Využitie duality v (ne)konvexnom programovaní na riešenie inverzného Wulffovho problému

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(Seminár) Aká si mi krásna v Banskej Bystrici

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Bagatella

Overture Optimization problem

Intermezzo Isoperimetric inequality, snowflakes and anisotropy

1 Act Quadratic optimization problem with linear matrix inequality constraints

2 Act Enhanced semidefinite relaxation method as the second dual to the Quadratic - linear augmented problem

3 Act Equivalence of the augmented primal and second dual problems

Finale Application of ESR method to the Inverse Wulff problem

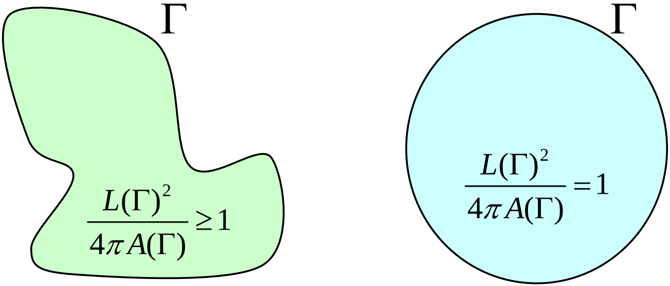
Optimization problem

$$\begin{aligned} \min_{x} \quad & x^T P_0 x + 2q_0^T x + r_0 \\ \text{s.t.} \quad & x^T P_l x + 2q_l^T x + r_l \le 0, \quad l = 1, \ldots, d, \\ & Ax = b, \\ & H_0 + \textstyle\sum_{j=1}^{n} x_j H_j \succeq 0 \end{aligned}$$

- $x \in \mathbb{R}^n$ is the variable
- data: $P_0, P_l \in \mathcal{S}^n$ are $n \times n$ real symmetric matrices
- $q_0, q_l \in \mathbb{R}^n$, $r_0, r_l \in \mathbb{R}$
- A is an $m \times n$ real matrix, $b \in \mathbb{R}^m$
- $H_0, H_1, \ldots, H_n \in \mathcal{H}^k$ are $k \times k$ complex Hermitian matrices.

The last constraint is a complex linear matrix inequality (LMI)

Isoperimetric inequality



$L(\Gamma)$ length of Γ $\quad$ $A(\Gamma)$ area enclosed by Γ

" . . . **the greatest plane figure of all those which have a given perimeter is the circle."**

Pappus of Alexandria (AD 290 – 350)

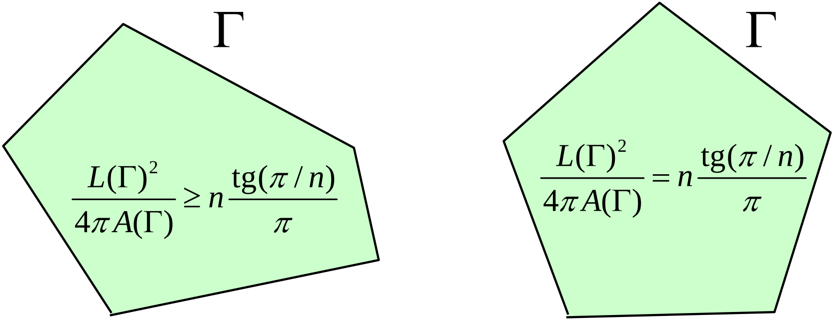

PAPPI
ALEXANDRINI
MATHEMATICAE
Collectiones.
A FEDERICO
COMMANDINO
VRBINATE
In Latinum Conuersæ, & Commentarijs
Illustratæ.

VENETIIS,
Apud Franciscum de Franciscis Senensem.
M. D. LXXXIX.

History of Isoperimetric inequality

"Bees, then, know just this fact which is useful to them, that the hexagon is greater than the square and the triangle and will hold more honey for the same expenditure of material used in constructing the different figures."

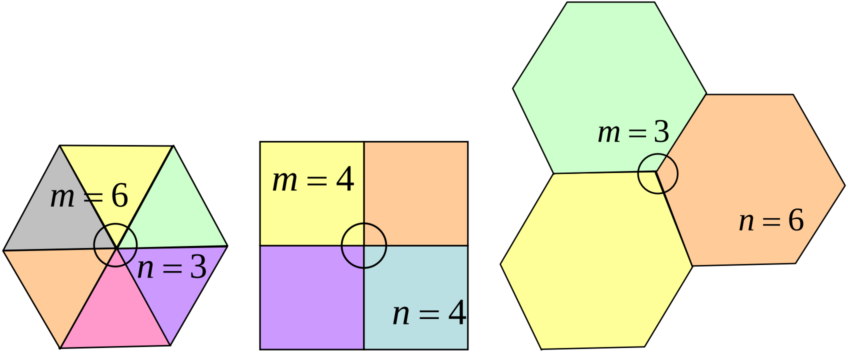
Discrete Isoperimetric inequality



$L(\Gamma)$ length of Γ $\quad$ $A(\Gamma)$ area enclosed by Γ

$$\frac{L^2}{4\pi A} \geq \frac{\tan(\pi/n)}{\pi/n}$$

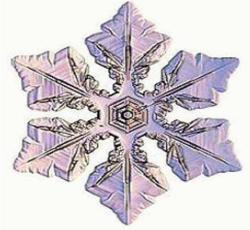
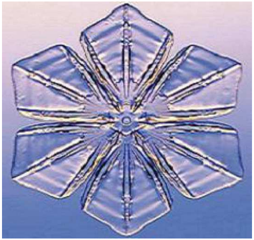
Isoperimetric inequality vs Optimal packing problem



$$2\pi = m\left(\pi - \frac{2\pi}{n}\right) \Rightarrow n = \frac{2m}{m-2}$$

$$m = 3, 4, 6$$

Isoperimetric ratios for hexagonal Bentley's snowflakes

$$\frac{L^2}{4\pi A} = 36.5 \qquad \frac{L^2}{4\pi A} = 8.49 \qquad \frac{L^2}{4\pi A} = 6.62$$

Isoperimetric ratios computed by Zosia Oravcová, 2012.

