Computing Maximum Likelihood Estimates for Gaussian Graphical Models with Macaulay2

joint work with Carlos Améndola, Luis David García Puente, Roser Homs, Olga Kuznetsova

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Overview

1. Graphical Models
2. Maximum Likelihood Estimation
3. Our Software Package
4. Examples

1. Graphical Models

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G is a mixed graph with undirected, directed and bidirected edges.

Figure: Food discovery in Uber Eats

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Graphs

We denote mixed graphs by $G = (V; E)$ with undirected edges $i \quad j$, directed edges $i \; ! \; j$ and bidirected edges $i \; \$ \; j$.

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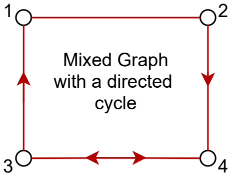
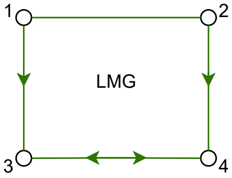
Loopless mixed graph (LMG)

An LMG is a mixed graph without loops or directed cycles.





2. Maximum Likelihood Estimation (MLE)

MLE is one of the major estimation tool in statistics.

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MLE is one of the major estimation tool in statistics.

Let $X^1;X^2;:::;X^n$ P be i.i.d r.v's according to some probability distribution P 2 P .

Goal

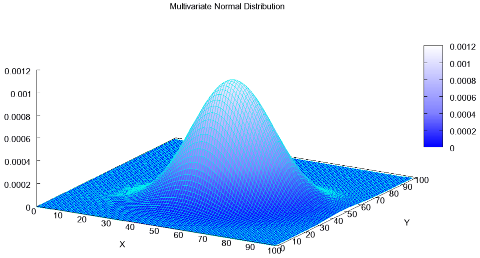
Find that best describes the data.

Multivariate Gaussian distribution

A r.v. $X = (X_1, X_2, \cdots, X_m) \sim N(\mu, \Sigma)$, if it follows this distribution:

$$p_{\mu,\Sigma}(x) = \frac{\exp\left(-\frac{1}{2}(x-\mu)^{\mathrm{T}}\Sigma^{-1}(x-\mu)\right)}{\sqrt{(2\pi)^m \det \Sigma}}, \quad x \in \mathbb{R}^m,$$

where $\mu \in \mathbb{R}^m$ and Σ is assumed to be p.d.



Optimisation problem

Let $N(\;\;;\Sigma)$ be a multivariate Gaussian distribution.

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$$\max_{\ 2\,\mathbb{R}^{m\ \ m}} \ \ell(\ ) = \ \log\det \ \ \mathrm{tr}(S\ \ ^{1})$$

$$\text{subject to:} \qquad 0$$

Gaussian Graphical Models

Graphical models where r.v. $X = (X_v j v \ 2 \ V) \quad N \ (; \ )$

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$$= (I \quad)^{T} \begin{pmatrix} K^{1} & 0 \\ 0 & \end{pmatrix} (I \quad)^{1};$$

where

$= [\;_{ij}]$ is such that $\;_{ij} = 0 \iff i \to j \notin E$
$K = [k_{ij}]$ is p.d. such that $k_{ij} = 0 \iff i \quad j \notin E$
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Example: $\;_{1;4} = k_{1;4} = \;_{1;4} = \;_{1;2} = \;_{1;2} = 0$

How to compute MLE?

We have to maximize the following objective function:

$$\max_{\Sigma \in \mathbb{R}^{m \times m}} \ell(\Sigma) = -\log\det\Sigma - \mathrm{tr}(S\Sigma^{-1})$$

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$$\max_{2\,\mathbb{R}^{m \quad m}} \quad `(\ ) = \quad \log\det \quad \operatorname{tr}(S \quad ^{1})$$

To nd critical points we rst compute the following partial derivatives:

$$\frac{@}{@(\ )}\det \quad \det \quad \frac{@}{@(\ )}\operatorname{tr}(S \quad ^{-1}) :$$

Let I be the ideal generated by the above equations.

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V (J) is the set of critical points of the objective function .

3. Our Software Package

Goal

To develop a software package for computing MLE of Gaussian models.

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GraphicalModelsMLE [AGHKM21]

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GraphicalModelsMLE [AGHKM21]

GraphicalModelsMLE computes MLE of Guassian graphical models.

