11.5 Evaluation of Expectation

Posterior distribution $f_{\theta|y}(\theta|y)$

$$\mathrm{E}(\theta|y) = \int \theta f_{\theta|y}(\theta|y)\mathrm{d}\theta = \frac{\int \theta f_{y|\theta}(y|\theta) f_\theta(\theta)\mathrm{d}\theta}{\int f_{y|\theta}(y|\theta) f_\theta(\theta)\mathrm{d}\theta}.$$

In the case where it is not easy to evaluate $\mathrm{E}(\theta|y)$, how do we do?

Bayesian Method = Evaluation of Integration (Too much to say?)

- Numerical Integration
- Monte Carlo Integration
- Random Number Generation from $f_{\theta|y}(\theta|y)$

11.5.1 Evaluation of Expectation: Numerical Integration

Univariate Case: Consider integration of a function $f(x)$.

Suppose that x is a scalar.

Let x_0, x_1, x_2, $\cdots$, x_n be n nodes, which are sorted by order of size but not necessarily equal intervals between x_{i-1} and x_i for $i = 1, 2, \cdots, n$.

Rectangular Approximation:

$$\int f(x)\mathrm{d}x \approx \sum_{i=1}^{n} f(x_i)(x_i - x_{i-1}) \quad \text{or} \quad \sum_{i=1}^{n} f(x_{i-1})(x_i - x_{i-1}).$$

Trapezoid Approximation:

$$\int f(x)\mathrm{d}x \approx \sum_{i=1}^{n} \frac{1}{2}(f(x_i) + f(x_{i-1}))(x_i - x_{i-1}).$$

Bivariate Case: Consider integration of a function $f(x, y)$.

Suppose that both x and y are scalars.

Let x_0, x_1, x_2, $\cdots$, x_n be n nodes, which are sorted by order of size not necessarily equal intervals between x_{i-1} and x_i for $i = 1, 2, \cdots, n$.
Let y_0, y_1, y_2, $\cdots$, y_m be m nodes.

Rectangular Approximation:

$$\int\int f(x, y)\mathrm{d}x\mathrm{d}y \approx \sum_{i=1}^{n}\sum_{j=1}^{m} f(x_i, y_j)(x_i - x_{i-1})(y_j - y_{j-1}).$$

Trapezoid Approximation:

$$\begin{aligned}&\int\int f(x.y)\mathrm{d}x\mathrm{d}y\\ &\approx \sum_{i=1}^{n}\sum_{j=1}^{m} \frac{1}{4}(f(x_i, y_j) + f(x_i, y_{j-1}) + f(x_{i-1}, y_j) + f(x_{i-1}, y_{j-1}))(x_i - x_{i-1})(y_j - y_{j-1}).\end{aligned}$$

Applying to Bayes Method (Rectangular Approximation):

$$\begin{aligned}\mathrm{E}(\theta|y) &= \frac{\int \theta f_{y|\theta}(y|\theta) f_\theta(\theta) \mathrm{d}\theta}{\int f_{y|\theta}(y|\theta) f_\theta(\theta) \mathrm{d}\theta} = \frac{\sum_{i=1}^{n} \theta_i f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)(\theta_i - \theta_{i-1})}{\sum_{i=1}^{n} f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)(\theta_i - \theta_{i-1})} \\ &= \frac{\sum_{i=1}^{n} \theta_i f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)}{\sum_{i=1}^{n} f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)} = \sum_{i=1}^{n} \theta_i \omega_i, \quad \text{for constant } \theta_i - \theta_{i-1},\end{aligned}$$

where

$$\omega_i = \frac{f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)}{\sum_{i=1}^{n} f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)}.$$

Problem of Numerical Integration:

1. Choice of initial and terminal values $\Longrightarrow$ Truncation errors
2. Accumulation of computational errors by computer
3. Increase of computational burden for large dimension.

   $\Longrightarrow$ k dimension, and n nodes for each dimension $\Longrightarrow$ n^k

11.5.2 Evaluation of Expectation: Monte Carlo Integration

Univariate Case: Consider integration of a function $f(x)$.

Suppose that x is a scalar.

Let $x_1, x_2, \cdots, x_n$ be n random draws generated from $g(x)$.

$$\int f(x)\mathrm{d}x = \int \frac{f(x)}{g(x)} g(x)\mathrm{d}x = \mathrm{E}\left(\frac{f(x)}{g(x)}\right) \approx \frac{1}{n}\sum_{i=1}^{n} \frac{f(x_i)}{g(x_i)}.$$

$\Longrightarrow$ **Importance Sampling (重点的サンプリング)**

Multivariate Case: Consider integration of a function $f(x)$.

Suppose that x is a vector.

Let $x_1, x_2, \cdots, x_n$ be n random draws generated from $g(x)$.

$$\int f(x)\mathrm{d}x = \int \frac{f(x)}{g(x)} g(x)\mathrm{d}x = \mathrm{E}\left(\frac{f(x)}{g(x)}\right) \approx \frac{1}{n}\sum_{i=1}^{n} \frac{f(x_i)}{g(x_i)},$$

which is exacly the same as the univariate case.

Computational burden: $\Longrightarrow$ Univariate case: n, Multivariate case: n

Precision of integration ???

Especially, when $g(x)$ is not close to $f(x)$, approximation is prror.

Applying to Bayes Method:

$$\mathrm{E}(\theta|y) = \frac{\int \theta f_{y|\theta}(y|\theta) f_\theta(\theta)\mathrm{d}\theta}{\int f_{y|\theta}(y|\theta) f_\theta(\theta)\mathrm{d}\theta} = \frac{\int \theta \dfrac{f_{y|\theta}(y|\theta) f_\theta(\theta)}{g(\theta)} g(\theta)\mathrm{d}\theta}{\int \dfrac{f_{y|\theta}(y|\theta) f_\theta(\theta)}{g(\theta)} g(\theta)\mathrm{d}\theta} = \frac{(1/n)\sum_{i=1}^{n} \theta_i \omega(\theta_i)}{(1/n)\sum_{i=1}^{n} \omega(\theta_i)},$$

where

$$\omega(\theta_i) = \frac{f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)}{g(\theta_i)}.$$

Choice of $g(\theta)$ — One Solution: Define $l(\theta) \equiv f_{y|\theta}(y|\theta) f_\theta(\theta)$.

$$\begin{aligned}
\log l(\theta) &\approx \log l(\tilde{\theta}) + \frac{1}{l(\tilde{\theta})} \frac{\partial l(\tilde{\theta})}{\partial \theta}(\theta - \tilde{\theta}) \\
&\quad + \frac{1}{2}(\theta - \tilde{\theta})' \Big(- \frac{1}{l(\tilde{\theta})^2} \frac{\partial l(\tilde{\theta})}{\partial \theta} \frac{\partial l(\tilde{\theta})}{\partial \theta'} + \frac{1}{l(\tilde{\theta})} \frac{\partial^2 l(\tilde{\theta})}{\partial \theta \partial \theta'} \Big) (\theta - \tilde{\theta}) \\
&= -\frac{1}{2}(\theta - \tilde{\theta})' \Big(- \frac{1}{l(\tilde{\theta})} \frac{\partial^2 l(\tilde{\theta})}{\partial \theta \partial \theta'} \Big) (\theta - \tilde{\theta}), \qquad \text{when } \tilde{\theta} \text{ is a mode of } l(\theta).
\end{aligned}$$

Thus, $N\Big(\tilde{\theta},\ \Big(- \frac{1}{l(\tilde{\theta})} \frac{\partial^2 l(\tilde{\theta})}{\partial \theta \partial \theta'} \Big)^{-1} \Big)$ might be taken as the importance density $g(\theta)$.

11.5.3 Evaluation of Expectation: Random Number Generation

Generate random draws of θ from the posterior distribution $f_{\theta|y}(\theta|y)$.

Then, $(1/n)\sum_{i=1}^{n}\theta_i$ is taken as a consistent estimator of $\mathrm{E}(\theta|y)$, where θ_i indicates the ith random draw generated from $f_{\theta|y}(\theta|y)$.

Note that $(1/n)\sum_{i=1}^{n}\theta_i \longrightarrow \mathrm{E}(\theta|y)$ under the condition $(1/n)\sum_{i=1}^{n}\theta_i < \infty$.

Bayesian confidence interval, median, quntiles and so on are obtained by sorting $\theta_1, \theta_2, \cdots, \theta_n$ in order of size.

$\Longrightarrow$ Sampling methods

11.6 Sampling Method I: Random Number Generation

Note that a lot of distribution functions are introduced in Kotz, Balakrishman and Johnson (2000a, 2000b, 2000c, 2000d, 2000e).

The random draws discussed in this section are based on uniform random draws between zero and one.

11.6.1 Uniform Distribution: $U(0, 1)$

Properties of Uniform Distribution: The most heuristic and simplest distribution is uniform.

The **uniform distribution** between zero and one is given by:

$$f(x) = \begin{cases} 1, & \text{for } 0 < x < 1, \\ 0, & \text{otherwise.} \end{cases}$$

Mean, variance and the moment-generating function are given by:

$$\mathrm{E}(X) = \frac{1}{2}, \qquad \mathrm{V}(X) = \frac{1}{12}, \qquad \phi(\theta) = \frac{e^{\theta} - 1}{\theta}.$$

Use L'Hospital's theorem to derive $\mathrm{E}(X)$ and $\mathrm{V}(X)$ using $\phi(\theta)$.

In the next section, we introduce an idea of generating uniform random draws, which in turn yield the other random draws by the transformation of variables, the inverse transform algorithm and so on.

Uniform Random Number Generators: It is no exaggeration to say that all the random draws are based on a uniform random number.

Once uniform random draws are generated, the various random draws such as exponential, normal, logistic, Bernoulli and other distributions are obtained by transforming the uniform random draws.

Thus, it is important to consider how to generate a uniform random number.

However, generally there is no way to generate exact uniform random draws.

As shown in Ripley (1987) and Ross (1997), a deterministic sequence that appears at random is taken as a sequence of random numbers.

First, consider the following relation:

$$m = k - [k/n]n,$$

where k, m and n are integers.

$[k/n]$ denotes the largest integer less than or equal to the argument.

In Fortran 77, it is written as `m=k-int(k/n)*n`, where $0 \leq m < n$.

m indicates the **remainder (余り)** when k is divided by n.

n is called the **modulus (商)**.

We define the right hand side in the equation above as:

$$k - [k/n]n \equiv k \bmod n.$$

Then, using the modular arithmetic we can rewrite the above equation as follows:

$$m = k \bmod n,$$

which is represented by: `m=mod(k,n)` in Fortran 77 and `m=k%n` in C language.

