Spectral Gap Optimization of Divergence Type Diffusion Operators

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***Abstract*— In this paper, we address the problem of maximizing the spectral gap of a divergence type diffusion operator. Our main application of interest is characterizing the distribution of a swarm of agents that evolve on a bounded domain in $\mathbb{R}^d$ according to a Markov process. A subclass of the divergence type operators that we introduce in this paper can describe the distribution of the swarm across the domain. We construct an operator that stabilizes target distributions that are bounded and strictly positive almost everywhere on the domain. Optimizing the spectral gap of the operator ensures fast convergence to this target distribution. The optimization problem is posed as the minimization of the second largest eigenvalue modulus (SLEM) of the operator (the largest eigenvalue is 0). We use the well-known *Courant-Fisher min-max* principle to characterize the SLEM. We also present a numerical scheme for solving the optimization problem, and we validate our optimization approach for two example target distributions.**

I. Introduction

Over the past two decades, there has been an increasing amount of research on the control of multi-agent systems. For agents whose dynamics can be described by a Markov process, controller design can be performed on a macroscopic abstraction of the swarm as a continuous spatio-temporal density field that evolves according to the *Kolmogorov forward equation*. In our previous works [3], [4], we constructed operators that stabilize a given target distribution for such a swarm and optimize the convergence rate of the swarm to this distribution. Both works considered swarms of agents whose dynamics evolve over a continuous state space in discrete time. However, except for a special case of the state space, the optimization problem posed in both works was not exact, meaning that it minimized only an upper bound on the eigenvalues of the operator rather than the eigenvalues themselves.

As a next step, in this paper we consider swarms of agents whose dynamics evolve over a continuous state space in continuous time; in particular, the dynamics of each agent can be modeled as a stochastic differential equation (SDE). The Kolmogorov forward equation in this case is a partial differential equation (PDE) that is commonly known as the *Fokker-Planck equation*. As in our earlier work [3], [4], we construct a partial differential operator that stabilizes target swarm distributions that are bounded and positive almost everywhere on the domain. In particular, the operator that we construct has a structure similar to the divergence form operator, which is known to be self-adjoint. The advantage in this case is that we can invoke the min-max principle to characterize the modulus of the second largest eigenvalue of the operator, which characterizes the asymptotic convergence rate of the swarm to the target distribution. Hence, unlike in our previous works, the optimization problem is exact. However, not all divergence form operators are Fokker-Planck equations; that is, they do not all give rise to SDEs. Instead of working with a restricted class of divergence form operators that do give rise to SDEs, we will work with general divergence form operators, and consider the SDE description of agent dynamics only formally. See [23] for a discussion on divergence type operators that correspond to diffusion semigroups.

We begin by briefly reviewing literature on the topic of using PDE models to predict and control the distribution of a swarm of agents. For a comprehensive survey of such works, see [5]. In [19], the authors design agent control parameters that stabilize the swarm to a target distribution. Works on mean-field game theory, which has only recently been applied to problems in swarm robotics [18], use optimal control techniques to construct policies for strategic decision-making in very large populations of interacting agents. In the field of multi-robot systems, a number of works utilize PDEs to model and control the collective behaviors of robotic swarms. The work [21] uses a PDE model with a constant velocity field to simulate a swarm of small robots performing an inspection task, and the model is validated experimentally. In [16], the authors design swarm control strategies that mimic fluid flow behavior by constructing state-feedback laws that are piecewise constant with respect to space. PDEs with feedback laws that are functions of population densities are used in [13] to model collective migration and collective perception in swarms. The work [6] applies optimal control of PDEs and PDE-constrained optimization to design time-dependent robot controllers for problems of stochastic spatial coverage and feature mapping by robotic swarms.

With regard to characterizing the spectral gap of Fokker-Planck equations or in general, diffusion equations, the *Bakry-Emery method* allows one to establish convex Sobolev inequalities and to compute exponential decay rates toward equilibrium for solutions of diffusion equations [2]. In [1], the authors quantify convergence rates of Fokker-Planck equations using convex Sobolev inequalities. In [15], the author poses the spectral optimization problem for a Fokker-

This work was supported by the Arizona State University Global Security Initiative. The work of Hans Mittelmann was supported in part by the Air Force Office of Scientific Research under grant FA9550-19-1-0070.

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Planck equation in $\mathbb{R}^1$ using the min-max principle. In contrast to our work, the domain is restricted to $\mathbb{R}^1$ and the constraint is posed in terms of minimizing the variance of the corresponding Markov process.

