Entropies et divergences
modélisation . statistique . algorithmique

Angular probability density reconstruction by maximum entropy

—

Towards air traffic complexity estimation

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Joint work with

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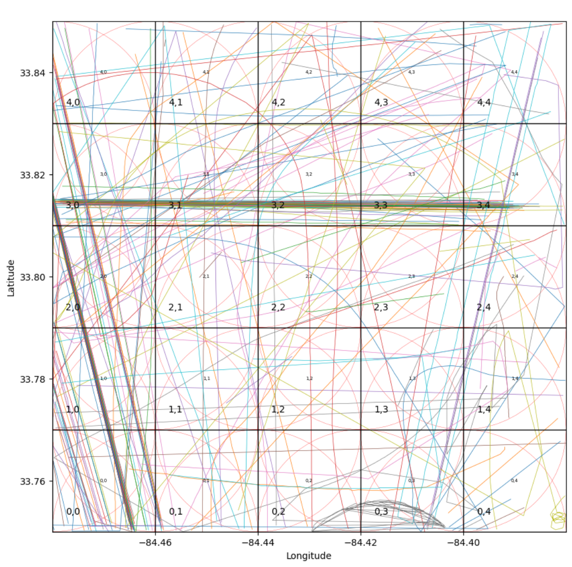

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4,0
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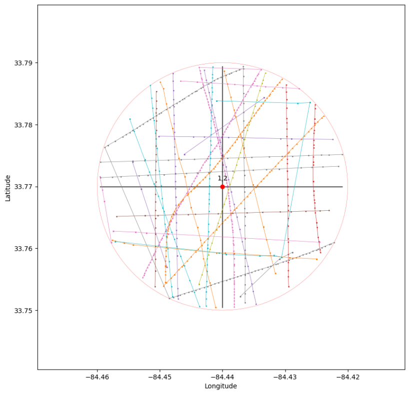
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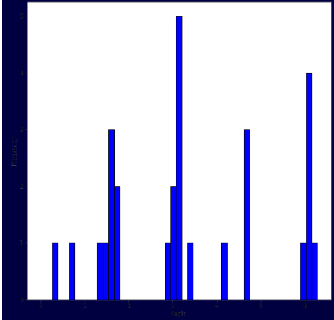
0
1
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6
Angle
Frequency

Some notation:

- S is the disc $\{(x,y) \in \mathbb{R}^2 | (x-u_1)^2 + (y-u_2)^2 \leq \delta^2\}$, in which $\mathbf{u} = (u_1, u_2)$ is the coordinate-vector of its center;

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- θ_j is the angle of $\mathscr{T}_j$ with respect to some fixed direction, at entrance point;
- we regard the θ_j's as realizations of a random variable θ, and we are then interested in estimating the probability density $p(\theta)$.

From the angular sampling θ_j, we may build a set of empirical moments. The Fourier coefficients of p are defined as

$$a_l = \frac{1}{\pi} \int_0^{2\pi} p(\theta) \cos(l\theta) \, \mathrm{d}\theta \quad \text{and} \quad b_l = \frac{1}{\pi} \int_0^{2\pi} p(\theta) \sin(l\theta) \, \mathrm{d}\theta.$$

The empirical coefficients

$$x_l = \frac{1}{\pi n} \sum_{j \in J} \cos(l\theta_j) \quad \text{and} \quad y_l = \frac{1}{\pi n} \sum_{j \in J} \sin(l\theta_j)$$

are regarded as statistical estimators of a_l and b_l, respectively.
Note in passing that the estimator x_0 gives the exact value $1/\pi$ of a_0.

