

# Tutorial on Information Geometry and Algebraic Statistics

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Algebraic Statistics

Genova, June 11, 2015

# Gradient Descent in Learning and Optimization

The use of **natural gradient descent** in statistics and machine learning was first proposed by Amari in 1998

- ▶ Policy Learning in Reinforcement Learning
- ▶ Neural Networks Training
- ▶ Bayesian Variational Inference
- ▶ **Stochastic Relaxation**

# Black-box Optimization

Suppose we want to optimize a function  $f : \Omega \rightarrow \mathbb{R}$ , **however**:

- ▶ you don't have direct access to an explicit formula for  $f$
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One naïve approach is a **local search**:

0. define a neighborhood function  $\mathcal{V}(\mathbf{x}) \subset \Omega$   
 $t = 0$   
 $\mathbf{x}_0$  chosen randomly
1.  $\mathbf{x}_{t+1} = \arg \max_{\mathbf{x} \in \mathcal{V}(\mathbf{x}_t)} f(\mathbf{x})$
2.  $t = t + 1$
3. repeat 1-2 until convergence

# Local Search Has Some Drawbacks

- ▶ For  $\Omega = \mathbb{R}^n$ , gradient **cannot** be evaluate directly, since  $f$  is unknown
- ▶ The choice of the  $\mathcal{V}(x)$  may determine **premature convergence** to local minima

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- ▶ For large  $\mathcal{V}(x)$ , the search space can be sampled: **random search**

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As an alternative approach, we can introduce a **statistical model** to **guide** the search for the optimum

A probability density function over  $\Omega$  can be used to concentrate probability mass around certain regions of the search space

## Some Notation: Finite Case

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- ▶  $\Delta_n$  the  $n$ -dimensional probability simplex
- ▶  $\mathcal{M} = \{p(\mathbf{x}; \boldsymbol{\xi}) : \boldsymbol{\xi} \in \Xi\} \subset \Delta$  a parametrized statistical model
- ▶  $\boldsymbol{\xi} = (\xi_1, \dots, \xi_d)$  a parameter vector for  $p$

# Stochastic Relaxation

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[Remark 2] Candidate solutions for P can be obtained by sampling

# Optimization over a Statistical Manifold

We introduce a chart  $\xi$  over  $\mathcal{M} = \{p(\boldsymbol{x}; \xi) : \xi \in \Xi\}$

Let  $F(\xi) = \mathbb{E}_{\xi}[f]$ , we have a **parametric representation** (in coordinates) of the SR

$$(\text{SR}) \quad \inf_{\xi \in \Xi} F(\xi)$$

## A Few Remarks

We move the search onto a statistical model, from a discrete optimization problem over  $\Omega$  to a **continuous** problem over  $\mathcal{M}$

In the parametric representation of  $F$ , the parameters  $\xi$  become the new **variables** of the SR

Since  $\xi \in \Xi$ , we may have a **constrained** formulation for the SR



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Since  $\xi \in \Xi$ , we may have a **constrained** formulation for the SR

[Remark 3] The SR **does not** provide **lower bounds** for P, indeed

$$\min_{\mathbf{x} \in \Omega} f(\mathbf{x}) \leq F(p) \leq \max_{\mathbf{x} \in \Omega} f(\mathbf{x})$$

Let  $\mathcal{M} = \Delta$ ,  $\min_{\mathbf{x} \in \Omega} f(\mathbf{x}) = \min_{p \in \Delta} F(p)$

More in general, for  $\mathcal{M} \subset \Delta$ ,  $\min_{\mathbf{x} \in \Omega} f(\mathbf{x}) \leq \inf_{p \in \mathcal{M}} F(p)$

## Closure of $\mathcal{M}$

We denote with  $\overline{\mathcal{M}}$  the **topological closure** of  $\mathcal{M}$ , i.e.,  $\mathcal{M}$  together with the limits of (weakly convergent) sequences of distributions

Moreover, we suppose  $\overline{\mathcal{M}}$  is **compact** so that by the extreme value theorem  $F(p)$  attains its minimum over  $\overline{\mathcal{M}}$

# Equivalence of P and SR

Let us denote the optimal solutions with:

- ▶  $\boldsymbol{x}^* \in \Omega^* = \arg \min_{\boldsymbol{x} \in \Omega} f(\boldsymbol{x})$
- ▶  $p^* \in P^* = \arg \min_{p \in \overline{\mathcal{M}}} F(p)$

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The SR is equivalent to P if  $p^*(\mathbf{x}^*) = 1$ , i.e., we can sample optimal solutions of P from optimal solutions of SR with probability one

In other words, there must exist a sequence  $\{p_t\}$  in  $\mathcal{M}$  such that

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A **sufficient condition** for the equivalence of SR and P is that all Dirac distribution  $\delta_x$  are included in  $\overline{\mathcal{M}}$

# How to solve the SR?

The SR in an optimization problem defined over a statistical model

It can be solved in many different ways, here we focus on **natural gradient descent**

$$\boldsymbol{\xi}^{t+1} = \boldsymbol{\xi}^t - \lambda \nabla F(\boldsymbol{\xi}), \quad \lambda > 0$$

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Some references:

- ▶ Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES), Hansen et al., 2001
- ▶ Natural Evolutionary Strategies (NES), Wierstra et al., 2008
- ▶ Stochastic Natural Gradient Descent (SNGD), M. et al., 2011
- ▶ Information Geometry Optimization (IGO), Arnold et al., 2011

## Which Model to Choose in the SR?

Let  $n$  be the cardinality of  $\Omega$ , to parametrize  $\Delta$  we need  $n - 1$  parameters

Minimizing  $F(p)$  with  $p \in \Delta$  is equivalent to an exhaustive search!



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We need a **low-dimensional** models in the SR

- ▶ The equivalence of P and SR can be easily guaranteed
- ▶ The **landscape** (number of local minima) of  $F(p)$  depends on the choice of  $\mathcal{M}$
- ▶ In practice we need to learn  $\mathcal{M}$ : **model selection**
- ▶ Often it is conveniente to employ graphical models

# Pseudo-Boolean Optimization

Consider the case where  $\Omega = \{+1, -1\}^n$ , where we use the **harmonic** encoding  $\{+1, -1\}$  for a binary variable

$$-1^0 = +1 \qquad -1^1 = -1$$

A **pseudo-Boolean function**  $f$  is a real-valued mapping

$$f(x) : \Omega = \{+1, -1\}^n \rightarrow \mathbb{R}$$

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$$f(\mathbf{x}) : \Omega = \{+1, -1\}^n \rightarrow \mathbb{R}$$

Any  $f$  can be expanded uniquely as a square free polynomial

$$f(\mathbf{x}) = \sum_{\alpha \in L} c_{\alpha} \mathbf{x}^{\alpha},$$

by employing a **multi-index** notation. Let  $L = \{0, 1\}^n$ , then  $\alpha = (\alpha_1, \dots, \alpha_n) \in L$  uniquely identifies the monomial  $\mathbf{x}^{\alpha}$  by

$$\alpha \mapsto \prod_{i=1}^n x_i^{\alpha_i}$$

# Monomial Representation of PS Functions

Let  $A^n = \underbrace{A^1 \otimes \dots \otimes A^1}_{n \text{ times}}$ , where  $\otimes$  denotes the Kronecker product

$$A^1 = \begin{matrix} & \begin{matrix} 0 & 1 \end{matrix} \\ \begin{matrix} + \\ - \end{matrix} & \begin{bmatrix} +1 & +1 \\ +1 & -1 \end{bmatrix} \end{matrix}$$

let  $\mathbf{a} = (f(\mathbf{x}))_{\mathbf{x} \in \Omega}$ , we have  $A^n \mathbf{c} = \mathbf{a}$ ,  $\mathbf{c} = (c_\alpha)_{\alpha \in L}$  and  $\mathbf{c} = 2^{-n} A^n \mathbf{a}$

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[Example] In case of two variables  $\mathbf{x} = (x_1, x_2)$ , we have

$$f(\mathbf{x}) = c_0 + c_1 x_1 + c_2 x_2 + c_{12} x_1 x_2$$

$x_1$	$x_2$	$f(\mathbf{x})$
+1	+1	$a_{++}$
+1	-1	$a_{+-}$
-1	+1	$a_{-+}$
-1	-1	$a_{--}$

