On optimization on the Euclidean unit sphere

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Optimization without Borders

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Based on :

Homogeneous polynomials and spurious local minima on the unit sphere arXiv:2010.07066

Optimization on the Euclidean unit sphere hal-03284041

• Homogeneous optimization on \mathbb{S}^{n-1}

Simple and complete characterization of first and second-order optimality conditions

• Sparse optimization on \mathbb{S}^{n-1}

(when the criterion to minimize is a function of a few linear forms)

I. Homogeneous polynomials & spurious local minima on the unit sphere

Let \mathbb{S}^{n-1} be the Euclidean unit sphere $\{\mathbf{x} : \|\mathbf{x}\| \leq 1\} \subset \mathbb{R}^n$, and \mathscr{E}_n the Euclidean unit ball $\{\mathbf{x} : \|\mathbf{x}\| \leq 1\}$.

Consider the optimization problem

P:
$$f^* = \min \{f(\mathbf{x}) : \mathbf{x} \in \mathbb{S}^{n-1}\}$$

where f is a homogeneous polynomial of degree t.

Problem **P** is **NP-hard** in general with several important applications, and in particular for some well-known combinatorial optimization problems.

- Finding the maximal cardinality $\alpha(G)$ of a stable set in a graph *G* reduces to minimizing a cubic form on \mathbb{S}^{n-1} .
- Deciding convexity of an *n*-variate form reduces to minimizing a form on \mathbb{S}^{n-1} .
- Deciding nonnegativity of an even-degree form reduces to minimizing this form on \mathbb{S}^{n-1} .
- Deciding copositivity of a symmetric matrix reduces to check whether some associated quartic form is nonnegative on S^{n-1} .
- In quantum information, the Best Separable State problem also relates to homogeneous polynomial optimization on S^{n-1} (Fawzi et al.)

In the first part of the talk, f is a form of degree t > 2.

This talk

A complete & simple characterization of Second-Order Necessary Optimality conditions (SONC) at $\mathbf{x}^* \in \mathbb{S}^{n-1}$ solely in terms of

- *f*(**x***)
- The first two smallest eigenvalues $\lambda_1(\nabla^2 f(\mathbf{x}^*))$ and $\lambda_2(\nabla^2 f(\mathbf{x}^*))$ of the Hessian $\nabla^2 f$ at $\mathbf{x}^* \in \mathbb{S}^{n-1}$.

First-Order Necessary Optimality Conditions (FONC)

A point $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (FONC) if and only if

 $abla f(\mathbf{x}^*) = t f(\mathbf{x}^*) \mathbf{x}^*$

Equivalently, if and only if

$$\|\nabla f(\mathbf{x}^*)\|^2 = t^2 f(\mathbf{x}^*)^2$$

Démonstration.

KKT-optimality conditions yield

$$\nabla f(\mathbf{x}^*) = 2 \lambda^* \mathbf{x}^*$$
, for some λ^*

Euler's identity for homogeneous functions yields

$$tf(\mathbf{x}^*) = \langle \mathbf{x}^*, \nabla f(\mathbf{x}^*) \rangle = 2 \lambda^* ||\mathbf{x}^*||^2 = 2 \lambda^*.$$

$$\Rightarrow \nabla f(\mathbf{x}^*) = tf(\mathbf{x}^*) \, \mathbf{x}^* \quad \text{and} \quad \|\nabla f(\mathbf{x}^*)\|^2 = t^2 f(\mathbf{x}^*)^2$$

Démonstration.

