Algebraic Optimization Degree

A Macaulay2 package

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Introduction

Introduction

Setting

Maximize/minimize an objective function Ψ over an algebraic variety X.

The algebraic degree of an optimization problem gives an algebraic measure of complexity of a problem

The algebraic degree of an optimization problem is an important invariant in applied algebraic geometry:

- nearest point problems (Draisma et al. 2016),
- maximum likelihood estimation (Catanese et al. 2006; Hoşten, Khetan, and Sturmfels 2005),
- semidefinite programming (Graf von Bothmer and Ranestad 2009).

A simple example

Let Y be a binomial random variable with 2 trials.

The probability mass function of Y is given by the map

$$p \mapsto ((1-p)^2, 2p(1-p), p^2) =: (p_0, p_1, p_2)$$

The Zariski closure of the image is the algebraic variety corresponding to the ideal

$$I = \langle 4p_0p_2 - p_1^2, 1 - p_0 - p_1 - p_2 \rangle \subseteq \mathbb{R}[p_0, p_1, p_2]$$

A simple example

Suppose we observe Y and collect the results in a vector (u_0, u_1, u_2).

The likelihood function is

$$\Psi(p_0, p_1, p_2) = p_0^{u_0} p_1^{u_1} p_2^{u_2}$$

Maximum likelihood estimation

Maximize Ψ subject to $(p_0, p_1, p_2) \in \mathbb{V}(I)$ and $0 \leq p_i \leq 1$ for $i \in \{1, 2, 3\}$.

Approach: find all complex critical points of Ψ. The number of critical points is the *maximum likelihood degree*.

General setting

- $X \subset \mathbb{C}^n$ an affine variety of codimension c
- $\Psi\colon X \to \mathbb{C}$ an objective function, with gradient $\nabla\Psi$

Definition

The critical ideal $\mathrm{Crit}_0(\Psi, X)$ is the ideal of the set of isolated critical points of Ψ on the regular locus of X. The degree of $\mathrm{Crit}_0(\Psi, X)$ is the optimization degree.

$$S := \left(\langle f_1, \ldots, f_N \rangle + \left\langle (c+1) \times (c+1) \text{ minors of } \begin{bmatrix} \nabla\Psi \\ \nabla f_1 \\ \vdots \\ \nabla f_N \end{bmatrix} \right\rangle \right) : I_{X_{\mathrm{sing}}}^{\infty},$$

where $f_1, \ldots, f_n$ generate the radical ideal of X. Let P denote the ideal of positive dimensional components of the variety of S. Then,

$$\mathrm{Crit}_0(\Psi, X) = S : P^{\infty}.$$

Euclidean distance degree

ED-degree

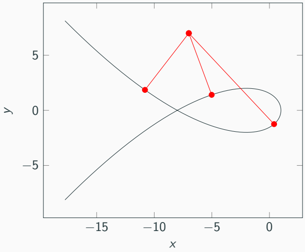
Problem

Given a variety $X \subseteq \mathbb{C}^n$ and a point $u \in \mathbb{C}^n$, find the point $x \in X$ that minimizes the Euclidean distance $\|x - u\|_2$.

The number of critical points of the Euclidean distance function for a *generic* point u is the Euclidean distance degree

Example

```
i1 : R = QQ[x,y];
i2 : I = ideal(27*y^2-(1-x)*(8+x)^2);
i3 : probabilisticEDDegree(I)
o3 = 5
i4 : symbolicEDDegree(I)
o4 = 5
```



ED-degree via projections

Let $X \subseteq \mathbb{P}^n$ have codimension ≥ 2. Let $\pi\colon \mathbb{P}^n \to \mathbb{P}^{n-1}$ be a rational map defined by a general linear map $\mathbb{C}^{n+1} \to \mathbb{C}^n$.

Theorem (Draisma et al. (2016))

The ED-degree of X is equal to the ED-degree of $\pi(X)$.

Example

```
i1 : R = ZZ/101[x_1..x_6]
i2 : M = genericSymmetricMatrix(R,3)
i3 : I = minors(2,M)
i4 : elapsedTime probabilisticEDDegree I
     -- 566.658 seconds elapsed
o4 = 13
i5 : elapsedTime projectionEDDegree I
     -- 0.115337 seconds elapsed
o5 = 13
```

Maximum likelihood degree

Introduction

- Probability simplex

$$\Delta_n := \{(p_0, \dots, p_n) : p_i \geq 0, \sum_i p_i = 1\}$$

- The statistical model is the solution set of homogeneous polynomials in $p_0, \dots, p_n$.
- Let V be the variety corresponding to the model.

Maximum Likelihood Estimation

Given a vector $u \in \mathbb{N}^{n+1}$ of observations, maximize

$$L = \frac{p_0^{u_0} + \cdots + p_n^{u_n}}{(p_0 + \cdots + p_n)^{u_0 + \cdots + u_n}}$$

subject to $(p_0, \dots, p_n) \in V \cap \Delta_n$.

Definition (Hoşten, Khetan, and Sturmfels (2005))

The ML-degree is the number of critical points of L for generic u.