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# The Independence Model

Let  $\mathcal{I}$  be the **independence model** for  $\mathbf{X} = (X_1, \dots, X_n)$

$$\mathcal{I} = \{p : p(\mathbf{x}) = \prod_{i=1}^n p_i(x_i)\}$$

with marginal probabilities  $p_i(x_i) = \mathbb{P}(X_i = x_i)$

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We parametrize  $\mathcal{I}$  using  $\{\pm 1\}$  Bernoulli distributions for  $X_i$

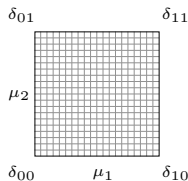
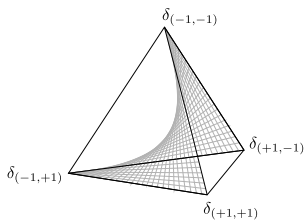
$$\begin{aligned} p(\mathbf{x}; \boldsymbol{\mu}) &= \prod_{i=1}^n \mu_i^{(1+x_i)/2} (1 - \mu_i)^{(1-x_i)/2} \\ &= \prod_{i=1}^n (2\mu_i x_i - x_i + 1) / 2 \end{aligned}$$

with  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n) \in [0, 1]^n$  and

$$\begin{aligned} \mu_i &= \mathbb{P}(X_i = +1) \\ 1 - \mu_i &= \mathbb{P}(X_i = -1) \end{aligned}$$



# Marginal Parameters for the Independence Model



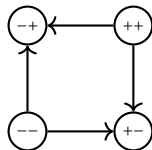
$\mathcal{I}$  is a  $n$ -dimensional manifold embedded in the  $2^n - 1$  dimensional probability simplex  $\Delta$

## A Toy Example

Let  $n = 2$ ,  $\Omega = \{-1, +1\}^2$ , we want to minimize

$$f(\mathbf{x}) = x_1 + 2x_2 + 3x_1x_2$$

$x_1$	$x_2$	$f$
+1	+1	6
+1	-1	-4
-1	+1	-2
-1	-1	0

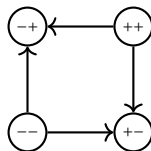


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The **gradient flow** is the solution of the differential equation

$$\dot{\xi} = \nabla F(\xi),$$

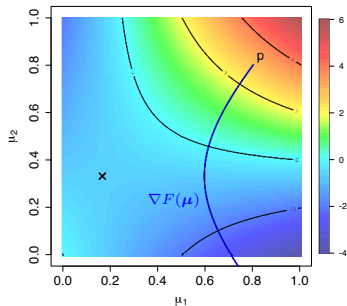
We are interested in studying gradient flows for different parameterization and different statistical models

# Gradient Flows on the Independence Model

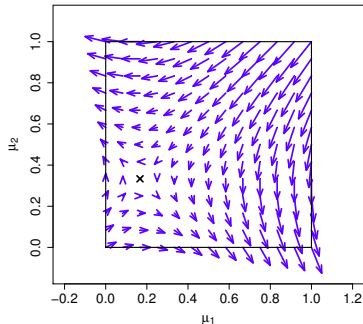
$$F(\boldsymbol{\mu}) = \sum_{\mathbf{x} \in \Omega} f(\mathbf{x}) p_1(x_1) p_2(x_2) = -4\mu_1 - 2\mu_2 + 12\mu_1\mu_2$$

$$\nabla F(\boldsymbol{\mu}) = (-4 + 12\mu_2, -2 + 12\mu_1)^T$$

Gradient flow in  $\boldsymbol{\mu}$



Gradient vector in  $\boldsymbol{\mu}$ ,  $\lambda = 0.025$

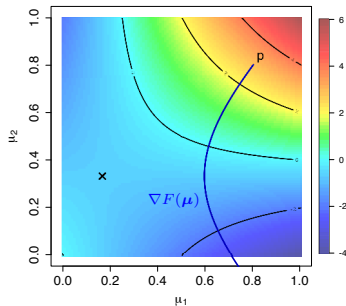


# Gradient Flows on the Independence Model

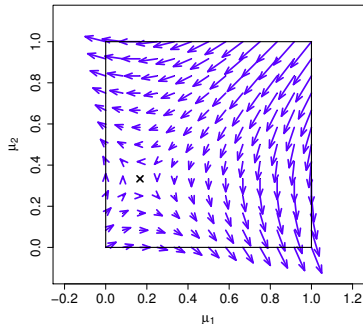
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Gradient flow in  $\boldsymbol{\mu}$



Gradient vector in  $\boldsymbol{\mu}$ ,  $\lambda = 0.025$



$\nabla F(\boldsymbol{\eta})$  does not converge to (local) optima, a projection over the hyperplanes given by the constraints is required

# Natural Parameters for the Independence Model

If we restrict to positive probabilities  $p > 0$ , we can represent the interior of the independence model as the **exponential family**

$$p(\mathbf{x}; \boldsymbol{\theta}) = \exp \left\{ \sum_{i=1}^n \theta_i x_i - \psi(\boldsymbol{\theta}) \right\}$$

where  $\psi(\boldsymbol{\theta}) = \ln Z(\boldsymbol{\theta})$  is the log partition function

The **natural parameters** of the independence model  $\mathcal{M}_1$  represented by an exponential family are  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_n) \in \mathbb{R}^n$ , with

$$p_i(x_i) = \frac{e^{\theta_i x_i}}{e^{\theta_i} + e^{-\theta_i}}$$

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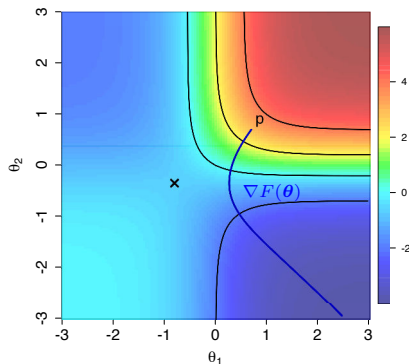
The mapping between **marginal probabilities** and **natural parameters** is one-to-one for  $p > 0$

$$\theta_i = (\ln(\mu_i) - \ln(1 - \mu_i)) / 2 \qquad \mu_i = \frac{e^{\theta_i}}{e^{\theta_i} + e^{-\theta_i}}$$

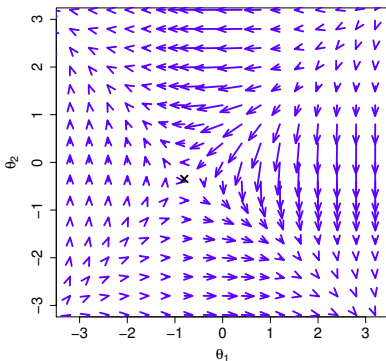
# Gradient Flows on the Independence Model

$$F(\boldsymbol{\theta}) = (-4e^{\theta_1 - \theta_2} - 2e^{-\theta_1 + \theta_2} + 6e^{\theta_1 + \theta_2})/Z(\boldsymbol{\theta})$$
$$\nabla F(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[f(\mathbf{X} - \mathbb{E}_{\boldsymbol{\theta}}[\mathbf{X}])] = \text{Cov}_{\boldsymbol{\theta}}(f, \mathbf{X})$$

Gradient flow in  $\boldsymbol{\theta}$



Gradient vectors in  $\boldsymbol{\theta}$ ,  $\lambda = 0.15$

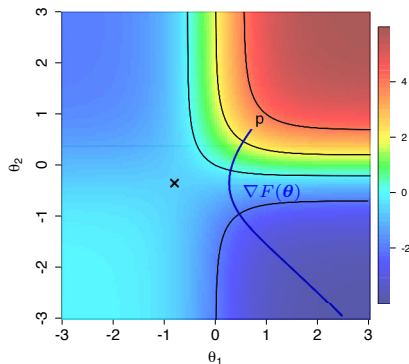




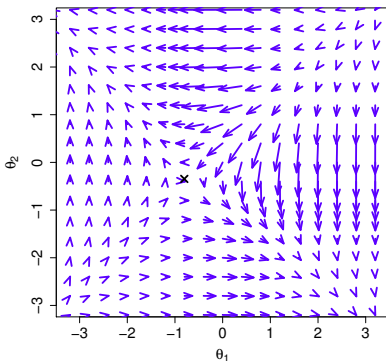
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Gradient flow in  $\boldsymbol{\theta}$



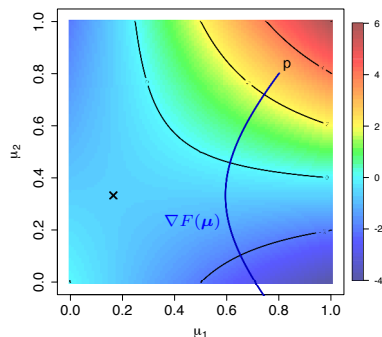
Gradient vectors in  $\boldsymbol{\theta}$ ,  $\lambda = 0.15$