(Continued) Conversely, suppose that $\|\nabla f(\mathbf{x}^*)\|^2 = t^2 f(\mathbf{x}^*)^2$. Then

$$\begin{aligned} \|\nabla f(\mathbf{x}^{*}) - tf(\mathbf{x}^{*}) \, \mathbf{x}^{*}\|^{2} &= \|\nabla f(\mathbf{x}^{*})\|^{2} - \underbrace{2tf(\mathbf{x}^{*})\langle \nabla f(\mathbf{x}^{*}), \mathbf{x}^{*} \rangle}_{= -2t^{2}f(\mathbf{x}^{*})^{2}} \\ &+ t^{2}f(\mathbf{x}^{*})^{2}\|\mathbf{x}^{*}\|^{2} \\ &= \|\nabla f(\mathbf{x}^{*})\|^{2} - t^{2}f(\mathbf{x}^{*})^{2} = 0 \\ \Rightarrow \nabla f(\mathbf{x}^{*}) &= tf(\mathbf{x}^{*}) \, \mathbf{x}^{*} \,, \end{aligned}$$

that is, **(FONC)** holds with $2\lambda^* = tf(\mathbf{x}^*)$.

Given
$$\mathbf{x} \in \mathbb{R}^n$$
, let
 $\mathbf{x}^{\perp} := \left\{ \mathbf{u} \in \mathbb{S}^{n-1} : \mathbf{u} \perp \mathbf{x}^* \right\}.$

Second-Order Necessary Optimality Conditions (SONC)

Definition : A point $\mathbf{x}^* \in \mathbb{S}^{n-1}$ which satisfies (FONC) satisfies (SONC) if

$$\langle \mathbf{u}, (\nabla^2 f(\mathbf{x}^*) - 2\,\lambda^*\,\mathbf{I})\,\mathbf{u} \rangle \ge 0\,, \quad \forall \mathbf{u} \perp \mathbf{x}^*\,.$$

Equivalently, if and only if

 $\langle \mathbf{u}, \nabla^2 f(\mathbf{x}^*) \, \mathbf{u} \rangle \geq \, 2 \, \lambda^* (= t f(\mathbf{x}^*)) \,, \quad \forall \mathbf{u} \in (\mathbf{x}^*)^\perp \,.$

Lemma

If $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (FONC) then \mathbf{x}^* is an eigenvector of $\nabla^2 f(\mathbf{x}^*)$ with associated eigenvalue $t(t-1)f(\mathbf{x}^*)$.

Démonstration.

Observe that $\mathbf{x} \mapsto \partial f(\mathbf{x}) / \partial x_i$ is homogeneous of degree t - 1, for every i = 1, ..., n, and therefore by Euler's identity

$$abla^2 f(\mathbf{x}) \, \mathbf{x} \,=\, (t-1) \,
abla f(\mathbf{x}) \,, \quad \forall \mathbf{x} \in \mathbb{R}^n \,.$$

So if $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (FONC) then

$$\nabla^2 f(\mathbf{x}^*) \, \mathbf{x}^* \,=\, (t-1) \nabla f(\mathbf{x}^*) \,=\, t \, (t-1) f(\mathbf{x}^*) \, \mathbf{x}^*.$$

Let

$$\tau(\mathbf{x}^*) \, := \, \min\left\{ \langle \mathbf{u}, (\nabla^2 f(\mathbf{x}^*) \, \mathbf{u} \rangle : \, \mathbf{u} \in (\mathbf{x}^*)^\perp \, \right\},\,$$

so that if $\mathbf{x}^* \in \mathbb{S}^{n-1}$ then

$$($$
SONC $) \Leftrightarrow \tau(\mathbf{x}^*) \geq tf(\mathbf{x}^*)$.

Lemma

If $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (FONC) then

$$\lambda_{1}(\nabla^{2} f(\mathbf{x}^{*})) = \min\left[t\left(t-1\right)f(\mathbf{x}^{*}), \tau(\mathbf{x}^{*})\right].$$

Démonstration.

