A generalized Gelfand-Yaglom formula

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Preliminaries

Consider a one dimensional quantum mechanic system with potential $V\big(q(t)\big)$. The action function on the space of paths is,

$$S(\gamma) = \int_0^T \left(\frac{m}{2}\dot{q}(t)^2 - V\big(q(t)\big)\right) dt$$

where $\gamma : [0, T] \to \mathbb{R}$, $t \mapsto q(t)$ is a path.

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where $\gamma : [0, T] \to \mathbb{R}$, $t \mapsto q(t)$ is a path. Let $\gamma_c = q_c(t)$ satisfy the Euler Lagrange equations,

$$m\ddot{q}_c(t) = -V'\big(q_c(t)\big)$$

with the boundary conditions,

$$q_c(0) = q \quad \dot{q}_c(0) = \frac{p}{m}$$

Preliminaries

Taking the second variation of the action at the critical point gives,

$$\delta^2 S(\gamma_c) = \int_0^T (\delta q) A(\delta q) dt$$

where A is the operator

$$A = -\frac{d^2}{dt^2} - \frac{1}{m} V''\big(q_c(t)\big)$$

acting on the domain

$$D(A) = \left\{ y(t) \in W^{2,2}(0,T) \, : \, y(0) = y(T) = 0 \right\}$$

The Gelfand-Yaglom formula

Theorem (The Gelfand-Yaglom formula)

Let A and $q_c(t)$ be as described, then

$$\frac{\partial q_c(T)}{\partial p} = \frac{1}{2m} \det{}_\zeta A$$

where $\det{}_\zeta A$ denotes the ζ-regularized determinant of A.

The Gelfand-Yaglom formula

The action written in the Hamiltonian formalism is,

$$\tilde{S}(\tilde{\gamma}; q, q') = \int_0^T \left(p(t)\dot{q}(t) - \frac{1}{2m}p(t)^2 + V\big(q(t)\big) \right) dt$$

where $\tilde{\gamma} : [0, T] \to T^*\mathbb{R}$, $t \mapsto \big(q(t), p(t)\big)$, $q = q(0)$, and $q' = q(T)$.

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where $\tilde{\gamma} : [0, T] \to T^*\mathbb{R}$, $t \mapsto \big(q(t), p(t)\big)$, $q = q(0)$, and $q' = q(T)$.

Corollary

For the operator A and the action functional described above,

$$\left(\frac{\partial \tilde{S}(\tilde{\gamma}_c; q, q')}{\partial q \partial q'} \right)^{-1} = \frac{1}{2m} \det{}_{\zeta} A$$

A generalized action functional

Consider the generalized Hamiltonian action functional,

$$\tilde{S}(\tilde{\gamma}; b_1, b_2) = \int_0^T \big(p(t)\dot{q}(t) - H\big(p(t), q(t)\big)\big)\, dt + f_1(q, b_1) - f_2(q', b_2)$$

where H is any twice differentiable Hamiltonian (for now) and f_1 and f_2 define the Lagrangian submanifolds

$$p = \frac{\partial f_1}{\partial q}(q, b_1) \quad p' = \frac{\partial f_2}{\partial q'}(q', b_2)$$

Critical points of the action are flow lines of the Hamiltonian vector field that connect the two submanifolds in time T.

The Hamilton-Jacobi operator

The Hamilton-Jacobi operator, $\tilde{A}$, that appears in the second variation of the action at the critical point has the form,

$$\tilde{A} = \begin{pmatrix} -\frac{\partial^2 H}{\partial p^2}(p_c, q_c) & \frac{d}{dt} - \frac{\partial^2 H}{\partial p \partial q}(p_c, q_c) \\ -\frac{d}{dt} - \frac{\partial^2 H}{\partial p \partial q}(p_c, q_c) & -\frac{\partial^2 H}{\partial q^2}(p_c, q_c) \end{pmatrix}$$

and has the domain,

$$D\left(\tilde{A}\right) = \left\{(x, y) \, : \, x, y \in W^{2,2}(0, T), \; x(0) = a_1 y(0), \; x(T) = a_2 y(T)\right\}$$

where we use the shorthand notation,

$$a_1 = \frac{\partial^2 f_1}{\partial q^2}(q_c, b_1) \quad a_2 = \frac{\partial^2 f_2}{\partial q'^2}(q'_c, b_2)$$

Motivating question

Question. Is there a similar Gelfand-Yaglom type formula for the action $\tilde{S}(\tilde{\gamma}_c; b_1, b_2)$ and the operator $\tilde{A}$?

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Answer. Sort of...

