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Spectral methods for identifying scalar diffusions

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Abstract

This paper shows how to identify nonparametrically scalar stationary diffusions from discrete-time data. The local evolution of the diffusion is characterized by a drift and diffusion coefficient along with the specification of boundary behavior. We recover this local evolution from two objects that can be inferred directly from discrete-time data: the stationary density and a conveniently chosen eigenvalue–eigenfunction pair of the conditional expectation operator over a unit interval of time. This construction also lends itself to a spectral characterization of the over-identifying restrictions implied by a scalar diffusion model of a discrete-time Markov process. © 1998 Elsevier Science S.A. All rights reserved.

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1. Introduction

The drift and diffusion coefficients of stationary, scalar diffusions are identifiable from discrete-time data without parametric restrictions (e.g., see Hansen and Scheinkman, 1995). In this paper we explore this identification more fully studying the relationship between two operators. One operator is the *infinitesimal generator* which captures the local evolution of the Markov process. This operator is a second-order differential operator with coefficients given by the

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local mean (drift) and local variance (diffusion coefficient) and appropriate boundary conditions. The other operator is the conditional expectation operator over a unit interval of time, which can be inferred from discrete-time data. Using this operator approach we answer two questions in this paper. How can we construct (or identify) the infinitesimal generator from information embodied in the conditional expectation operator? What are the overidentifying restrictions?

We answer these questions using spectral decompositions. Under appropriate boundary protocol, stationary scalar diffusions are reversible. This implies that the infinitesimal generator, when defined on an appropriate Hilbert space, is self-adjoint. As a consequence the infinitesimal generator has real eigenvalues and eigenfunctions that are mutually orthogonal, where orthogonality is defined using the stationary distribution of the diffusion. Conveniently, the infinitesimal generator and the conditional expectation operator share eigenfunctions, and the eigenvalues for the conditional expectation operator are obtained by exponentiating the eigenvalues of the generator. These simple relations make spectral methods attractive for our analysis. Previously, spectral methods have proved useful in investigating identification of Markov chains e.g. see Singer and Spilerman (1977), and in characterizing the transition densities of polynomial models of diffusions (see Wong 1964).¹

Using spectral methods, we will show that the generator for a scalar diffusion can be constructed from the stationary density and a single eigenfunction–eigenvalue pair of the conditional expectation operator. One such eigenfunction is identified as the maximally autocorrelated function of the Markov state. As we will see, this construction of the scalar diffusion exploits specific features of the eigenfunctions, including the location and number of zeros and the boundary behavior. Hence, we will be obliged to characterize fully these features. Since the generator can be constructed from a single eigenvalue–eigenfunction pair, there is an extensive set of overidentifying restrictions. Thus, we will provide a spectral characterization of the sense in which a scalar diffusion model is restrictive.

Although our analysis is devoted to the study of scalar diffusions, it is a common-place in the literature on bond prices to use independent scalar diffusions as building blocks for multivariate bond price processes (e.g., see Duffie and Kan, 1993). Portions of our analysis extend directly to these multivariate ‘factor models’. We will also show that with minor modifications our analysis is directly applicable to a class of subordinated diffusions advocated by Bochner (1960), Clark (1973) and others whereby the time clock for the diffusion is modified or distorted in a random fashion. Discrete-time samples of

¹ In independent work, Kessler and Sorenson (1996) construct estimators of scalar diffusions that are parameterized by their eigenfunctions.

subordinated diffusions are formally equivalent to randomizing the interval of time that elapses between observations. Hence, we will investigate the ramifications of random sampling and permitting the sampling intervals to be temporally dependent.

2. Overview

Suppose we have a scalar stationary and ergodic discrete-time Markov process $\{x_{jt}\}$ with stationary distribution Q . Consistent with our interest in diffusion models, we assume that Q has a density q with respect to Lebesgue measure. We presume this discrete-time process is reversible (see Florens et al., (1995) for a discussion of the observable implications of reversibility). Our focus is on discrete-time Markov processes that are obtained by sampling continuous-time diffusions. The diffusion models we consider are specified formally in Section 3. Let \mathcal{T} denote the one-period conditional expectation operator defined on the space $L^2(Q)$ of Borel measurable *test functions* with finite second moments. That is

$$\mathcal{T}\psi(y) = E[\psi(x_{t+1}) \mid x_t = y].$$

When the Markov process is reversible, the conditional expectation operator is self-adjoint. In other words,

$$\langle \mathcal{T}\psi \mid \psi^* \rangle = \langle \psi \mid \mathcal{T}\psi^* \rangle,$$

where $\langle \psi^* \mid \psi \rangle = \int \psi^* \psi \, dQ = E[\psi^*(x_t) \psi(x_t)]$. Under some additional conditions, \mathcal{T} has a *spectral representation*:

$$\mathcal{T}\psi = \sum_{j=0}^{\infty} \lambda_j \langle \psi_j \mid \psi \rangle \psi_j,$$

where $\{\psi_j\}$ is an orthonormal family of eigenfunctions of the conditional expectation operator, and $\{\lambda_j\}$ is the corresponding family of eigenvalues. In Section 4 we present sufficient conditions on the local evolution of the diffusion to guarantee this spectral representation.

Because the conditional expectation operator \mathcal{T} is self-adjoint, its eigenvalues are all real. For this operator to correspond to a discrete-time sample of a continuous-time Markov process, the eigenvalues of \mathcal{T} all must lie between 0 and 1. Further, if the eigenvalues λ_j are ordered so that $1 = \lambda_0 > \lambda_1 > \dots > \lambda_j > \lambda_{j+1} > \dots$, then ψ_0 is a constant and for each $j \geq 1$, ψ_j solves:

$$\max\{\langle \psi \mid \mathcal{T}\psi \rangle : \langle \psi \mid \psi \rangle = 1, \langle \psi \mid \psi_k \rangle = 0, \text{ for } 0 \leq k < j\}. \quad (2.1)$$

Using the Law of Iterated Expectations, the criteria in Eq. (2.1) are equivalent to maximizing $E\psi(x_t)\psi(x_{t+1})$ subject to the same norm and orthogonality

conditions. Thus, ψ_1 is the function of the Markov state with *maximal* autocorrelation. More generally, the eigenfunctions and eigenvalues are identifiable from discrete-time data by solving a sequence of maximum correlation problems.

Our task in this paper is to characterize the restrictions on the eigenvalues and eigenfunctions when it is known that the discrete-time process is obtained by sampling a continuous-time diffusion. In doing so, we will work with the infinitesimal generator \mathcal{B} of the process. Roughly speaking, an infinitesimal generator is an operator used to characterize the local evolution of the Markov process. Section 3 gives the formal construction of this operator as a second-order differential operator defined for functions ψ in an appropriate domain:

$$\mathcal{B}\psi = \mu\psi' + \frac{1}{2}\sigma^2\psi'',$$

where μ and σ^2 are the drift and diffusion coefficients associated with the Markov diffusion. Its relation to the conditional expectation operator is given by taking the operator counterpart to a logarithm:

$$\mathcal{B}\psi = \sum_{j=0}^{\infty} -\delta_j \langle \psi_j | \psi \rangle \psi_j,$$

where $-\delta_j = \log \lambda_j$. In particular, the ψ_j identified as solving a maximum correlation problem also solve the second-order differential equation:

$$\frac{1}{2}\sigma^2\psi_j'' + \mu\psi_j' + \delta_j\psi_j = 0,$$

subject to boundary restrictions made explicit in Section 3.

An important consequence of our analysis is an alternative way to parameterize a diffusion. Instead of modeling the drift and diffusion coefficients, we suggest specifying a conveniently chosen eigenfunction along with the stationary density. As we will see in Section 5, this identification scheme can be viewed as extensions of identification schemes proposed by Ait-Sahalia (1996a), Demoura (1993) and Kessler and Sorenson (1996). As in Hansen and Scheinkman (1995), the identification method is robust to the presence of possibly temporarily dependent randomization of the sample size interval. Hence, the identification scheme allows for the possibility that *economic time* differs from the calendar time observed by the econometrician.

In Sections 4 and 6 we give a complete characterization of the restrictions on $\{\lambda_j\}$ and $\{\psi_j\}$ for \mathcal{B} to be the generator of a diffusion. Thus, we provide a spectral characterization of when a stationary scalar diffusion with a generator whose spectrum is discrete can be *embedded* in a one-period conditional expectation operator. In addition, we study the extent to which these embeddability restrictions continue to apply when the sampling scheme is randomized.

As we noted previously, spectral characterizations of embeddability are familiar from the literature on finite state Markov chains. The Markov chain models

most closely tied to scalar diffusions are finite-state birth and death processes. For such processes Karlin and McGregor (1959) established *total positivity* as a necessary condition for a one-period transition matrix to be embeddable in a time-homogeneous birth and death process. As shown by Frydman and Singer (1979) the total positivity restrictions only become sufficient when time homogeneity is relaxed. Karlin (1968) has deduced the analogous total positivity restrictions for transition densities to be embeddable in scalar diffusions (see also Karlin and Taylor, 1981, p. 167).² In contrast to the spectral restrictions we derive, the total positivity restrictions are known to be sufficient only when they can be checked at arbitrarily small time intervals. On the other hand, these total positivity restrictions are applicable as necessary conditions to a more general class of diffusion models including ones that are nonstationary.