Observe that any $\mathbf{z} \in \mathbb{S}^{n-1}$ reads

$$\mathbf{z} = \alpha \, \mathbf{x}^* \oplus \beta \, \mathbf{u} : \, \mathbf{u} \in (\mathbf{x}^*)^\perp ; \, \alpha^2 + \beta^2 = 1$$

and observe that if $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (FONC)

$$\langle \mathbf{u}, \nabla^2 f(\mathbf{x}^*) \, \mathbf{x}^* \rangle = t \, (t-1) f(\mathbf{x}^*) \, \langle \mathbf{u}, \mathbf{x}^* \rangle = 0.$$

Démonstration.

Hence

$$\begin{split} \lambda_1(\nabla^2 f(\mathbf{x}^*)) &= \min \left\{ \langle \mathbf{z}, \nabla^2 f(\mathbf{x}^*) \, \mathbf{z} \rangle : \, \mathbf{z} \in \mathbb{S}^{n-1} \right\} \\ &= \min \left\{ \langle (\alpha \mathbf{x}^* + \beta \mathbf{u}), \nabla^2 f(\mathbf{x}^*) \, (\alpha \mathbf{x}^* + \beta \mathbf{u}) \rangle : \, \alpha^2 + \beta^2 = 1 \right\} \\ &= \min \left\{ \, \alpha^2 \, t \, (t-1) f(\mathbf{x}^*) + \beta^2 \, \tau(\mathbf{x}^*) : \, \alpha^2 + \beta^2 = 1 \right\} \\ &= \min \left[\, t \, (t-1) f(\mathbf{x}^*) \, , \, \tau(\mathbf{x}^*) \right]. \end{split}$$

In particular

If $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (**FONC**) then :

$$\lambda_1(\nabla^2 f(\mathbf{x}^*)) = t(t-1)f(\mathbf{x}^*) \Rightarrow \tau(\mathbf{x}^*) = \lambda_2(\nabla^2 f(\mathbf{x}^*))$$

and (SONC) $\Leftrightarrow \lambda_2(\nabla^2 f(\mathbf{x}^*)) \ge tf(\mathbf{x}^*) = \frac{\lambda_1(\nabla^2 f(\mathbf{x}^*))}{t-1}.$

Theorem

Let $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfy (FONC). Then \mathbf{x}^* satisfies (SONC) if and only if

 $\begin{array}{lll} \lambda_1(\nabla^2 f(\mathbf{x}^*)) & \geq & tf(\mathbf{x}^*) & iff(\mathbf{x}^*) \geq 0\\ \lambda_2(\nabla^2 f(\mathbf{x}^*)) & \geq & tf(\mathbf{x}^*) & iff(\mathbf{x}^*) < 0. \end{array}$

So all (SONC) points $\mathbf{x}^* \in \mathbb{S}^{n-1}$ are characterized by : - the value $f(\mathbf{x}^*)$, and

- The first and second smallest eigenvalues of $\nabla^2 f$ at \mathbf{x}^* .

In particular

If $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfies (**FONC**) and $f(\mathbf{x}^*) < 0$ then :

$$(\mathbf{SONC}) \Leftrightarrow \lambda_2(\nabla^2 f(\mathbf{x}^*)) \geq \frac{\lambda_1(\nabla^2 f(\mathbf{x}^*))}{t-1}$$

and \mathbf{x}^* is the eigenvector associated with $\lambda_1(\nabla^2 f(\mathbf{x}^*))$.

Solution $\lambda_2(\nabla^2 f(\mathbf{x}^*))$ is significantly larger than $\lambda_1(\nabla^2 f(\mathbf{x}^*))$.

The case of odd degree forms

The only interesting local minima are negative since if $\mathbf{x} \in \mathbb{S}^{n-1}$ with $f(\mathbf{x}) > 0$ then $\mathbf{u} := -\mathbf{x} \in \mathbb{S}^{n-1}$ with value $f(\mathbf{u}) = -f(\mathbf{x}) < 0$.

So in this case

a negative local minimizer $\mathbf{x}^* \in \mathbb{S}^{n-1}$ is necessarily the eigenvector of the Hessian $\nabla^2 f(\mathbf{x}^*)$ associated with the SMALLEST EIGENVALUE $\lambda_1(\nabla^2 f(\mathbf{x}^*)) = t(t-1)f(\mathbf{x}^*)$.