1. In the discrete setting there are no issues, so that is where we will start.
2. In the continuous setting the operator $\tilde{A}$ causes difficulties, but we have no problems when using A.
3. How does the discrete case compare to the continuous one in the continuum limit?

The discrete action

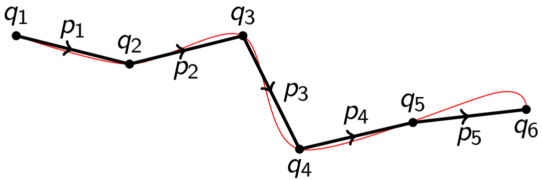

Figure: A discretization of a path into $N = 6$ position vectors and $N - 1 = 5$ momentum vectors.

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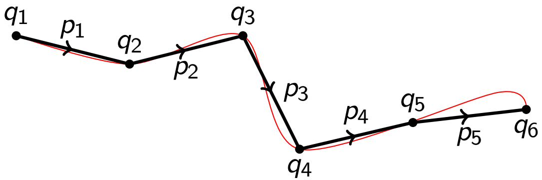

Figure: A discretization of a path into $N = 6$ position vectors and $N - 1 = 5$ momentum vectors.

In the one dimensional case we propose the discrete action functional,

$$\tilde{S}_d(\tilde{\gamma}_d; b_1, b_2) = \sum_{i=1}^{N-1} p_i(q_{i+1} - q_i) - \sum_{i=1}^{N-1} H(p_i, q_i) - f_2(q_N, b_2) + f_1(q_1, b_1)$$

The discrete Hamilton-Jacobi operator

The discrete analog of the operator $\tilde{A}$ is the $(2N-1) \times (2N-1)$ matrix operator with block form,

$$\tilde{A}_N = \begin{pmatrix} D_1 & D_2 \\ D_3 & D_4 \end{pmatrix}$$

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$$D_1 = \begin{pmatrix} -\frac{\partial^2 H}{\partial p_1^2} & & \\ & \ddots & \\ & & -\frac{\partial^2 H}{\partial p_{N-1}^2} \end{pmatrix} \quad D_4 = \begin{pmatrix} a_1 - \frac{\partial^2 H}{\partial q_1^2} & & & & \\ & -\frac{\partial^2 H}{\partial q_2^2} & & & \\ & & \ddots & & \\ & & & -\frac{\partial^2 H}{\partial q_{N-1}^2} & \\ & & & & -a_2 \end{pmatrix}$$

$$D_2 = D_3^T = \begin{pmatrix} -1 - \frac{\partial^2 H}{\partial p_1 \partial q_1} & 1 & & & \\ & & \ddots & & \\ & & \ddots & 1 & \\ & & & -1 - \frac{\partial^2 H}{\partial p_{N-1} \partial q_{N-1}} & 1 \end{pmatrix}$$

Discrete Gelfand-Yaglom theorem

In the discrete setting, the critical path solves a discrete version of Hamilton's equations

$$q_{i+1} - q_i - \frac{\partial H}{\partial p_i}(p_i, q_i) = 0, \quad p_i - p_{i-1} + \frac{\partial H}{\partial q_i}(p_i, q_i) = 0$$

and the same Lagrangian boundary conditions as earlier.

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Theorem

For the discrete action functional at the critical path, $\tilde{S}_d(\tilde{\gamma}_{d,c}; b_1, b_2)$ and discrete Hamilton-Jacobi operator, $\tilde{A}_N$, the following Gelfand-Yaglom type formula holds (in the one dimensional case)

$$\frac{\partial^2 \tilde{S}_d(\tilde{\gamma}_{d,c}; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\frac{\partial^2 f_1(q_1, b_1)}{\partial q_1 \partial b_1} \cdot \frac{\partial^2 f_2(q_N, b_2)}{\partial q_N \partial b_2}}{\det \tilde{A}_N} \cdot \prod_{i=1}^{N-1} \left(- \frac{\partial^2 H(p_i, q_i)}{\partial p_i \partial q_i} - 1 \right)$$

Proof outline

For this proof we assume $1 + \dfrac{\partial^2 H(p_i, q_i)}{\partial p_i \partial q_i} \neq 0$ for all i. The proof follows the steps...