$$
(\mathscr{P}_\circ)\quad
\begin{array}{|rl}
\text{Minimize} & H(p) := \displaystyle\int_0^{2\pi} p(\theta)\ln p(\theta)\,\mathrm{d}\theta \\
\text{s.t.} & p \in L^1([0,2\pi)), \\
& 1 = \displaystyle\int_0^{2\pi} p(\theta)\,\mathrm{d}\theta, \\
& x_l = \dfrac{1}{\pi}\displaystyle\int_0^{2\pi} p(\theta)\cos(l\theta)\,\mathrm{d}\theta,\ l \in \{1,\ldots,N\}, \\
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Relaxation:

$$(\mathscr{P})\quad \left|\quad \begin{aligned} \text{Minimize}\quad & H(p) + \frac{\alpha}{2}\|\mathbf{z} - \mathbb{A}p\|^2_{\Sigma^{-1}} \\ \text{s.t.}\quad & 1 = \int_0^{2\pi} p(\theta)\,\mathrm{d}\theta, \end{aligned}\right.$$

- $\|\cdot\|_{\Sigma^{-1}}$ denotes the function given by

$$\|\mathbf{z}'\|_{\Sigma^{-1}} = \sqrt{\langle \mathbf{z}', \Sigma^{-1}\mathbf{z}' \rangle},$$

in which Σ denotes the covariance matrix of random vector Z of components $X_1, \ldots, X_N, Y_1, \ldots, Y_N$, with

$$X_l = \frac{1}{n}\sum_{j \in J} \frac{1}{\pi}\cos(l\theta_j) \quad \text{and} \quad Y_l = \frac{1}{n}\sum_{j \in J} \frac{1}{\pi}\sin(l\theta_j);$$

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- $\mathbf{z} = (x_1, \ldots, x_N, y_1, \ldots, y_N)$ is the data vector;
- $\mathbb{A} : L^1([0, 2\pi)) \to \mathbb{R}^{2N}$ is the linear mapping defined by

$$(\mathbb{A}p)_m = \int_0^{2\pi} p(\theta)\cos(m\theta)\,\mathrm{d}\theta \quad \text{if} \quad m \in \{1, \ldots, N\},$$

$$(\mathbb{A}p)_m = \int_0^{2\pi} p(\theta)\sin((m-N)\theta)\,\mathrm{d}\theta \quad \text{if} \quad m \in \{N+1, \ldots, 2N\}.$$

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- In Problem $(\mathscr{P})$, the squared Mahalanobis distance between $\mathbb{A}p$ and $\mathbf{z}$ is penalized, as a *model fitting* requirement.

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  $\hookrightarrow$ *degenerate* version of the Mahalanobis distance:

$$\|\mathbf{z}'\|^2_{\Sigma^\dagger} = \begin{cases} \langle \mathbf{z}', \Sigma^\dagger \mathbf{z}' \rangle & \text{if } \mathbf{z}' \in \operatorname{ran} \Sigma, \\ \infty & \text{otherwise,} \end{cases}$$

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- The infinite value of the corresponding penalization is, of course, equivalent to a sharp constraint in problem $(\mathscr{P})$.

- *Constraint function:*

$$\boldsymbol{\gamma}(\theta) = (\cos\theta, \ldots, \cos(N\theta), \sin\theta, \ldots, \sin(N\theta)).$$

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- Problem $(\mathscr{P})$ pertains to *partially finite convex programming*.

- L real vector space;
- $f : L \to [-\infty, \infty]$;
- $\operatorname{epi} f := \{\, (x, \alpha) \in L \times \mathbb{R} \mid f(x) \le \alpha \,\}$;
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Definition

- *f is said to be convex if its epigraph is a convex subset of $L \times \mathbb{R}$. It is said to be proper convex if it never takes the value $-\infty$ and it is not identically equal to ∞.*
- *A function $g : L \to [-\infty, \infty]$ is said to be concave if $-g$ is convex, and proper concave if $-g$ is proper convex. Thus g is concave if and only if its hypograph is convex.*

Definition

The effective domain of a convex function f is the set

$$\operatorname{dom} f = \left\{ x \in L \,\middle|\, f(x) < \infty \right\}.$$

The effective domain of a concave function g is the set

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In optimization, we use *indicator functions* to encode constraints. The indicator function of a subset $C \subset L$ is the function

$$\delta_C(x) := \begin{cases} 0 & \text{if } x \in C, \\ \infty & \text{otherwise.} \end{cases}$$

