Basis Expansion Monte Carlo

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Abstract

We introduce Basis Expansion Monte Carlo, which studies a Gibbs or Metropolis-Hastings sampler to infer the underlying transition kernel. To make inference about the steady state, we compute the steady-state of the approximate kernel. Results show ...

1 Introduction

In many statistical models, it is impossible to find a closed form for the distribution of interest (we will call this π). One work-around, originating in computational physics, relies on the fact that for points x_1 and x_2 in the parameter space, $\pi(x_1)/\pi(x_2)$ may still be calculable, though $\pi(x_1)$ and $\pi(x_2)$ are not. This fact is exploited to produce a Markov chain whose steady-state distribution is guaranteed to be π .

More and references about history, background, and/or tutorials on monte carlo methods. One popular method, the Metropolis-Hastings scheme consists of the following procedure.

Algorithm 1: Metropolis-Hastings algorithm

```
Set x_0 = 0, i = 0
Repeat ad nauseum:
Increment i
Draw x from a proposal distribution q(x|x_{i-1})
Set \alpha(x|x_{i-1}) = 1 - \min(1, \frac{\pi(x)q(x_{i-1}|x)}{\pi(x_{i-1})q(x|x_{i-1})})
Draw u from a uniform density on [0,1]. Set x_i = x with probability 1 - \alpha, i.e. if u > \alpha, and x_i = x_{i-1} otherwise.
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Suppose this MCMC algorithm produces a chain $x_1, x_2, x_3, ...$ of samples. Because the algorithm is stochastic, these samples can be viewed as realizations of random variables $X_1, X_2, X_3, ...$ with marginal density functions f_1, f_2, f_3 , etc. If you initialize deterministically, then X_1 is just a constant. Because X_i is independent of past draws given X_{i-1} , we can write $f_i(x_i) = \int f_{i|i-1}(x_i, x_{i-1})f_{i-1}(x_{i-1})dx_{i-1}$ using the conditional density of X_i given X_{i-1} . Noting that $f_{i|i-1}$ doesn't depend on i, we can replace it with a function K so that $f_i(x_i) = \int K(x_i, x_{i-1})f_{i-1}(x_{i-1})dx_{i-1}$. This function K, called the Markov kernel, is analogous to the transition probability matrices of discrete-space Markov chain theory. We refer to the linear operator of integrating against K as L, so that $f_i = Lf_{i-1}$. The object of interest is the steady state of this operator, an eigenfunction π that has eigenvalue 1 so that for any x, $\pi(x) = \int K(x,t)\pi(t)dt$. In MCMC methods, chains are usually left to run until the Markov chain reaches its steady state. In BEMC, we approximate L, then compute π from the approximation.

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1.1 Stage one: approximating the kernel

Our estimator is parametric, using a fixed set of functions $\{h_i\}_{i=1}^B$ from Ω to \mathbb{R} . We will choose them to be orthogonal with respect to an L_2 inner product, i.e. $\int_{\Omega} h_i(x)h_j(x)dx = 0$ when $i \neq j$. For $\Omega = \mathbb{R}^n$, we use Hermite functions, which are exponentially-weighted orthogonal polynomials. We will attempt to estimate a matrix M in $\mathbb{R}^{B \times B}$ such that $L \approx \hat{L}$, where $(\hat{L}f)(x) = \sum_{i,j=1}^B h_i(x)M_{ij} \int h_j(x)f(x)dx$. Equivalently, we approximate K as $\hat{K}(x,y) = \sum_{i,j=1}^B M_{ij}h_i(x)h_j(y)$.

This approximation can imitate continuous kernels, i.e. situations where $\int K(x_i, x_{i-1}) f_{i-1}(x_{i-1}) dx_{i-1}$ can be done with respect to the Lebesgue measure. This presents an obstacle, because with positive probability, the Metropolis-Hastings algorithm will reject a proposed sample and stay in place. As a workaround, we approximate the kernel not of a single M-H iteration but of ℓ iterations for ℓ around 10 or 20. The probability of ℓ consecutive rejections is much smaller, forcing the true kernel closer to the subspace in which we approximate it. In section 1.3, we discuss a variant that explicitly models rejection events.

