Applications of an algorithm for solving Fredholm equations of the first kind^{*}

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Abstract

In this paper we use an iterative algorithm for solving Fredholm equations of the first kind. The basic algorithm is known and is based on an EM algorithm when involved functions are non-negative and integrable. With this algorithm we demonstrate two examples involving the estimation of a mixing density and a first passage time density function involving Brownian motion. We also develop the basic algorithm to include functions which are not necessarily non-negative and again present illustrations under this scenario. A self contained proof of convergence of all the algorithms employed is presented.

Keywords: Brownian motion first passage time; convergence; expectation–maximization; iterative algorithm; mixture model.

1 Introduction

An important problem in statistics and applied mathematics is the solution to a so-called *Fredholm* equation of the first kind, i.e., given a probability density function f(x) on $\mathbb{X} \subset \mathbb{R}$ and a nonnegative kernel $k(x, \theta)$ which is a probability density function in x for each θ , find the probability

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density function $p(\theta)$ such that

$$f(x) = \int_{\Theta} k(x,\theta) \, p(\theta) \, \mathrm{d}\theta. \tag{1}$$

Such equations have a wide range of applications across a variety of fields, including signal processing, physics, and statistics. See Ramm (2005) for a general introduction, and Vangel (1992) for statistical applications. We will also consider problems where the density and non-negativity constraints are relaxed.

Given the importance of this problem, it should be no surprise that there is a substantial literature on the theoretical and computational aspects of solving (1); see, for example, Corduneanu (1994); Groetsch (2007); Hansen (1999); Morozov (1984); Wing (1990). Existence of a unique solution to (1) is a relevant question, though we will not speak directly on this issue here. One important case for which there is a well-developed existence theory is when the operator $p \mapsto \int k(\cdot, \theta) p(\theta) d\theta$ is compact, a consequence of square-integrability of $k(x, \theta)$ with respect to $dx \times d\theta$. In this case, there exists a singular value system (σ_j, u_j, v_j) for which $(u_j(x))$ and $(v_j(\theta))$ are orthogonal bases in $L_2(\mathbb{X})$ and $L_2(\Theta)$, respectively, and

$$\int_{\Theta} k(x,\theta) v_j(\theta) \,\mathrm{d}\theta = \sigma_j u_j(x).$$

Then f can be expressed as $f(x) = \sum_{j} \lambda_{j} u_{j}(x)$ for some (λ_{j}) , and it follows that

$$p(\theta) = \sum_{j} (\lambda_j / \sigma_j) v_j(\theta),$$

which exists and is square-integrable if $\sum_{j} (\lambda_j / \sigma_j)^2 < \infty$. Of course, the above formula for p is not of direct practical value since computing all the eigenvalues and eigenfunctions is not feasible. Computationally efficient approximations are required.

The classic iterative algorithm for finding p is given by

$$p_m(\theta) = p_{m-1}(\theta) + \int_{\mathbb{X}} k(x,\theta) \left(f(x) - f_{m-1}(x) \right) \mathrm{d}x, \tag{2}$$

where

$$f_m(x) = \int_{\Theta} k(x,\theta) p_m(\theta) \,\mathrm{d}\theta.$$

Convergence properties of (2) are detailed in Landweber (1951). An issue here is that, under the constraint that p and $k(\cdot, \theta)$ are density functions, there is no guarantee that the sequence of approximations (p_m) coming from (2) are density functions. An alternative is to apply a discretization-based method. That is, specify grid points (θ_j, x_i) and approximate the original problem (1) via a discrete system

$$f(x_j) = \sum_i w_i \, p(\theta_i) \, k(x_j, \theta_i),$$

where the (w_i) are weighting coefficients for a quadrature formula. One then solves the linear system of equations to get an approximation for p. See for example, Phillips (1962). Of course, there is no guarantee here either that the solution p will be a density.

As an alternative to the additive updates in (2), in this paper we focus on a multiplicative version, described in Section 2, that can guarantee the sequence of approximations are density functions. Moreover, the theoretical convergence analysis of this multiplicative algorithm turns out to be rather straightforward for the case where there exists a unique solution to equation (1). For the general case, where a solution may not exist, the asymptotic behavior of the algorithm can still be determined, and, in Section 3, we provide a characterization of this algorithm as an *alternating minimization* algorithm, and employ the powerful tools developed in Csiszzár and Tusnády (1984) to study its convergence. The remainder of the paper focuses on three applications of this algorithm. The first, in Section 4, is estimating a smooth mixing density based on samples X_1, \ldots, X_n from the density f in (1). The second, in Section 5, is computing the density of the first passage time for Brownian motion hitting an upper boundary, where the boundary need not be concave. The third, in Section 6, is solving general Fredholm equations where the density function constraints are relaxed. Finally, some concluding remarks are given in Section 7.