The interfacial energy functional and the Wulff shape

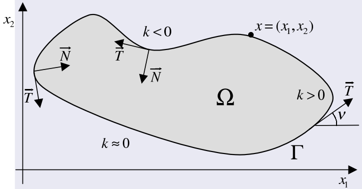
From Euclidean curve length to Finsler relative metric curve length

$$L(\Gamma) = \int_\Gamma ds$$

$$\Downarrow$$

$$L_\sigma(\Gamma) = \int_\Gamma \sigma(\nu)\, ds$$

- $\sigma(\nu)$ is the anisotropy function, ν is the tangent vector (σ corresponds to the relative Finsler geometry of the plane)
- $\mathbf{t} = (\cos(\nu), \sin(\nu))^T, \quad \mathbf{n} = (-\sin(\nu), \cos(\nu))^T$



v is the normal velocity
k is the curvature of Γ at $x \in \Gamma$
ν is the tangent angle of Γ at $x \in \Gamma$

Isoperimetric and Anisoperimetric Wulff problem

Find a plane closed Jordan curve Γ, minimizing the anisoperimetric ratio

$$\min_{\Gamma} \frac{L(\Gamma)^2}{4\pi A(\Gamma)} \qquad \min_{\Gamma} \frac{L_\sigma(\Gamma)^2}{4|W_\sigma|A(\Gamma)}$$

The anisotropy function σ is given

Anisoperimetric ratio

$$\Pi_\sigma(\Gamma) := \frac{L_\sigma(\Gamma)^2}{4|W_\sigma|A(\Gamma)}, \qquad \Longrightarrow \Pi_\sigma(\Gamma) \geq 1, \quad \Pi_\sigma(\partial W_\sigma) = 1$$

The minimizer of $\Pi_\sigma(\Gamma)$ is a curve $\Gamma \propto \partial W_\sigma$ of the Wulff shape

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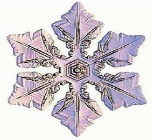
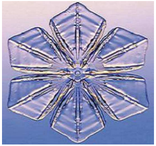
* G. Wulff, “Zür Frage der Geschwindigkeit des Wachstums und der Auflösung der Kristallfläschen”, *Zeitschrift für Kristallographie*, Vol. 34, pp. 449–530, 1901.
* A. Dinghas, “Über einen geometrischen Satz von Wulff für die Gleichgewichtsform von Kristallen”, *Zeitschrift für Kristallographie*, Vol. 105, pp. 304–314, 1944.
* DS and S.Yazaki: On a gradient flow of plane curves minimizing the anisoperimetric ratio, *IAENG Journal of Appl. Mathematics, 43(3) 2013, 160-171*

Inverse Wulff problem statement

Given a plane Jordan curve Γ, find the optimal anisotropy function σ minimizing the anisoperimetric ratio for Γ

$$\min_{\sigma} \frac{L_{\sigma}(\Gamma)^2}{4|W_{\sigma}|A(\Gamma)}$$

under the constraint the Wulff shape W_σ is convex ($\sigma \in \mathcal{K}$ - cone)

What is the optimal anisotropy function σ for those snowflakes?

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* DS, M.Trnovská: Solution to the Inverse Wulff Problem by Means of the Enhanced Semidefinite Relaxation Method, Journal of Inverse and Ill Posed Problems, 2014, www.arxiv.org/abs/1402.5668

General Quadratic optimization problem with LMI

$$\begin{aligned}
\min_{x} \quad & x^T P_0 x + 2q_0^T x + r_0 \\
\text{s.t.} \quad & x^T P_l x + 2q_l^T x + r_l \leq 0, \quad l = 1, \dots, d, \\
& Ax = b, \\
& H_0 + \textstyle\sum_{j=1}^{n} x_j H_j \succeq 0
\end{aligned}$$

- $x \in \mathbb{R}^n$ is the variable
- data: $P_0, P_l \in \mathcal{S}^n$ are $n \times n$ real symmetric matrices
- $q_0, q_l \in \mathbb{R}^n$, $r_0, r_l \in \mathbb{R}$
- A is an $m \times n$ real matrix, $b \in \mathbb{R}^m$
- $H_0, H_1, \dots, H_n \in \mathcal{H}^k$ are $k \times k$ complex Hermitian matrices.

The last constraint is a complex linear matrix inequality (LMI)

Quadratic-linear (Q-L) enhancement of linear constraints

$$\begin{aligned} \hat{p}_1 := \min_x \quad & x^T P_0 x + 2q_0^T x + r_0 \\ \text{s.t.} \quad & x^T P_l x + 2q_l^T x + r_l \leq 0, \quad l = 1, \dots, d, \\ & Ax = b, \\ & A\, xx^T = bx^T, \\ & H_0 + \sum_{j=1}^n x_j H_j \succeq 0 \end{aligned}$$

- Equality $Ax = b$ is augmented with quadratic-linear constraint $A\, xx^T = bx^T$.

