Computational Information Geometry and Graphical Models

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Workshop on Graphical Models:
Mathematics, Statistics and Computer Science
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Overview

- Information Geometry - our embedding approach
- Focus on computation (CIG)
- Boundaries - essential for graphical models
- MCMC - geometric approach
- Curvature and mixture models
- Simplicial asymptotics - lack of uniformity

Acknowledgements

- Paul Vos
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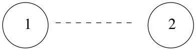
- Simon Byrne
- EPSRC
- NSERC

Information Geometry

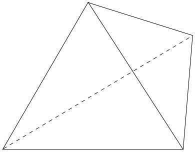
- Information geometry (M, g, ∇^{α}) [20] intrinsic
- We work by embedding in ‘space of all possible models’
- Models can be simplicial rather than manifolds: non-constant dimension
- Operational means finite dimensional
- Computational Information Geometry on extended multinomials

Discrete models

- Basic model have set of binary random variables



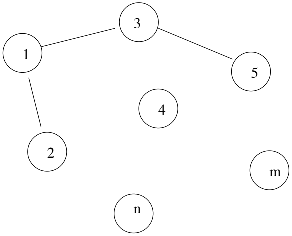
- Look at all possible joint distributions: simplex



- Models are sub-families of simplex

Extended Multinomial

- Look at discrete graphical models



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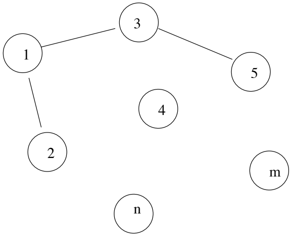
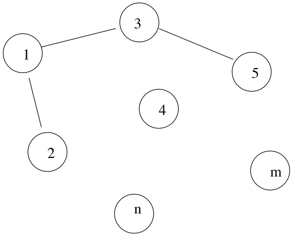


- Look at discrete graphical models
- Space of distributions simplicial

Extended Multinomial



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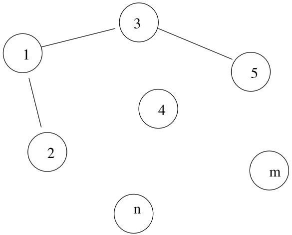
- Space of distributions simplicial
- Boundaries where probabilities are zero

Extended Multinomial



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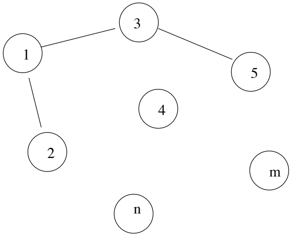
- Space of distributions simplicial
- Boundaries where probabilities are zero
- Information geometry of extended multinomial models

Extended Multinomial



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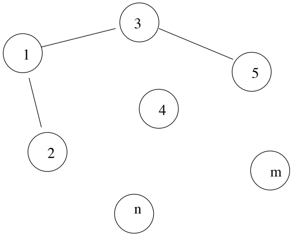
- applications to graphical models and elsewhere

Extended Multinomial



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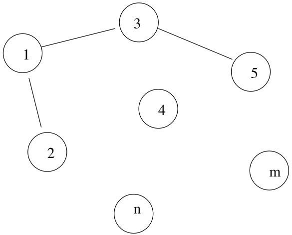
Extended Multinomial



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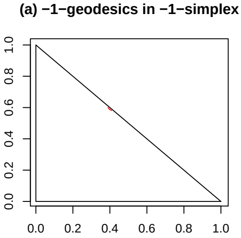
- proxy for space of all models
- IG all explicit

Information Geometry

- How to connect two probability density or mass functions $f(x)$ and $g(x)$ in some space of models?
  - -1: $\rho f(x) + (1-\rho)g(x)$
  - +1: $\frac{f(x)^{\rho} g(x)^{1-\rho}}{C(\rho)}$
- Two different affine structures used simultaneously
  - -1: Mixture affine geometry on unit measures
  - +1: Exponential affine geometry on positive measures
- Fisher Information's roles
  - measures angles and lengths
  - maps between $+1$ and -1 representations of tangent vectors, [3], [4], [19]

Visualising IG: extended trinomial example



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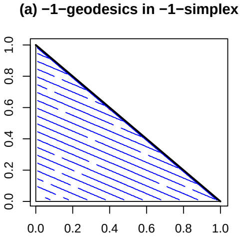

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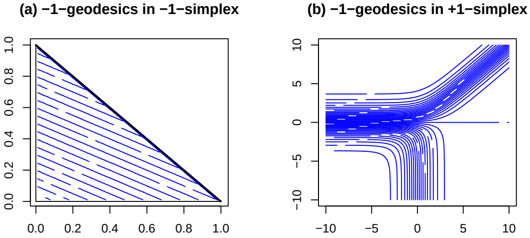

