On the Contraction Coefficient of the Schrödinger Bridge for Stochastic Linear Systems

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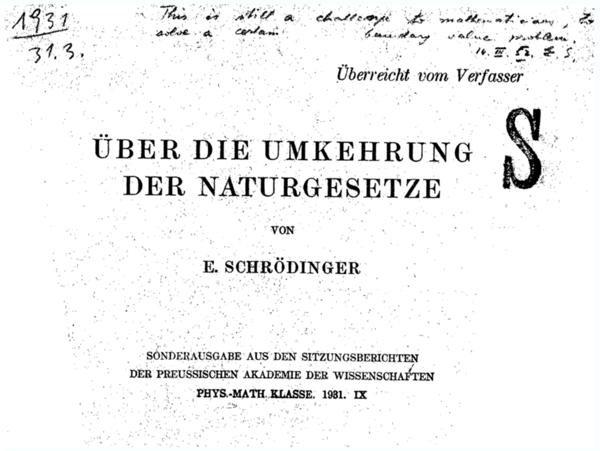
What is a Schrödinger Bridge Problem (SBP)



1931
31.3.

This is still a challenge to mathematicians, to solve a certain boundary value problem.
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Überreicht vom Verfasser

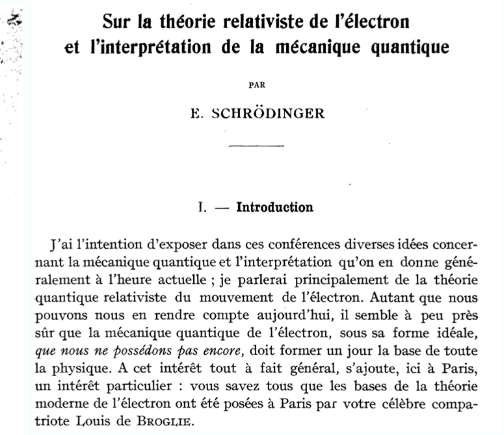
S

ÜBER DIE UMKEHRUNG
DER NATURGESETZE

VON

E. SCHRÖDINGER

SONDERAUSGABE AUS DEN SITZUNGSBERICHTEN
DER PREUSSISCHEN AKADEMIE DER WISSENSCHAFTEN
PHYS.-MATH. KLASSE. 1931. IX



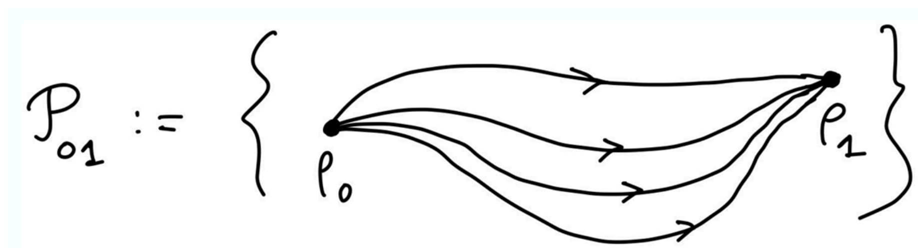
Sur la théorie relativiste de l'électron
et l'interprétation de la mécanique quantique