3. The general framework

3.1. Scale and speed densities

Let $\{W_t, t \geq 0\}$ be a scalar Brownian motion, and consider a continuous semi-martingale (the sum of a local martingale and an adapted process of bounded variation) $\{x_t, t \geq 0\}$ satisfying in (ℓ, r) the stochastic differential equation:

$$dx_t = \mu(x_t) dt + \sigma(x_t) dW_t. \quad (3.1)$$

We assume that the functions μ and σ are continuous in (ℓ, r) and that $\sigma(x) > 0$ for $x \in (\ell, r)$. Either boundary ℓ or r can be infinite. We follow Karlin and Taylor (1981) and others by introducing a *scale function* S and its derivative:

$$S(x) = \int_{x_0}^x s(y) dy, \quad \ell < x_0 < r \quad (3.2)$$

$$s(x) = \exp \left[- \int_{x_0}^x \frac{2\mu(y)}{\sigma^2(y)} dy \right], \quad (3.3)$$

and a *speed density*:

$$m(x) = \frac{1}{s(x)\sigma^2(x)}, \quad \ell < x < r. \quad (3.4)$$

² See a recent manuscript by Ait-Sahalia (1996b) for the development and application of a statistical test of these total positivity restrictions.

Since

$$\frac{s'(x)}{s(x)} = -2 \frac{\mu(x)}{\sigma^2(x)}, \quad (3.5)$$

we can deduce the corresponding drift and diffusion coefficients from the scale and speed densities.

The scale function is unique up to an increasing affine transformation, and appears naturally in the study of the hitting times of the process:

$$\Pr \{T_b < T_a \mid x_0 = x\} = \frac{S(x) - S(a)}{S(b) - S(a)}, \quad \ell < a < x < b < r,$$

where $T_y = \inf \{t \geq 0: x_t = y\}$ is the first hitting time of y starting from x . The boundary r is said to be *attracting* if $S(r) = \lim_{b \uparrow r} S(b) < \infty$. If r is not attracting, then $S(r) = \lim_{b \uparrow r} S(b) = +\infty$, and thus $\Pr\{T_b < T_r \mid x_0 = x\} = 1$ for any $b, x \in (\ell, r)$. The corresponding definition holds for the boundary ℓ .

To ensure the existence of a stationary measure, we assume that the speed density is integrable,

Assumption 1. $\int_{\ell}^r m(x) dx < \infty$.

Under this assumption, attracting barriers are also attainable. We use the measure Q with density:

$$q(x) = \frac{m(x)}{\int_{\ell}^r m(y) dy}, \quad \ell < x < r \quad (3.6)$$

to initialize the process. Then under appropriate boundary conditions, the Markov process $\{x_t, t \geq 0\}$ that satisfies the stochastic differential equation given by Eq. (3.1) satisfies:

Assumption 2. $\{x_t, t \geq 0\}$ is stationary and time reversible.

We will have more to say about the boundary restrictions needed for reversibility. We will refer to the stochastic processes described in this subsection as (reversible) stationary diffusions. This reference will be justified in Section 3.3.

3.2. Transforming to the natural scale

Next, we use a standard trick for analyzing a scalar diffusion. We transform the original process into a local martingale by applying scale function. Let $u_t = S(x_t)$. Since S is at least twice continuously differentiable, Ito's formula implies that the scalar process $\{u_t\}$ is a continuous semi-martingale that satisfies in $(S(\ell), S(r))$:

$$du_t = \theta(u_t) dW_t, \quad (3.7)$$

where

$$\theta^2(v) = s^2[S^{-1}(v)] \sigma^2 [S^{-1}(v)].$$

The transformed boundaries are $S(\ell)$ and $S(r)$, which are finite when the original boundaries are attracting. The transformed process is referred to as being in the *natural scale*.

In the natural scale, the speed density is just the reciprocal of the diffusion coefficient and specifies how much the process must be *sped up* to convert it to a Brownian motion. The stationary distribution, P , of the transformed process has a density, p , that is again proportional to the speed density:

$$p(v) = \frac{1/\theta^2(v)}{\int_{S(\ell)}^{S(r)} dv/\theta^2(v)} = \frac{q[S^{-1}(v)]}{s[S^{-1}(v)]}.$$

Notice that we opted to start with a continuous semi-martingale that satisfies a stochastic differential equation. Conversely, we could have started with Eq. (3.7) or Eq. (3.1) and appropriate boundary conditions and established that there exist a solution $\{u_t\}$ that is a continuous semi-martingale. For instance, when $S(\ell) = -\infty$, $S(r) = +\infty$, and θ is continuous and positive, there exists a weak solution to Eq. (3.7) with initial distribution P , which is a continuous local martingale (e.g. Karatzas and Shreve 1988, p. 332).

3.3. Infinitesimal generator

We represent the local evolution of the process with an operator called the *infinitesimal generator*. We denote by $L^2(P)$ the Hilbert space of (equivalence classes of) measurable functions ϕ defined on $(S(\ell), S(r))$ for which $\int_{S(\ell)}^{S(r)} |\phi(v)|^2 p(v) dv < \infty$. The scalar product on $L^2(P)$ is $\langle \phi | \varphi \rangle_P = \int_{S(\ell)}^{S(r)} \phi(v) \varphi(v) p(v) dv$. Also, we denote by $\{\mathcal{U}_t, t \geq 0\}$ the semigroup of conditional expectation operators associated with the process $\{u_t, t \geq 0\}$ defined by

$$\mathcal{U}_t \phi(u) = E [\phi(u_t) | u_0 = u], \quad \phi \in L^2(P).$$

The focus of this paper is on the infinitesimal generator \mathcal{A} induced by the semigroup of linear operators $\{\mathcal{U}_t, t \geq 0\}$. For $\phi \in L^2(P)$, $\mathcal{A}\phi$ is defined as the limit in the sense of $L^2(P)$ of $(1/t)[\mathcal{U}_t \phi - \phi]$ as $t \downarrow 0$, whenever this limit exists. The domain $D(\mathcal{A})$ of this generator is the family of functions $\phi \in L^2(P)$ for which $\mathcal{A}\phi$ is well defined.

To characterize the domain of the generator, we initially consider two spaces of functions. The first space contains the domain of the generator and the second space is contained in it. Define:

$$\bar{D} \equiv \{\phi \in L^2(P): \phi' \text{ is absolutely continuous and } \theta^2 \phi'' \in L^2(P)\} \tag{3.8}$$

and

$$\underline{D} \equiv \{\phi \in \overline{D} : \phi' \text{ has compact support in } (S(\ell), S(r))\}. \quad (3.9)$$

To show that the smaller space \underline{D} is contained in $D(\mathcal{A})$, we apply a generalized version of Ito's formula for continuous semi-martingales (see Revuz and Yor, 1994, Remark 3 p. 215):

$$\phi(u_t) = \phi(u_0) + \int_0^t \mathcal{L}\phi(u_s) ds + \int_0^t \phi'(u_s)\theta(u_s) dW_s \quad (3.10)$$

for $\phi \in \underline{D}$, where

$$\mathcal{L}\phi(u) \equiv \frac{1}{2} \theta^2(u)\phi''(u).$$

The contribution from any finite boundary is zeroed out for any ϕ in \underline{D} . Note that the process $\{\theta(u_t)\phi'(u_t)\}$ is bounded so that $\{\int_0^t \phi'(u_s)\theta(u_s) dW_s\}$ is a martingale. Taking conditional expectations on both sides of Eq. (3.10), and using Fubini's Theorem we obtain

$$\mathcal{U}_t\phi(u_0) - \phi(u_0) = \int_0^t \mathcal{U}_s \mathcal{L}\phi(u_0) ds. \quad (3.11)$$

If ϕ is twice continuously differentiable and with a compact support in $(S(\ell), S(r))$, Eq. (3.11) establishes that $\mathcal{U}_t\phi \rightarrow \phi$ as t goes to zero in the $L^2(P)$ norm. Since \mathcal{U}_t is a semi-group of contractions and the space of C^2 functions with a compact support in $(S(\ell), S(r))$ is dense in $L^2(P)$, the semigroup $\{\mathcal{U}_t, t \geq 0\}$ is strongly continuous. Further, Eq. (3.11) implies that:

$$\begin{aligned} & \left\{ \int_{S(\ell)}^{S(r)} \left[\frac{1}{t} (\mathcal{U}_t\phi(u) - \phi(u)) - \mathcal{L}\phi(u) \right]^2 p(u) du \right\}^{1/2} \\ &= \left\{ \int_{S(\ell)}^{S(r)} \left[\frac{1}{t} \int_0^t (\mathcal{U}_s \mathcal{L}\phi(u) - \mathcal{L}\phi(u)) ds \right]^2 p(u) du \right\}^{1/2} \\ &\leq \frac{1}{t} \int_0^t \left[\int_{S(\ell)}^{S(r)} (\mathcal{U}_s \mathcal{L}\phi(u) - \mathcal{L}\phi(u))^2 p(u) du \right]^{1/2} ds \end{aligned} \quad (3.12)$$

Since \mathcal{U}_s is strongly continuous, we have that $\mathcal{L}\phi = \mathcal{A}\phi$ for ϕ in \underline{D} and, hence, $\underline{D} \subset D(\mathcal{A})$. In particular, the domain of the infinitesimal generator $D(\mathcal{A})$

is dense in $L^2(P)$, and \mathcal{A} is a closed linear operator (see Pazy, 1983, Corollary 2.5, p. 5).