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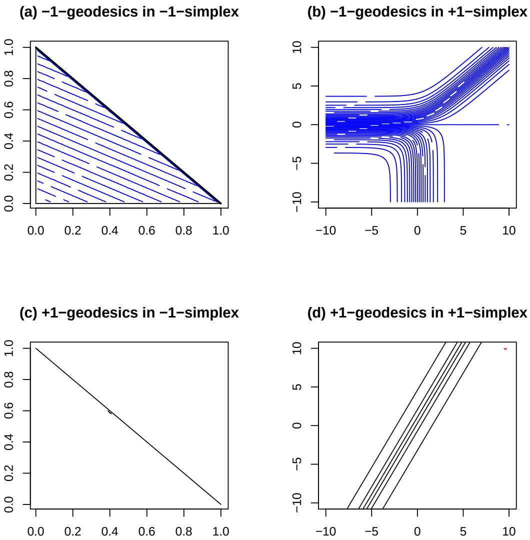

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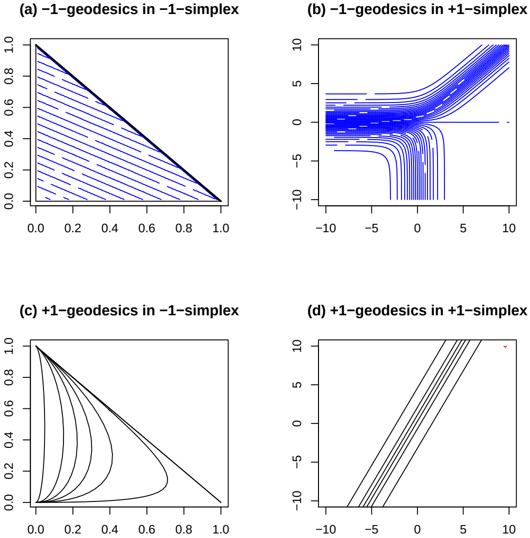

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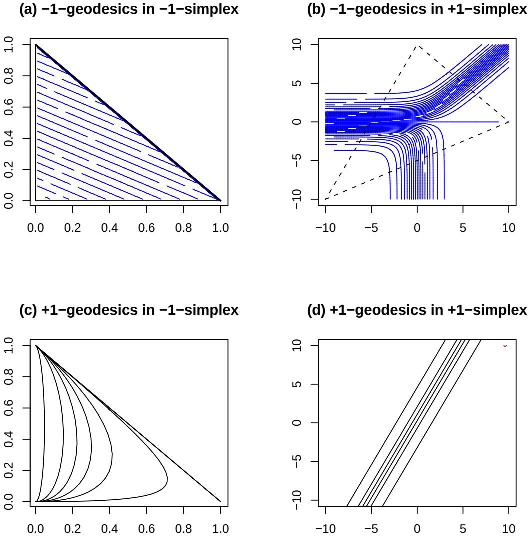
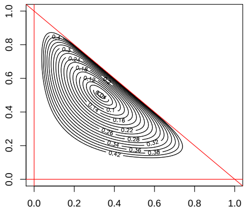


Riemannian Geometry

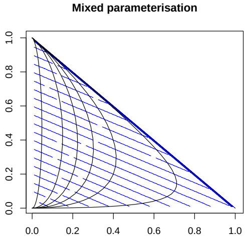
- The 0-geometry defined by the Fisher information metric
- Look at 0-geodesic spheres in simplex



- These are smoothly attached to boundary: *c.f.* ± 1-geodesics
- Can use this smooth structure in MCMC

Duality

- There exists a mixed parameterisation [6] as solution of differential equation



- -1-geodesics Fisher orthogonal to $+1$-geodesics
- Limit of mixed parameters give extended exponential family
- Key to structural theorem [3] and idea of inferential cuts

Geometry of likelihood

For sparse extended multinomial models:

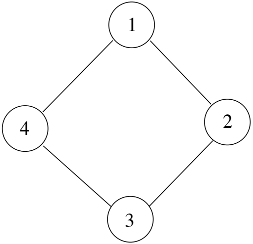
- Quadratic approximations to log-likelihood fail globally
- Many -1-flat directions
- MCMC
- Asymptotics

Examples: Graphs, Networks and IG

- Full exponential families [17]
- Very high-dimensional models [21] - MCMC is one tool here
- Curved exponential families - curvature can be very high
- Closure of exponential families- boundaries