2 The algorithm

Following Vardi and Lee (1993), an alternative to the algorithms described above for iteratively solving (1) is to fix an initial guess p_0 and then repeat

$$p_m(\theta) = p_{m-1}(\theta) \int_{\mathbb{X}} \frac{k(x,\theta) f(x)}{f_{m-1}(x)} \, \mathrm{d}x, \quad m \ge 1.$$
(3)

This algorithm was also studied in Shyamalkumr (1996). First note that, if f_0 is well-defined, then it follows immediately from the multiplicative structure of the algorithm, and Fubini's theorem, that p_m is also a density for $m \ge 1$. This overcomes the difficulty faced with using (2). Second, for a comparison with (2), we see that (3) operates in roughly the same way, but on the log-scale:

$$\log p_m(\theta) = \log p_{m-1}(\theta) + \log \int_{\mathbb{X}} \frac{k(x,\theta) f(x)}{f_{m-1}(x)} \,\mathrm{d}x.$$
(4)

This logarithmic version will be helpful when we discuss convergence in Section 3.

The sequence (3) also has a Bayesian interpretation. Indeed, if, at iteration m, we had seen an observation X from the distribution with density f, then the Bayes update of "prior" $p_{m-1}(\cdot)$ to "posterior" $p_m(\cdot \mid X)$ would be given by

$$p_m(\theta \mid X) = p_{m-1}(\theta) \frac{k(X,\theta)}{f_{m-1}(X)}$$

But without such an X, yet knowing X comes from f, the natural choice now is to use the "average update"

$$p_m(\theta) = \int_{\mathbb{X}} p_m(\theta \mid x) f(x) \, \mathrm{d}x,$$

which is exactly (3).

For a quick proof-of-concept, consider a Pareto density $f(x) = a(x + 1)^{-(a+1)}$, supported on $(0, \infty)$, with a > 0. It is easy to check that f is a gamma mixture of exponentials, i.e., $f(x) = \int k(x,\theta)p(\theta) \,d\theta$, where $k(x,\theta) = \theta e^{-\theta x}$ is an exponential density and $p(\theta) = \Gamma(a)^{-1}\theta^{a-1}e^{-\theta}$ is a gamma density. We can apply algorithm (3) to solve the above equation for p. Figure 1 shows a plot of the estimate from (3), with a = 5, based on 200 iterations and p_0 a half-Cauchy starting density, along with the true gamma density p(x). Clearly, the approximation is quite accurate over most of the support.

Before formally addressing the convergence properties of (3), it will help to provide some intuition as to why it should work. The argument presented in Vardi and Lee (1993) proceeds by considering i.i.d. samples X_1, \ldots, X_n from the distribution with density f. Replacing the f(x) dxin (3) with $d\hat{F}(x)$, where \hat{F} is the empirical distribution based on X_1, \ldots, X_n , gives the algorithm

$$\widehat{p}_m(\theta) = \widehat{p}_{m-1}(\theta) \int_{\mathbb{X}} \frac{k(x,\theta)}{f_{m-1}(x)} \,\mathrm{d}\widehat{F}(x).$$
(5)

It turns out that this is precisely an EM algorithm to compute the nonparametric maximum likelihood estimator of p, see e.g., Laird (1978). This connection to likelihood-based estimation gives the algorithm (5) some justification for a fixed sample X_1, \ldots, X_n . The dependence on a particular sample can be removed by allowing $n \to \infty$ and applying the law of large numbers to



Figure 1: Plot of the mixing density p_{200} (black) from (3) and the true gamma density (gray).

get convergence of (5) to (3), hence motivation for the latter. However, despite the identification of (5) as an EM algorithm, no formal convergence proof has been given that the iterates \hat{p}_m in (5) converge to the nonparametric maximum likelihood estimator, but see Chae et al. (2017).

