Information Geometry of Polytopes

general theory and applications to stochastic matrices

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Notation

Simplex of probability measures

$$\mathbb{R}^{\mathscr{X}} \;:=\; \text{real valued functions on a finite set } \mathscr{X}$$

$$\delta_x \in \left(\mathbb{R}^{\mathscr{X}}\right)^*, \quad x \in \mathscr{X}, \qquad \text{(dual of the canonical basis)}$$

$$\mathcal{P} \;:=\; \left\{ \sum_x p_x\, \delta_x \in \left(\mathbb{R}^{\mathscr{X}}\right)^* \;:\; p_x > 0, \quad \sum_x p_x = 1 \right\}$$

Quotient vector space

$$\mathcal{C} \;:=\; \text{subspace of constant functions}$$

$$\mathbb{R}^{\mathscr{X}}/\mathcal{C} \;=\; \left\{ f + \mathcal{C} \;:\; f \in \mathbb{R}^{\mathscr{X}} \right\}$$

$\mathcal{P}$ as a Manifold

Tangent and cotangent space of $\mathcal{P}$

- Tangent space of $\mathcal{P}$:

$$\mathcal{T} \;:=\; \left\{\varphi \in \left(\mathbb{R}^{\mathscr{X}}\right)^* \;:\; \varphi(f) = 0 \text{ for all } f \in \mathcal{C}\right\}$$

- Cotangent space of $\mathcal{P}$:

$$\mathbb{R}^{\mathscr{X}}/\mathcal{C} \;\cong\; \mathcal{T}^*$$

$$\mathbb{R}^{\mathscr{X}}/\mathcal{C} \;\to\; \mathcal{T}^*, \qquad f + \mathcal{C} \;\mapsto\; \left(\varphi \;\mapsto\; \varphi(f)\right)$$

Remark

$$\mathcal{U} \;\subseteq\; \mathcal{V}, \qquad \mathcal{U}^0 := \{\varphi \in \mathcal{V}^* \;:\; \varphi(f) = 0 \text{ for all } f \in \mathcal{U}\}$$

$$\Rightarrow \qquad \mathcal{V}^*/\mathcal{U}^0 \;\to\; \mathcal{U}^*, \quad \varphi + \mathcal{U}^0 \;\mapsto\; \varphi|_{\mathcal{U}}, \quad \text{natural isomorphism}$$

$\mathcal{P}$ as a Riemannian Manifold

- Scalar product on $\mathbb{R}^{\mathscr{X}}/\mathcal{C}$:

$$\langle f + \mathcal{C}, g + \mathcal{C} \rangle_p \; := \; \mathrm{cov}(f, g) \; = \; \langle f \cdot g \rangle_p - \langle f \rangle_p \cdot \langle g \rangle_p$$

- Identification of $\mathbb{R}^{\mathscr{X}}/\mathcal{C}$ and $\mathcal{T}$ with respect to $\langle \cdot, \cdot \rangle_p$:

$$\phi_p : \; \mathbb{R}^{\mathscr{X}}/\mathcal{C} \; \to \; \mathcal{T}, \qquad f + \mathcal{C} \; \mapsto \; \sum_x p_x \left(f_x - \langle f \rangle_p \right) \delta_x$$

- Natural bundle isomorphism:

$$T^*\mathcal{P} = \mathcal{P} \times (\mathbb{R}^{\mathscr{X}}/\mathcal{C}) \; \stackrel{\phi}{\longrightarrow} \; \mathcal{P} \times \mathcal{T} = T\mathcal{P}$$

- Fisher metric, Shahshahani inner product:

$$\langle \cdot, \cdot \rangle_p : \mathcal{T} \times \mathcal{T} \to \mathbb{R}, \qquad \langle A, B \rangle_p \; := \; \sum_x \frac{1}{p_x} A_x B_x$$

