Modified Equations for Variational Integrators

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Continuous

- Action: $S = \int_a^b \mathcal{L}(x(t), \dot{x}(t)) \, \mathrm{d}t$
- Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial x}(x(t), \dot{x}(t)) - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{x}}(x(t), \dot{x}(t)) = 0.$$

Discrete

- Action: $S_{\mathrm{disc}} = \sum_{j=1}^n h L_{\mathrm{disc}}(x_{j-1}, x_j)$, with

$$L_{\mathrm{disc}}\big(x((t-h), x(t)\big) \approx \mathcal{L}(x(t), \dot{x}(t)),$$

- Euler-Lagrange equation:

$$\mathrm{D}_2 L_{\mathrm{disc}}(x_{j-1}, x_j) + \mathrm{D}_1 L_{\mathrm{disc}}(x_j, x_{j+1}) = 0.$$

Preliminaries: consistency

Definition

(a) *A discrete quantity* $\Psi_h(x_j, x_{j+1})$ *is a* consistent discretization *of a continuous quantity* $f(x, \dot{x})$ *if for any smooth curve* x

$$\Psi_h(x(t), x(t+h)) = f(x(t), \dot{x}(t)) + \mathcal{O}(h) \qquad \text{for } h \to 0.$$

(b) $\Psi_h(x_{j-1}, x_j, x_{j+1})$ *is a* consistent discretization *of* $f(x, \dot{x}, \ddot{x})$ *if*

$$\Psi_h(x(t-h), x(t), x(t+h)) = f(x(t), \dot{x}(t), \ddot{x}(t)) + \mathcal{O}(h).$$

Proposition

If L_{disc} is a consistent discretization of $\mathcal{L}$, then the discrete Euler-Lagrange equation is a consistent discretization of the continuous Euler-Lagrange equation,

$$\begin{aligned}&\mathrm{D}_2 L_{\mathrm{disc}}(x(t-h),x(t)) + \mathrm{D}_1 L_{\mathrm{disc}}(x(t),x(t+h)) \\ &= \frac{\partial \mathcal{L}}{\partial x(t)}(x(t),\dot{x}(t)) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial x(t)}(x(t),\dot{x}(t))\right) + \mathcal{O}(h).\end{aligned}$$

Modified Equations

Definition (First order equations)

Let $\Psi_h(x_j, x_{j+1})$ *be a consistent discretization of some* $g(x(t), \dot{x}(t))$*, where* $\det \frac{\partial g}{\partial \dot{x}} \neq 0$*. The differential equation* $\dot{x} = f_h(x)$*, where*

$$f_h(x) \simeq f_0(x) + hf_1(x) + h^2 f_2(x) + \dots$$

is a modified equation for the difference equation $\Psi_h(x_j, x_{j+1}) = 0$ *if, for every* k*, every solution of the truncated differential equation*

$$\dot{x} = \mathcal{T}_k\left(f_h(x)\right)$$

satisfies $\Psi_h(x(t), x(t+h)) = \mathcal{O}(h^{k+1})$ *for all* t*.*

Definition (Second order equations)

Let $\Psi_h(x_{j-1}, x_j, x_{j+1})$ *be a consistent discretization of some* $g(x(t), \dot{x}(t), \ddot{x}(t))$, *where* $\det \frac{\partial g}{\partial \ddot{x}} \neq 0$. *The differential equation* $\ddot{x} = f_h(x, \dot{x})$, *where*

$$f_h(x, \dot{x}) \simeq f_0(x, \dot{x}) + h f_1(x, \dot{x}) + h^2 f_2(x, \dot{x}) + \ldots$$

is a modified equation for the second order difference equation $\Psi_h(x_{j-1}, x_j, x_{j+1}) = 0$ *if, for every* k, *every solution of the truncated differential equation*

$$\ddot{x} = \mathcal{T}_k\left(f_h(x, \dot{x})\right)$$

satisfies $\Psi_h(x(t-h), x(t), x(t+h)) = \mathcal{O}(h^{k+1})$ *for all* t.

Example.

- Differential equation: $\ddot{x} = -g(x)$
- Discretization: $x_{j+1} - 2x_j + x_{j-1} = -h^2 g(x_j)$.

The modified equation is of the form

$$\ddot{x} = f_h(x) = f_0(x, \dot{x}) + h^2 f_2(x, \dot{x}) + \mathcal{O}(h^4).$$

If $x(t) = x_j$, then $x_{j\pm1} = x(t \pm h) = x \pm h\dot{x} + \frac{h^2}{2}\ddot{x} \pm \frac{h^3}{6}x^{(3)} + \ldots$.