Remark 1. The above reasoning applies whenever $\phi \in \overline{D}$, has vanishing derivatives at boundaries and $\{\int_0^t \phi'(u_s)\theta(u_s) dW_s\}$ is a martingale. Hence, any such ϕ is actually in $D(\mathcal{A})$, and $\mathcal{A}\phi = \mathcal{L}\phi$.

A simple integration by parts argument shows that $(\mathcal{L}, \underline{D})$ is symmetric (i.e. $\langle \mathcal{L}\varphi|\phi \rangle_P = \langle \varphi|\mathcal{L}\phi \rangle_P$ for all φ, ϕ in \underline{D}). Since $\{x_t\}$ is time reversible, so is $\{u_t\}$ and, hence, the generator \mathcal{A} is a self-adjoint extension of $(\mathcal{L}, \underline{D})$ (in $L^2(P)$). Such an extension exists by Theorem 8.9 of Weidmann (Weidmann, 1980, p. 235). Moreover, it follows from Theorem 8.22 of Weidmann (Weidmann, 1980, p. 250) that any self-adjoint extension of $(\mathcal{L}, \underline{D})$ must be a restriction on $(\mathcal{L}, \overline{D})$.³ Therefore, \mathcal{A} is the restriction of \mathcal{L} to a domain $D(\mathcal{A})$, which satisfies $\underline{D} \subset D(\mathcal{A}) \subset \overline{D}$. In the appendix we show that reversibility restricts the test function derivatives to be zero at the boundaries. More precisely,

$$D(\mathcal{A}) = \left\{ \phi \in \overline{D}: \lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(r)} \phi'(v) = 0 \right\}.$$

Remark 2. When confronted with a family of generators, as it is the case in econometric investigations, it is often useful to characterize a common subset of the domains of generators in the family, that is ‘large’ enough. (see e.g. Hansen and Scheinkman (1995) and Conley et al., 1997.) The proof of Theorem 8.29 in Weidmann (Weidmann, 1980, p. 256) can be used straightforwardly to show that \mathcal{A} is the closure of $(\mathcal{L}, \underline{D})$, that is, that \underline{D} is a Core for \mathcal{A} . Further, as shown in Weidmann (Weidmann, 1987, p. 42), since θ^2 is continuous in $(S(\ell), S(r))$, the closure of \mathcal{L} , when restricted to C^2 functions with compact support $K \subset (S(\ell), S(r))$ contains $(\mathcal{L}, \underline{D})$. Hence, the space of twice continuously differentiable functions with a compact support contained in $(S(\ell), S(r))$ is a Core for \mathcal{A} .

Remark 3. Suppose that r is a natural boundary, that is $S(r) = +\infty$ and

$$\int_v^{S(r)} \frac{u}{\theta^2(u)} du = +\infty. \tag{3.13}$$

³ This follows because $(\mathcal{L}, \underline{D})$ is a (symmetric) extension of minimal operator defined in Weidmann (1980).

It follows from Lemma A.1 and the proof of Lemma A.2, that the boundary restriction $\lim_{v \uparrow S(r)} \phi'(v) = 0$ is automatically satisfied for any $\phi \in \bar{D}$.⁴ Therefore, when both ℓ and r are natural boundaries, $D(\mathcal{A}) = \bar{D}$.

Remark 4. Recall that when $S(r)$ is finite, the right boundary is attracting. The restriction $\phi'(S(r)) = 0$ corresponds to making r a reflecting barrier.

We conclude this discussion by describing briefly how our results for a process in the natural scale extend to the original process. The generator \mathcal{B} for the original process satisfies:

$$\begin{aligned} \mathcal{B}\psi(y) &= \lim_{h \searrow 0} \mathbb{E} \left[\frac{\psi(x_h) - \psi(x_0)}{h} \middle| x_0 = y \right] \\ &= \lim_{h \searrow 0} \mathbb{E} \left[\frac{\psi[S^{-1}(u_h)] - \psi[S^{-1}(u_0)]}{h} \middle| u_0 = S(y) \right] \\ &= \mathcal{A}(\psi \circ S^{-1})[S(y)] \end{aligned} \tag{3.14}$$

for each ψ such that $\psi \circ S^{-1}$ is in $D(\mathcal{A})$. [Recall that $u_t = S(x_t)$.] Hence for any such ψ , \mathcal{B} is given by

$$\begin{aligned} \mathcal{B}\psi(y) &= \frac{\theta^2[S(y)]}{2} \left[\frac{\psi''(y)}{s^2(y)} - \frac{\psi'(y)s'(y)}{s^3(y)} \right] \\ &= \frac{1}{2m(y)} \left[\frac{\psi'(y)}{s(y)} \right]' \\ &= \mu(y)\psi'(y) + \frac{\sigma^2(y)}{2} \psi''(y), \end{aligned} \tag{3.15}$$

and the domain of \mathcal{B} is

$$D(\mathcal{B}) \equiv \{ \psi: \psi \circ S^{-1} \in D(\mathcal{A}) \}.$$

Therefore, the domain $D(\mathcal{B})$ consists of all functions ψ such that:

1. ψ' is absolutely continuous;
2. $\psi \in L^2(Q)$;
3. $\mu\psi' + \frac{\sigma^2}{2} \psi'' \in L^2(Q)$;
4. $\lim_{y \downarrow \ell} \frac{\psi'(y)}{s(y)} = \lim_{y \uparrow r} \frac{\psi'(y)}{s(y)} = 0$.

⁴From Lemma A.1, we know that ϕ' has a limit. If this limit is different from zero, then $\lim_{u \nearrow S(r)} \phi(u)\phi'(u) = \pm \infty$. Eq. (A.6) implies that this limit cannot be $-\infty$. From the proof of Lemma A.2, it is easy to see that if $\lim_{u \nearrow S(r)} \phi(u)\phi'(u) = +\infty$ and Eq. (3.13) is satisfied, then $\phi \notin L^2(P)$.

Remark 5. Suppose μ and σ are continuous functions in (ℓ, r) , with $\sigma > 0$. For each subset I of the extended real line we write $C_I(C_I^2)$ for the set of continuous (resp. twice continuously differentiable) real-valued functions in I . For $\psi \in C_{[\ell, r]} \cap C_{(\ell, r)}^2$, let

$$\mathcal{G}\psi(x) = \mu(x)\psi'(x) + \frac{1}{2}\sigma^2(x)\psi''(x). \tag{3.16}$$

Often a diffusion in $[\ell, r]$ is defined as a stochastic process with: (a) continuous sample paths; and (b) a semi-group of conditional expectations operators (defined in $C_{[\ell, r]}$ with the sup-norm) generated by \mathcal{G} on a restriction of the set of functions $\psi \in C_{[\ell, r]} \cap C_{(\ell, r)}^2$ for which $\mathcal{G}\psi \in C_{[\ell, r]}$. The appropriate restriction is given by boundary conditions (see e.g. Mandl, 1968, p. 66) or (Ethier and Kurtz, 1986, p. 366). Our characterization of $\mathcal{D}(\mathcal{B})$ shows that the process $\{x_t\}$ defined in Section 3.1 satisfies property (a) and property (b'), that coincides with (b) except that the space $L^2(Q)$ replaces $C_{[\ell, r]}$ and the restricted domain of \mathcal{G} is given by conditions (i)–(iv) above. Condition (iv) imposes the boundary restrictions. In what follows, we will refer to a reversible diffusion as a stochastic process satisfying (a) and (b').

Given the continuity of the coefficients of the second-order operator, one may show that the stochastic processes treated here are, in fact, diffusions in the sense used by Mandl (1968). However, our characterization of the domain of the generator in subsets of $L^2(Q)$ is needed for our subsequent use of spectral decompositions.

4. Spectrum

In this section we study the spectral representation of the generator \mathcal{A} . This operator is known to be negative semi-definite, and, as a consequence its eigenvalues are real and nonpositive. In other words, the only solutions (δ, ϕ) to the equation

$$\mathcal{A}\phi = -\delta\phi \tag{4.1}$$

with $\phi \in D(\mathcal{A})$ are ones for which $\delta \geq 0$. We derive two alternative sufficient conditions for the generator \mathcal{A} to be representable in terms of a countable number of eigenvalues and eigenfunctions:

$$\mathcal{A}\phi = \sum_{j=0}^{\infty} -\delta_j \langle \phi_j | \phi \rangle_P \phi_j,$$

where (δ_j, ϕ_j) solves the eigenvalue problem given by Eq. (4.1). This representation is referred to as the spectral representation and is analogous to the spectral representation of a symmetric matrix. When such a representation exists, the generator is said to have a *discrete spectrum*, and the eigenvalues can be ordered

so that $\{\delta_j\}$ is strictly increasing and unbounded. The constant function ϕ_0 is an eigenfunction corresponding to an eigenvalue of zero. More generally, the ϕ_j eigenfunction associated with δ_j crosses the zero axis precisely j times (see Weidmann, 1987, Theorem 14.10, p. 225).