Graphical models: FEF

- Consider the example from [14] of the cyclic graph of order 4 with binary values at each node



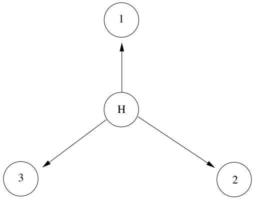
- Models lie in 15-dimensonal simplex, but with constraints imposed by conditional independence
- Constraints linear in $+1$-affine parameters

$$\eta_i + \eta_j = \eta_k + \eta_l$$

- So get 7-dimensional full exponential family

DAG with hidden variables

- In multinomials independence is expressible as a finite set of polynomial equalities
- Add hidden variables



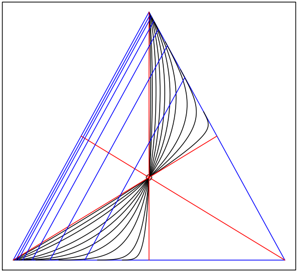
- Example lies in 7 dimensional simplex- mixes over a 3 dimensional CEF
- The model space is not a manifold but a variety- union of different dimensional manifolds- extended exponential family

Attaching to the boundaries

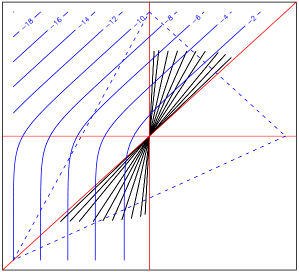
- Models are low-dimensional families within high dimensional simplexes
- Need to understand how models are attached to boundaries
- Extended exponential families: see also [30], [9]
- Need to be able to compute limit points in computationally efficient way
- Use linear programming and convex geometry techniques
- The following plot is generic

Attaching to the boundaries

Minus 1 plot



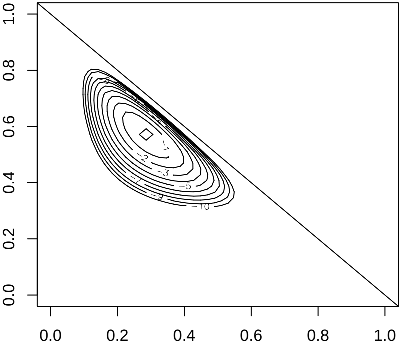
Plus 1 plot



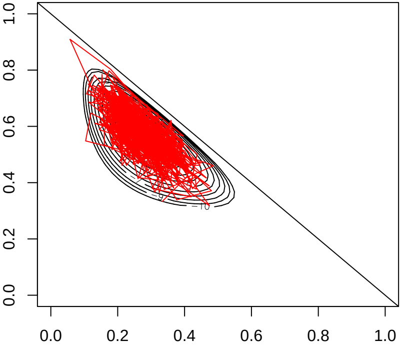
Geometric MCMC

- When doing MCMC on models the boundaries matter
- Riemann manifold Metropolis adjusted Langevin algorithm, [13] uses Fisher metric structure.
- Use a Metropolis-Hastings where the random-walk proposals have variance determined by Fisher metric
- Have seen how the 0-geometry smoothly attaches the boundaries
- Other geometric approaches are under active development - cuts and mixed parameterisations

Geometric MCMC



Geometric MCMC



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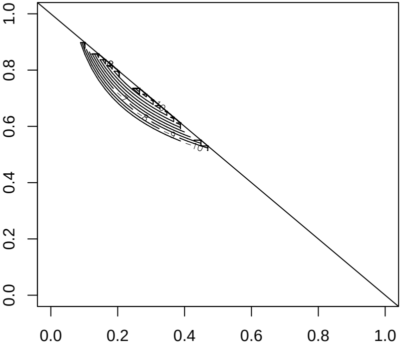

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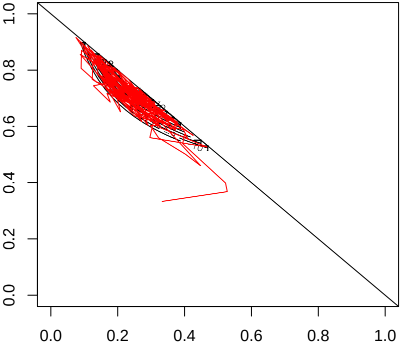
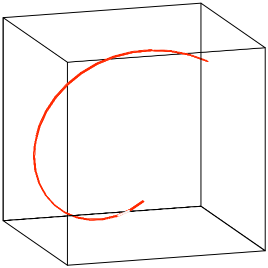
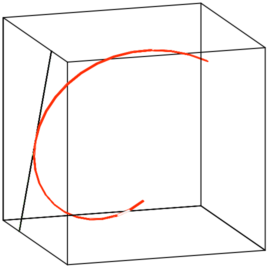