Plugging this into the difference equation we find that (with $v = \dot{x}$)

$$\begin{aligned}
-h^2 g(x) &= h^2 \ddot{x} + \frac{h^4}{12} x^{(4)} + \mathcal{O}(h^6) \\
&= h^2(f_0 + h^2 f_2) + \frac{h^4}{12}\big(f_{0,xx}(v, v) + 2f_{0,xv}(f_0, v) + f_{0,x} f_0 \\
&\qquad + f_{0,vv}(f_0, f_0) + f_{0,v} f_{0,x} v + f_{0,v} f_{0,v} f_0\big) + \mathcal{O}(h^6)
\end{aligned}$$

Example (continued). We have

$$
\begin{aligned}
-h^2 g(x) &= h^2 \ddot{x} + \frac{h^4}{12} x^{(4)} + \mathcal{O}(h^6) \\
&= h^2 (f_0 + h^2 f_2) + \frac{h^4}{12} \big(f_{0,xx}(v,v) + 2 f_{0,xv}(f_0, v) + f_{0,x} f_0 \\
&\qquad + f_{0,vv}(f_0, f_0) + f_{0,v} f_{0,x} v + f_{0,v} f_{0,v} f_0 \big) + \mathcal{O}(h^6)
\end{aligned}
$$

- The h^2-term of this equation gives us $f_0(x,v) = -g(x)$. In particular, partial derivatives of f_0 with respect to v are zero.
- The h^4-term then reduces to $f_2 = \frac{1}{12}(g_{xx}(v,v) - g_x g)$.

We find that the modified equation is

$$
\ddot{x} = -g(x) + \frac{h^2}{12}(g_{xx}(\dot{x},\dot{x}) - g_x g) + \mathcal{O}(h^4).
$$

Question

From now on we consider Lagrangian equations

$$\mathcal{L} = \frac{1}{2}\langle \dot{x}\,, \dot{x} \rangle - U(x) \qquad \Rightarrow \qquad \ddot{x} = -U'(x)$$

and variational integrators.

Are their modified equations are Lagrangian as well?

The truncated modified equation from our Example

$$\ddot{x} = -U' + \frac{h^2}{12}\big(U'''(\dot{x}, \dot{x}) - U''U'\big).$$

is not an Euler-Lagrange equation.

However, we will see that it can be obtained from an EL equation by solving it for $\ddot{x}$ and truncating the resulting power series.

General idea

Look for a modified Lagrangian $\mathcal{L}_{\mathrm{mod}}(x, \dot{x})$ such that the discrete Lagrangian L_{disc} is its exact discrete Lagrangian, i.e.

$$\int_{(j-1)h}^{jh} \mathcal{L}_{\mathrm{mod}}(x(t), \dot{x}(t)) \mathrm{d}t = hL_{\mathrm{disc}}\big(x((j-1)h), x(jh)\big).$$

The Euler-Lagrange equation of $\mathcal{L}_{\mathrm{mod}}$ will then be the modified equation.

The best we can hope for is to find such a modified Lagrangian up to an error of arbitrarily high order.

We can write the discrete Lagrangian as a function of x and its derivatives, all evaluated at the point $jh - \frac{h}{2}$,

$$\begin{aligned}\mathcal{L}_{\mathrm{disc}}[x] &:\simeq L_{\mathrm{disc}}\Bigg(x - \frac{h}{2}\dot{x} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \ddot{x} - \ldots, \\ &\qquad\qquad\qquad x + \frac{h}{2}\dot{x} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \ddot{x} + \ldots \Bigg). \\ &\simeq L_{\mathrm{disc}}(x_{j-1}, x_j)\end{aligned}$$

Here and in the following:

- we evaluate at $t = jh - \frac{h}{2}$ whenever we omit the variable t, i.e. $x := x\left(jh - \frac{h}{2}\right)$,
- $x_j = x(jh)$ and $x_{j-1} = x((j-1)h)$.

We want to write the discrete action

$$S_{\mathrm{disc}} = \sum_{j=1}^{n} h L_{\mathrm{disc}}(x_{j-1}, x_j) \simeq \sum_{j=1}^{n} h \mathcal{L}_{\mathrm{disc}} \left[x \left(jh - \tfrac{h}{2} \right) \right]$$

as an integral.

