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.
```

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 $E_h[f] \approx \frac{c_+}{N_+}\sum f(z_{n+}) - \frac{c_-}{N_-}\sum f(z_{n-})$.

To take care of one last detail, suppose ϕ is Lh for some h, and we can only sample from ϕ by running an M-H iteration on samples from h. We need to know we can sample from ϕ_+ 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

```
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 $h_{b_{in}(w_n)}/N$.
```

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:

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

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.

Algorithm 3: BEMC-R algorithm–stage one

```
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 $b_{out} = 1 : B$
    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 $T$.
```

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. They are generated by setting $\phi_{n+1} = \sqrt{\frac{2}{n+1}}\left[x\phi_n - \sqrt{\frac{n}{2}}\phi_{n-1}\right]$, with $\phi_0 = \pi^{-\frac{1}{4}}e^{\frac{-x^2}{2}}$ and $\phi_1 = \sqrt{2}\pi^{-\frac{1}{4}}xe^{\frac{-x^2}{2}}$. They are orthogonal: $\int_{\mathbf{R}} \phi_i\phi_j = 1$ if $i = j$ and 0 otherwise.

When the sample space is $\mathbf{R}^n$, 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 $h_{35}(x_1, x_2) = \phi_3(x_1)\phi_5(x_2)$. 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 ϕ_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 [1], which is implemented in the R package `fastGHQuad` [2]. The number of positive regions scales exponentially with the dimension, so we need to simplify the sum. We spend a paragraph setting up notation.

Suppose we are dealing with a basis that looks like $h_{J_1J_2...J_D}(x_1, x_2, ..., x_D) = \prod_{d=1}^D \phi_{J_d}(x_d)$, and suppose x_{dj} is the jth root of the J_dth order Hermite polynomial. Index the roots from 1 so that if the factor on the first dimension is $\phi_1 = \sqrt{2}\pi^{-\frac{1}{4}}xe^{\frac{-x^2}{2}}$, 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. Letting $A_{\gamma,d} = \sum_{(k_1 \bmod 2)=\gamma} \int_{I_{1,J_d-k_d}} \phi_{J_d}(x_d)$ and $B_{D_0\gamma} = \sum_{(\sum_{d=D_0}^D k_d \bmod 2)=\gamma} \int_{I_{1,J_{D_0}-k_{D_0}}} \phi_{J_2}(x_2) \int ... \int_{I_{D,J_D-k_D}} \phi_{J_D}(x_D)$, $B_{0\gamma}$ is what we seek.

$$
\begin{aligned}
B_{0\gamma} &= \sum_{(\sum_{d=1}^D k_d \bmod 2)=\gamma} \int_{I_{1,J_1-k_1}} \phi_{J_1}(x_1) \int ... \int_{I_{D,J_D-k_D}} \phi_{J_D}(x_D) \\
&= \sum_{(\sum_{d=0}^D k_d \bmod 2)=\gamma} \int_{I_{1,J_1-k_1} \times ... \times I_{D,J_D-k_D}} h_{J_1J_2...J_D} \\
&= c_+ \text{ if } \gamma = 0 \text{ and } c_- \text{ otherwise.}
\end{aligned}
$$

We have the following recursive relation.

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

This motivates an economical 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 $\sum_{K-D \text{ even}} \int_{I_{D,J_D-k_D}} \phi_{J_D}(x_D)$ Initialize $B_{D,1}$ to
```

We'll then need to integrate terms of the form $cx^k \exp(\frac{-x^2}{2})$, a task we can rewrite using gamma densities. Below, Y is a Gamma random variable with shape $a = (k+1)/2$ and rate $b = -1/2$; F_Y is its cumulative distribution function (CDF). The variables x_0 and x_1 are roots of whichever Hermite polynomial we are working with.

$$
\begin{aligned}
\int_{x_0}^{x_1} cx^k \exp(\frac{-x^2}{2})dx &= \int_{x_0^2}^{x_1^2} \frac{c}{2} y^{(\frac{k-1}{2})} \exp(\frac{-y}{2})dy \\
&= \frac{c}{2}\frac{\Gamma(a)}{b^a} \int_{x_0^2}^{x_1^2} \frac{b^a}{\Gamma(a)} y^{(a-1)} \exp(-by)dy \\
&= \frac{c}{2}\frac{\Gamma(a)}{b^a}(F_Y(x_1^2) - F_Y(x_1^2))
\end{aligned}
$$

Another way to phrase this trick: the square root of a Gamma random variable with the right parameters has a density function proportional to $x^k \exp(\frac{-x^2}{2})$. This is also called the Nakagami distribution, and the `R` package `VGAM` has functions `rnaka()` (for sampling) and `pnaka()` for evaluating the CDF. To match $x^k \exp(\frac{-x^2}{2})$, the shape parameter should be $(k+1)/2$ and the rate $k+1$. The normalizing constant is $\frac{(\frac{1}{2})^{\frac{k-1}{2}}}{\Gamma(k+1)}$.

2.2 Sampling

The Nakagami distribution is supported only on $\mathbb{R}_+$, so we will need modify our calculations to reflect half the mass onto the negative numbers. We will call this a double Nakagami distribution. Since some multiple of the double Nakagami density dominates ϕ_{J+} and ϕ_{J-}, we can use rejection sampling with a Nakagami$((J+1)/2, J+1)$ proposal to draw samples from basis function ϕ_J. Rather than separately sampling ϕ_{J+} and ϕ_{J-}, we can employ the following trick.

Algorithm 5: Rejection sampling from ϕ_J. Let h

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] Golub, G.H., Welsch, J.H.: Calculation of Gauss quadrature rules. Math. Comp. **23**(106) (1969) 221–230 Loose microfiche suppl. A1–A10.

[2] Blocker, A.W.: fastGHQuad: Fast Rcpp implementation of Gauss-Hermite quadrature. (2014) R package version 0.2.