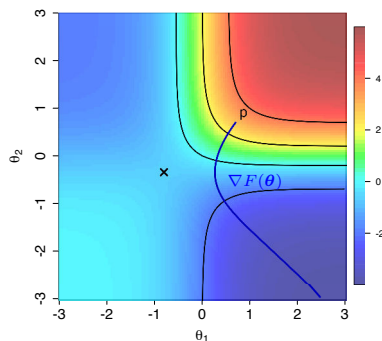
In the  $\boldsymbol{\theta}$  parameters,  $\nabla F(\boldsymbol{\theta})$  vanishes over the plateaux

# Gradient Flows on the Independence Model

Marginal probabilities  $\mu$

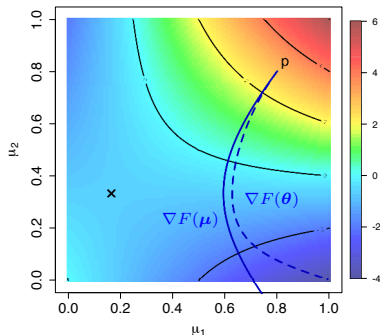


Natural parameters  $\theta$

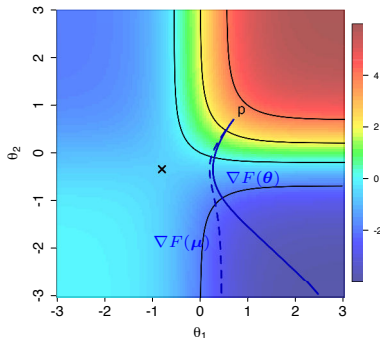


# Gradient Flows on the Independence Model

Marginal probabilities  $\mu$



Natural parameters  $\theta$



Gradient flows  $\nabla F(\xi)$  depend on the parameterization

In the  $\eta$  parameters,  $\nabla F(\eta)$  does not converge to the expected distribution  $\delta_{x^*}$  over an optimum

# The Exponential Family

In the following, we consider models in the **exponential family**  $\mathcal{E}$

$$p(\mathbf{x}, \boldsymbol{\theta}) = \exp\left(\sum_{i=1}^m \theta_i T_i(\mathbf{x}) - \psi(\boldsymbol{\theta})\right)$$

- ▶ sufficient statistics  $\mathbf{T} = (T_1(\mathbf{x}), \dots, T_m(\mathbf{x}))$
- ▶ natural parameters  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_m) \in \Theta \subset \mathbb{R}^m$
- ▶ log-partition function  $\psi(\boldsymbol{\theta})$

# The Exponential Family

In the following, we consider models in the **exponential family**  $\mathcal{E}$

$$p(\mathbf{x}, \boldsymbol{\theta}) = \exp\left(\sum_{i=1}^m \theta_i T_i(\mathbf{x}) - \psi(\boldsymbol{\theta})\right)$$

- ▶ sufficient statistics  $\mathbf{T} = (T_1(\mathbf{x}), \dots, T_m(\mathbf{x}))$
- ▶ natural parameters  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_m) \in \Theta \subset \mathbb{R}^m$
- ▶ log-partition function  $\psi(\boldsymbol{\theta})$

Several statistical models belong to the exponential family, both in the continuous and discrete case, among them

- ▶ the independence model
- ▶ Markov random fields
- ▶ multivariate Gaussians

# Markov Random Fields

[Recall] The monomials  $\{\mathbf{x}^\alpha\}, \alpha \in L$ , define a basis for  $f$

By choosing a **subset** of  $\{\mathbf{x}^\alpha\}$  as sufficient statistics, we can identify a low-dimensional exponential family parametrized by  $\theta$

$$p(\mathbf{x}; \theta) = \exp \left( \sum_{\alpha \in M \subset L_0} \theta_\alpha \mathbf{x}^\alpha - \psi(\theta) \right), \quad L_0 = L \setminus \{0\}$$

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We have an interpretation for the topology of the model

- ▶ The absence of edges in an undirected graphical model implies conditional independence among variables
- ▶ Joint probability distributions factorize over the cliques

# Dual Parameterization for the Exponential Family

$$p(\mathbf{x}; \boldsymbol{\theta}) = \exp \left( \sum_{i=1}^m \boldsymbol{\theta}_i T_i(\mathbf{x}) - \psi(\boldsymbol{\theta}) \right)$$

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- ▶ Let  $\varphi(\boldsymbol{\eta})$  be the negative entropy of  $p$ , then  $\boldsymbol{\theta}$  and  $\boldsymbol{\eta}$  are connected by the Legendre transform

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The **natural parameters**  $\theta = (\theta_\alpha)$ ,  $\alpha \in L$ , can be obtained from raw probabilities, with the constraint  $\theta_0 = -\log \mathbb{E}_\theta[\exp \sum_{\alpha \in L \setminus \{0\}} \theta_\alpha x^\alpha]$

$$\ln \rho = 2^{-n} A^n \theta \qquad \theta = A^n \ln \rho$$

# Mixed Parametrization for Markov Random Fields

An exponential family  $\mathcal{M}$  given by the sufficient statistics  $\{\boldsymbol{x}^\alpha\}, \alpha \in M$ , identifies a submanifold in  $\Delta$ , parametrized by  $\boldsymbol{\theta} = ((\boldsymbol{\theta})_{\alpha \in M}; \mathbf{0})$

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Due to the **duality** between  $\boldsymbol{\theta}$  and  $\boldsymbol{\eta}$ , we can employ a **mixed parametrization** for  $\mathcal{M}$  and parametrize the model as  $(\boldsymbol{\eta}_{\alpha \in M}; \mathbf{0})$

# Algebraic Statistics: Invariants in $\rho$ and $\eta$

[Example] Let  $n = 2$ , we consider the independence model parametrized by  $(\theta_1, \theta_2; 0)$ , with  $\theta_{12} = 0$

The same model can be parametrized by  $(\eta_1, \eta_2; 0)$ , we show  $\eta_{12} = \eta_1 \eta_2$

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The same model can be parametrized by  $(\eta_1, \eta_2; 0)$ , we show  $\eta_{12} = \eta_1 \eta_2$

Since  $\theta = A^n \ln \rho$ , by imposing  $\theta_{12} = 0$  we have

$$\ln \rho_{++} + \ln \rho_{--} = \ln \rho_{+-} + \ln \rho_{-+}$$

$$\rho_{++}\rho_{--} = \rho_{+-}\rho_{-+}$$

$$\begin{bmatrix} \rho_{++} \\ \rho_{+-} \\ \rho_{-+} \\ \rho_{--} \end{bmatrix} = \frac{1}{4} \times \begin{matrix} & \begin{matrix} 00 & 10 & 01 & 11 \end{matrix} \\ \begin{matrix} ++ \\ +- \\ -+ \\ -- \end{matrix} & \begin{bmatrix} +1 & +1 & +1 & +1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & -1 & -1 & +1 \end{bmatrix} \end{matrix} \begin{bmatrix} 1 \\ \eta_1 \\ \eta_2 \\ \eta_{12} \end{bmatrix}$$

$$(1 + \eta_1 + \eta_2 + \eta_{12})(1 - \eta_1 - \eta_2 + \eta_{12}) = (1 + \eta_1 - \eta_2 - \eta_{12})(1 - \eta_1 + \eta_2 - \eta_{12})$$

$$\eta_{12} = \eta_1 \eta_2$$

# Marginal Polytope

The range of the expectation parameters  $\boldsymbol{\eta} = \mathbb{E}_{\boldsymbol{\theta}}[\boldsymbol{T}]$  identifies a polytope  $M$  in  $\mathbb{R}^m$  called the **marginal polytope**

The marginal polytope can be obtained as the convex hull of  $\boldsymbol{T}(\Omega)$ , there  $\boldsymbol{T}$  is the vector of sufficient statistics of the model

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[Example] Let  $n = 2$ ,  $\boldsymbol{T} = (x_1, x_1x_2)$

$$A = \begin{array}{cc} & \begin{array}{cc} x_1 & x_1x_2 \end{array} \\ \begin{array}{c} ++ \\ +- \\ -+ \\ -- \end{array} & \left[ \begin{array}{cc} -1 & +1 \\ +1 & -1 \\ +1 & +1 \\ -1 & -1 \end{array} \right] \end{array}$$

Convex hull of

$(+1, +1)$

$(+1, -1)$

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The marginal polytope corresponds to the domain for the  $\eta$  parameters in the SR