Moreover

all negative local minima of f on \mathbb{S}^{n-1} are all negative local minima of f on the Euclidean ball \mathcal{E}_n .

It is then much easier to minimize f on the convex set \mathcal{E}_n rather than on the "nasty" non-convex set \mathbb{S}^{n-1} .

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Homogeneous polynomials & spurious local minima on the unit sphere

The case of cubic forms

For instance if t = 3 (i.e., f is a cubic form) then

- $\nabla^2 f(\mathbf{x}^*)$ is a matrix whose entries are linear forms, and so
- $\mathbf{x} \mapsto \lambda_1(\nabla^2 f(\mathbf{x}))$ is a **CONCAVE** function
- $\mathbf{x} \mapsto \lambda_1(\nabla^2 f(\mathbf{x})) + \lambda_2(\nabla^2 f(\mathbf{x}))$ is also a **CONCAVE** function.

Hence the (SONC) condition

$$\lambda_{2}(\nabla^{2} f(\mathbf{x}^{*})) \geq \frac{\lambda_{1}(\nabla^{2} f(\mathbf{x}^{*}))}{t-1}$$

is equivalent to the condition

$$\lambda_{\mathbf{1}}(\nabla^2 f(\mathbf{x}^*)) + \lambda_{\mathbf{2}}(\nabla^2 f(\mathbf{x}^*)) \ge \frac{3\,\lambda_{\mathbf{1}}(\nabla^2 f(\mathbf{x}^*))}{2}$$

Theorem

An odd degree-t form f (with t > 1) has no spurious negative local minimum if the system

$$\nabla^2 f(\mathbf{x}) \mathbf{x} = t (t-1) f(\mathbf{x}) \mathbf{x}$$
$$\lambda_2 (\nabla^2 f(\mathbf{x})) \geq \frac{\lambda_1 (\nabla^2 f(\mathbf{x}))}{t-1}$$

has a unique solution \mathbf{x} *with* $f(\mathbf{x}) < 0$

One may also relate the critical points of f on \mathbb{S}^{n-1} with the sub-varieties of a certain gradient ideal.

Let $f \in \mathbb{R}[\mathbf{x}]$ be homogeneous of degree *t*, and define $g \in \mathbb{R}[\mathbf{x}]$ by :

$$\mathbf{x} \mapsto \mathbf{g}(\mathbf{x}) := f(\mathbf{x}) \left(1 - \frac{t \|\mathbf{x}\|^2}{t+2}\right), \quad \mathbf{x} \in \mathbb{R}^n.$$

Proposition

On
$$\mathbb{S}^{n-1}$$
: $\nabla g(\mathbf{x}) = 0 \quad \Leftrightarrow \quad \nabla f(\mathbf{x}) = tf(\mathbf{x}) \mathbf{x}$

and so all (FONC) points of f are critical points of g and conversely.

$$V_{grad}(g) := \{ \mathbf{z} \in \mathbb{C}^n : \nabla g(\mathbf{x}) = 0 \}$$
$$= W_0 \cup W_1 \ldots \cup W_p$$

where each W_i is an irreducible subvariety and g is constant on each W_i .

^{IEF} Hence *f* has no spurious local minimum on \mathbb{S}^{n-1} if all the **(SONC)** points belong to a single $W_j \cap \mathbb{S}^{n-1}$ for some index j^* .

😰 an algebraic characterization

Homogeneous polynomials & spurious local minima on the unit sphere

II. Sparse optimization on \mathbb{S}^{n-1}

Consider the problem

$$\mathbf{P}: \quad f^* = \min \{h(\mathbf{x}) : \mathbf{x} \in \mathbb{S}^{n-1} \}$$

where $h(\mathbf{x}) = f((\ell_1 \cdot \mathbf{x}), (\ell_2 \cdot \mathbf{x}), \dots, (\ell_m \cdot \mathbf{x}))$

- for some *m* linear forms $\ell_1, \ldots, \ell_m : \mathbb{R}^n \to \mathbb{R}$, and - some function $f : \mathbb{R}^m \to \mathbb{R}$.

