Extremal functional determinants: progress in the Dirichlet and periodic cases

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Workshop on Optimal control theory
Rouen, June 2022

Motivation

Sturm-Liouville (Schrödinger) operators. Consider the 1D linear differential operator

$$T := \sum_{k=0}^{p} a_k(x) D^k, \quad D := -i\frac{\mathrm{d}}{\mathrm{d}x}$$

with domain $\mathrm{H}^p(0,1)$ (+ boundary conditions).

We are interested in the particular case of order $p = 2$ associated with a potential V,

$$T = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$$

with Dirichlet or periodic boundary conditions on $[0,1]$.

Motivation

Determinant. For smooth V, let $\lambda_1, \lambda_2, \ldots$ be the eigenvalues of T,

$$-u''(x) + V(x)u(x) = \lambda\, u(x), \quad x \in (0,1),$$

$$+ \text{ boundary conditions}$$

and define for $\mathrm{Re}(s) > 1/2$

$$\zeta_T(s) := \sum_{\lambda_j > 0} \frac{1}{\lambda_j^s}.$$

ζ_T has a meromorphic extension to the complex plane, regular at $s = 0$. After Ray-Singer'1971, define the determinant of T according to

$$\det T := \exp(-\zeta_T'(0)).$$

Remarks. (i) Equal to the product of eigenvalues when finitely many of them. (ii) Regularises the divergent infinite product.

Motivation

Theorem. (Levit-Smilansky'1977, Burghelea-Friedlander-Kappeler'1995) For a smooth potential V, for Dirichlet boundary conditions $\det T = 2y(1)$ where y is the solution of

$$-y''(x) + V(x)y(x) = 0, \quad x \in (0,1),$$
$$y(0) = 0, \quad y'(0) = 1.$$

Variational problem. Extremise the determinant wrt. the potential under various constraints (positivity, bounds...)

Remark. Contrary to other spectral problems (extremization of first or second eigenvalue, *e.g.*—see Harrell'1984), the problem is global (involves the whole spectrum).

Motivation

Extension to $\mathbf{L^1}$ potentials.

Lemma. The endpoint mapping $V \mapsto y(1)$ is well-defined and Lipschitz on bounded subsets of $L^1(0,1)$.

Proof. For $x := (y, y')$, write

$$x' = C(V)x, \quad x(0) = (0,1),$$

$$C(V) := \left[\begin{array}{cc} 0 & 1 \\ V & 0 \end{array} \right],$$

and use Gronwall to prove that

$$|x(1) - z(1)| \le e^{2(1+\rho)} \|V - W\|_1$$

where x is associated with $V \in L^1$ (*resp.* z with W), and $\|V\|_1$, $\|W\|_1 \le \rho$. $\square$

The determinant, that coincides with the endpoint mapping on smooth functions, has a unique continuous extension to L^1 (thus equal to the endpoint mapping).

Motivation

Theorem. For Dirichlet boundary conditions, existence and uniqueness of maximisers hold under L^q constraints, for all q in $[1, \infty]$.

In particular, (i) for $q = \infty$ the maximising potential is constant; (ii) for $q = 1$, there exists $\delta(A) \in (0, 1)$ (analytically depending on $A > 0$) such that the unique maximising potential is $A/\delta(A)$ times the characteristic function of the interval of length $\delta(A)$ centered at $1/2$.

- Aldana, C.; Caillau, J.-B.; Freitas, P. Maximal determinants of Schrödinger operators on bounded intervals. *J. Ec. polytech. Math.* **7** (2020), 803–829.

Open questions. (i) Minimisation for Dirichlet BC (ongoing work)
(ii) Extremisation for periodic boundary conditions (change of geometry)

Main result

Theorem. For periodic boundary conditions, existence and uniqueness of maximisers and minimisers hold under L^∞ constraints.

Outline.

