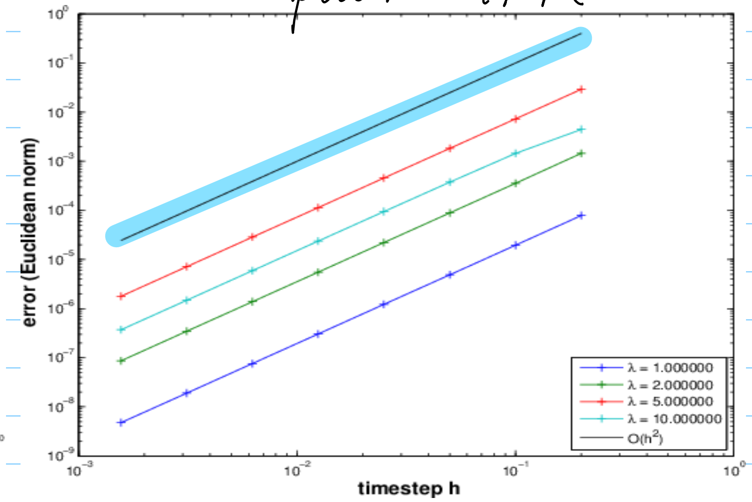
◁ Alg. cvg., rate 1

Observation: Order q ▷ rate q

Implicit MPR



implicit Euler method



Rate 1   Rate 2

(4)

smoothness assumption

Theorem 9.2.6.14. Convergence of single-step methods

Let $\mathbf{u}^{(j)} \in \mathbb{R}^N$, $j = 1,\dots,M$, be the sequence of pointwise approximations of the solution of the initial value problem

$$\text{seek} \quad \mathbf{u}: I \to V_0: \quad \dot{\mathbf{u}}(t) = \mathbf{f}(t,\mathbf{u}(t)) \quad \forall t \in I \quad , \quad \mathbf{u}(t_0) = \mathbf{u}_0\,, \tag{9.2.5.7}$$

on a time interval $[t_0, T]$ with fixed final time $T > t_0$ generated by a single step method of order $q \in \mathbb{N}$ on a temporal mesh $t_0 < t_1 < t_2 < \ldots < t_M = T$.
If $\mathbf{f} \in C^{q+1}(I \times \mathbb{R}^N)$, then

$$\max_{j=1,\dots,M} \left\| \mathbf{u}^{(j)} - \mathbf{u}(t_j) \right\| \le C\tau^q \quad \text{for} \quad \tau := \max_{j=1,\dots,M} |t_j - t_{j-1}|\,, \tag{9.2.6.15}$$

with $C > 0$ independent of the t_j. ↳ Alg. cvg. rate q !

9.2.6.4. Collocation SSM

Idea: Polynomial approximation of the solution of $\dot{\mathbf{u}} = \mathbf{f}(t,\mathbf{u})$, $\mathbf{u}(t_0) = \mathbf{u}_0$, on $[t, t+\tau]$.

$\tilde{u} \in (\mathcal{P}_s(\mathbb{R}))^N =: \mathcal{P}_s$

▷ Relax ODE to finitely many collocation condition: $\tilde{u}$ is to solve ODE at isolated points:

$\dot{\tilde{u}}(t+c_j\tau) = f(t+c_j\tau, \tilde{u}_s(t+c_j\tau))$

for $0 \le c_1 < c_2 < \ldots < c_s \le 1$

Discrete evolution operator by polynomial collocation

Given $t \in I$, $\tau \in \mathbb{R}$ with $t+\tau \in I$, $\mathbf{u}_0 \in \mathbb{R}^N$, $s \in \mathbb{N}$, and interpolation nodes $0 \le c_1 < c_2 < \cdots < c_s \le 1$, we set

$$\mathbf{\Psi}^{t,t+\tau}\mathbf{u}_0 = \tilde{\mathbf{u}}_s(t+\tau)\,,$$

where $\tilde{\mathbf{u}}_s \in \mathcal{P}_s(\mathbb{R})$ satisfies

ODE satisfied at s points

$$\tilde{\mathbf{u}}_s(t) = \mathbf{u}_0\,, \tag{9.2.6.21}$$
$$\dot{\tilde{\mathbf{u}}}_s(t+c_j\tau) = \mathbf{f}(t+c_j\tau, \tilde{\mathbf{u}}_s(t+c_j\tau))\,, \quad j = 1,\dots,s\,. \tag{9.2.6.22}$$

The equations (7.1.6.22) are called collocation conditions. (CC)

Explicit formulas:

Lagrange Polynomials: $L_j \in \mathcal{P}_{s-1}(\mathbb{R})$: $L_j(c_k) = \delta_{kj} = \begin{cases} 1 & \text{, if } k = j\,, \\ 0 & \text{else,} \end{cases} \quad 1 \le k,j \le s\,.$

▷ $\dot{\tilde{u}}(t+\xi\tau) = \sum_{j=1}^{s} k_j L_j(\xi)$, $k_j \in \mathbb{R}^N$, $\xi \in \mathbb{R}$

(CC) ▷ $k_j = f(t+c_j\tau, \tilde{u}_s(t+c_j\tau))$

↳ increment

(7.1.6.22)

▶ $\dot{\tilde{\mathbf{u}}}_s(t+\xi\tau) = \sum_{j=1}^{s} \mathbf{k}_j L_j(\xi)$ with increments $\mathbf{k}_j := f(t+c_j\tau, \tilde{\mathbf{u}}_s(t+c_j\tau))$.