A basic idea of the uniform random draw is as follows.

Given x_{i-1}, x_i is generated by:

$$x_i = (ax_{i-1} + c) \bmod n,$$

where $0 \leq x_i < n$.

a and c are positive integers, called the **multiplier** and the **increment**, respectively.

The generator above have to be started by an initial value, which is called the **seed**.

$u_i = x_i/n$ is regarded as a uniform random number between zero and one.

This generator is called the **linear congruential generator (線形合同法)**.

Especially, when $c = 0$, the generator is called the **multiplicative linear congruential generator**.

This method was proposed by Lehmer in 1948 (see Lehmer, 1951).

If n, a and c are properly chosen, the period of the generator is n.

However, when they are not chosen very carefully, there may be a lot of serial correlation among the generated values.

Therefore, the performance of the congruential generators depend heavily on the choice of (a, c).

There is a great amount of literature on uniform random number generation.

See, for example, Fishman (1996), Gentle (1998), Kennedy and Gentle (1980), Law and Kelton (2000), Niederreiter (1992), Ripley (1987), Robert and Casella (1999), Rubinstein and Melamed (1998), Thompson (2000) and so on for the other congruential generators.

However, we introduce only two uniform random number generators.

Wichmann and Hill (1982 and corrigendum, 1984) describe a combination of three congruential generators for 16-bit computers.

The generator is given by:

$$x_i = 171x_{i-1} \bmod 30269,$$

$$y_i = 172y_{i-1} \bmod 30307,$$

$$z_i = 170z_{i-1} \bmod 30323,$$

and

$$u_i = \left(\frac{x_i}{30269} + \frac{y_i}{30307} + \frac{z_i}{30323}\right) \bmod 1.$$

We need to set three seeds, i.e., x_0, y_0 and z_0, for this random number generator.

u_i is regarded as a uniform random draw within the interval between zero and one.

The period is of the order of 10^{12} (more precisely the period is 6.95×10^{12}).

The source code of this generator is given by `urnd16(ix,iy,iz,rn)`, where `ix`, `iy` and `iz` are seeds and `rn` represents the uniform random number between zero and one.

`urnd16(ix,iy,iz,rn)`

```
1:        subroutine urnd16(ix,iy,iz,rn)
2: c
3: c  Input:
4: c    ix, iy, iz:  Seeds
5: c  Output:
6: c    rn: Uniform Random Draw U(0,1)
7: c
8:      1 ix=mod( 171*ix,30269 )
9:        iy=mod( 172*iy,30307 )
10:       iz=mod( 170*iz,30323 )
11:       rn=ix/30269.+iy/30307.+iz/30323.
12:       rn=rn-int(rn)
13:       if( rn.le.0 ) go to 1
14:       return
15:       end
```

We exclude one in Line 12 and zero in Line 13 from rn.

That is, $0 <$ rn < 1 is generated in urnd16(ix,iy,iz,rn).

Zero and one in the uniform random draw sometimes cause the complier errors in programming, when the other random draws are derived based on the transformation of the uniform random variable.

De Matteis and Pagnutti (1993) examine the Wichmann-Hill generator with respect to the higher order autocorrelations in sequences, and conclude that the Wichmann-Hill generator performs well.

For 32-bit computers, L'Ecuyer (1988) proposed a combination of k congruential generators that have prime moduli n_j, such that all values of $(n_j - 1)/2$ are relatively prime, and with multipliers that yield full periods.

Let the sequence from jth generator be $x_{j,1}, x_{j,2}, x_{j,3}, \cdots$.

Consider the case where each individual generator j is a maximum-period multiplicative linear congruential generator with modulus n_j and multiplier a_j, i.e.,

$$x_{j,i} \equiv a_j x_{j,i-1} \bmod n_j.$$

Assuming that the first generator is a relatively good one and that n_1 is fairly large, we form the ith integer in the sequence as:

$$x_i = \sum_{j=1}^{k} (-1)^{j-1} x_{j,i} \bmod (n_1 - 1),$$

where the other moduli n_j, $j = 2, 3, \cdots, k$, do not need to be large.

The normalization takes care of the possibility of zero occurring in this sequence:

$$u_i = \begin{cases} \dfrac{x_i}{n_1}, & \text{if } x_i > 0, \\ \dfrac{n_1 - 1}{n_1}, & \text{if } x_i = 0. \end{cases}$$

As for each individual generator j, note as follows.

Define $q = [n/a]$ and $r \equiv n \bmod a$, i.e., n is decomposed as $n = aq + r$, where $r < a$.

Therefore, for $0 < x < n$, we have:

$$\begin{aligned} ax \bmod n &= (ax - [x/q]n) \bmod n \\ &= \Big(ax - [x/q](aq + r)\Big) \bmod n \\ &= \Big(a(x - [x/q]q) - [x/q]r\Big) \bmod n \\ &= \Big(a(x \bmod q) - [x/q]r\Big) \bmod n. \end{aligned}$$

Practically, L'Ecuyer (1988) suggested combining two multiplicative congruential generators, where $k = 2$, $(a_1, n_1, q_1, r_1) = (40014, 2147483563, 53668, 12211)$ and $(a_2, n_2, q_2, r_2) = (40692, 2147483399, 52774, 3791)$ are chosen.

Two seeds are required to implement the generator.

The source code is shown in `urnd(ix,iy,rn)`, where `ix` and `iy` are inputs, i.e., seeds, and `rn` is an output, i.e., a uniform random number between zero and one.

urnd(ix,iy,rn)

```
      subroutine urnd(ix,iy,rn)
c
c  Input:
c    ix, iy:  Seeds
c  Output:
c    rn: Uniform Random Draw U(0,1)
c
     1 kx=ix/53668
       ix=40014*(ix-kx*53668)-kx*12211
       if(ix.lt.0) ix=ix+2147483563
c
       ky=iy/52774
       iy=40692*(iy-ky*52774)-ky*3791
       if(iy.lt.0) iy=iy+2147483399
c
       rn=ix-iy
       if( rn.lt.1.) rn=rn+2147483562
       rn=rn*4.656613e-10
       if( rn.le.0.) go to 1
c
       return
       end
```

The period of the generator proposed by L'Ecuyer (1988) is of the order of 10^{18} (more precisely

2.31×10^{18}), which is quite long and practically long enough.

L'Ecuyer (1988) presents the results of both theoretical and empirical tests, where the above generator performs well.

Furthermore, L'Ecuyer (1988) gives an additional portable generator for 16-bit computers.

Also, see L'Ecuyer(1990, 1998).

To improve the length of period, the above generator proposed by L'Ecuyer (1988) is combined with the shuffling method suggested by Bays and Durham (1976), and it is introduced as `ran2` in Press, Teukolsky, Vetterling and Flannery (1992a, 1992b).

However, from relatively long period and simplicity of the source code, hereafter the subroutine `urnd(ix,iy,rn)` is utilized for the uniform random number generation method, and we will obtain various random draws based on the uniform random draws.

11.6.2 Transforming $U(0, 1)$: Continuous Type

In this section, we focus on a continuous type of distributions, in which density functions are derived from the uniform distribution $U(0, 1)$ by transformation of variables.

Normal Distribution: $N(0,1)$**:** The normal distribution with mean zero and variance one, i.e, the standard normal distribution, is represented by:

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2},$$

for $-\infty < x < \infty$.

Mean, variance and the moment-generating function are given by:

$$\mathrm{E}(X) = 0, \qquad \mathrm{V}(X) = 1, \qquad \phi(\theta) = \exp\left(\frac{1}{2}\theta^2\right).$$

The normal random variable is constructed using two independent uniform random variables.

This transformation is well known as the Box-Muller (1958) transformation and is shown as follows.

Let U_1 and U_2 be uniform random variables between zero and one.

Suppose that U_1 is independent of U_2.

Consider the following transformation:

$$\begin{aligned} X_1 &= \sqrt{-2\log(U_1)}\cos(2\pi U_2), \\ X_2 &= \sqrt{-2\log(U_1)}\sin(2\pi U_2). \end{aligned}$$

where we have $-\infty < X_1 < \infty$ and $-\infty < X_2 < \infty$ when $0 < U_1 < 1$ and $0 < U_2 < 1$.

Then, the inverse transformation is given by:

$$u_1 = \exp\left(-\frac{x_1^2 + x_2^2}{2}\right), \qquad u_2 = \frac{1}{2\pi} \arctan \frac{x_2}{x_1}.$$

We perform transformation of variables in multivariate cases.

From this transformation, the Jacobian is obtained as:

$$\begin{aligned} J &= \begin{vmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} \end{vmatrix} = \begin{vmatrix} -x_1 \exp\left(-\frac{1}{2}(x_1^2 + x_2^2)\right) & -x_2 \exp\left(-\frac{1}{2}(x_1^2 + x_2^2)\right) \\ \frac{1}{2\pi} \frac{-x_2}{x_1^2 + x_2^2} & \frac{1}{2\pi} \frac{x_1}{x_1^2 + x_2^2} \end{vmatrix} \\ &= -\frac{1}{2\pi} \exp\left(-\frac{1}{2}(x_1^2 + x_2^2)\right). \end{aligned}$$

Let $f_x(x_1, x_2)$ be the joint density of X_1 and X_2 and $f_u(u_1, u_2)$ be the joint density of U_1 and U_2.

Since U_1 and U_2 are assumed to be independent, we have the following:

$$f_u(u_1, u_2) = f_1(u_1) f_2(u_2) = 1,$$

where $f_1(u_1)$ and $f_2(u_2)$ are the density functions of U_1 and U_2, respectively.

Note that $f_1(u_1) = f_2(u_2) = 1$ because U_1 and U_2 are uniform random variables between zero and one.

Accordingly, the joint density of X_1 and X_2 is:

$$\begin{aligned} f_x(x_1, x_2) &= |J| f_u\Big(\exp(-\frac{x_1^2 + x_2^2}{2}), \frac{1}{2\pi} \arctan \frac{x_2}{x_1}\Big) \\ &= \frac{1}{2\pi} \exp\Big(-\frac{1}{2}(x_1^2 + x_2^2)\Big) \\ &= \frac{1}{\sqrt{2\pi}} \exp\Big(-\frac{1}{2}x_1^2\Big) \times \frac{1}{\sqrt{2\pi}} \exp\Big(-\frac{1}{2}x_2^2\Big), \end{aligned}$$

which is a product of two standard normal distributions.

Thus, X_1 and X_2 are mutually independently distributed as normal random variables with mean zero and variance one.