- Determinant on the circle (after Burghelea-Friedlander-Kappeler'91)
- Maximisation, minimisation

Determinant on the circle

Theorem. (Burghelea-Friedlander-Kappeler'1991) For periodic boundary conditions,

$$\det T = -\det(I_2 - X(1))$$

where $X(1)$ is the monodromy of the system

$$X'(x) = \begin{bmatrix} 0 & 1 \\ V(x) & 0 \end{bmatrix} X(x), \quad X(0) = I_2.$$

The state X lives in the Lie group $SL(2, \mathbf{R})$ so

$$\det T = -(1 - \operatorname{tr} X(1) + \det X(1)) = \operatorname{tr} X(1) - 2.$$

As a result we have a bilinear optimal control problem on $SL(2, \mathbf{R})$:

$$\operatorname{tr} X(1) \to \max \text{ or } \min, \quad |V| \le A \text{ a.e. on } [0, 1].$$

Maximisation

The trace of the monodromy is equal to $z(1)+y'(1)$ where

$$-z''+V(x)z=0, \quad z(0)=1, \quad z'(0)=0,$$

$$-y''+V(x)y=0, \quad y(0)=0, \quad y'(0)=1.$$

Proposition. Let V_1 and V_2 be two potentials in $L^1_{\mathrm{loc}}(\mathbf{R}_+)$, $V_1 \geq |V_2|$ a.e., and let y_1 and y_2 satisfy

$$-y_i''+V_i(x)y_i=0, \quad i=1,2.$$

If $y_1(0) \geq |y_2(0)|$ and $y_1'(0) \geq |y_2'(0)|$, then $y_1(x) \geq |y_2(x)|$ and $y_1'(x) \geq |y_2'(x)|$ for all $x \geq 0$.

Maximisation

Proof. (i) First assume V_1 and V_2 constant, $V_1 \equiv A$ and $V_2 \equiv B$ with A and B two reals such that $A \geq |B|$. One has

$$y_1(x) = y_1(0)\cosh(\alpha x) + xy_1'(0)\mathrm{sinhc}(\alpha x)$$

where $\alpha = \sqrt{A}$, and where we denote $\mathrm{sinhc}(x) = \sinh(x)/x$ if $x \neq 0$, $\mathrm{sinhc}(0) = 1$. If B is nonnegative, let $\beta := \sqrt{B} \leq \alpha$; one has

$$\begin{aligned} |y_2(x)| &= |y_2(0)\cosh(\beta x) + xy_2'(0)\mathrm{sinhc}(\beta x)| \\ &\leq |y_2(0)|\cosh(\beta x) + x|y_2'(0)|\mathrm{sinhc}(\beta x) \\ &\leq y_1(0)\cosh(\alpha x) + xy_1'(0)\mathrm{sinhc}(\alpha x) = y_1(x) \end{aligned}$$

for $x \geq 0$ since both cosh and sinhc are nondecreasing functions on $\mathbf{R}_+$ (and $\beta \leq \alpha$). Similarly, for $x \geq 0$,

$$\begin{aligned} |y_2'(x)| &= |\beta y_2(0)\sinh(\beta x) + y_2'(0)\cosh(\beta x)| \\ &\leq \alpha y_1(0)\sinh(\alpha x) + y_1'(0)\cosh(\alpha x) = y_1'(x). \end{aligned}$$

Same argument for negative B.

Maximisation

Proof (continued). (ii) Take now some positive x, and assume V_1 and V_2 are piecewise constant on $[0,x]$; there exists a common subdivision $0 = x_0 < x_1 < \ldots < x_N = x$, $N \geq 1$, such that on every $[x_i, x_{i+1}[$ both V_1 and V_2 are constant, with $V_1 \geq |V_2|$. A simple recurrence using step (i) allows to conclude that $y_1(x) \geq |y_2(x)|$ and $y_1'(x) \geq |y_2'(x)|$.

(iii) Pass to the limit for general locally integrable potentials using the fact that, for all $x > 0$, the mapping $V \mapsto (y(x), y'(x))$ (where y is the solution of $-y'' + Vy = 0$, $y(0) = y_0$, $y'(0) = y_0'$) is continuous from $L^1(0,x)$ to $\mathbf{R}^2$. $\square$

Corollary. For V in $L^\infty(0,1)$, let y and z denote the solutions of

$$-y'' + V(x)y = 0, \quad y(0) = 0, \quad y'(0) = 1,$$

$$-z'' + V(x)z = 0, \quad z(0) = 1, \quad z'(0) = 0.$$

Then, for any positive bound A, the constant potential $V \equiv A$ is the unique function maximising both $y(1)$, $y'(1)$, $z(1)$ and $z'(1)$ over essentially bounded potentials such that $\|V\|_\infty \leq A$.

