

Maximum entropy reconstruction using derivative information part 2: computational results

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Summary. Maximum entropy density estimation, a technique for reconstructing an unknown density function on the basis of certain measurements, has applications in various areas of applied physical sciences and engineering. Here we present numerical results for the maximum entropy inversion program based on a new class of information measures which are designed to control derivative values of the unknown densities.

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1. Introduction

To begin with, let us consider the following Fourier inversion problem. We wish to reconstruct an unknown function $x(t) \geq 0$ on $[-\pi, \pi]$ on the basis of a finite number of known Fourier coefficients

$$(1.1) \quad b_k := \int_{-\pi}^{\pi} x(t) \exp\{ikt\} dt, \quad k = 0, \dots, n.$$

Problem (1.1) is most conveniently solved by calculating the truncated Fourier series, often via discretizing and using the fast Fourier transform (FFT). While this approach is generally trouble-free, there are a variety of situations where it may have serious drawbacks. For instance, in nuclear magnetic resonance spectroscopy (NMR), due to a poor signal-to-noise ratio, a low resolution in the data b_k may cause artificial effects in the estimated spectra $x(t)$. Sensitivity, that is the ability to detect weak resonances by distinguishing them from noise, may be low, and noisy or corrupted data may easily propagate into the reconstruction. Generally speaking, with only sparse data b_k , similar phenomena may arise in various other problems of Fourier spectroscopy, or in the analysis of stationary time series.

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The maximum entropy method offers a potentially more intelligent approach to the processing of the data (1.1). Among the infinitely many solutions of (1.1) it selects the estimate $x(t)$ which maximizes a given measure of entropy $H(x)$. The resulting mathematical model is the following *best entropy density estimation* program

$$\begin{aligned}
 & \text{minimize} && I(x) = -H(x) := \int_T \phi(x(t), x'(t)) dt \\
 (P) & \text{ subject to} && x \geq 0, x \in \mathcal{A}(T), \\
 & && \int_T a_k(t)x(t) dt = b_k \text{ for } k = 0, \dots, n.
 \end{aligned}$$

Here, besides the trigonometric case $a_k(t) = \exp\{ikt\}$ on $[-\pi, \pi]$, the weight functions may be algebraic polynomials (orthonormalized), $a_k(t) = t^k$ on $T = [0, 1]$, in which case the b_k would be known Hausdorff (Legendre) moments of the unknown $x(t)$, or as is the case in many applications like for instance in image reconstruction, seismology, or in small angle neutron scattering or other problems in plasma physics (see [12]), the a_k might be an appropriate wavelet basis, in which case the b_k would be known wavelet coefficients of $x(t)$. Here, $\mathcal{A}(T)$ denotes the space of absolutely continuous functions on the interval T .

In Part I of this paper [10], we began with a constrained optimization problem of type (P) and transformed it to a dual problem (P)* which we were then able to convert to an optimization problem with constraints given in terms of a boundary value problem for an ODE. This result is quite surprising. In this paper we describe how this dual problem can be solved computationally and demonstrate that the resulting reconstructed functions are comparable in quality to other entropy methods. We do conjecture that our present method of reconstruction is less likely to introduce spurious spikes since the objective (1.2) below pays a heavy price for such functions.

An important aspect of the best entropy method (P), which has found much attention in the applied literature, is the choice of the entropy measure $H(x)$. The entropy functions most frequently encountered in practice are the *Boltzmann-Shannon entropy* and the *Burg entropy*, whose integrands $\phi(x)$ do *not* depend on derivative values of the densities and are defined respectively as

$$\phi(x) := \begin{cases} x \log x & \text{for } x > 0 \\ 0 & \text{for } x = 0 \\ +\infty & \text{for } x < 0 \end{cases} \quad \text{resp.} \quad \phi(x) := \begin{cases} -\log x & \text{for } x > 0 \\ +\infty & \text{for } x \leq 0 \end{cases} .$$

Another density which is encountered in power spectrum estimation is the *positive L² entropy* defined by

$$\phi(x) := \begin{cases} \frac{1}{2}x^2 & x \geq 0 \\ +\infty & \text{else} \end{cases} .$$

The purpose of our present investigation is to discuss extended entropy-information models (P) which attempt to control derivative values of the densities. In particular we discuss a model based on the *Fisher information measure* which is defined by

$$(1.2) \quad \phi(x, x') := \begin{cases} \frac{x'^2}{x} & \text{for } x > 0 \\ 0 & \text{for } x = x' = 0 \\ +\infty & \text{else} \end{cases} .$$

More generally, we consider a class of information measures called *Csiszár distances*, which have been used in related situations (see [14], [6] and [10]), and which are defined by the integrands of the form

$$(1.3) \quad \phi(x, x') := \begin{cases} x\psi\left(\frac{x'}{x}\right) & \text{for } x > 0 \\ 0^+\psi(x') & \text{for } x = 0 \\ +\infty & \text{for } x < 0 \end{cases} .$$

Here $\psi : \mathbb{R} \rightarrow \mathbb{R}$ is a real convex function, and $0^+\psi$ denotes its recession function, see [31]. The case of the Fisher information is recovered from (1.3) by choosing $\psi(v) = v^2$. The use of the Fisher information for the inference problem of type (P) was proposed in [35] and [18], and the mathematical aspects of the corresponding model (P) have been discussed in [10].