If the generator \mathcal{A} has a discrete spectrum, then so will the generator \mathcal{B} and conversely. In fact the eigenvalues of the two operators coincide and the eigenfunctions of \mathcal{B} can be constructed directly from those of \mathcal{A} via: $\phi_j \circ S^{-1}$. In other words,

$$\mathcal{B}\phi = \sum_{j=0}^{\infty} -\delta_j \langle \phi_j \circ S^{-1} | \phi \rangle \phi_j \circ S^{-1}. \tag{4.2}$$

Since ϕ_j crosses the zero axis j times, the same can be said of $\phi_j \circ S^{-1}$. For this reason our results obtained using the natural scale have direct implications for the generator of the original diffusion.

We begin by studying the solutions to:

$$\phi'' + \delta \frac{2}{\theta^2} \phi = 0. \tag{4.3}$$

We will draw a distinction between a *solution to the eigenvalue problem* (that is a solution to Eq. (4.3) for a particular δ) and an *eigenfunction* for \mathcal{A} with eigenvalue $-\delta$. In addition to solving Eq. (4.3) for some δ , an eigenfunction is restricted to be in the domain $D(\mathcal{A})$ and, hence, its derivatives must converge to zero at the boundaries.

Consider for the moment any nonempty compact interval $[\underline{v}, \bar{v}] \subset (S(\ell), S(r))$. The function $2/\theta^2$ is continuous and positive on this finite interval. Given a point $v \in [\underline{v}, \bar{v}]$ and the initial conditions:

$$\phi(v) = c, \phi'(v) = d, \tag{4.4}$$

differential equation given by Eq. (4.3) is known from Sturm–Louville theory to have a unique solution on $[\underline{v}, \bar{v}]$. This solution crosses the zero axis at most a finite number of times (e.g. see Birkhoff and Rota, 1989, Theorem 7, p. 189 for existence, and Theorem 3, p. 41 for uniqueness and the discussion on p. 313 for the finite number of zero crossings). To show that the spectrum of \mathcal{A} is discrete, it suffices to verify that for any positive δ , there exists solutions to Eq. (4.3) that cross the zero axis only a finite number of times once we extend the domain to $(S(\ell), S(r))$ (see Weidmann, 1987, Theorem 14.9, p. 225). We now investigate this question for alternative boundary behavior.

4.1. Entrance and attracting boundaries

In this section we treat the case in which the stationary density in the natural scale has a finite first moment, that is:

Assumption 3. $\int_{S(\ell)}^{S(r)} |u| p(u) du < \infty$.

The counterpart to this assumption in the original scale is that $S(x_t)$ have a finite moment. This assumption is clearly satisfied when $S(\ell)$ and $S(r)$ are both finite, in which case both ℓ and r are reflecting barriers. We are particularly interested in cases in which at least one of the boundaries is not attracting. Assumption 3 restricts any such boundary to be an entrance boundary (see Karlin and Taylor, 1981, p. 234). Although an entrance boundary is not attracting, it is still possible to initialize the diffusion at such a boundary.

Theorem 4.1. When Assumption 3 is satisfied, every solution to Eq. (4.3) for $\delta > 0$ has a finite number of zeros.

Proof. If $v \in (S(\ell), S(r))$, the number of zeros in $[v, S(r))$ is bounded by $\int_v^{S(r)} (u - v) \delta(2/\theta^2) du + 1$. An analogous bound exists for the number of zeroes in $(S(\ell), v]$. (See Hartman, 1973, p. 347). \square

Hence, the spectrum of the corresponding generator is discrete.

Assumption 3 is the weakest moment condition possible for the spectrum to be discrete. In the natural scale, if an absolute moment of order less than one exists, every solution to Eq. (4.3) when $\delta > 0$ has an infinite number of zeroes (see Hartman, 1973, p. 368). As we will see in the next subsections there are many examples of processes where Assumption 3 fails to hold but the spectrum of the generator is discrete.

4.2. Natural boundaries

When Assumption 3 is not satisfied at least one of the boundaries must be natural. A diffusion cannot escape from a natural boundary. Some processes with natural boundaries are known to have a discrete spectrum. Others are known to have a spectrum that also contains a continuous portion beyond some critical value η . For δ 's in the continuous portion of the spectrum, the operators $(\mathcal{L} + \delta\mathcal{A})$ is one-to-one, dense but not onto. Beyond η , solutions to the eigenvalue problem (for Sturm-Louville operators) are known to cross the zero axis an infinite number of times. Non-constant eigenfunctions may still exist for processes with a mixed spectrum. As a consequence, it is of interest to obtain a characterization of the critical value of δ . When this critical value is infinite, the spectrum is discrete and when this critical value is zero, the constant function is the only eigenfunction of the generator.

Assumption 4. $S(\ell) = -\infty$ and $S(r) = +\infty$. θ is continuously differentiable on $(S(\ell), S(r))$, $\lim_{u \nearrow +\infty} \theta'(u)$ exists and $\lim_{u \searrow -\infty} \theta'(u)$ exists.

We permit the limits in Assumption 4 to be $\pm \infty$. Define $\gamma(u) \equiv [\theta'(u)]^2/8$. In light of Assumption 4, $\gamma(-\infty)$ and $\gamma(+\infty)$ are well defined. The function γ can

be represented using the coefficients of the original diffusion. Since $\theta = s\sigma$ and $s'/s = -2\mu/\sigma^2$, it can be shown that

$$\gamma(u) = \frac{1}{8} \left[\sigma'(y) - \frac{2\mu(y)}{\sigma(y)} \right]^2, \tag{4.5}$$

where $y = S^{-1}(u)$.

We will now see that the spectrum of the operator \mathcal{A} (and hence \mathcal{B}) must be discrete in the interval:

$$(-\eta, 0],$$

and no $-\delta < -\eta$ can be an eigenvalue of \mathcal{A} (and hence \mathcal{B}) where

$$\eta = \min\{\gamma(-\infty), \gamma(+\infty)\}.$$

Theorem 4.2. When Assumption 4 is satisfied, any solution to the eigenvalue problem crosses the zero axis a finite number of times if $\delta < \eta$ and an infinite number of times if $\delta > \eta$.

Proof. By L'Hospital's rule, $\lim_{u \rightarrow +\infty} u/\theta(u) = 1/\theta'(+\infty)$. Hence,

$$\lim_{u \rightarrow +\infty} u^2 \frac{2\delta}{\theta^2(u)} = \frac{\delta}{4\gamma(+\infty)}.$$

From (Hartman 1973, Theorem 7.1, p. 347), it follows that if $0 < \delta < \gamma(+\infty)$, then a solution to Eq. (4.3) has a finite number of zeroes in $[0, \infty)$, while if $\delta > \gamma(+\infty)$, then a solution to Eq. (4.3) has an infinite number of zeroes in $[0, \infty)$. Applying a symmetric reasoning to $(-\infty, 0]$, we obtain the result. \square

One standard way of characterizing the temporal dependence of a stochastic process is through its ρ mixing coefficients. Recall that for a stationary Markov process, these coefficients are defined as

$$\rho(s) = \sup_{\phi \in L^2(P), \phi \perp 1} \frac{E[\phi(x_{t+s})\phi(x_t)]}{E\phi^2(x_t)}.$$

Previously, Hansen and Scheinkman (1995) used $\eta > 0$ as a sufficient condition for geometric ergodicity, that is for the exponential decay of the ρ mixing coefficients. When $\eta > 0$ there exists a gap on the spectrum to the left of zero, that is $\mathcal{A} + \varepsilon\mathcal{I}$ is invertible for all $\varepsilon > 0$ sufficiently small. Hence, Theorem 4.2 extends the results of Hansen and Scheinkman (1995) by giving a more precise role for η in characterizing the spectrum and, consequently, the temporal dependence. When $\eta = 0$ the process is strongly dependent – the ρ mixing coefficients are identically equal to one for all s .

Theorem 4.3. When Assumption 4 is satisfied, the operator \mathcal{B} has at least one nonzero eigenvalue if there exists a ϕ in $\mathcal{D}(\mathcal{B})$ such that

$$\frac{\langle \phi | \mathcal{B} \phi \rangle}{\langle \phi | \phi \rangle - \langle \phi | 1 \rangle^2} > -\eta. \quad (4.6)$$

Proof. As argued by Hansen and Scheinkman (1995), when Assumption 4 is satisfied, the operator \mathcal{B} has a spectral gap to the left of zero. The magnitude of the gap is given by

$$\varepsilon = \inf_{\phi \in \mathcal{D}} - \frac{\langle \phi | \mathcal{B} \phi \rangle}{\langle \phi | \phi \rangle - \langle \phi | 1 \rangle^2}.$$

Since this gap is less than η , $-\varepsilon$ is an eigenvalue of \mathcal{B} . \square

4.3. Mixed boundaries

We comment briefly on how to combine the analysis in the previous two subsections to handle processes with one natural boundary and the other either an entrance or a reflecting boundary. For definiteness assume that the right boundary is the natural boundary. The first part of the proof of Theorem 4.3 actually establishes that if the left boundary is reflexive and $\gamma(+\infty) = \infty$, then we have a discrete spectrum. For the case where the left boundary is an entrance boundary select a point y in (ℓ, r) . Form two processes with the same diffusion and drift coefficients, one concentrated on $[\ell, y]$ and the other on $[y, r]$, both with a reflecting barrier at y . As long as the two newly formed processes have a discrete spectrum, so will the original one. This follows because solutions to the eigenvalue problem for the original process can be obtained by pasting together smoothly two solutions to the eigenvalue problems for the two newly constructed processes. If the latter two solutions only cross the zero axis a finite number of times, the same must be true of the pasted together solution.