- ▶ For the independence model  $M = [-1, 1]^n$
- ▶ For the saturated model  $M = \Delta$
- ▶ In the other cases, things can get very “nasty”, indeed the number of its faces can grow more than exponentially in  $n$

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[Example] Let  $n = 3$ , consider the exponential model with sufficient statistics given by

$$\{x_1, x_2, x_3, x_{12}, x_{23}, x_{13}\}$$

then the number of hyperplanes of  $M$  is 16



# Information Geometry

The geometry of statistical models is not Euclidean

We need tools from [differential geometry](#) to define notions such as tangent vectors, shortest paths and distances between distributions

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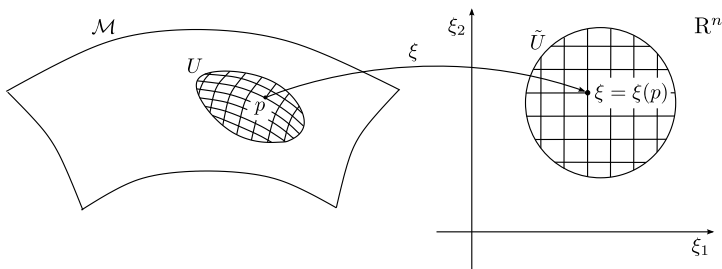
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Why  $\tilde{\nabla}_{\xi} F(\xi)$  and not just  $\nabla_{\xi} F(\xi)$  ?

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[Short answer]

The geometry of  $\mathcal{M}$  is not Euclidean

$\tilde{\nabla}_{\xi} F(\xi)$  is the **natural gradient**, i.e., the direction of **steepest descent** evaluated over a statistical model

In general  $\tilde{\nabla}_{\xi} F(\xi)$  does not coincide with the vector of **partial derivatives** with respect to  $\xi$  denoted by  $\nabla_{\xi} F(\xi)$

# Amari's Natural Gradient

[Longer answer]

Let  $\mathcal{M}$  be a **statistical manifold** endowed with the metric  $I = [g_{ij}]$ ,  
and let  $F(p) : \mathcal{M} \mapsto \mathbb{R}$  be smooth function

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Let  $\mathcal{M}$  be a **statistical manifold** endowed with the metric  $I = [g_{ij}]$ , and let  $F(p) : \mathcal{M} \mapsto \mathbb{R}$  be smooth function

For each vector field  $U$  over  $\mathcal{M}$ , the **natural gradient**  $\tilde{\nabla} F$ , is the unique vector that satisfies

$$\langle \tilde{\nabla} F, U \rangle_g = D_U F,$$

where  $D_U F$  is the **directional derivative** of  $F$  in the direction of  $U$

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Given a **coordinate chart** (a parameterization)  $\xi$  for  $\mathcal{M}$ , the representation in coordinates of  $\tilde{\nabla}_\xi F(\xi)$  reads

$$\tilde{\nabla}_\xi F(\xi) = \sum_{i=1}^k \sum_{j=1}^k g^{ij} \frac{\partial F(\xi)}{\partial \xi_i} \frac{\partial}{\partial \xi_j} = I_\xi(\xi)^{-1} \nabla_\xi F(\xi)$$



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The metric for  $\mathcal{M}$  is the **Fisher information matrix**

# Geometry of the Exponential Family

In case of a finite sample space  $\Omega$ , we have

$$p(\mathbf{x}; \boldsymbol{\theta}) = \exp\left(\sum_{i=1}^m \theta_i T_i(\mathbf{x}) - \psi(\boldsymbol{\theta})\right) \quad \boldsymbol{\theta} \in \mathbb{R}^m$$

and

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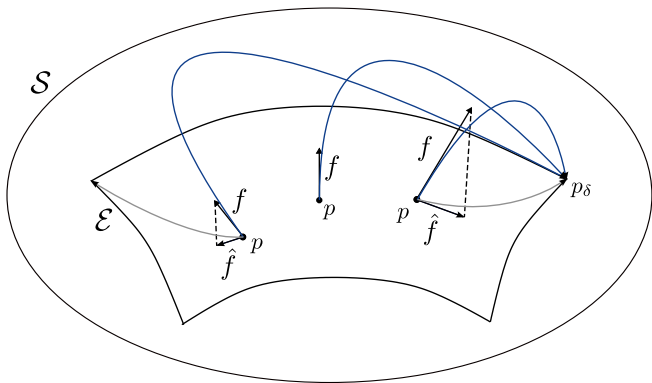
Since  $\nabla F(\boldsymbol{\theta}) = \text{Cov}_{\boldsymbol{\theta}}(f, T)$ , if  $f \in \mathbb{T}_p$ , the steepest direction is given by  $f - \mathbb{E}_{\boldsymbol{\theta}}[f]$ , otherwise we take the projection  $\widehat{f}$  of  $f$  onto  $\mathbb{T}_p$

$$\widehat{f} = \sum_{i=1}^m \widehat{a}_i (T_i(\mathbf{x}) - \mathbb{E}_{\boldsymbol{\theta}}[T_i]),$$

and obtain  $\widehat{f}$  by solving a system of linear equations

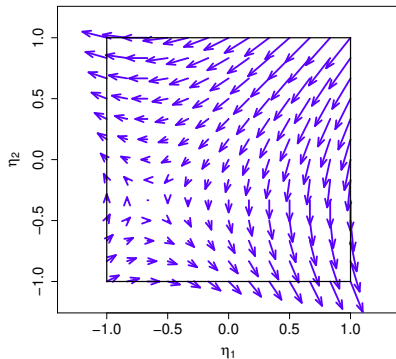
# The Big Picture

If  $f \notin T_p$ , the projection  $\hat{f}$  may vanish, and local minima may appear



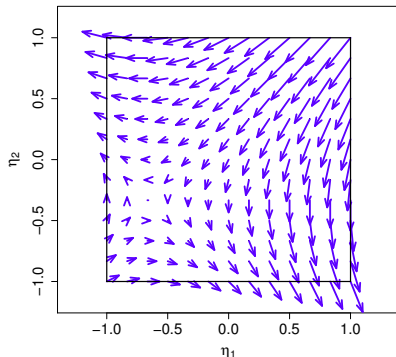
# Vanilla vs Natural Gradient: $\eta, \lambda = 0.05$

Vanilla gradient  $\nabla F(\eta)$

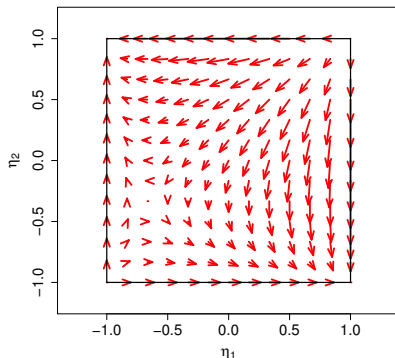


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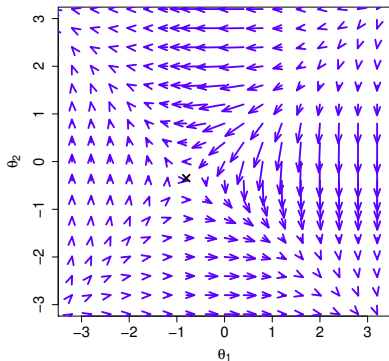
Natural gradient  $\tilde{\nabla} F(\eta)$



In both cases there exist two basins of attraction, however  $\tilde{\nabla} F(\eta)$  converges to  $\delta_x$  distributions, which are local optima for  $F(\eta)$  and where  $\tilde{\nabla} F(\delta_x) = 0$

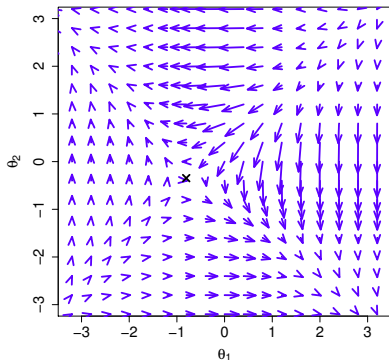
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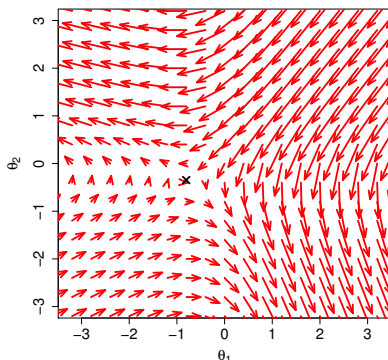