■ If $m \ll n$ then **P** can be view a sparse optimization problem as in *h*, the coupling of variables only occurs through the *m* linear forms $(\ell_j)_{j \in [m]}$. ■ Sometimes *h* is said to be *low-rank*

However the constraint $\mathbf{x} \in \mathbb{S}^{n-1}$ is not expressed through the ℓ_j 's.

Take home message

Problem **P** is in fact equivalent to an *m* variables problem on the Euclidean unit ball $\mathscr{E}_m := \{ \mathbf{x} \in \mathbb{R}^m : \|\mathbf{x}\| \le 1 \}$ of \mathbb{R}^m .

• Let $\ell \in \mathbb{R}^{m \times n}$ be the real matrix with rows $(\ell_i)_{i \in [m]}$.

• $\mathcal{L} := \ell \ell^T \in \mathbb{R}^{m \times m}$, and $\mathbf{L} := \mathcal{L}^{1/2}$,

and consider the problem

$$\mathbf{Q}: \qquad \min_{\mathbf{y}} \left\{ f((\mathbf{L}_1 \cdot \mathbf{y}), \ldots, (\mathbf{L}_m \cdot \mathbf{y})) : \mathbf{y} \in \mathscr{E}_m \right\}.$$

Theorem

Assume that the ℓ_j are linearly independent. (i) Let $\mathbf{x}^* \in \mathbb{S}^{n-1}$ satisfy (SONC) for problem **P**. Then there exists $\mathbf{y}^* \in \mathscr{E}_m$ which satisfies (SONC) for problem **Q** and with same value

$$f((\mathbf{L}_1\cdot\mathbf{y}^*),\ldots,(\mathbf{L}_m\cdot\mathbf{y}^*))=f(\boldsymbol{\ell}\,\mathbf{x}^*)\,=\,h(\mathbf{x}^*)\,.$$

(ii) Conversely, let $\mathbf{y}^* \in \mathscr{E}_m$ satisfy (SONC) for problem **Q**. Then there exists $\mathbf{x}^* \in \mathbb{S}^{n-1}$ which satisfies (SONC) for problem **P** and with same value

$$h(\mathbf{x}^*) = f(\boldsymbol{\ell} \, \mathbf{x}^*) = f((\mathbf{L}_1 \cdot \mathbf{y}^*), \dots, (\mathbf{L}_m \cdot \mathbf{y}^*)).$$

• Let $\ell \in \mathbb{R}^{m \times n}$ be the real matrix with rows $(\ell_j)_{j \in [m]}$.

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$$f((\mathbf{L}_1 \cdot \mathbf{y}^*), \ldots, (\mathbf{L}_m \cdot \mathbf{y}^*)) = f(\boldsymbol{\ell} \mathbf{x}^*) = h(\mathbf{x}^*).$$

(ii) Conversely, let $\mathbf{y}^* \in \mathscr{E}_m$ satisfy (SONC) for problem **Q**. Then there exists $\mathbf{x}^* \in \mathbb{S}^{n-1}$ which satisfies (SONC) for problem **P** and with same value

$$h(\mathbf{x}^*) = f(\boldsymbol{\ell} \, \mathbf{x}^*) = f((\mathbf{L}_1 \cdot \mathbf{y}^*), \dots, (\mathbf{L}_m \cdot \mathbf{y}^*)).$$

Key observation

The KKT-optimality conditions at $\mathbf{x}^* \in \mathbb{S}^{n-1}$ read :

$$\boldsymbol{\ell}^T \nabla f((\boldsymbol{\ell}_1 \cdot \mathbf{x}^*), \ldots, (\boldsymbol{\ell}_m \cdot \mathbf{x}^*)) = 2 \,\lambda^* \mathbf{x}^*,$$

for some λ^* .