II. Notation

We define $\bar{\mathbb{R}}_+ := [0, \infty)$, $\mathbb{R}_+ := (0, \infty)$. We denote the state space by $\Omega \subset \mathbb{R}^d$, an open, bounded connected set. The boundary of Ω will be denoted by $\partial\Omega$, which is assumed to be *Lipschitz continuous* [12].

We define $L^p(\Omega)$, where $p \in [1, \infty)$, as the space $\{f : \Omega \to \mathbb{R};\ f \text{ is measurable and } \|f\|_p < \infty\}$, where $\|f\|_p = (\int |f|^p dx)^{1/p}$. We also define $L^\infty(\Omega, m) = \{f : \mathcal{X} \to \mathbb{R};\ f \text{ is measurable and } \|f\|_\infty < \infty\}$, where $\|f\|_\infty = \operatorname{ess\,sup}_{x\in\Omega} |f(x)|$. The space $L^2(\Omega)$ is a Hilbert space equipped with the standard inner product $\langle \cdot, \cdot \rangle_2 : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$ given by $\langle f, g \rangle_2 = \int_\Omega f(x)g(x)dx$, for all $f, g \in L^2(\Omega)$. The symbol $\|\cdot\|_2$ will be reserved for the $L^2(\cdot)$ norm. For a given real-valued function $h \in L^\infty(\Omega)$, (weighted) $L^2_h(\Omega)$ refers to the set of all functions f such that $\int_\Omega |f(x)|^2 |h(x)| dx < \infty$. In this case, $L^2_h(\Omega)$ is a Hilbert space with respect to the weighted inner product $\langle \cdot, \cdot \rangle_h : L^2_h(\Omega) \times L^2_h(\Omega) \to \mathbb{R}$ given by $\langle f, g \rangle_h = \int_\Omega f(x)g(x)h(x)dx$. We let $\|\cdot\|_F$ stand for the weighted L^2_F norm.

Let f_{x_i} denote the first-order weak partial derivative of the function f with respect to coordinate x_i. We define the Sobolev space $H^1(\Omega)$ of $L^2(\Omega)$ functions whose partial derivatives, in the weak sense, are also in $L^2(\Omega)$. This is a Hilbert space with the norm: $\|f\|_{H^1} = \|f\|_2^2 + \left(\sum_{i=1}^d \|f_{x_i}\|_2^2\right)^{1/2}$ for $f \in H^1(\Omega)$. Correspondingly, for $h \in L^\infty(\Omega)$ we define the space $H^1_h(\Omega) = \left\{f \in L^2_h(\Omega) : (fh)_{x_i} \in L^2(\Omega) \text{ for } 1 \le i \le d\right\}$, equipped with the norm $\|f\|_{H^1_a} = \left(\|f\|_a^2 + \sum_{i=1}^d \|(af)_{x_i}\|_2^2\right)^{1/2}$.

Let $\mathcal{X}$ be a Hilbert space. Let A be a closed linear operator that is densely defined on a subset $\mathcal{D}(A) \subset \mathcal{X}$, the domain of the operator. If A is a bounded operator, then $\|A\|_{op}$ will denote the operator norm induced by the norm defined on $\mathcal{X}$. The spectrum $\sigma(A)$ of A is the non-void compact set of complex numbers λ for which $A - \lambda I$ does not have a continuous inverse on $\mathcal{X}$. The operator A is said to be *positive*, denoted by $A > 0$, if for $x \in \mathcal{X}$, $x \ge 0$ implies that $Ax \ge 0$.

III. Problem Formulation

We begin by setting up the problem that we address in this paper. Let $F \in L^\infty(\Omega)$ such that $F(x) > 0$ *a.e.* be the target steady-state probability density function for a swarm of robots. Then F must satisfy the condition $\int_\Omega F(x)dx = 1$. Define $\Omega_{T_f} = \Omega \times (0, T_f)$ for some fixed final time T_f. Let $p : \Omega_{T_f} \to \mathbb{R}^n$ denote a probability density function. The forward Kolmogorov equation, also called the Fokker-Planck equation, gives the evolution of probability densities on the state space Ω. In continuous time and continuous space, this equation is a partial differential equation (PDE) of the form:

$$\frac{\partial}{\partial t} p(x,t) = \frac{1}{2} \sum_{i,j=1}^d \frac{\partial^2}{\partial x_i \partial x_j} [D_{ij}(x,t)p(x,t)] - \sum_{i=1}^d \frac{\partial}{\partial x_i} [a_i(x,t)p(x,t)]. \quad (1)$$

Here, the coefficients D_{ij} and a_{ij} represent diffusion and advection parameters, respectively. In this paper, however, we will not be working with such a general formulation. For reasons that will be made clear later, we require the partial differential operator associated with the PDE to be self-adjoint. This is not true for the PDE (1). We will therefore introduce an operator, formally, which is self-adjoint.