The best entropy method has been applied in such diverse areas as astronomy and geophysics, tomography, signal processing, in problems of spectroscopy or crystallography, and in the analysis of stationary time series. For a survey containing an abundance of references see [13, 16, 17, 19, 22, 26, 27, 34, 44, 45, 46], and also [5, 6, 7, 8, 9, 10, 29].

Efficient numerical codes for the Boltzmann-Shannon and Burg entropy models have been used for several years, see [7, 4, 2, 18] for example. The programs (P) for the Fisher information (1.2) and the Csiszár distances (1.3) are different in nature and our approach for solving them resembles models in convex optimal control. While these kinds of control problems are often solved by means of Galerkin or Ritz-Treffts methods, cf. [20], our present approach is based on a different idea which uses convexity methods, motivated in particular by the *partially finite programming* technique as discussed for instance in [5, 6] or [34].

While the numerical results we present are for the case of algebraic and trigonometric polynomials a_k , the mathematical models (Sects. 2 and 3) nevertheless encompass much more general classes of weight functions, and one might in particular use wavelets. While the latter are typically used in the time-frequency analysis of signals occurring in image reconstruction, a great variety of applications of the reconstruction problem of type (1.1) still arise as problems of classical spectral analysis, with the b_k representing the Fourier coefficients of an unknown physical entity like an electron density, or a spectral density of a stationary time series, obtained by means of a physical measurement or from a series of observations, and this shows that the numerical procedures presented here are of practical relevance.

The structure of the paper is the following. In Sects. 2 and 3 we present the theoretical background for the treatment of program (P) using the objectives (1.2) and (1.3). Sections 4 and 5 give the details of the numerical results which we obtained using the duality approach previously documented [10].

Let us fix some notations. For a convex function ψ , the Young-Fenchel conjugate ψ^* is as usual defined by the formula $\psi^*(y) = \sup_x x \cdot y - \psi(x)$, see [31]. By $\phi(x, y)$ we shall always denote a lower semi-continuous proper convex function on \mathbb{R}^2 . The associated integral functional is

$$I(x, y) = \int_T \phi(x(t), y(t)) dt,$$

and we keep the notation $I(x)$ for $I(x, x')$. Given the weight functions a_0, \dots, a_n , we let A denote the operator $Ax = (\int_T a_0x, \dots, \int_T a_nx)$, and we let $b = (b_0, \dots, b_n)$.

2. Duality

We need the following minimal requirement on the weight functions a_k . We assume that $\{a_0, \dots, a_n\}$ is a *pseudo-Haar* family, which means that $a_0|_M, \dots, a_n|_M$ is linearly independent on any set M of positive measure (see [5] for this notion). In particular, this is the case for any Tchebysheff system in the sense of [26], and in particular, for the trigonometric or algebraic polynomial systems. Equally, it would be fulfilled e.g. for a_k representing an appropriate wavelet basis. Also, we assume $a_k \in \mathcal{L}_\infty(T)$, and for convenience that $a_0 \equiv 1$ on T .

The first question for program (P) regards feasibility. This is answered by the following:

Proposition 2.1. *Suppose there exists $\hat{x} \in \mathcal{L}_1(T)$ such that $\hat{x} \geq 0$, $\hat{x} \neq 0$, and having $\int_T a_k(t)\hat{x}(t) dt = b_k$ for $k = 0, \dots, n$. Then problem (P) is feasible for any of the Csiszár objectives (1.3). Even more, the following constraint qualification is satisfied:*

$$(CQ) \quad \exists \tilde{x} \in \mathcal{C}^1(T) \quad \tilde{x} > 0 \quad \text{and} \quad \int_T a_k(t)\tilde{x}(t) dt = b_k \quad \text{for } k = 0, \dots, n.$$

Proof. Observe first that (CQ) certainly implies feasibility of (P), since $\phi(\tilde{x}, \tilde{x}') = \tilde{x}\psi(\tilde{x}'/\tilde{x})$ is integrable for \tilde{x} as in (CQ).