Next we integrate* and use $\tilde{\mathbf{u}}_s(t) = \mathbf{u}_0$: * w.r.t. ξ [introduces τ-factor]

▶ $\tilde{\mathbf{u}}_s(t+c_i\tau) = \mathbf{u}_0 + \tau \sum_{j=1}^{s} \mathbf{k}_j \int_0^{c_i} L_j(\xi)\,\mathrm{d}\xi\,, \quad 0 \le c_i \le 1\,.$

⑤ ▷ $N\cdot s$ equ. for $N\cdot s$ unknowns

$$\mathbf{k}_i = f(t + c_i\tau, \mathbf{u}_0 + \tau\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,,\qquad \text{where}\quad a_{ij} := \int_0^{c_i} L_j(\xi)\,\mathrm{d}\xi\,,$$

$$\Psi^{t,t+\tau}\mathbf{u}_0 := \tilde{\mathbf{u}}_s(t+\tau) = \mathbf{u}_0 + \tau\sum_{i=1}^{s} b_i\mathbf{k}_i\,.\qquad b_i := \int_0^1 L_i(\xi)\,\mathrm{d}\xi\,. \tag{7.3.2.6}$$

Theorem 9.2.6.29. Order of collocation single step method

Provided that $\mathbf{f} \in C^p(I \times \mathbb{R}^N)$, the order (→ Def. 7.1.6.2) of an s-stage collocation single step method according to (7.1.6.26) agrees with the order (→) of the quadrature formula on $[0,1]$ with nodes c_j and weights b_j, $j = 1,\dots,s$.

▷ Order $2s$ Gauss-collocation SSM

$$\dot{\tilde{u}}_s(t+\xi\tau) = f(\xi)$$

$$\tilde{u}_s(\sigma) = \tilde{u}_s(t) + \int_t^\sigma \dot{\tilde{u}}_s(v)\,dv$$

$v := \xi\tau$, $dv = \tau\, d\xi$

$$= u_0 + \int_0^{\sigma - t} \dot{\tilde{u}}_s(v+t)\,dv$$

$$\tilde{u}_s(t + c_i\tau) = u_0 + \tau\int_0^{(\sigma-t)/\tau = c_i} \underbrace{\dot{\tilde{u}}_s(t+\xi\tau)}_{=\sum_{j=1} k_j L_j(\xi)}\,d\xi$$

9.2.6.5 Runge-Kutta SSM

Definition 7.3.3. 1. General Runge-Kutta method →

For coefficients $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{s} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, the discrete evolution $\Psi^{s,t}$ of an s-stage Runge-Kutta single step method (RK-SSM) for the ODE $\dot{\mathbf{u}} = \mathbf{f}(t,\mathbf{u})$, is defined by

$$\mathbf{k}_i := \mathbf{f}(t + c_i\tau, \mathbf{u} + \tau\sum_{j=1}^{s} a_{ij}\mathbf{k}_j)\,,\quad i = 1,\dots,s\quad,\quad \Psi^{t,t+\tau}\mathbf{u} := \mathbf{u} + \tau\sum_{i=1}^{s} b_i\mathbf{k}_i\,.$$

The $\mathbf{k}_i \in V_0$ are called increments.

Notation: Butcher schemes

$$\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} \;\hat{=}\; \begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & \ddots & & a_{2s} \\ \vdots & \vdots & & \ddots & \vdots \\ c_s & a_{s1} & \dots & & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}\,,\quad \mathbf{c},\mathbf{b} \in \mathbb{R}^s,\quad \mathfrak{A} \in \mathbb{R}^{s,s}\,. \tag{7.3.3.3'}$$

$$\begin{array}{c|cc} \frac{1}{2} - \sqrt{3}/6 & \frac{1}{4} & \frac{1}{4} - \sqrt{3}/6 \\ \frac{1}{2} + \sqrt{3}/6 & \frac{1}{4} + \sqrt{3}/6 & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

2-stage Gauss SSM, order 4

$s = 2$

$$\begin{array}{c|ccc} \frac{1}{2} - \sqrt{15}/10 & \frac{5}{36} & \frac{2}{9} - \sqrt{15}/15 & \frac{5}{36} - \sqrt{15}/30 \\ \frac{1}{2} & \frac{5}{36} + \sqrt{15}/24 & \frac{2}{9} & \frac{5}{36} - \sqrt{15}/24 \\ \frac{1}{2} + \sqrt{15}/10 & \frac{5}{36} + \sqrt{15}/30 & \frac{2}{9} + \sqrt{15}/15 & \frac{5}{36} \\ \hline & \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \end{array}$$

3-stage Gauss SSM, order 6

$s = 3$

6 Review questions 9.2.6.31:

A:

Explain, why the condition $\sum_{i=1}^{s} b_i = 1$ has to be satisfied for the coefficient for a general Runge-Kutta method according to Def. 6.2.6.31.

Definition 6.2.6.31. General Runge-Kutta method

For coefficients $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{s} a_{ij}$, $i, j = 1, \ldots, s$, $s \in \mathbb{N}$, the discrete evolution $\boldsymbol{\Psi}^{s,t}$ of an s-stage Runge-Kutta single step method (RK-SSM) for the ODE $\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u})$, is defined by

$$\mathbf{k}_i := \mathbf{f}(t + c_i\tau, \mathbf{u} + \tau \sum_{j=1}^{s} a_{ij}\mathbf{k}_j) \ , \quad i = 1, \ldots, s \quad , \quad \boldsymbol{\Psi}^{t,t+\tau}\mathbf{u} := \mathbf{u} + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i \ .$$

The $\mathbf{k}_i \in V_0$ are called increments.