Theorem. The unique maximiser of the determinant on the circle is the constant potential $V \equiv A$.

Minimisation

Let us now minimise $\operatorname{tr} X(1)$ under the constraints

$$X'(x) = F_0 X(x) + V F_1 X(x), \quad |V(x)| \leq A,$$

$$X(0) = I_2,$$

with linear vector fields

$$F_0 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad F_1 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \in sl(2, \mathbf{R}).$$

As for maximisation, existence holds (Filippov). Pontrjagin Maximum Principle ensures that any minimising potential V is associated with some $P : [0,1] \to M(2, \mathbf{R})$, $P(x) \in T_{X(x)} SL(2, \mathbf{R})$, such that

$$P'(x) = -\nabla_X H(X(x), P(x), V(x)), \quad P(1) = -I_2,$$

where the Hamiltonian in Mayer form is

$$H(X, P, V) = H_0(X, P) + V H_1(X, P), \quad H_i(X, P) = (P|F_i X), \quad i = 0, 1,$$

and the maximisation condition holds a.e.:

$$H(X(x), P(x), V(x)) = \max_{|W| \leq A} H(X(x), P(x), W).$$

Minimisation

Lemma. Minimising potentials are bang-bang.

Sketch of proof. Notice that

$$F_0 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad F_1 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \text{ and } F_{01} = [F_0, F_1] = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

form an sl_2-triple as (dim 3 Lie algebra)

$$F_{001} = [F_0, F_{01}] = -2F_0, \quad F_{101} = [F_1, F_{01}] = 2F_1.$$

Since

$$\dot{H}_1 = H_{01}, \quad \dot{H}_{01} = H_{001} + VH_{101},$$

singular arcs are excluded, and switchings must be of order 1 or 2. As a result, switching points are isolated. $\square$

Remark. The problem is well-posed for controls in $L^\infty(\mathbf{S}^1)$ (invariance by translation). In particular, switchings come in pair.

Theorem. For any ess. bound A, there is a unique minimising potential in $L^\infty(\mathbf{S}^1)$: (i) for $A \leq \pi^2$, the minimising potential is constant, $V \equiv -A$ (ii) for $A > \pi^2$, the minimising potential has exactly two switchings, and $V \equiv A$ on a subarc of $\mathbf{S}^1$ whose length depends analytically on A.

Conclusion and ongoing work

- Complete solution on the circle in the L^∞ case
- Compare with minimisers for Dirichlet boundary conditions (ongoing, L^q constraints with $q \in [1, \infty])$
- Matrix potential on the circle (dimension $N \geq 1$)
- Open questions: are optimal potentials symmetric, or even diagonal?

$$T = -I_N \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \quad V(x) \in M_N(\mathbf{R}), \quad x \in \mathbf{S}^1$$

References

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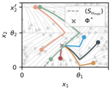
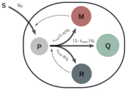
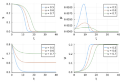