Suppose now \hat{x} is given as above. Then according to [5, Thm. 2.9] there exists $\bar{x} \in \mathcal{L}_\infty(T)$ such that $\bar{x} \geq \epsilon > 0$ for some $\epsilon > 0$ and still $A\bar{x} = b$, where A denotes the operator $Ax = (\int_T a_0x, \dots, \int_T a_nx)$, and $b = (b_0, \dots, b_n)$. Now observe that A is surjective and hence open as an operator $\mathcal{C}^1(T) \rightarrow \mathbb{R}^{n+1}$, since the a_i are pseudo-Haar and so in particular independent. So there exists $\delta > 0$ such that any $v \in \mathbb{R}^{n+1}$ with $|v| < \delta$ may be written as $v = Ax$ for some $x \in \mathcal{C}^1(T)$ with $\|x\|_\infty \leq \epsilon/8$, say. Fix a sequence (x_k) in $\mathcal{C}^1(T)$ having $x_k \geq \epsilon/2$ which converges to \bar{x} in \mathcal{L}_1 -norm. Then $Ax_k \rightarrow A\bar{x} = b$. Find k such that $v = A(\bar{x} - x_k)$ has $|v| < \delta$, and let $v = Ax$ with x as above. Setting $\tilde{x} = x_k + x \in \mathcal{C}^1(T)$, then $A\tilde{x} = A(x_k + x) = b$, and $\tilde{x} \geq \epsilon/2 - \epsilon/8 > \epsilon/8$. But notice that $\tilde{x} \in \text{dom}I_\phi$ for any of the integrands ϕ of type (1.3), since $\tilde{x}\psi(\tilde{x}'/\tilde{x})$ is integrable. This shows that problem (P) is feasible for any of the Csiszár distances, and that the constraint qualification (CQ) is satisfied. \square

For algebraic or trigonometric moments a_k , the feasibility condition in Proposition 2.1 above has an explicit algebraic formulation. For $a_k(t) = t^k$ on $T = [0, 1]$, and with $b = (b_0, \dots, b_n) \neq 0$, problem (P) is feasible, (and therefore, the constraint qualification (CQ) is satisfied) if and only if

- (a) For $n = 2m$, the matrices $(b_{i+j})_{0 \leq i, j \leq m}$ and $(b_{i+j+1} - b_{i+j+2})_{0 \leq i, j \leq m-1}$ are positive definite;
- (b) For $n = 2m + 1$, the matrices $(b_{i+j+1})_{0 \leq i, j \leq m}$ and $(b_{i+j} - b_{i+j+1})_{0 \leq i, j \leq m}$ are positive definite.

In fact, in this case, the feasibility condition is equivalent to $b = (b_0, \dots, b_n)$ being an interior point of the moment cone \mathcal{M}_{n+1} in the sense of [26], and the latter may be expressed by (a),(b) above. See [26, p. 106], and [27] for details including even more general pseudo-Haar systems. Similarly, for the trigonometric moment case, $a_k(t) = \exp ikt$ on $T = [-\pi, \pi]$, program (P) is feasible (and hence (CQ) is satisfied) if and only if

- (c) the Toeplitz matrix $(b_{k-l})_{0 \leq k, l \leq n}$ is positive definite.

See [1] and also [27] for the details of the formulation in these cases.

With the question of feasibility of program (P) settled, let us now discuss the existence and uniqueness of its solution, and the duality result used to calculate it. This has been presented in full detail in the first part [10] of this paper, and we recall the relevant facts here.

On recognizing problem (P) as an infinite dimensional convex optimization program, the basic idea is to apply methods of convex duality. This requires a Lagrangian formulation. As in similar situations, see [10] or [32, 33, 21], we define the *Lagrangian* as

$$(2.1) \quad L(x, y; v, \lambda) := \int_T \phi(x, y) dt + \int_T v(x' - y) dt + \sum_{k=0}^n \lambda_k \left(\int_T a_k x dt - b_k \right) \\ = I(x, y) + \langle v, x' - y \rangle + \langle \lambda, Ax - b \rangle,$$

with $x \in \mathcal{A}(T)$, $y \in \mathcal{L}_1(T)$, $v \in \mathcal{A}(T)$, $\lambda \in \mathbb{R}^{n+1}$. Then program (P) clearly has the equivalent formulation

$$(P) \quad \inf_{x, y} \sup_{v, \lambda} L(x, y; v, \lambda),$$

and one defines the corresponding *dual program* as

$$(P)^* \quad \sup_{v, \lambda} \inf_{x, y} L(x, y; v, \lambda).$$

The constraint qualification (CQ) is then needed to prove the equivalence of both programs. In particular, in [10], we proved the following:

Proposition 2.2. *Suppose ψ is strictly convex and coercive (that is $\psi(t)/t \rightarrow +\infty$ as $|t| \rightarrow \infty$). Let (P) be the problem with corresponding integrand ϕ given in (1.3), and suppose (P) is feasible. Then:*

