

NOTES ON ROA PROJECT

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1. CONSTRAINT EQUATION

Let $\psi(t), \nu(t) \in L^2(M)$ for $t \in [0, T]$. Then observe that

$$\begin{aligned}\langle \psi(T), \nu(T) \rangle_{L^2} &= \langle \psi(0), \nu(0) \rangle_{L^2} + \int_0^T \frac{d}{dt} \langle \psi(t), \nu(t) \rangle dt \\ &= \langle \psi(0), \nu(0) \rangle_{L^2} + \int_0^T \langle \partial_t \psi, \nu \rangle_{L^2} + \langle \psi, \partial_t \nu \rangle_{L^2} dt\end{aligned}$$

Let A be an anti-symmetric operator on $L^2(M)$. Then $\psi(t)$ satisfies

$$(1) \quad \partial_t \psi + A[\psi] = 0$$

if and only if

$$\langle \partial_t \psi + A[\psi], \nu \rangle_{L^2} = 0$$

for all $\nu \in L^2(M)$. Invoking the anti-symmetry of A we find that the above equation holds if and only if

$$\langle \partial_t \psi, \nu \rangle = \langle \psi, A[\nu] \rangle_{L^2}$$

for all ν .

Thus ψ satisfies (1) if and only if

$$\langle \psi(T), \nu(T) \rangle_{L^2} = \langle \psi(0), \nu(0) \rangle_{L^2} + \int_0^T \langle \psi, \partial_t \nu + A[\nu] \rangle_{L^2} dt$$

for all $\nu(t) \in L^2(M)$ with $t \in [0, 1]$.

In our case $A[\psi](x) := X^i(x) \partial_i \psi(x) + \frac{1}{2} \partial_i X^i(x) \psi(x)$ and we use weak-derivatives if needed.

2. CONTROLS

We wish to solve for the region of attraction under the controlled dynamics

$$\dot{x} = X_0(x) + \sum_{k=1}^c u^k X_k(x).$$

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where X_0, X_1, \dots, X_c are vector fields. Define the unbounded Hermetian operators $\hat{H}_i \in \text{Herm}(L^2(M))$ by

$$\hat{H}_i \cdot \psi := i \sum_{\alpha=1}^d \frac{1}{2} \partial_\alpha X_i^\alpha \psi + X_i^\alpha \partial_\alpha \psi,$$

for $i = 0, 1, \dots, c$. Then the dynamics of a half-density evolve under the controlled Schrodinger equation

$$\dot{\psi} = i \hat{H} \cdot \psi + i \sum_{k=1}^c u^k \hat{H}_k \cdot \psi = i \hat{H}(u) \cdot \psi.$$

where $\hat{H}(u) = \hat{H}_0 + u^k \hat{H}_k$. Let $\pi_M : U \times M \rightarrow M$ be the cartesian projection onto M . We can define the operator $\hat{J} : L^2(M) \rightarrow L^2(M \times U)$ given by $(\hat{J} \cdot \psi)(x, u) = (\hat{H}(u) \cdot \psi)(x) \sqrt{du}$ or more concisely $\hat{J} = \hat{H}(\cdot) \otimes \sqrt{u}$. From here we may compute the dual operator $\hat{J}^\dagger : L^2(U \times M) \rightarrow L^2(M)$. Explicitly \hat{J}^\dagger takes the the form

$$(\hat{J}^\dagger \cdot \phi)(x) := \int_U \hat{H}(u) \phi(x, u) du$$

Inspired by Henrion-Korda we should be able to obtain the ROA by solving the primal QP

$$p^* = \sup_{\substack{\delta_T \otimes \psi_T - \delta_0 \otimes \psi_0 = \int_0^T \hat{J}^\dagger \cdot \phi dt \\ -1 \leq \psi_T \leq 1}} \|\psi\|_{L^2(M)}^2$$

where the decision variables are $\phi \in H^1([0, T]; L^2(U \times M))$, and $\psi_T \in L^2(M)$.