Vector Fields and Differential Equations

Replicator equations

Consider a map $f : \mathcal{P} \to \mathbb{R}^{\mathscr{X}}$ and the induced section

$$\mathcal{P} \to \mathbb{R}^{\mathscr{X}}/\mathcal{C}, \qquad p \mapsto f(p) + \mathcal{C}.$$

in $T^*\mathcal{P}$. This can be identified with the vector field

$$\mathcal{P} \to \mathcal{T}, \qquad p \mapsto \sum_x p_x \left(f_x(p) - \langle f(p) \rangle_p \right) \delta_x$$

and the corresponding differential equations

$$\dot{p}_x = p_x \Big(f_x(p) - \langle f(p) \rangle_p \Big), \qquad x \in \mathscr{X}.$$

These equations are known as *replicator equations*.

Observation

Replicator equations are nothing but ordinary differential equations expressed in terms of a section in the cotangent bundle $T^*\mathcal{P}$ instead of a section in the tangent bundle $T\mathcal{P}$.

Gradient fields

Consider a function $F : \mathcal{P} \to \mathbb{R}$. Then the gradient of F with respect to the Fisher metric is given by

$$(\mathrm{grad}_p F)_x \;=\; p_x \left(\partial_x F(p) - \sum_{x'} p_{x'} \, \partial_{x'} F(p) \right)$$

- J. Hofbauer & K. Sigmund. *Evolutionary Games and Population Dynamics.* Cambridge University Press 2002.
- N. Ay & I. Erb. *On a Notion of Linear Replicator Equations.* Journal of Dynamics and Differential Equations 2005.

Example: Darwinian selection, "survival of the fittest"

Consider a function $f : \mathscr{X} \to \mathbb{R}$ (f_x is called *fitness of species x*) and

$$\dot{p}_x \;=\; p_x\Big(f_x - \langle f\rangle_p\Big) \;=\; \mathrm{grad}_p\langle f\rangle, \qquad p(0) \;=\; p.$$

Solution curves satisfy the Price-equation and Fisher's fundamental theorem of natural selection:

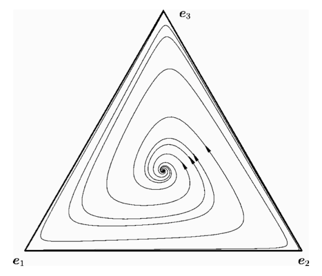
$$\frac{d}{dt}\langle g\rangle_{p(t)} \;=\; \mathrm{cov}(f,g) \qquad\qquad \frac{d}{dt}\langle f\rangle_{p(t)} \;=\; \mathrm{var}(f)$$

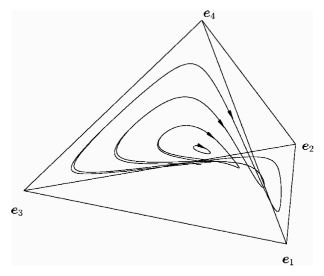
Solution curves: $t \;\mapsto\; p(t) = \frac{p\,e^{tf}}{\left\langle e^{tf}\right\rangle_p}$

$$\lim_{t\to-\infty} p(t) \;=\; \begin{cases} \frac{p_x}{\sum_{x\in\mathrm{argmin}(f)} p_x}, & \text{falls } x \in \mathrm{argmin}(f) \\ 0, & \text{sonst} \end{cases}$$

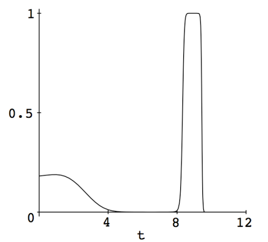
$$\lim_{t\to\infty} p(t) \;=\; \begin{cases} \frac{p_x}{\sum_{x\in\mathrm{argmax}(f)} p_x}, & \text{falls } x \in \mathrm{argmax}(f) \\ 0, & \text{sonst} \end{cases}$$