The above argument giving intuitive support for algorithm (3) is not fully satisfactory because it does not give any indication that the algorithm will converge to a solution of (1). For a more satisfactory argument, note that, *if the algorithm converges* to a limit p_{∞} , then we must have

$$\int_{\mathbb{X}} \frac{k(x,\theta)}{f_{\infty}(x)} f(x) \, \mathrm{d}x = 1 \quad \forall \ \theta \in \mathrm{supp}(p_{\infty}),$$

where $f_{\infty}(x) = \int k(x,\theta) p_{\infty}(\theta) d\theta$. According to Lemma 2.1 in Patilea (2001) or Lemma 2.3 in Kleijn and van der Vaart (2006), the above condition implies that

$$D(f, f_{\infty}) = \inf_{P} D(f, f_{P}), \tag{6}$$

where $D(f,g) = \int \log(f/g) f \, dx$ is the Kullback-Leibler divergence and the infimum is over all densities of the form $\int k(x,\theta) \, dP(\theta)$ for some probability measure P on Θ . So, if there exists a solution to (1), then the limit p_{∞} would have to be one of them. Even if there is no solution to (1), p_{∞} will be such that the corresponding f_{∞} is closest to f in the Kullback-Leibler sense. To make this argument fully rigorous, we need to establish that algorithm (3) does indeed converge.

3 Convergence properties

In Section 3.4 of Vardi and Lee (1993), the authors consider (1), but with some restrictions. The first is that p is a finite measure, i.e., point masses on a finite number of atoms, and the second is that the solution p is piecewise constant. Our arguments here do not require such restrictions.

To assess the properties of (2), let p be a solution to (1). Multiply (4) by $p(\theta)$ throughout, and then integrate over θ to get

$$\int p(\theta) \log p_m(\theta) \,\mathrm{d}\theta = \int p(\theta) \log p_{m-1}(\theta) \,\mathrm{d}\theta + \int p(\theta) \log \int \frac{k(x,\theta) f(x)}{f_{m-1}(x)} \,\mathrm{d}x \,\mathrm{d}\theta$$

By Jensen's inequality, the last term is lower bounded by $D(f, f_{m-1})$, the Kullback–Leibler divergence of f_{m-1} from f. Since D is non–negative, we can deduce that

$$D(p, p_m) \le D(p, p_{m-1}) - D(f, f_{m-1})$$

This implies that $D(p, p_m)$ is a non-negative and non-increasing sequence, hence has a limit, say, $c \ge 0$, which, in turn, implies $f_m \to f$ strongly in the D or L_1 sense. Therefore, in agreement with Landweber (1951) for the additive algorithm (2), we have that p_m is converging to a set \mathbb{S} where $D(p, \tilde{p}) = c$ for all $\tilde{p} \in \mathbb{S}$. Of course, if p is a unique solution to (1) then $p_m \to p$ strongly. A similar argument for convergence of (3) is presented in Shyamalkumr (1996), with some generalizations.

On the other hand, if (1) does not have a solution, then, as discussed above, we expect that p_m in algorithm (3) will converge to a density with limit p_{∞} such that the corresponding mixture f_{∞} satisfies (6). This can be proved by considering (3) as an *alternating minimization* procedure; see, for example, Csiszár (1975); Csiszzár and Tusnády (1984); Dykstra (1985).

In the following, define the joint densities on $\mathbb{X} \times \Theta$,

$$q_m(x,\theta) = p_m(\theta)k(x,\theta) \quad \text{and} \quad \pi_m(x,\theta) = \frac{f(x)q_{m-1}(x,\theta)}{\int q_{m-1}(x,\theta')d\theta'}.$$
(7)

Theorem 3.1. For an initial solution $p_0 > 0$, let (p_m) be obtained via (3). Assume there exists a sequence $(p_s^*)_{s\geq 1}$ of densities such that

$$D(f, f_s^*) \to \inf_P D(f, f_P)$$

and $D(\pi_s^*, q_m) < \infty$ for some $m \ge 0$, where $f_s^*(x) = \int k(x, \theta) p_s^*(\theta) d\theta$ and

$$\pi_s^*(x,\theta) = \frac{f(x)p_s^*(\theta)k(x,\theta)}{\int p_s^*(\theta')k(x,\theta')d\theta'}$$

Then, $D(f, f_m)$ decreases to $\inf_P D(f, f_P)$.

Proof. Let \mathcal{P} be the set of all bivariate densities π on $\mathbb{X} \times \Theta$ with x-marginal f, i.e., such that $\int \pi(x,\theta) \, \mathrm{d}\theta = f(x)$. Similarly, let \mathcal{Q} be the set of all bivariate densities q on $\mathbb{X} \times \Theta$ such that $q(x,\theta) = k(x,\theta) p(\theta)$ for some density p. Note that q_m and π_m in (7) satisfy $q_m \in \mathcal{Q}$ and $\pi_m \in \mathcal{P}$.