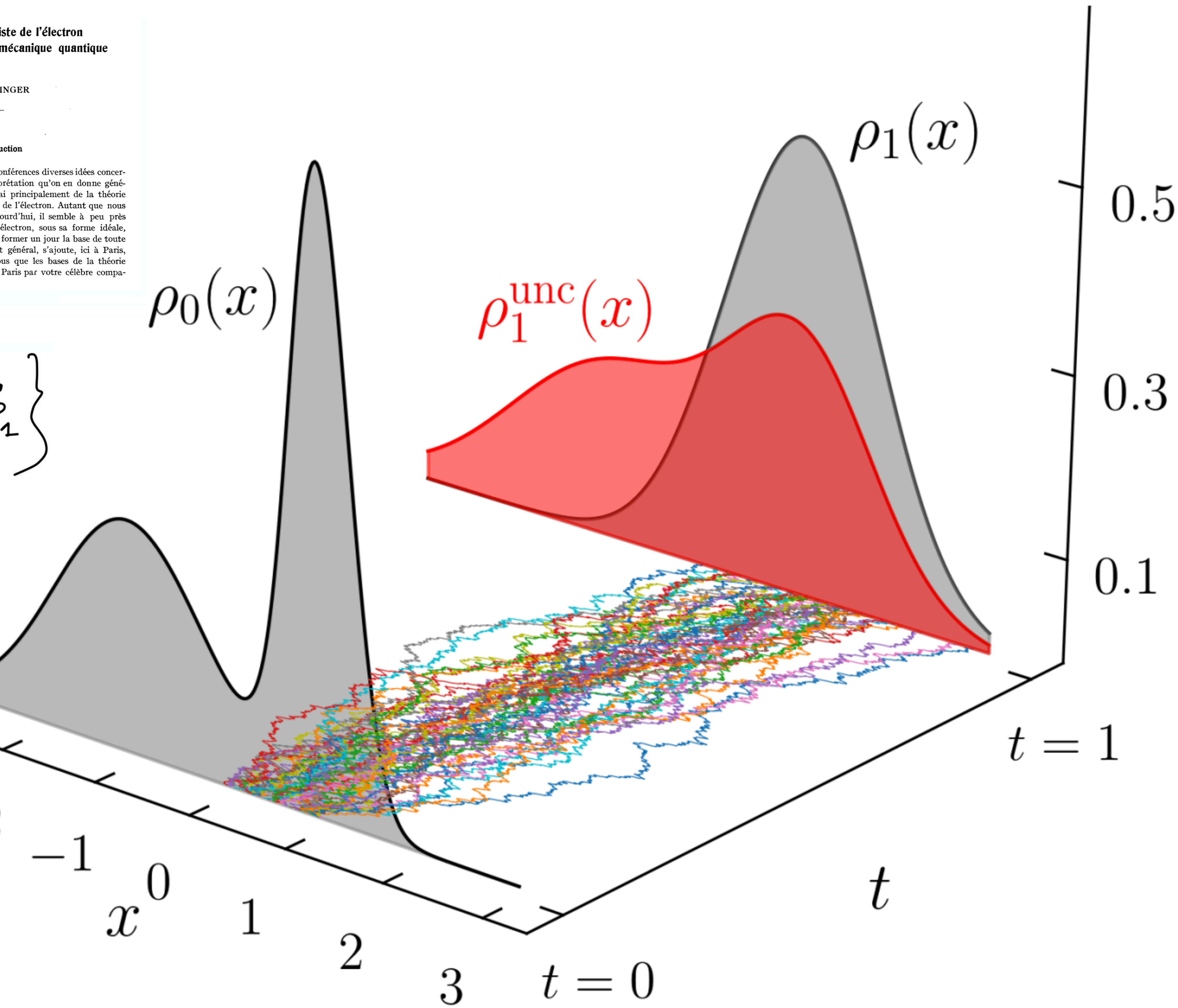
PAR

E. SCHRÖDINGER

I. — **Introduction**

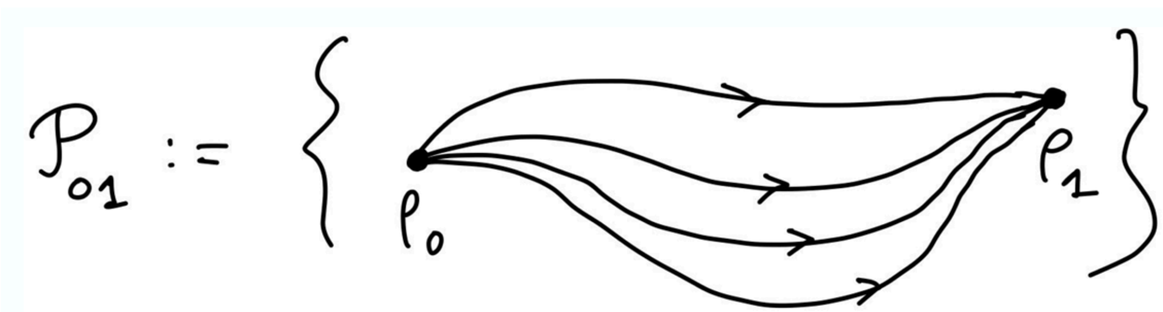
J'ai l'intention d'exposer dans ces conférences diverses idées concernant la mécanique quantique et l'interprétation qu'on en donne généralement à l'heure actuelle ; je parlerai principalement de la théorie quantique relativiste du mouvement de l'électron. Autant que nous pouvons nous en rendre compte aujourd'hui, il semble à peu près sûr que la mécanique quantique de l'électron, sous sa forme idéale, *que nous ne possédons pas encore*, doit former un jour la base de toute la physique. A cet intérêt tout à fait général, s'ajoute, ici à Paris, un intérêt particulier : vous savez tous que les bases de la théorie moderne de l'électron ont été posées à Paris par votre célèbre compatriote Louis de Broglie.

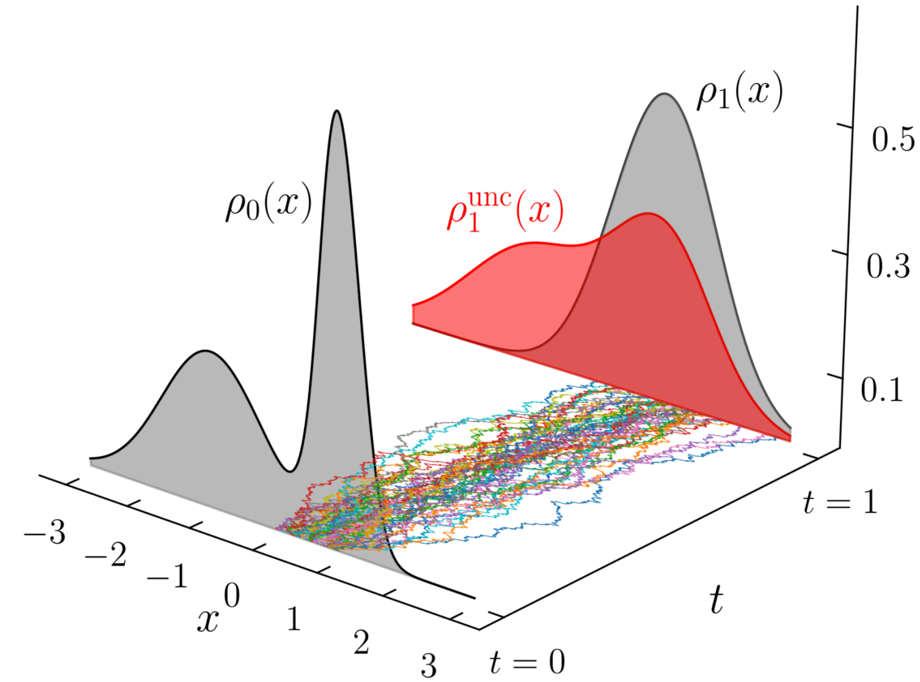




Most likely evolution between 2 distributional snapshots

Classical SBP





$$\underset{(\rho,\boldsymbol{v})\in\mathcal{P}_{01}\times\mathcal{V}}{\operatorname{arginf}} \int_{t_0}^{t_1}\int_{\mathbb{R}^n} \frac{1}{2}|\boldsymbol{v}|^2\rho(\boldsymbol{x},t)\mathrm{d}\boldsymbol{x}\mathrm{d}t$$