Let $a_{ij} : \Omega \to \mathbb{R}^d$ for $i, j = 1, \ldots, d$, with $a_{ij} = a_{ji}$, be in $L^\infty(\Omega)$. Further, we assume that the coefficients satisfy the uniform *ellipticity* condition; that is, there exists a constant α such that for every vector $\xi \in \mathbb{R}^d$ and every $x \in \Omega$, $\sum_{i,j=1}^d a_{ij}(x)\xi_i\xi_j \ge \alpha|\xi|^2$. Consider the following *unbounded* operator,

$$\mathcal{L}_F u = \sum_{i,j=1}^d \frac{\partial}{\partial x_i} \left(a_{ij}(x) \frac{\partial (u/F)}{\partial x_j} \right). \quad (2)$$

We note that this operator has the advantage of being self-adjoint. Moreover, the operator is almost in the standard divergence form [9]; however, the inclusion of F makes it non-standard. It is clear that the inclusion of F ensures that $\mathcal{L}_F F = 0$; that is, the PDE generated by this operator has F as an equilibrium point. Without the inclusion of F, there are only a few special cases in which Eq. (2) can be rewritten as Eq. (1), and vice versa.

Remark III.1. *We note that the operator* (2) *is not defined rigorously. This is because the L^∞ condition on the coefficients a_{ij} makes it impossible to define the operator on $H^1(\Omega)$ or $H^2(\Omega)$ (defined similarly to $H^1(\Omega)$, but comprised of functions that are twice weakly differentiable and are in L^2); either space is not necessarily preserved under the multiplication of an L^∞ function and an H^1 or H^2 function. Therefore, in order to proceed, we will instead define a weak formulation of the operator* (2) *via forms.*

Note that according to our notation in Section II, as per standard definitions, H^1_F and L^2_F norms entail a multiplication by F; that is, $\|f\|_F = \int_\Omega |f|^2|F|$. However, in this paper, the norm entails a division by F; that is, $\|f\|_F = \int_\Omega |f|^2|1/F|$.

We define a *bilinear form* $B_F[u, v] : H^1_F(\Omega) \times H^1_F(\Omega) \to \mathbb{R}$ as follows:

$$B_F[u,v] = \int_\Omega \sum_{i,j=1}^d a_{ij}(x) \frac{\partial (u/F)}{\partial x_j} \frac{\partial (v/F)}{\partial x_i} dx \quad (3)$$

The space $H^1_F(\Omega)$ is called the domain of B_F, $\mathcal{D}(B_F)$. We associate with the form B an operator $\hat{\mathcal{L}} : \mathcal{D}(\hat{\mathcal{L}}_F) \subset L^2_F(\Omega) \to L^2_F(\Omega)$, defined as $\hat{\mathcal{L}}_F u = f$ if $B_F[u, v] = \langle f, v \rangle_F$ for all $v \in H^1_F(\Omega)$ and $u \in \mathcal{D}(\hat{\mathcal{L}}_F) = \{g \in H^1_F(\Omega) :$

$\exists h \in L^2_F(\Omega)$ $s.t.$ $B_F[g,\varphi] = \langle h, \varphi\rangle$ $\forall$ $\varphi \in H^1_F(\Omega)\}$. The operator $\hat{\mathcal{L}}_F$ so defined is a weak formulation of the operator (2). Defining $\hat{\mathcal{L}}_F$ via the bilinear form B_F is similar in spirit to the formulation of weak solutions to elliptic equations. A detailed treatment of the interplay between forms and operators is provided in [22]. In the specific case where the coefficients a_{ij} and the function F are uniformly Lipschitz functions, then $\hat{\mathcal{L}}_F$ coincides with the operator (2), with $H^2(\Omega)$ as its domain [12].