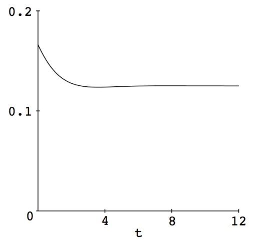
Hypercycle dynamics (Eigen und Schuster) with three and four species

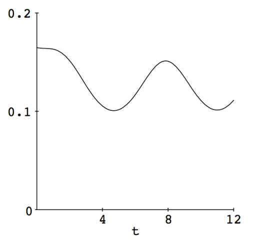




Hypercycle dynamics with eight species for different initial conditions







Natural Connections

Mixture Connection

$$\overset{m}{\Pi}_{p,q}\colon\ T_p\mathcal{P} \longrightarrow T_q\mathcal{P}, \qquad (p, A) \longmapsto (q, A)$$

Exponential Connection

$$\overset{e}{\Pi}_{p,q}\colon\ T_p^*\mathcal{P} \longrightarrow T_q^*\mathcal{P}, \qquad (p, f + \mathcal{C}) \longmapsto (q, f + \mathcal{C})$$

$$\overset{e}{\Pi}_{p,q}\colon\ T_p\mathcal{P} \longrightarrow T_q\mathcal{P}, \qquad (p, A) \longmapsto (q, (\phi_q \circ {\phi_p}^{-1})(A))$$

Duality

$$\left\langle \overset{e}{\Pi}_{p,q} A, \overset{m}{\Pi}_{p,q} B \right\rangle_q = \langle A, B \rangle_p$$

Differential version

$$\overset{m,e}{\nabla}_A B\Big|_p \;:=\; \lim_{t\to 0}\frac{1}{t}\left(\overset{m,e}{\Pi}_{\gamma(t),p}\left(B_{\gamma(t)}\right) - B_p\right) \;\in\; T_p\mathcal{P}.$$

Geodesics satisfying $\overset{m,e}{\gamma}(0) = p$ and $\overset{m,e}{\gamma}(1) = q$

1. *m*-geodesics:

$$\overset{m}{\gamma}_{p,q}\colon\; [0,1] \to \mathcal{P}, \qquad t \mapsto (1-t)\,p + t\,q$$

2. *e*-geodesics:

$$\overset{e}{\gamma}_{p,q}\colon\; [0,1] \to \mathcal{P}, \qquad t \mapsto \frac{p^{1-t}q^{t}}{\sum_x p_x^{1-t}q_x^{t}}$$

Corresponding exponential maps

1. *m*-exponential map:

$$\overset{m}{\exp}: \ \left\{(p, q-p) \in T\mathcal{P} \ : \ p, q \in \mathcal{P}\right\} \ \to \ \mathcal{P}, \qquad (p, A) \ \mapsto \ p + A,$$

2. *e*-exponential map:

$$\overset{e}{\exp}: \ T\mathcal{P} \ \to \ \mathcal{P}, \qquad (p, A) \ \mapsto \ \frac{p\, e^{\frac{A}{p}}}{\sum_x p_x\, e^{\frac{A_x}{p_x}}}$$

Relative entropy

$$D(p \,\|\, q) \ = \ \begin{cases} \sum_x p_x \ln \frac{p_x}{q_x}, & \text{if } \operatorname{supp}(p) \subseteq \operatorname{supp}(q) \\ +\infty \quad , & \text{otherwise} \end{cases}$$

$$\overset{m}{\exp}_q{}^{-1}(p) \ = \ -\operatorname{grad}_q D(p \,\|\, \cdot) \qquad \overset{e}{\exp}_q{}^{-1}(p) \ = \ -\operatorname{grad}_q D(\cdot \,\|\, p)$$

Motivation of the previous relations

- Squared distance from q:

$$D_q : \mathbb{R}^n \to \mathbb{R}, \qquad p \mapsto \frac{1}{2}\|q-p\|^2 = \frac{1}{2}\sum_{i=1}^{n}(q_i - p_i)^2$$