See Hogg and Craig (1995, pp.177 – 178).

The source code of the standard normal random number generator shown above is given by `snrnd(ix,iy,r`

snrnd(ix,iy,rn)

```
1:          subroutine snrnd(ix,iy,rn)
2:  c
```

```
3: c  Use "snrnd(ix,iy,rn)"
4: c  together with "urnd(ix,iy,rn)".
5: c
6: c  Input:
7: c    ix, iy:  Seeds
8: c  Output:
9: c    rn: Standard Normal Random Draw N(0,1)
10: c
11:       pi= 3.1415926535897932385
12:       call urnd(ix,iy,rn1)
13:       call urnd(ix,iy,rn2)
14:       rn=sqrt(-2.0*log(rn1))*sin(2.0*pi*rn2)
15:       return
16:       end
```

`snrnd(ix,iy,rn)` should be used together with the uniform random number generator `urnd(ix,iy,rn)` shown in Section 11.6.1 (p.290).

`rn` in `snrnd(ix,iy,rn)` corresponds to X_2.

Conventionally, one of X_1 and X_2 is taken as the random number which we use.

Here, X_1 is excluded from consideration.

`snrnd(ix,iy,rn)` includes the sine, which takes a lot of time computationally.

Therefore, to avoid computation of the sine, various algorithms have been invented (Ahrens and Dieter (1988), Fishman (1996), Gentle (1998), Marsaglia, MacLaren and Bray (1964) and so on).

Standard Normal Probabilities When $X \sim N(0,1)$, we have the case where we want to approximate p such that $p = F(x)$ given x, where $F(x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t = P(X < x)$.

Adams (1969) reports that

$$P(X > x) = \int_x^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}t^2}\,\mathrm{d}t = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}\left(\frac{1}{x+}\frac{1}{x+}\frac{2}{x+}\frac{3}{x+}\frac{4}{x+}\cdots\right),$$

for $x > 0$, where the form in the parenthesis is called the continued fraction, which is defined as follows:

$$\frac{a_1}{x_1+}\frac{a_2}{x_2+}\frac{a_3}{x_3+}\cdots = \cfrac{a_1}{x_1 + \cfrac{a_2}{x_2 + \cfrac{a_3}{x_3 + \cdots}}}.$$

A lot of approximations on the continued fraction shown above have been proposed.

See Kennedy and Gentle (1980), Marsaglia (1964) and Marsaglia and Zaman (1994).

Here, we introduce the following approximation (see Takeuchi (1989)):

$$P(X > x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}(b_1 t + b_2 t^2 + b_3 t^3 + b_4 t^4 + b_5 t^5), \qquad t = \frac{1}{1 + a_0 x},$$

$$a_0 = 0.2316419, \quad b_1 = 0.319381530, \quad b_2 = -0.356563782,$$
$$b_3 = 1.781477937, \quad b_4 = -1.821255978, \quad b_5 = 1.330274429.$$

In `snprob(x,p)` below, $P(X < x)$ is shown.

That is, `p` up to Line 19 is equal to $P(X > x)$ in `snprob(x,p)`.

In Line 20, $P(X < x)$ is obtained.

`snprob(x,p)`

```
1:        subroutine snprob(x,p)
2:  C
3:  C  Input:
4:  C    x:  N(0,1) Percent Point
5:  C  Output:
6:  C    p:  Probability corresponding to x
7:  C
8:        pi= 3.1415926535897932385
9:        a0= 0.2316419
10:       b1= 0.319381530
11:       b2=-0.356563782
12:       b3= 1.781477937
13:       b4=-1.821255978
14:       b5= 1.330274429
```

```
15: C
16:       z=abs(x)
17:       t=1.0/(1.0+a0*z)
18:       pr=exp(-.5*z*z)/sqrt(2.0*pi)
19:       p=pr*t*(b1+t*(b2+t*(b3+t*(b4+b5*t))))
20:       if(x.gt.0.0) p=1.0-p
21: C
22:       return
23:       end
```

The maximum error of approximation of p is 7.5×10^{-8}, which practically gives us enough precision.

Standard Normal Percent Points When $X \sim N(0, 1)$, we approximate x such that $p = F(x)$ given p, where $F(x)$ indicates the standard normal cumulative distribution function, i.e., $F(x) = P(X < x)$, and p denotes probability.

As shown in Odeh and Evans (1974), the approximation of a percent point is of the form:

$$x = y + \frac{S_4(y)}{T_4(y)} = y + \frac{p_0 + p_1 y + p_2 y^2 + p_3 y^3 + p_4 y^4}{q_0 + q_1 y + q_2 y^2 + q_3 y^3 + q_4 y^4},$$

where $y = \sqrt{-2 \log(p)}$.

$S_4(y)$ and $T_4(y)$ denote polynomials degree 4.

The source code is shown in `snperpt(p,x)`, where x is obtained within $10^{-20} < p < 1 - 10^{-20}$.

snperpt(p,x)

```
      subroutine snperpt(p,x)
c
c  Input:
c    p:  Probability
c       (err<p<1-err, where err=1e-20)
c  Output:
c    x:  N(0,1) Percent Point corresponding to p
c
       p0=-0.322232431088
       p1=-1.0
       p2=-0.342242088547
       p3=-0.204231210245e-1
       p4=-0.453642210148e-4
       q0= 0.993484626060e-1
       q1= 0.588581570495
       q2= 0.531103462366
       q3= 0.103537752850
       q4= 0.38560700634O-2
       ps=p
       if( ps.gt.0.5 ) ps=1.0-ps
       if( ps.eq.0.5 ) x=0.0
       y=sqrt( -2.0*log(ps) )
       x=y+((((y*p4+p3)*y+p2)*y+p1)*y+p0)
      &   /((((y*q4+q3)*y+q2)*y+q1)*y+q0)
```

```
25:         if( p.lt.0.5 ) x=-x
26:         return
27:         end
```

The maximum error of approximation of x is 1.5×10^{-8} if the function is evaluated in double precision and 1.8×10^{-6} if it is evaluated in single precision.

The approximation of the form $x = y + S_2(y)/T_3(y)$ by Hastings (1955) gives a maximum error of 4.5×10^{-4}.

To improve accuracy of the approximation, Odeh and Evans (1974) proposed the algorithm above.

Normal Distribution: $N(\mu, \sigma^2)$: The normal distribution denoted by $N(\mu, \sigma^2)$ is represented as follows:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2},$$

for $-\infty < x < \infty$.

μ is called a **location parameter** and σ^2 is a **scale parameter**.

Mean, variance and the moment-generating function of the normal distribution $N(\mu, \sigma^2)$ are given by:

$$\mathrm{E}(X) = \mu, \qquad \mathrm{V}(X) = \sigma^2, \qquad \phi(\theta) = \exp\left(\mu\theta + \frac{1}{2}\sigma^2\theta^2\right).$$

When $\mu = 0$ and $\sigma^2 = 1$ are taken, the above density function reduces to the standard normal distribution in Section 11.6.2.

$X = \sigma Z + \mu$ is normally distributed with mean μ and variance σ^2, when $Z \sim N(0, 1)$.

Therefore, the source code is represented by `nrnd(ix,iy,ave,var,rn)`, where `ave` and `var` correspond to μ and σ^2, respectively.

`nrnd(ix,iy,ave,var,rn)`

```
1:        subroutine nrnd(ix,iy,ave,var,rn)
2: c
3: c  Use "nrnd(ix,iy,ave,var,rn)"
4: c  together with "urnd(ix,iy,rn)"
5: c            and  "snrnd(ix,iy,rn)".
6: c
7: c  Input:
8: c    ix, iy:  Seeds
9: c    ave: Mean
```

```
c     var: Variance
c   Output:
c     rn: Normal Random Draw N(ave,var)
c
        call snrnd(ix,iy,rn1)
        rn=ave+sqrt(var)*rn1
        return
        end
```

`nrnd(ix,iy,ave,var,rn)` should be used together with `urnd(ix,iy,rn)` and `snrnd(ix,iy,rn)`.

It is possible to replace `snrnd(ix,iy,rn)` by `snrnd2(ix,iy,rn)` or `snrnd3(ix,iy,rn)`.

Exponential Distribution: The exponential distribution with parameter β is written as:

$$f(x) = \begin{cases} \frac{1}{\beta} e^{-\frac{x}{\beta}}, & \text{for } 0 < x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

for $\beta > 0$.

β indicates a scale parameter.

Mean, variance and the moment-generating function are obtained as follows:

$$\mathrm{E}(X) = \beta, \qquad \mathrm{V}(X) = \beta^2, \qquad \phi(\theta) = \frac{1}{1-\beta\theta}.$$

The relation between the exponential random variable the uniform random variable is shown as follows:

When $U \sim U(0,1)$, consider the following transformation:

$$X = -\beta \log(U).$$

Then, X is an exponential distribution with parameter β.

Because the transformation is given by $u = \exp(-x/\beta)$, the Jacobian is:

$$J = \frac{\mathrm{d}u}{\mathrm{d}x} = -\frac{1}{\beta}\exp\left(-\frac{1}{\beta}x\right).$$

By transforming the variables, the density function of X is represented as:

$$f(x) = |J| f_u\left(\exp(-\frac{1}{\beta}x)\right) = \frac{1}{\beta}\exp\left(-\frac{1}{\beta}x\right),$$

where $f(\cdot)$ and $f_u(\cdot)$ denote the probability density functions of X and U, respectively.

Note that $0 < x < \infty$ because of $x = -\beta \log(u)$ and $0 < u < 1$.

Thus, the exponential distribution with parameter β is obtained from the uniform random draw between zero and one.

exprnd(ix,iy,beta,rn)

```
      subroutine exprnd(ix,iy,beta,rn)
C
C  Use "exprnd(ix,iy,beta,rn)"
C  together with "urnd(ix,iy,rn)".
C
C  Input:
C    ix, iy:  Seeds
C    beta: Parameter
C  Output:
C    rn: Exponential Random Draw
C        with Parameter beta
C
       call urnd(ix,iy,rn1)
       rn=-beta*log(rn1)
       return
       end
```

`exprnd(ix,iy,beta,rn)` should be used together with `urnd(ix,iy,rn)`.

When $\beta = 2$, the exponential distribution reduces to the chi-square distribution with 2 degrees of freedom.

Gamma Distribution: $G(\alpha,\beta)$: The gamma distribution with parameters α and β, denoted by $G(\alpha,\beta)$, is represented as follows:

$$f(x) = \begin{cases} \dfrac{1}{\beta^{\alpha}\Gamma(\alpha)} x^{\alpha-1} e^{-\frac{x}{\beta}}, & \text{for } 0 < x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

for $\alpha > 0$ and $\beta > 0$, where α is called a **shape parameter** and β denotes a scale parameter.