Although considering the divergence form operator (2) or the bilinear form (3) simplifies the analysis owing to the fact that they can be used to construct operators, we lose the guarantee that the generated PDE corresponds to a stochastic differential equation. Only in the case where the coefficients a_{ij} are uniformly Lipschitz continuous does the operator (2) give rise to a forward equation [11]. However, one can make sense of the stochastic differential equations that divergence form operators give rise to in a non-classical way; see [17] for this description.

We consider the following PDE generated by the operator $\mathcal{L}_F$ in (2). Note that this is only a formal statement because of the explanation in the previous paragraphs.

$$\frac{\partial p}{\partial t} = -\mathcal{L}_F p \text{ on } \Omega_{T_f} \tag{4}$$

$$\sum_{i,j=1}^{d} a_{ij}\frac{\partial(p/F)}{\partial x_j} n_i = 0 \text{ on } \partial\Omega \times (0, T_f) \tag{5}$$

$$p(x,0) = p_0(x) \text{ on } \Omega. \tag{6}$$

Equation (5) represents the zero flux boundary condition, also called the *Neumann* boundary condition; n_i is the ith unit normal vector to Ω, pointing outward.

We now state the problem that we solve in this paper. To address this problem, in the next section we will prove that 0 is the unique largest eigenvalue of the operator $-\hat{\mathcal{L}}_F$, with all other eigenvalues located in the left half-plane. Therefore, the convergence rate of the PDE (4) to its equilibrium is characterized by the L^2_F spectral gap. First, however, we will need to prove the existence of this spectral gap for $\hat{\mathcal{L}}_F$.

Problem III.2. *Given F, determine whether there exist time-independent, spatially-dependent parameters $a_{ij} : \Omega \to \mathbb{R}^n$, for $i,j \in 1\ldots d$, such that F is an exponentially stable equilibrium point for the PDE* (4)*. Toward this end, determine whether the following optimization problem admits a solution.*

$$\min_{a_{ij}} |\lambda_2(\hat{\mathcal{L}}_F)|$$

Due to the definition of the operator $\hat{\mathcal{L}}$, we need not impose the condition $\hat{\mathcal{L}}_F F = 0$ as a constraint. In Section V, we will characterize the eigenvalues of $\hat{\mathcal{L}}_F$ via the min-max principle, which is only true for a self-adjoint operator. We chose to work with divergence form operators in order to be able to characterize their eigenvalues via this principle.

IV. Analytical Properties of $\hat{\mathcal{L}}_F$

We begin by proving a few properties of the operator $\hat{\mathcal{L}}_F$; proofs for general functions F and general domains Ω are given in [7]. Therefore, only those parts of the proofs that are specific to our case are detailed below.

Proposition IV.1. *The operator $\hat{\mathcal{L}}_F$ is closed, densely defined, self-adjoint, and positive. Moreover, the operator $\hat{\mathcal{L}}_F$ has a purely discrete spectrum.*

Proof. First we prove that the bilinear form (3) is closed; that is, the space $\mathcal{D}(B_F) = H^1_F(\Omega)$ equipped with the norm $\|u\|_B = (\|u\|^2_F + B_F[u,u])^{1/2}$ for each $u \in \mathcal{D}(B_F)$ must be complete [22]. To see this, we note that by the uniform ellipticity condition on the coefficients a_{ij}, we have that

$$B_F[u,u] = \int_\Omega \left[\tfrac{\partial(u/F)}{\partial x}\right] A \left[\tfrac{\partial(u/F)}{\partial x}\right]^T \geq \int_\Omega \alpha \left|\frac{\partial(u/F)}{\partial x}\right|^2,$$

where $A = [a_{ij}]$. We also have that

$$\|A\|_\infty \int_\Omega \left|\frac{\partial(u/F)}{\partial x}\right|^2 \geq B_F[u,u].$$

Therefore, the norm $\|\cdot\|_B$ is equivalent to $\|u\|_{H^1_F}$. It has been shown in [7] that $H^1_F(\Omega)$ is complete. Therefore, B_F is closed.

Next, from [7], we can show that B_F is densely defined; that is, $\mathcal{D}(B_F)$ must be dense in $L^2_F(\Omega)$, which is true in this case. Furthermore, B_F is *symmetric*, that is, $B_F[u,v] = \overline{B_F[v,u]}$ for each $u,v \in \mathcal{D}(B_F)$, and B_F is *semibounded*, that is, $B_F[u,u] \geq m\|u\|^2_F$ for some $m \in \mathbb{R}$, for each $u \in \mathcal{D}(B_F)$. The latter property is true for $m = 0$. By Theorem 10.7 of [22], these properties imply that $\hat{\mathcal{L}}_F$ is self-adjoint, which further implies that $\hat{\mathcal{L}}_F$ is also closed and densely defined.