- The differential $d_p D_q \in (\mathbb{R}^n)^*$:

$$d_p D_q : \mathbb{R}^n \to \mathbb{R}, \qquad v \mapsto \frac{\partial D_q}{\partial v}(p)$$

- Identification of the differential with a vector in $\mathbb{R}^n$:

$$-\mathrm{grad}_p\, D_q = -\mathrm{grad}\big(d_p D_q\big) = q - p = \overrightarrow{p\,q}$$

$\mathcal{P}$ as an Affine Space

Note that $\overset{e}{\exp}$ is not an affine action:

$$\overset{e}{\exp}\left(\overset{e}{\exp}(p, A), B\right) \neq \overset{e}{\exp}(p, A + B)$$

Consider instead the composition

$$\mathrm{t}: \; \mathcal{P} \times (\mathbb{R}^{\mathscr{X}}/\mathcal{C}) = T^*\mathcal{P} \;\; \xrightarrow{\phi} \;\; T\mathcal{P} \xrightarrow{\overset{e}{\exp}} \mathcal{P},$$

$$(p, f + \mathcal{C}) \;\mapsto\; \frac{p\, e^f}{\langle e^f \rangle_p}$$

This is an affine action with difference vector

$$\mathrm{vec}: \mathcal{P} \times \mathcal{P} \to \mathbb{R}^{\mathscr{X}}/\mathcal{C}, \qquad (p, q) \mapsto \mathrm{vec}(p, q) = \ln\left(\frac{q}{p}\right) + \mathcal{C}$$

and $\mathcal{P}$ is an affine space over $\mathbb{R}^{\mathscr{X}}/\mathcal{C}$.

Definition: Exponential families

An affine subspace $\mathcal{E}$ of $\mathcal{P}$ with respect to t is called *exponential family*. Given a probability measure q and a linear subspace $\mathcal{L}$ of $\mathbb{R}^{\mathscr{X}}$, the following submanifold of $\mathcal{P}$ is an exponential family:

$$\mathcal{E}(q, \mathcal{L}) \quad := \quad \left\{ \frac{q\, e^f}{\langle e^f \rangle_q} \; : \; f \in \mathcal{L} \right\}$$

Clearly, all exponential families are of this structure. We always assume $\mathcal{C} \subseteq \mathcal{L}$ and thereby ensure uniqueness of $\mathcal{L}$. Furthermore, with this assumption we have $\dim(\mathcal{E}) = \dim(\mathcal{L}) - 1$.

Remark

An exponential family can be identified with a polytope via the expectation value map.

Extension to Polytopes
work in progress with Johannes Rauh

Consider a polytope $\bar{\mathcal{C}} \subset \mathbb{R}^d$, and its set $\mathrm{ext}(\bar{\mathcal{C}})$ of extreme points.

$$\bar{\mathcal{C}} \;=\; \left\{ \sum_{x \in \mathrm{ext}(\bar{\mathcal{C}})} p(x)\, x \;\in\; \mathbb{R}^d \;:\; p \in \bar{\mathcal{P}}(\mathrm{ext}(\bar{\mathcal{C}})) \right\}$$

$$\varphi : \bar{\mathcal{P}}(\mathrm{ext}(\bar{\mathcal{C}})) \;\to\; \bar{\mathcal{C}}, \qquad p \;\mapsto\; \varphi(p) \;:=\; \sum_{x \in \mathrm{ext}(\bar{\mathcal{C}})} p(x)\, x$$

The set $\varphi^{-1}(\{\kappa\})$ is a convex set. Choose that member p_κ that has maximal entropy. This corresponds to the canonical representation.