- We compute MLE, the ideal J of score equations, critical points of the objective function, and ML-degree.
- Our running examples:

Example 1 (MLE of undirected 4-cycle)

```
i1 : loadPackage "GraphicalModelsMLE";
i2 : G=graph{{1,2},{2,3},{3,4},{4,1}};
i3 : S=matrix {{.105409, -.0745495, -.0186132, .0621907},
               {-.0745495, .0783734,-.00844503,-.0872842},
               {-.0186132, -.00844503, .128307, .0230245},
               {.0621907, -.0872842, .0230245,.109849}};
i4 : solverMLE(G,S,SampleData=>false)
o4 = (6.62005, | .105409    -.0745495   .0124099    .0621907   |, 5)
               | -.0745495  .0783734    -.00844503  -.0439427  |
               | .0124099   -.00844503  .128307     .0230245   |
               | .0621907   -.0439427   .0230245    .109849    |
```

Example 1 (Ideal of score equations for 4-cycle)

```
i5 : U=matrix{{3,5,9,5},{1,6,1,5},{2,9,6,6},{2,5,0,4}};
i6 : J=scoreEquations(gaussianRing G,U);
o6 : Ideal of QQ[k   , k   , k   , k   , k   , k   , k   , k   ]
                  1,1   2,2   3,3   4,4   1,2   1,4   2,3   3,4
i7 : dim J
o7 = 0
```

The score ideal is generated by 4 linear polynomials and 10 quadratic polynomials such as

$$1312002k_{3,4}^2 \quad 387081k_{1,2} + 109860k_{1,4} + 1972025k_{2,3} \quad 898518k_{3,4} \quad 291556.$$

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Example 1 (ML-degree of 4-cycle)

ML-degree of 4-cycle

```
i2 : G=graph{{1,2},{2,3},{3,4},{4,1}};
i3 : MLdegree(gaussianRing G)
o3 = 5
```

Example 2 (MLE of LMG on 4 vertices)

```
i2 : G = mixedGraph(graph{{1,2}},digraph{{1,3},{2,4}},bigraph{{3,4}});
i3 : S=matrix {{34183/50000, 716539/10000000, 204869/250000, 12213/25000},
              {716539/10000000, 112191/500000, 309413/1000000, 1803/4000},
              {204869/250000, 309413/1000000, 3849/3125,15172/15625},
              {12213/25000, 1803/4000, 15172/15625, 4487/4000}};
i4 : solverMLE(G,S,SampleData=>false)
o4 = (9.36624, {| .68366   .0716539 1.00282   .234375   |}, 5)
                | .0716539 .224382  .105105   .733937   |
                | 1.00282  .105105  1.76955   -.0700599 |
                | .234375  .733937  -.0700599 2.97432   |
```

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Example 2 (Critical points for LMG on 4 vertices)

```
i5 : R = gaussianRing G;
i6 : (J,Sigma)=scoreEquations(R,S,SampleData=>false,CovarianceMatrix=>true);
i7 : dim J, degree J
o7 = (0, 5)
i8 : sols=zeroDimSolve(J);
i9 : checkPD(apply(sols,i->sub(Sigma,matrix{coordinates(i)})))
| .68366   .0716539 1.00282   .234375   |, | .68366   .0716539 .467724   .070198 |,
| .0716539 .224382  .105105   .733937   |  | .0716539 .224382  .0490218 .219823 |
| 1.00282  .105105  1.76955   -.0700599 |  | .467724  .0490218 .75038   .429714 |
| .234375  .733937  -.0700599 2.97432   |  | .070198  .219823  .429714  .66928  |
                       | .68366   .0716539 .675787  .117978 |
                       | .0716539 .224382  .0708287 .369443 |
                       | .675787  .0708287 .947611  .211905 |
                       | .117978  .369443  .211905  .854009 |
```

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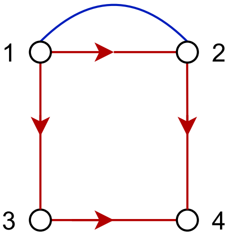
Example 3 (Non-identifiable model)

```
i2: G=mixedGraph(digraph{{1,3},{1,2},{2,4},{3,4}},
graph{{1,2}});
i3: MLdegree(gaussianRing G)
error: the ideal of score equations has dimension 1 > 0,
so ML degree is not well-defined. The degree of this ideal is 2.
```



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References

The work presented here is based on:

Amendola C, Garc a-Puente LD, Homs R, Kuznetsova O, Motwani HJ. **Computing Maximum Likelihood Estimates for Gaussian Graphical Models with Macaulay2.** arXiv:2012.11572.

GraphicalModelsMLE: http://www2.macaulay2.com/Macaulay2/doc/Macaulay2/share/doc/Macaulay2/GraphicalModelsMLE/html/index.html

Additional references:

Daniel R. Grayson, and Michael E. Stillman, Macaulay2, a software system for research in algebraic geometry. http://www.math.uiuc.edu/Macaulay2/

Sullivant S. Algebraic statistics. American Mathematical Soc; 2018

Lauritzen SL. Graphical models. Clarendon Press; 1996