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# Superconvergence of Galerkin Variational Integrators

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# Contents

# Lagrangian mechanics

Lagrangian $\mathcal{L} : TQ \to \mathbb{R}$ on a vector space $Q$. Action $\mathfrak{S}[q] = \int_a^b \mathcal{L}(q(t), \dot{q}(t)) \, \mathrm{d}t$.

A curve $q$ is critical if $\left. \frac{\partial}{\partial \alpha} \mathfrak{S}[q + \alpha \delta q] \right|_{\alpha=0} = 0$ for all $\delta q : [a, b] \to Q$ with $\delta q(a) = \delta q(b) = 0$.

A curve $q$ is critical if the Euler-Lagrange equation holds: $\frac{\partial \mathcal{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{q}} = 0$

Assume the Lagrangian is non-degenerate: $\det \left( \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^2} \right) \neq 0$. Then

- the Euler-Lagrange equation is a second order ODE
- the Legendre transform $TQ \to T^* Q : (q, \dot{q}) \mapsto (q, p) = \left( q, \frac{\partial \mathcal{L}}{\partial \dot{q}} \right)$ is invertible.
- the Euler-Lagrange equation is equivalent to the Hamiltonian system

$$\dot{q} = \frac{\partial \mathcal{H}(q, p)}{\partial p}, \qquad \dot{p} = -\frac{\partial \mathcal{H}(q, p)}{\partial q}$$

  with Hamiltonian $\mathcal{H}(q, p) = p\dot{q} - \mathcal{L}(q, \dot{q})$.

# Variational integrators

Discrete Lagrange function $L : Q \times Q \times (0, \infty) \to \mathbb{R}$.

Discrete action for a discrete curve $q = (q_0, q_1, \ldots, q_N)$ with step size $h$:

$$\mathfrak{S}_d(q) = \sum_{i=1}^{N} L(q_{i-1}, q_i; h).$$

Discrete Euler-Lagrange equation

$$\mathrm{D}_2 L(q_{i-1}, q_i; h) + \mathrm{D}_1 L(q_i, q_{i+1}; h) = 0$$

for $i \in \{1, \ldots, N-1\}$, where $\mathrm{D}_1$ and $\mathrm{D}_2$ denote the partial derivatives of $L$.

Discrete EL equation implies equality of the two formulas for the discrete momentum,

$$p_i = \mathrm{D}_2 L(q_{i-1}, q_i; h) \qquad \text{and} \qquad p_i = -\mathrm{D}_1 L(q_i, q_{i+1}; h).$$

This gives a natural implementation of the discrete Euler-Lagrange equation as a one-step method $\Phi_h : (q_i, p_i) \mapsto (q_{i+1}, p_{i+1})$ which is a symplectic integrator.

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Marsden, West. Discrete mechanics and variational integrators. Acta Numerica, 2001.

# Variational error analysis

Assume that there exists a unique smooth minimizer of the action subject to $q(0) = q_0$ and $q(h) = q_1$. The minimal value of the action is called the exact discrete Lagrangian:

$$L_{exact}(q_0, q_1, h) = \min_q \int_0^h \mathcal{L}(q, \dot{q}) \, \mathrm{d}t.$$

The order of a variational integrator can be determined by comparing its discrete Lagrangian to the exact discrete Lagrangian.

If

$$L(q(0), q(h), h) - L_{exact}(q(0), q(h), h) = \mathcal{O}(h^{\ell+1}),$$

then the variational integrator defined $L$ (in its symplectic form $\Phi_h$) is of order $\ell$:

$$\Phi_h(q, p) - \varphi_h(q, p) = \mathcal{O}(h^{\ell+1}),$$

where $\varphi_h$ is the flow over time $h$ of the continuous Hamiltonian system.

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Marsden, West. Discrete mechanics and variational integrators. Acta Numerica, 2001.

Patrick, Cuell. Error analysis of variational integrators of unconstrained Lagrangian systems. Numerische Mathematik, 2009.

# Galerkin variational integrators

Replace the space of smooth curves by a finite dimensional space of polynomials

$$\mathcal{P}^s([0,h],Q) = \{q : [0,h] \to Q \text{ polynomial of degree at most } s\}$$

($\mathcal{P}^s([0,h],Q)$ can be paremeterized by the values of $q$ at $s+1$ control points.)