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1. Compute the mixed (boundary) derivative of the action at the critical value,

$$\frac{\partial^2 \tilde{S}(\tilde{\gamma}_{d,c}; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\partial^2 f_1}{\partial q \partial b_1} \frac{\partial q}{\partial b_2}$$

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1. Compute the mixed (boundary) derivative of the action at the critical value,
$$\frac{\partial^2 \tilde{S}(\tilde{\gamma}_{d,c}; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\partial^2 f_1}{\partial q \partial b_1} \frac{\partial q}{\partial b_2}$$
2. Take derivatives of the Hamilton's equations with respect to b_2 and write the (linear) system as a recursive system.
$$\frac{\partial q_{i+1}}{\partial b_2} - \frac{\partial q_i}{\partial b_2} - \frac{\partial^2 H}{\partial p_i^2}(p_i, q_i)\frac{\partial p_i}{\partial b_2} - \frac{\partial^2 H}{\partial p_i \partial q_i}(p_i, q_i)\frac{\partial q_i}{\partial b_2} = 0$$
$$\frac{\partial p_i}{\partial b_2} - \frac{\partial p_{i-1}}{\partial b_2} + \frac{\partial^2 H}{\partial q_i^2}(p_i, q_i)\frac{\partial q_i}{\partial b_2} + \frac{\partial^2 H}{\partial q_i \partial p_i}(p_i, q_i)\frac{\partial p_i}{\partial b_2} = 0$$

Proof outline

2. Express the determinant of $\tilde{A}_N$ as a recursive system, using the fact that,

$$\det \tilde{A}_N = \det D_1 \det(D_4 - D_3 D_1^{-1} D_2)$$

and the matrix $D_4 - D_3 D_1^{-1} D_2$ is tri-diagonal.

Proof outline

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   and the matrix $D_4 - D_3 D_1^{-1} D_2$ is tri-diagonal.
3. Recognize these systems are almost the same after gauge transformation.

The same steps apply in the n-dimensional case as well.

Specializations

For the rest of this talk we will make a few assumptions...

1. $H(p_i, q_i) = \frac{1}{2m} p_i^2 + V(q_i)$ where V is a twice differentiable function.
2. N is odd.

Specializations

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1. $H(p_i, q_i) = \frac{1}{2m} p_i^2 + V(q_i)$ where V is a twice differentiable function.
2. N is odd.

And so the statement from the theorem simplifies to,

$$\frac{\partial^2 \tilde{S}_d(\tilde{\gamma}_{d,c}; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\frac{\partial^2 f_1(q_1, b_1)}{\partial q_1 \partial b_1} \frac{\partial^2 f_2(q_N, b_2)}{\partial q_N \partial b_2}}{\det \tilde{A}_N}$$

Convergence of $\tilde{A}_N$

Theorem

The operator $\tilde{A}_N$ weakly converges to the operator $\tilde{A}$.

To prove this theorem we need to be careful with epsilons (as opposed to letting $\epsilon = 1$).

Using the discrete generalized Gelfand-Yaglom formula we have,

$$\lim_{N\to\infty} \det \tilde{A}_N = \frac{\frac{\partial^2 f_1(q_1,b_1)}{\partial q_1 \partial b_1} \frac{\partial^2 f_2(q_N,b_2)}{\partial q_N \partial b_2}}{\frac{\partial^2 \tilde{S}_d(\tilde{\gamma}_{d,c};b_1,b_2)}{\partial b_1 \partial b_2}}$$

so the limit is finite and well-defined*.

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Instead, we computed a generalized (continuous) Gelfand-Yaglom formula using A. Recall,

$$A = -\frac{d^2}{dt^2} - \frac{1}{m} V''(q_c(t))$$

and the boundary conditions take the form,

$$\dot{y}(0) = \frac{a_1}{m} y(0) \quad \dot{y}(T) = \frac{a_2}{m} y(T)$$

Generalized Gelfand-Yaglom formula

Let $L = -\frac{d^2}{dt^2} + u(t)$ where $u(t) \in C^1([0, T], \mathbb{R})$ and

$$D(L) = \left\{ y(t) \in W^{2,2}(0, T) \ : \ \dot{y}(0) = \frac{a_1}{m} y(0), \ \dot{y}(T) = \frac{a_2}{m} y(T) \right\}$$

Theorem

The ζ-regularized determinant of the operator L satisfies the following equation,

$$\det{}_\zeta L = \dot{y}_1(T) - \frac{a_2}{m} y_1(T)$$

where $y_1(t)$ is the solution to the initial value problem,

$$-\ddot{y}(t) + u(t) y(t) = 0, \ y(0) = 1, \ \dot{y}(0) = \frac{a_1}{m}$$

Generalized Gelfand-Yaglom formula

The proof is very similar to the proof of the original Gelfand-Yaglom formula. The outline goes,

1. Consider two solutions of the equation $-\ddot{y} + u(t)y = \lambda y$ with boundary conditions,
    1. $y_1(0) = 1$, $\dot{y}_1(0) = a_1/m$
    2. $y_2(T) = 1$, $\dot{y}_2(T) = a_2/m$

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2. Use the two solutions to simplify the expression $\mathrm{Tr}\, R_\lambda$, therefore simplifying the expression

$$\log \det{}_\zeta(L - \lambda I) = -\mathrm{Tr}\, R_\lambda$$

to

$$\log \det{}_\zeta(L - \lambda I) = C\left(\dot{y}_1(T) - \frac{a_2}{m} y_1(T)\right)$$

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3. Using asymptotics compute that $C = 1$.