4.4. Examples

We conclude this section with four examples.

Example 1. (A process with natural boundaries and a discrete spectrum). The Ornstein–Uhlenbeck process (σ^2 constant and μ linear with a negative slope) is known to have a discrete spectrum (see Wong, 1964). It can be shown that both endpoints ($-\infty$ and $+\infty$) are natural boundaries and that γ diverges at both of these boundaries.

Example 2. (A generator with a linear eigenfunction with non-discrete spectrum). Consider a process with a drift $\mu(y) = -\alpha y$ for $\alpha > \frac{1}{2}$ and a diffusion coefficient $\sigma^2(y) = 1 + y^2$. The generator for this process has $-\alpha$ as an eigenvalue. For sufficiently large δ , the solutions to the eigenvalue problem are known to cross the axis an infinite number of times (see Wong, 1964). Notice that $\gamma(+\infty) = \gamma(-\infty) = (2\alpha + 1)^2/8 > \alpha$. Thus, Theorem 4.3 is applicable.

Example 3. (A process without a spectral gap). Consider a process suggested by Bouc and Pardoux (1984) on the positive half-line with $\mu(y) = -y^{-1/2}$ and $\sigma^2(y) = 1$. For this process, γ converges to zero at the right boundary. All of the solutions to the eigenvalue problem for $\delta > 0$ cross the zero axis an infinite number of times. The process is stationary and ergodic but its generator does not have a spectral gap.

Example 4. (A parameterized family of local martingales). Suppose that μ is zero, implying that the process is in the natural scale. Let $\sigma^2(y) = \theta^2(y) = (1 + y^2)^\alpha$ where $\alpha > \frac{1}{2}$, and consider the resulting diffusion defined on the entire real line. This process has entrance barriers at both boundaries when $\alpha > 1$ and hence has a discrete spectrum. For $\frac{1}{2} < \alpha < 1$, all solutions to the eigenvalue problem for $\delta > 0$ cross the zero axis an infinite number of times. Hence, the discrete spectrum is reduced to $\{0\}$. For $\alpha = 1$, $\gamma(-\infty) = \gamma(+\infty) = \frac{1}{8}$. Hence, for $\delta > \frac{1}{8}$, all solutions to the eigenvalue problem cross the zero axis an infinite number of times. On the other hand, the spectrum is discrete in $[0, \frac{1}{8}]$.

5. An alternative parameterization of a scalar diffusion

In Section 3, we described two ways to specify a scalar diffusion. The first and most common way is to specify a drift-diffusion coefficient pair (μ, σ^2) , and the second is to specify a scale-speed density pair (s, m) . In this section we use our previous results to suggest an alternative way to specify a scalar diffusion that is stationary and geometrically ergodic. We start with the stationary density q , an increasing function π that integrates to zero under the stationary density and a positive number κ to represent the scalar diffusion. We show how to construct another representation of the diffusion in terms of the triple (q, π, κ) and how to identify these latter three objects in practice.

To guarantee that q can be interpreted as a density, we assume:

Assumption 5. q is a nonnegative Borel measurable function that integrates to one with respect to Lebesgue measure and is strictly positive on (ℓ, r) .

As we know from the formula given by Eq. (3.6), q should be proportional to the speed density m . Since the scale density is determined only up to scale, the

same is true of the speed density (see Eqs. (3.3) and (3.4)). Hence, we are free to take m to be equal to q .

We construct the scale density s or alternatively the diffusion coefficient σ^2 in terms of the function π and the scalar κ . These latter objects are restricted as follows:

Assumption 6. π is a Borel measurable function such that (i) π' is absolutely continuous, (ii) $\pi' > 0$ on (ℓ, r) , (iii) $\int_{\ell}^r \pi |^2 q < \infty$, and (iv) $\int_{\ell}^r \pi q = 0$.

Assumption 7. $\kappa > 0$.

Form:

$$s(x) = \frac{\pi'(x)}{\kappa \int_x^r \pi q} \tag{5.1}$$

Notice that the right-hand side of Eq. (5.1) is positive except possibly at the boundary points ℓ and r . Using Eq. (3.4) we see that the implied formula for the diffusion coefficient is

$$\sigma^2(x) = \frac{\kappa \int_x^r \pi q}{\pi'(x)q(x)} \tag{5.2}$$

The logarithmic derivative of s is

$$\frac{s'(x)}{s(x)} = \frac{\pi''(x)}{\pi'(x)} + \frac{\pi(x)q(x)}{\int_x^r \pi q}$$

Using Eq. (3.5) it follows that μ is given by

$$\mu(x) = - \frac{\sigma^2(x)s'(x)}{2s(x)} = - \frac{\sigma^2(x)\pi''(x)}{2\pi'(x)} - \frac{\kappa\pi(x)}{2\pi'(x)} \tag{5.3}$$

By design the pair (π, κ) solves the eigenvalue problem:

$$\mu\psi' + \frac{1}{2}\sigma^2 \psi'' = - \delta\psi$$

and

$$\lim_{x \nearrow r} \frac{\pi'(x)}{s(x)} = \lim_{x \searrow \ell} \frac{\pi'(x)}{s(x)} = 0.$$

where $-\kappa$ is the eigenvalue and π is the eigenfunction. Since π only crosses the zero axis once, $-\kappa$ is the closest nonzero eigenvalue to zero and π is the maximally autocorrelated function of discretely sampled observations on the Markov state.⁵

⁵ Without additional restrictions, the spectrum of the resulting generator is not necessarily discrete.

When condition (iii) is replaced by the weaker requirement that π be integrable with respect to the stationary density, the resulting process remains geometrically ergodic. In this case, π might no longer be an eigenfunction because it may fail to be in the domain of the generator. Geometric ergodicity is preserved because the continuous range of the spectrum of the generator must be to the left of $-\kappa$ (again see Weidmann, 1987, Theorem 14.9, p. 225).

There exists an extensive literature on estimating densities using time series obtained from observing a stationary and ergodic process. Parametric, local nonparametric (kernel) and global nonparametric (sieve) methods have been justified and can be applied directly to estimate q . Either parametric or sieve methods may also be employed to estimate the eigenfunction π and the eigenvalue $-\kappa$ of the generator. For instance, let Π_N be some (possibly sample size dependent) parameter space of functions which satisfy the restrictions (i)–(iv) of Assumption 6. Since restrictions (iii) and (iv) make reference to the stationary density, the estimated density may be used when imposing these restrictions. The eigenfunction π is estimable by solving the sample counterpart to the maximal autocorrelation problem:

$$\max_{\{\psi \in \Pi_N\}} \frac{1}{N} \sum_{j=1}^N \psi(x_j) \psi(x_{j-1}),$$

which is in the form of an M-estimation problem. Thus, the estimated eigenfunction is extracted as the most persistent function in the sample among the admissible functions in Π_N . Since $-\kappa$ is the corresponding eigenvalue of the generator, κ may be estimated by the negative of the logarithm of the maximized criterion function.

This approach yields a positive estimate of the local variance because of the imposition of conditions (ii) and (iv) when building the parameter space Π_N . Notice that π' is also present in the formula given by Eq. (5.2) for the diffusion coefficient σ^2 and formula [Eq. (5.1)] for the scale density s . Thus, if a sieve method is to be employed it must be designed to approximate first derivatives as well as levels (integrated against the estimated density) of the eigenfunction. Furthermore, in light of formula given by Eq. (5.3) for μ , the second derivative of the eigenfunction must also be approximated to infer the drift from the stationary density and an eigenfunction.

In the remainder of this section, we compare this alternative parameterization to other related approaches.

5.1. Demoura

Demoura (1993) suggested identifying the drift and the diffusion from two eigenfunctions inferred from discrete-time data. Let $(-\delta_1, \psi_1)$ and $(-\delta_2, \psi_2)$

denote two such solutions. Then Demoura suggests deducing the drift and diffusion coefficient from the two linear equations:

$$\begin{bmatrix} \psi'_1 & \psi''_1 \\ \psi'_2 & \psi''_2 \end{bmatrix} \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix} = \begin{bmatrix} -\delta_1 \psi_1 \\ -\delta_2 \psi_2 \end{bmatrix}.$$

While the linear equation formulation is convenient, without additional restrictions on the estimated functions ψ_1 and ψ_2 , the resulting estimate of σ^2 may fail to be positive.

5.2. Ait-Sahalia

Ait-Sahalia (1996a) proposed an identification scheme that entails constructing the diffusion coefficient from the drift and the stationary density. He implements this scheme in the case in which the drift is a linear function of the Markov state. This approach presumes that there is a linear test function in the domain of the generator. Notice that if $\mu(y) = -\alpha y + \beta$, $\alpha > 0$, is in the domain of the generator, then

$$\mathcal{B}\mu = -\alpha\mu.$$

In other words, $(-\alpha, \mu)$ solves the eigenvalue problem. Since the derivative of μ does not change signs, $(-\alpha, \mu)$ coincides with our parameterization $(-\delta, -\pi)$. Therefore, we can view our parameterization as an extension of the one proposed by Ait-Sahalia (1996a) in the case of linear drift.