Information geometry of polytopes, the main idea

The image of the map $\kappa \mapsto p_\kappa$ is the closure of an exponential family $\mathcal{E} = \mathcal{E}(\mathcal{C})$. Take the push-forward of the induced geometry $(\mathcal{E}, g|_{\mathcal{E}}, \overset{m}{\nabla}|_{\mathcal{E}}, \overset{e}{\nabla}|_{\mathcal{E}})$. In particular,

$$D(\kappa \,\|\, \sigma) \;:=\; D(p_\kappa \,\|\, p_\sigma).$$

Application of this idea to the setting of Markov kernels

Polytope of Markov kernels

$$\bar{\mathcal{C}} \;:=\; \bar{\mathcal{C}}(\mathscr{X};\mathscr{Y}) \;=\; \left\{\kappa \in \mathbb{R}^{\mathscr{X}\times\mathscr{Y}} \;:\; \kappa(x;y) \geq 0, \quad \sum_y \kappa(x;y) = 1\right\}$$

$$f \in \mathscr{Y}^{\mathscr{X}}, \quad \kappa_f(x;y) \;:=\; \delta_{f(x)}(y), \qquad \mathrm{ext}(\bar{\mathcal{C}}) = \left\{\kappa_f \;:\; f \in \mathscr{Y}^{\mathscr{X}}\right\}$$

$$\varphi : \bar{\mathcal{P}}(\mathscr{Y}^{\mathscr{X}}) \;\to\; \bar{\mathcal{C}}, \qquad p \;\mapsto\; \varphi(p) \;:=\; \sum_f p(f)\,\kappa_f$$

Corresponding exponential family

$$\mathcal{E} = \mathcal{E}(\mathcal{C}) = \frac{e^{\sum_{x,y} \theta_{x,y} \kappa_{\cdot}(x;y)}}{\sum_{f \in \mathscr{Y}^{\mathscr{X}}} e^{\sum_{x,y} \theta_{x,y} \kappa_f(x;y)}}$$

Proposition

The restriction $\varphi|_{\bar{\mathcal{E}}}$ *has the inverse*

$$\varphi^{-1} : \bar{\mathcal{C}} \to \bar{\mathcal{E}}, \qquad \kappa \mapsto p_\kappa := \bigotimes_{x \in \mathscr{X}} \kappa(x;\cdot).$$

Example: Structural equation model and Markov kernels

Structural equation model

Consider $\mathscr{Z}$ and $F : \mathscr{X} \times \mathscr{Z} \to \mathscr{Y}$

$$y \;=\; F(x,z), \quad z \text{ disturbance with distribution } p$$

$$\leadsto \qquad \kappa(x;y) \;:=\; \sum_{z \in \mathscr{Z}} p(z)\, \delta_{F(x,z)}(y) \;=\; \sum_{z \in \mathscr{Z}} p(z)\, \delta_{F_z(x)}(y)$$

$$\Rightarrow \qquad \kappa(x;\cdot) \;\in\; \bar{\mathcal{P}}(\mathscr{Y}) \quad \text{for all } x$$

Canonical representation

Given κ, choose $\mathscr{Z} := \mathscr{Y}^{\mathscr{X}}$,

$$F : \mathscr{X} \times \mathscr{Y}^{\mathscr{X}} \;\to\; \mathscr{Y}, \qquad (x,f) \;\mapsto\; f(x), \qquad \text{and}$$

$$p_\kappa(f) \;:=\; \prod_{x \in \mathscr{X}} \kappa(x; f(x))$$

Fisher metric

$$g_\kappa(A, B) \;:=\; \sum_{x,y} \frac{1}{\kappa(x;y)} A(x;y)\, B(x;y)$$

m-Geodesics

$$\gamma^{(m)}(t) \;:=\; (1-t)\,\kappa(x;y) + t\,\sigma(x;y)$$

e-Geodesics

$$\gamma^{(e)}(t) \;:=\; \frac{\kappa(x;y)^{1-t}\sigma(x;y)^t}{\sum_{y'} \kappa(x;y')^{1-t}\sigma(x;y')^t}$$