How will we choose M? Notice that the orthogonality of the basis functions implies $\int h_i(x)(\hat{L}h_j)(x)dx = M_{ij}$. This can be written as an expectation $M_{ij} = E_{Lh_j}[h_i]$, which motivates us to sample from Lh_j and approximate M_{ij} as a sum. All we need to do is sample z from h_j , run an M-H iteration on z to get w, and retain w as our sample.

How do we "sample" from h, a basis function that sometimes takes negative values? How do we formally take an expectation? The important property to preserve is the law of large numbers: sample averages of should still converge to their expectation. We use a classic tactic from analysis. Let $h_+(x)$ be defined as $\frac{1}{c_+} \max(h(x), 0)$ and let $h_-(x)$ be defined as $\frac{-1}{c_-} \min(h(x), 0)$, with c_+ and c_- chosen so h_+ and h_- each integrate to one. Then define $E_h[f]$ as $c_+E_{h_+}[f]-c_-E_{h_-}[f]$. We can approximate this expectation by sampling z_{n+} from $h_+, n=1...N_+$ and $z_{n-}, n=1...N_-$ from h_- . We would then compute $E_h[f] \approx \frac{c_+}{N_+} \sum_{n=1}^{\infty} f(z_{n+}) - \frac{c_-}{N_-} \sum_{n=1}^{\infty} f(z_{n-})$.

To take care of one last detail, suppose ψ is Lh for some h, and we can only sample from ψ by running an M-H iteration on samples from h. We need to know we can sample from ψ_+ by sampling from h_+ and applying an M-H iteration. In fact, we can, because L will not change the sign of a function.

Algorithm 2: BEMC algorithm-stage one

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Set M to a matrix of all zeroes. For b_{in}=1:B For b_{out}=1:B For n=1:N Draw a sample z_n from h_{b_{in}}. Run the M-H sampler for \ell rounds on z_n. Call the result w_n. Increment M_{b_{out},b_{in}} by h_{b_{in}(w_n)}/N.
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1.2 BEMC-G, a Gibbs sampling variant

This approximation can also be adapted to Gibbs sampling, a ubiquitous MCMC variant.

1.3 BEMC-R, a variant modeling rejections

As we mention in section 1.1, our scheme is able to model continuous kernels. On the other hand, the Metropolis-Hastings algorithm sometimes rejects proposed samples, so its kernel will have a component shaped like a Dirac delta function. In this section, we introduce a variant of BEMC that explicitly models rejections by the sampler.

Let us look at the Metropolis-Hastings kernel in more detail. Going back to the algorithm, the quantity $\alpha(x|x_{i-1})$ is the probability of rejecting a move from x_{i-1} to x. For convenience, let $\alpha(x_{i-1})$ denote the (overall) probability of rejecting a move from x_{i-1} . Splitting up the next draw as an alternative between moving and staying put, we can write $K(x_2, x_1) = \alpha(x_1)\delta_{x_1}(x_2) + (1 - \alpha(x_1))r(x_2|x_1)$. In this expression, $r(x_2|x_1)$ is the conditional density of x_2 given that our move out of x_1 was not rejected. This is not the

same as $q(x_2|x_1)$, since the lack of rejection informs us that we have more likely moved into a region of higher probability. To set up the last line below, define D_{α} from α so that $(D_{\alpha}f)(x) \equiv \alpha(x)f(x)$, and let $(L_{acc}f)(x) \equiv \int r(x|y)(1-\alpha(y))f(y)dy$. Then:

$$\begin{split} f_2(x_2) &= \int K(x_2,x_1) f_1(x_1) dx_1 \\ &= \int (\alpha(x_1) \delta_{x_1}(x_2) + (1-\alpha(x_1)) r(x_2|x_1)) f_1(x_1) dx_1 \\ &= \int \alpha(x_1) \delta_{x_2}(x_1) f_1(x_1) dx_1 + \int (1-\alpha(x_1)) r(x_2|x_1) f_1(x_1) dx_1 \\ &= \alpha(x_2) f_1(x_2) + \int (1-\alpha(x_1)) r(x_2|x_1) f_1(x_1) dx_1 \\ &= (D_{\alpha} f_1)(x_2) + (L_{acc} f_1)(x_2) \end{split}$$

We can sample from a pdf proportional to $D_{\alpha}f$ by sampling z from f(x), then running an M-H iteration on z to get w and retaining the sample z if $w \neq z$. We can sample from a pdf proportional to $L_{acc}f$ by doing nearly the same steps, but retaining w if $w \neq z$. These facts will be useful as we attempt to estimate L_{acc} .