As discrete Lagrangian, we want

$$L(q_0, q_1; h) \approx \min_{\substack{q \in \mathcal{P}^s([0,h],Q), \\ q(0)=q_0, q(h)=q_1}} \left( \int_0^h \mathcal{L}(q(t), \dot{q}(t)) \, \mathrm{d}t \right)$$

Approximation using a quadrature rule with points $c_i \in [0,1]$ and weights $b_i \in \mathbb{R}$:

$$L(q_0, q_1; h) = \min_{\substack{q \in \mathcal{P}^s([0,h],Q), \\ q(0)=q_0, q(h)=q_1}} \left( h \sum_i b_i \mathcal{L}(q(hc_i), \dot{q}(hc_i)) \right)$$

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Marsden, West. Discrete mechanics and variational integrators. Acta Numerica, 2001.

Leok, Shingel. General techniques for constructing variational integrators. Frontiers of Mathematics in China, 2012

# Superconvergence

## Previous result*

Let $L$ be a Galerkin discretization of a Lagrangian $\mathcal{L}$, based on polynomials of degree $s$ and a quadrature rule of degree $u$. Assume that all discrete and continuous critical curves minimize their respective actions. Then the corresponding symplectic integrator is of order $\min(s, u)$.

Numerical evidence suggested superconvergence: order of up to $2s$[†].

Superconvergence has been proved for some particular cases[‡].

## Our result

The corresponding symplectic integrator is of order $\min(2s, u)$.

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*Hall, Leok. Spectral variational integrators. Numerische Mathematik, 2015.

†Ober-Blöbaum, Saake. Construction and analysis of higher order Galerkin variational integrators Advances in Computational Mathematics, 2015.

‡Ober-Blöbaum. Galerkin variational integrators and modified symplectic Runge-Kutta methods, IMA Journal of Numerical Analysis, 2017.

# Superconvergence: sketch of proof

By variational error analysis, it suffices to show that for any smooth $q$

$$L_{\mathrm{exact}}(q(0), q(h); h) - L(q(0), q(h); h) = \mathcal{O}\left(h^{\min(2s,u)+1}\right) \qquad (*)$$

Consider three curves:

- $q_{\mathrm{EL}}$: minimizer of the continuous action with $q_{\mathrm{EL}}(0) = q(0)$ and $q_{\mathrm{EL}}(h) = q(h)$.
- $\hat{q}$: polynomial that agrees with $q_{\mathrm{EL}}$ at control points $0 = hd_0, hd_1, \ldots, hd_s = h$.
- $\tilde{q}$: polynomial that minimizes $h \sum_i b_i \mathcal{L}(q(hc_i), \dot{q}(hc_i))$.

Then $(*)$ is equivalent to

$$\int_0^h \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})\,\mathrm{d}t - h \sum_i b_i \mathcal{L}(\tilde{q}(hc_i), \dot{\tilde{q}}(hc_i)) = \mathcal{O}\left(h^{\min(2s,u)+1}\right)$$

or

$$\left( \int_0^h \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})\,\mathrm{d}t - \int_0^h \mathcal{L}(\hat{q}, \dot{\hat{q}}) \right) + \left( \int_0^h \mathcal{L}(\hat{q}, \dot{\hat{q}}) - h \sum_i b_i \mathcal{L}(\tilde{q}(hc_i), \dot{\tilde{q}}(hc_i)) \right) = \mathcal{O}\left(h^{\min(2s,u)+1}\right)$$