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Natural gradient  $\tilde{\nabla} F(\theta)$

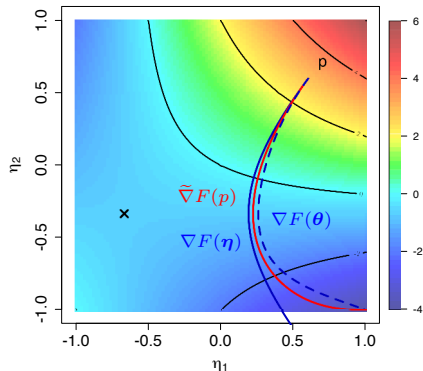


In both cases there exist two basins of attraction, however in the natural parameters  $\tilde{\nabla} F(\theta)$  “speeds up” over the plateaux

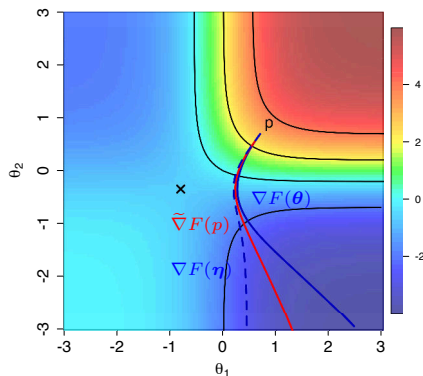


# Vanilla vs Natural Gradient

Expectation parameters  $\eta$



Natural parameters  $\theta$



Vanilla gradient  $\nabla F$  vs Natural gradient  $\tilde{\nabla} F$

The natural gradient flow is invariant to parameterization

# Stochastic Natural Gradient Descent

In the exponential family, the **natural gradient descent** updating rule reads

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \lambda I(\boldsymbol{\theta})^{-1} \nabla F(\boldsymbol{\theta}), \quad \lambda > 0$$

Unfortunately, exact gradients **cannot be computed efficiently**

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As a consequence, **stochastic natural gradient** can be estimated by replacing exact gradients with empirical estimates, so that

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \lambda \widehat{\text{Cov}}_{\boldsymbol{\theta}^t}(\mathbf{T}, \mathbf{T})^{-1} \widehat{\text{Cov}}_{\boldsymbol{\theta}^t}(f, \mathbf{T}), \quad \lambda > 0$$

## Back to the Toy Example

The landscape of  $F(\boldsymbol{\eta})$  changes according to  $f$  and  $\mathcal{M}$

[Example] Natural gradient flows in the  $\boldsymbol{\eta}$  are given by

$$\dot{\eta}_1 = (1 - \eta_1^2)(a_1 + a_{12}\eta_2)$$

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The natural gradient vanishes over

- ▶ the vertices of the marginal polytope  $\mathbf{M}$
- ▶  $\mathbf{c} = (-a_2/a_{12}, -a_1/a_{12})^T$

The **nature** of the critical points can be determined by studying the **eigenvalues** of the Hessian

$$M = \begin{bmatrix} -2\eta_1(a_1 + a_{12}\eta_2) & a_{12}(1 - \eta_1^2) \\ a_{12}(1 - \eta_2^2) & -2\eta_2(a_2 + a_{12}\eta_1) \end{bmatrix}$$

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Let  $v \in \{-1, +1\}^2$  be a vertex of  $M$ , the eigenvalues of  $H$  are

$$\lambda_1 = -2v_1(a_{12}v_2 + a_1)$$

$$\lambda_2 = -2v_2(a_{12}v_1 + a_2)$$

According to the signs of  $\lambda_1$  and  $\lambda_2$ , each vertex can be either a stable node (SN), an unstable node (UN) or a saddle point (SP)

## Back to the Toy Example: Critical Points

The solutions of the differential equations associated to the flows can be studied for every value of  $\eta$ , even outside of  $M$

Let  $v \in \{-1, +1\}^2$  be a vertex of  $M$ , the eigenvalues of  $H$  are

$$\lambda_1 = -2v_1(a_{12}v_2 + a_1)$$

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According to the signs of  $\lambda_1$  and  $\lambda_2$ , each vertex can be either a stable node (SN), an unstable node (UN) or a saddle point (SP)

For  $c = (-a_2/a_{12}, -a_1/a_{12})^T$

$$\lambda_{1,2} = \pm \sqrt{(a_{12}^2 - a_2^2)(a_{12}^2 - a_1^2)}/a_{12}^2$$

Follows that  $c$  is saddle point for

$(|a_{12}| \geq |a_1| \wedge |a_{12}| \geq |a_2|) \vee (|a_{12}| \leq |a_1| \wedge |a_{12}| \leq |a_2|)$ , in the other cases, it is a center (C)

## Back to the Toy Example: Bifurcation Diagram

We can interpret  $|a_{12}|$  as  
the **strength** of the  
interaction among  $x_1$  and  
 $x_2$

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For  $|a_{12}| \neq 0$ ,  $\mathbf{c}$  is a saddle point in the shaded regions, where there exist

- ▶ strong interactions,  
 $|a_{12}| > |a_1| \wedge |a_{12}| > |a_2|$ , i.e.  $\mathbf{c} \in M$
- ▶ weak interactions,  
 $|a_{12}| < |a_1| \wedge |a_{12}| < |a_2|$ , i.e.,  $\mathbf{c} \notin M$

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In the remaining cases  $\mathbf{c}$  is a center

# Back to the Toy Example: Bifurcation Diagram

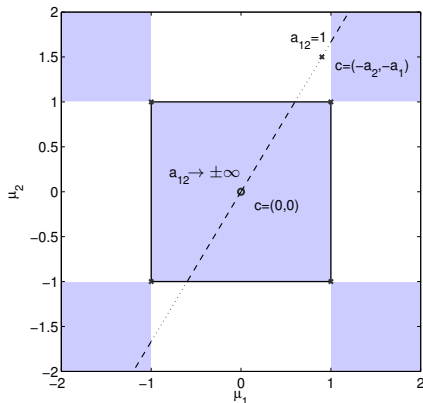
We can interpret  $|a_{12}|$  as the **strength** of the interaction among  $x_1$  and  $x_2$

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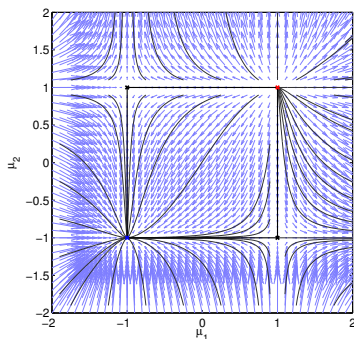
Projection of the bifurcation diagram  $(\eta_1, a_{12})$  over  $(\eta_1, \eta_2)$  for arbitrary  $a_1, a_2$  and  $0 \leq a_{12} < \infty$



The coordinates of  $\mathbf{c}$  depends on  $a_{12}$ ,  $\mathbf{c}$  is a SP on the dashed lines and a **C** on the dotted line; for  $a_{12} \rightarrow \infty$ ,  $\mathbf{c}$  converges to the center of  $M$

# Back to the Toy Example (M. et al., 2014)

Natural Gradient Flows over  $(\eta_1, \eta_2)$  for fixed  $a_{12}$

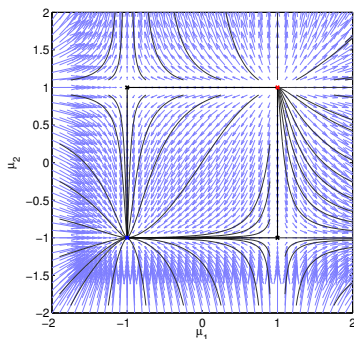


$(a_{12} = 0)$  1 SN, 1 UN, 2 SPs

No critical points besides the vertices of  $M$ , all trajectories in  $M$  converge to the global optimum

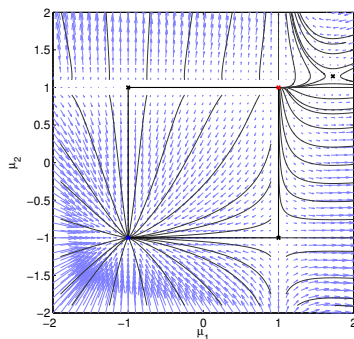
# Back to the Toy Example (M. et al., 2014)

Natural Gradient Flows over  $(\eta_1, \eta_2)$  for fixed  $a_{12}$



( $a_{12} = 0$ ) 1 **SN**, 1 **UN**, 2 SPs

No critical points besides the vertices of  $M$ , all trajectories in  $M$  converge to the global optimum



