Geometry of ML estimation in Gaussian graphical models

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SIAM Conference on Applied Algebraic Geometry

October 8, 2011

Motivation

Current statistical applications:

- Number of variables >> Number of observations
- Example: Genetic networks

  Gene expression data of a few individuals to model interaction between large number of genes

➡ **Gaussian graphical models** widely used in this context

? Minimum number of observations for existence of MLE (maximum likelihood estimator) in Gaussian graphical model?

Gaussian graphical models

- $G = ([m], E)$ undirected graph with $(\alpha, \alpha) \in E \ \ \forall \alpha \in [m]$.
- $X_1, \ldots, X_n \in \mathbb{R}^m$ i.i.d. sample from $\mathcal{N}_m(0, \Sigma)$
- $\Sigma \in \mathbb{S}^m_{\succ 0}$ covariance matrix on $[m]$ satisfying

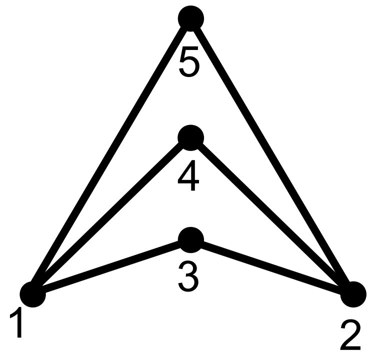
  $(\Sigma^{-1})_{\alpha,\beta} = 0, \ \ \forall\, (\alpha, \beta) \notin E.$

- $S := \frac{1}{n} \sum_{i=1}^n X_i X_i^T \in \mathbb{S}^m_{\succeq 0}$ sample covariance matrix
- $S_G = (S_{\alpha,\beta} \mid (\alpha, \beta) \in E)$ sufficient statistics

- S_G **partial matrix** with entries at positions corresponding to edges E

Example $K_{2,3}$

- The Gaussian graphical model on $K_{2,3}$ consists of multivariate Gaussians satisfying

$G =$ 

$$\Sigma^{-1} = \begin{pmatrix} \lambda_{11} & 0 & \lambda_{13} & \lambda_{14} & \lambda_{15} \\ 0 & \lambda_{22} & \lambda_{23} & \lambda_{24} & \lambda_{25} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & 0 & 0 \\ \lambda_{14} & \lambda_{24} & 0 & \lambda_{44} & 0 \\ \lambda_{15} & \lambda_{25} & 0 & 0 & \lambda_{55} \end{pmatrix}$$

- Given a sample covariance matrix S, the sufficient statistic is

$$S_G = \begin{pmatrix} s_{11} & ? & s_{13} & s_{14} & s_{15} \\ ? & s_{22} & s_{23} & s_{24} & s_{25} \\ s_{13} & s_{23} & s_{33} & ? & ? \\ s_{14} & s_{24} & ? & s_{44} & ? \\ s_{15} & s_{25} & ? & ? & s_{55} \end{pmatrix}$$

MLE, a special PD completion

Theorem *(Dempster, 1972)*:

In a Gaussian graphical model on G the MLE $\hat{\Sigma}$ exists, if and only if the partial sample covariance matrix S_G can be completed to a positive definite matrix.

Then the MLE $\hat{\Sigma}$ is the unique completion, whose inverse satisfies

$$(\hat{\Sigma}^{-1})_{\alpha,\beta} = 0, \ \forall\ (\alpha, \beta) \notin E.$$

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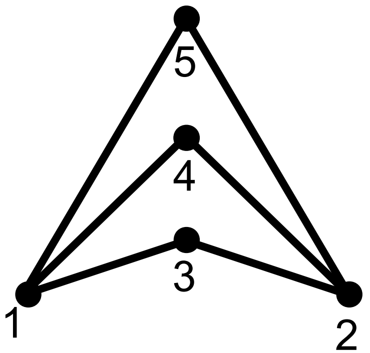
$G =$ 

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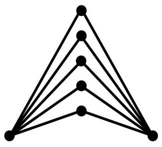
- Existence of MLE in Gaussian graphical models is special **PD matrix completion problem** with rank constraint given by the number of observations.