- (1) *problem (P) has a unique optimal solution \bar{x} which is strictly positive on $T = [t_0, t_1]$ and satisfies $\bar{x}'(t_0) = \bar{x}'(t_1) = 0$;*
- (2) *problem (P)* has the equivalent formulation*

$$(P)^* \quad \begin{aligned} & \text{maximize} && - \sum_{j=0}^n \lambda_j b_j \\ & \text{subject to} && v' + \psi^*(v) = \sum_{j=0}^n \lambda_j a_j, \\ & && v(t_0) = v(t_1) = 0, \quad v \in \mathcal{C}^1(T). \end{aligned}$$

- (3) *problem (P)* has a unique optimal solution $(\bar{v}, \bar{\lambda})$, and the primal optimal solution \bar{x} may be recovered from the latter by means of the formulae*

$$(2.2) \quad \frac{\bar{x}'(t)}{\bar{x}(t)} = \psi^*(\bar{v}(t)) \quad \text{and} \quad A\bar{x} = b.$$

Proof. The results are covered by [10]. Statement (1) is Theorem 2.4 and Corollary 4.8, while statement (2) is Proposition 4.5 and Example 4.1. Formula (2.2) above is formula (4.11) in [10]. \square

It is worth noting that for a_k and ψ^* of class \mathcal{C}^k , the solution \bar{x} is of class \mathcal{C}^{k+2} . In particular, for the Fisher information, and for the a_k algebraic or trigonometric polynomials, \bar{x} is a \mathcal{C}^∞ function.

3. Numerical formulation

In this section we obtain a numerically tractable formulation for the dual program $(P)^*$. We assume throughout that ψ is strictly convex and coercive. This implies that the conjugate function ψ^* is differentiable and $\text{dom } \psi^* = \mathbb{R}$. We start by considering the differential equation with initial condition

$$(3.1) \quad v'(t) + \psi^*(v(t)) = \sum_{j=0}^n \lambda_j a_j(t), \quad v(t_0) = 0.$$

Notice that in the Fisher case $\psi(v) = v^2$, $\psi^*(v) = \frac{1}{4}v^2$, (3.1) is a Riccati equation. Now let Ω denote the set of all $\lambda \in \mathbb{R}^{n+1}$ for which (3.1) has a unique solution $v(\lambda, \cdot)$ defined on the whole interval $T = [t_0, t_1]$. Clearly $0 \in \Omega$, and it is well-known that Ω is an open domain in \mathbb{R}^{n+1} , see for instance [22, p. 95]. Let $k : \Omega \rightarrow \mathbb{R}$ be defined as

$$(3.2) \quad k(\lambda) := v(\lambda, t_1),$$

then k is of class \mathcal{C}^1 on Ω , see [22, p. 95]. The dual program $(P)^*$ obtained in Proposition 2.2(2) now takes the equivalent finite dimensional form

$$(P)^* \quad \begin{array}{ll} \text{maximize} & - \sum_{j=0}^n \lambda_j b_j \\ \text{subject to} & \lambda \in \Omega, \quad k(\lambda) = 0. \end{array}$$

Notice that in this formulation, $(P)^*$ has an optimal solution $\bar{\lambda}$ by Proposition 2.2(3), with the corresponding $\bar{v} := v(\bar{\lambda}, \cdot)$ satisfying $\bar{v}(t_1) = v(\bar{\lambda}, t_1) = k(\bar{\lambda}) = 0$.

Let us consider the Lagrangian for problem $(P)^*$:

$$L(\lambda, r) = - \sum_{j=0}^n \lambda_j b_j + r k(\lambda).$$

Then the optimal solution $\bar{\lambda}$ gives rise to a saddle point $(\bar{\lambda}, \bar{r})$ of $L(\lambda, r)$. Here the Kuhn-Tucker conditions must be satisfied, and these take the form

$$(3.3) \quad \begin{array}{ll} -b_j + \bar{r} \frac{\partial}{\partial \lambda_j} k(\bar{\lambda}) = 0 & \text{for } j = 0, \dots, n \\ k(\bar{\lambda}) = 0 \end{array}.$$

Assuming again that $b = (b_0, \dots, b_n) \neq 0$, we must have $\bar{r} \neq 0$. Also, since problem (P) is feasible and $a_0 = 1$, we must have $b_0 > 0$, which implies $\text{sgn } \bar{r} = \text{sgn } \frac{\partial}{\partial \lambda_0} k(\bar{\lambda})$.