$\Gamma(\cdot)$ is called the **gamma function**, which is the following function of α:

$$\Gamma(\alpha) = \int_0^{\infty} x^{\alpha-1} e^{-x}\, \mathrm{d}x.$$

The gamma function has the following features:

$$\Gamma(\alpha+1) = \alpha\Gamma(\alpha), \qquad \Gamma(1) = 1, \qquad \Gamma\left(\frac{1}{2}\right) = 2\Gamma\left(\frac{3}{2}\right) = \sqrt{\pi}.$$

Mean, variance and the moment-generating function are given by:

$$\mathrm{E}(X) = \alpha\beta, \qquad \mathrm{V}(X) = \alpha\beta^2, \qquad \phi(\theta) = \frac{1}{(1-\beta\theta)^{\alpha}}.$$

The gamma distribution with $\alpha = 1$ is equivalent to the exponential distribution shown in Section 11.6.2.

This fact is easily checked by comparing both moment-generating functions.

Now, utilizing the uniform random variable, the gamma distribution with parameters α and β are derived as follows.

The derivation shown in this section deals with the case where α is a positive integer, i.e., $\alpha = 1, 2, 3, \cdots$.

The random variables Z_1, Z_2, $\cdots$, Z_α are assumed to be mutually independently distributed as exponential random variables with parameter β, which are shown in Section 11.6.2.

Define $X = \sum_{i=1}^{\alpha} Z_i$.

Then, X has distributed as a gamma distribution with parameters α and β, where α should be an

integer, which is proved as follows:

$$\phi_x(\theta) = \mathrm{E}(e^{\theta X}) = \mathrm{E}(e^{\theta \sum_{i=1}^{\alpha} Z_i}) = \prod_{i=1}^{\alpha} \mathrm{E}(e^{\theta Z_i}) = \prod_{i=1}^{\alpha} \phi_i(\theta) = \prod_{i=1}^{\alpha} \frac{1}{1-\beta\theta}$$
$$= \frac{1}{(1-\beta\theta)^{\alpha}},$$

where $\phi_x(\theta)$ and $\phi_i(\theta)$ represent the moment-generating functions of X and Z_i, respectively.

Thus, sum of the α exponential random variables yields the gamma random variable with parameters α and β.

Therefore, the source code which generates gamma random numbers is shown in `gammarnd(ix,iy,alpha`

gammarnd(ix,iy,alpha,beta,rn)

```
1:        subroutine gammarnd(ix,iy,alpha,beta,rn)
2: c
3: c  Use "gammarnd(ix,iy,alpha,beta,rn)"
4: c  together with "exprnd(ix,iy,beta,rn)"
5: c            and  "urnd(ix,iy,rn)".
6: c
7: c  Input:
8: c    ix, iy:   Seeds
```

```
c    alpha:    Shape Parameter (which should be an integer)
c    beta:     Scale Parameter
c  Output:
c    rn: Gamma Random Draw with alpha and beta
c
       rn=0.0
        do 1 i=1,nint(alpha)
       call exprnd(ix,iy,beta,rn1)
     1 rn=rn+rn1
       return
       end
```

`gammarnd(ix,iy,alpha,beta,rn)` is utilized together with `urnd(ix,iy,rn)` and `exprnd(ix,iy,rn)`

As pointed out above, α should be an integer in the source code.

When α is large, we have serious problems computationally in the above algorithm, because α exponential random draws have to be generated to obtain one gamma random draw with parameters α and β.

When $\alpha = k/2$ and $\beta = 2$, the gamma distribution reduces to the chi-square distribution with k degrees of freedom.

Chi-Square Distribution: $\chi^2(k)$: The chi-square distribution with k degrees of freedom, denoted by $\chi^2(k)$, is written as follows:

$$f(x) = \begin{cases} \dfrac{1}{2^{k/2}\Gamma\left(\frac{k}{2}\right)} x^{\frac{k}{2}-1} e^{-\frac{1}{2}x}, & \text{for } 0 < x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

where k is a positive integer.

The chi-square distribution is equivalent to the gamma distribution with $\beta = 2$ and $\alpha = k/2$.

The chi-square distribution with $k = 2$ reduces to the exponential distribution with $\beta = 2$, shown in Section 11.6.2.

Mean, variance and the moment-generating function are given by:

$$\mathrm{E}(X) = k, \qquad \mathrm{V}(X) = 2k, \qquad \phi(\theta) = \frac{1}{(1-2\theta)^{k/2}}.$$

F Distribution: $F(m, n)$: The F distribution with m and n degrees of freedom, denoted by $F(m, n)$, is represented as:

$$f(x) = \begin{cases} \dfrac{\Gamma\left(\frac{m+n}{2}\right)}{\Gamma\left(\frac{m}{2}\right)\Gamma\left(\frac{n}{2}\right)}\left(\dfrac{m}{n}\right)^{\frac{m}{2}} x^{\frac{m}{2}-1}\left(1+\dfrac{m}{n}x\right)^{-\frac{m+n}{2}}, & \text{for } 0 < x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

where m and n are positive integers.

Mean and variance are given by:

$$\mathrm{E}(X) = \frac{n}{n-2}, \qquad \text{for } n > 2,$$
$$\mathrm{V}(X) = \frac{2n^2(m+n-2)}{m(n-2)^2(n-4)}, \qquad \text{for } n > 4.$$

The moment-generating function of F distribution does not exist.

One F random variable is derived from two chi-square random variables.

Suppose that U and V are independently distributed as chi-square random variables, i.e., $U \sim \chi^2(m)$ and $V \sim \chi^2(n)$.

Then, it is shown that $X = \dfrac{U/m}{V/n}$ has a F distribution with (m, n) degrees of freedom.

***t* Distribution: $t(k)$:** The t distribution (or Student's t distribution) with k degrees of freedom, denoted by $t(k)$, is given by:

$$f(x) = \frac{\Gamma\left(\frac{k+1}{2}\right)}{\Gamma\left(\frac{k}{2}\right)} \frac{1}{\sqrt{k\pi}} \left(1 + \frac{x^2}{k}\right)^{-\frac{k+1}{2}},$$

for $-\infty < x < \infty$, where k does not have to be an integer but conventionally it is a positive integer.

When k is small, the t distribution has fat tails.

The t distribution with $k = 1$ is equivalent to the Cauchy distribution.

As k goes to infinity, the t distribution approaches the standard normal distribution, i.e., $t(\infty) = N(0, 1)$, which is easily shown by using the definition of e, i.e.,

$$\left(1 + \frac{x^2}{k}\right)^{-\frac{k+1}{2}} = \left(1 + \frac{1}{h}\right)^{-\frac{hx^2+1}{2}} = \left(\left(1 + \frac{1}{h}\right)^{h}\right)^{-\frac{1}{2}x^2} \left(1 + \frac{1}{h}\right)^{-\frac{1}{2}} \longrightarrow e^{-\frac{1}{2}x^2},$$

where $h = k/x^2$ is set and h goes to infinity (equivalently, k goes to infinity).

Thus, a kernel of the t distribution is equivalent to that of the standard normal distribution.

Therefore, it is shown that as k is large the t distribution approaches the standard normal distribution.

Mean and variance of the t distribution with k degrees of freedom are obtained as:

$$\mathrm{E}(X) = 0, \qquad \text{for } k > 1,$$

$$\mathrm{V}(X) = \frac{k}{k-2}, \qquad \text{for } k > 2.$$

In the case of the t distribution, the moment-generating function does not exist, because all the moments do not necessarily exist.

For the t random variable X, we have the fact that $\mathrm{E}(X^p)$ exists when p is less than k.

Therefore, all the moments exist only when k is infinity.

One t random variable is obtained from chi-square and standard normal random variables.

Suppose that $Z \sim N(0, 1)$ is independent of $U \sim \chi^2(k)$.

Then, $X = Z/\sqrt{U/k}$ has a t distribution with k degrees of freedom.

Marsaglia (1984) gives a very fast algorithm for generating t random draws, which is based on a transformed acceptance/rejection method, which will be discussed later.

11.6.3 Inverse Transform Method

In Section 11.6.2, we have introduced the probability density functions which can be derived by transforming the uniform random variables between zero and one.

In this section, the probability density functions obtained by the inverse transform method are presented and the corresponding random number generators are shown.

The inverse transform method is represented as follows.

Let X be a random variable which has a cumulative distribution function $F(\cdot)$.

When $U \sim U(0,1)$, $F^{-1}(U)$ is equal to X.

The proof is obtained from the following fact:

$$P(X < x) = P\Big(F^{-1}(U) < x\Big) = P\Big(U < F(x)\Big) = F(x).$$

In other words, let u be a random draw of U, where $U \sim U(0,1)$, and $F(\cdot)$ be a distribution function of X.

When we perform the following inverse transformation:

$$x = F^{-1}(u),$$

x implies the random draw generated from $F(\cdot)$.

The inverse transform method shown above is useful when $F(\cdot)$ can be computed easily and the inverse distribution function, i.e., $F^{-1}(\cdot)$, has a closed form.

For example, recall that $F(\cdot)$ cannot be obtained explicitly in the case of the normal distribution because the integration is included in the normal cumulative distribution (conventionally we approximate the normal cumulative distribution when we want to evaluate it).

If no closed form of $F^{-1}(\cdot)$ is available but $F(\cdot)$ is still computed easily, an iterative method such as the Newton-Raphson method can be applied.

Define $k(x) = F(x) - u$.

The first order Taylor series expansion around $x = x^*$ is:

$$0 = k(x) \approx k(x^*) + k'(x^*)(x - x^*).$$

Then, we obtain:

$$x = x^* - \frac{k(x^*)}{k'(x^*)} = x^* - \frac{F(x^*) - u}{f(x^*)}.$$

Replacing x and x^* by $x^{(i)}$ and $x^{(i-1)}$, we have the following iteration:

$$x^{(i)} = x^{(i-1)} - \frac{F(x^{(i-1)}) - u}{f(x^{(i-1)})},$$

for $i = 1, 2, \cdots$.

The convergence value of $x^{(i)}$ is taken as a solution of equation $u = F(x)$.

Thus, based on u, a random draw x is derived from $F(\cdot)$.

However, we should keep in mind that this procedure takes a lot of time computationally, because we need to repeat the convergence computation shown above as many times as we want to generate.