This time around, we will try to estimate a function $\hat{\alpha}$ and a matrix M so that $\hat{\alpha} \approx \alpha$ and $L_{acc} \approx \hat{L}_{acc}$, where $(\hat{L}_{acc}f)(x) = \sum_{i,j=1}^{B} h_i(x) M_{ij} \int h_j(x) f(x) dx$. Even if the parameters were chosen optimally, L may not take the same form as $\hat{L}_{\alpha} + \hat{L}_{M}$, so the estimate $\hat{\pi}$ will not be correct. EMK: Need some results answering "in what sense is your method correct?"

For this variant, we need still need to estimate M with the added complication of trying to infer $\hat{\alpha}$ at the same time. Fortunately, it is easy to tell when the sampler rejects and when it doesn't, and this provides a way to tease out information about α . Suppose for a moment that we start the sampler at a point z and it takes a single step to w. If $w \neq z$, then the sampler has shown less of a tendency to reject starting from z, and we label z with a 0. If w = z, we label z with a 1. Once the sample space is covered in zeroes and ones, there are many probabilistic classifier methods that could give an estimate of $\hat{\alpha}$, which at any given point is just the probability of labeling with a one. Meanwhile, whenever the sampler moves, we gain information about L_{acc} , and we can update M as before.

This strategy still throws away useful information. To see why, recall that the Metropolis-Hastings algorithm makes a proposal, computes an rejection probability, flips a proverbial coin with that probability, and then discards the rejection probability. When drawing a chain of samples, the rejection probability serves no further purpose, so discarding it is natural. In BEMC-R, though, it provides a more efficient estimate of α . If the rejection probability when proposing a move to w from z is p, then the better procedure is to label z with p. Likewise, instead of updating the estimate of M_{ij} with sample of weight 1 with probability p, we can update it with a sample of weight p.

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Algorithm 3: BEMC-R algorithm-stage one
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Set M to 0.

Set a scalar W to zero. W is the effective number of samples in an estimate of an entry of M.

Set T = \{\}. T will be the training set for \hat{\alpha}.

For b_{in} = 1: B

For n = 1: N

Draw a sample z_n from h_{b_{in}}.

Draw a proposal w_n and compute its rejection probability p.

Add (z_n, p) to T.

Increment M_{b_{out},b_{in}} by ph_{b_{in}(w_n)}.

Increment W by p.

Divide M_{b_{out},b_{in}} by W.

Train \hat{\alpha} on T.
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For one further refinement, we could include some prior information about M. Since L_{acc} mimics the action of the sampler as it moves, it should resemble the action of the proposal alone, with no rejections. That would mean $M_{ij} \approx \int h_i(x)q(x|y)h_j(y)dydx$. For simple proposal distributions like a uniform or normal centered on the current value, this integral may be easy to find as a convolution.