Idea of semidefinite relaxation

$$x^T P x = tr(PX)$$

where

$$X = xx^T$$

is a matrix and $tr(PX)$ is a trace of the product PX, i.e. the Frobenius inner product of matrices P and X

SDP relaxation

Replace (relax) nonconvex constraint $X = xx^T$
by a convex constraint $X \succeq xx^T$

Systematic way of derivation of the SDP relaxation is based

- on construction of the second Lagrangian dual problem
- showing equivalence between optimal values of the primal and second dual problem

Primal augmented problem

$$
\begin{aligned}
\hat{p}_1 := \min_{x} \quad & x^T P_0 x + 2q_0^T x + r_0 \\
\text{s.t.} \quad & x^T P_l x + 2q_l^T x + r_l \le 0, \quad l = 1, \dots, d, \\
& Ax = b, \\
& A\,xx^T = bx^T, \\
& H_0 + \textstyle\sum_{j=1}^n x_j H_j \succeq 0
\end{aligned}
$$

Dual augmented problem

$$
\begin{aligned}
\hat{p}_2 := \min_{x,X} \quad & \mathrm{tr}(P_0 X) + 2q_0^T x + r_0 \\
\text{s. t.} \quad & \mathrm{tr}(P_l X) + 2q_l^T x + r_l \le 0, \quad l = 1, \dots, d, \\
& Ax = b, \\
& AX = bx^T, \\
& X \succeq xx^T \\
& H_0 + \textstyle\sum_{j=1}^n x_j H_j \succeq 0
\end{aligned}
$$

First Lagrangian dual

Lagrangian function $\mathcal{L}^1 = \mathcal{L}^1(x; \lambda, u, V, Z)$:

$$\begin{aligned}
\mathcal{L}^1 &= x^T P_0 x + 2q_0^T x + r_0 \\
&\quad + \sum_{l=1}^{d} \lambda_l [x^T P_l x + 2q_l^T x + r_l] \\
&\quad + u^T (Ax - b) + \underbrace{\operatorname{tr}(V^T (Axx^T - bx^T)}_{V \bullet (Axx^T - bx^T)} \\
&\quad \underbrace{- \operatorname{tr}(Z^T (H_0 + \sum_{j=1}^{n} x_j H_j))}_{Z \bullet (H_0 + \sum_{j=1}^{n} x_j H_j)},
\end{aligned}$$

where $0 \leq \lambda \in \mathbb{R}^d, u \in \mathbb{R}^n$, V is an $m \times n$ real matrix and Z is a $k \times k$ Hermitian matrix

$$\inf_x \mathcal{L}^1(x; \lambda, u, V, Z)$$

The first Lagrangian dual

$$\begin{array}{rl} \hat{d}_1 := \max & \gamma \\ \text{s. t.} & M_0 + \sum_{l=1}^{d} \lambda_l M_l + M_*(V, u) - \sum_{j=0}^{n} z_j N_j - \gamma N_0 \succeq 0, \\ & Z \succeq 0, \ \ \lambda \geq 0, \\ & z_j = \mathrm{tr}(Z^T \tilde{H}_j), \ \ j = 0, 1, \ldots, n. \end{array}$$

Here we have denoted

$$M_j = \begin{pmatrix} P_l & q_l \\ q_l^T & r_l \end{pmatrix}, \ M_*(V, u) = \frac{1}{2} \begin{pmatrix} V^T A + A^T V & A^T u - V^T b \\ u^T A - b^T V & -2u^T b \end{pmatrix},$$

$$N_0 = \begin{pmatrix} 0_{n\times n} & 0_n \\ 0_n^T & 1 \end{pmatrix}, \quad N_j = \frac{1}{2} \begin{pmatrix} 0_{n\times n} & e_j \\ e_j^T & 0 \end{pmatrix},$$

Second Lagrangian dual

Define $\mathcal{L}^2(\gamma, \lambda, Z, V, u, z; W, \beta, \tilde{X}, \alpha)$ function as follows:

$$\begin{aligned}\mathcal{L}^2 \;=\;& \gamma + \mathrm{tr}(ZW) + \lambda\beta + \mathrm{tr}(\tilde{X}(M_0 + \sum_{l=1}^{d} \lambda_l M_l + M_*(u, V) \\ & - \sum_{j=0}^{n} z_j N_j - \gamma N_0)) + \sum_{j=0}^{n} \alpha_j (z_j - \mathrm{tr}(Z^* H_j))\end{aligned}$$

with dual variables

$W \succeq 0, \tilde{X} = \begin{pmatrix} X & x \\ x^T & \varphi \end{pmatrix} \succeq 0,\ \beta \geq 0,\ \alpha_j \in \mathbb{R},\ j = 0, 1, \ldots, n.$

$$\sup_{\gamma,\lambda,Z,V,u,z} \mathcal{L}^2(\gamma, \lambda, Z, V, u, z; W, \beta, \tilde{X}, \alpha).$$

$$\begin{array}{rl} \min & \mathrm{tr}(P_0 X) + 2q_0^T x + r_0 \\ \text{s. t.} & \mathrm{tr}(P_l X) + 2q_l^T x + r_l \leq 0, \quad l = 1, \ldots, d, \\ & Ax = b,\ AX = bx^T,\ X \succeq xx^T, \\ & H_0 + \sum_{j=1}^{n} x_j H_j \succeq 0. \end{array}$$