11.6.4 Using $U(0, 1)$: Discrete Type

In Sections 11.6.2 and 11.6.3, the random number generators from continuous distributions are discussed, i.e., the transformation of variables in Section 11.6.2 and the inverse transform method in Section 11.6.3 are utilized.

Based on the uniform random draw between zero and one, in this section we deal with some discrete distributions and consider generating their random numbers.

As a representative random number generation method, we can consider utilizing the inverse transform method in the case of discrete random variables.

Suppose that a discrete random variable X can take $x_1, x_2, \cdots, x_n$, where the probability which X takes x_i is given by $f(x_i)$, i.e., $P(X = x_i) = f(x_i)$.

Generate a uniform random draw u, which is between zero and one.

Consider the case where we have $F(x_{i-1}) \leq u < F(x_i)$, where $F(x_i) = P(X \leq x_i)$ and $F(x_0) = 0$.

Then, the random draw of X is given by x_i.

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11.7 Sampling Method II: Random Number Generation

11.7.1 Rejection Sampling (棄却法)

We want to generate random draws from $f(x)$, called the **target density (目的密度)**, but we consider the case where it is hard to sample from $f(x)$.

Now, suppose that it is easy to generate a random draw from another density $f_*(x)$, called the **sampling density (サンプリング密度)** or **proposal density (提案密度)**.

In this case, random draws of X from $f(x)$ are generated by utilizing the random draws sampled from $f_*(x)$.

Let x be the the random draw of X generated from $f(x)$.

Suppose that $q(x)$ is equal to the ratio of the target density and the sampling density, i.e.,

$$q(x) = \frac{f(x)}{f_*(x)}. \tag{19}$$

Then, the target density is rewritten as:

$$f(x) = q(x)f_*(x).$$

Based on $q(x)$, the acceptance probability is obtained.

Depending on the structure of the acceptance probability, we have three kinds of sampling techniques, i.e., **rejection sampling (棄却法)** in this section, **importance resampling (重点的リサンプリング法)** in Section 11.7.2 and the **Metropolis-Hastings algorithm (メトロポリスーハスティング・アルゴリズム)** in Section 11.7.4.

See Liu (1996) for a comparison of the three sampling methods.

Thus, to generate random draws of x from $f(x)$, the functional form of $q(x)$ should be known and random draws have to be easily generated from $f_*(x)$.

In order for rejection sampling to work well, the following condition has to be satisfied:

$$q(x) = \frac{f(x)}{f_*(x)} < c,$$

where c is a fixed value.

That is, $q(x)$ has an upper limit.

As discussed below, $1/c$ is equivalent to the acceptance probability.

If the acceptance probability is large, rejection sampling computationally takes a lot of time.

Under the condition $q(x) < c$ for all x, we may minimize c.

That is, since we have $q(x) < \sup_x q(x) \leq c$, we may take the supremum of $q(x)$ for c.

Thus, in order for rejection sampling to work efficiently, c should be the supremum of $q(x)$ with respect to x, i.e., $c = \sup_x q(x)$.

Let x^* be the random draw generated from $f_*(x)$, which is a candidate of the random draw generated from $f(x)$.

Define $\omega(x)$ as:

$$\omega(x) = \frac{q(x)}{\sup_z q(z)} = \frac{q(x)}{c},$$

which is called the **acceptance probability** (採択確率).

Note that we have $0 \leq \omega(x) \leq 1$ when $\sup_z q(z) = c < \infty$.

The supremum $\sup_z q(z) = c$ has to be finite.

This condition is sometimes too restrictive, which is a crucial problem in rejection sampling.

A random draw of X is generated from $f(x)$ in the following way:

(i) Generate x^* from $f_*(x)$ and compute $\omega(x^*)$.

(ii) Set $x = x^*$ with probability $\omega(x^*)$ and go back to (i) otherwise.

In other words, generating u from a uniform distribution between zero and one, take $x = x^*$ if $u \leq \omega(x^*)$ and go back to (i) otherwise.

The above random number generation procedure can be justified as follows.

Let U be the uniform random variable between zero and one, X be the random variable generated from the target density $f(x)$,

X^* be the random variable generated from the sampling density $f_*(x)$, and x^* be the realization (i.e., the random draw) generated from the sampling density $f_*(x)$.

Consider the probability $P\Big(X \leq x | U \leq \omega(x^*)\Big)$, which should be the cumulative distribution of X, $F(x)$, from Step (ii).

The probability $P\Big(X \le x | U \le \omega(x^*)\Big)$ is rewritten as follows:

$$P\Big(X \le x | U \le \omega(x^*)\Big) = \frac{P\Big(X \le x, U \le \omega(x^*)\Big)}{P\Big(U \le \omega(x^*)\Big)},$$

where the numerator is represented as:

$$\begin{aligned} P\Big(X \le x, U \le \omega(x^*)\Big) &= \int_{-\infty}^{x} \int_{0}^{\omega(t)} f_{u,*}(u,t)\, \mathrm{d}u\, \mathrm{d}t = \int_{-\infty}^{x} \int_{0}^{\omega(t)} f_u(u) f_*(t)\, \mathrm{d}u\, \mathrm{d}t \\ &= \int_{-\infty}^{x} \Big(\int_{0}^{\omega(t)} f_u(u)\, \mathrm{d}u \Big) f_*(t)\, \mathrm{d}t = \int_{-\infty}^{x} \Big(\int_{0}^{\omega(t)} \mathrm{d}u \Big) f_*(t)\, \mathrm{d}t \\ &= \int_{-\infty}^{x} \Big[u \Big]_{0}^{\omega(t)} f_*(t)\, \mathrm{d}t = \int_{-\infty}^{x} \omega(t) f_*(t)\, \mathrm{d}t = \int_{-\infty}^{x} \frac{q(t)}{c} f_*(t)\, \mathrm{d}t = \frac{F(x)}{c}, \end{aligned}$$

and the denominator is given by:

$$P\Big(U \le \omega(x^*)\Big) = P\Big(X \le \infty, U \le \omega(x^*)\Big) = \frac{F(\infty)}{c} = \frac{1}{c}.$$

In the numerator, $f_{u,*}(u, x)$ denotes the joint density of random variables U and X^*.

Because the random draws of U and X^* are independently generated in Steps (i) and (ii) we have $f_{u,*}(u, x) = f_u(u) f_*(x)$, where $f_u(u)$ and $f_*(x)$ denote the marginal density of U and that of X^*.

The density function of U is given by $f_u(u) = 1$, because the distribution of U is assumed to be uniform between zero and one.

Thus, the first four equalities are derived.

Furthermore, in the seventh equality of the numerator, since we have:

$$\omega(x) = \frac{q(x)}{c} = \frac{f(x)}{c f_*(x)},$$

$\omega(x) f_*(x) = f(x)/c$ is obtained.

Finally, substituting the numerator and denominator shown above, we have the following equality:

$$P\Big(X \leq x | U \leq \omega(x^*)\Big) = F(x).$$

Thus, the rejection sampling method given by Steps (i) and (ii) is justified.

The rejection sampling method is the most efficient sampling method in the sense of precision of the random draws, because using rejection sampling we can generate mutually independently distributed random draws.

However, for rejection sampling we need to obtain the c which is greater than or equal to the supremum of $q(x)$.

If the supremum is infinite, i.e., if c is infinite, $\omega(x)$ is zero and accordingly the candidate x^* is never accepted in Steps (i) and (ii).

Moreover, as for another remark, note as follows.

Let N_R be the average number of the rejected random draws.

We need $(1 + N_R)$ random draws in average to generate one random number from $f(x)$.

In other words, the acceptance rate is given by $1/(1 + N_R)$ in average, which is equal to $1/c$ in average because of $P\Big(U \leq \omega(x^*)\Big) = 1/c$.

Therefore, to obtain one random draw from $f(x)$, we have to generate $(1 + N_R)$ random draws from $f_*(x)$ in average.

See, for example, Boswell, Gore, Patil and Taillie (1993), O'Hagan (1994) and Geweke (1996) for rejection sampling.

To examine the condition that $\omega(x)$ is greater than zero, i.e., the condition that the supremum of $q(x)$ exists, consider the case where $f(x)$ and $f_*(x)$ are distributed as $N(\mu, \sigma^2)$ and $N(\mu_*, \sigma_*^2)$, respectively.

$q(x)$ is given by:

$$
\begin{aligned}
q(x) = \frac{f(x)}{f_*(x)} &= \frac{(2\pi\sigma^2)^{-1/2}\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)}{(2\pi\sigma_*^2)^{-1/2}\exp\left(-\frac{1}{2\sigma_*^2}(x-\mu_*)^2\right)} \\
&= \frac{\sigma_*}{\sigma}\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2 + \frac{1}{2\sigma_*^2}(x-\mu_*)^2\right) \\
&= \frac{\sigma_*}{\sigma}\exp\left(-\frac{1}{2}\frac{\sigma_*^2-\sigma^2}{\sigma^2\sigma_*^2}\left(x - \frac{\mu\sigma_*^2-\mu_*\sigma^2}{\sigma_*^2-\sigma^2}\right)^2 + \frac{1}{2}\frac{(\mu-\mu_*)^2}{\sigma_*^2-\sigma^2}\right).
\end{aligned}
$$

If $\sigma_*^2 < \sigma^2$, $q(x)$ goes to infinity as x is large.

In the case of $\sigma_*^2 > \sigma^2$, the supremum of $q(x)$ exists, which condition implies that $f_*(x)$ should be more broadly distributed than $f(x)$.

In this case, the supremum is obtained as:

$$
c = \sup_x q(x) = \frac{\sigma_*}{\sigma}\exp\left(\frac{1}{2}\frac{(\mu-\mu_*)^2}{\sigma_*^2-\sigma^2}\right).
$$

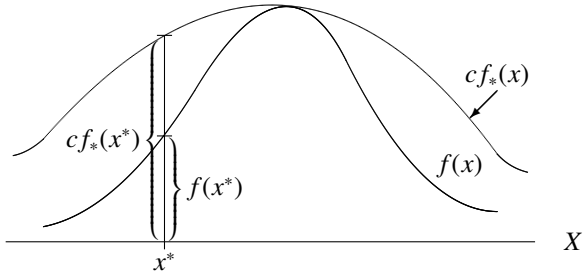
When $\sigma^2 = \sigma_*^2$ and $\mu = \mu_*$, we have $q(x) = 1$, which implies $\omega(x) = 1$.

That is, a random draw from the sampling density $f_*(x)$ is always accepted as a random draw from the target density $f(x)$, where $f(x)$ is equivalent to $f_*(x)$ for all x.