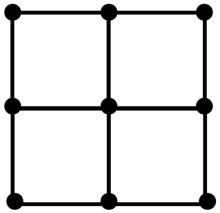
Outline

- Geometry of Dempster's theorem
  - Characterization of minimal number of observations needed

- Examples
  - Bipartite graphs $K_{2,m}$

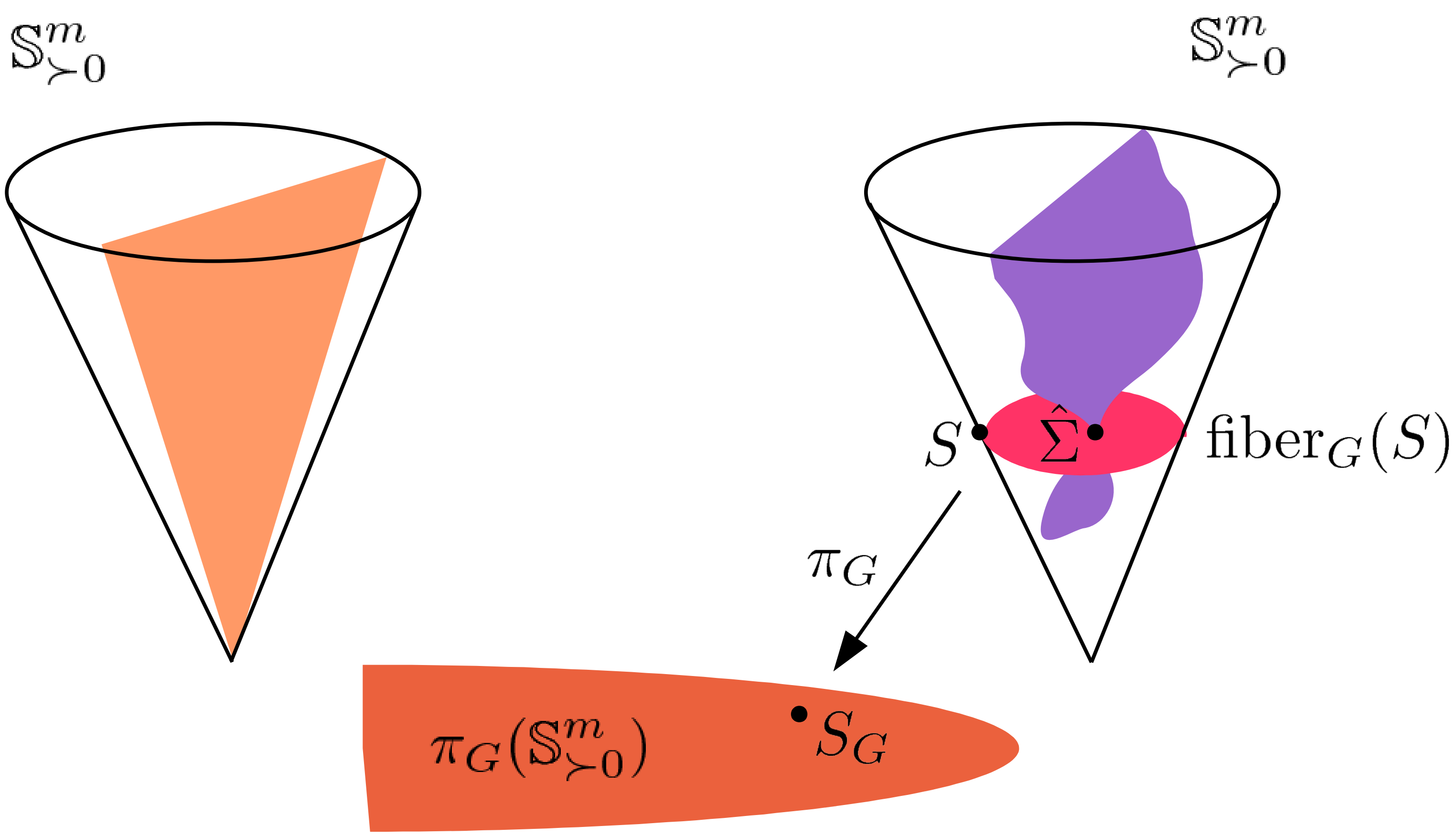


  - 3-by-3 grid



Geometry of Dempster's theorem

Concentration matrices: $K = \Sigma^{-1}$ Covariance matrices: Σ



$$\mathrm{fiber}_G(S) := \{\Sigma \in \mathbb{S}^m_{\succ 0} \mid \Sigma_G = S_G\}$$