Semidefinite relaxation of a nonconvex quadratic problem

$$
\begin{aligned}
\hat{p}_2 := \min_{x,X} \quad & \mathrm{tr}(P_0 X) + 2q_0^T x + r_0 \\
\text{s. t.} \quad & \mathrm{tr}(P_l X) + 2q_l^T x + r_l \leq 0, \quad l = 1, \ldots, d, \\
& Ax = b, \\
& AX = bx^T, \\
& X \succeq xx^T \\
& H_0 + \textstyle\sum_{j=1}^{n} x_j H_j \succeq 0
\end{aligned}
$$

- The semidefinite relaxation constraint $X \succeq xx^T$ can be rewritten using Schur complement theorem as:

$$
\begin{pmatrix} X & x \\ x^T & 1 \end{pmatrix} \succeq 0
$$

- Shor type of Q-L enhancement allows for convexification of the problem on the contrained set $Ax = b$

Equivalence of problems (harder part)

Lemma

Let $M \succeq 0$ and $X \succeq xx^T$. Then $\mathrm{tr}(MX) \geq x^T Mx$.

Assumption (A)

$P_l \succeq 0$ for $l = 1, \ldots, d$ and there exists a real $m \times n$ matrix V such that

$$M \equiv P_0 + \frac{1}{2}(V^T A + A^T V) \succeq 0.$$

Let (x, X) be a feasible solution to the 2nd dual. Then

$$x^T P_l x + 2q_l^T x + r_l \leq \mathrm{tr}(P_l X) + 2q_l^T x + r_l \leq 0, \quad l = 1, \ldots, d.$$

Hence x is a feasible solution to the primal problem

$$\mathrm{tr}((V^T A + A^T V)(X - xx^T)) = 2\mathrm{tr}(V^T (AX - Axx^T)) = 0$$

for any (x, X) feasible to 2nd dual. By Lemma we have $x^T P_0 x + 2q_0^T x + r_0 \leq \mathrm{tr}(P_0 X) + 2q_0^T x + r_0$. Hence $\hat{p}_1 \leq \hat{p}_2$.

Equivalence of problems (easier part)

- Let x be feasible for primal problem.
- Then the pair (x, X) where $X = xx^T$ is feasible for the 2nd dual
- Since $x^T P_j x = \text{tr}(P_j xx^T), j = 0, 1, \ldots, d$

$$\hat{p}_2 = \min_{(x,X)} \text{tr}(P_0 X) + 2q_0^T x + r_0 \leq x^T P_0 x + 2q_0^T x + r_0$$

- $$\hat{p}_2 \leq \min_x x^T P_0 x + 2q_0^T x + r_0 = \hat{p}^1$$
- Hence $\hat{p}_2 \leq \hat{p}_1$ and so $\hat{p}_2 \equiv \hat{p}_1$

Application to the Inverse Wulff problem

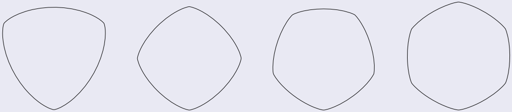
The interfacial energy functional and the Wulff shape

$$L_\sigma(\Gamma) = \int_\Gamma \sigma(\nu)\, ds$$

$$W_\sigma = \bigcap_{\nu \in [0,2\pi]} \left\{ \mathbf{x} \in \mathbb{R}^2,\ -\mathbf{x}^T \mathbf{n} \le \sigma(\nu) \right\}.$$

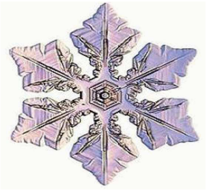
$$\partial W_\sigma = \left\{ \mathbf{x}\ | \mathbf{x} = -\sigma(\nu)\mathbf{n} + \sigma'(\nu)\mathbf{t},\ \nu \in [0, 2\pi] \right\}.$$

- $\mathbf{t} = (\cos(\nu), \sin(\nu))^T, \quad \mathbf{n} = (-\sin(\nu), \cos(\nu))^T$
- the curvature is given by $\kappa = [\sigma(\nu) + \sigma''(\nu)]^{-1}$ on ∂W_σ
- $\sigma \equiv const$ means that the Wulff shape W_σ is a circle

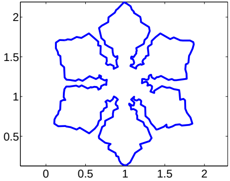


$m = 3$ $m = 4$ $m = 5$ $m = 6$

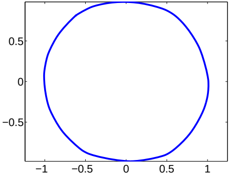
Wulff shape corresponding to $\sigma(\nu) = 1 + \varepsilon \cos(m\nu)$ and $\varepsilon \le 1/(m^2 - 1)$.