1.4 Computing the steady state in BEMC-R

Given \hat{M} , $\hat{\alpha}$, and an initial state f_0 , we want to compute $[D_{\hat{\alpha}} + \hat{L}_{acc}]^P(f_0)$ for some moderately high exponent P. To simplify the problem, suppose we set f_0 to h_1 , one of the initial B basis functions. Also, suppose that we restrict $\hat{\alpha}$ to a form where for any of our basis functions h_i , we can expand $\hat{\alpha}h_i$ as a sum $\sum_{i=1}^B c_i h_i$. Because of the orthogonality, computing $\hat{L}_{acc}(f_0)$ is simple: $\hat{L}_{acc}(f_0) = \sum_{i=1}^B \hat{L}_{acc}(c_i h_i) = \sum_{i=1}^B [\hat{M}c]_i h_i$. The difficulty lies in finding a representation of $D_{\hat{\alpha}}(f_0)$ in this basis, i.e. evaluating or quickly approximating integrals of the form $\int_{\Omega} h_i(x)h_j(x)\hat{\alpha}(x)dx$. EMK: Maybe we'll choose a crafty form for $\hat{\alpha}$ and do this analytically.

2 Implementation details

At this point, we will introduce a family of basis functions and begin to work in specifics. We will at first discuss the scenario where the sample space Ω is \mathbf{R} . Our basis of choice is the Hermite functions, line (46) of [1]. To describe them, it's easiest to first define the nth-degree physicists' Hermite polynomial, $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$. (This definition in terms of derivatives is called a Rodriguez formula.) As the name suggests, this boils down to a polynomial in x. Then, the nth Hermite function is $\psi_n(x) = (\pi^{1/2} n! 2^n)^{-1/2} H_n(x) e^{-x^2/2}$, an exponentially decaying polynomial. The Hermite functions are orthogonal: $\int_{\mathbf{R}} \psi_i \psi_j = 1$ if i = j and 0 otherwise (line (48) of [1]). In fact, this orthogonality is preserved even if we alter the definition to include a scale factor so that $\psi_n(x) = \sqrt{\frac{a}{(\pi^{1/2} n! 2^n)}} H_n(ax) e^{-\frac{(ax)^2}{2}}$.

When the sample space is \mathbb{R}^n , we will use products of Hermite functions. This means it may be more convenient to index the basis with D coordinates if the sample space is D-dimensional; for example, we might write $h_{35}(x_1, x_2) = \psi_3(x_1)\psi_5(x_2)$. In order to fit the BEMC mold, we need to separate the positive and negative parts for each function, find their normalizing constants c_+ and c_- , and sample from densities proportional to the positive and negative parts.

2.1 Computing c_+ and c_-

The sign changes of ψ_k are just the roots of the kth Hermite polynomial. In the one-dimensional case, these roots are few in number and can be found via the Golub-Welsch algorithm [2], which is implemented in the R package fastGHQuad [3]. The number of positive regions scales exponentially with the dimension, so we need to simplify the sum. We take the next paragraph to set up notation.

Suppose we are dealing with a basis that looks like $h_{J_1J_2...J_D}(x_1, x_2, ..., x_D) = \prod_{d=1}^D \psi_{J_d}(x_d)$, and suppose x_{dj} is the jth root of the J_d th order Hermite polynomial. Index the roots from 1 so that if the factor on the first dimension is $\psi_1 = \sqrt{2}\pi^{-\frac{1}{4}}xe^{\frac{-x^2}{2}}$, then $x_{11} = 0$. Let I_{dj} be the interval from x_{dj} to $x_{d,j+1}$, and use the convention that $x_{d0} = -\infty$ and $x_{d,J_{d+1}} = \infty$. Then $h_{J_1J_2...J_D}$ is positive on $I_{1J_1} \times ... \times I_{DJ_D}$, and it is positive on $I_{1,J_1-k_1} \times ... \times I_{D,J_D-k_D}$ iff $\sum_{d=1}^D k_d$ is even. (Every time we cross a hyperplane $x_d = x_{dj}$, one of the k's changes, and so does the sign of h. This connects the parity of $\sum_{d=1}^D k_d$ to the sign of the basis element.) Letting $A_{\gamma,d} = \sum_{(k_1 \mod 2)=\gamma} \int_{I_{1,J_d-k_d}} \psi_{J_d}(x_d)$ and $B_{D_0\gamma} = \sum_{(\sum_{d=D_0}^D k_d \mod 2)=\gamma} \int_{I_{1,J_D-k_D}} \psi_{J_2}(x_2) \int ... \int_{I_{D,J_D-k_D}} \psi_{J_D}(x_D)$, then $B_{0\gamma}$ is what we seek, and the others are useful intermediaries.