$$\frac{\partial\rho}{\partial t} + \nabla_{\boldsymbol{x}}\cdot(\rho\boldsymbol{v}) = \varepsilon\Delta_{\boldsymbol{x}}\rho, \quad \varepsilon > 0,$$

$$\rho(\boldsymbol{x}, t = t_0) = \rho_0, \quad \rho(\boldsymbol{x}, t = t_1) = \rho_1,$$

Controlled sample path dynamics

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{v}(\boldsymbol{x},t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}\boldsymbol{w}(t)$$

Solution to the Classical SBP

The pair $(\rho_\varepsilon^{\text{opt}}, \boldsymbol{v}_\varepsilon^{\text{opt}})$ solves the coupled PDEs

Value function

$$\frac{\partial \psi_\varepsilon}{\partial t} + \frac{1}{2}\left|\nabla_x \psi_\varepsilon\right|^2 + \varepsilon \Delta_x \psi_\varepsilon = 0,$$

$$\frac{\partial \rho_\varepsilon^{\text{opt}}}{\partial t} + \nabla_x \cdot \left(\rho_\varepsilon^{\text{opt}} \nabla_x \psi_\varepsilon\right) = \varepsilon \Delta_x \rho_\varepsilon^{\text{opt}}$$

Hopf-Cole transform

$$\varphi_\varepsilon := \exp\left(\frac{\psi_\varepsilon}{2\varepsilon}\right), \quad \widehat{\varphi}_\varepsilon := \rho_\varepsilon^{\text{opt}} \exp\left(-\frac{\psi_\varepsilon}{2\varepsilon}\right)$$

Schrödinger factors

Optimally controlled joint state PDF: $\rho_\varepsilon^{\text{opt}}(\cdot, t) = \widehat{\varphi}_\varepsilon(\cdot, t)\varphi_\varepsilon(\cdot, t)$

Optimal control: $\boldsymbol{v}_\varepsilon^{\text{opt}}(\cdot, t) = 2\varepsilon \nabla_{\boldsymbol{x}} \log \varphi_\varepsilon(\cdot, t)$

Schrödinger factors

Algorithm

Fixed point recursion over pair $\left(\varphi_{\varepsilon,1}, \widehat{\varphi}_{\varepsilon,0}\right)$

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
\widehat{\varphi}_{\varepsilon,0}(\cdot) \arrow[r, "\int \mathcal{L}_{\text{forward}} \widehat{\varphi}"] & \widehat{\varphi}_{\varepsilon}(\cdot, t = t_1) \arrow[d, "\rho_1(\cdot) / \widehat{\varphi}_{\varepsilon}(\cdot, t = t_1)"] \\
\varphi_{\varepsilon}(\cdot, t = t_0) \arrow[u, "\rho_0(\cdot) / \varphi_{\varepsilon}(\cdot, t = t_0)"] & \varphi_{\varepsilon,1}(\cdot) \arrow[l, "\int \mathcal{L}_{\text{backward}} \varphi"]
\end{tikzcd}
$$

Schrödinger system

Markov kernel

$$\rho_0(\boldsymbol{x}) = \widehat{\varphi}_{\varepsilon,0}(\boldsymbol{x}) \int_{\mathbb{R}^n} k(t_0, \boldsymbol{x}, t_1, \boldsymbol{y}) \varphi_{\varepsilon,1}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y}$$

$$\rho_1(\boldsymbol{x}) = \varphi_{\varepsilon,1}(\boldsymbol{x}) \int_{\mathbb{R}^n} k(t_0, \boldsymbol{y}, t_1, \boldsymbol{x}) \widehat{\varphi}_{\varepsilon,0}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y}$$

Coupled nonlinear integral equations

Contraction Coefficient γ in Classical SBP

Let

$$\tilde{\alpha}_{\mathrm{B}} := \max_{\boldsymbol{x}_0 \in \mathcal{X}_0, \boldsymbol{x}_1 \in \mathcal{X}_1} |\boldsymbol{x}_0 - \boldsymbol{x}_1|^2 \quad \text{and} \quad \tilde{\beta}_{\mathrm{B}} := \min_{\boldsymbol{x}_0 \in \mathcal{X}_0, \boldsymbol{x}_1 \in \mathcal{X}_1} |\boldsymbol{x}_0 - \boldsymbol{x}_1|^2$$

Then

$$\boxed{\gamma_{\mathrm{B}} = \tanh^2\left(\frac{\tilde{\alpha}_{\mathrm{B}} - \tilde{\beta}_{\mathrm{B}}}{8\varepsilon}\right) \in (0,1)}$$

Chen, Georgiou, Pavon, ***SIAM J. Applied Math, 2016***

Linear SBP

$$\underset{(\rho,\boldsymbol{v})\in\mathcal{P}_{01}\times\mathcal{V}}{\arg\inf} \quad \int_{t_0}^{t_1}\int_{\mathbb{R}^n} \frac{1}{2}|\boldsymbol{v}|^2\rho(\boldsymbol{x},t)\,d\boldsymbol{x}\,dt$$

$$\frac{\partial\rho}{\partial t} + \nabla_{\boldsymbol{x}}\cdot(\rho(\boldsymbol{A}(t)\boldsymbol{x}+\boldsymbol{B}(t)\boldsymbol{v})) = \varepsilon\langle\text{Hess}, \boldsymbol{B}(t)\boldsymbol{B}(t)^\top\rho\rangle$$

resp. compact supports $\mathcal{X}_0, \mathcal{X}_1$

$$\rho(\boldsymbol{x},t=t_0) = \rho_0, \quad \rho(\boldsymbol{x},t=t_1) = \rho_1$$