Let now L and Λ be vector spaces paired by some bilinear mapping

$$\begin{array}{rccc} \langle\cdot,\cdot\rangle : & L\times\Lambda & \longrightarrow & \mathbb{R} \\ & (x,\xi) & \longmapsto & \langle x,\xi\rangle . \end{array}$$

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An standard example is $L=\mathbb{R}^d=\Lambda$ with the usual Euclidean scalar product. Another example is obtained by taking $L=L^1(V)$ and $\Lambda=L^\infty(V)$ with V a subset of $\mathbb{R}^n$.

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Definition

The convex conjugate of a function f (convex or not) is defined as the function

$$f^\star(\xi) = \sup \left\{ \langle x, \xi \rangle - f(x) \;\middle|\; x \in X \right\}, \quad \xi \in \Lambda.$$

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$$f_\star(\xi) = \inf \left\{ \langle x, \xi \rangle - f(x) \;\middle|\; x \in X \right\}, \quad \xi \in \Lambda.$$

A remarkable fact is that convex conjugacy acts as an involution on certain classes of functions. For example, if $f\colon \mathbb{R}^d \to [-\infty, \infty]$ is a lower-semicontinuous proper convex function, then

$$f^{\star\star} := (f^\star)^\star = f.$$

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Given a convex subset $C \in \mathbb{R}^d$, we call relative interior *of C the interior of C with respect to its* affine hull $\operatorname{aff} C$. *Recall that* $\operatorname{aff} C$ *is the smallest affine subspace that contains C. The relative interior of C is denoted by* $\operatorname{ri} C$.

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It can be shown that the relative interior of a nonempty convex set is necessarily nonempty.

Theorem (Fenchel)

Let f and g be functions on $\mathbb{R}^d$ respectively proper convex and proper concave such that

$$\operatorname{ri}\operatorname{dom} f \cap \operatorname{ri}\operatorname{dom} g \neq \emptyset.$$

Then

$$\eta := \inf_{\mathbf{x}\in\mathbb{R}^d} \{f(\mathbf{x}) - g(\mathbf{x})\} = \sup_{\boldsymbol{\xi}\in\mathbb{R}^d} \{g_\star(\boldsymbol{\xi}) - f^\star(\boldsymbol{\xi})\}$$

and the supremum is attained.

Theorem

Let be given:

- L *and* Λ*, real vector spaces;*
- $\langle \cdot, \cdot \rangle$*, a bilinear form on* $L \times \Lambda$*;*
- $\mathbb{A} \colon L \to \mathbb{R}^d$*, a linear mapping;*
- $F \colon L \to (-\infty, \infty]$*, a proper convex function;*
- $g \colon \mathbb{R}^d \to [-\infty, \infty)$*, a proper concave function.*

Assume that $\mathbb{A}$ *admits a formal adjoint mapping* $\mathbb{A}^\star$*, that is, a linear mapping* $\mathbb{A}^\star \colon \mathbb{R}^d \to \Lambda$ *such that* $\langle \mathbb{A}x, \mathbf{y} \rangle = \langle x, \mathbb{A}^\star \mathbf{y} \rangle$ *for every* $x \in L$ *and every* $\mathbf{y} \in \mathbb{R}^d$*. Then, under the qualification condition*

$$(QC) \quad \operatorname{ri}(\mathbb{A} \operatorname{dom} F) \cap \operatorname{ri}(\operatorname{dom} g) \neq \emptyset,$$

one has

$$\eta := \inf_{x \in X} \left\{ F(x) - g(\mathbb{A}x) \right\} = \max_{\boldsymbol{\lambda} \in \mathbb{R}^d} \left\{ g_\star(\boldsymbol{\lambda}) - F^\star(\mathbb{A}^\star \boldsymbol{\lambda}) \right\}.$$