Observe next that for $i, j = 0, \dots, n$

$$(3.4) \quad \begin{array}{ll} \frac{\partial}{\partial \lambda_i} k(\lambda) & = \frac{\partial}{\partial \lambda_i} v(\lambda, t_1) =: v_i(\lambda, t_1), \\ \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} k(\lambda) & = \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} v(\lambda, t_1) =: v_{ij}(\lambda, t_1), \end{array}$$

and that the functions $v_i(\lambda, \cdot)$ so defined solve the initial value problems

$$(3.5) \quad v_i'(\lambda, t) + \psi^{*'}(v(\lambda, t)) v_i(\lambda, t) = a_i(t), \quad v_i(\lambda, t_0) = 0,$$

for $i = 0, \dots, n$. Similarly, the functions $v_{ij}(\lambda, \cdot)$ solve the initial value problems

$$(3.6) \quad \begin{aligned} v'_{ij}(\lambda, t) + \psi^{*''}(v(\lambda, t)) v_i(\lambda, t) v_j(\lambda, t) + \psi^{*'}(v(\lambda, t)) v_{ij}(\lambda, t) &= 0, \\ v_{ij}(\lambda, t_0) &= 0 \end{aligned}$$

for $0 \leq i, j \leq n$. Let us now define

$$(3.7) \quad \alpha(t) := \exp \left\{ \int_{t_0}^t \psi^{*'}(\bar{v}(s)) ds \right\},$$

where $\bar{v} = v(\bar{\lambda}, \cdot)$, then $\alpha(t_0) = 1$, $\alpha(t_1) > 0$, and $\alpha'/\alpha = \psi^{*'}(\bar{v})$. Therefore, α is an integrating factor for each of the equations (3.5), and we obtain

$$\alpha' v_i + v'_i \alpha = a_i \alpha, \quad i = 0, \dots, n.$$

On integrating over $T = [t_0, t_1]$, we get

$$(3.8) \quad \int_{t_0}^{t_1} \alpha(s) a_i(s) ds = \alpha v_i \Big|_{t_0}^{t_1} = \alpha(t_1) \frac{\partial}{\partial \lambda_i} k(\bar{\lambda}) = \frac{\alpha(t_1) b_i}{\bar{r}}.$$

Choosing $i = 0$ therefore gives $\bar{r} > 0$. Let us summarize:

Proposition 3.1. *Suppose problem (P)* has optimal solution $\bar{\lambda}$. Then problem (P) has optimal solution \bar{x} with the explicit form*

$$(3.9) \quad \bar{x}(t) = C \exp \left\{ \int_{t_0}^t \psi^{*'}(\bar{v}(s)) ds \right\},$$

where $C = \bar{r}/\alpha(t_1) > 0$, $\bar{v} = v(\bar{\lambda}, \cdot)$, and where $(\bar{\lambda}, \bar{r})$ is a Kuhn-Tucker point of (P)*.

Let us continue by noticing that $\alpha(t)$ is in addition an integrating factor for the equations (3.6), and leads to

$$(3.10) \quad -\alpha \psi^{*''}(v) v_i v_j = \alpha' v_{ij} + \alpha v'_{ij}.$$

On integrating over T we obtain

$$(3.11) \quad -\int_{t_0}^{t_1} \frac{\alpha}{\alpha(t_1)} \psi^{*''}(v) v_i v_j ds = \frac{1}{\alpha(t_1)} \alpha v_{ij} \Big|_{t_0}^{t_1} = v_{ij}(\lambda, t_1) = \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} k(\lambda).$$

Using this formula, we may now establish the following:

Proposition 3.2. *Suppose ψ is differentiable and ψ^* is of class \mathcal{C}^2 . Then k is strictly concave on its domain Ω .*

Proof. It follows from (3.11) that the associated Hessian quadratic form for k at $\lambda \in \Omega$ is given by

$$(3.12) \quad \sum_{i=0}^n \sum_{j=0}^n \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} k(\lambda) \mu_i \mu_j = -\int_{t_0}^{t_1} \frac{\alpha}{\alpha(t_1)} \psi^{*''}(v) \left(\sum_{k=0}^n \mu_k v_k \right)^2 ds \leq 0,$$

for every $\mu \in \mathbb{R}^{n+1}$, and it suffices to show that, with the possible exception of the point $\lambda = (\psi^*(0), 0, \dots, 0)$, the term (3.12) is strictly negative for $\mu \neq 0$ [30, Thm. (2.3.7)].

Suppose (3.12) equals 0 for some $\mu \neq 0$. Suppose first that $\psi^{*''}(v(\lambda, \cdot)) > 0$ on a set M of positive measure. Then $\sum_{k=0}^n \mu_k v_k = 0$ on M , and hence is zero on some interval $I = (r, s)$ in which M is dense; (notice that $\psi^{*''}$ is continuous). Differentiating with respect to t implies $\sum_{k=0}^n \mu_k v'_k = 0$ on I , and equation (3.5) then implies $\sum_{k=0}^n \mu_k a_k = 0$ on I . Since the a_k are linearly independent on I , this gives $\mu = 0$, which is impossible, so we must have $\psi^{*''}(v(\lambda, \cdot)) = 0$ almost everywhere on T in order that (3.12) equal 0 for nonzero μ .