Generalized Gelfand-Yaglom formula

We can put this in the context of the operator A to get,

Corollary

For the operator A with mixed boundary conditions we have the generalized Gelfand-Yaglom formula,

$$\det{}_\zeta A = \frac{\partial \dot{q}_c(T)}{\partial q} - \frac{a_2}{m}\frac{\partial q_c(T)}{\partial q}$$

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After taking some derivative we get,

$$\frac{\partial^2 \tilde{S}(\tilde{\gamma}_c; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\frac{\partial^2 f_1(q_1, b_1)}{\partial q_1 \partial b_1}\frac{\partial^2 f_2(q_N, b_2)}{\partial q_N \partial b_2}}{m \det{}_{\zeta} A}$$

The operator A_N

So far we have,

$$\frac{\partial^2 \tilde{S}_d(\tilde{\gamma}_{d,c}; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\frac{\partial^2 f_1(q_1, b_1)}{\partial q_1 \partial b_1} \frac{\partial^2 f_2(q_N, b_2)}{\partial q_N \partial b_2}}{\lim_{N\to\infty} \det \tilde{A}_N}$$

and

$$\frac{\partial^2 \tilde{S}(\tilde{\gamma}_c; b_1, b_2)}{\partial b_1 \partial b_2} = \frac{\frac{\partial^2 f_1(q_1, b_1)}{\partial q_1 \partial b_1} \frac{\partial^2 f_2(q_N, b_2)}{\partial q_N \partial b_2}}{m \det_\zeta A}$$

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and

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One would hope that $\lim_{N\to\infty} \det \tilde{A}_N = \det_\zeta \tilde{A}$, so we would suspect

$$\det{}_\zeta \tilde{A} = m \det{}_\zeta A$$

The operator A_N

Well we have this* in the discrete case...

Theorem

The determinants of the discrete operators A_N and $\tilde{A}_N$ satisfy the relation

$$\det \tilde{A}_N = (-1)^{N-1} m \det A_N$$

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The operator A_N has the form,

$$A_4 = \begin{pmatrix} \frac{a_1}{m} + 1 - \frac{1}{m} V''(q_c(t_1)) & -1 & 0 & 0 \\ -1 & 2 - \frac{1}{m} V''(q(t_2)) & -1 & 0 \\ 0 & -1 & 2 - \frac{1}{m} V''(q(t_2)) & -1 \\ 0 & 0 & -1 & -\frac{a_2}{m} + 1 \end{pmatrix}$$

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This theorem is then obvious once you observe,

$$mA_N = D_4 - D_3 D_1^{-1} D_2$$

The operator A_N

We also have,

Theorem

The operator A_N weakly converges to the operator A.

As before, the limit is well-defined (no asterisk!) and finite

$$\lim_{N\to\infty} A_N = \frac{\frac{\partial^2 f_1(q_1,b_1)}{\partial q_1 \partial b_1} \frac{\partial^2 f_2(q_N,b_2)}{\partial q_N \partial b_2}}{m \frac{\partial^2 \tilde{S}_d(\tilde{\gamma}_{d,c};b_1,b_2)}{\partial b_1 \partial b_2}}$$

Obviously, one has to be careful about epsilons to prove this.

Lattice regularization

Since the determinant of A_N and $\tilde{A}_N$ exist in the continuum limit and converge to A and $\tilde{A}$, respectively, we define,

Definition

We define the lattice regularized determinants of A and $\tilde{A}$ by,

$$\det{}_{\text{reg}} A = \lim_{N\to\infty} \det A_N$$

$$\det{}_{\text{reg}} \tilde{A} = \lim_{N\to\infty} \det \tilde{A}_N$$

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And we see from everything that,

$$\det{}_{\text{reg}} A = \det{}_{\zeta} A$$

Concluding remarks

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2. Something more complex is going on in the case of mixed second derivatives of H, which probably warrants more investigation.
3. Thank you for listening!