Finally, we have that $H^1_F(\Omega) = \mathcal{D}(B_F)$ equipped with the norm $\|\cdot\|_B$ is *compactly embedded* in $L^2(\Omega)$. By Proposition 10.6 of [22], this condition is sufficient for the operator $\hat{\mathcal{L}}_F$ to have a discrete spectrum. □

Proposition IV.2. *The spectrum of the operator $\hat{\mathcal{L}}_F$ satisfies $\sigma(\hat{\mathcal{L}}_F) \in (\infty, 0]$. Furthermore, 0 is a unique eigenvalue of $\hat{\mathcal{L}}_F$.*

Proof. From the definition of the bilinear form, we observe that the operator $-\hat{\mathcal{L}}_F$ must be negative semidefinite. Hence, $\sigma(-\hat{\mathcal{L}}_F) \in (\infty, 0]$. Consider the bilinear form (3) with $F = \mathbf{1}$. In this case, it is clear that $\hat{\mathcal{L}}_{\mathbf{1}}\mathbf{1} = 0$; that is, $\mathbf{1}$ is an eigenvector corresponding to the eigenvalue 0. To prove the uniqueness of 0, we use the *Poincaré inequality* [9]: there exists a constant C such that $\int_\Omega |u(x) - u_\Omega| dx \leq C \int_\Omega |\nabla u(x)|^2$, where $u_\Omega = \frac{1}{m(\Omega)}\int_\Omega u(x)dx$, and $m(\Omega)$ stands for the Lebesgue measure of the set Ω. Using the uniform ellipticity condition and assuming that $\alpha \geq C$, we have that

$$\begin{aligned}\int_\Omega |u(x) - u_\Omega| dx &\leq \alpha \int_\Omega |\nabla u(x)|^2 \\ &\leq \alpha B_F[u,u] = \alpha \int_\Omega \left[\tfrac{\partial u}{\partial x}\right] A(x) \left[\tfrac{\partial u}{\partial x}\right]^T.\end{aligned} \tag{7}$$

If u is an eigenvector other than $\mathbf{1}$, then the right-hand side of the inequality above evaluates to 0 while the left-hand side is positive, leading to a contradiction. Therefore, the eigenvalue

0 must be unique. For general F we define the multiplication map $M_F : L^2(\Omega) \to L^2_F(\Omega)$ that takes a function $u \in L^2_F(\Omega)$ to $u/F \in L^2(\Omega)$. Note that $\hat{\mathcal{L}}_F = \hat{\mathcal{L}}_{\mathbf{1}} M_F$. From this observation we can infer that $\mathbf{1}$ is an eigenvector of $\hat{\mathcal{L}}_{\mathbf{1}}$ for the eigenvalue 0 if and only if F is an eigenvector of $\hat{\mathcal{L}}_F$.

In the case where $\alpha \leq C$, we can replace α by C/α in equation (7), and the analysis remains the same. □

Due to the lack of smoothness of the functions a_{ij} and F, the PDE (4) might not have solutions that are continuously differentiable in the classical sense, or even solutions that are weakly twice differentiable. Using the above properties, one can show that the PDE (4) has a *mild solution* [8], which can be represented as a *semigroup* of linear operators. This follows from the *Lumer-Phillips theorem* by noting that the operator $\hat{\mathcal{L}}_F$ is self-adjoint and dissipative. See [7] for details. Since $\mathcal{D}(\hat{\mathcal{L}}_F)$ is a subset of $H^1_F(\Omega)$, it follows that if the initial condition is in $\mathcal{D}(\hat{\mathcal{L}}_F)$, then the mild solution lies in $H^1_F(\Omega)$ for all time $t \geq 0$. One can also show that the semigroup is analytic, and hence has regularizing properties. This implies that even if the initial condition is known to be only in $L^2(\Omega)$, the solution of the PDE (4) lies in $H^1_F(\Omega)$ for all $t > 0$.

V. Formulation of the Optimization Problem

Recall the conditions on F, the desired density function: it is in $L^\infty(\Omega)$ and is strictly positive almost everywhere. We have established that F is a unique eigenvector of the operator $-\hat{\mathcal{L}}$ corresponding to the largest eigenvalue 0. Furthermore, we have showed the existence of a spectral gap of $\hat{\mathcal{L}}$. In this section, we solve Problem III.2.