Embedding curvature and affine approximation



- Curvature(s) key part(s) of differential geometry
- Tangent space gives best linear approximation
- Tangent and curvature gives best two dimensional affine embedding space

Embedding curvature and affine approximation



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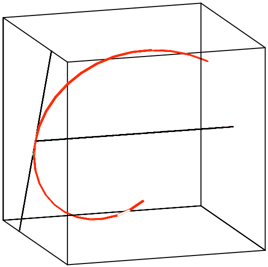

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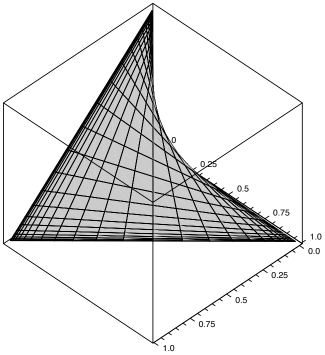
Curvature and Dimension Reduction

- Dimension reduction (best approximating subspaces) via tangent and curvature
- Different affine geometries give different dimension reduction
- Low dimensional $+1$-affine spaces give approximate sufficient statistics [28]
- Low dimensional -1 approximations give limits to identification and computation in mixture models [27], [2]

Example: tripod and bipod

- Use -1-affine approximations
- tri and bi pod example are ruled surfaces: exploit this for computing 2-hull



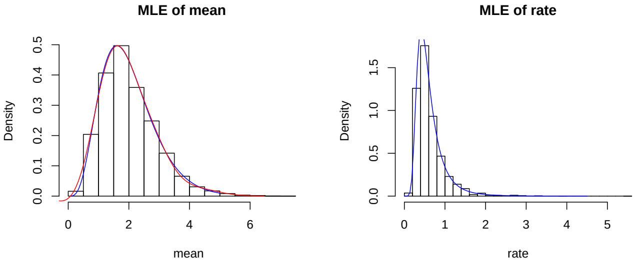
- IG gives ways to explore convex hull efficiently

Mixing paradox

- There is a paradoxical aspect to mixing in high dimensional extended multinomial model
- The convex hull of any open interval of a one-dimensional exponential family is of full dimension $\cdots$
- This is due to total positivity
- $\cdots$ But, there exist low dimensional approximations to this convex hull based on curvature, [2]

Asymptotic expansions

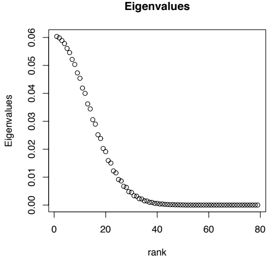
- Strong links between IG and higher order asymptotic expansions [7]
- Can apply Edgeworth, saddlepoint or Laplace expansions [32]



- Flexible, tractable given IG, invariance properties clear [3]

Asymptotic expansions

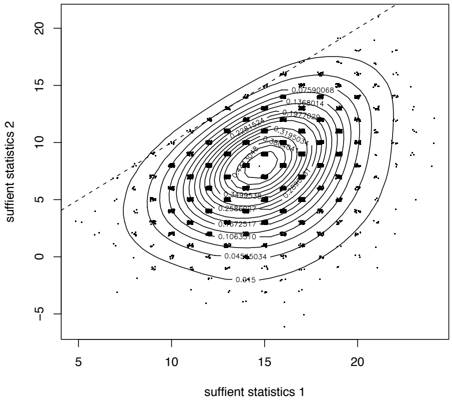
- High dimensional calculus through tensor analysis, McCullagh [29]
- Many terms need to be computed in high dimensional problems
- Singularity of Fisher information matters



- Fisher information can be singular (or infinite) [24]

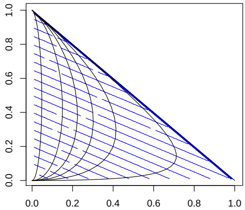
Asymptotic expansions

- Works in high dimensional examples
- Edgeworth: boundaries and discretisation effects
- Laplace expansion can be problematic in high-dimension- spectrum of FI



Asymptotic expansions

- First order Normal approximations require controlling statistical curvature
- As near boundary statistical curvature can be unbounded - most asymptotic formula not uniform across simplex



- Higher order corrections define the area where first order formula can be used
- Note centre of very high-dimensional simplex also problematic- get discretisation effects

Summary

- Information Geometry - our embedding approach
- Focus on computation (CIG)
- Boundaries - essential for graphical models
- MCMC - geometric approach
- Curvature and mixture models
- Simplicial asymptotics - lack of uniformity
- CIG useful generally in statistical modelling

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