Relative entropy

$$D(\kappa \,\|\, \sigma) \;:=\; D(p_\kappa \,\|\, p_\sigma) \;=\; \sum_{x,y} \kappa(x;y) \ln \frac{\kappa(x;y)}{\sigma(x;y)}$$

Affine action

$f, g \in \mathbb{R}^{\mathscr{X} \times \mathscr{Y}}$:

$$f \sim g \quad :\Leftrightarrow \quad f - g \in \mathbb{R}^{\mathscr{X}}$$

$$\mathcal{V} := \mathbb{R}^{\mathscr{X} \times \mathscr{Y}} / \mathbb{R}^{\mathscr{X}}$$

$$\mathcal{C} \times \mathcal{V} \to \mathcal{C}, \qquad (\kappa, f + \mathbb{R}^{\mathscr{X}}) \mapsto \frac{\kappa\, e^{f}}{\sum_y \kappa(\cdot; y)\, e^{f(\cdot;y)}}$$

Proposition

The affine subspaces of $\mathcal{C}(\mathscr{X};\mathscr{Y})$ are the exponential families in $\mathcal{C}(\mathscr{X};\mathscr{Y})$. Given a subspace $\mathcal{L}$ of dimension $|\mathscr{X}| + d$ with $\mathbb{R}^{\mathscr{X}} \subseteq \mathcal{L} \subseteq \mathbb{R}^{\mathscr{X} \times \mathscr{Y}}$, and given a reference element κ, the following subfamily is a d-dimensional exponential family:

$$\mathcal{E}(\kappa, \mathcal{L}) := \left\{ \frac{\kappa\, e^{f}}{\sum_y \kappa(\cdot; y)\, e^{f(\cdot;y)}} \; : \; f \in \mathcal{L} \right\}$$

Maximization of Entropy Distance from Exponential Families

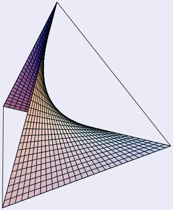
based on Ay 2002, Matúš & Ay 2003

Multi-Information as an Example

Family of product distributions

$$\otimes : \ \bar{\mathcal{P}}(\mathscr{X}_1) \times \cdots \times \bar{\mathcal{P}}(\mathscr{X}_N) \ \rightarrow \ \bar{\mathcal{P}}(\mathscr{X}_1 \times \cdots \times \mathscr{X}_N)$$

$$(p_1, \ldots, p_N) \ \mapsto \ p_1 \otimes \cdots \otimes p_N$$



Definition of multi-information

$$I : \ \bar{\mathcal{P}}(\mathscr{X}_1 \times \cdots \times \mathscr{X}_N) \rightarrow \mathbb{R}, \qquad p \mapsto I(p) := \inf_{q \in \mathrm{im}(\otimes)} D(p \,\|\, q)$$

General problem

Given an exponential family $\mathcal{E}$, maximize the function

$$D_{\mathcal{E}} : \bar{\mathcal{P}} \to \mathbb{R}, \qquad p \mapsto \inf_{q \in \mathcal{E}} D(p \,\|\, q).$$

Results

1. Support bound: Let p be a local maximizer of $D_{\mathcal{E}}$. Then

$$|\text{supp}(p)| \leq \dim(\mathcal{E}) + 1$$

   In particular, $H(p) \leq \ln(\dim(\mathcal{E}) + 1)$.

2. Extended exponential families: There exists an exponential family $\widetilde{\mathcal{E}}$ of dimension

$$\dim\left(\widetilde{\mathcal{E}}\right) \leq 3\dim(\mathcal{E}) + 2$$

   that contains $\mathcal{E}$ and all local maximizers of $D_{\mathcal{E}}$ in its closure.