5.3. Kessler and Sorenson

Kessler and Sorenson (1996) suggested using eigenvalues of parameterized versions of (μ, σ^2) to construct estimating equations. Since the conditional expectation of an eigenfunction satisfies:

$$E[\psi(x_{t+j})|x_t] = \exp(-\delta j)\psi(x_t) \quad (5.4)$$

for any discrete time interval j , knowledge of an eigenfunction can be translated directly into a set of conditional moment conditions to be used in estimation. Whenever eigenfunctions of a finitely parameterized family of generators are easy to compute, Kessler and Sorenson (1996) show how to use the resulting conditional moment restrictions to deduce nearly efficient parameter estimators of the generator. The parameterization suggested in this section is also suited to exploit conditional moment restriction [Eq. (5.4)]. However, in general it may be difficult to compute the implied eigenfunctions from the parameterized drift

and diffusion coefficients. For this reason, directly parameterizing an eigenfunction may be an attractive alternative.

6. Restrictions across eigenfunctions

In this section we derive necessary and sufficient conditions for there to exist a scalar diffusion model consistent with the one-period conditional expectation operator of a discrete-time Markov process. The restrictions are depicted using the spectral representations of the respective operators. As such, they are restrictions across the eigenfunctions and eigenvalues of the conditional expectation operator. Prior to presenting these restrictions, we use the zeroes of the eigenfunctions to partition the state space of the diffusion.

6.1. Partitioning the state space

As we remarked earlier, when the spectrum is discrete the eigenvalues can be ordered so as to make $\{\delta_j\}$ an unbounded increasing sequence where the eigenfunction ϕ_j of \mathcal{A} associated with the eigenvalue $-\delta_j$ has precisely j zeros. Between every zero, the derivative of an eigenfunction has precisely one zero (see Birkhoff and Rota, 1989, p. 314). In the interval to the right of the largest interior zero of ϕ_j the eigenfunction is either strongly convex or strongly concave. Since ϕ_j' is zero at the right boundary, it cannot be zero elsewhere in this region. Similarly, ϕ_j' cannot be zero to the left of the smallest zero of ϕ_j except at $S(\ell)$. Therefore, ϕ_j' has precisely $j + 1$ zeroes in $[S(\ell), S(r)]$.

Let $v_{j,k}$ for $k = 1, \dots, j - 1$ denote the $j - 1$ interior zeroes of the derivative of eigenfunction ϕ_j delineated in ascending order and $v_{j,0} = S(\ell)$ and $v_{j,j} = S(r)$. Consider a diffusion restricted to a particular subinterval $[v_{j,k-1}, v_{j,k}]$, and impose a reflecting barrier at any endpoint except possibly $S(\ell)$ and $S(r)$. The stationary distribution of this restricted diffusion is the probability measure with density proportional to p but restricted to the interval $[v_{j,k-1}, v_{j,k}]$. The function, ϕ_j , appropriately restricted, is an eigenfunction for the generator of this process associated with an eigenvalue δ_j . Since ϕ_j has mean zero against the restriction of p , ϕ_j must cross the zero axis at least once in $(v_{j,k-1}, v_{j,k})$. It can only cross once because ϕ_j' does not change signs. Thus δ_j is the eigenvalue closest to zero for this restricted process.

When we convert the process back to the original scale we preserve the number of interior zeros but not their location. In other words, the derivative ψ_j' of eigenfunction $\psi_j = \phi_j \circ S^{-1}$ in the original scale has precisely $j - 1$ zeros in (ℓ, r) . Again we use the zeroes of ψ_j' to partition the state space $[\ell, r]$. Let $y_{j,k}$ for $k = 1, 2, \dots, j - 1$ denote the interior zeroes of ψ_j' , and define $y_{j,0} = \ell$ and $y_{j,j} = r$. Then ψ_j crosses the zero axis exactly once in the subinterval $(y_{j,k-1}, y_{j,k})$,

its derivative does not change signs in that same interval, (δ_j, ψ_j) solves the eigenvalue problem for the restricted domain, and $\int_{y_{j,k-1}}^{y_{j,k}} \psi_j(y)q(y) dy = 0$.

6.2. Necessary conditions

We now use the partitioning of the zeroes of the derivatives of the eigenfunction to represent the restrictions on the eigenfunctions of a generator of a scalar diffusion. Eq. (3.15) can be written as:

$$\frac{1}{2m(y)} \left[\frac{\psi'_j(y)}{s(y)} \right]' = -\delta_j \psi_j(y).$$

Multiplying by the speed measure m and integrating between consecutive zeroes of ψ'_j we get

$$\frac{\psi'_j(y)}{2s(y)} = -\delta_j \int_{y_{j,k-1}}^y \psi_j(z) m(z) dz + C \tag{6.1}$$

for $y \in (y_{j,k-1}, y_{j,k})$ where C is an arbitrary constant. Taking limits of both sides of Eq. (6.1) as $y \rightarrow y_{j,k}$, it follows that $C = 0$ because m is proportional to q . Moreover, as before, we may normalize m to be q and define s accordingly. Consequently, it follows from, Eq. (6.1) that

Theorem 6.1. For any of the eigenvalue–eigenfunction pair $(-\delta_j, \psi_j)$ of the generator \mathcal{B} (except $\psi_j \equiv 1$), and $y \in (y_{j,k-1}, y_{j,k})$,

$$s(y) = \frac{\psi'_j(y)}{-2\delta_j \int_{y_{j,k-1}}^y \psi_j(z)q(z) dz}. \tag{6.2}$$

Moreover,

$$s(y_{j,k}) = \frac{\psi''_j(y_{j,k})}{-2\delta_j \psi_j(y_{j,k})q(y_{j,k})}.$$

Notice that the scale density function is overidentified. In particular, s can be deduced from any of the eigenvalue–eigenfunction pairs of the generator \mathcal{B} . Moreover, these restrictions must hold even if the spectrum of the generator is not discrete. As we remarked earlier, it is possible for the generator to have multiple eigenvalues without the entire spectrum being discrete. Theorem 6.1 is

still applicable to eigenvalue–eigenfunction pairs associated with the discrete portion of the spectrum.⁶

6.3. Sufficient conditions

So far, we have only established that restrictions given by Eq. (6.2) are necessary. We now establish sufficiency when the spectrum of the conditional expectation operator is discrete. In what follows, \mathcal{T} denotes a conditional expectation operator with a stationary distribution Q with density q in an interval (ℓ, r) . Moreover, there exists a sequence of eigenvalues and eigenfunctions $\{(\exp(-\delta_j), \psi_j)\}$ such that \mathcal{T} has spectral representation:

$$\mathcal{T}\psi = \sum_{j=0}^{\infty} \exp(-\delta_j) \langle \psi | \psi_j \rangle \psi_j.$$

The sequence of eigenfunctions $\{\psi_j\}$ forms an orthonormal basis for $L^2(Q)$. The implied generator satisfies:

$$\hat{\mathcal{B}}\psi = - \sum_{j=0}^{\infty} \delta_j \langle \psi | \psi_j \rangle \psi_j$$

which is a well defined $L^2(Q)$ limit when:

$$\sum_{j=0}^{\infty} (\delta_j)^2 \langle \psi | \psi_j \rangle^2 < \infty.$$

The operator $\hat{\mathcal{B}}$ is clearly closed and symmetric on this domain.

Recall that as stated in Remark 5, for our purposes a reversible diffusion in $[\ell, r]$ is a stochastic process with continuous sample paths with a generator that is an appropriately restricted second-order operator. Our proof strategy will again entail transforming the process to the natural scale. With this in mind,

Theorem 6.2. Suppose that each of the eigenfunctions ψ_j of \mathcal{T} is twice continuously differentiable and ψ'_j has a finite number (K_j) of interior zeroes: $y_{j,1} < y_{j,2} < \dots < y_{j,K_j}$. In addition, suppose that there exists a function s positive on (ℓ, r) such that each ψ_j satisfies:

$$s(y) = \frac{\psi'_j(y)}{-2 \delta_j \int_{y_{j,k-1}}^y \psi_j(z) q(z) dz} \quad \text{for } y \in (y_{j,k-1}, y_{j,k}),$$

$$s(y_{j,k}) = \frac{\psi''_j(y_{j,k})}{-2 \delta_j \psi_j(y_{j,k}) q(y_{j,k})},$$

⁶ Any self-adjoint generator of a semigroup has a spectral representation, but not necessarily of the form of Eq. (4.2).

where $\ell = y_{j,0}$ and $r = y_{j,K_j+1}$. Then there exists a reversible diffusion process for which \mathcal{F} is the conditional expectation operator over a unit time interval.