Suppose alternatively we had $\psi^{*''} = 0$ on some interval. Then ψ^* is linear there, and hence is not strictly convex, contradicting the assumption that ψ is differentiable. So $\{t : \psi^{*''}(t) = 0\}$ does not contain an interval, and by continuity, this implies that $v(\lambda, \cdot)$ has constant value, which is 0 by the initial condition in (3.1). Now equation (3.1) tells that this is only possible for $\lambda_0 = \psi^*(0)$, $\lambda_1 = \dots = \lambda_n = 0$, as claimed. This proves the fact that k is strictly concave on its domain Ω . \square

As a consequence of Proposition 3.2, we see that program $(P)^*$ is equivalent to the concave program

$$\begin{aligned}
 (\tilde{P})^* \quad & \text{maximize} && - \sum_{j=0}^n \lambda_j b_j \\
 & \text{subject to} && \lambda \in \Omega, \quad k(\lambda) \geq 0.
 \end{aligned}$$

Indeed, any optimal solution for $(\tilde{P})^*$ is attained at a boundary point of the constraint set, and hence is admissible for program $(P)^*$. But now, as a consequence of the concavity, the Kuhn-Tucker conditions (3.3) fully characterize the optimal solution of $(P)^*$.

4. Algorithms

The straight forward approach is to solve the dual program $(P)^*$ by solving the nonlinear equations (3.3) directly using Newton’s method. This requires the first and second order partial derivatives of k at every step. These are obtained by first solving the equations (3.1), (3.5) using a standard ODE solver to compute the value $k(\lambda)$ and the gradient $\nabla k(\lambda)$. The second order partial derivatives may then be obtained by first computing α via (3.7) and then applying formula (3.11), which requires another $(n+1)(n+2)/2$ quadratures. As an initial vector $\lambda^{(0)}$ we may choose $\lambda^{(0)} = 0$, which is always a feasible point. The primal solution \bar{x} is finally calculated from the dual data $\bar{\lambda}$ and \bar{r} by numerical integration using (3.9). In the case of the Fisher information, $\psi^{*'}(v) = v/2$ is known explicitly and does not need an extra numerical procedure. We then have the following Algorithm 1:

1. Initialize $\lambda^{(0)} = 0$; $j = 0$.
2. Solve the initial value problems, (3.1), (3.5) in order to compute $k(\lambda^{(j)})$, $\nabla k(\lambda^{(j)})$. Then use (3.11) to compute $\nabla^2 k(\lambda^{(j)})$.
3. Use Newton’s method with an Armijo-Goldstein line search to update $\lambda^{(j)} \rightarrow \lambda^{(j+1)}$.
4. Stop when $|k(\lambda^{(j+1)})| \leq \epsilon$ and reconstruct \bar{x} by computing (3.9).

There is an alternative way which makes a more explicit use of the fact that program $(P)^*$ resp. $(\tilde{P})^*$ is concave. Using the concave Young-Fenchel conjugate k_* of k , that is, $k_*(y) := \inf_{x \in \mathbb{R}} yx - k(x)$, we have

$$L(r) := \sup_{\lambda} L(\lambda, r) = \sup_{\lambda} r k(\lambda) - \langle \lambda, b \rangle = -r k_*(b/r).$$

Therefore, the derivative $L'(r)$ is available, namely,

$$L'(r) = k(\lambda_r) \quad \text{where} \quad \lambda_r \quad \text{solves} \quad r \nabla k(\lambda) = b.$$

This leads to the following Algorithm 2:

1. Initialize $r^{(0)} > 0; j = 0$.
2. Calculate $L(r^{(j)}) = \sup_{\lambda} r^{(j)} k(\lambda) - \langle \lambda, b \rangle$ using step 2 in Algorithm 1 above. Let $\lambda^{(j)}$ be the solution.
3. Update $r^{(j)} \rightarrow r^{(j+1)}$ using the value $L'(r^{(j)}) = k(\lambda^{(j)})$.
4. Stop when $|k(\lambda^{(j)})| \leq \epsilon$ and reconstruct \bar{x} using (3.9).