The optimization problems

$$\text{Minimize } (F - g \circ \mathbb{A}) \quad \text{and} \quad \text{Maximize } (g_\star - F^\star \circ \mathbb{A}^\star)$$

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The function $D := g_\star - F^\star \circ \mathbb{A}^\star$ is referred to as the *dual function.*

Theorem (Primal attainment)

With the notation and assumptions of the previous theorem, assume in addition that

$$(QC^\star) \quad \operatorname{ri}\operatorname{dom} g_\star \cap \operatorname{ri}\operatorname{dom}(F^\star \circ \mathbb{A}^\star) \neq \emptyset.$$

Suppose further that

(a) $F^{\star\star} = F$ and $g_{\star\star} = g$;

(b) *there exists* $\bar{\boldsymbol{\lambda}}$ *dual optimal and* $\bar{x} \in \partial F^\star(\mathbb{A}^\star \bar{\boldsymbol{\lambda}})$ *such that* $F^\star \circ \mathbb{A}^\star$ *has gradient* $\mathbb{A}\bar{x}$ *at* $\bar{\boldsymbol{\lambda}}$.

Then $\bar{x}$ *is primal optimal.*

Definition

An integral functional is a functional of the form

$$\mathscr{H}(p) = \int_V h\big(p(\mathbf{x}),\mathbf{x}\big)\,\mathrm{d}\mu(\mathbf{x}), \quad u \in L.$$

Here, V is assumed to be endowed with a σ-algebra of measurable sets and with a measure denoted by μ; the function h is called the integrand, and the argument p is assumed to pertain to some space of measurable functions L.

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In our case:

- $L = L^1$,
- $h\big(p(\mathbf{x}),\mathbf{x}\big) = h_\circ\big(p(\mathbf{x})\big)$, with

$$h_\circ(t) = \begin{cases} t\ln t & \text{if } t > 0, \\ 0 & \text{if } t = 0, \\ \infty & t < 0. \end{cases}$$

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Definition

We say that a space L of measurable functions is decomposable *if it is stable under bounded alteration on sets of finite measure. Otherwise expressed, L is decomposable if and only if it contains all functions of the form*

$$\mathbb{1}_T \cdot p_\circ + \mathbb{1}_{T^c} \cdot p,$$

in which T has finite measure, $p_\circ$ is a measurable function such that the set $p_\circ(T)$ is bounded, and p is any member of L.

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One can easily see that the familiar L^p-spaces are decomposable, which includes our workspace $L^1(V, \mathscr{B}, \mathrm{d}\mathbf{x})$.

Theorem (Rockafellar)

Let L and Λ be spaces of measurable functions on Ω paired by means of the standard integral bilinear form

$$\langle f, \varphi \rangle = \int_V f(\mathbf{x})\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x}.$$

Let $\mathscr{H}$ be the functional of integrand $h_\circ$, that is,

$$\mathscr{H}(p) = \int_V h_\circ(p(\mathbf{x}))\,\mathrm{d}\mathbf{x},$$

with $h_\circ$ proper convex and lower semi-continuous. Assume that L is decomposable and that $\mathscr{H}$ has nonempty effective domain. Then

$$\mathscr{H}^\star(\varphi) = \int h_\circ^\star(\varphi(\mathbf{x}))\,\mathrm{d}\mathbf{x}$$

for every $\varphi \in \Lambda$, and $\mathscr{H}^\star$ is convex on Λ.