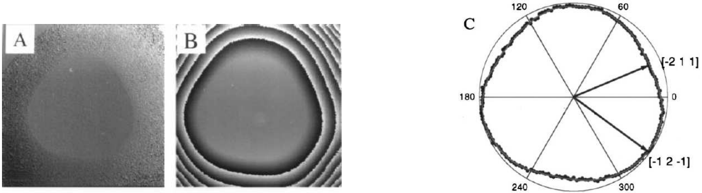
Hexagonal snowflake



Contour curve Γ



Expected hexagonal Wulff shape



a three-fold anisotropy function can be found as a shape of the (111) facet of Pb particles, prepared and equilibrated on Cu(111) under ultrahigh vacuum conditions

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* K. Arenhold, et al.(1998): Scanning tunneling microscopy of equilibrium crystal shape of Pb particles: test of universality, Surface Science 417(2-3),160–165.

Application of ESR method to Inverse Wulff problem

Using the expression for the Wulff shape area

$$
\begin{aligned}
|W_\sigma| &= \frac{1}{2} L_\sigma(\partial W_\sigma) = \frac{1}{2}\int_\Gamma \sigma(\nu)\,ds = \frac{1}{2}\int_0^{2\pi} \sigma(\nu)[\sigma(\nu) + \sigma''(\nu)]\,d\nu \\
&= \frac{1}{2}\int_0^{2\pi} |\sigma(\nu)|^2 - |\sigma'(\nu)|^2\,d\nu
\end{aligned}
$$

Equivalent formulation of the inverse Wulff problem statement

Given a plane Jordan curve Γ, find the optimal anisotropy function $\sigma(\nu)$ minimizing the anisoperimetric ratio for Γ

$$
\min_{\sigma} \frac{1}{2}\int_0^{2\pi} |\sigma'(\nu)|^2 - |\sigma(\nu)|^2\,d\nu
$$

under the constraints: $L_\sigma(\Gamma) = L(\Gamma)$ and $\sigma \geq 0, \sigma + \sigma'' \geq 0$.

This is an nonconvex optimization problem, in general

Fourier series representation

- Let $\sigma : \mathbb{R} \to \mathbb{R}$ be a smooth 2π-periodic function. It can be represented by its complex Fourier series

$$\sigma(\nu) = \sum_{n=-\infty}^{\infty} \sigma_n e^{in\nu}, \quad \text{where } \sigma_n = \frac{1}{2\pi} \int_0^{2\pi} e^{-in\nu} \sigma(\nu) \mathrm{d}\nu$$

  are complex Fourier coefficients.
- Since $\sigma(\nu)$ is a real function we have $\sigma_{-n} = \bar{\sigma}_n$ for any $n \in \mathbb{Z}$ and $\sigma_0 \in \mathbb{R}$.

Positivess of Fourier series

What are necessary and sufficient conditions guaranteering non-negativity of the Fourier series?

Fourier series representation, Bochner theorem

Given $N \in \mathbb{N}$ let us construct the following circulant Toeplitz matrix

$$Q^N = \begin{pmatrix} \sigma_0 & \bar{\sigma}_1 & \cdots & \bar{\sigma}_{N-1} \\ \sigma_1 & \sigma_0 & \cdots & \bar{\sigma}_{N-2} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{N-1} & \sigma_{N-2} & \cdots & \sigma_0 \end{pmatrix}$$

i.e. $Q^N_{kj} = \sigma_{k-j}$. The matrix $Q = Q^N$ is Hermitian, $Q^* = Q$.

Bochner theorem

A complex Fourier series

$$\sigma(\nu) \equiv \sum_{n=-\infty}^{\infty} \sigma_n e^{in\nu} \geq 0$$

if and only if $Q^N \succeq 0$ is positive definite Hermitian matrix $\forall N \in \mathbb{N}$.

Analogously, $\sigma(\nu) + \sigma''(\nu) \equiv \sum_{n=-\infty}^{\infty}(1 - n^2)\sigma_n e^{in\nu} \geq 0$ if and only if $S^N \succeq 0$ is positive definite $\forall N \in \mathbb{N}$ where $S^N_{kj} = (1 - (k-j)^2)\sigma_{k-j}$

Fourier series representation, McLean theorem

McLean criterion for nonnegativity of partial F-series

Let $\sigma_0 \in \mathbb{R}, \sigma_k = \bar{\sigma}_{-k} \in \mathbb{C}$ for $k = 1, \ldots, N-1$. Then the finite Fourier series expansion

$$\sigma(\nu) = \sum_{k=-N+1}^{N-1} \sigma_k e^{ik\nu} \geq 0$$

if and only if there exists a p.s.d. Hermitian matrix $F \succeq 0$, such that

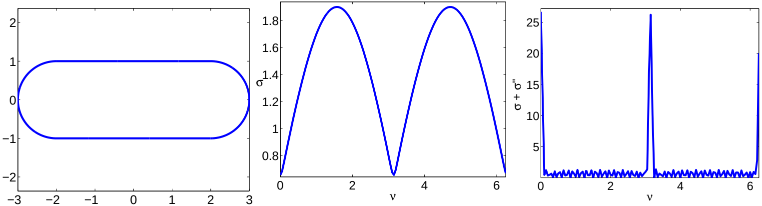
$$\sum_{p=k+1}^{N} F_{p,p-k} = \sigma_k,$$

for each $k = 0, 1, \ldots, N-1$

* J. W. McLean, H. J. Woerdeman (2001): Spectral Factorizations and Sums of Squares Representations via Semidefinite Programming, SIAM. J. Matrix Appl., 23(3)
* B. A. Dumitrescu (2007): Positive trigonometric polynomials and signal processing applications, Springer Verlag, New York, Berlin.