Cones

Def: $\mathcal{C} \subset \mathbb{R}^k$ is a **convex cone** if

$$ax + by \in \mathcal{C} \quad \text{for all} \quad a, b \geq 0, \ \ x, y \in \mathcal{C}.$$

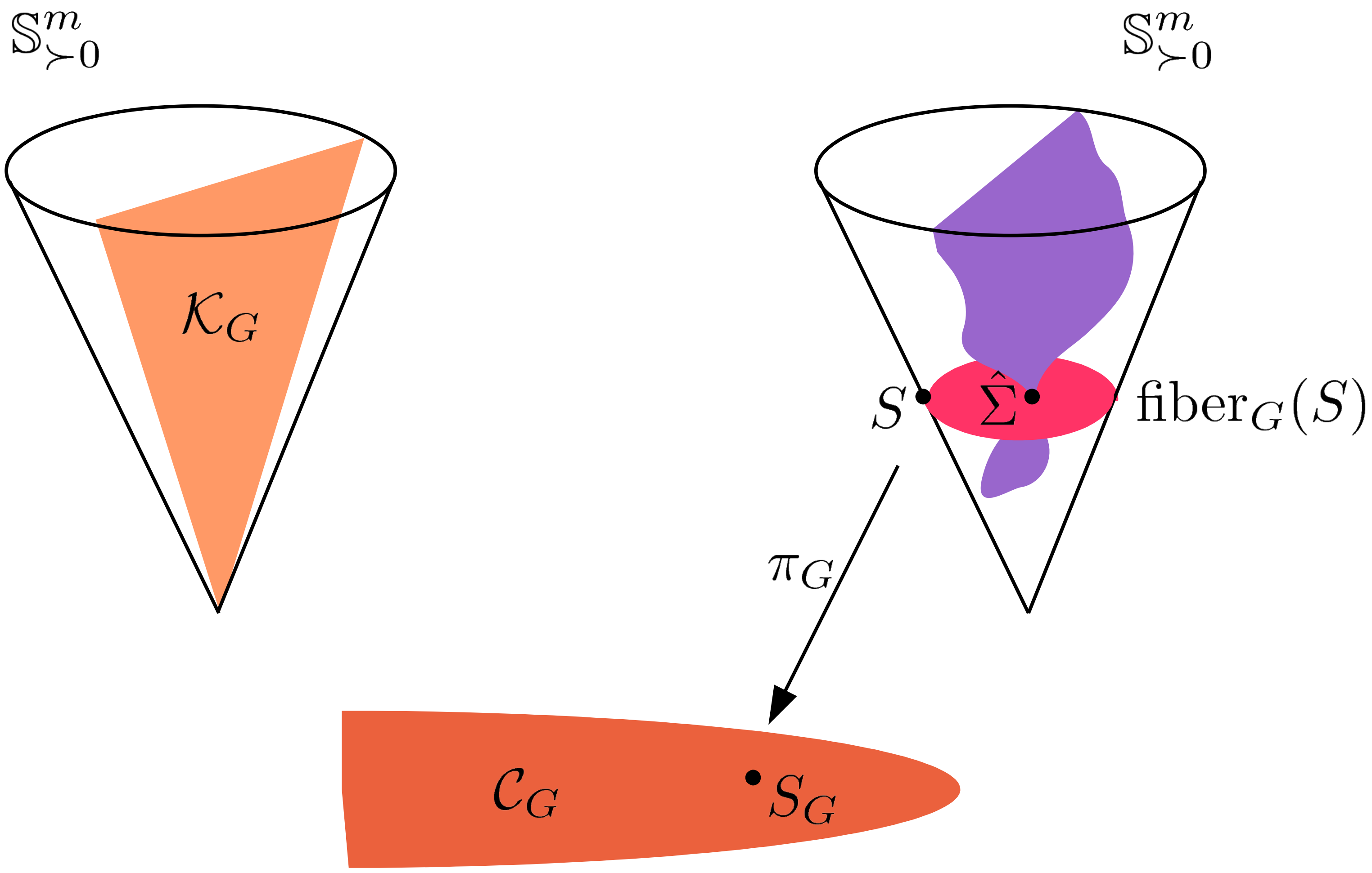
Ex: $\mathbb{R}^m_+, \ \ \mathbb{S}^m_{\succeq 0}$