We first claim that (q_m) and (π_m) are obtained by the alternating minimization procedure of Csiszzár and Tusnády (1984) with the objective function $D(\pi, q)$, where π and q ranges over \mathcal{P} and \mathcal{Q} , respectively. To see this, note that $D(\pi_m, q_{m-1}) = D(f, f_{m-1}) \leq D(\pi, q_{m-1})$ for every $\pi \in \mathcal{P}$; the inequality holding since f and f_{m-1} are marginal densities of π and q_{m-1} , respectively. It follows that $\pi_m = \operatorname{argmin}_{\pi \in \mathcal{P}} D(\pi, q_{m-1})$. Also, note that

$$D(\pi_m, q) = \iint \pi_m(x, \theta) \log \frac{\pi_m(x, \theta)}{q(x, \theta)} d\theta dx$$

= $C - \int \log p(\theta) \int \pi_m(x, \theta) dx d\theta$
= $C - \int \log p(\theta) \int \frac{f(x)q_{m-1}(x, \theta)}{\int q_{m-1}(x, \theta')d\theta'} dx d\theta$
= $C - \int \log p(\theta) \int \frac{k(x, \theta)p_{m-1}(\theta)}{\int k(x, \theta')p_{m-1}(\theta') d\theta'} f(x) dx d\theta$
= $C - \int \log p(\theta) dP_m(\theta),$

where C does not depend on p. The last integral is maximized at p_m , so $q_m = \operatorname{argmin}_{q \in \mathcal{Q}} D(\pi_m, q)$. Since \mathcal{P} and \mathcal{Q} are convex, we have

$$D(f, f_{m-1}) = D(\pi_m, q_{m-1}) \searrow \inf_{p \in \mathcal{P}_0, q \in \mathcal{Q}} D(\pi, q),$$

by Theorem 3 in Csiszzár and Tusnády (1984), with $\mathcal{P}_0 = \{\pi \in \mathcal{P} : D(\pi, q_m) < \infty \text{ for some } m\}$. We have $D(\pi, q) = D(f, f_p)$, and and the assumption $D(\pi_s^*, q_m) < \infty$ for some m implies that $\inf_{p \in \mathcal{P}_0} \inf_{q \in \mathcal{Q}} D(\pi, q) \leq \inf_P D(f, f_P)$. Since $D(f, f_m) \geq \inf_P D(f, f_P)$, we conclude that $D(f, f_m) \searrow \inf_P D(f, f_P)$.

Two remarks are in order. First, the integrability condition $D(\pi_s^*, q_m) < \infty$ for some $m \ge 0$ is not especially strong. For example, assume there exists P^* which minimizes $D(f, f_P)$ and has a density p^* . Such a minimizer exists under a mild identifiability condition; see Lemma 3.1 of Kleijn and van der Vaart (2006). Then $D(\pi^*, q_m) < \infty$ for some m implies the required integrability condition, where

$$\pi^*(x,\theta) = \frac{f(x)p^*(\theta)k(x,\theta)}{\int p^*(\theta')k(x,\theta')\mathrm{d}\theta'}.$$

Second, if Θ is compact and the minimizer P^* is unique, every subsequence of (p_m) has a further subsequence weakly converging to P^* , so (p_m) converges to P^* .

It is also worth noting that the monotonicity property of $D_m = D(f, f_m)$ from the theorem can be used to define a stopping rule. For example, one could terminate algorithm (3) when D_m itself and/or the difference $D_m - D_{m-1}$ falls below a certain user-specified tolerance.

4 Smooth mixing density estimation

Suppose we observe X_1, \ldots, X_n as i.i.d. from a distribution with density f as in (1), and we wish to estimate a smooth version of p. The nonparametric maximum likelihood estimator of p is known to be discrete, so is not fully satisfactory for our purposes. One idea for a smooth estimate of pis to maximize a penalized likelihood. The proposal in Liu et al. (2009) is to define a penalized log-likelihood function

$$\ell(\eta) = n^{-1} \sum_{i=1}^{n} \log \int k(X_i, \theta) e^{\eta(\theta)} \,\mathrm{d}\theta - \log \int e^{\eta(\theta)} \,\mathrm{d}\theta - \lambda \,\int [\eta''(\theta)]^2 \,\mathrm{d}\theta,$$

where $\lambda > 0$ is a smoothing parameter, and η determines the mixing density

$$p(\theta) = \frac{e^{\eta(\theta)}}{\int e^{\eta(\theta)} \,\mathrm{d}\theta}.$$

The right-most integral in the expression for $\ell(\eta)$ measures the curvature of η , so maximizing ℓ will encourage solutions which are "less curved," i.e., more smooth. An EM algorithm is available to produce an estimate of η and, hence, of p. However, each iteration requires solving a non-trivial functional differential equation.