Lemma

For any smooth function $f : \mathbb{R} \to \mathbb{R}^N$ we have

$$\begin{aligned} \sum_{j=1}^{n} h f\left(jh - \frac{h}{2} \right) &\simeq \int_0^{nh} \sum_{i=0}^{\infty} h^{2i} \left(2^{1-2i} - 1 \right) \frac{B_{2i}}{(2i)!} f^{(2i)}(t) \,\mathrm{d}t \\ &\simeq \int_0^{nh} \left(f(t) - \frac{h^2}{24} \ddot{f}(t) + 7 \frac{h^4}{5760} f^{(4)}(t) + \dots \right) \mathrm{d}t, \end{aligned}$$

where B_i are the Bernoulli numbers.

Proof (sketch). The h^2-term can easily be obtained by Taylor expansion. We have

$$\begin{aligned}
\int_0^h f(t)\,\mathrm{d}t &= \int_0^h f\left(\tfrac{h}{2}\right) + \left(t-\tfrac{h}{2}\right)\dot{f}\left(\tfrac{h}{2}\right) + \frac{1}{2}\left(t-\tfrac{h}{2}\right)^2 \ddot{f}\left(\tfrac{h}{2}\right) + \mathcal{O}(t^3)\,\mathrm{d}t \\
&= hf\left(\tfrac{h}{2}\right) + \frac{h^3}{24}\ddot{f}\left(\tfrac{h}{2}\right) + \mathcal{O}(h^4) \\
&= hf\left(\tfrac{h}{2}\right) + \int_0^h \frac{h^2}{24}\ddot{f}\left(\tfrac{h}{2}\right)\,\mathrm{d}t + \mathcal{O}(h^4) \\
&= hf\left(\tfrac{h}{2}\right) + \int_0^h \frac{h^2}{24}\Big(\ddot{f}(t) + \mathcal{O}(t)\Big)\,\mathrm{d}t + \mathcal{O}(h^4) \\
&= hf\left(\tfrac{h}{2}\right) + \int_0^h \frac{h^2}{24}\ddot{f}(t)\,\mathrm{d}t + \mathcal{O}(h^4).
\end{aligned}$$

Two proof strategies:

- iterate this,
- use Euler-Maclaurin formula. ■

Definition

We call

$$\mathcal{L}_{\mathrm{mod}}[x(t)] :\simeq \mathcal{L}_{\mathrm{disc}}[x(t)] + \sum_{i=1}^{\infty} \left(2^{1-2i} - 1\right) \frac{h^{2i} B_{2i}}{(2i)!} \frac{\mathrm{d}^{2i}}{\mathrm{d}t^{2i}} \mathcal{L}_{\mathrm{disc}}[x(t)]$$

$$\simeq \mathcal{L}_{\mathrm{disc}}[x(t)] - \frac{h^2}{24} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \mathcal{L}_{\mathrm{disc}}[x(t)] + \frac{7h^4}{5760} \frac{\mathrm{d}^4}{\mathrm{d}t^4} \mathcal{L}_{\mathrm{disc}}[x(t)] + \dots$$

the modified Lagrangian of L_{disc}.

Lemma

$$\mathcal{L}_{\mathrm{mod}}[x] = \mathcal{L}(x, \dot{x}) + \mathcal{O}(h).$$

Towards a first order Lagrangian

The modified Lagrangian

$$\mathcal{L}_{\mathrm{disc}}[x(t)] - \frac{h^2}{24}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{L}_{\mathrm{disc}}[x(t)] + \frac{7h^4}{5760}\frac{\mathrm{d}^4}{\mathrm{d}t^4}\mathcal{L}_{\mathrm{disc}}[x(t)] + \dots$$

is an asymptotic power series in h and contains derivatives $x^{(i)}$ of every order i.

For every truncation of the power series $\mathcal{L}_{\mathrm{mod}}$ we will construct an equivalent Lagrangian that is of first order, i.e. that depends only on x and $\dot{x}$.

For any $k \in \mathbb{N}$ we define first order Lagrangians

$$\mathcal{L}_{\mathrm{mod},k}(x,\dot{x}) = \mathscr{L}_0(x,\dot{x}) + h\mathscr{L}_1(x,\dot{x}) + \ldots + h^k \mathscr{L}_k(x,\dot{x}),$$

where the coefficients $\mathcal{L}_i(x,\dot{x})$ will be defined recursively below.