- **Cone of concentration matrices:** $\mathcal{K}_G \ := \ \mathcal{G} \cap \mathbb{S}^m_{\succ 0}$
- **Cone of sufficient statistics:** $\mathcal{C}_G \ := \ \pi_G(\mathbb{S}^m_{\succ 0})$

where $\pi_G : \mathbb{S}^m \to \mathbb{R}^E, \quad S \mapsto S_G$

Geometry of ML estimation

Concentration matrices: $K = \Sigma^{-1}$ Covariance matrices: Σ



Cones and maximum likelihood estimation

Def: Let $\mathcal{C}$ be a convex cone. The **dual cone** is

$$C^* = \{w \mid \langle v, w\rangle \geq 0 \quad \text{for all } v \in \mathcal{C}\}.$$

Ex: $\mathbb{R}^m_+, \quad \mathbb{S}^m_{\succeq 0}$ are self-dual

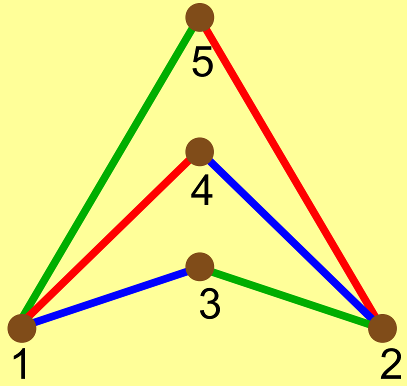
Theorem *(Sturmfels & U., 2010)*:
$\mathcal{C}_G$ is the convex dual to $\mathcal{K}_G$. Furthermore, $\overline{\mathcal{K}_G}$ and $\overline{\mathcal{C}_G}$ are closed convex cones which are dual to each other with

$$\overline{\mathcal{K}_G} = \mathcal{G} \cap \mathbb{S}^m_{\succeq 0} \qquad \text{and} \qquad \overline{\mathcal{C}_G} = \pi_G(\mathbb{S}^m_{\succeq 0}).$$

- Used this duality to find an algebraic characterization of the cone of sufficient statistics

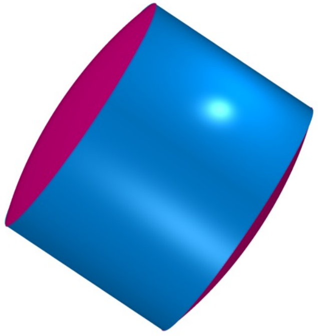
Example $K_{2,3}$

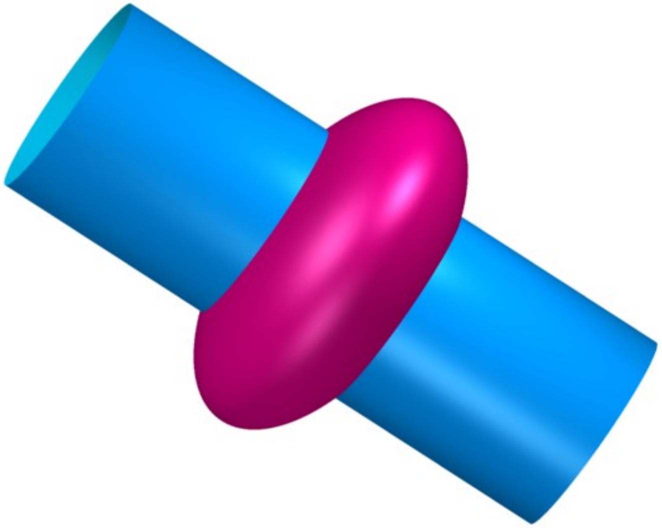
Example:



$$K = \begin{pmatrix} \lambda_1 & 0 & \lambda_2 & \lambda_3 & \lambda_4 \\ 0 & \lambda_1 & \lambda_4 & \lambda_2 & \lambda_3 \\ \lambda_2 & \lambda_4 & \lambda_1 & 0 & 0 \\ \lambda_3 & \lambda_2 & 0 & \lambda_1 & 0 \\ \lambda_4 & \lambda_3 & 0 & 0 & \lambda_1 \end{pmatrix}$$

$\mathcal{K}_G$:





Example $K_{2,3}$

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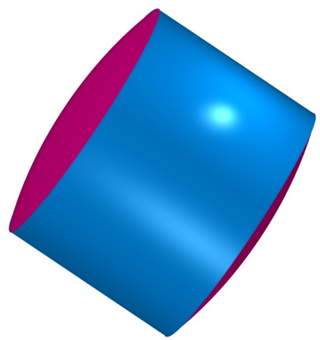
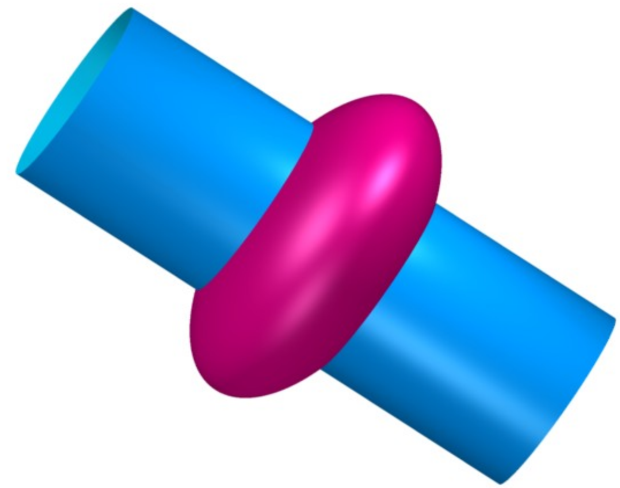
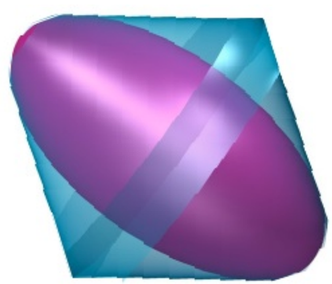
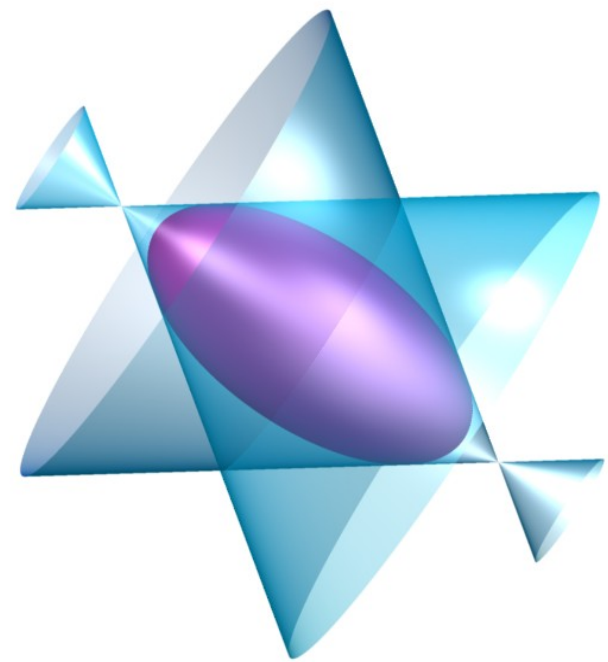




$\mathcal{C}_G$:





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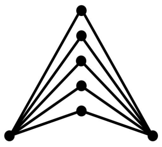