$$B_{0\gamma} = \sum_{\left(\sum_{d=1}^{D} k_d \bmod 2\right) = \gamma} \int_{I_{1,J_1 - k_1}} \psi_{J_1}(x_1) \int \dots \int_{I_{D,J_D - k_D}} \psi_{J_D}(x_D) dx_1 \dots dx_D$$

$$= \sum_{\left(\sum_{d=0}^{D} k_d \bmod 2\right) = \gamma} \int_{I_{1,J_1 - k_1} \times \dots \times I_{D,J_D - k_D}} h_{J_1 J_2 \dots J_D}(x_1, \dots, x_D) dx_1 \dots dx_D$$

$$= c_+ \text{ if } \gamma = 0 \text{ and } c_- \text{ otherwise.}$$

We have the following recursive relation.

$$\begin{split} B_{D_0\gamma_1} &= \sum_{\left(\sum_{d=1}^D k_d \bmod 2\right) = \gamma_1} \int_{I_{1,J_1-k_1}} \psi_{J_1}(x_1) \int \dots \int_{I_{D,J_D-k_D}} \psi_{J_D}(x_D) \\ &= \sum_{\gamma_2 \in \{0,1\}} \sum_{(k_1 \bmod 2) = \gamma_1 - \gamma_2} \int_{I_{1,J_{D_0}-k_{D_0}}} \psi_{J_{D_0}}(x_{D_0}) \sum_{\left(\sum_{d=D_0+1}^D k_d \bmod 2\right) = \gamma_2} \int_{I_{1,J_2-k_2}} \psi_{J_2}(x_2) \int \dots \int_{I_{D,J_D-k_D}} \psi_{J_D}(x_D) \\ &= \sum_{\gamma_2 \in \{0,1\}} A_{\gamma_1 - \gamma_2, D_0} B_{D_0+1,\gamma_2} \end{split}$$

This motivates a feasible procedure to compute c_{+} and c_{-} .

Algorithm 4: Computing c_+ and c_-

Input: a set of indices $J_1,...J_D$ for a basis function on a D-dimensional space.

Initialize $B_{D,0}$ to $\sum_{k_D \text{ even}} \int_{I_{D,J_D-k_D}} \psi_{J_D}(x_D)$

Initialize $B_{D,1}$ to $\sum_{k_D \text{ odd}} \int_{I_{D,J_D-k_D}} \psi_{J_D}(x_D)$

For d from D-1 to 1:

For γ in $\{0,1\}$:

Compute $A_{\gamma,d} = \sum_{(k \mod 2) = \gamma} \int_{I_{1,J_d-k}} \psi_{J_d}(x_d)$ For γ_1 and γ_2 in $\{0,1\}^2$: Compute $B_{d,\gamma_1} = \sum_{\gamma_2 \in \{0,1\}} A_{\gamma_1-\gamma_2,d} B_{d+1,\gamma_2}$ Return B_{00} for c_+ and B_{01} for c_- .

We'll then need to integrate these Hermite functions. We start by using integration by parts with the

Rodriguez formula. In the last line, we use equation (4) c.f. [4].