Solve the Euler-Lagrange equation

$$\frac{\partial \mathscr{L}_0}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}_0}{\partial \dot{x}} + \ldots + h^k \left(\frac{\partial \mathscr{L}_k}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}_k}{\partial \dot{x}} \right) = 0$$

for $\ddot{x}$. This gives us an expression of the form

$$\ddot{x} = F_0^2(x,\dot{x}) + hF_1^2(x,\dot{x}) + \ldots + h^k F_k^2(x,\dot{x}) + \mathcal{O}(h^{k+1}).$$

Similar expressions for the higher derivatives follow

$$\begin{aligned} x^{(3)} &= F_0^3(x,\dot{x}) + hF_1^3(x,\dot{x}) + \ldots + h^k F_k^3(x,\dot{x}) + \mathcal{O}(h^{k+1}), \\ x^{(4)} &= F_0^4(x,\dot{x}) + hF_1^3(x,\dot{x}) + \ldots + h^k F_k^4(x,\dot{x}) + \mathcal{O}(h^{k+1}), \\ &\vdots \end{aligned}$$

We want that $\mathcal{L}_{\text{mod},k}(x, \dot{x}) = \mathcal{L}_{\text{mod}}[x] + \mathcal{O}(h^{k+1})$ for critical curves. This is the case if and only if for any k there holds

$$\begin{aligned}
\mathcal{L}_{\text{mod},k}(x, \dot{x}) &= \mathscr{L}_0(x, \dot{x}) + \ldots + h^k \mathscr{L}_k(x, \dot{x}) \\
&= \mathcal{L}_{\text{mod}}[x] \Big|_{\substack{\ddot{x} = F_0^2(x,\dot{x}) + \ldots + h^{k-1} F_{k-1}^2(x,\dot{x}) \\ x^{(3)} = F_0^3(x,\dot{x}) + \ldots + h^{k-1} F_{k-1}^3(x,\dot{x}) \\ \ldots}} + \mathcal{O}(h^{k+1}) \\
&= \mathcal{L}_{\text{mod}}[x] \Big|_{\text{EL equations of } \mathcal{L}_{\text{mod},k-1}} + \mathcal{O}(h^{k+1}).
\end{aligned}$$

This gives us a recurrence relation for the $\mathcal{L}_{\text{mod},k}$.

Definition

(a) *A curve* $x : [a, b] \to \mathbb{R}$ *is* *k-critical* *for some action* $S = \int_a^b \mathcal{L}\,\mathrm{d}t$ *if for any variation of* x *there holds*

$$\delta S = \mathcal{O}\big(h^{k+1}\,\|\delta x\|\big),$$

where $\|\delta x\| = \int_a^b |\delta x(t)| \mathrm{d}t$ *is the usual 1-norm.*

(b) *A discrete curve* $(x_j)_j$ *is* *k-critical* *for some action* $S_{\mathrm{disc}} = \sum_j L_{\mathrm{disc}}(x_j, x_{j+1})$ *if for any variation of* $(x_j)_j$ *there holds*

$$\delta S = \mathcal{O}\big(h^{k+1}\,\|(\delta x_j)_j\|\big),$$

where $\|(\delta x_j)_j\| = \sum h|\delta x_j|$.

The scaling is chosen such that $\|\delta x\| = \big(1 + \mathcal{O}(h)\big)\|(\delta x(jh))_j\|$.

We can characterize k-critical curves by the fact that they satisfy the Euler-Lagrange equations up to a certain order.

Lemma

(a) *A curve $x : [a, b] \to \mathbb{R}$ is k-critical for the action $S = \int_a^b \mathcal{L} \,\mathrm{d}t$ if and only if it satisfies the corresponding Euler-Lagrange equations up to order k.*

(b) *A discrete curve $(x_j)_j$ is k-critical for the action $S_{\mathrm{disc}} = \sum_j L_{\mathrm{disc}}(x_j, x_{j+1})$ if and only if it satisfies the corresponding discrete Euler-Lagrange equations up to order k.*

Lemma

The Euler-Lagrange equations of $\mathcal{L}_{\mathrm{mod}}[x]$ and of the first order Lagrangian $\mathcal{L}_{\mathrm{mod},k}(x,\dot{x})$ are equivalent up to order k.

Proof. We need to show that both Lagrangians have the same k-critical curves,

$$\mathcal{C}_k(\mathcal{L}_{\mathrm{mod}}) = \mathcal{C}_k(\mathcal{L}_{\mathrm{mod},k}).$$

We use induction on k.

Obviously a curve is 0-critical for $\mathcal{L}_{\mathrm{mod}}[x]$ if and only if it is 0-critical for $\mathcal{L}_{\mathrm{mod},0}(x,\dot{x}) = \mathcal{T}_0\left(\mathcal{L}_{\mathrm{mod}}[x]\right)$.