Controlled sample path dynamics

$$\mathrm{d}\boldsymbol{x}(t) = (\boldsymbol{A}(t)\boldsymbol{x}(t)+\boldsymbol{B}(t)\boldsymbol{v}(\boldsymbol{x},t))\mathrm{d}t + \sqrt{2\varepsilon}\boldsymbol{B}(t)\mathrm{d}\boldsymbol{w}(t)$$

State transition matrix $\boldsymbol{\Phi}_{t\tau} := \boldsymbol{\Phi}(t,\tau) \quad \forall t_0\leq\tau\leq t\leq t_1$

Assume controllability: $\boldsymbol{M}_{10} := \int_{t_0}^{t_1}\boldsymbol{\Phi}_{t_1\tau}\boldsymbol{B}(\tau)\boldsymbol{B}^\top(\tau)\boldsymbol{\Phi}_{t_1\tau}^\top\mathrm{d}\tau \succ \boldsymbol{0}$

Structure of the Solution for Linear SBP

Optimally controlled joint state PDF: $\rho_{\varepsilon}^{\text{opt}}(\cdot, t) = \widehat{\varphi}_{\varepsilon}(\cdot, t)\varphi_{\varepsilon}(\cdot, t)$

Optimal control: $\boldsymbol{v}_{\varepsilon}^{\text{opt}}(\cdot, t) = 2\varepsilon \boldsymbol{B}(t)^{\top}\nabla_{\boldsymbol{x}} \log \varphi_{\varepsilon}(\cdot, t)$

Schrödinger factors

Define: $\widehat{\varphi}_{\varepsilon,0}(\cdot) := \widehat{\varphi}_{\varepsilon}(\cdot, t = t_0), \quad \varphi_{\varepsilon,1}(\cdot) := \varphi_{\varepsilon}(\cdot, t = t_1)$

Schrödinger system

Markov kernel

$$\rho_0(\boldsymbol{x}) = \widehat{\varphi}_{\varepsilon,0}(\boldsymbol{x}) \int_{\mathbb{R}^n} \underbrace{k(t_0, \boldsymbol{x}, t_1, \boldsymbol{y})}_{\text{Markov kernel}} \varphi_{\varepsilon,1}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y}$$

$$\rho_1(\boldsymbol{x}) = \varphi_{\varepsilon,1}(\boldsymbol{x}) \int_{\mathbb{R}^n} k(t_0, \boldsymbol{y}, t_1, \boldsymbol{x}) \widehat{\varphi}_{\varepsilon,0}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y}$$

Coupled nonlinear integral equations

Here

$$k(t_0, \boldsymbol{x}_0, t_1, \boldsymbol{x}_1) := \frac{\exp\left(-\frac{\left(\boldsymbol{\Phi}_{t_1 t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1\right)^{\top} \boldsymbol{M}_{10}^{-1} \left(\boldsymbol{\Phi}_{t_1 t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1\right)}{4\varepsilon}\right)}{\sqrt{(4\pi\varepsilon)^n \det(\boldsymbol{M}_{10})}}$$

Contractive Fixed Point Algorithm

Fixed point recursion over pair $(\varphi_{\varepsilon,1}, \widehat{\varphi}_{\varepsilon,0})$

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\widehat{\varphi}_{\varepsilon,0}(\cdot) \arrow[r, "\int", "\text{IVP forward in time}"'] & \widehat{\varphi}_{\varepsilon}(\cdot, t = t_1) \arrow[d, "\rho_1(\cdot)/\widehat{\varphi}_{\varepsilon}(\cdot, t = t_1)"] \\
\varphi_{\varepsilon}(\cdot, t = t_0) \arrow[u, "\rho_0(\cdot)/\varphi_{\varepsilon}(\cdot, t = t_0)"] & \varphi_{\varepsilon,1}(\cdot) \arrow[l, "\text{IVP backward in time}"', "\int"]
\end{tikzcd}$$

Guaranteed linear convergence with contraction rate $\kappa \in (0,1)$

But exact rate depends on problem data $(\mathcal{X}_0, \mathcal{X}_1, \varepsilon, \boldsymbol{A}(t), \boldsymbol{B}(t))$

Worst case contraction coefficient $\gamma := \sup\limits_{\text{Linear SBPs with fixed } (\mathcal{X}_0, \mathcal{X}_1, \varepsilon, \boldsymbol{A}(t), \boldsymbol{B}(t))} \kappa$

Contraction Coefficient γ in Linear SBP

Thm. (informal)

State transition matrix   Controllability Gramian

Let

$$\tilde{\alpha}_{\mathrm{L}} := \max_{\boldsymbol{x}_0 \in \mathcal{X}_0, \boldsymbol{x}_1 \in \mathcal{X}_1} (\boldsymbol{\Phi}_{t_1 t_0} \boldsymbol{x}_0 - \boldsymbol{x}_1)^\top \boldsymbol{M}_{10}^{-1} (\boldsymbol{\Phi}_{t_1 t_0} \boldsymbol{x}_0 - \boldsymbol{x}_1)$$

$$\tilde{\beta}_{\mathrm{L}} := \min_{\boldsymbol{x}_0 \in \mathcal{X}_0, \boldsymbol{x}_1 \in \mathcal{X}_1} (\boldsymbol{\Phi}_{t_1 t_0} \boldsymbol{x}_0 - \boldsymbol{x}_1)^\top \boldsymbol{M}_{10}^{-1} (\boldsymbol{\Phi}_{t_1 t_0} \boldsymbol{x}_0 - \boldsymbol{x}_1)$$