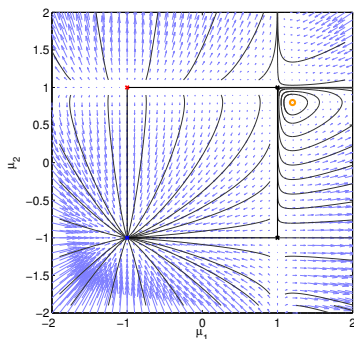
( $a_{12} = 0.85$ ) 1 **SN**, 1 **UN**, 3 SPs

The interaction is weak,  $c$  is a SP and is outside of  $M$  so that all flows converge to the global optimum



# Back to the Toy Example (M. et al., 2014)

Natural Gradient Flows over  $(\eta_1, \eta_2)$  for fixed  $a_{12}$

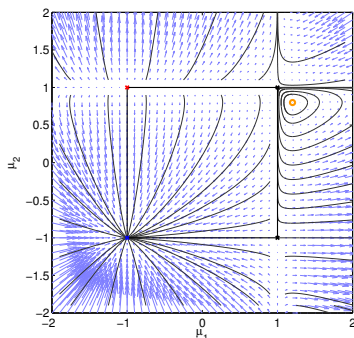


$(a_{12} = 1.25)$  1 SN, 1 UN, SPs, 1 C

The interaction is not strong enough to have  $c \in M$  and to generate local minima, we have period solutions

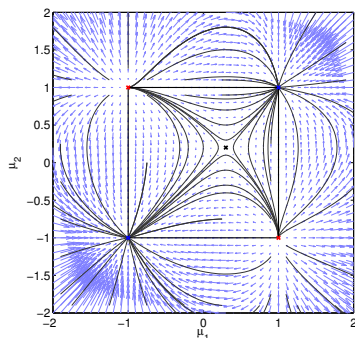
# Back to the Toy Example (M. et al., 2014)

Natural Gradient Flows over  $(\eta_1, \eta_2)$  for fixed  $a_{12}$



( $a_{12} = 1.25$ ) 1 **SN**, 1 **UN**, SPs, 1 **C**

The interaction is not strong enough to have  $c \in M$  and to generate local minima, we have period solutions



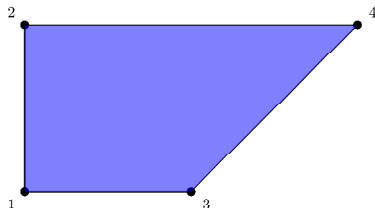
( $a_{12} = 5$ ) 2 **SN**s, 2 **UN**s, 1 SP

The interaction is strong,  $c$  is a SP and belongs to  $M$ , flows converge to either local or global optimum

## A Second Toy Example

Consider the exponential family over  $\Omega = \{1, 2, 3, 4\}$  given by the sufficient statistics  $T_1, T_2$ :

$\Omega$	$T_1$	$T_2$
1	0	0
2	0	1
3	1	0
4	2	1



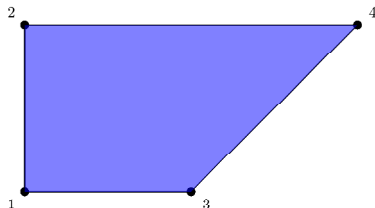
Marginal Polytope

$$p_{\boldsymbol{\theta}} = \exp(\theta_1 T_1 + \theta_2 T_2 - \psi(\boldsymbol{\theta})), \quad \psi(\boldsymbol{\theta}) = \log(1 + e^{\theta_2} + e^{\theta_1} + e^{2\theta_1 + \theta_2})$$

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We are interested in natural gradient flows in the mixture geometry

# Stochastic Relaxation

We generate a basis for all  $f : \Omega \rightarrow \mathbb{R}$

$$\{1, x_1, x_2, x_{12}\}$$

Any  $f$  can be written as

$$f = c_0 + c_1 x_1 + c_2 x_2 + c_{12} x_1 x_2$$

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Any  $f$  can be written as

$$f = c_0 + c_1 x_1 + c_2 x_2 + c_{12} x_1 x_2$$

We move to the SR with respect to the model identified by  $T_1, T_2$

$$F(\boldsymbol{\eta}) = \mathbb{E}_{\boldsymbol{\eta}}[f] = c_0 + c_1 \eta_1 + c_2 \eta_2 + c_{12} \mathbb{E}_{\boldsymbol{\eta}}[x_1 x_2]$$

How do express  $\mathbb{E}_{\boldsymbol{\eta}}[x_1 x_2]$  as a function of  $\eta_1, \eta_2$ ?

# Orthogonal Space and Markov Basis

Notice that the exponential family is a **toric model**

We can derive a Markov basis  $\{T_3\}$  the orthogonal space of the space spanned by  $\{1, T_1, T_2\}$

$\Omega$	1	$T_1$	$T_2$	$T_3$
1	1	0	0	-2
2	1	0	1	1
3	1	1	0	2
4	1	2	1	-1

## Derivation of the Invariant

From the exponential family  $\log p_{\boldsymbol{\theta}} \in \text{Span}(\{1, T_1, T_2\})$

$$\log p_{\boldsymbol{\theta}} = \theta_1 T_1 + \theta_2 T_2 - \psi(\boldsymbol{\theta}) ,$$

and thus  $\log p_{\boldsymbol{\theta}} \perp T_3$

Let  $T_3 = T_3^+ - T_3^- = (0, 1, 2, 0) - (2, 0, 0, 1)$ , orthogonality can be rewritten as

$$\begin{aligned} 0 &= \sum_{x=1}^4 \log p(x) T_3(x) \\ &= \sum_{x: T_3(x) > 0} \log p(x) T_3^+(x) - \sum_{x: T_3(x) < 0} \log p(x) T_3^-(x) \\ &= \log \left( \prod_{x: T_3(x) > 0} p(x)^{T_3^+(x)} \right) - \log \left( \prod_{x: T_3(x) < 0} p(x)^{T_3^-(x)} \right) \end{aligned}$$



## Derivation of the Invariant (cont.)

Remember that  $T_3 = T_3^+ - T_3^- = (0, 1, 2, 0) - (2, 0, 0, 1)$ , by dropping the log in

$$0 = \log \left( \prod_{x: T_3(x) > 0} p(x)^{T_3^+(x)} \right) - \log \left( \prod_{x: T_3(x) < 0} p(x)^{T_3^-(x)} \right),$$

we obtain the polynomial invariant

$$p_1^2 p_4 - p_2 p_3^2 = 0$$

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we obtain the polynomial invariant

$$p_1^2 p_4 - p_2 p_3^2 = 0$$

Our exponential family for positive probabilities is equivalently described by

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

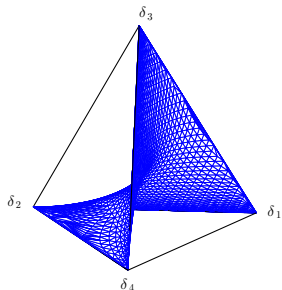
$$p_1^2 p_4 - p_2 p_3^2 = 0$$

# A Surface in the Probability Simplex

The model identifies a surface in the probability simplex

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

$$p_1^2 p_4 - p_2 p_3^2 = 0$$



Probability Simplex  $\Delta_3$

Notice, the surface is **not** the independence model as in the previous example

## Expectation Parameters

We introduce the following matrix:

$$B = \begin{array}{c} \mathbf{1} \quad T_1 \quad T_2 \quad T_3 \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{bmatrix} 1 & 0 & 0 & -2 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 \\ 1 & 2 & 1 & -1 \end{bmatrix} \end{array}$$

In the simplex, probabilities maps into expected values one-to-one

$$\begin{bmatrix} 1 \\ \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 2 \\ 0 & 1 & 0 & 1 \\ -2 & 1 & 2 & -1 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix}$$

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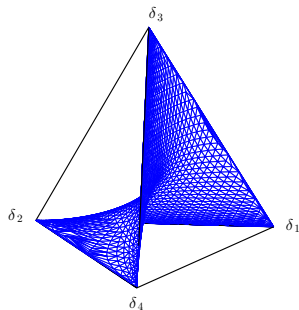
In the simplex, probabilities maps into expected values one-to-one

$$\begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix} = \begin{bmatrix} \frac{3}{5} & -\frac{1}{5} & -\frac{2}{5} & -\frac{1}{5} \\ \frac{1}{5} & -\frac{2}{5} & \frac{7}{10} & \frac{1}{10} \\ \frac{2}{5} & \frac{1}{5} & -\frac{3}{5} & \frac{1}{5} \\ -\frac{1}{5} & \frac{2}{5} & \frac{3}{10} & -\frac{1}{10} \end{bmatrix} \begin{bmatrix} 1 \\ \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}$$