Proof (continued). Now suppose that $\mathcal{C}_k(\mathcal{L}_{\mathrm{mod}}) = \mathcal{C}_k(\mathcal{L}_{\mathrm{mod},k})$ for some fixed k. The higher derivatives of $x \in \mathcal{C}_k(\mathcal{L}_{\mathrm{mod},k})$ are given by

$$\begin{aligned} \ddot{x} &= F_0^2(x,\dot{x}) + \ldots + h^k F_k^2(x,\dot{x}) + \mathcal{O}(h^{k+1}), \\ x^{(3)} &= F_0^3(x,\dot{x}) + \ldots + h^k F_k^3(x,\dot{x}) + \mathcal{O}(h^{k+1}), \\ &\vdots \end{aligned}$$

so we can conclude from the recurrence relation

$$\begin{aligned} \mathcal{L}_{\mathrm{mod},k+1}(x,\dot{x}) &= \mathscr{L}_0(x,\dot{x}) + \ldots + h^{k+1}\mathscr{L}_{k+1}(x,\dot{x}) \\ &= \mathcal{L}_{\mathrm{mod}}[x]\Big|_{\substack{\ddot{x}=F_0^2(\mathscr{L}_0)+\ldots+h^k F_l^2(\mathscr{L}_0,\ldots,\mathscr{L}_k) \\ x^{(3)}=F_0^3(\mathscr{L}_0)+\ldots+h^k F_l^3(\mathscr{L}_0,\ldots,\mathscr{L}_k) \\ \ldots}} + \mathcal{O}(h^{k+2}). \end{aligned}$$

that for any $x \in \mathcal{C}_k(\mathcal{L}_{\mathrm{mod},k})$,

$$\mathcal{L}_{\mathrm{mod},k+1}(x,\dot{x}) = \mathcal{L}_{\mathrm{mod}}[x] + \mathcal{O}(h^{k+2}).$$

Proof (continued). For every k-critical curve x we have

$$\int_a^b \mathcal{L}_{\mathrm{mod},k+1}(x(t),\dot{x}(t))\,\mathrm{d}t = \int_a^b \mathcal{L}_{\mathrm{mod}}[x(t)]\,\mathrm{d}t + \mathcal{O}(h^{k+2}).$$

Now observe that:

- every $(k+1)$-critical curve for $\mathcal{L}_{\mathrm{mod}}$ is also a k-critical curve, i.e. $\mathcal{C}_{k+1}(\mathcal{L}_{\mathrm{mod}}) \subset \mathcal{C}_k(\mathcal{L}_{\mathrm{mod}})$.
- $\mathcal{T}_k(\mathcal{L}_{\mathrm{mod},k+1}) = \mathcal{L}_{\mathrm{mod},k}$ so $\mathcal{C}_{k+1}(\mathcal{L}_{\mathrm{mod},k+1}) \subset \mathcal{C}_k(\mathcal{L}_{\mathrm{mod},k})$
- any sufficiently small variation of a k-critical curve is still k-critical.

To determine if a curve is $(k+1)$-critical, it is sufficient to consider variations in the set of k-critical curves.

Therefore $\mathcal{C}_{k+1}(\mathcal{L}_{\mathrm{mod},k+1}) = \mathcal{C}_{k+1}(\mathcal{L}_{\mathrm{mod}})$. ∎

Main result

Theorem

For a discrete Lagrangian L_{disc} that is a consistent discretization of some $\mathcal{L}$, the k-th truncation of the Euler-Lagrange equation of $\mathcal{L}_{\mathrm{mod},k}(x,\dot{x})$ is the k-th truncation of the modified equation.

Compare:

"This example illustrates that the modified equation corresponding to a separable Hamiltonian (i.e., $H(p,q) = T(p) + U(q)$) is in general not separable. Moreover, it shows that the modified equation of a second order differential equation $q'' = \nabla U(q)$ (or equivalently, $q' = p$, $p' = \nabla U(q)$) is in general not a second order equation."

Hairer, Lubich, Wanner (2006), Example IX.3.4

Proof. Let x be a solution of the Euler-Lagrange equation for $\mathcal{L}_{\mathrm{mod},k}(x,\dot{x})$, truncated after order k. Consider the discrete curve $(x_j)_j := (x(jh))_j$.