If $\sigma^2 = \sigma_*^2$ and $\mu \neq \mu_*$, the supremum of $q(x)$ does not exists.

Accordingly, the rejection sampling method does not work in this case.

Figure 1: Rejection Sampling



From the definition of $\omega(x)$, we have the inequality $f(x) \leq cf_*(x)$.

$cf_*(x)$ and $f(x)$ are displayed in Figure 1.

The ratio of $f(x^*)$ and $cf_*(x^*)$ corresponds to the acceptance probability at x^*, i.e., $\omega(x^*)$.

Thus, for rejection sampling, $cf_*(x)$ has to be greater than or equal to $f(x)$ for all x, which implies that

the sampling density $f_*(x)$ needs to be more widely distributed than the target density $f(x)$.

Finally, note that the above discussion holds without any modification even though $f(x)$ is a kernel of the target density, i.e., even though $f(x)$ is proportional to the target density, because the constant term is canceled out between the numerator and denominator (remember that $\omega(x) = q(x)/\sup_z q(z)$).

Normal Distribution: $N(0, 1)$: First, denote the half-normal distribution by:

$$f(x) = \begin{cases} \dfrac{2}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}, & \text{for } 0 \leq x < \infty, \\ 0, & \text{otherwise.} \end{cases}$$

The half-normal distribution above corresponds to the positive part of the standard normal probability density function.

Using rejection sampling, we consider generating standard normal random draws based on the half-normal distribution.

We take the sampling density as the exponential distribution:

$$f_*(x) = \begin{cases} \lambda e^{-\lambda x}, & \text{for } 0 \leq x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

where $\lambda > 0$. Since $q(x)$ is defined as $q(x) = f(x)/f_*(x)$, the supremum of $q(x)$ is given by:

$$c = \sup_x q(x) = \frac{2}{\lambda\sqrt{2\pi}} e^{\frac{1}{2}\lambda^2}.$$

which depends on parameter λ.

Remember that $P(U \leq \omega(x^*)) = 1/c$ corresponds to the acceptance probability.

Since we need to increase the acceptance probability to reduce computational time, we want to obtain the λ which minimizes $\sup_x q(x)$ with respect to λ.

Solving the minimization problem, $\lambda = 1$ is obtained.

Substituting $\lambda = 1$, the acceptance probability $\omega(x)$ is derived as:

$$\omega(x) = e^{-\frac{1}{2}(x-1)^2},$$

for $0 < x < \infty$.

Remember that $-\log U$ has an exponential distribution with $\lambda = 1$ when $U \sim U(0, 1)$.

Therefore, the algorithm is represented as follows.

(i) Generate two independent uniform random draws u_1 and u_2 between zero and one.

(ii) Compute $x^* = -\log u_2$, which indicates the exponential random draw generated from the target density $f_*(x)$.

(iii) Set $x = x^*$ if $u_1 \leq \exp(-\frac{1}{2}(x^* - 1)^2)$, i.e., $-2\log(u_1) \geq (x^* - 1)^2$, and return to (i) otherwise.

x in Step (iii) yields a random draw from the half-normal distribution.

To generate a standard normal random draw utilizing the half-normal random draw above, we may put the positive or negative sign randomly with x.

Therefore, the following Step (iv) is additionally put.

(iv) Generate a uniform random draw u_3 between zero and one, and set $z = x$ if $u_3 \leq 1/2$ and $z = -x$ otherwise.

z gives us a standard normal random draw.

Note that the number of iteration in Step (iii) is given by $c = \sqrt{2e/\pi} \approx 1.3155$ in average, or equivalently, the acceptance probability in Step (iii) is $1/c \approx 0.7602$.

The source code for this standard normal random number generator is shown in `snrnd6(ix,iy,rn)`.

snrnd6(ix,iy,rn)

```
      subroutine snrnd6(ix,iy,rn)
c
c  Use "snrnd6(ix,iy,rn)"
c  together with "urnd(ix,iy,rn)".
c
c  Input:
c    ix, iy:   Seeds
c  Output:
c    rn: Normal Random Draw N(0,1)
c
     1 call urnd(ix,iy,rn1)
       call urnd(ix,iy,rn2)
       y=-log(rn2)
       if( -2.*log(rn1).lt.(y-1.)**2 ) go to 1
       call urnd(ix,iy,rn3)
         if(rn3.le.0.5) then
       rn= y
         else
       rn=-y
         endif
       return
       end
```

Note that snrnd6(ix,iy,rn) should be used together with urnd(ix,iy,rn).

Thus, utilizing rejection sampling, we have the standard normal random number generator, which is based on the half-normal distribution.

Gamma Distribution: $G(\alpha, 1)$ for $0 < \alpha \leq 1$ and $1 < \alpha$: In this section, utilizing rejection sampling we show an example of generating random draws from the gamma distribution with parameters α and $\beta = 1$, i.e., $G(\alpha, 1)$.

When $X \sim G(\alpha, 1)$, the density function of X is given by:

$$f(x) = \begin{cases} \dfrac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}, & \text{for } 0 < x < \infty, \\ \\ 0, & \text{otherwise.} \end{cases}$$

Ahrens and Dieter (1974) consider the case of $0 < \alpha \leq 1$, which is discussed in this section.

The case of $\alpha > 1$ will be discussed later.

Using the rejection sampling, the composition method and the inverse transform method, we consider generating random draws from $G(\alpha, 1)$ for $0 < \alpha \leq 1$.

The sampling density is taken as:

$$f_*(x) = \frac{e}{\alpha + e} \alpha x^{\alpha-1} I_1(x) + \frac{\alpha}{\alpha + e} e^{-x+1} I_2(x),$$

where both $I_1(x)$ and $I_2(x)$ denote the indicator functions defined as:

$$I_1(x) = \begin{cases} 1, & \text{if } 0 < x \leq 1, \\ 0, & \text{otherwise,} \end{cases} \qquad I_2(x) = \begin{cases} 1, & \text{if } 1 < x, \\ 0, & \text{otherwise.} \end{cases}$$

Random number generation from the sampling density above utilizes the composition method and the inverse transform method.

The cumulative distribution related to $f_*(x)$ is given by:

$$F_*(x) = \begin{cases} \dfrac{e}{\alpha + e} x^{\alpha}, & \text{if } 0 < x \leq 1, \\ \dfrac{e}{\alpha + e} + \dfrac{\alpha}{\alpha + e}(1 - e^{-x+1}), & \text{if } x > 1. \end{cases}$$

Note that $0 < \alpha \leq 1$ is required because the sampling density for $0 < x \leq 1$ has to satisfy the property that the integration is equal to one.

The acceptance probability $\omega(x) = q(x)/\sup_z q(z)$ for $q(x) = f(x)/f_*(x)$ is given by:

$$\omega(x) = e^{-x} I_1(x) + x^{\alpha - 1} I_2(x).$$

Moreover, the mean number of trials until success, i.e., $c = \sup_z q(z)$ is represented as:

$$c = \frac{\alpha + e}{\alpha e \Gamma(\alpha)},$$

which depends on α and is not greater than 1.39.

Note that $q(x)$ takes a maximum value at $x = 1$.

The random number generation procedure is given by:

(i) Generate a uniform random draw u_1 from $U(0, 1)$, and set $x^* = \left((\alpha/e+1)u_1\right)^{1/\alpha}$ if $u_1 \leq e/(\alpha+e)$ and $x^* = -\log\Big((1/e + 1/\alpha)(1 - u_1)\Big)$ if $u_1 > e/(\alpha + e)$.

(ii) Obtain $\omega(x^*) = e^{-x^*}$ if $u_1 \leq e/(\alpha + e)$ and $\omega(x^*) = x^{*\alpha-1}$ if $u_1 > e/(\alpha + e)$.

(iii) Generate a uniform random draw u_2 from $U(0, 1)$, and set $x = x^*$ if $u_2 \leq \omega(x^*)$ and return to (i) otherwise.

In Step (i) a random draw x^* from $f_*(x)$ can be generated by the inverse transform method discussed in Section 11.6.3.

gammarnd2(ix,iy,alpha,rn)

```
1:        subroutine gammarnd2(ix,iy,alpha,rn)
2: c
3: c  Use "gammarnd2(ix,iy,alpha,rn)"
4: c  together with "urnd(ix,iy,rn)".
```

```
c
c  Input:
c    ix, iy: Seeds
c    alpha:  Shape Parameter (0<alpha \le 1)
c  Output:
c    rn: Gamma Random Draw
c        with Parameters alpha and beta=1
c
       e=2.71828182845905
     1 call urnd(ix,iy,rn0)
       call urnd(ix,iy,rn1)
            if( rn0.le.e/(alpha+e) ) then
       rn=( (alpha+e)*rn0/e )**(1./alpha)
       if( rn1.gt.e**(-rn) ) go to 1
            else
       rn=-log((alpha+e)*(1.-rn0)/(alpha*e))
       if( rn1.gt.rn**(alpha-1.) ) go to 1
            endif
       return
       end
```

Note that `gammarnd2(ix,iy,alpha,rn)` should be used with `urnd(ix,iy,rn)`.

In `gammarnd2(ix,iy,alpha,rn)`, the case of $0 < \alpha \leq 1$ has been shown.

Now, using rejection sampling, the case of $\alpha > 1$ is discussed in Cheng (1977, 1998).

The sampling density is chosen as the following cumulative distribution:

$$F_*(x) = \begin{cases} \dfrac{x^\lambda}{\delta + x^\lambda}, & \text{for } x > 0, \\ 0, & \text{otherwise,} \end{cases}$$

which is sometimes called the **log-logistic distribution**.

Then, the probability density function, $f_*(x)$, is given by:

$$f_*(x) = \begin{cases} \dfrac{\lambda\delta x^{\lambda-1}}{(\alpha + x^\lambda)^2}, & \text{for } x > 0, \\ 0, & \text{otherwise.} \end{cases}$$

By the inverse transform method, the random draw from $f_*(x)$, denoted by x, is generated as follows:

$$x = \left(\frac{\delta u}{1-u}\right)^{1/\lambda},$$

where u denotes the uniform random draw generated from $U(0, 1)$.

For the two parameters, $\lambda = \sqrt{2\alpha - 1}$ and $\delta = \alpha^\lambda$ are chosen, taking into account minimizing $c = \sup_x q(x) = \sup_x f(x)/f_*(x)$ with respect to δ and λ (note that λ and δ are approximately taken, since it is not possible to obtain the explicit solution of δ and λ).