$$\begin{split} \int_{a}^{b} \psi_{n}(x) dx &= \int_{a}^{b} \sqrt{\frac{1}{\sqrt{\pi n! 2^{n}}}} H_{n}(x) e^{\frac{-x^{2}}{2}} dx \\ &= \sqrt{\frac{1}{\sqrt{\pi n! 2^{n}}}} \int_{a}^{b} (-1)^{n} e^{\frac{-x^{2}}{2}} e^{x^{2}} \frac{d^{n}}{dx^{n}} e^{-x^{2}} dx \\ &= \sqrt{\frac{1}{\sqrt{\pi n! 2^{n}}}} (-1)^{n} \left[e^{\frac{x^{2}}{2}} \frac{d^{n-1}}{dx^{n-1}} e^{-x^{2}} \Big|_{a}^{b} - \int_{a}^{b} \frac{d}{dx} (e^{\frac{x^{2}}{2}}) \frac{d^{n-1}}{dx^{n-1}} e^{-x^{2}} dx \right] \\ &= \sqrt{\frac{1}{\sqrt{\pi n! 2^{n}}}} (-1)^{n} \left[\sqrt{\sqrt{\pi} (n-1)! 2^{(n-1)}} (-1)^{(n-1)} \psi_{n-1} \Big|_{a}^{b} - \int_{a}^{b} (\frac{d}{dx} e^{\frac{x^{2}}{2}}) (\frac{d^{n-1}}{dx^{n-1}} e^{-x^{2}}) dx \right] \\ &= \sqrt{\frac{1}{\sqrt{\pi n! 2^{n}}}} (-1)^{n} \left[\sqrt{\sqrt{\pi} (n-1)! 2^{(n-1)}} (-1)^{(n-1)} \psi_{n-1} \Big|_{a}^{b} - \int_{a}^{b} (x e^{\frac{x^{2}}{2}}) (-1)^{n-1} e^{-x^{2}} H_{n-1}(x) dx \right] \\ &= \sqrt{\frac{1}{\sqrt{\pi n! 2^{n}}}} (-1)^{n} \left[\sqrt{\sqrt{\pi} (n-1)! 2^{(n-1)}} (-1)^{(n-1)} \psi_{n-1} \Big|_{a}^{b} - \int_{a}^{b} \sqrt{\sqrt{\pi} (n-1)! 2^{(n-1)}} (-1)^{n-1} x \psi_{n-1}(x) dx \right] \\ &= -\sqrt{\frac{1}{2n}} \left[\psi_{n-1} \Big|_{a}^{b} - \int_{a}^{b} x \psi_{n-1}(x) dx \right] \\ &= -\sqrt{\frac{1}{2n}} \left[\psi_{n-1} \Big|_{a}^{b} - \int_{a}^{b} \sqrt{\frac{n-1}{2}} \psi_{n-2}(x) + \sqrt{\frac{n}{2}} \psi_{n}(x) dx \right] \end{split}$$

Rearranging the last line, we have a recurrence relation for the integrals we need.

$$(1 - \sqrt{\frac{n}{2}}) \int_{a}^{b} \psi_{n}(x) dx = \sqrt{\frac{1}{2n}} \left[-\psi_{n-1} \Big|_{a}^{b} + \int_{a}^{b} \sqrt{\frac{n-1}{2}} \psi_{n-2}(x) dx \right]$$

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Algorithm 5: Computing \int_a^b \psi_n(x) dx
If a = -\infty or b = \infty, set a flag. If n is 0:
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Set $I = \int_a^b \pi^{-\frac{1}{4}} e^{\frac{-x^2}{2}} dx$ by re-scaling output from a built-in normal distribution CDF calculator.

Set $I = \int_a^b \sqrt{2}\pi^{-\frac{1}{4}}xe^{\frac{-x^2}{2}}dx$ by re-scaling output from a built-in Nakagami distribution CDF

If n > 1:

Follow this routine to compute $I_{n-2} = \int_a^b \psi_{n-2}(x) dx$.