Bistable gene-regulatory networks



Optimal resource allocation in microbial growth



Biomass maximization with substrate depletion

- ct.gitlabpages.inria.fr/gallery

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Direct solve

[1]:

```julia
using JuMP, Ipopt, Plots, MINPACK

#JuMP model, Ipopt solver
sys = Model(optimizer_with_attributes(Ipopt.Optimizer,"print_level"=> 5))
set_optimizer_attribute(sys,"tol",1e-8)
set_optimizer_attribute(sys,"constr_viol_tol",1e-6)
set_optimizer_attribute(sys,"max_iter",1000)

# Parameters
Cd = 310.0
Tmax = 3.5
β = 500.0
b = 2.0
N = 100
t0 = 0.0
r0 = 1.0
v0 = 0.0
vmax = 0.1
m0 = 1.0
x0 = [ r0, v0, m0 ]
mf = 0.6

# Variables (some state constraints have been added to ease convergence)
@variables(sys, begin
    0.0 ≤ Δt                    # time step (unknown as tf is free)
    r[1:N+1] ≥ r0               # r
    0 ≤ v[1:N+1] ≤ vmax         # v
    mf ≤ m[1:N+1] ≤ m0          # m
    0.0 ≤ u[1:N+1] ≤ 1.0        # u
end)

# Objective
@objective(sys, Max, r[N+1])

# Boundary constraints
@constraints(sys, begin
    con_r0, r[1] == r0
    con_v0, v[1] == v0
    con_m0, m[1] == m0
end)

# Dynamics
@NLexpressions(sys, begin
    # D = Cd v^2 exp(-β(r-1))
    D[i = 1:N+1], Cd * v[i]^2 * exp(-β * (r[i] - 1.0))
    # r'= v
    dr[i = 1:N+1], v[i]
    # v' = (Tmax.u-D)/m - 1/r^2
    dv[i = 1:N+1], (Tmax*u[i]-D[i])/m[i] - 1/r[i]^2
    # m' = -b.Tmax.u
    dm[i = 1:N+1], -b*Tmax*u[i]
end)

# Crank-Nicolson scheme
@NLconstraints(sys, begin
    con_dr[i = 1:N], r[i+1] == r[i] + Δt * (dr[i] + dr[i+1])/2.0
    con_dv[i = 1:N], v[i+1] == v[i] + Δt * (dv[i] + dv[i+1])/2.0
    con_dm[i = 1:N], m[i+1] == m[i] + Δt * (dm[i] + dm[i+1])/2.0
end)
```

Indirect solve

[4]:

```julia
include("flow.jl")

# Dynamics
function F0(x)
    r, v, m = x
    D = Cd * v^2 * exp(-β*(r-1.0))
    F = [ v, -D/m-1.0/r^2, 0.0 ]
    return F
end

function F1(x)
    r, v, m = x
    F = [ 0.0, Tmax/m, -b*Tmax ]
    return F
end

# Computation of singular control of order 1
H0(x, p) = p' * F0(x) # passer en H0(x, p) =
H1(x, p) = p' * F1(x)
H01 = Poisson(H0, H1)
H001 = Poisson(H0, H01)
H101 = Poisson(H1, H01)
us(x, p) = -H001(x, p)/H101(x, p)

# Computation of boundary control
c(x) = x[2]-vmax # v - vmax ≤ 0
ub(x) = -Lie(F0, c)(x) / Lie(F1, c)(x)
μb(x, p) = -H01(x, p) / Lie(F1, c)(x)

# Hamiltonians (regular, singular, boundary) and associated flows
H(x, p, u, μ) = H0(x, p) + u*H1(x, p) - μ*c(x)
Hr(x, p) = H(x, p, 1.0, 0.0)
Hs(x, p) = H(x, p, us(x, p), 0.0)
Hb(x, p) = H(x, p, ub(x), μb(x, p))

f0 = Flow(H0)
fr = Flow(Hr)
fs = Flow(Hs)
fb = Flow(Hb);
```

[5]:

```julia
# Shooting function
function shoot(p0, t1, t2, t3, tf) # B+ S C B0 structure

    x1, p1 = fr(t0, x0, p0, t1)
    x2, p2 = fs(t1, x1, p1, t2)
    x3, p3 = fb(t2, x2, p2, t3)
    xf, pf = f0(t3, x3, p3, tf)
    s = zeros(eltype(p0), 7)
    s[1:2] = pf[1:2] - [ 1.0, 0.0 ]
    s[3] = xf[3] - mf # supposed to be active
    s[4] = H1(x1, p1)
    s[5] = H01(x1, p1)
    s[6] = c(x2)
    s[7] = H0(xf, pf) # free tf

    return s

end
```

- Numerics for finite-dimensional optimal control problems, preprint (Caillau, J.-B.; Ferretti, R.; Trélat, E.; Zidani, H.)

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