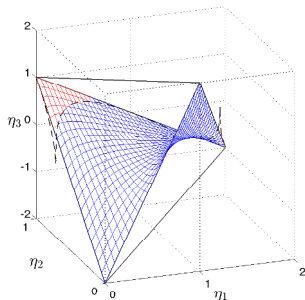
## A Surface in the Full Marginal Polytope

Then, in the  $\eta$  parameters  $p_1^2 p_4 - p_2 p_3^2 = 0$  becomes

$$(4\eta_1 + 3\eta_2 - \eta_3 - 2)(\eta_1 + 2\eta_2 + \eta_3 - 3)^2 + (4\eta_1 - 7\eta_2 - \eta_3 - 2)(\eta_1 - 3\eta_2 + \eta_3 + 2)^2 = 0$$



Probability simplex  $\Delta_3$



Full marginal polytope

The surface on the right has been plotted by evaluating the **unique real root** in the interior of the marginal polytope

## Back to the Stochastic Relaxation

We stopped at

$$F(\boldsymbol{\eta}) = c_0 + c_1\eta_1 + c_2\eta_2 + c_{12}\mathbb{E}_{\boldsymbol{\eta}}[x_1x_2]$$

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$$F(\boldsymbol{\eta}) = c_0 + c_1\eta_1 + c_2\eta_2 + c_{12}\mathbb{E}_{\boldsymbol{\eta}}[x_1x_2]$$

We have  $T_3 = 4x_1 + 3x_2 - 5x_1x_2 - 2$  and  $\eta_3 = \mathbb{E}[T_3]$ , so that

$$\mathbb{E}[x_1x_2] = \frac{1}{5}(4\eta_1 + 3\eta_2 - \eta_3 - 2) ,$$



## Back to the Stochastic Relaxation

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$$\mathbb{E}[x_1x_2] = \frac{1}{5}(4\eta_1 + 3\eta_2 - \eta_3 - 2) ,$$

which implies

$$F_{\eta}(\boldsymbol{\eta}) = c_0 - \frac{2}{5}c_{12} + \left(c_1 + \frac{4}{5}c_{12}\right)\eta_1 + \left(c_2 + \frac{3}{5}c_{12}\right)\eta_2 - \frac{1}{5}c_{12}\eta_3 ,$$

where  $\eta_3$  is the unique real root as a function of  $\eta_1, \eta_2$

[Remark] The solution of the problem relies on being able to find real root of the invariant

**Mauro C. Beltrametti  
Ettore Carletti  
Dionisio Gallarati  
Giacomo Monti Bragadin**

## **Lectures on Curves, Surfaces and Projective Varieties**

**A Classical View of Algebraic Geometry**

Translated from the Italian  
by Francis Sullivan

Mauro C. Beltrametti  
Ettore Carletti  
Dionisio Gallarati  
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## Lectures on Curves, Surfaces and Projective Varieties

A Classical View of Algebraic Geometry

Translated from the Italian  
by Francis Sullivan

**5.8.15.** Let  $\mathcal{F}$  be the surface with equation  $x_0^2 x_1 - x_2^2 x_3 = 0$ . Noting that  $\mathcal{F}$  has a double line and then observing that it is a ruled surface, find the singular generators and the pinch-points on the double line.

It is a well-known result that  $p_1^2 p_4 - p_2 p_3^2 = 0$  is a ruled surface in  $\Delta_3$

# Algebraic Varieties

In the polynomial ring  $\mathbb{Q}[p_1, p_2, p_3, p_4]$ , the **model ideal**

$$I = \langle p_1 + p_2 + p_3 + p_4 - 1, p_1^2 p_4 - p_2 p_3^2 \rangle$$

consists of all the polynomials of the form

$$A(p_1 + p_2 + p_3 + p_4 - 1) + B(p_1^2 p_4 - p_2 p_3^2), \quad \forall A, B \in \mathbb{Q}[p_1, p_2, p_3, p_4]$$

The algebraic variety  $I$  uniquely extends the exponential family outside of  $\Delta_3$ , by means of the **Zarinski closure**

# Exploiting Ruled Surfaces

Let us discuss in more detail the ruled parameterization of the toric variety

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

$$p_1^2 p_4 - p_2 p_3^2 = 0$$

# Exploiting Ruled Surfaces

Let us discuss in more detail the ruled parameterization of the toric variety

$$\begin{aligned}p_1 + p_2 + p_3 + p_4 - 1 &= 0 \\ p_1^2 p_4 - p_2 p_3^2 &= 0\end{aligned}$$

The Jacobian matrix is

$$J = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2p_1p_4 & -p_3^2 & -2p_2p_3 & p_1^2 \end{bmatrix}$$

It has rank one, that is, there is a singularity, if, and only if

$$2p_1p_4 = -p_3^2 = -2p_2p_3 = p_1^2 ,$$

which is equivalent to  $p_1^2 = p_3^2 = 0$

# Exploiting Ruled Surfaces

The subspace  $p_1^2 = p_3^2 = 0$  intersects the model along a **double critical line**  $\mathcal{C}$ , and the simplex along the edge  $\delta_2 \leftrightarrow \delta_4$

If we take a **sheaf of planes** through  $\mathcal{C}$ , by the Bezout theorem, it intersects the cubic surface along  $\mathcal{C}$  and on a space of degree  $3 - 2 = 1$

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If we take a **sheaf of planes** through  $\mathcal{C}$ , by the Bezout theorem, it intersects the cubic surface along  $\mathcal{C}$  and on a space of degree  $3 - 2 = 1$

That is, the system of equations

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

$$p_1^2 p_4 - p_2 p_3^2 = 0$$

$$\alpha p_1 + \beta p_3 = 0$$

admits as a solution  $\mathcal{C}$  and a line



# Lowering the Degree on the Invariant

The system of equations

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

$$p_1^2 p_4 - p_2 p_3^2 = 0$$

$$\alpha p_1 + \beta p_3 = 0$$

can be reduced to

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

$$\alpha p_1 + \beta p_3 = 0$$

$$-\alpha^2 p_2 + \beta^2 p_4 = 0$$

## A New Parametrization for the Model

In parametric form, the line in becomes

$$p_1([\alpha : \beta], t) = \beta t$$

$$p_2([\alpha : \beta], t) = \frac{\beta^2}{\alpha^2 + \beta^2} + \frac{\beta^2(\alpha - \beta)}{\alpha^2 + \beta^2} t$$

$$p_3([\alpha : \beta], t) = -\alpha t$$

$$p_4([\alpha : \beta], t) = \frac{\alpha^2}{\alpha^2 + \beta^2} + \frac{\alpha^2(\alpha - \beta)}{\alpha^2 + \beta^2} t$$

By setting  $\alpha = \beta - 1$ ,  $0 < t < 1$ ,  $-1 < \alpha < 0$ , we get:

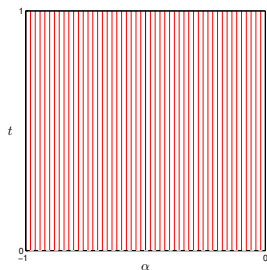
$$p_1(\alpha, t) = (\alpha + 1)t$$

$$p_2(\alpha, t) = \frac{\alpha^2 - (\alpha^2 + 2\alpha + 1)t + 2\alpha + 1}{2\alpha^2 + 2\alpha + 1}$$

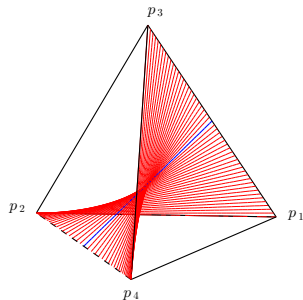
$$p_3(\alpha, t) = -\alpha t$$

$$p_4(\alpha, t) = -\frac{\alpha^2 t - \alpha^2}{2\alpha^2 + 2\alpha + 1}$$

# The Ruled Surface in $\Delta_3$



$(\alpha, t)$  parameterization

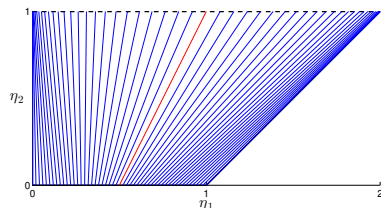


Probability simplex  $\Delta_3$

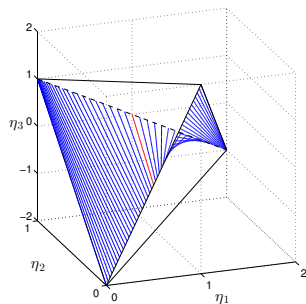
The critical line  $\mathcal{C}$  is the dashed line