Here we propose a more direct approach, namely, to use algorithm (3) with the true density freplaced by, say, a kernel density estimate of f. For some h > 0, define the kernel estimate

$$f^{h}(x) = \frac{1}{nh} \sum_{i=1}^{n} \phi\left(\frac{x - X_{i}}{h}\right)$$

where $\phi(x) = \exp(-\frac{1}{2}x^2)/\sqrt{2\pi}$ is the standard normal density function. The bandwidth h can be selected in a variety of ways. One option is the traditional approach (Sheather and Jones (1991)) of minimizing asymptotic mean integrated square error, which gives h of order $n^{-1/5}$. Another



Figure 2: Mixing and mixture density estimates based on algorithm (3) with a kernel density plugin for the galaxy data. In Panel (b), solid line is the kernel estimate and dashed is the mixture corresponding to the mixing density in Panel (b).

idea is to get the nonparametric maximum likelihood estimator \hat{P} of P, define the corresponding mixture

$$\widehat{f}(x) = \int k(x,\theta) \,\mathrm{d}\widehat{P}(\theta)$$

and then choose the bandwidth $\hat{h} = \arg \min d(f^h, \hat{f})$, where d is, say, the L_1 distance. Finally, our proposal is to estimate p by running algorithm (3) with f replaced by $f^{\hat{h}}$. Since $f^{\hat{h}}$ is smooth, so too will be our estimate of p.

As a quick real-data illustration, consider the well-known galaxy data set, available in the MASS package in R (R Core Team (2015)). We estimate the mixture density f with the Gaussian kernel method described above, using the default settings in **density**. Then we estimate the mixing density via the procedure just described above. In this case, we used 25 iterations of (3) and the results are displayed in Figure 2. Panel (a) shows p_{25} from (3), and Panel (b) shows the data histogram, the kernel density estimator (solid), and the mixture corresponding to p_{25} . Both densities in Panel (b) fit the data well, and the fact that the two are virtually indistinguishable suggests that the density p in Panel (a) is indeed a solution to the mixture equation.

Next, for further investigation into the performance of the proposed mixing density estimation procedure, we present some examples with simulated data. We start by considering a deconvolution problem, where $k(\cdot, \theta)$ is the normal density with mean θ and standard deviation $\sigma = 0.05$. Two mixing densities on the unit interval [0,1] are illustrated;

$$p_1(\theta) \propto \theta^4 (1-\theta)^4$$

$$p_2(\theta) \propto \phi \left(\frac{\theta-0.3}{0.1}\right) + 2\phi \left(\frac{\theta-0.7}{0.1}\right).$$

With a sample of size n = 300, we first obtained a kernel density estimator f^h , using the Gaussian kernel, with bandwidth as in Sheather and Jones (1991), and then ran (3). As suggested above, monotonicity of $D_m = D(f^h, f_m)$ suggests a stopping rule, and we terminated the algorithm when $D_m - D_{m-1} < 10^{-5}$. The number of iterations used were m = 8 for p_1 and m = 14 for p_2 . The estimates of the mixing and corresponding mixture densities are depicted in Figure 3. As can be seen in the right figures, the f_m and \hat{f} are indistinguishable; that is, D_m are effectively zero after a few iterations.

Next, we consider scale mixtures of normal distributions where $k(\cdot, \theta)$ is the centered normal density with variance θ . For the mixing density, two well–known distributions on the positive real line, the inverse-gamma and gamma densities, are considered, i.e.,

$$p_1(\theta) \propto \theta^{-3} e^{-1/\theta}$$
 and $p_2(\theta) \propto e^{-5\theta}$.

With a sample of size n = 300, the estimator of the mixing density is obtained as previously. The number of iterations are m = 57 for p_1 and m = 78 for p_2 , and the estimates of p and f are illustrated in Figure 4. Although the density estimates, f^h and f_m , are close to the true f, there are deviations between p and p_m , in particular for the inverse–gamma case. This is mainly due to the ill–posedness of the problem.