Theorem (Primal-dual relationship)

With the notation and assumptions of the general Fenchel Theorem, assume in addition that $\operatorname{dom} D$ *has nonempty interior, that* $\mathscr{H}$ *is an integral functional of integrand* h *such that conjugacy through the integral sign is permitted. Assume that, as requested in the primal attainment theorem,* $\mathscr{H}^{\star\star} = \mathscr{H}$ and $g_{\star\star} = g$*. Assume finally that the conjugate integrand* $h^{\star}$ *is differentiable over* $\mathbb{R}$*, and that there exists some dual-optimal vector* $\bar{\boldsymbol{\lambda}}$ *in* $\operatorname{int}\operatorname{dom} D$*. If*

$$\bar{p}(\mathbf{x}) := h^{\star\prime}\left([\mathbb{A}^{\star}\bar{\boldsymbol{\lambda}}](\mathbf{x}), \mathbf{x}\right) \in L,$$

then $\bar{p}$ *is a primal solution.*

$$(\mathscr{P}) \quad \left| \begin{array}{rl} \text{Minimize} & H(p) + \dfrac{\alpha}{2} \|\mathbf{z} - \mathbb{A}p\|^2_{\Sigma^{-1}} \\ \text{s.t.} & 1 = \displaystyle\int_0^{2\pi} p(\theta)\, \mathrm{d}\theta, \end{array} \right.$$

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Problem $(\mathscr{P})$ can be written as

$$\text{Minimize} \quad H(p) - g_\circ(\mathbb{A}_\circ p)$$

where

$$\mathbb{A}_\circ p = (\mathbb{I}p; \mathbb{A}p) \in \mathbb{R} \times \mathbb{R}^{2N} = \mathbb{R}^{1+2N}$$

and

$$g_\circ(\eta_\circ, \boldsymbol{\eta}) = -\frac{\alpha}{2}\|\mathbf{z} - \boldsymbol{\eta}\|^2_{\Sigma^{-1}} - \delta_{\{1\}}(\eta_\circ).$$

The adjoint mapping $\mathbb{A}_\circ^\star\colon \mathbb{R}^{1+2N} \to L^\infty([0,2\pi))$ is given by

$$\mathbb{A}_\circ^\star(\lambda_\circ, \boldsymbol{\lambda})(\theta) = \lambda_\circ + \langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle.$$

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$$(g_\circ)_\star(\lambda_\circ, \boldsymbol{\lambda}) = \lambda_\circ + \langle \mathbf{z}, \boldsymbol{\lambda} \rangle - \frac{1}{2\alpha} \| \boldsymbol{\lambda} \|_\Sigma^2.$$

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Accounting for *conjugacy through the integral sign*, the dual problem reads:

$$(\mathscr{D}) \quad \text{Maximize} \quad \lambda_\circ + \langle \boldsymbol{\lambda}, \mathbf{z} \rangle - \frac{1}{2\alpha} \| \boldsymbol{\lambda} \|_\Sigma^2 - \exp(\lambda_\circ - 1) \int_0^{2\pi} \exp\langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta.$$

The dual function is concave, finite and differentiable on $\mathbb{R}^{1+2N}$.

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Optimality system:

$$\begin{cases} 0 & = & 1 - \exp(\bar{\lambda}_\circ - 1) \displaystyle\int_0^{2\pi} \exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta, \\ \mathbf{0} & = & \mathbf{z} - \dfrac{1}{\alpha} \Sigma \bar{\boldsymbol{\lambda}} - \exp(\bar{\lambda}_\circ - 1) \displaystyle\int_0^{2\pi} \boldsymbol{\gamma}(\theta) \exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta, \end{cases}$$

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The system reduces to

$$\mathbf{0} = \mathbf{z} - \frac{1}{\alpha} \Sigma \bar{\boldsymbol{\lambda}} - \frac{\displaystyle\int_0^{2\pi} \boldsymbol{\gamma}(\theta) \exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta}{\displaystyle\int_0^{2\pi} \exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta}.$$

The above system is also the optimality system of the problem

$$(\tilde{\mathscr{D}}) \quad \text{Maximize } \langle \boldsymbol{\lambda}, \mathbf{z} \rangle - \frac{1}{2\alpha} \| \boldsymbol{\lambda} \|_\Sigma^2 - \ln \int_0^{2\pi} \exp\langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta$$