3. DISCRETIZATION OF VECTOR-FIELDS AS OPERATORS

Let $X(x, t) = f^\alpha(x, t) \frac{\partial}{\partial x^\alpha}$. We wish to discretize the operator

$$\rho(X)[\psi] = \frac{1}{2} (\partial_\alpha (f^\alpha \cdot \psi) + f^\alpha \partial_\alpha \psi)$$

To do this, let us note that

$$\rho(f \cdot X) = \frac{1}{2} \left(\hat{f} \cdot \rho(X) + \widehat{X[f]} \right) = \frac{1}{2} \left(\hat{f} \cdot \rho(X) + [\hat{f}, \rho(X)] \right) = \hat{f} \rho(X) - \frac{1}{2} \rho(X) \hat{f}$$

What we could do is construct the operator $\widehat{\partial_\alpha}$ and the multiplication operator $\hat{f}^\alpha : \psi(\cdot) \mapsto f^\alpha(\cdot) \cdot \psi(\cdot)$ given in matrix form by

$$[\hat{f}^\alpha]^i_j = \langle w_i | \hat{f}^\alpha | w_j \rangle.$$

My hope is that the operator $\frac{1}{2}([\widehat{f^\alpha}]_n \cdot [\widehat{\partial_\alpha}]_n + [\widehat{\partial_\alpha}]_n \cdot [\widehat{f^\alpha}]_n)$ is a good approximation of $\rho(X)$ when $[\widehat{f^\alpha}]_n$ a least squares projection of \hat{f}^α and $[\widehat{\partial_\alpha}]_n$ is a least squares projection of $\widehat{\partial_\alpha}$ onto some finite-dimensional subspace V_n . The following two (yet to be proven) lemmas would give us this result.

Lemma 3.1. *Let $f \in L^\infty$, $n \in \mathbb{N}$, and $\{e_0, e_1, \dots\}$ a Hilbert basis for L^2 . Let $V_n = \text{span}(e_0, e_1, \dots, e_n)$ and let $\pi_n : L^2 \rightarrow V_n$ be the orthogonal projection. Then the operator $[\hat{f}]_n = \pi_n \circ \hat{f} \circ \pi_n$ satisfies the error bound*

$$\|\hat{f} - [\hat{f}]_n\|_{L^2} = \epsilon_1(n)$$

for some function $\epsilon_1(n)$ which vanishes at infinity.

Lemma 3.2. *The operator $[\widehat{\partial_\alpha}]_n = \pi_n \circ \widehat{\partial_\alpha} \circ \pi_n$ satisfies the error bound*

$$\|\widehat{\partial_\alpha}|_{H^1} - [\widehat{\partial_\alpha}]_n\|_{L^2} = \epsilon_2(n)$$

for some function $\epsilon_1(n)$ which vanishes at infinity.

Proposition 3.3. *The operator $\frac{1}{2}([\widehat{f^\alpha}]_n \cdot [\widehat{\partial_\alpha}]_n + [\widehat{\partial_\alpha}]_n \cdot [\widehat{f^\alpha}]_n)$ approximates the operator $\rho(X) = \frac{1}{2}(\widehat{f^\alpha} \widehat{\partial_\alpha} + \widehat{\partial_\alpha} \widehat{f^\alpha})$ on H^1 with an error bound proportional to $\epsilon(n) = \max(\epsilon_1(n), \epsilon_2(n))$.*

Proof. The proof comes down to the following computation for any two operators A and B with approximations A_n and B_n .

$$\begin{aligned} \|AB - A_n B_n\| &= \|AB - A_n B + A_n B - A_n B_n\| \\ &\leq \|AB - A_n B\| + \|A_n B - A_n B_n\| \\ &\leq \|B\| \|A - A_n\| + \|A_n\| \|B - B_n\|. \end{aligned}$$