Then, the number of rejections in average is given by:

$$c = \frac{4\alpha^{\alpha} e^{-\alpha}}{\Gamma(\alpha)\sqrt{2\alpha - 1}},$$

which is computed as:

1.47 when $\alpha = 1$, 1.25 when $\alpha = 2$, 1.17 when $\alpha = 5$,

1.15 when $\alpha = 10$, 1.13 when $\alpha = \infty$.

Thus, the average number of rejections is quite small for all α.

The random number generation procedure is given by:

(i) Set $a = 1/\sqrt{2\alpha - 1}$, $b = \alpha - \log 4$ and $c = \alpha + \sqrt{2\alpha - 1}$.

(ii) Generate two uniform random draws u_1 and u_2 from $U(0, 1)$.

(iii) Set $y = a \log \dfrac{u_1}{1 - u_1}$, $x^* = \alpha e^y$, $z = u_1^2 u_2$ and $r = b + cy - x$.

(iv) Take $x = x^*$ if $r \geq \log z$ and return to (ii) otherwise.

To avoid evaluating the logarithm in Step (iv), we put Step (iii)' between Steps (iii) and (iv), which is as follows:

(iii)' Take $x = x^*$ if $r \geq 4.5z - d$ and go to (iv) otherwise.

d is defined as $d = 1 + \log 4.5$, which has to be computed in Step (i).

Note that we have the relation: $\theta z - (1 + \log \theta) \geq \log z$ for all $z > 0$ and any given $\theta > 0$, because $\log z$ is a concave function of z. According to Cheng (1977), the choice of θ is not critical and the suggested value is $\theta = 4.5$, irrespective of α.

The source code for Steps (i) – (iv) and (iii)' is given by `gammarnd3(ix,iy,alpha,rn)`.

gammarnd3(ix,iy,alpha,rn)

```
      subroutine gammarnd3(ix,iy,alpha,rn)
C
C  Use "gammarnd3(ix,iy,alpha,rn)"
C  together with "urnd(ix,iy,rn)".
C
C  Input:
C    ix, iy: Seeds
C    alpha:  Shape Parameter (1<alpha)
C  Output:
C    rn: Gamma Random Draw
C        with Parameters alpha and beta=1
C
       e=2.71828182845905
       a=1./sqrt(2.*alpha-1.)
       b=alpha-log(4.)
```

```
16:       c=alpha+sqrt(2.*alpha-1.)
17:       d=1.+log(4.5)
18:     1 call urnd(ix,iy,u1)
19:       call urnd(ix,iy,u2)
20:       y=a*log(u1/(1.-u1))
21:       rn=alpha*(e**y)
22:       z=u1*u1*u2
23:       r=b+c*y-rn
24:       if( r.ge.4.5*z-d ) go to 2
25:       if( r.lt.log(z)  ) go to 1
26:     2 return
27:       end
```

Note that `gammarnd3(ix,iy,alpha,rn)` requires `urnd(ix,iy,rn)`.

Line 24 corresponds to Step (iii)', which gives us a fast acceptance.

Taking into account a recent progress of a personal computer, we can erase Lines 17 and 24 from `gammarnd3`, because evaluating the `if(...)` sentences in Lines 24 and 25 sometimes takes more time than computing the logarithm in Line 25.

Thus, using both `gammarnd2` and `gammarnd3`, we have the gamma random number generator with parameters $\alpha > 0$ and $\beta = 1$.

11.7.2 Importance Resampling (重点的リサンプリング)

The **importance resampling** method also utilizes the sampling density $f_*(x)$, where we should choose the sampling density from which it is easy to generate random draws.

Let x_i^* be the ith random draw of x generated from $f_*(x)$.

The acceptance probability is defined as:

$$\omega(x_i^*) = \frac{q(x_i^*)}{\sum_{j=1}^n q(x_j^*)},$$

where $q(\cdot)$ is represented as equation (19).

To obtain a random draws from $f(x)$, we perform the following procedure:

(i) Generate x_j^* from the sampling density $f_*(x)$ for $j = 1, 2, \cdots, n$.

(ii) Compute $\omega(x_j^*)$ for all $j = 1, 2, \cdots, n$.

(iii) Generate a uniform random draw u between zero and one and take $x = x_j^*$ when $\Omega_{j-1} \leq u < \Omega_j$, where $\Omega_j = \sum_{i=1}^j \omega(x_i^*)$ and $\Omega_0 \equiv 0$.

The x obtained in Step (iii) represents a random draw from the target density $f(x)$.

In Step (ii), all the probability weights $\omega(x_j^*)$, $j = 1, 2, \cdots, n$, have to be computed for importance resampling.

Thus, we need to generate n random draws from the sampling density $f_*(x)$ in advance.

When we want to generate more random draws (say, N random draws), we may repeat Step (iii) N times.

In the importance resampling method, there are n realizations, i.e., $x_1^*, x_2^*, \cdots, x_n^*$, which are mutually independently generated from the sampling density $f_*(x)$.

The cumulative distribution of $f(x)$ is approximated by the following empirical distribution:

$$P(X \le x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t = \int_{-\infty}^{x} \frac{f(t)}{f_*(t)} f_*(t)\,\mathrm{d}t = \frac{\int_{-\infty}^{x} q(t) f_*(t)\,\mathrm{d}t}{\int_{-\infty}^{\infty} q(t) f_*(t)\,\mathrm{d}t}$$
$$\approx \frac{(1/n)\sum_{i=1}^{n} q(x_i^*) I(x, x_i^*)}{(1/n)\sum_{j=1}^{n} q(x_j^*)} = \sum_{i=1}^{n} \omega(x_i^*) I(x, x_i^*),$$

where $I(x, x_i^*)$ denotes the indicator function which satisfies $I(x, x_i^*) = 1$ when $x \ge x_i^*$ and $I(x, x_i^*) = 0$ otherwise.

$P(X = x_i^*)$ is approximated as $\omega(x_i^*)$.

See Smith and Gelfand (1992) and Bernardo and Smith (1994) for the importance resampling proce-

dure.

As mentioned in Section 11.7.1, for rejection sampling, $f(x)$ may be a kernel of the target density, or equivalently, $f(x)$ may be proportional to the target density.

Similarly, the same situation holds in the case of importance resampling.

That is, $f(x)$ may be proportional to the target density for importance resampling, too.

To obtain a random draws from $f(x)$, importance resampling requires n random draws from the sampling density $f_*(x)$, but rejection sampling needs $(1 + N_R)$ random draws from the sampling density $f_*(x)$.

For importance resampling, when we have n different random draws from the sampling density, we pick up one of them with the corresponding probability weight.

The importance resampling procedure computationally takes a lot of time, because we have to compute all the probability weights Ω_j, $j = 1, 2, \cdots, n$, in advance even when we want only one random draw.

When we want to generate N random draws, importance resampling requires n random draws from the sampling density $f_*(x)$, but rejection sampling needs $n(1 + N_R)$ random draws from the sampling density $f_*(x)$.

Thus, as N increases, importance resampling is relatively less computational than rejection sampling. Note that $N < n$ is recommended for the importance resampling method.

In addition, when we have N random draws from the target density $f(x)$, some of the random draws take the exactly same values for importance resampling, while all the random draws take the different values for rejection sampling.

Therefore, we can see that importance resampling is inferior to rejection sampling in the sense of precision of the random draws.

Normal Distribution: $N(0, 1)$: Again, we consider an example of generating standard normal random draws based on the half-normal distribution:

$$f(x) = \begin{cases} \dfrac{2}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}, & \text{for } 0 \le x < \infty, \\ 0, & \text{otherwise.} \end{cases}$$

We take the sampling density as the following exponential distribution:

$$f_*(x) = \begin{cases} e^{-x}, & \text{for } 0 \le x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

which is exactly the same sampling density as in Section 11.7.1.

Given the random draws x_i^*, $i = 1, \cdots, n$, generated from the above exponential density $f_*(x)$, the acceptance probability $\omega(x_i^*)$ is given by:

$$\omega(x_i^*) = \frac{q(x_i^*)}{\sum_{j=1}^n q(x_j^*)} = \frac{f(x_i^*)/f_*(x_i^*)}{\sum_{j=1}^n f(x_j^*)/f_*(x_j^*)} = \frac{\exp(-\frac{1}{2}x_i^{*2} + x_i^*)}{\sum_{j=1}^n \exp(-\frac{1}{2}x_j^{*2} + x_j^*)}.$$

Therefore, a random draw from the half-normal distribution is generated as follows.

(i) Generate uniform random draws $u_1, u_2, \cdots, u_n$ from $U(0, 1)$.

(ii) Obtain $x_i^* = -\log(u_i)$ for $i = 1, 2, \cdots, n$.

(iii) Compute $\omega(x_i^*)$ for $i = 1, 2, \cdots, n$.

(iv) Generate a uniform random draw v_1 from $U(0, 1)$.

(v) Set $x = x_j^*$ when $\Omega_{j-1} \leq v_1 < \Omega_j$ for $\Omega_j = \sum_{i=1}^j \omega(x_i^*)$ and $\Omega_0 = 0$.

x is taken as a random draw generated from the half-normal distribution $f(x)$.

In order to have a standard normal random draw, we additionally put the following step.

(vi) Generate a uniform random draw v_2 from $U(0, 1)$, and set $z = x$ if $v_2 \leq 1/2$ and $z = -x$ otherwise.

z represents a standard normal random draw.

Note that Step (vi) above corresponds to Step (iv) in Section 11.7.1.

Steps (i) – (vi) shown above represent the generator which yields one standard normal random draw.

When we want N standard normal random draws, Steps (iv) – (vi) should be repeated N times.

In Steps (iv) and (v), a random draw from $f(x)$ is generated based on Ω_j for $j = 1, 2, \cdots, n$.

Gamma Distribution: $G(\alpha, 1)$ for $0 < \alpha \leq 1$: When $X \sim G(\alpha, 1)$, the density function of X is given by:

$$f(x) = \begin{cases} \dfrac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}, & \text{for } 0 < x < \infty, \\ 0, & \text{otherwise.} \end{cases}$$

The sampling density is taken as:

$$f_*(x) = \frac{e}{\alpha + e} \alpha x^{\alpha-1} I_1(x) + \frac{\alpha}{\alpha + e} e^{-x+1} I_2(x),$$

which is the same function as in `gammarnd2` of Section 11.7.1, where both $I_1(x)$ and $I_2(x)$ denote the indicator functions defined in Section 11.7.1.