- x is k-critical for the action $\int \mathcal{L}_{\mathrm{mod},k}(x,\dot{x})\,\mathrm{d}t$.
- By the Lemma, x is k-critical for the action $\int \mathcal{L}_{\mathrm{mod}}[x]\,\mathrm{d}t$.
- By construction, the actions $S_{\mathrm{disc}} = \sum_j L_{\mathrm{disc}}(y(jh), y((j+1)h))$ and $S = \int_a^b \mathcal{L}_{\mathrm{mod}}[y(t)]\,\mathrm{d}t$ are equal for any smooth curve y.
- Therefore the discrete curve $(x(jh))_j$ is k-critical for the discrete action S_{disc}. Hence

$$\mathrm{D}_2 L_{\mathrm{disc}}(x(t-h), x(t)) + \mathrm{D}_1 L_{\mathrm{disc}}(x(t), x(t+h)) = \mathcal{O}(h^{k+1}). \qquad \blacksquare$$

Example: Störmer-Verlet discretization

$$\mathcal{L}(x,\dot{x}) = \frac{1}{2}\langle \dot{x}\,,\dot{x}\rangle - U(x)$$

$$L_{\mathrm{disc}}(x_j,x_{j+1}) = \frac{1}{2}\left\langle \frac{x_{j+1}-x_j}{h}\,,\frac{x_{j+1}-x_j}{h}\right\rangle - \frac{1}{2}U\left(x_j\right) - \frac{1}{2}U\left(x_{j+1}\right).$$

Its Euler-Lagrange equation is

$$\frac{x_{j+1}-2x_j+x_{j-1}}{h^2} = -U'(x_j).$$

We have

$$\mathcal{L}_{\mathrm{disc}}[x] \simeq \left\langle \dot{x} + \tfrac{h^2}{24}x^{(3)} + \ldots\,,\dot{x} + \tfrac{h^2}{24}x^{(3)} + \ldots\right\rangle$$
$$- \tfrac{1}{2}U\left(x - \tfrac{h}{2}\dot{x} + \tfrac{1}{2}\left(\tfrac{h}{2}\right)^2\ddot{x} - \ldots\right) - \tfrac{1}{2}U\left(x + \tfrac{h}{2}\dot{x} + \tfrac{1}{2}\left(\tfrac{h}{2}\right)^2\ddot{x} + \ldots\right).$$

$$\mathcal{L}_{\mathrm{disc}}[x] = \frac{1}{2}\langle \dot{x}, \dot{x}\rangle - U + \frac{h^2}{24}\left(\left\langle \dot{x}, x^{(3)}\right\rangle - 3U'\ddot{x} - 3U''(\dot{x},\dot{x})\right) + \mathcal{O}(h^4),$$

From this we calculate the modified Lagrangian,

$$\begin{aligned}
\mathcal{L}_{\mathrm{mod}}[x] &= \mathcal{L}_{\mathrm{disc}}[x] - \frac{h^2}{24}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{L}_{\mathrm{disc}}[x] + \mathcal{O}(h^4) \\
&= \frac{1}{2}\langle \dot{x}, \dot{x}\rangle - U + \frac{h^2}{24}\left(\left\langle \dot{x}, x^{(3)}\right\rangle - 3U'\ddot{x} - 3U''(\dot{x},\dot{x})\right) \\
&\qquad - \frac{h^2}{24}\left(\langle \ddot{x}, \ddot{x}\rangle + \left\langle \dot{x}, x^{(3)}\right\rangle - U'\ddot{x} - U''(\dot{x},\dot{x})\right) + \mathcal{O}(h^4) \\
&= \frac{1}{2}\langle \dot{x}, \dot{x}\rangle - U + \frac{h^2}{24}\left(-\langle \ddot{x}, \ddot{x}\rangle - 2U'\ddot{x} - 2U''(\dot{x},\dot{x})\right) + \mathcal{O}(h^4).
\end{aligned}$$

Eliminate second derivatives using $\ddot{x} = -U' + \mathcal{O}(h^2)$,

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \frac{1}{2}\langle \dot{x}, \dot{x}\rangle - U + \frac{h^2}{24}\left(U'U' - 2U''(\dot{x},\dot{x})\right).$$

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \frac{1}{2}\langle \dot{x}\,,\dot{x}\rangle - U + \frac{h^2}{24}\left(U'U' - 2U''(\dot{x},\dot{x})\right).$$

Observe that this Lagrangian is not separable for general U.