Proposition

The function

$$\tilde{D}(\boldsymbol{\lambda}) := \langle \boldsymbol{\lambda}, \mathbf{z} \rangle - \frac{1}{2\alpha} \| \boldsymbol{\lambda} \|_{\Sigma}^2 - \ln \int_0^{2\pi} \exp\langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta$$

to be maximized in Problem $(\tilde{\mathscr{D}})$ *is concave, smooth and everywhere finite. Its gradient is given by*

$$\nabla \tilde{D}(\boldsymbol{\lambda}) = \mathbf{z} - \frac{1}{\alpha} \Sigma \boldsymbol{\lambda} - \frac{\displaystyle\int_0^{2\pi} \boldsymbol{\gamma}(\theta) \exp\langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta}{\displaystyle\int_0^{2\pi} \exp\langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta}.$$

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The function $h_\circ^\star(\tau) = \exp(\tau - 1)$ obviously meets the requirements of the primal-dual relationship theorem. Provided we can obtain a dual solution $(\bar{\lambda}_\circ, \bar{\boldsymbol{\lambda}})$, the optimal density is then given by

$$\bar{p}(\theta) = \exp\left[\bar{\lambda}_\circ - 1 + \langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle\right] = \frac{\exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle}{\displaystyle\int_0^{2\pi} \exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta}.$$

Algorithm 1 Computing maximum entropy densities

1: **Input**: the range N, that is, the number of *empirical* (complex) Fourier coefficients to be taken into account, and the data vector $\mathbf{z} \in \mathbb{R}^{2N}$

2: **Output**: The maximum entropy probability angular distributions in the cell under consideration

3: Maximize the dual functions

$$\tilde{D}(\boldsymbol{\lambda}) := \langle \boldsymbol{\lambda}, \mathbf{z} \rangle - \frac{1}{2\alpha} \|\boldsymbol{\lambda}\|_{\Sigma}^{2} - \ln \int_{0}^{2\pi} \exp\langle \boldsymbol{\lambda}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta$$

4: From the dual optimal solutions $\bar{\boldsymbol{\lambda}}$ obtained in the previous step, form the optimal densities

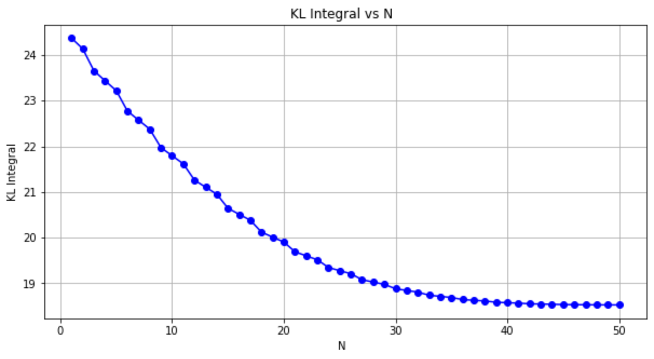
$$\bar{p}(\theta) = \frac{\exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle}{\displaystyle\int_{0}^{2\pi} \exp\langle \bar{\boldsymbol{\lambda}}, \boldsymbol{\gamma}(\theta) \rangle \, \mathrm{d}\theta}$$

In the maximum entropy problem, the *attach term*

$$\frac{\alpha}{2}\|\mathbf{z} - \mathbb{A}p\|^2_{\Sigma^{-1}}$$

depends of the choice of the highest frequency N to be accounted for, on the estimation of the covariance matrix Σ and on the choice of the *regularization parameter* α.

We observe that the Kullback-Leibler entropy of the true density $p_\circ$ relative to the reconstructed density p decreases as N increases, and stabilizes beyond some value of N.



Here, we see that there is no gain beyond $N = 50$.