The *Courant-Fisher min-max principle* provides a way to formulate the objective function of the optimization problem in Problem III.2. Let $(T, \mathcal{D}(T))$ be a lower-semibounded, self-adjoint operator on a Hilbert space H with a purely discrete spectrum. Let $(\lambda_n(T))_n$ be the increasing sequence of eigenvalues of T, counted with multiplicities. The min-max principle gives a variational characterization for the eigenvalues that are below the bottom of the essential spectrum [22]. Let E_k be a linear subspace of H of dimension k. Then the eigenvalues λ_k can be defined as:

$$\lambda_k(T) = \max_{E_k} \min_{\substack{v \in \mathcal{D}(T), \|v\|=1, \\ v \in E_k^\perp}} \langle Tv, v \rangle.$$

The inner product in this definition is called the Rayleigh quotient.

In our case, the operator $\hat{\mathcal{L}}_F$ satisfies the properties listed above, and therefore we can characterize the second largest eigenvalue of $\hat{\mathcal{L}}$ by restricting $\hat{\mathcal{L}}$ to the subspace obtained after removing the eigenspace F corresponding to the eigenvalue 0. The objective function is hence formulated as,

$$\lambda_2(-\hat{\mathcal{L}}_F) = \lambda_1(-\hat{\mathcal{L}}_F \circ \mathrm{Proj}_{F^\perp}) = \min_{\substack{v \in \mathcal{D}(\hat{\mathcal{L}}),\ \|v\|_F=1 \\ \int_\Omega v = 0}} \langle -\hat{\mathcal{L}}_F v, v \rangle_F. \tag{8}$$

Here $\mathrm{Proj}(\cdot)$ is the projection operator onto a subspace. We note that removing the negative sign changes the minimization problem to a maximization problem. Further, the outer optimization, that is, the maximization can be omitted, since $E_0 \subset \mathcal{D}(\mathcal{L})$ is just $\{0\}$. The integral constraint in the equation above represents the projection onto $F^\perp$. To see this, let $v \in F^\perp$; then $\langle v, F \rangle_F = 0$, and this is exactly the integral $\int_\Omega v = 0$.

The constraints of the optimization problem are listed below.

$$a_{ij} \leq c, \text{ for some } c > 0 \tag{9}$$

$$a_{ij} = a_{ji} \tag{10}$$

$$\sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j \geq \alpha|\xi|^2, \ \forall \xi \in \mathbb{R}^d. \tag{11}$$

Constraint (9) ensures that the coefficients are bounded in the L^∞ norm. Constraint (11) ensures that the coefficients satisfy the uniform ellipticity condition. Equations (8)-(11) formulate the optimization problem that we will solve in this paper.

The set of decision variables is given by

$$\mathscr{A} = \{(a_{ij}) \in (L^\infty(\Omega))^{d(d+1)/2} : a_{ij} \leq c$$
$$\sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j \geq \alpha|\xi|^2, \forall \xi \in \mathbb{R}^d, \ i,j \in 1 \ldots n\}, \tag{12}$$

where $d(d+1)/2$ is the number of upper triangular elements in the coefficient matrix.

In the next result we prove the continuity of eigenvalues of the operator $\hat{\mathcal{L}}_F$ with respect to the coefficients following the approach outlined in [14], where the authors consider the special case when $F = \mathbf{1}$.

Theorem V.1. *Let $\hat{\mathcal{L}}^n_F$ be the sequence of operators corresponding to a sequence of functions a^n_{ij} that is bounded in $L^\infty(\Omega)$ for each i and j, such that the functions converge almost everywhere to a function a_{ij} for each i and j. Let $\hat{\mathcal{L}}_F$ be the elliptic operator as defined in* (2) *by the functions a_{ij}. Then each eigenvalue of $\hat{\mathcal{L}}^n_F$ converges to the corresponding eigenvalue of $\hat{\mathcal{L}}_F$.*