The corresponding Euler-Lagrange equation is

$$\begin{aligned} 0 &= -\ddot{x} - U' + \frac{h^2}{24}\left(2U''U' - 2U'''(\dot{x},\dot{x}) + 4\frac{\mathrm{d}}{\mathrm{d}t}\left(U''\dot{x}\right)\right) \\ &= -\ddot{x} - U' + \frac{h^2}{24}\left(2U''U' - 2U'''(\dot{x},\dot{x}) + 4U'''(\dot{x},\dot{x}) + 4U''\ddot{x}\right). \end{aligned}$$

Solving this for $\ddot{x}$ we find the modified equation

$$\ddot{x} = -U' + \frac{h^2}{12}\left(U'''(\dot{x},\dot{x}) - U''U'\right) + \mathcal{O}(h^4).$$

The Kepler problem

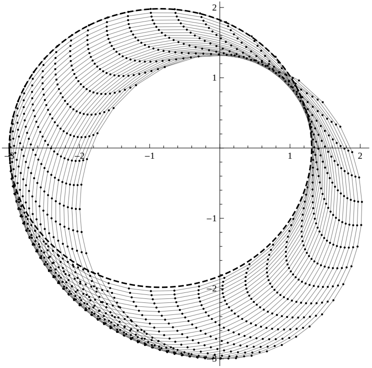
Potential: $U(x) = -\dfrac{1}{|x|}$.

Lagrangian: $\mathcal{L} = \dfrac{1}{2}\langle \dot{x}\,, \dot{x}\rangle + \dfrac{1}{|x|}$.

Equation of motion $\ddot{x} = -\dfrac{x}{|x|^3}$.

Störmer-Verlet discretization:

$$\frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -U'(x_j).$$



The modified Lagrangian of the Störmer-Verlet discretization is

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \frac{1}{2}\langle \dot{x}\,,\dot{x}\rangle - U + \frac{h^2}{24}\left(U'U' - 2U''(\dot{x},\dot{x})\right).$$

For the Kepler problem we have $U(x) = -\frac{1}{|x|}$, hence

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \langle \dot{x}\,,\dot{x}\rangle + \frac{1}{|x|} + \frac{h^2}{24}\left(\frac{1}{|x|^4} - 2\frac{\langle \dot{x},\dot{x}\rangle}{|x|^3} + 6\frac{\langle x,\dot{x}\rangle^2}{|x|^5}\right).$$

Up to higher order terms, we can consider this as a perturbation of the potential:

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \langle \dot{x}\,,\dot{x}\rangle + \frac{1}{|x|} + \frac{h^2}{24}\left(\frac{9}{|x|^4} + 8\frac{\mathbb{E}}{|x|^3} - 6\frac{\mathbb{L}^2}{|x|^5}\right) + \mathcal{O}(h^4),$$

where $\mathbb{E}$ and $\mathbb{L}$ are the constant energy and angular momentum of the unperturbed problem.

From Hamiltonian perturbation theory:

Lemma

The precession rate (in radians per period) for the perturbed Lagrangian

$$\mathcal{L} = \frac{1}{2} \langle \dot{x} , \dot{x} \rangle + \frac{1}{|x|} + \Delta U(x),$$

is given in first order approximation by

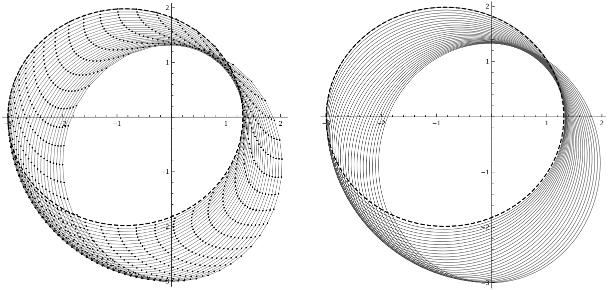
$$2\pi a^2 \frac{\partial \langle \Delta U(x) \rangle}{\partial b},$$

where a and b are the semimajor and semiminor axes of the orbit respectively, and $\langle \cdot \rangle$ denotes the time-average along the unperturbed orbit.

Proposition

The numerical precession rate of the Störmer-Verlet method is

$$\frac{\pi}{24}\left(15\frac{a^3}{b^6} - 3\frac{a}{b^4}\right)h^2 + \mathcal{O}(h^4)$$



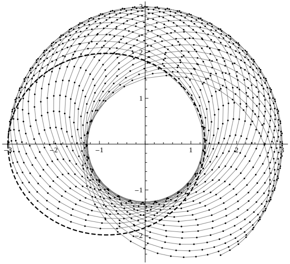
Predicted: 0.0673 rad per revolution.

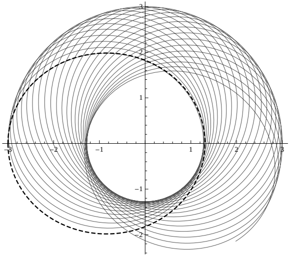
Measured: 0.0659 rad per revolution.