Proof. Since the eigenfunctions satisfy the embeddability restrictions for some positive function s , we construct a candidate scale function S , by integrating s . Transform the problem to natural scale, and construct the resulting operator:

$$\hat{\mathcal{A}}\phi = - \sum_{j=0}^{\infty} \delta_j \langle \phi | \phi_j \rangle_P \phi_j,$$

where $\phi_j = \psi_j \circ S$ and the inner product is now defined using the transformed probability density $p = \frac{a}{s} \circ S$. Build the local operator:

$$\mathcal{L}\phi = \frac{1}{2p} \phi''.$$

Notice in particular that

$$\mathcal{L}\phi_j = -\delta_j \phi_j.$$

Construct the candidate domain:

$$\hat{D} \equiv \left\{ \phi \in \bar{D}: \lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(l)} \phi'(v) = 0 \right\}.$$

For $\phi \in \hat{D}$, integration by parts and Lemma A.3 yield:

$$\langle \phi | \phi_j \rangle_P = \int_{S(\ell)}^{S(r)} \phi \phi_j p = - \frac{1}{\delta_j} \int_{S(\ell)}^{S(r)} \phi (\mathcal{L}\phi_j) p = - \frac{1}{2\delta_j} \int_{S(\ell)}^{S(r)} \phi \phi_j'' = - \frac{1}{2\delta_j} \int_{S(\ell)}^{S(r)} \phi'' \phi_j.$$

Therefore,

$$\sum_{j=0}^{\infty} (\delta_j)^2 \langle \phi | \phi_j \rangle_P^2 = \sum_{j=0}^{\infty} \langle \mathcal{L}\phi | \phi_j \rangle_P^2 < \infty,$$

and

$$\hat{\mathcal{A}}\phi = \sum_{j=0}^{\infty} \langle \mathcal{L}\phi | \phi_j \rangle_P \phi_j = \mathcal{L}\phi.$$

In other words, $\hat{\mathcal{A}}$ coincides with \mathcal{L} on \hat{D} . From the results in Weidmann (Weidmann, 1980, Chapter 8), \mathcal{L} restricted to \hat{D} is self-adjoint. Since $\hat{\mathcal{A}}$ is self-adjoint, $\hat{\mathcal{A}}$ is \mathcal{L} restricted \hat{D} . From the results in Chapter 3 of Mandl (1968), there exists a process $\{u_t\}$, with continuous sample paths and with conditional expectations operators determined by \mathcal{L} , when viewed as an operator on the subspace of $C_{[\ell,r]}$ with the sup-norm (see Remark 5 above for a detailed

definition). Since the continuous bounded functions are dense in $L^2(Q)$, the conditional operators must coincide with that generated by \mathcal{L} on \hat{D} and hence by $\hat{\mathcal{A}}$. Since s is continuously differentiable, S^{-1} is twice continuously differentiable and hence $\{S^{-1}(u_t)\}$ is a diffusion. \square

Remark 6. We actually showed in this proof that \mathcal{T} is the conditional expectations operator of a diffusion process as it is usually defined (cf. Remark 5). One could further use the results of (Revuz and Yor 1994, Section VII.2) to show that there exists a Brownian motion on an appropriate probability space such that $\{x_t\}$ satisfies the stochastic differential equation given by Eq. (3.1), in (ℓ, r) .

6.4. Subordination

We now consider the impact of sampling the process $\{x_t\}$ at random points in time. Formally, we model this sampling as an increasing process $\{\tau_t\}$ with stationary increments and independent of $\{x_t\}$. The sampling increments are permitted to be temporally dependent. In other words, we study the stationary process:

$$y_t = x_{\tau_t}$$

which we refer to as a *subordinated process*. The process $\{y_t\}$ is stationary but not necessarily Markovian. Subordination does not alter the stationary distribution, so the distribution induced by y_t is still Q . Let \mathcal{V} denote the one-period conditional expectation operator:

$$\mathcal{V}\psi = E [\psi(y_{t+1}) | y_t = x]$$

defined on $L^2(Q)$. Then this operator has a spectral representation with the same eigenvector structure as \mathcal{T} , but with different eigenvalues. In particular,

$$\mathcal{V}\psi = \sum_{j=0}^{\infty} \rho_j \langle \psi | \psi_j \rangle \psi_j,$$

where

$$\rho_j = E \{ \exp[- \delta_j (\tau_{t+1} - \tau_t)] \}. \tag{6.3}$$

As a consequence, the eigenfunctions should still satisfy the embeddability restrictions, but the eigenvalues are distorted. In other words the parameter δ_j in Eq. (6.2) is not given by $-\log(\rho_j)$. The eigenvalues $\{\delta_j\}$ can still be identified up to scale. Once we adopt a scale normalization (and hence identify the eigenvalues), relation Eq. (6.3) provides information about the moment generating function for the random variable $\tau_{t+1} - \tau_t$ evaluated at the generator for the diffusion $\{x_t\}$.

Hansen and Scheinkman (1995) show how to use test functions to check for many of the overidentifying restrictions. In fact, Hansen and Scheinkman (1995), use a version of formula given by Eq. (6.2) applied to ‘approximating’ diffusions with a reflexive barrier to establish their identification result. As emphasized by Conley et al. (1997), this test function approach is particularly suitable for subordinated Markov processes since the sampling interval in Hansen and Scheinkman can be randomized.⁷ In the application in this paper, the test function approach is designed to check whether the remaining eigenvalues of the parameterized generator match those of the operator \mathcal{V} constructed in the previous section. In particular, Hansen and Scheinkman (1995) show that their moments-based test function criterion is equivalent to checking whether \mathcal{V} commutes with \mathcal{B} . Self-adjoint operators with discrete spectra commute if, and only if, they share eigenfunctions. Thus Hansen and Scheinkman’s results can be used to avoid formally computing additional eigenfunctions of the parameterized generator.

7. Concluding remarks

In this paper we have studied identification of scalar diffusions using spectral methods. In particular, exact identification can be achieved using the parameterization of a diffusion proposed in Section 5. This parameterization is based on the most persistent nondegenerate eigenfunction. Alternatively, other eigenfunctions could be used in conjunction with the stationary density to infer the parameters of the diffusion. These other eigenfunctions are more tedious to parameterize because they must satisfy a more complicated set of restrictions. Constructing estimators based on the first (nondegenerate) eigenfunction may be appealing for reasons other than computational tractability. Fitting to the low-frequency time-series movements may be attractive for reasons similar to those used to justify low-frequency analysis of linear times models. By focusing on low-frequency movements, we may tolerate, at least approximately, high-frequency contamination of the diffusion model. This rationale has as antecedents (a) the use of cointegration methods which abstract from transient departures when identifying a linear relation among a vector of time series; and (b) the omission of seasonal frequencies from the frequency decomposition of a Gaussian likelihood function to permit the analysis of stochastic process models which are not designed to capture seasonality.

⁷ Duffie and Glynn (1996) develop a family of GMM estimators for parameters of continuous-time processes, for particular forms of subordination.

As is evident from our analysis and previous work, spectral methods are also valuable in characterizing the long run dependence of a scalar diffusion. For instance, Banon (1978) showed that a diffusion process is geometrically ergodic (and hence ρ -mixing) when there exists a gap in the spectrum to the left of zero. Hence the existence of a nonconstant eigenfunction is a slight strengthening of weak dependence. Discreteness of the spectrum, however, is considerably more restrictive than geometric ergodicity. For this reason we provided sufficient conditions on the drift and diffusion coefficients for the spectrum to be discrete. Our characterization is simpler, and in some cases more general, than the one suggested by Banon (1978).⁸ Discreteness of the spectrum is also used by Conley et al. (1997) and Kessler and Sorenson (1996) to justify martingale approximations for alternative estimators of scalar diffusions. Finally, when there is no spectral gap, the diffusion is strongly dependent (with ρ -mixing coefficients equal to unity). A byproduct of our analysis is a characterization of the tail properties of the drift and diffusion coefficients that imply this strong dependence.

There are two important extensions that are left out of this paper. First, we only considered identification and did not explore formally estimation and inference. Converting our alternative parameterization of a diffusion into an operational estimation method requires parameterizing the maximally autocorrelated eigenfunction. Recall that we showed that this eigenfunction has a non-zero derivative at all interior points in the state space. Sieve methods or other related global approximation methods in statistics and econometrics are, in principle, applicable to this problem; however, it remains to work out their formal properties. Second, our paper only studies scalar diffusions. As we remarked in the introduction, factor models of bond prices are often multivariate diffusions built from independent scalar diffusions. Our identification results are directly extendable to this class of models. In principle, spectral methods are applicable to the more general class of multivariate stationary diffusions that are time reversible. However, we are not aware of full characterizations of eigenfunctions of the generators of such processes.

Appendix A. Intermediate results

In this appendix we establish three intermediate results. First, we show that

$$D(\mathcal{A}) \subset \left\{ \phi \in \bar{D}: \lim_{v \downarrow S(l)} \phi'(v) = \lim_{v \uparrow S(l)} \phi'(v) = 0 \right\}. \quad (\text{A.1})$$

⁸ For instance, Banon's condition involve second derivatives of the drift and diffusion coefficients and does not consider separately the case of entrance barriers.

Lemma A.1. For any $\phi \in \overline{D}$, $\lim_{v \downarrow S(\ell)} \phi'(v)$ and $\lim_{v \uparrow S(r)} \phi'(v)$ are finite. For any $\phi \in D(\mathcal{A})$, $\lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(r)} \phi'(v) = 0$.