Fourier series representation, McLean theorem

- This criterion is a consequence of the classical Riesz-Fejer factorization theorem:
  a polynomial $p(\nu)$ is nonnegative iff it is a square of another polynomial, $p(\nu) = |q(\nu)|^2$ with complex coefficients



The capsule curve ∂W_σ. The functions $\sigma(\nu)$ and $\sigma(\nu) + \sigma''(\nu)$ containing 50 Fourier modes fulfilling McLean criterion for $N = 50$

Fourier series representation of the optimization problem

- The Wulff area representation

$$|W_\sigma| = \frac{1}{2}\int_0^{2\pi} |\sigma(\nu)|^2 - |\sigma'(\nu)|^2 d\nu = \pi \sum_{n=-\infty}^{\infty} (1-n^2)|\sigma_n|^2$$

- The interface energy

$$L_\sigma(\Gamma) = \int_\Gamma \sigma(\nu) ds = \sum_{n=-\infty}^{\infty} \bar{c}_n \sigma_n$$

where

$$c_n = \int_\Gamma e^{-in\nu} ds = \int_\Gamma (t_1 - it_2)^n ds$$

where $\mathbf{t} = (t_1, t_2)^T$ is a tangent vector to Γ.

- as the anisotropy function $\sigma(\nu)$ is real valued, thus

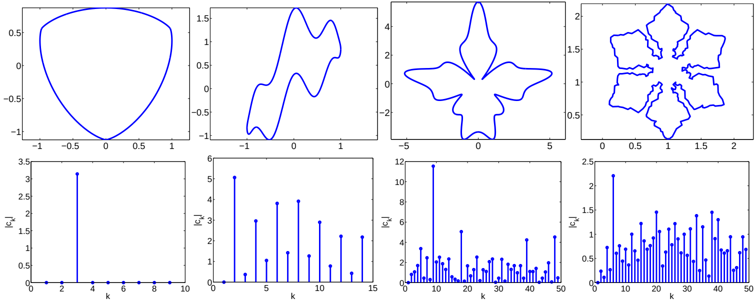
$$\sigma_0 = \frac{1}{2\pi}\int_0^{2\pi} \sigma(\nu) d\nu \in \mathbb{R}, \qquad \text{and} \quad \sigma_{-k} = \bar{\sigma}_k$$

Fourier length spectrum of a curve

Let Γ be a C^1 smooth (Jordan) curve in the plane. By the complex Fourier length spectrum of Γ we mean the set $\{c_k, k \in \mathbb{Z}\}$ of all Fourier complex coefficients defined as follows:

$$c_k = \int_\Gamma e^{-ik\nu} ds = \int_\Gamma (t_1 - it_2)^k ds \,,$$

$\mathbf{t} = (t_1, t_2)^T = (\cos(\nu), \sin(\nu))^T$ is the unit tangent vector to Γ.



DS, M.Trnovská: Solution to the Inverse Wulff Problem by Means of the Enhanced Semidefinite Relaxation Method, Journal of Inverse and Ill Posed Problems, 2014, www.arxiv.org/abs/1402.5668

Finite number Fourier modes approximation

Discretization with $N \in \mathbb{N}$ finite

$$\min_{\sigma} \sum_{k=-N+1}^{N-1} (k^2 - 1)|\sigma_k|^2$$

subject to:

$$\sum_{k=-N+1}^{N-1} \bar{c}_k \sigma_k = L(\Gamma)$$

$$\sum_{k=-N+1}^{N-1} \sigma_k e^{ik\nu} \geq 0$$

$$\sum_{k=-N+1}^{N-1} \sigma_k (1 - k^2) e^{ik\nu} \geq 0$$

- This is a nonconvex optimization problem (indefinite quadratic)

Nonconvex quadratic optimization problem with LMI

Realification of the problem for complex vector
$\sigma = (\sigma_0, \sigma_1, \cdots, \sigma_{N-1})^T \in \mathbb{C}^N \qquad x = [\Re(\sigma); \Im(\sigma)] \in \mathbb{R}^{2N}$

$$
\begin{array}{rl}
\min_x & x^T P_0 x \\
\text{s.t.} & Ax = b, \\
& \sum_{p=k+1}^{N} F_{p,p-k} = x_k^R + i x_k^I, \quad \forall k \\
& \sum_{p=k+1}^{N} G_{p,p-k} = (1-k^2)(x_k^R + i x_k^I), \\
& F, G \succeq 0
\end{array}
$$

- The matrix P_0 is symmetric real matrix representing the indefinite quadratic form $\sum_{k=-N+1}^{N-1} (k^2-1)|\sigma_k|^2$
- A is a $1 \times 2N$ matrix representing constraints $\mathbf{c}^* \boldsymbol{\sigma} = L(\Gamma)$