To obtain a good initial value for r using Hausdorff (or an equivalent orthogonalized system) moments, we can exploit the structure of the equations. On the interval $[0, 1]$, a simple transformation of (3.9) results in,

$$\bar{x}(t) = \bar{r} \exp \left\{ - \int_t^1 \psi^{*'}(\bar{v}(s)) ds \right\}.$$

Using integration by parts twice on the moments,

$$b_{N-1} = \int_0^1 \bar{x}(t) t^{N-1} dt \quad \text{and} \quad b_N = \int_0^1 \bar{x}(t) t^N dt$$

(assuming \bar{x} is \mathcal{C}^2) we obtain

$$\begin{aligned} N(N+1)b_{N-1} &= (N+1)\bar{x}(1) - \dot{\bar{x}}(1) + \int_0^1 \ddot{\bar{x}}(t) t^{N+1} dt \\ (N+1)(N+2)b_N &= (N+2)\bar{x}(1) - \dot{\bar{x}}(1) + \int_0^1 \ddot{\bar{x}}(t) t^{N+2} dt. \end{aligned}$$

Subtracting the two equations, we obtain asymptotically

$$\bar{r} = \bar{x}(1) \approx (N+1)(N+2)b_N - N(N+1)b_{N-1}$$

which can be used as an initial approximation for r . In order to obtain a good initial value for λ in an N -moment problem, the solution to the easier problem using the first M moments ($M < N$) can be computed and then used to initialize λ for the more difficult N -moment problem. This emphasizes one of the advantages of the dual approach, namely a dual vector λ calculated for a reconstruction with $M < N$ moments is a feasible point for the N -moment reconstruction, a fact which is not true for the corresponding primal programs.

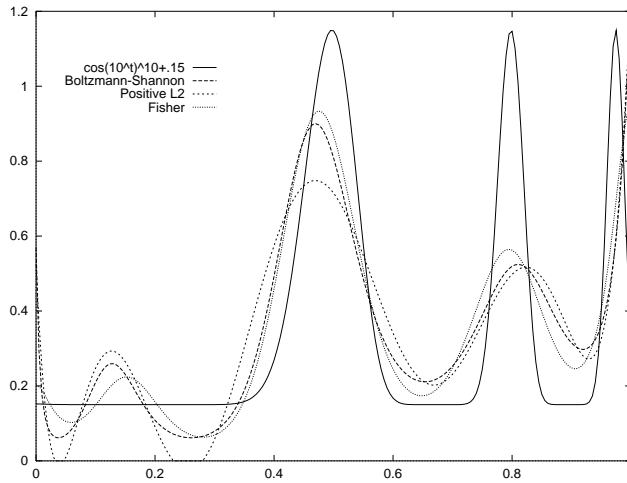


Fig. 1. $x(t) = \cos^{10}(10t) + .15$ with 10 Legendre moments

5. Numerical Results

In this section we compare reconstructions using the Fisher Algorithm 2 with the Boltzmann-Shannon and positive L^2 methods for several examples. All computations were written in C and run on SGI machines in double precision. Tests for the Burg entropy are not included since in [3] it was shown that Boltzmann-Shannon and positive L^2 methods very generally produced better reconstructions than Burg (see however [28]).

In Figs. 1, 2 and 3 we compare the reconstructions using each method with the original known function which was used to generate the moments. Visually, the reconstructions appear to be fairly comparable. They all locate the spikes, yet have trouble finding the height of the original spikes and oscillate along flat regions.

In Tables 1, 2, and 3 various measures of how well each method reconstructed the original function are shown. The L^2 -norm of the difference between the estimated function \bar{x} and the original test function x ,

$$L^2\text{-error} = \int (\bar{x} - x)^2,$$

and the L^∞ norm of the difference,

$$L^\infty\text{-error} = \max_{t \in T} |\bar{x}(t) - x(t)|$$

both measure how well the reconstruction of the original function was performed. The moment error,

$$\text{mom-error} = \frac{\sum_{k=0}^n |b_k - \bar{b}_k|}{n + 1}$$

(where \bar{b}_k are the reconstructed moments) measures how well each method succeeded in reconstructing the given moments.

The implementation of the Fisher Algorithm involved a combination of numerical optimization techniques and ODE methods and, as a result, posed an interesting