Then

$$\gamma_{\mathrm{L}} = \tanh^2 \left(\frac{\tilde{\alpha}_{\mathrm{L}} - \tilde{\beta}_{\mathrm{L}}}{8\varepsilon} \right)$$

Control-theoretic Interpretation for γ_{L}

$$\tilde{\alpha}_{\mathrm{L}} := \max_{\boldsymbol{x}_0 \in \mathcal{X}_0, \boldsymbol{x}_1 \in \mathcal{X}_1} (\boldsymbol{\Phi}_{t_1 t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1)^{\top} \boldsymbol{M}_{10}^{-1} (\boldsymbol{\Phi}_{t_1 t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1)$$

$$\tilde{\beta}_{\mathrm{L}} := \min_{\boldsymbol{x}_0 \in \mathcal{X}_0, \boldsymbol{x}_1 \in \mathcal{X}_1} (\boldsymbol{\Phi}_{t_1 t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1)^{\top} \boldsymbol{M}_{10}^{-1} (\boldsymbol{\Phi}_{t_1 t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1)$$

$$\begin{aligned}
&\underset{\boldsymbol{v}}{\text{minimum}} \int_{t_0}^{t_1} \frac{1}{2} |\boldsymbol{v}|^2 dt \\
&\text{subject to} \quad \dot{\boldsymbol{x}} = \boldsymbol{A}(t)\boldsymbol{x} + \boldsymbol{B}(t)\boldsymbol{v} \\
&\qquad\qquad\quad \boldsymbol{x}(t = t_0) = \boldsymbol{x}_0, \boldsymbol{x}(t = t_1) = \boldsymbol{x}_1
\end{aligned}$$

Minimum cost for deterministic OCP

Control-theoretic Interpretation for γ_{L}

Range of optimal state transfer cost

$$\gamma_{\mathrm{L}} = \tanh^2\left(\frac{\tilde{\alpha}_{\mathrm{L}} - \tilde{\beta}_{\mathrm{L}}}{8\varepsilon}\right)$$

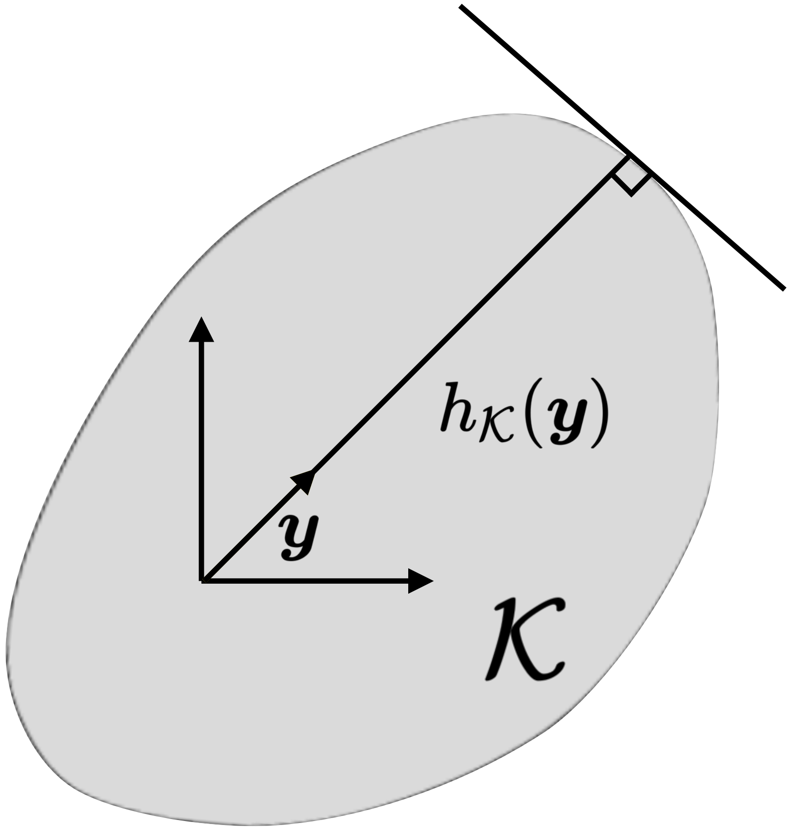
Process noise

Intuitive:

$$\boxed{\varepsilon \uparrow \quad \Rightarrow \quad \gamma_{\mathrm{L}} \downarrow}$$

$$\boxed{\tilde{\alpha}_{\mathrm{L}} - \tilde{\beta}_{\mathrm{L}} \uparrow \quad \Rightarrow \quad \gamma_{\mathrm{L}} \uparrow}$$