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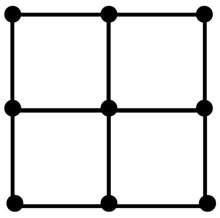
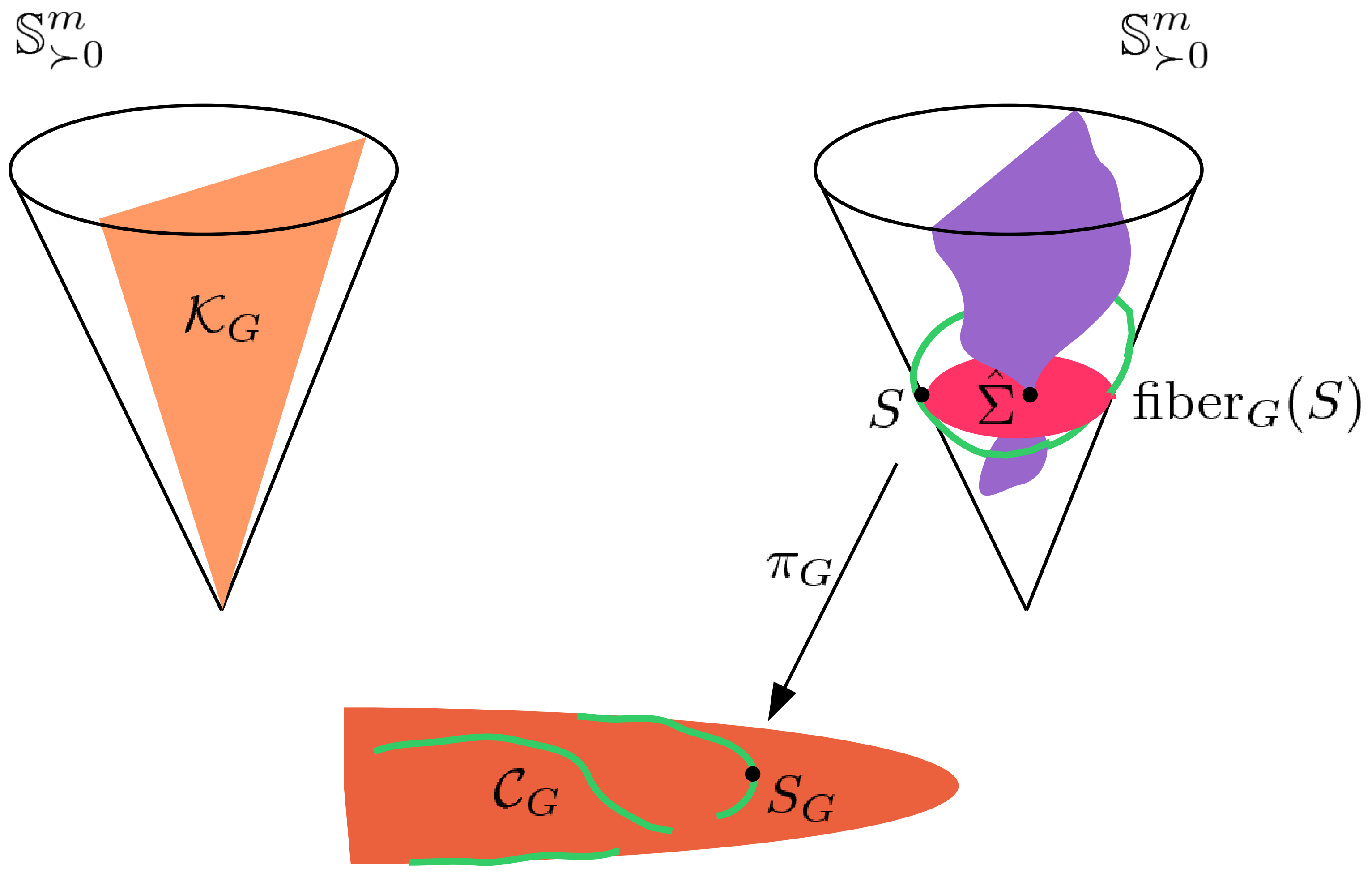


Geometry of ML estimation

Concentration matrices: $K = \Sigma^{-1}$ Covariance matrices: Σ



Sufficient condition for existence of MLE

Elimination Criterion *(U. 2010)*:

Let I_n be the ideal of $(n+1)\times(n+1)$ minors of a symmetric $m\times m$ matrix of unknowns S. Let $I_{G,n}$ be the elimination ideal obtained from I_n by eliminating all unknowns corresponding to non-edges in the graph. If

$$I_{G,n} = 0,$$

then the MLE exists with probability 1 for n observations.

- I_n corresponds to all symmetric matrices of rank $\leq n$
- Elimination corresponds to projection onto $\mathcal{C}_G$
- $I_{G,n} = 0$ means that the projection is full-dimensional