We use the Morozov discrepancy principle:

> *the regularization parameter* α *should be such that the corresponding solution* $\bar{p}$ *should give a residual* $\|\mathbf{z} - \mathbb{A}\bar{p}\|$ *equal to a number strictly greater than, but close to, the estimated size* ρ *of the error on the data.*

Algorithm 2 Determining α using the Morozov discrepancy principle

Input: ρ, condition (e.g. $1.095\rho \leq \text{residual} \leq 1.105\rho$), μ (e.g. μ =1.2), maximum number of iterations $N_{\max}$
Output: Morozov value of α
Set $i = 0$, $\alpha_{\min} = 0$, $\alpha_{\max} = \infty$, $\alpha_0 = 1$
while condition is not satisfied and $i < N_{\max}$ **do**
    Compute the maximum entropy solution $\bar{p}_{\alpha_i}$
    Compute the residual $\|\mathbf{z} - \mathbf{A}\bar{p}_{\alpha_i}\|$
    if residual $< 1.095\rho$ **then**
        Set $\alpha_{\max} = \alpha_i$
        Set $\alpha_{i+1} = \frac{\alpha_{\min}+\alpha_{\max}}{2}$
    end if
    if residual $> 1.105\rho$ **then**
        Set $\alpha_{\min} = \alpha_i$
        Set $\alpha_{i+1} = \begin{cases} \frac{\alpha_{\min}+\alpha_{\max}}{2} & \text{if } \alpha_{\max} < \infty \\ \mu\alpha_i & \text{otherwise} \end{cases}$
    end if
    Set $i = i + 1$
end while

Choose the appropriate value for α:

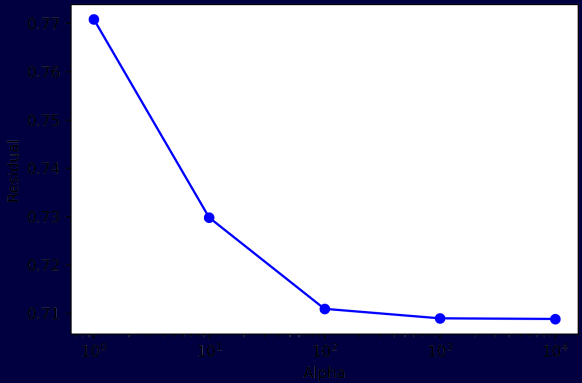


Figure: Residual values when α values from 1 to 10000.

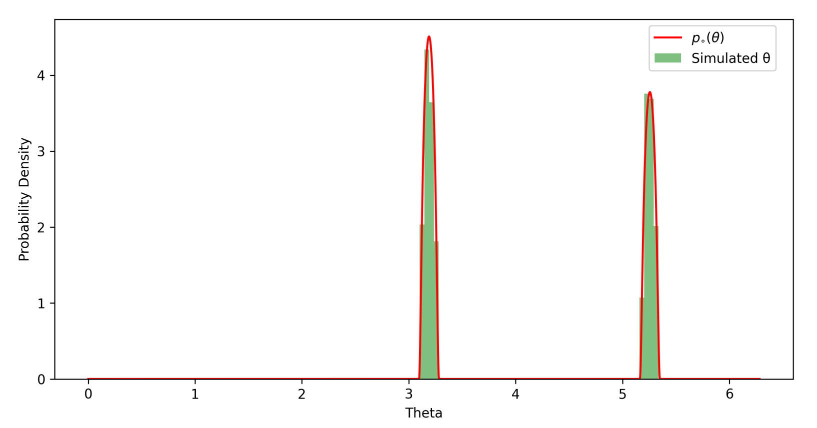
We start by performing simulations. We shall:

(a) Generate an angular sample following a probability $p_\circ$;

(b) Compute the corresponding empirical Fourier coefficients;

(c) Compute the maximum entropy density that is compatible, in the relaxed setting described above, with our empirical Fourier coefficients.

Given a specific simulation example based on the original probability $p_\circ(\theta)$ with 2 peaks and $\beta = 0.1$.



For reconstruction between original and optimal densities with two peaks.