Support Function

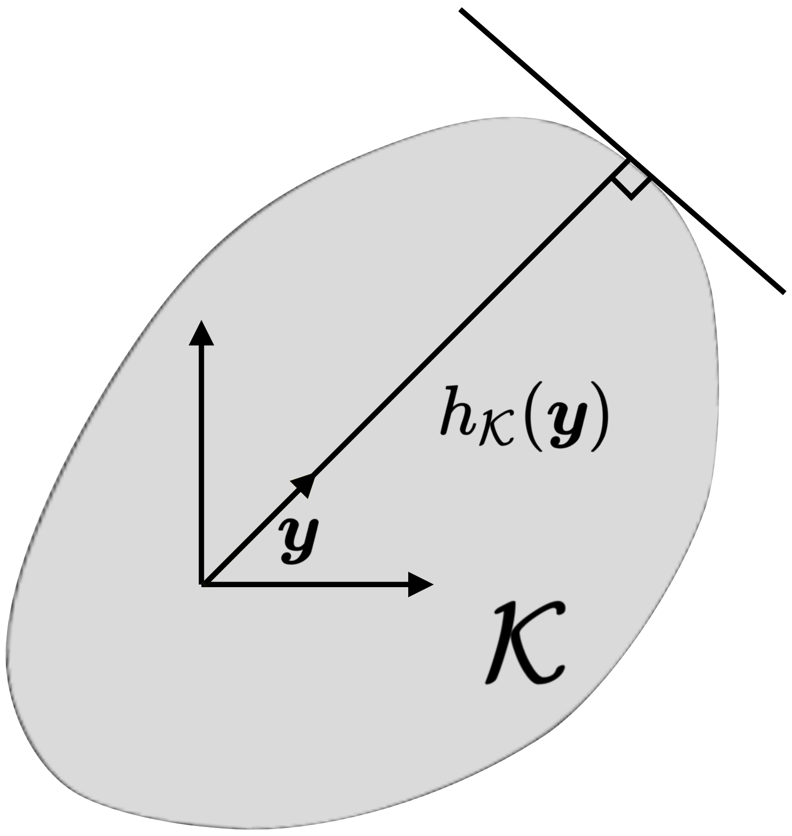


The support function $h_{\mathcal{K}}(\cdot)$ for closed convex set $\mathcal{K}$ is

$$h_{\mathcal{K}}(\boldsymbol{y}) := \sup_{\boldsymbol{x} \in \mathcal{K}} \langle \boldsymbol{y}, \boldsymbol{x} \rangle, \quad \boldsymbol{y} \in \mathbb{R}^n$$

e.g., distance from the origin to a supporting hyperplane of $\mathcal{K}$ with normal in direction of $\boldsymbol{y}$

Geometric Interpretation for γ_{L}



$$\gamma_{\mathrm{L}} = \tanh^2\left(\frac{\tilde{\alpha}_{\mathrm{L}} - \tilde{\beta}_{\mathrm{L}}}{8\varepsilon}\right)$$

$$\tilde{\alpha}_{\mathrm{L}} = \{\max_{\boldsymbol{y}\in\mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\boldsymbol{\Phi}_{t_1 t_0}^{\top}\boldsymbol{M}_{10}^{-1/2}\boldsymbol{y}) + h_{\mathcal{X}_1}(-\boldsymbol{M}_{10}^{-1/2}\boldsymbol{y}))\}^2$$

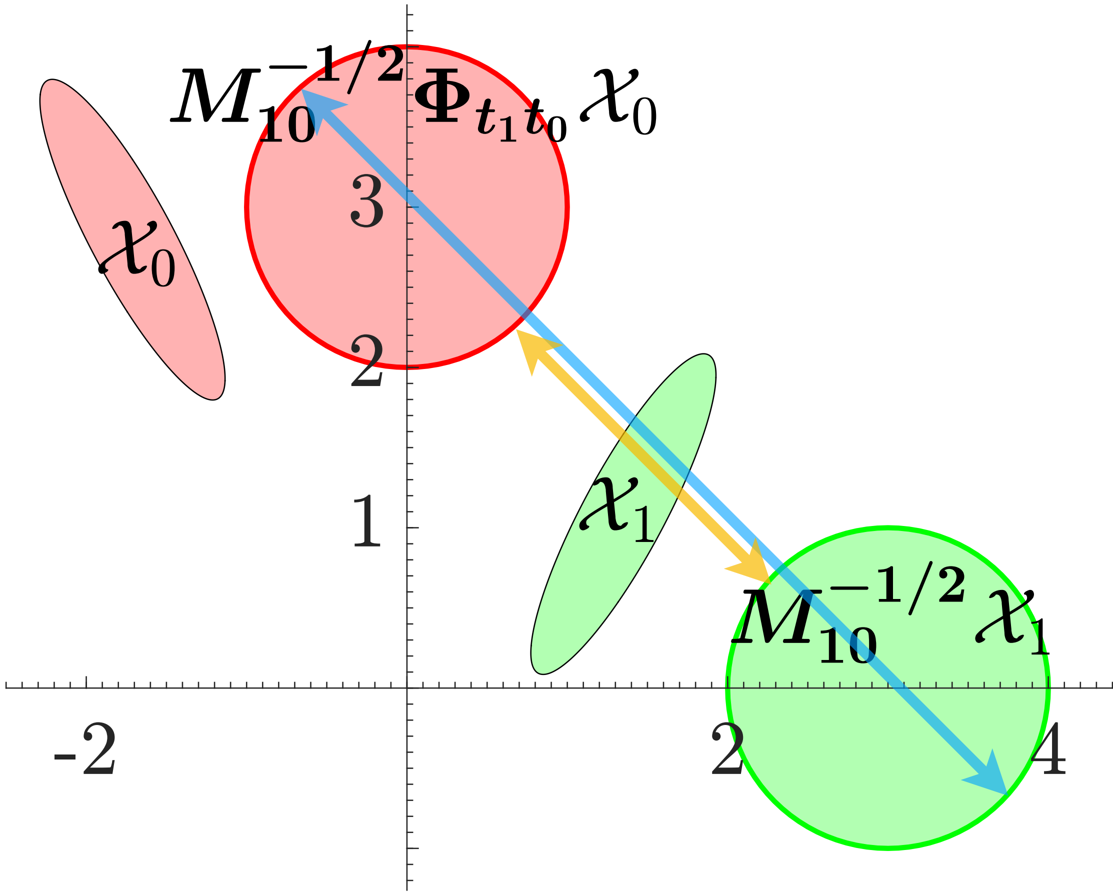
$$\tilde{\beta}_{\mathrm{L}} = \{\min_{\boldsymbol{y}\in\mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\boldsymbol{\Phi}_{t_1 t_0}^{\top}\boldsymbol{M}_{10}^{-1/2}\boldsymbol{y}) + h_{\mathcal{X}_1}(-\boldsymbol{M}_{10}^{-1/2}\boldsymbol{y}))\}^2$$