2^{nd} Lagrangian dual - Q-L enhancement and Semidefinite relaxation

$$\min_{x,X} \; tr(P_0 X) \qquad \Longleftarrow \text{Maximization of } |W_\sigma|$$

s. t.:

$$Ax = b \qquad \Longleftarrow \text{Constraint } L_\sigma(\Gamma) = L(\Gamma)$$

$$AX = bx^T \qquad \Longleftarrow \text{Q-L enhancement}$$

$$X \succeq xx^T \qquad \Longleftarrow \text{Semidefinite relaxation}$$

$$\sum_{p=k+1}^{N} F_{p,p-k} = x_k^R + ix_k^I, \qquad \Longleftarrow \sigma \geq 0$$

$$\sum_{p=k+1}^{N} G_{p,p-k} = (1-k^2)(x_k^R + ix_k^I) \Longleftarrow \sigma + \sigma'' \geq 0$$

$$F, G \succeq 0 \qquad \Longleftarrow \text{McLean constraints}$$

Here: $\sigma_k = x_k^R + ix_k^I$

Equivalence of the primal and second dual problems

$$\hat{p}_1 = \min_{x} x^T P_0 x + 2q_0^T x + r_0$$
$$\text{s.t.} \quad Ax = b, \quad A\,xx^T = bx^T, \quad x \in \mathcal{K}$$

$$\hat{p}_2 = \min_{x,X} \operatorname{tr}(P_0 X) + 2q_0^T x + r_0$$
$$\text{s.t.} \quad Ax = b, \quad AX = bx^T, \quad X \succeq xx^T, \quad x \in \mathcal{K}$$

The primal Q-L augmented problem and its second enhanced relaxation yield the same optimal values $\hat{p}_1 = \hat{p}_2$ if

- function $x \mapsto x^T P_0 x$ is convex on the null space $Ax = 0$ $\iff$ Finsler condition $P_0 + \varrho A^T A \succeq 0$ for all $\varrho \gg 1$.

Theorem

$P_0 = \mathrm{diag}(p_0, p_1, \ldots, p_{N-1}, q_0, q_1, \ldots, q_{N-1})$
$p_0 < 0, q_0 \le 0, p_1 = q_1 = 0$, and $p_k, q_k > 0$, for $k \ge 2$.
$A = \begin{pmatrix} \alpha^T & \beta^T \end{pmatrix}, \quad \alpha_1 = \beta_1 = 0$ and

$$\frac{1}{\varrho} + \sum_{k=2}^{N-1} \left(\frac{\alpha_k^2}{p_k} + \frac{\beta_k^2}{q_k} \right) \le \frac{\alpha_0^2}{-p_0} + \frac{\beta_0^2}{-q_0}.$$

Then the matrix $P_0 + \varrho A^T A$ is positive semidefinite.

Proof is based on:

- properties of the Schur complement for the matrix $P_0 + \varrho A^T A$
- Morrison-Sherman formula for inversion of the Schur complement

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In our application: $p_k = q_k = 2(k^2 - 1), p_0 = q_0 = -1, \quad \alpha_k + i\beta_k = 2c_k, \alpha_0 = c_0, \beta_0 = 0$

Proof

- $$P_0 + \varrho A^T A = \begin{pmatrix} p_0 + \varrho\alpha_0^2 & \varrho\alpha_0 v^T \\ \varrho\alpha_0 v & D + \varrho v v^T \end{pmatrix},$$
- $P_0 + \varrho A^T A \succeq 0$ if and only if the Schur complement is nonnegative

$$0 \le p_0 + \varrho\alpha_0^2 - \varrho^2\alpha_0^2\, v^T (D + \varrho v v^T)^{-1} v.$$

where $D = \mathrm{diag}(p_2, \dots, p_{N-1}, q_0 + \varrho, q_2, \dots, q_{N-1})$
- Morrison-Sherman: $(D + \varrho v v^T)^{-1} = D^{-1} - \frac{\varrho}{1+\varrho\gamma} D^{-1} v v^T D^{-1}$ where we have denoted $\gamma = v^T D^{-1} v \ge 0$.
- The previous inequality is equivalent with assumption of the theorem

Theorem

Let $\{c_k, k \in \mathbb{Z}\}$ be the Fourier length spectrum of a Jordan curve. Then

1. $R = \text{Toep}(c_0, c_1, \ldots, c_{N-1}) \succeq 0$ is a p.s.d. matrix $\forall N \in \mathbb{N}$
2. $$\sum_{k=2}^{N-1} \frac{|c_k|^2}{k^2-1} \leq \frac{c_0^2}{2}\left(1 - \frac{1}{N}\right).$$

Proof is based on:

- positive semidefinitness:

$$\begin{aligned} z^* R z &= \sum_{k,m=1}^{N} \bar{z}_k c_{k-m} z_m = \int_\Gamma \sum_{k,m=1}^{N} \bar{z}_k \exp(-i(k-m)\nu) z_m \, d\nu \\ &= \int_\Gamma \left| \sum_{k=1}^{N} z_k \exp(ik\nu) \right|^2 d\nu \geq 0, \end{aligned}$$

- properties of main minors of the p.s.d. matrix $R \succeq 0$

Convergence of finite dimensional approximations

Theorem

Let $\sigma^N(\nu) = \sum_{k=-N+1}^{N-1} \sigma_k e^{ik\nu} \in \mathcal{K}^N \subset \mathcal{K}$ be a minimizer of the anisoperimetric ratio resolved by the method of Enhanced SDP relaxation, where

$$\mathcal{K} = \{\sigma \in W^{2,2}_{per}(0, 2\pi) \mid \sigma(\nu) \geq 0, \sigma(\nu) + \sigma''(\nu) \geq 0\}.$$