Applied to multi-information

1. Let p be a local maximizer of the multi-information. Then

$$|\mathrm{supp}(p)| \;\leq\; \sum_{i=1}^{N}(|\mathscr{X}_i| - 1) + 1 \quad (= \; N + 1 \;\ll\; 2^N \text{ for binary nodes})$$

In particular

$$H(p) \;\leq\; \ln\left(\sum_{i=1}^{N}(|\mathscr{X}_i| - 1) + 1\right).$$

2. There exists an exponential family of dimension at most

$$3\sum_{i=1}^{N}(|\mathscr{X}_i| - 1) \;+\; 2 \qquad (3\,N \;+\; 2 \;\ll\; 2^N - 1 \text{ for binary nodes})$$

that contains all local maximizers of the multi-information in its closure.

Multi-Information for Kernels

Factorized kernels

Consider a set $[N]$ of nodes with input symbols $\mathscr{X}_i$ and output symbols $\mathscr{Y}_i$ and denote with $\mathscr{X}$ and $\mathscr{Y}$ the products.

$$\otimes : \quad \prod_{i \in [N]} \bar{\mathcal{C}}(\mathscr{X}_i; \mathscr{Y}_i) \;\hookrightarrow\; \bar{\mathcal{C}}(\mathscr{X}; \mathscr{Y})$$

$$(\kappa_i)_i \;\mapsto\; (\otimes_i \kappa_i)(x; y) := \kappa_1(x_1; y_1) \cdots \kappa_N(x_N; y_N)$$

This is the closure of an exponential family in $\mathcal{C}(\mathscr{X}; \mathscr{Y})$ of dimension

$$\sum_{i=1}^{N} |\mathscr{X}_i|(|\mathscr{Y}_i| - 1)$$

Multi-information

$$I(\kappa) \;:=\; \inf_{\sigma \in \mathrm{im}(\otimes)} D(\kappa \,\|\, \sigma)$$

Local maximizers

Let κ be a local maximizer of I. Then the dimension of the face $F(\kappa)$ of $\bar{\mathcal{C}}(\mathscr{X};\mathscr{Y})$ in which κ is contained is upper bounded by

$$d \;:=\; \sum_{i=1}^{N} |\mathscr{X}_i|(|\mathscr{Y}_i| - 1) \qquad (d = 2\,N \text{ for binary nodes})$$

The theorem of Carathéodory implies there are at most $d+1$ functions so that κ can be written as their convex combination:

$$\kappa \;=\; \sum_{f} p(f)\,\kappa_f$$

This implies

$$|\mathrm{supp}\,\kappa(x;\cdot)| \;\leq\; d+1$$

and therefore $H(Y\,|\,X) \leq \ln(d+1)$ for any distribution of X.

Low-dimesional exponential families

There exists an exponential family $\mathcal{E}$ of dimension at most $3\,d + 2$ such that all maximizers of the multi-information are contained in the set

$$\left\{ \sum_{f \in \mathscr{Y}^{\mathscr{X}}} p(f)\,\kappa_f \;:\; p \in \bar{\mathcal{E}} \right\} \;\subseteq\; \bar{\mathcal{C}}(\mathscr{X};\mathscr{Y})$$

A second approach based on Stephan Weis' dissertation, University of Erlangen Nuremberg 2009

A different way to see the previous approach

The previous geometry can also be obtained by the affine embedding

$$\bar{\mathcal{C}}(\mathscr{X};\mathscr{Y}) \hookrightarrow \bar{\mathcal{P}}(\mathscr{X} \times \mathscr{Y}), \qquad \kappa \mapsto \frac{1}{|\mathscr{X}|}\,\kappa$$

The more general affine embedding:

$$\kappa \mapsto p \otimes \kappa, \qquad (p \otimes \kappa)(x;y) := p(x)\,\kappa(x;y).$$

It does change the geometry but does not change the results on maximizers of multi-information.