Geometric Interpretation for γ_{L}

$$\gamma_{\mathrm{L}} = \tanh^2\left(\frac{\tilde{\alpha}_{\mathrm{L}} - \tilde{\beta}_{\mathrm{L}}}{8\varepsilon}\right)$$

$$\tilde{\alpha}_{\mathrm{L}} := \max_{\boldsymbol{x}_0 \in \boldsymbol{M}_{10}^{-1/2}\boldsymbol{\Phi}_{10}\mathcal{X}_0,\ \boldsymbol{x}_1 \in \boldsymbol{M}_{10}^{-1/2}\mathcal{X}_1} |\boldsymbol{x}_0 - \boldsymbol{x}_1|^2$$

$$\tilde{\beta}_{\mathrm{L}} := \min_{\boldsymbol{x}_0 \in \boldsymbol{M}_{10}^{-1/2}\boldsymbol{\Phi}_{10}\mathcal{X}_0,\ \boldsymbol{x}_1 \in \boldsymbol{M}_{10}^{-1/2}\mathcal{X}_1} |\boldsymbol{x}_0 - \boldsymbol{x}_1|^2$$



$\tilde{\alpha}_{\mathrm{L}}$ and $\tilde{\beta}_{\mathrm{L}}$ are the maximum and the minimum separation of the sets

$M_{10}^{-1/2}\boldsymbol{\Phi}_{t_1t_0}\mathcal{X}_0$ and $M_{10}^{-1/2}\mathcal{X}_1$

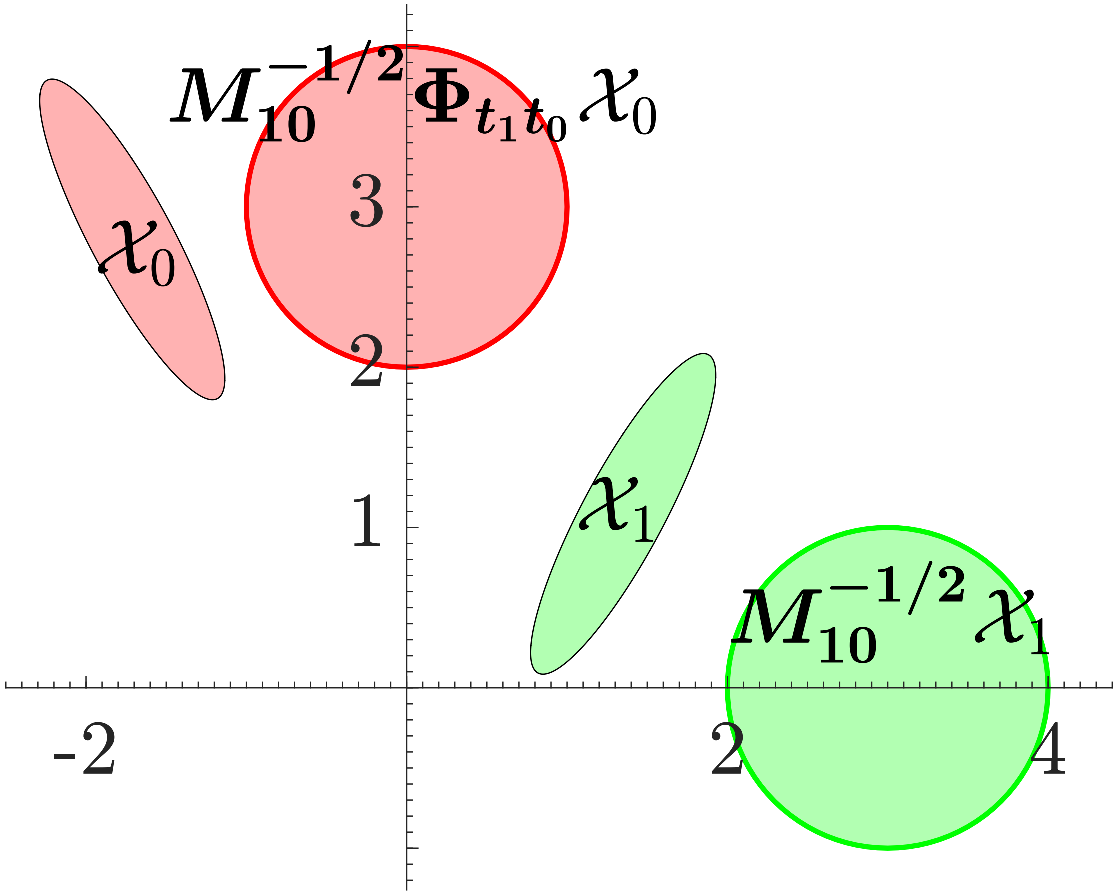
Applications to Preconditioning

Preconditioning to improve optimal transport algorithms
~ Kuang and Tabak, *SIAM J. Scientific Computing*, 2017