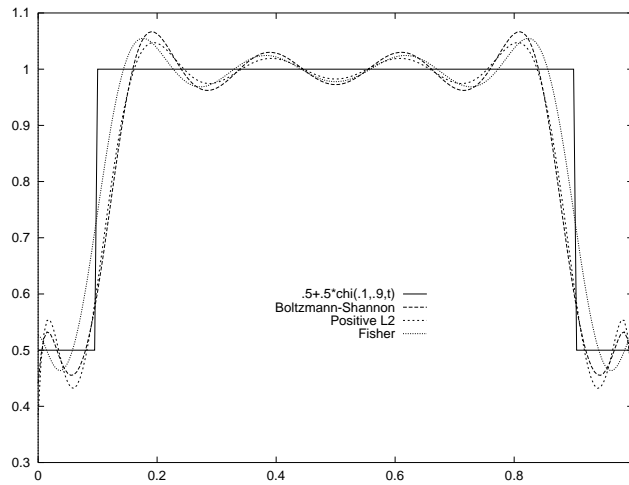


Fig. 2. $x(t) = .5 + .5\chi_{[.1,.9]}(t)$ with 14 Legendre moments

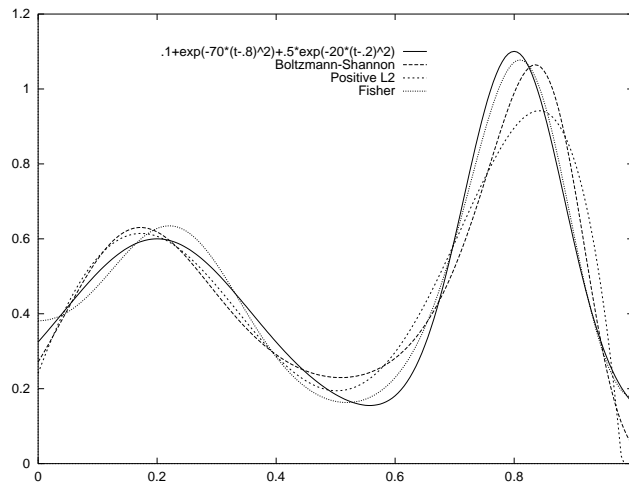


Fig. 3. $x(t) = .1 + e^{-70(t-.8)^2} + .5e^{-20(t-.2)^2}$ with 6 Legendre moments

Table 1. Various Comparisons, $x(t) = \cos^{10}(10^t) + .15$

	Fisher	B-S	L^2
L^∞ -error	6.3×10^{-1}	6.3×10^{-1}	6.5×10^{-1}
L^2 -error	2.8×10^{-2}	3.8×10^{-2}	4.9×10^{-2}
mom-error	8.1×10^{-6}	9.7×10^{-15}	2.0×10^{-4}

Table 2. Various Comparisons, $x(t) = .5 + .5\chi_{[.1, .9]}(t)$

	Fisher	B-S	L^2
L^∞ -error	2.5×10^{-1}	3.9×10^{-1}	3.8×10^{-1}
L^2 -error	3.6×10^{-3}	7.2×10^{-3}	6.2×10^{-3}
mom-error	1.8×10^{-6}	1.7×10^{-11}	2.0×10^{-2}

Table 3. Various Comparisons, $x(t) = .1 + e^{-70(t-.8)^2} + .5e^{-20(t-.2)^2}$

	Fisher	B-S	L^2
L^∞ -error	5.8×10^{-2}	5.3×10^{-2}	7.2×10^{-2}
L^2 -error	9.8×10^{-4}	2.2×10^{-4}	4.9×10^{-4}
mom-error	6.0×10^{-6}	2.5×10^{-13}	1.0×10^{-3}

computational challenge. A double iteration method was used and at each iteration of the Lagrange multiplier, r , an optimal value for λ was determined using a Newton iteration. Further, at each of these Newton steps, for an N -moment problem it was necessary to solve an ODE to compute $k(\lambda)$, then N variational ODE's to compute the gradient of k , and finally $(N^2 + N)/(N^2 + N)/2$ integrations to compute the Hessian of k . As might be expected, the entire computation is quite slow. However, early tests of a Galerkin-like heuristic method for computing the Fisher algorithm indicate that we will be able to improve the speed of the algorithm dramatically by using the heuristic to calculate a good initial vector for the Newton iteration. We are able to solve a typical 14-moment problem using the new heuristic method written in C on an SGI machine in 1.6 user seconds, see [11].

A further computational difficulty is that the solution to the ODE becomes increasingly unstable as the number of moments is increased. In addition, the iterations are sensitive to both the initial value of r and of λ and did not converge well for test functions which were close to zero. We have found that both iterations were considerably more stable and the algorithm converged for more difficult problems when the Legendre moments were used, i.e., when the sequence a_0, \dots, a_n is orthonormal. In practice this makes an immense difference. Despite these computational difficulties, we want to emphasize that the approach we used here was a straight forward implementation of an unusual and quite surprisingly explicit duality theory.

The reconstruction programs based on the Boltzmann-Shannon and the positive L^2 -entropies have been implemented using a partially finite programming duality approach as in [7, 34]. See [1, 8] for details, and also [3] for a comparison of these methods.

We have found a variety of examples where the Fisher information performs better than the more standard Boltzmann-Shannon entropy. Along with a more detailed comparison of these methods, those will be presented in a forthcoming paper [11]. In particular, there we will present numerical results for a Galerkin-like heuristic method for solving the same Fisher entropy problem. Early test results indicate that the heuristic method is more stable and produces comparable reconstructions in a very small fraction of the time. We conclude that the Fisher entropy method produces comparable results to other entropy methods and will continue to explore its use in

situations when it is important to minimize oscillatory behavior often exhibited in other methods.

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