Implicit form

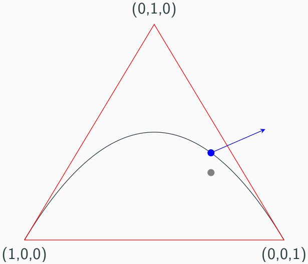
Example

Binomial random variable with 2 trials. Say we observe $u = (2, 5, 9)$.

```
i1 : R = QQ[p_0..p_2]
i2 : P = ideal(4*p_0*p_2-p_1^2)
i3 : MLequationsIdeal(P, {2,5,9})

o3 = ideal (23p  - 18p , 529p  - 81p )
               1      2       0      2

i4 : MLequationsDegree(P)
o4 = 1
```



Toric models

Definition

The scaled toric variety is the Zariski closure of the map $\phi_{A,c} : (\mathbb{C}^*)^d \to (\mathbb{C}^*)^r$ in $\mathbb{C}^r$ given by

$$\phi_{A,c}(\theta_1, \ldots, \theta_d) = (c_1\theta^{a_1}, \ldots, c_r\theta^{a_r}).$$

Example

```
i1 : A = matrix {{1,1,1,0,0,0,0,0,0}, {0,0,0,1,1,1,0,0,0},
{0,0,0,0,0,0,1,1,1},{1,0,0,1,0,0,1,0,0},{0,1,0,0,1,0,0,1,0}}
i2 : c = {1,2,3,1,1,1,1,1,1};
i3 : elapsedTime toricMLDegree(A, c)
     -- 0.00849565 seconds elapsed
o3 = 3
```

The corresponding computation using `MLequationsDegree` took 228 seconds.

Optimizations and future

Fritz John and Lagrange multipliers

- Let $A \in \mathbb{C}[x]^{m \times n}$ be a (generically) full-rank matrix, $m \geq n$.
- Computing $\langle n \times n$ minors of $A\rangle$ may be difficult.
- Lagrange/Fritz John:

$$\begin{bmatrix} z_1 & \cdots & z_n \end{bmatrix} A = 0$$

$$\sum_i c_i z_i = 1$$

Example

```
i1 : R = QQ[x_1..x_6];
i2 : M = genericSymmetricMatrix(R,3);
i3 : I = minors(2, M);
i4 : probabilisticEDDegree I
     -- 179.771 seconds elapsed
o4 = 13
i5 : probabilisticFritzJohnEDDegree I
     -- 4.95628 seconds elapsed
o5 = 13
```

Numerical algebraic geometry

Future: push beyond the boundaries of symbolic methods with numerical algebraic geometry

- Compute all critical points
- Find the optimal point
- Parametric homotopy
- `MonodromySolver`

Conclusion

Package features

- General optimization problem
  - Ideal
  - Largrange
- Euclidean Distance Degree
  - Probabilistic
  - Symbolic
  - Projective
    - Multidegree
    - Projections
    - Sections
  - Fritz John
- Maximum Likelihood degree
  - Symbolic
  - Parametric
  - Toric

Package available at
`https://github.com/Macaulay2/Workshop-2020-Cleveland/tree/ISSAC-AlgOpt/alg-stat/AlgebraicOptimization`

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For more questions, join the link

https://bluejeans.com/550710311

on Jul 21, 18:00 EET

References

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Backup slides

ED-degree via multidegree

Theorem (Draisma et al. (2016))

The ED-degree of X is the sum of the polar classes of $\mathcal{N}$

Example

```
i1: R = QQ[x_0..x_3]
i2: J = ideal det(matrix{
  {x_0, x_1, x_2},
  {x_1, x_0, x_3},
  {x_2, x_3, x_0}});
i3: symbolicMultidegreeEDDegree J
     -- 0.263975 seconds elapsed
o3 = 13
i4: probabilisticMultidegreeEDDegree J
     -- 0.264061 seconds elapsed
o4 = 13
```

Projective varieties

The ED-degree of a projective variety $X \subseteq \mathbb{P}^n$ is the ED-degree of its affine cone in $\mathbb{C}^{n+1}$.

Definition

- The conormal variety $\mathcal{N}$ is the closure of the set

$$\{(x, u) \in \mathbb{P}^n \times (\mathbb{P}^n)^* : x \in X \setminus X_{\mathrm{sing}}, u \in T_x X\}$$

- We say X is in general position if $\mathcal{N}$ does not intersect the diagonal $\Delta \subseteq \mathbb{P}^n \times (\mathbb{P}^n)^*$.

Throughout the rest of the section, X is a projective variety in general position.

ED-degree via linear sections

Theorem

$$\mathrm{EDdegree}(X) = \begin{cases} \mathrm{EDdegree}(X \cap H), & \textit{if } \mathrm{codim}(X^*) \geq 2 \\ \mathrm{EDdegree}(X \cap H) + \deg(X^*), & \textit{if } \mathrm{codim}(X^*) = 1 \end{cases}$$

Notes

- Requires computing the projective dual X^*, i.e. the projection of $\mathcal{N}$ onto its second factor.
- Iterated application requires computation of $(X \cap H)^*$

Theorem (Holme (1988))

Let H be a hyperplane. If X^* has codimension ≥ 2, then

$$(X \cap H)^* = \pi_H(X^*),$$

where π_H is the projection with center point $H \in (\mathbb{P}^n)^*$

ML-degree of parametric models

In many applications, the statistical model is given as the image of a polynomial map

Example

```
i1 : R = QQ[p]
i2 : param = {(1-p)^2, 2*p*(1-p), p^2}
i3 : parametricMLIdeal(param, {2,5,9})
o3 = ideal(32p - 23)
i4 : parametricMLDegree(param)
o4 = 1
```