Proposition

The numerical precession rate of the midpoint rule is

$$-\frac{\pi}{12}\left(15\frac{a^3}{b^6} - 3\frac{a}{b^4}\right) h^2 + \mathcal{O}(h^4)$$





Predicted: -0.134 rad per revolution.

Measured: -0.152 rad per revolution.

Let's look at those expressions again

Störmer-Verlet: $\dfrac{\pi}{24}\left(15\dfrac{a^3}{b^6} - 3\dfrac{a}{b^4}\right) h^2 + \mathcal{O}(h^4)$

Midpoint rule: $-\dfrac{\pi}{12}\left(15\dfrac{a^3}{b^6} - 3\dfrac{a}{b^4}\right) h^2 + \mathcal{O}(h^4)$

Proposition

The numerical precession rate of the method with Lagrangian

$$L(x_j, x_{j+1}) = \frac{2}{3} L_{SV}(x_j, x_{j+1}) + \frac{1}{3} L_{MP}(x_j, x_{j+1})$$

is of order $\mathcal{O}(h^4)$.

This is an implicit method, given by

$$
\begin{aligned}
&x_{j+1} - 2x_j + x_{j-1} \\
&\qquad = -\frac{2h^2}{3} U'(x_j) - \frac{h^2}{6} U'\left(\frac{x_{j-1} + x_j}{2}\right) - \frac{h^2}{6} U'\left(\frac{x_j + x_{j+1}}{2}\right).
\end{aligned}
$$

Other options: compose two Störmer-Verlet-steps with one midpoint-step

- Either on the level of second order difference equations $(x_{j-1}, x_j) \mapsto (x_j, x_{j+1})$,
- or on the level of a symplectic map $(x_j, p_j) \mapsto (x_{j+1}, p_{j+1})$.

They are not equivalent because the Legendre transformation depends on the ever-changing Lagrangian.

This is an implicit method, given by

$$x_{j+1} - 2x_j + x_{j-1} = -\frac{2h^2}{3} U'(x_j) - \frac{h^2}{6} U'\left(\frac{x_{j-1}+x_j}{2}\right) - \frac{h^2}{6} U'\left(\frac{x_j + x_{j+1}}{2}\right).$$

Other options: compose two Störmer-Verlet-steps with one midpoint-step

- Either on the level of second order difference equations $(x_{j-1}, x_j) \mapsto (x_j, x_{j+1})$,
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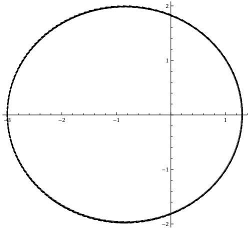
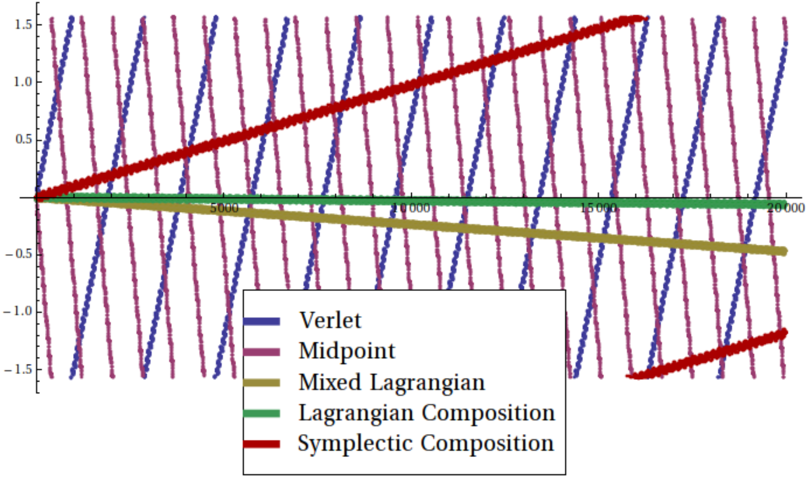


They are not equivalent because the Legendre transformation depends on the ever-changing Lagrangian.

Comparison of precession angles



Summary

- Truncations of the modified equations are not Euler-Lagrange equations.
- But they are truncations of EL equations solved for $\ddot{x}$.
- Obtaining a high-order modified Lagrangian $\mathcal{L}_{\mathrm{mod}}[x]$ is relatively straighforward.
- From $\mathcal{L}_{\mathrm{mod}}[x]$ a first order Lagrangians $\mathcal{L}_{\mathrm{mod},k}(x, \dot{x})$ can be found recursively.
- Standard perturbation theory applied to these Lagrangians can lead us to better integrators.

Reference. Mats Vermeeren. Modified Equations for Variational Integrators. `arXiv:1505.05411 [math.NA]`