Proof. From the Cauchy–Schwarz Inequality, the limits are finite because $\int_{S(\ell)}^{S(r)} \theta^2(u) [\phi''(u)]^2 du$ and $\int_{S(\ell)}^{S(r)} \frac{1}{\theta(u)^2} du$ are both finite. Since \mathcal{A} is self-adjoint,

$$\int_{S(\ell)}^{S(r)} \phi''(v) \psi(v) dv = \int_{S(\ell)}^{S(r)} \phi(v) \psi''(v) dv. \tag{A.2}$$

Employing integration by parts,

$$\int_{S(\ell)}^{S(r)} \phi''(v) \psi(v) dv = \lim_{v \searrow S(\ell), w \nearrow S(r)} \left[- \int_v^w \phi'(v) \psi'(v) dv + \phi'(w) \psi(w) - \phi'(v) \psi(v) \right].$$

Given any nonempty closed interval $[v_1, v_2] \subset (S(\ell), S(r))$, there exists $\psi \in \underline{D} \subset D(\mathcal{A})$ such that $\psi(v) = 0$ for $v \leq v_1$ and $\psi(v) = 1$ for $v \geq v_2$. For such a ψ ,

$$\lim_{v \searrow S(\ell), w \nearrow S(r)} \phi'(w) \psi(w) - \phi'(v) \psi(v) = \lim_{w \uparrow S(r)} \phi'(w).$$

Consequently,

$$\int_{S(\ell)}^{S(r)} \phi''(v) \psi(v) dv = - \int_{S(\ell)}^{S(r)} \phi'(v) \psi'(v) dv + \lim_{w \uparrow S(r)} \phi'(w). \tag{A.3}$$

Using similar logic, it follows that

$$\int_{S(\ell)}^{S(r)} \phi(v) \psi''(v) dv = - \int_{S(\ell)}^{S(r)} \phi'(v) \psi'(v) dv. \tag{A.4}$$

Substituting Eq. (A.3) and Eq. (A.4) into Eq. (A.2), we obtain the conclusion. \square

Our next task is to show that \subset can be replaced by equality in the relation given by Eq. (A.1). In other words,

$$D(\mathcal{A}) = \left\{ \phi \in \overline{D}: \lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(r)} \phi'(v) = 0 \right\}. \tag{A.5}$$

As we stated in Remark 1 it suffices to show that for any function ϕ on the right-hand side of Eq. (A.1) the local martingale $\{M_t\}$ defined by the stochastic integral

$$M_t = \int_0^t \theta(u_t)\phi'(u_t) dW_t$$

is a square integrable martingale. The quadratic variation of this local martingale is $\int_0^t \theta^2(u_s)\phi'(u_s)^2 ds$. By Corollary 1.25 of Revuz and Yor (Revuz and Yor 1994, p. 124),

$$\infty > E \int_0^t \theta^2(u_s) \phi'(u_s)^2 ds = t E \theta^2(u_0)\phi'(u_0)^2.$$

Therefore, equality holds in the relation given by Eq. (A.1) provided $\theta\phi' \in L^2(P)$ whenever the derivative ϕ' vanishes at the boundaries.

Lemma A.2. If $\phi \in \bar{D}$ and $\lim_{u \nearrow S(r)}\phi'(u) = \lim_{u \searrow S(\ell)}\phi'(u) = 0$, then $\int_{S(\ell)}^{S(r)}\phi(u)'^2 du < \infty$.

Proof. Suppose that $\phi \in \bar{D}$. From the Cauchy–Schwarz Inequality, we know that

$$\int_{S(\ell)}^{S(r)} \phi(u)\phi''(u) du < \infty.$$

Applying integration by parts, it follows that

$$+ \infty > \int_v^{S(r)} \phi(u)\phi''(u) du = - \int_v^{S(r)} \phi'^2(u) du + \phi(u)\phi'(u)|_v^{S(r)} \tag{A.6}$$

for some arbitrary $v > S(\ell)$. We will now show that whenever $\lim_{u \nearrow S(r)}\phi(u)\phi'(u) = + \infty$, then $\int_v^{S(r)}\phi'^2(u) du < + \infty$, and similarly for the left boundary. Putting together the results for the two boundaries, it then follows that $\int_{S(\ell)}^{S(r)}\phi'^2(u) du < + \infty$.

Without loss of generality, we take ϕ and ϕ' to be positive for sufficiently large v . For sufficiently large v , there exists a $c > 0$ such that for $u \geq v$,

$$\phi'(u) \geq \frac{c}{\phi(u)}.$$

It follows that for $u \geq v$,

$$\phi(u) \geq c^*(u + \underline{c})^{1/2}.$$

where $c^* = (2c)^{1/2}$ and \underline{c} is chosen to match initial conditions at v . Since $\phi \in L^2(P)$,

$$\int_v^{S(r)} \frac{u}{\theta^2(u)} du < +\infty. \quad (\text{A.7})$$

Also, $\psi \equiv \theta^2 \phi''$ satisfies:

$$\int_v^{S(r)} \frac{\psi^2(u)}{\theta^2(u)} du < +\infty. \quad (\text{A.8})$$

Since ϕ' converges to zero at the right boundary, we may represent this derivative as:

$$\phi'(v) = - \int_v^{S(r)} \frac{\psi(u)}{\theta^2(u)} du.$$

By the Cauchy–Schwarz Inequality:

$$|\phi'(v)|^2 \leq \int_v^{S(r)} \frac{\psi^2(u)}{\theta^2(u)} du \int_v^{S(r)} \frac{1}{\theta^2(u)} du.$$

Consequently, since

$$\int_v^{S(r)} \frac{\psi^2(u)}{\theta^2(u)}$$

is monotone decreasing as a function of v ,

$$\int_v^{S(r)} |\phi'(u)|^2 du \leq \int_v^{S(r)} \frac{\psi^2(u)}{\theta^2(u)} du \int_v^{S(r)} H(u) du, \quad (\text{A.9})$$

where

$$H(v) = \int_v^{S(r)} \frac{1}{\theta^2(u)} du.$$

In light of Eq. (A.8), the left-hand side of Eq. (A.9) is finite if $\int_v^{S(r)} H(u) du$ is finite. To show that this integral is finite, we again employ integration by parts:

$$\int_v^{S(r)} H(u) du = \int_v^{S(r)} \frac{u}{\theta^2(u)} du + uH(u)|_v^{S(r)}. \tag{A.10}$$

Note that

$$uH(u) \leq \int_u^{S(r)} \frac{w}{\theta^2(w)} dw.$$

Since Eq. (A.7) is satisfied, the right-hand side of Eq. (A.10) is finite. Thus,

$$\int_v^{S(r)} |\phi'(u)|^2 du < \infty.$$

The argument for the left boundary is identical. \square

Characterization [Eq. (A.5)] follows from combining relation depicted in Eq. (A.1) and Lemma A.2.

Remark A.1. Another way to show that $D(\mathcal{A}) = \{\phi \in \bar{D}: \lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(\ell)} \phi'(v) = 0\}$ is to use Theorem 8.29 in Weidmann (Weidmann, 1980, p. 256), to show that \mathcal{L} restricted to $\{\phi \in \bar{D}: \lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(\ell)} \phi'(v) = 0\}$ is a self-adjoint extension to \mathcal{L} restricted to \underline{D} . Since \mathcal{A} is also a self-adjoint extension of $(\mathcal{L}, \underline{D})$, they must coincide. We chose here to explicitly prove Lemma A.2 for completeness.

Finally, we prove an intermediate result referred to in the proof of Theorem 6.2. Recall that

$$\hat{D} \equiv \left\{ \phi \in \bar{D}: \lim_{v \downarrow S(\ell)} \phi'(v) = \lim_{v \uparrow S(\ell)} \phi'(v) = 0 \right\}.$$

Lemma A.3. For any pair of functions ϕ and φ in \hat{D} , $\lim_{v \nearrow S(r)} \phi(v)\varphi'(v) = \lim_{v \searrow S(\ell)} \phi(v)\varphi'(v) = 0$.

Proof. Since

$$(\phi\varphi')^2 + (\phi'\varphi)^2 = [(\phi + \varphi)(\phi + \varphi)' - \phi\phi' - \varphi\varphi']^2 - 2(\phi\phi')(\varphi\varphi'),$$

we need only to verify that for any ϕ in \hat{D} ,

$$\lim_{v \nearrow S(r)} \phi(v) \phi'(v) = \lim_{v \searrow S(l)} \phi(v) \phi'(v) = 0.$$

The limit at the right boundary is finite because

$$\lim_{u \uparrow S(r)} \phi(u) \phi'(u) = \int_v^{S(r)} \phi' \phi' + \int_v^{S(r)} \phi \phi'' + \phi(v) \phi'(v).$$

The integrals on the right-hand side are finite because of Lemma A.2 and the Cauchy–Schwarz Inequality. The argument of Lemma A.2 is easily modified to show that $\lim_{v \nearrow S(r)} \phi(v) \phi'(v) \leq 0$. If $\lim_{v \nearrow S(r)} \phi(v) \phi'(v) < 0$, we may assume, without loss of generality, that ϕ is positive and decreasing for large v , and hence ϕ converges as v goes to $S(r)$. However, in this case, $\lim_{v \nearrow S(r)} \phi(v) \phi'(v) = 0$.

The argument for the left boundary is identical. \square

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