In other words, whenever $\lambda^* \neq 0$

any candidate local minimizer $\mathbf{x}^* \in \mathbb{S}^{n-1}$ necessarily satisfies

$$\mathbf{x}^* \in \operatorname{Span}(\boldsymbol{\ell}_1,\ldots,\boldsymbol{\ell}_m)$$

For It is enough to search in Span $(\ell_1, \ldots, \ell_m) \cap \mathbb{S}^{n-1}$!

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It is enough to search in $\text{Span}(\ell_1, \ldots, \ell_m) \cap \mathbb{S}^{n-1}$!

(i) Let $\mathbf{x}^* \in \mathbb{S}^{n-1}$ be such that $\lambda^* \neq 0$. Then letting $\mathbf{z} = (z_j)$,

$$\mathbf{x}^* = \sum_{j=1}^m z_j \, \boldsymbol{\ell}_j \quad \text{and} \quad \mathbf{y}^* := \mathbf{L} \, \mathbf{z} \Rightarrow \|\mathbf{y}^*\| = 1 \,,$$

so that $\mathbf{y}^* \in \mathscr{E}_n$ and $f((\mathbf{L}_1 \cdot \mathbf{y}^*), \dots, (\mathbf{L}_m \cdot \mathbf{y}^*)) = h(\mathbf{x}^*)$.

• $\boldsymbol{\ell} \mathbf{x}^* = \boldsymbol{\ell} \boldsymbol{\ell}^T \mathbf{u} = \mathbf{L} \mathbf{L} \mathbf{u} = \mathbf{L} \mathbf{y}^*$, and therefore

$$h(\mathbf{x}^*) = f(\boldsymbol{\ell} \, \mathbf{x}^*) = f(\mathbf{L} \, \mathbf{y}^*), \quad \text{with } \mathbf{y}^* \in \mathscr{E}_m.$$

For the converse, similar calculations yield the desired result.

Hence

solving **P** on \mathbb{S}^{n-1} is equivalent to solving **Q** on \mathscr{E}_m and the latter problem is lower-dimensional on the CONVEX SET \mathscr{E}_m , a significant progress.

The case m = 1

If m = 1 (so that $\ell \in \mathbb{R}^n$) then Problem **P** reduces to the easy to solve univariate problem

$$\mathbf{Q}: \quad f^* = \min_{\mathbf{y}} \{ f(\|\boldsymbol{\ell}\|\,\mathbf{y}): \, \mathbf{y} \in [-1,1] \}$$

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Q:
$$f^* = \min_{y} \{ f(||\boldsymbol{\ell}|| y) : y \in [-1, 1] \}$$

The case m = 1 (continued) If m = 1 and h is a quasi-convex polynomial then $f^* = \min[f(||\boldsymbol{\ell}||), f(-||\boldsymbol{\ell}||)]$

and so *h* has no spurious local minimum on \mathbb{S}^{n-1} .

^{ISF} *h* quasi-convex implies $h(\mathbf{x}) = f(\boldsymbol{\ell} \cdot \mathbf{x})$ for some $\boldsymbol{\ell} \in \mathbb{R}^n$ and some monotonic univariate polynomial *f* (Ahmadi et al. (2013), Math. Program.).

Finally if *h* has the low-rank formulation

$$h(\mathbf{x}) = f(\boldsymbol{\ell} \mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n,$$

for some *hidden* $\ell \in \mathbb{R}^{m \times n}$ then by sufficiently many evaluations of ∇f at randomly chosen points $(\mathbf{x}(i))_{i \in J}$ (e.g. $\mathbf{x}(i) \in \mathbb{S}^{n-1}$) one may recover ℓ .

Happy Birthday !