is the cone of admissible anisotropis. Then

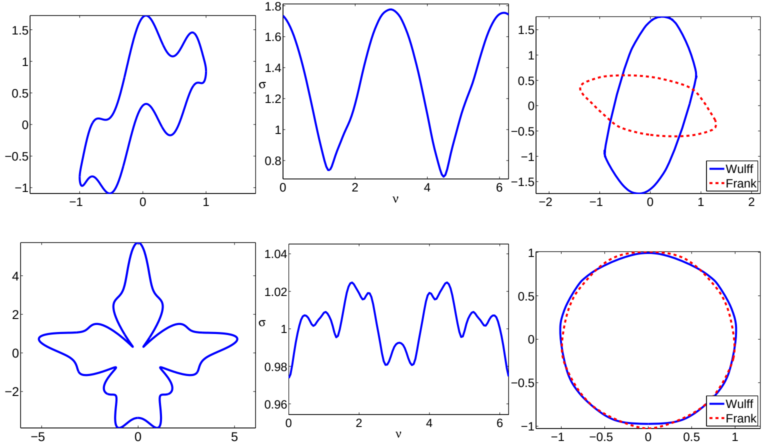
- $1 \leq \lim_{N\to\infty} \Pi_{\sigma^N}(\Gamma) = \inf_{\sigma\in\mathcal{K}} \Pi_\sigma(\Gamma)$
- $\sigma^N \rightharpoonup \sigma$ weakly in $W^{1,2}_{per}(0, 2\pi)$
- $\sigma^N \to \sigma$ strongly in $C^{1/2}_{per}(0, 2\pi)$, as $N \to \infty$

Proof relies on:

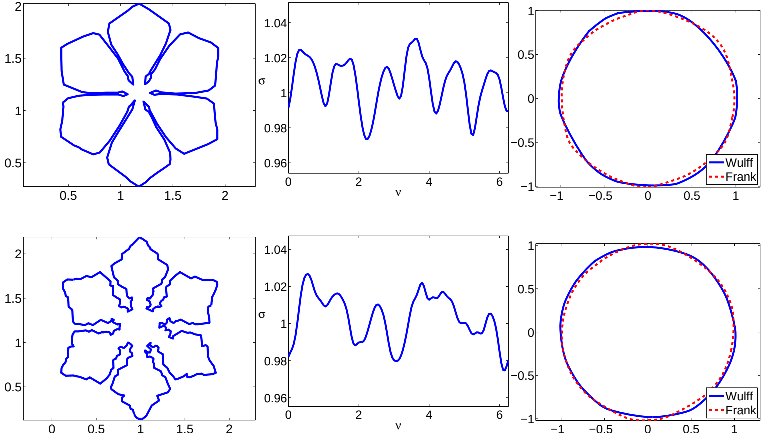
- monotonicity of optimal values $|W_{\sigma^N}| \leq |W_{\sigma^{N+1}}| \leq C_\infty < \infty$.
- density of $\mathcal{K}^N$ in $\mathcal{K}$ for $N \to \infty$ and continuity of $\Pi_\sigma(\Gamma)$ in the $W^{1,2}_{per}(0, 2\pi)$ topology,
- boundedness of σ^N in $W^{1,2}_{per}(0, 2\pi)$ and $W^{1,2}_{per} \hookrightarrow\hookrightarrow C^{1/2}$

Code snippet of a code in CVX using SeDuMi solver

```
cvx_begin sdp
cvx_solver sedumi

variable sigma(N) complex
variable F(N,N), G(N,N) hermitian
variable sreal(N), simag(N), x(2*N)
variable X(2*N,2*N) symmetric

% Objective function
minimize( trace(P0 * X) )

sreal==real(sigma)
simag==imag(sigma)
x == [sreal;simag]

% Build Toeplitz matrix
for k=1:N
        sum (diag(F,-k+1)) == sigma(k)
        sum (diag(G,-k+1)) == (1-(k-1)^2)*sigma(k)
end


A=[ real([c(1);2*c(2:N)])', imag([c(1);2*c(2:N)])'; elong'];
b=[LGamma; 0];
% Constraint A*x=b  <-> L_sigma(Gamma) = L(Gamma)
% Constraint A*X = b*x'
A*x == b
A*X == b*x'

% Semidefinite relaxation
[X, x;
x', 1] >=0

% Toeplitz matrices are positive semidefinite
F>=0
G>=0

cvx_end

```



The curve (left), the optimal anisotropy function σ (middle), the Wulff shape and Frank diagram (right).



The curve (left), the optimal anisotropy function σ (middle), the Wulff shape and Frank diagram (right).

Thank you for your attention

1 D. Ševčovič and M.Trnovská: Solution to the Inverse Wulff Problem by Means of the Enhanced Semidefinite Relaxation Method, Journal of Inverse and Ill Posed Problems, 2014, www.arxiv.org/abs/1402.5668

2 D. Ševčovič and M.Trnovská: Construction of the Optimal Anisotropy Function by the Enhanced Semidefinite Relaxation Method, IAENG International Journal of Applied Mathematics 2014.

3 D. Ševčovič and S.Yazaki: Computational and qualitative aspects of motion of plane curves with a curvature adjusted tangential velocity, *Mathematical Methods in the Applied Sciences*, 35(15) (2012), 1784-1798.

4 D. Ševčovič and S.Yazaki: Evolution of plane curves with a curvature adjusted tangential velocity, *Japan J. Indust. Appl. Math.* 28(3) 2011, 413-442.

5 D. Ševčovič and S.Yazaki: On a gradient flow of plane curves minimizing the anisoperimetric ratio, *IAENG International Journal of Applied Mathematics*, 43(3) 2013, 160-171

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