# Superconvergence: sketch of proof

Since $q_{EL}$ and $\hat{q}$ agree at $s+1$ control points in $[0,h]$ there holds $q_{EL} - \hat{q} = \mathcal{O}(h^{s+1})$ and $\dot{q}_{EL} - \dot{\hat{q}} = \mathcal{O}(h^s)$. Hence

$$
\begin{aligned}
&\int_0^h \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})\,\mathrm{d}t - \int_0^h \mathcal{L}(\hat{q}, \dot{\hat{q}})\,\mathrm{d}t \\
&\quad = \int_0^h \left( \frac{\partial \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})}{\partial q}(q_{\mathrm{EL}} - \hat{q}) + \frac{\partial \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})}{\partial \dot{q}}(\dot{q}_{\mathrm{EL}} - \dot{\hat{q}}) + \mathcal{O}\left(h^{2s}\right) \right)\mathrm{d}t \\
&\quad = \int_0^h \left( \left( \frac{\partial \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})}{\partial \dot{q}} \right)(q_{\mathrm{EL}} - \hat{q}) + \mathcal{O}\left(h^{2s}\right) \right)\mathrm{d}t \\
&\qquad + \left( \frac{\partial \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})}{\partial \dot{q}}(q_{\mathrm{EL}} - \hat{q}) \right)\Bigg|_0^h .
\end{aligned}
$$

Note that $\hat{q}(0) = q_{\mathrm{EL}}(0)$ and $\hat{q}(h) = q_{\mathrm{EL}}(h)$ and $q_{\mathrm{EL}}$ solves the EL equation, so

$$
\int_0^h \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})\,\mathrm{d}t - \int_0^h \mathcal{L}(\hat{q}, \dot{\hat{q}})\,\mathrm{d}t = \int_0^h \mathcal{O}\left(h^{2s}\right)\,\mathrm{d}t = \mathcal{O}\left(h^{2s+1}\right).
$$

# Superconvergence: sketch of proof

- Using the calculus of variations we found

$$\int_0^h \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})\,\mathrm{d}t - \int_0^h \mathcal{L}(\hat{q}, \dot{\hat{q}})\,\mathrm{d}t = \mathcal{O}\left(h^{2s+1}\right).$$

- From the assumption that critical curves are minimizers, it follows that $\hat{q}$ and $\tilde{q}$ are close to each other. In particcular,

$$\int_0^h \mathcal{L}(\hat{q}, \dot{\hat{q}}) - h \sum_i b_i \mathcal{L}(\tilde{q}(hc_i), \dot{\tilde{q}}(hc_i)) = \mathcal{O}\left(h^{\min(2s,u)+1}\right).$$

Hence

$$\begin{aligned} L_{\mathrm{exact}}(q(0), q(h); h) - L(q(0), q(h); h) &= \int_0^h \mathcal{L}(q_{\mathrm{EL}}, \dot{q}_{\mathrm{EL}})\,\mathrm{d}t - h \sum_i b_i \mathcal{L}(\tilde{q}(hc_i), \dot{\tilde{q}}(hc_i)) \\ &= \mathcal{O}\left(h^{\min(2s,u)+1}\right). \end{aligned}$$

By variational error analysis, this proves that the integrator is of order $\min(2s, u)$. ■

# Possible extension to forced systems

External forces can be accommodated by doubling the dimension[*]: consider the extended Lagrangian

$$\mathcal{L}^{\mathrm{f}}(q, Q, \dot{q}, \dot{Q}) = \mathcal{L}(Q, \dot{Q}) - \mathcal{L}(q, \dot{q}) + \tfrac{1}{2}(f(Q, \dot{Q}) + f(q, \dot{q}))(Q - q).$$

First taking variations with respect to $Q$, then imposing $Q = q$ we find

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

Good news: we can use this to apply variational error analysis to forced systems.[†]

Bad news: our superconvergence result requires that critical curves of are minimizers, but this does not hold for $\mathcal{L}^{\mathrm{f}}$.

We needed this assumption to show that the minimizing polynomial $\tilde{q}$ is close to the polynomial interpolating the continuous solution $\hat{q}$.

Workaround? Without this assumption, can we still expect the difference $\hat{q} - \tilde{q}$ will be small in a generic case?

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[*] Galley. Classical mechanics of nonconservative systems. Physical review letters, 2013.

[†] De Diego, de Almagro. Variational order for forced Lagrangian systems. Nonlinearity, 2018.

# Conclusions

- Under mild assumptions (minimality of critical curves) Galerkin variational integrators based on polynomials of degree $s$ are of order $2s$.

  Proof is inspired on the calculus of variations itself.

- Forced systems pose an interesting challenge.

- The foundational result on variational error analysis is subtle. Can we provide a more insightful proof using modified Lagrangians?

Thank you for your attention!