Set I to $(1-\sqrt{\frac{n}{2}})^{-1}\sqrt{\frac{1}{2n}}\left[\psi_{n-1}(a)-\psi_{n-1}(b)+\sqrt{\frac{n-1}{2}}I_{n-2}\right]$. If there is a flag set for $a=-\infty$ or $b=\infty$, set $\psi_{n-1}(a)$ or $\psi_{n-1}(b)$ to zero as needed instead of calculating them.

Return I.

2.2Sampling

To compute β , $\sup_x |\psi_J(x)|/f(x)$ is the greater of $\sup_x \psi_J(x)/f(x)$ and $-\inf_x \psi_J(x)/f(x)$. Either way, we can take derivatives and set them to 0. Below, f is a mixture density with coefficient ν for the normal component

Algorithm 6: Rejection sampling from ψ_J .

On initialization:

Suppose x_j is the jth root of ψ_J . Using the convention that $x_0 = -\infty$ and $x_{J+1} = \infty$,

For j = 1, ...J: Set $p_j = \int_{x_j}^{x_{j+1}} |\psi_J(x)| dx/(c_+ + c_-)$.

For j = 1, ...J, generate three abcissae ξ_{j1} , ξ_{j2} , and ξ_{j3} on a grid between x_j and x_{j+1} .

Evaluate $\psi_J(\xi_{j1})$, $\psi_J(\xi_{j2})$, and $\psi_J(\xi_{j3})$.

Find a quadratic of best fit.

For one sample:

Draw $u_1 \sim \text{unif}(0,1)$.

and $1 - \nu$ for the double Nakagami((J+1)/2, J+1), i.e. $f(x) = (1 - \nu) \frac{(\frac{1}{2})^{\frac{k+1}{2}}}{\Gamma(k+1)} x^k \exp(\frac{-x^2}{2}) + \nu \frac{1}{\sqrt{2\pi}} \exp(\frac{-x^2}{2})$. Then $\frac{df}{dx}$ is $(1 - \nu) \frac{(\frac{1}{2})^{\frac{k+1}{2}}}{\Gamma(k+1)} \left[kx^{(k-1)} \exp(\frac{-x^2}{2}) - x^{k+1} \exp(\frac{-x^2}{2}) \right] - \nu \frac{1}{\sqrt{2\pi}} x \exp(\frac{-x^2}{2})$.

$$\frac{d}{dx}\psi_J(x)/f(x) = \frac{f(x)\psi_J'(x) - f'(x)\psi_J(x)}{f(x)^2}$$

3 **Proof of Correctness**

In stage 1, we will suffer some error while estimating M and α from. The true transition kernel cannot always be represented in the finite-dimensional form we impose, which is a second source of error. In stage two of BEMC-R, we incur a third source, namely that $D_{\hat{\alpha}}(f_0)$ does not necessarily take the form $\sum_{i=1}^{B} c_i h_i$, especially if $\hat{\alpha}$ is also represented in the same basis. For example, if the basis were Gaussian-weighted polynomials up to degree 15, the degree of $D_{\hat{\alpha}}(f_0)$ would quickly exceed 15, and the variance of the Gaussian would change.

References

- [1] Weisstein, E.W.: Hermite polynomial. From MathWorld-A Wolfram Web Resource. (December 2014)
- [2] Golub, G.H., Welsch, J.H.: Calculation of Gauss quadrature rules. Math. Comp. 23(106) (1969) 221–230 Loose microfiche suppl. A1–A10.
- [3] Blocker, A.W.: fastGHQuad: Fast Rcpp implementation of Gauss-Hermite quadrature. (2014) R package version 0.2.
- [4] Bunck, B.: A fast algorithm for evaluation of normalized hermite functions. Bit Numer Math 49(2) (2009) 281-295