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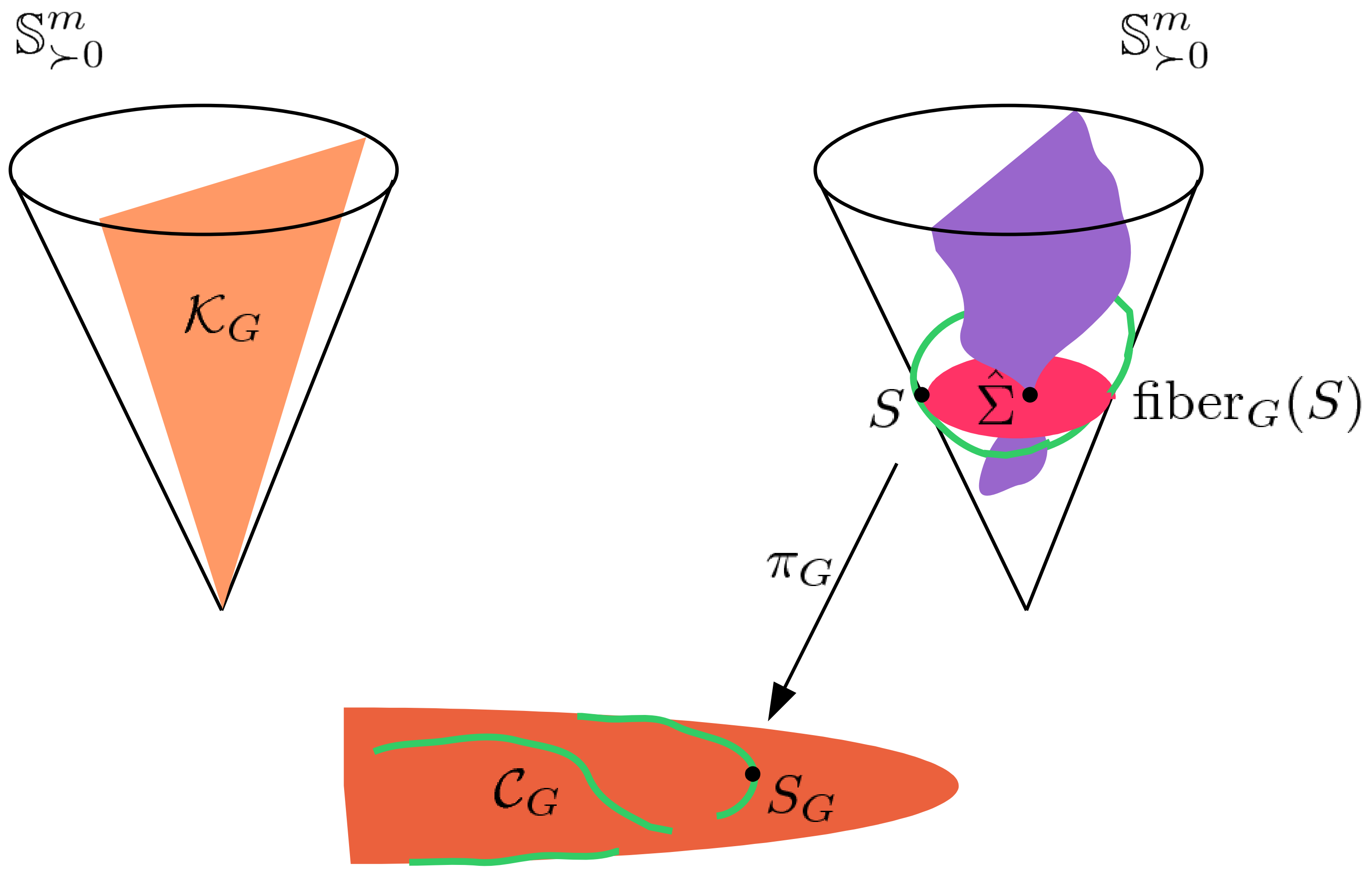

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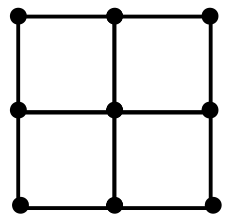
$G =$ 

Theorem (U. 2010):

The MLE on the 3-by-3 grid exists with probability 1 if $n \geq 3$ and does not exist if $n = 1$. For $n = 2$ the MLE exists with probability $\in (0, 1)$.

Solves Steffen Lauritzen's open problem

- Sturmfels & U.: Multivariate Gaussians, semidefinite matrix completion, and convex algebraic geometry (AISM 62, 2010)
- U.: Geometry of maximum likelihood estimation in Gaussian graphical models (submitted, arXiv:1012.2643v1)

Thank you!

- I am looking for a postdoc starting in September 2012 at the Institute of Science and Technology Austria.