5 First passage time for Brownian motion

The second example is computing the stopping time density for Brownian motion hitting a boundary function. For example, since Breiman (1966) there has been substantial interest in the first passage time distribution of Brownian motion passing a square root boundary. To set the scene, denote $(B(t))_{t\geq 0}$ as standard Brownian motion started at 0, let $h(t) : (0, \infty) \to \mathbb{R}$ be a continuous function with h(0) > 0, the boundary function, and define

$$\tau = \inf\{t > 0 : B(t) \ge h(t)\}.$$



Figure 3: Estimate of mixing density with location mixtures of normals. Left plots are the true (black) and estimated (red) mixing density. Right plots are the true (black), kernel estimator (red) and the one obtained by smooth NPMLE (green).



Figure 4: Estimate of mixing density with scale mixtures of normals. Left plots are the true (black) and estimated (red) mixing density. Right plots are the true (black), kernel estimator (red) and the one obtained by smooth NPMLE (green).

Then Peskir et al. (2002) provides an equation satisfied by the density p of τ , in particular,

$$1 - \Phi\left(\frac{h(t)}{\sqrt{t}}\right) = F(t) - \int_0^t \Phi\left(\frac{h(t) - h(s)}{\sqrt{t - s}}\right) \,\mathrm{d}P(s),$$

where Φ and P are the probability measures/cumulative distribution functions corresponding to ϕ and p, respectively. This leads to a Volterra equation and Peskir et al. (2002) demonstrates solutions when h is constant and linear. When h is increasing and concave and $h(t) \leq h(0) + b\sqrt{t}$ then Peskir et al. (2002) proves that

$$P(t) = m(t) + \int_0^t R(t,s) m(s) \,\mathrm{d}s$$

where

$$m(t) = 2 - 2\Phi\left(\frac{h(t)}{\sqrt{t}}\right)$$
 and $R(t,s) = \sum_{m=1}^{\infty} K_m(t,s),$

with

$$K_m(t,s) = \int_s^t K_1(t,r) K_{m-1}(r,s) \,\mathrm{d}r,$$

and

$$K_1(t,s) = \frac{1}{\sqrt{t-s}} \phi\left(\frac{h(t)-h(s)}{\sqrt{t-s}}\right) \left(2h'(s) - \frac{h(t)-h(s)}{t-s}\right)$$

Clearly $h(t) = a + b\sqrt{t}$ meets the requirements for this result.

On the other hand, we can solve using (3) after setting up a suitable Fredholm equation for h(t) increasing and bounded by $a + b\sqrt{t}$, but not necessarily concave. Define, for any x > 0, the martingale

$$X_t = \exp\left\{x B(t) - \frac{1}{2}x^2t\right\}.$$

With $\theta = T_{a,b} = \inf\{t > 0 : B(t) \ge a + b h(t)\}$ with a, b > 0, h(0) = 0 and $h(t) \le \sqrt{t}$, we have that $X_{t \land T_{a,b}}$ is a martingale and, from the optional stopping theorem, that $E(X_{t \land T_{a,b}}) = E(X_0) = 1$.

Now it is easy to show that $X_{t \wedge T_{a,b}} \leq \exp\{xa + \frac{1}{2}b^2h^2(t)/t\}$, which is bounded and, hence, from the dominated convergence theorem,

$$E(X_{T_{a,b}}) = \lim_{t \to \infty} E(X_{t \wedge T_{a,b}}) = E(X_0) = 1.$$

Effectively, we are also using the result that $T_{a,b} < \infty$ almost surely. Hence,

$$\int \exp\left\{xa + xbh(\theta) - \frac{1}{2}x^2\theta\right\} \, p(\theta) \, \mathrm{d}\theta = 1$$

which after some algebra yields the Fredholm equation

$$\int_0^\infty k(x,\theta)\,\widetilde{p}(\theta)\,\mathrm{d}\theta = a\,e^{-xa} = f(x),\tag{8}$$

where $k(x,\theta)$ is the normal density with mean $b h(\theta)/\theta$ and variance $1/\theta$, constrained on \mathbb{R}_+ , and

$$a\sqrt{2\pi} e^{\frac{1}{2}b^2h^2(\theta)/\theta} \Psi(-bh(\theta)/\sqrt{\theta}) p(\theta) = \sqrt{\theta} \,\widetilde{p}(\theta)$$

and $\Psi(\cdot) = 1 - \Phi(\cdot)$. Now (8) can be readily solved by algorithm (3).

The approach here is closely related to work appearing in Valov (2009). This considers first passage times which are almost surely finite and of the type $\tau = \inf\{t > 0 : B(t) \leq b_{\alpha}(t) = b(t) + \alpha t\}$, where $b_{\alpha}(t) > -c$ for some c > 0. While Valov (2009) constructs a Fredholm equation using Girsanov's theorem, as we do, this is quite different and each equation depends on the type of boundary, whereas ours is always based on the half-normal and exponential distributions.