# The Ruled Surface in the (Full) Marginal Polytope

By the linear mapping between  $p$  and  $\eta$ , lines map to lines



Marginal polytope



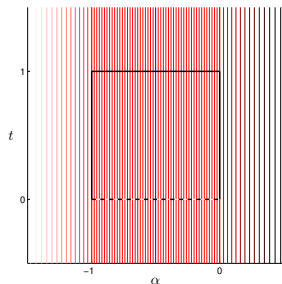
Full marginal polytope

Each line intersects  $\delta_2 \leftrightarrow \delta_4$  and  $\delta_1 \leftrightarrow \delta_3$  in

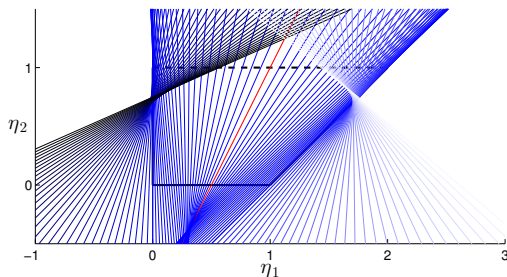
$$\mathbf{a} = \left( \frac{2\alpha^2}{2\alpha^2 + 2\alpha + 1}, 1, \frac{2\alpha + 1}{2\alpha^2 + 2\alpha + 1} \right) \quad \mathbf{b} = (-\alpha, 0, -4\alpha - 2)$$

# Extension of the Model

Lines can be extended outside of  $\Delta_3$  and of the marginal polytope

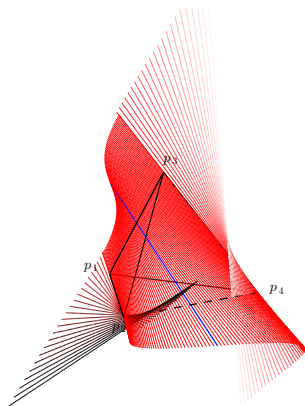


$(\alpha, t)$  parameterization

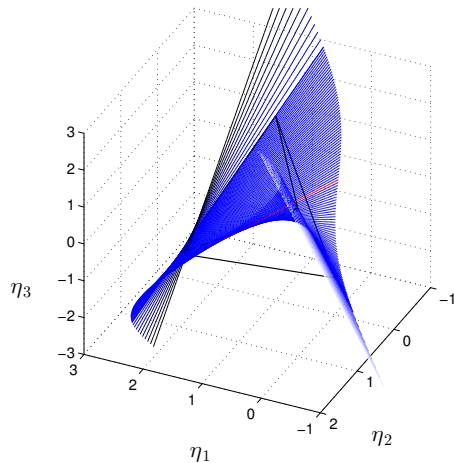


Marginal polytope

# Extension of the Model



Probability Simplex  $\Delta_3$



Full marginal polytope

## Back to the SR

The expectation parameters become rational functions of  $(\alpha, t)$

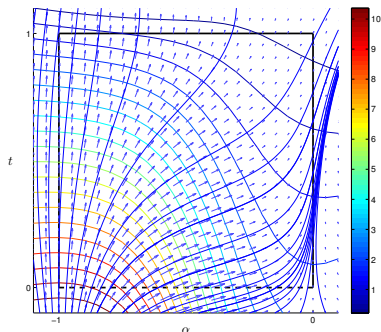
$$\begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} = \begin{bmatrix} -\alpha \\ 0 \\ -4\alpha - 2 \end{bmatrix} + t \begin{bmatrix} \frac{2\alpha^3 + 4\alpha^2 + \alpha}{2\alpha^2 + 2\alpha + 1} \\ 1 \\ \frac{8\alpha^3 + 12\alpha^2 + 10\alpha + 3}{2\alpha^2 + 2\alpha + 1} \end{bmatrix}$$

The same applies to the (inverse) Fisher Information matrix and the natural gradient, which now can be computed by

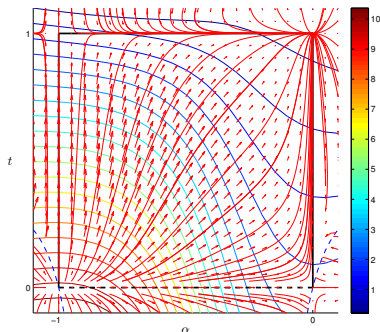
$$\tilde{\nabla} F_{\eta}(\alpha, t) = I_{\eta}(\alpha, t)^{-1} \nabla F_{\eta}(\alpha, t)$$

## Case 1: Gradient Flows in $(\alpha, t)$

Consider the case with  $c_0 = 0, c_1 = 1, c_2 = 2, c_3 = 3$



Vanilla gradient



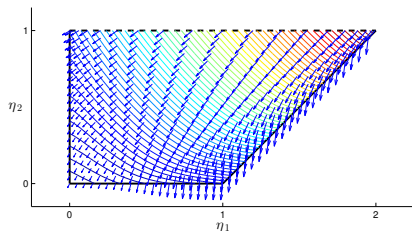
Natural gradient

The function  $f$  admits one global minima

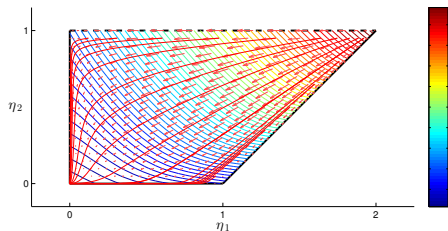


## Case 1: Gradient Flows on the Marginal Polytope

Consider the case with  $c_0 = 0, c_1 = 1, c_2 = 2, c_3 = 3$



Vanilla gradient

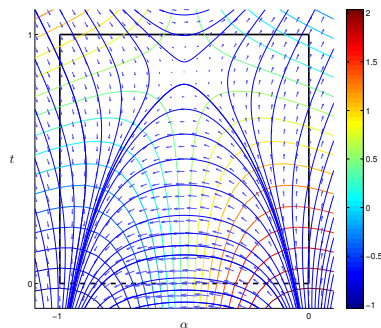


Natural gradient

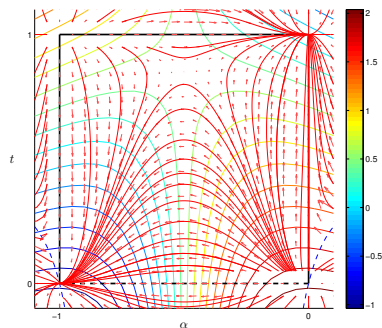
The function  $f$  admits one global minima

## Case 2: Gradient Flows in $(\alpha, t)$

Consider the case with  $c_0 = 0, c_1 = 1, c_2 = 2, c_3 = -5/2$



Vanilla gradient

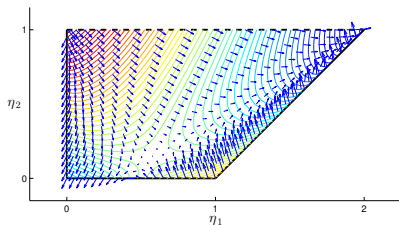


Natural gradient

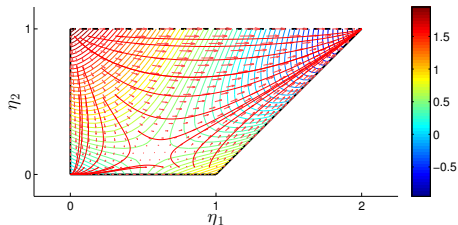
The function  $f$  admits two local minima

## Case 2: Gradient Flows on the Marginal Polytope

Consider the case with  $c_0 = 0, c_1 = 1, c_2 = 2, c_3 = -5/2$



Vanilla gradient



Natural gradient

The function  $f$  admits two local minima

## Some Remarks

By exploiting the fact that surface in the probability simplex given by the invariant is a ruled surface, we introduced a new parametrization for the model

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By exploiting the fact that surface in the probability simplex given by the invariant is a ruled surface, we introduced a new parametrization for the model

In the new parametrization, the natural gradient is given by a rational formula

The model can be extended, the Fisher information matrix, and the natural gradient can be evaluated also for negative probabilities

The approach is more general than this specific example, and is based on the evaluation of the Markov basis for the orthogonal space and on the intersection of sheaf of planes on exposed faces of the model

Work in progress: the tutorial example is going to appear on Entropy this month, another paper is in preparation