Proof. From [14][Theorem 2.3.3] it is known that under the convergence conditions on the function a^n_{ij}, for each fixed $f \in L^2(\Omega)$, $(\hat{\mathcal{L}}^n_{\mathbf{1}})^{-1} f$ converges to $(\hat{\mathcal{L}}_{\mathbf{1}})^{-1} f$ in norm. To prove the result in our modified case we let $M_F : L^2(\Omega) \to L^2_F(\Omega)$ be the multiplication map that takes $u \in L^2_F\Omega$ to $u/F \in L^2(\Omega)$. Since $\hat{\mathcal{L}}^n_F = \hat{\mathcal{L}}^n_{\mathbf{1}} M_F$, we can infer that for each fixed $f \in L^2(\Omega)$, $(\hat{\mathcal{L}}^n_F)^{-1} f$ converges to $(\hat{\mathcal{L}}_F)^{-1} f$ in norm. From this, we can conclude that the resolvents of the operators $\hat{\mathcal{L}}^n_F$ strongly converge to the resolvent of the operator $\hat{\mathcal{L}}_F$ [14][Theorem 2.3.2]. The operators $\hat{\mathcal{L}}^n_F$ and $\hat{\mathcal{L}}_F$ have a compact resolvent since $H^1_F(\Omega)$ is compactly embedded in $L^2_F(\Omega)$. Therefore, it follows from [14][Theorem 2.3.1] that the eigenvalues of the operators $\hat{\mathcal{L}}^n_F$ converge to the respective eigenvalues of the operator $\hat{\mathcal{L}}_F$. □

VI. Numerical Optimization

In this section, we numerically solve the optimization problem. Instead of working with a discrete version of the operator $\hat{\mathcal{L}}_F$, we directly discretize the inner product in the objective function. Discretizing this inner product, rather than discretizing the operator $\hat{\mathcal{L}}$ and substituting it into the objective function, significantly reduces the computational complexity of solving the optimization problem. From the bilinear form (3), we have that for $u \in \mathcal{D}(\hat{\mathcal{L}}_F)$, $B_F[u,u] = \langle \hat{\mathcal{L}}_F u, u\rangle_F$. Therefore, the objective function can be recast as the following expression:

$$\langle -\hat{\mathcal{L}}_F u, u\rangle_F = -\int_\Omega \sum_{i,j=1}^{d} \left(a_{ij}(x) \frac{\partial(u/F)}{\partial x_j} \frac{\partial(u/F)}{\partial x_i} \right) dx \tag{13}$$

We demonstrate our numerical optimization procedure for a domain $\Omega \subset \mathbb{R}^2$. In this case, the above equation can be simplified to:

$$-\int_\Omega \begin{bmatrix} \frac{\partial v(x,y,t)}{\partial x} & \frac{\partial v(x,y,t)}{\partial y} \end{bmatrix} A(x,y) \begin{bmatrix} \frac{\partial v(x,y,t)}{\partial x} \\ \frac{\partial v(x,y,t)}{\partial y} \end{bmatrix} dxdy, \tag{14}$$

where $v = u/F$ and $A = [a_{ij}]$ is the coefficient matrix in $\mathbb{R}^{2\times 2}$.

In our example, we define $\Omega = [0,1]\times[0,1]$. We partition Ω into an $N \times N$ grid and define $h = 1/N$. Let I be the index set $\{1,\ldots,N\}$. Then $\Omega = \cup_{i,j\in I}\widetilde{\Omega}_{ij}$, where $\widetilde{\Omega}_{ij} = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]\times[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}]$ for $i,j \in I$. Let $w_{ij}(t) = v(x_i, y_j, t)$ be evaluated at the midpoint of each grid cell $\widetilde{\Omega}_{ij}$. Let $\widetilde{F}(i,j) = F(x_i, y_j)$. Note that we can remove the negative sign in the objective function (8) and pose the optimization problem as a maximization problem. The finite-dimensional optimization problem that is equivalent to (8)-(11) can be stated as:

$$\max_w \frac{1}{N^2} \sum_{i=1}^{N-1}\sum_{j=1}^{N-1} \begin{bmatrix} \frac{w_{i+1,j}-w_{i,j}}{h} \\ \frac{w_{i,j+1}-w_{i,j}}{h} \end{bmatrix}^T A(i,j) \begin{bmatrix} \frac{w_{i+1,j}-w_{i,j}}{h} \\ \frac{w_{i,j+1}-w_{i,j}}{h} \end{bmatrix} \tag{15}$$

subject to

$$\sum_{i,j}^{N} w_{ij}\widetilde{F}(i,j) = 0 \tag{16}$$

$$\|w\widetilde{F}\|_F^2 = \|w\sqrt{\widetilde{F}}\|_2^2 = 1 \tag{17}$$

$$\text{Equations (9)} - \text{(11)}$$

Constraint (16) ensures that the vector u (before discretization) is perpendicular to F. Constraint (17) ensures that the weighted 2-norm of u is 1. The objective function (15) is nonlinear. Further, it is difficult to prove that it is convex. Therefore, the nonlinear optimization solver KNITRO [20] was used to solve this problem. This solver implements both interior-point and active-set methods for solving nonlinear optimization problems. The problem was solved in AMPL (A Mathematical Programming Language) [10]. We ran two test cases, described below.