Stationarity and the Kirchhoff polytope

Consider

$$\otimes : \bar{\mathcal{P}}(\mathscr{X}) \times \bar{\mathcal{C}}(\mathscr{X};\mathscr{X}) \rightarrow \bar{\mathcal{P}}(\mathscr{X} \times \mathscr{X}),$$

$$(p,\kappa) \mapsto (p \otimes \kappa)(x;x') := p(x)\,\kappa(x;x')$$

Remark: This map is surjective but at the boundary not injective.

Assume stationarity:

$$\bar{\mathcal{S}}(\mathscr{X}) := \left\{ p \in \bar{\mathcal{P}}(\mathscr{X} \times \mathscr{X}) \,:\, \sum_{x'} p(x,x') = \sum_{x'} p(x',x) \right\}$$

We have the following correspondence:

$$\mathcal{S}(\mathscr{X}) \longleftrightarrow \mathcal{C}(\mathscr{X};\mathscr{X})$$

Multi-information

Consider N nodes with state sets $\mathscr{X}_i$ and the following map:

$$\otimes : \;\; \bar{\mathcal{S}}(\mathscr{X}_1) \times \cdots \times \bar{\mathcal{S}}(\mathscr{X}_N) \;\; \to \;\; \bar{\mathcal{S}}(\mathscr{X}_1 \times \cdots \times \mathscr{X}_N)$$

Note that $\mathrm{im}(\otimes)$ is not an exponential family. It is the intersection of an exponential family with a convex set.

$$I(p) \;:=\; \inf_{q \in \mathrm{im}(\otimes)} D(p \,\|\, q)$$

Extreme points of $\bar{\mathcal{S}}(\mathscr{X})$

Consider a set $\emptyset \neq \mathscr{U} \subseteq \mathscr{X}$ and a cyclic permutation $\pi : \mathscr{U} \to \mathscr{U}$.

$$c(\mathscr{U}, \pi)(x, x') := \frac{1}{|\mathscr{U}|} \cdot \begin{cases} 1, & \text{if } \pi(x) = x' \\ 0, & \text{otherwise} \end{cases}$$

The number of extreme points

$$|\mathrm{ext}(\bar{\mathcal{S}}(\mathscr{X}))| = \sum_{k=1}^{|\mathscr{X}|} \binom{|\mathscr{X}|}{k} (k-1)! \leq |\mathscr{X}|^{|\mathscr{X}|} = |\mathrm{ext}(\bar{\mathcal{C}}(\mathscr{X};\mathscr{X}))|$$

$\lvert\mathscr{X}\rvert$	dim	$\lvert\mathrm{ext}(\bar{\mathcal{S}}(\mathscr{X}))\rvert$	$\lvert\mathrm{ext}(\bar{\mathcal{C}}(\mathscr{X};\mathscr{X}))\rvert$
2	2	3	4
3	6	8	27
4	12	24	256
5	20	89	3125

Local maximizers

Each local maximizer p of I satisfies

$$\dim\big(F(p)\big) \;\leq\; \sum_{i=1}^{N} (|\mathscr{X}_i|^2 - |\mathscr{X}_i|) \qquad (=\; 2\,N \text{ for binary nodes})$$

With the Carathéodory theorem there are at most $\sum_{i=1}^{N}(|\mathscr{X}_i|^2 - |\mathscr{X}_i|) + 1$ cycles so that p can be represented as convex combination of them. This implies that for all x with $\sum_{x'} p(x,x') > 0$:

$$|\mathrm{supp} p(\cdot\,|\,x)| \;\leq\; \sum_{i=1}^{N} (|\mathscr{X}_i|^2 - |\mathscr{X}_i|) + 1,$$

which implies

$$H(X'\,|\,X) \;\leq\; \ln\left(\sum_{i=1}^{N} (|\mathscr{X}_i|^2 - |\mathscr{X}_i|) + 1\right)$$

Next IGAIA

Information Geometry and its Applications III

August 2 - 6, 2010 MPI for Mathematics in the Sciences, Leipzig, Germany

http://www.mis.mpg.de/calendar/conferences/2010/infgeo.html