Here we demonstrate the algorithm for solving the Fredholm equation for the hitting time density with a square root boundary; specifically $a + b\sqrt{t}$ with a = 1 and b = 0.1. We start with a grid of points $\theta_j = hj$, where h = 0.05 and $j = 1, \ldots, 1000$. The starting density is $p_0(\theta) = 0.01 e^{-0.01\theta}$ and at each iteration we evaluate $p_m(\theta_j)$. Due to the ease of sampling from an exponential density, we evaluate

$$\int_0^\infty \frac{k(x,\theta_j) f(x)}{f_m(x)} \,\mathrm{d}x$$

using Monte Carlo methods, i.e.,

$$N^{-1} \sum_{i=1}^{N} \frac{k(X_i, \theta_j)}{f_m(X_i)}$$

where the (X_i) are iid from the exponential distribution with mean 1/a, and we take N = 5000. The $f_m(X_i)$ is evaluated using the trapezoidal rule using the $\tilde{p}_m(\theta_j)$ values, so

$$f_m(X_i) \approx \frac{h}{2} \sum_{j=1}^M \left[k(X_i, \theta_{j-1}) \, \widetilde{p}_m(\theta_{j-1}) + k(X_i, \theta_j) \, \widetilde{p}_m(\theta_j) \right],$$

where $\theta_0 = 0$. Consequently, we have numerically,

$$\widetilde{p}_{m+1}(\theta_j) = N^{-1} \sum_{i=1}^N \frac{2 k(X_i, \theta_j) \widetilde{p}_m(\theta_j)}{h \sum_{j=1}^M \left[k(X_i, \theta_{j-1}) \widetilde{p}_m(\theta_{j-1}) + k(X_i, \theta_j) \widetilde{p}_m(\theta_j) \right]}.$$

The estimated $p(\theta)$, obtained by transforming $\tilde{p}(\theta)$, is given in Figure 5, based on 200 iterations of algorithm (3).



Figure 5: Estimate of hitting time density for square root boundary

6 General Fredholm equation

Algorithm (3) can be applied to solve general Fredholm equations of the first kind, where f, p and $k(\cdot, \theta)$ are not necessarily probability density functions. Assume first that f, p and $k(\cdot, \theta)$ in (1) are non-negative functions, but not necessarily probability densities. Then equation (1) can be rewritten as

$$f(x) = \int_{\Theta} \widetilde{k}(x,\theta) q(\theta) d\theta,$$

where $\tilde{k}(x,\theta) = k(x,\theta) / \int k(x,\theta) dx$ and $q(\theta) = p(\theta) \int k(x,\theta) dx$. Thus, the update (3) can be replaced with

$$p_m(\theta) = \frac{p_{m-1}(\theta)}{\int_{\mathbb{X}} k(x,\theta) \,\mathrm{d}x} \int_{\mathbb{X}} \frac{k(x,\theta) f(x)}{f_{m-1}(x)} \,\mathrm{d}x,\tag{9}$$

which was also considered in Vardi and Lee (1993). Here it is assumed that $\sup_x \int k(x,\theta) d\theta$ and $\sup_{\theta} \int k(x,\theta) dx$ are both finite.

Next, assume that the solution p and f may not be necessarily non-negative functions. In this case, instead of the original equation (1), we solve an equivalent non-negative equation

$$\widetilde{f}(x) = \int_{\Theta} k(x,\theta) \, \widetilde{p}(\theta) \, \mathrm{d}\theta, \tag{10}$$

where $\tilde{p}(\theta) = p(\theta) + t$, $\tilde{f}(x) = f(x) + t \int_{\Theta} k(x, \theta) d\theta$, and t > 0 is a constant to be specified. Since

k is non-negative, so are both \tilde{f} and \tilde{p} for a sufficiently large t. As illustrated below, the value of t rarely affects the convergence rate in practice. Therefore, t can be chosen as a very large number.