In the first case, F was defined as the uniform distribution $\mathbf{1}$. Four different grid sizes $N \times N$ and two different values of c, $c = 1$ and $c = 10$, were tested. The eigenvalue $-\lambda_2$ was computed for each combination of grid size and c value, and the results are tabulated in Table I. This table shows that as the discretization becomes finer, the eigenvalue converges. Note that for $c = 1$, the computed eigenvalue, which is close to -12, yields a faster asymptotic convergence rate to the target distribution than the second-largest eigenvalue of the Neumann Laplacian, which is $-\pi^2 \approx -9.87$.

TABLE I

Eigenvalue $-\lambda_2$ for the case $F = \mathbf{1}$

$N \times N$	$c = 1$	$c = 10$
20×20	11.9	154.604
40×40	11.97	155.65
80×80	11.99	155.9
100×100	11.995	155.94

In the second case, F was defined as the non-uniform distribution $F = (\sin(2\pi i/N))^2 + (\sin(2\pi j/N))^2 + \epsilon$, where ϵ was chosen to be 0.1 to ensure strict positivity of F over Ω. In this case, we also investigate how the eigenvalue changes in magnitude with respect to the $L^\infty(\Omega)$ bound c on the parameters a_{ij}. Table II shows the eigenvalue $-\lambda_2$ that was computed for each combination of nine different grid sizes $N \times N$ and three different values of c, and Fig. 1 graphs the data in this table. We observe that the magnitude of the eigenvalue depends on the magnitude of the parameter c, and that the convergence rate of the eigenvalue in this case is much slower than in the case where $F = \mathbf{1}$.

TABLE II

Eigenvalue $-\lambda_2$ for the non-uniform F case

$N \times N$	$c = 1$	$c = 2$	$c = 5$
20×20	71.82	163.15	437.386
40×40	91.74	211.5	570.883
60×60	102.64	237.58	642.505
80×80	108.96	252.72	684.042
100×100	113.06	262.52	710.958
140×140	118.03	274.44	743.7
200×200	121.979	283.91	769.75
240×240	123.568	287.73	780.25
300×300	125.189	291.62	790.95

VII. Conclusion

In this paper, we have presented an approach to optimizing the rate at which a PDE generated by a divergence type operator converges to a desired function. The desired function must satisfy certain properties; namely, it must be bounded in the L^∞ norm and positive almost everywhere on the domain. Since the operator in this case is self-adjoint, the optimization problem can be posed exactly as the maximization of the modulus of the operator's second largest eigenvalue. We described a numerical procedure for solving this optimization problem and validated it for systems on a two-dimensional domain.

As future work, we plan to investigate the existence of an optimal solution to this problem. Demonstrating the existence of this solution would entail proving that the set of decision

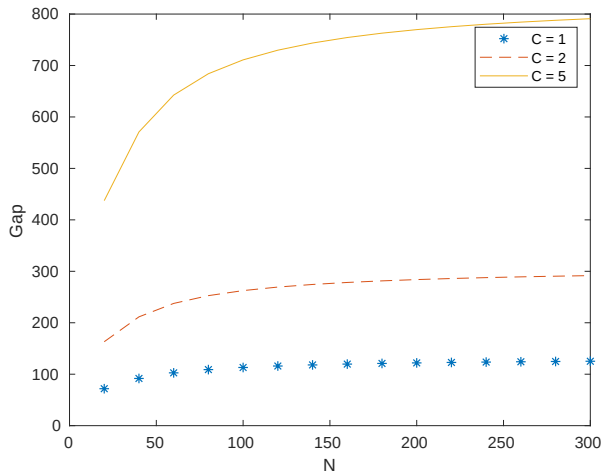

Fig. 1. Plots of the eigenvalue $-\lambda_2$ as a function of c and N for the non-uniform F case.

variables is compact in some topology and that the objective function is continuous on this set with respect to the chosen topology. Here, we have shown only that the eigenvalues of the operator vary continuously with respect to the coefficients of the operator.

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