□

APPENDIX A. CONSTRUCTION OF OPERATORS

Let $\{e_0, e_1, \dots\}$ be a Hilbert basis for $L^2(\mathbb{R})$ and compute the coefficients

$$a^i_j = \int_{\mathbb{R}} e_i(x) \frac{de_j}{dx}(x) dx$$

In n -dimensions we may consider the basis elements for $L^2(\mathbb{R}^n)$ computed as tensor products of the one-dimensional case. That is to say, we use a basis of the form $e_{\mathbf{i}}(\mathbf{x}) := e_{i_1}(x^1) e_{i_2}(x^2) \cdots e_{i_n}(x^n)$ where $\mathbf{i} = (i_1, i_2, \dots, i_n)$ and $\mathbf{x} = (x^1, \dots, x^n)$. In this bases the operator $\widehat{\partial_\alpha}$ is computed entry-wise to be

$$\begin{aligned} [\widehat{\partial_\alpha}]_{\mathbf{j}}^{\mathbf{i}} &= \langle e_{\mathbf{i}} | \widehat{\partial_\alpha} | e_{\mathbf{j}} \rangle = \int_{\mathbb{R}^n} e_{\mathbf{i}}(\mathbf{x}) \frac{\partial e_{\mathbf{j}}}{\partial x^\alpha} d\mathbf{x} \\ &= \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \left(\prod_{\beta \neq \alpha} e_{i_\beta}(x^\beta) e_{j_\beta}(x^\beta) \right) \cdot e_{i_\alpha}(x^\alpha) \frac{de_{j_\alpha}}{dx}(x^\alpha) dx^1 \cdots dx^n \\ &= \left(\prod_{\beta \neq \alpha} \delta^{i_\beta}_{j_\beta} \right) a^{i_\alpha}_{j_\alpha} \end{aligned}$$

where the indices are $\mathbf{i} = (i_1, \dots, i_n)$ and $\mathbf{j} = (j_1, \dots, j_n)$. Similarly, for a L^∞ function f the operator \hat{f} is given entry-wise by

$$\left[\hat{f}\right]_{\mathbf{j}}^{\mathbf{i}} = \langle e_{\mathbf{i}} \mid \hat{f} \mid e_{\mathbf{j}} \rangle = \int_{\mathbb{R}^n} e_{\mathbf{i}}(\mathbf{x}) f(\mathbf{x}) e_{\mathbf{j}}(\mathbf{x}) d\mathbf{x}$$

You can probably compute this using your existing code by first decomposing $f(\mathbf{x})$ into a wavelet basis as $f(\mathbf{x}) = \sum_{\mathbf{k}} f_{\mathbf{k}} e_{\mathbf{k}}(\mathbf{x})$ for some real coefficients $f_{\mathbf{k}}$. Then we'd find

$$\left[\hat{f}\right]_{\mathbf{j}}^{\mathbf{i}} = \sum_{\mathbf{k}} f_{\mathbf{k}} \int_{\mathbb{R}^n} e_{\mathbf{i}}(\mathbf{x}) e_{\mathbf{k}}(\mathbf{x}) e_{\mathbf{j}}(\mathbf{x}) d\mathbf{x}$$

and we can use your pre-computation of integrals of the above form.

In the case of a vector-field $X = f^\alpha \partial_\alpha$, the corresponding operator on half-densities is given by $(f^\alpha \cdot \partial_\alpha + \partial_\alpha \circ f^\alpha)/2$ and so we are going to use the operator

$$\rho(X) = \frac{1}{2} \left(\widehat{f^\alpha} \cdot \widehat{\partial_\alpha} + \widehat{\partial_\alpha} \cdot \widehat{f^\alpha} \right)$$

given entry-wise by

$$[\rho(X)]_{\mathbf{j}}^{\mathbf{i}} = \frac{1}{2} \sum_{\mathbf{k}} \left(\left[\widehat{f^\alpha}\right]_{\mathbf{k}}^{\mathbf{i}} \left[\widehat{\partial_\alpha}\right]_{\mathbf{j}}^{\mathbf{k}} + \left[\widehat{\partial_\alpha}\right]_{\mathbf{k}}^{\mathbf{i}} \left[\widehat{f^\alpha}\right]_{\mathbf{j}}^{\mathbf{k}} \right)$$