Finally, assume that k is not necessarily non-negative, and write $k = k^+ - k^-$, where $k^+, k^- \ge 0$. This case can also be solved by transforming the original equation to a non-negative one. For convenience, assume that $\Theta = [0, 1]$, then the original equation (1) can be written as

$$f(x) = \int_0^1 k^+(x,\theta)p(\theta)d\theta - \int_0^1 k^-(x,\theta)p(\theta)d\theta.$$

Note that

$$\int_{0}^{1} k^{-}(x,\theta)p(\theta)d\theta - \int_{1}^{2} k^{-}(x,\theta-1)p(\theta-1)d\theta = 0,$$
(11)

and therefore, by adding the last two display equations, we have

$$f(x) = \int_0^1 k^+(x,\theta)p(\theta)d\theta + \int_1^2 k^-(x,\theta-1)\{-p(\theta-1)\}d\theta.$$

Let

$$\widetilde{k}(x,\theta) = \begin{cases} k^+(x,\theta) & \text{if } \theta \in [0,1] \\ k^-(x,\theta-1) & \text{if } \theta \in (1,2] \end{cases}$$

and

$$\widetilde{p}(\theta) = \begin{cases} p(\theta) & \text{if } \theta \in [0, 1] \\ -p(\theta - 1) & \text{if } \theta \in (1, 2], \end{cases}$$

then we have the Fredholm equation

$$f(x) = \int_0^2 \widetilde{k}(x,\theta) \widetilde{p}(\theta) d\theta$$
(12)

with a non-negative kernel, which can be solved as previously described.

Note that \tilde{k} and \tilde{p} may have discontinuities; but this does not cause any problem once (12) has the unique solution. If there is another solution to (12), say \bar{p} , and (11) is not satisfied, the restriction of \bar{p} on [0,1] may not be a solution of the original equation. In this case we may apply another decomposition of k. In many examples, however, the simple approach (12) works well.

For illustration, consider the equation (1), where $k(\cdot, \theta)$ is the normal density with mean θ and standard deviation $\sigma = 0.05$, and p has both positive and negative components. In particular, we consider two examples

$$p_1(\theta) = b_{2,5}(\theta) - b_{4,1}(\theta)$$

$$p_2(\theta) = b_{10,1}(\theta) - b_{1,10}(\theta),$$

where $b_{a,b}(\cdot)$ is the density of Beta(a, b) distribution. In both cases, a transformed equation (10) is solved with t = 50 and the results are illustrated in Figure 6. It can be easily seen that the true solution and p_m are nearly the same. Different values of t (5 × 10^k with $k \leq 4$) have been tried, and in any case, the algorithm has been stopped in 10 iterations yielding nearly the same solution.



Figure 6: Illustration with a positive kernel $k(x, \theta) = \phi_{\sigma}(x - \theta)$ and general solutions $p_1(\cdot)$ (top) and $p_2(\cdot)$ (bottom).



Figure 7: Illustration with a general kernel $k(x, \theta) = \phi_{\sigma}(x - \theta) - \phi_{\sigma}(x + \theta)$ for $p_1(\cdot)$ (top) and $p_2(\cdot)$ (bottom).

Next, we consider a general kernel $k(x,\theta) = \phi_{\sigma}(x-\theta) - \phi_{\sigma}(x+\theta)$ with $\sigma = 0.05$ and

$$p_1(\theta) = b_{2,3}(\theta) - b_{3,2}(\theta)$$
$$p_2(\theta) = b_{2,7}(\theta) + b_{3,4}(\theta) - 1,$$

where $\phi_{\sigma}(x) = \phi(x/\sigma)/\sigma$. The equations are solved by setting $k^+(x,\theta) = \phi_{\sigma}(x-\theta)$, $k^-(x,\theta) = \phi_{\sigma}(x+\theta)$ and t = 50. For both examples, the algorithm stopped in 5 iterations. Results are illustrated in Figure 7.

7 Conclusion

In this paper, we focused on an algorithm for solving Fredholm integral equations of the first kind, its properties, and some applications. For the mixing density estimation application described in Section 4, we did not address the question of whether the estimate based on plugging in a kernel density estimator for f in (3) would be consistent in the statistical estimation sense. The *predictive recursion* method of Newton (2002) can also quickly produce a smooth estimator of the mixing density, and it was shown in Tokdar et al. (2009) and Martin et al. (2009) that the estimator is consistent, but non-standard arguments are needed because of its dependence on the data order. We are optimistic that the estimator described in Section 4, through the simple formula (3) for the updates, and the well-known behavior of the kernel density estimator, can have even stronger convergence properties than those demonstrated for predictive recursion.

In Section 5 we were able to extend the class of boundary function for which the hitting time density can be solved using a novel Fredholm equation. Future work would consider upper and lower boundaries. Section 6 we were able to extend the basic algorithm, which was set up for density functions, to non-negative functions.

SUPPLEMENTAL MATERIALS

Rcpp code: It contains code to perform the iterative algorithm proposed in this paper and numerical experiments.

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