Example: Linear SBP:

$$d\boldsymbol{x}(t) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \boldsymbol{x}(t)dt + \sqrt{2\varepsilon} \begin{bmatrix} 0 \\ 1 \end{bmatrix} d\boldsymbol{w}(t)$$

$$\boldsymbol{\Phi}_{t_1 t_0} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad \boldsymbol{M}_{10}^{-1} = \begin{bmatrix} 12 & -6 \\ -6 & 4 \end{bmatrix}.$$



No Preconditioning:

$$\tilde{\alpha}_{\mathrm{L}} = 2 + 2\sqrt{3} \qquad \tilde{\beta}_{\mathrm{L}} = -2 + 2\sqrt{3} \longrightarrow \gamma_{\mathrm{L}} = \tanh^2(1) \approx 0.580$$

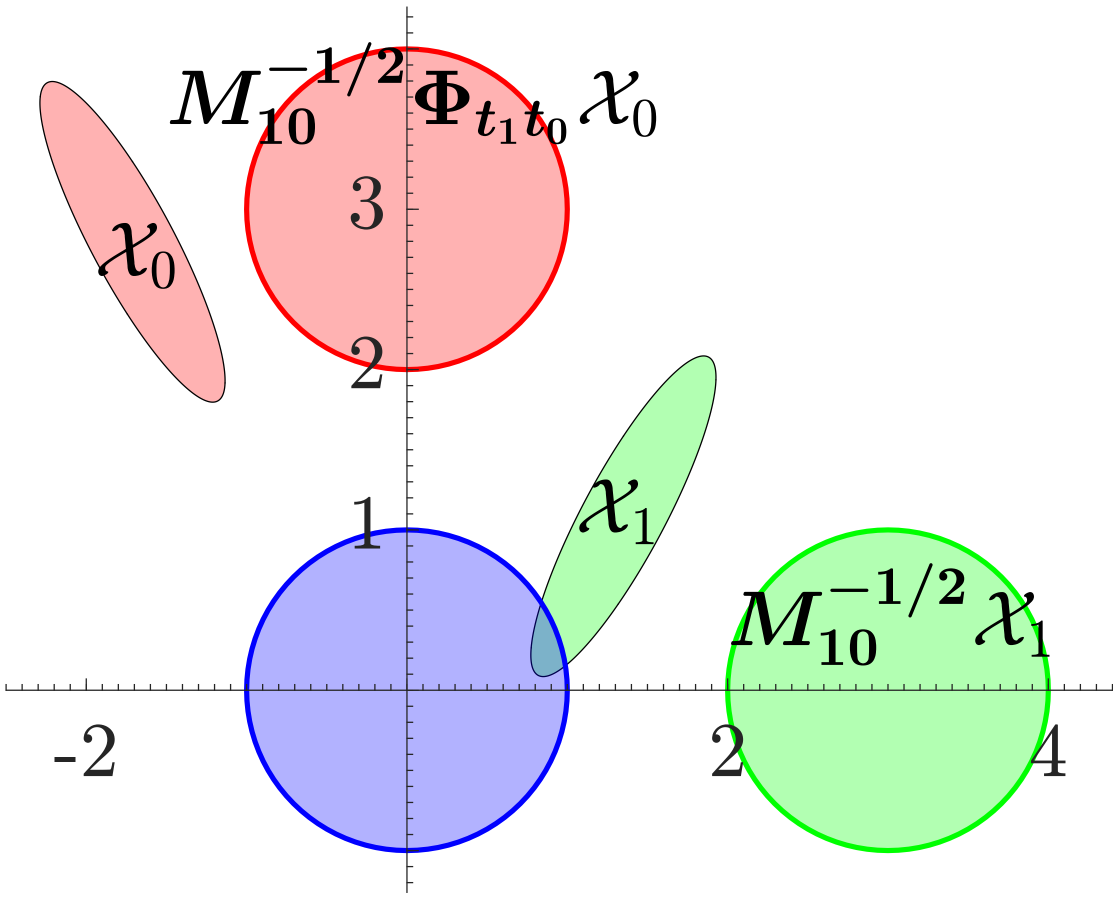
Applications to Preconditioning

Preconditioning to improve optimal transport algorithms
~ Kuang and Tabak, *SIAM J. Scientific Computing*, 2017

Example: Linear SBP:

$$d\boldsymbol{x}(t) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \boldsymbol{x}(t)dt + \sqrt{2\varepsilon} \begin{bmatrix} 0 \\ 1 \end{bmatrix} d\boldsymbol{w}(t)$$

$$\boldsymbol{\Phi}_{t_1 t_0} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad \boldsymbol{M}_{10}^{-1} = \begin{bmatrix} 12 & -6 \\ -6 & 4 \end{bmatrix}.$$



With Preconditioning:

$$\tilde{\alpha}_{\mathrm{L}}^{\mathrm{precond}} = 2, \ \tilde{\beta}_{\mathrm{L}}^{\mathrm{precond}} = 0 \quad \longrightarrow \quad \gamma_{\mathrm{L}}^{\mathrm{precond}} = \tanh^2(0.5) = 0.214$$

Avenues of Future Research

Preconditioning:

—> Demonstrate effectiveness of proposed methods

—> Inform the construction of new methods

Additional Generalizations of SBP:

—> Current: Quadratic state cost

—> Future: Keplerian state cost

Thank You

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