The probability weights are given by:

$$\omega(x_i^*) = \frac{q(x_i^*)}{\sum_{j=1}^n q(x_j^*)} = \frac{f(x_i^*)/f_*(x_i^*)}{\sum_{j=1}^n f(x_j^*)/f_*(x_j^*)}$$

$$= \frac{x_i^{*\alpha-1}e^{-x_i^*}/\left(x_i^{*\alpha-1}I_1(x_i^*) + e^{-x_i^*}I_2(x_i^*)\right)}{\sum_{j=1}^n x_j^{*\alpha-1}e^{-x_j^*}/\left(x_j^{*\alpha-1}I_1(x_j^*) + e^{-x_j^*}I_2(x_j^*)\right)},$$

for $i = 1, 2, \cdots, n$.

The cumulative distribution function of $f_*(x)$ is represented as:

$$F_*(x) = \begin{cases} \dfrac{e}{\alpha+e}x^\alpha, & \text{if } 0 < x \le 1, \\ \dfrac{e}{\alpha+e} + \dfrac{\alpha}{\alpha+e}(1 - e^{-x+1}), & \text{if } x > 1. \end{cases}$$

Therefore, x_i^* can be generated by utilizing both the composition method and the inverse transform method.

Given x_i^*, compute $\omega(x_i^*)$ for $i = 1, 2, \cdots, n$, and take $x = x_i^*$ with probability $\omega(x_i^*)$.

Summarizing above, the random number generation procedure for the gamma distribution is given by:

(i) Generate uniform random draws u_i, $i = 1, 2, \cdots, n$, from $U(0, 1)$, and set $x_i^* = \left((\alpha/e + 1)u_i\right)^{1/\alpha}$

and $\omega(x_i^*) = e^{-x_i^*}$ if $u_i \le e/(\alpha + e)$ and take $x_i^* = -\log\Big((1/e + 1/\alpha)(1 - u_i)\Big)$ and $\omega(x_i^*) = x_i^{*\alpha-1}$ if $u_i > e/(\alpha + e)$ for $i = 1, 2, \cdots, n$.

(ii) Compute $\Omega_i = \sum_{j=1}^{i} \omega(x_j^*)$ for $i = 1, 2, \cdots, n$, where $\Omega_0 = 0$.

(iii) Generate a uniform random draw v from $U(0, 1)$, and take $x = x_i^*$ when $\Omega_{i-1} \le v < \Omega_i$.

As mentioned above, this algorithm yields one random draw.

If we want N random draws, Step (iii) should be repeated N times.

Beta Distribution: The beta distribution with parameters α and β is of the form:

$$f(x) = \begin{cases} \dfrac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}, & \text{for } 0 < x < 1, \\ 0, & \text{otherwise.} \end{cases}$$

The sampling density is taken as:

$$f_*(x) = \begin{cases} 1, & \text{for } 0 < x < 1, \\ 0, & \text{otherwise,} \end{cases}$$

which represents the uniform distribution between zero and one.

The probability weights $\omega(x_i^*)$, $i = 1, 2, \cdots, n$, are given by:

$$\omega(x_i^*) = \frac{q(x_i^*)}{\sum_{j=1}^n q(x_j^*)} = \frac{f(x_i^*)/f_*(x_i^*)}{\sum_{j=1}^n f(x_j^*)/f_*(x_j^*)} = \frac{x_i^{*\alpha-1}(1-x_i^*)^{\beta-1}}{\sum_{j=1}^n x_j^{*\alpha-1}(1-x_j^*)^{\beta-1}}.$$

Therefore, to generate a random draw from $f(x)$, first generate x_i^*, $i = 1, 2, \cdots, n$, from $U(0, 1)$, second compute $\omega(x_i^*)$ for $i = 1, 2, \cdots$,n, and finally take $x = x_i^*$ with probability $\omega(x_i^*)$.

We have shown three examples of the importance resampling procedure in this section.

One of the advantages of importance resampling is that it is really easy to construct a Fortran source code.

However, the disadvantages are that (i) importance resampling takes quite a long time because we have to obtain all the probability weights in advance and (ii) importance resampling requires a great amount of storages for x_i^* and Ω_i for $i = 1, 2, \cdots, n$.

11.7.3 Metropolis-Hastings Algorithm (メトロポリスーハスティングス・アルゴリズム)

This section is based on Geweke and Tanizaki (2003), where three sampling distributions are compared with respect to precision of the random draws from the target density $f(x)$.

The **Metropolis-Hastings algorithm** is also one of the sampling methods to generate random draws from any target density $f(x)$, utilizing sampling density $f_*(x)$, even in the case where it is not easy to generate random draws from the target density.

Let us define the acceptance probability by:

$$\omega(x_{i-1}, x^*) = \min\left(\frac{q(x^*)}{q(x_{i-1})}, 1\right) = \min\left(\frac{f(x^*)/f_*(x^*)}{f(x_{i-1})/f_*(x_{i-1})}, 1\right),$$

where $q(\cdot)$ is defined as equation (19).

By the Metropolis-Hastings algorithm, a random draw from $f(x)$ is generated in the following way:

(i) Take the initial value of x as x_{-M}.

(ii) Generate x^* from $f_*(x)$ and compute $\omega(x_{i-1}, x^*)$ given x_{i-1}.

(iii) Set $x_i = x^*$ with probability $\omega(x_{i-1}, x^*)$ and $x_i = x_{i-1}$ otherwise.

(iv) Repeat Steps (ii) and (iii) for $i = -M + 1, -M + 2, \cdots, 1$.

In the above algorithm, x_1 is taken as a random draw from $f(x)$.

When we want more random draws (say, N), we replace Step (iv) by Step (iv)', which is represented as follows:

(iv)' Repeat Steps (ii) and (iii) for $i = -M + 1, -M + 2, \cdots, N$.

When we implement Step (iv)', we can obtain a series of random draws x_{-M}, x_{-M+1}, $\cdots$, x_0, x_1, x_2, $\cdots$, x_N, where x_{-M}, x_{-M+1}, $\cdots$, x_0 are discarded from further consideration.

The last N random draws are taken as the random draws generated from the target density $f(x)$.

Thus, N denotes the number of random draws.

M is sometimes called the **burn-in period**.

We can justify the above algorithm given by Steps (i) – (iv) as follows.

The proof is very similar to the case of rejection sampling in Section 11.7.1.

We show that x_i is the random draw generated from the target density $f(x)$ under the assumption x_{i-1} is generated from $f(x)$.

Let U be the uniform random variable between zero and one, X be the random variable which has the density function $f(x)$ and x^* be the realization (i.e., the random draw) generated from the sampling density $f_*(x)$.

Consider the probability $P\Big(X \leq x | U \leq \omega(x_{i-1}, x^*)\Big)$, which should be the cumulative distribution of X, i.e., $F(x)$.

The probability $P\Big(X \le x | U \le \omega(x_{i-1}, x^*)\Big)$ is rewritten as follows:

$$P\Big(X \le x | U \le \omega(x_{i-1}, x^*)\Big) = \frac{P\Big(X \le x, U \le \omega(x_{i-1}, x^*)\Big)}{P\Big(U \le \omega(x_{i-1}, x^*)\Big)},$$

where the numerator is represented as:

$$\begin{aligned}
P\Big(X \le x, U \le \omega(x_{i-1}, x^*)\Big) &= \int_{-\infty}^{x} \int_{0}^{\omega(x_{i-1},t)} f_{u,*}(u,t)\, \mathrm{d}u\, \mathrm{d}t \\
&= \int_{-\infty}^{x} \int_{0}^{\omega(x_{i-1},t)} f_u(u) f_*(t)\, \mathrm{d}u\, \mathrm{d}t = \int_{-\infty}^{x} \Big(\int_{0}^{\omega(x_{i-1},t)} f_u(u)\, \mathrm{d}u \Big) f_*(t)\, \mathrm{d}t \\
&= \int_{-\infty}^{x} \Big(\int_{0}^{\omega(x_{i-1},t)} \mathrm{d}u \Big) f_*(t)\, \mathrm{d}t = \int_{-\infty}^{x} \Big[u \Big]_{0}^{\omega(x_{i-1},t)} f_*(t)\, \mathrm{d}t \\
&= \int_{-\infty}^{x} \omega(x_{i-1}, t) f_*(t)\, \mathrm{d}t = \int_{-\infty}^{x} \frac{f_*(x_{i-1}) f(t)}{f(x_{i-1})}\, \mathrm{d}t = \frac{f_*(x_{i-1})}{f(x_{i-1})} F(x)
\end{aligned}$$

and the denominator is given by:

$$P\Big(U \le \omega(x_{i-1}, x^*)\Big) = P\Big(X \le \infty, U \le \omega(x_{i-1}, x^*)\Big) = \frac{f_*(x_{i-1})}{f(x_{i-1})} F(\infty) = \frac{f_*(x_{i-1})}{f(x_{i-1})}.$$

The density function of U is given by $f_u(u) = 1$ for $0 < u < 1$.

Let X^* be the random variable which has the density function $f_*(x)$.

In the numerator, $f_{u,*}(u, x)$ denotes the joint density of random variables U and X^*.

Because the random draws of U and X^* are independently generated, we have $f_{u,*}(u, x) = f_u(u)f_*(x) = f_*(x)$.

Thus, the first four equalities are derived.

Substituting the numerator and denominator shown above, we have the following equality:

$$P\Big(X \leq x | U \leq \omega(x_{i-1}, x^*)\Big) = F(x).$$

Thus, the x^* which satisfies $u \leq \omega(x_{i-1}, x^*)$ indicates a random draw from $f(x)$.

We set $x_i = x_{i-1}$ if $u \leq \omega(x_{i-1}, x^*)$ is not satisfied. x_{i-1} is already assumed to be a random draw from $f(x)$.

Therefore, it is shown that x_i is a random draw from $f(x)$.

See Gentle (1998) for the discussion above.

As in the case of rejection sampling and importance resampling, note that $f(x)$ may be a kernel of the target density, or equivalently, $f(x)$ may be proportional to the target density.

The same algorithm as Steps (i) – (iv) can be applied to the case where $f(x)$ is proportional to the target density, because $f(x^*)$ is divided by $f(x_{i-1})$ in $\omega(x_{i-1}, x^*)$.

As a general formulation of the sampling density, instead of $f_*(x)$, we may take the sampling density as the following form: $f_*(x|x_{i-1})$, where a candidate random draw x^* depends on the $(i-1)$th random draw, i.e., x_{i-1}.

For choice of the sampling density $f_*(x|x_{i-1})$, Chib and Greenberg (1995) pointed out as follows.

$f_*(x|x_{i-1})$ should be chosen so that the chain travels over the support of $f(x)$, which implies that $f_*(x|_{i-1})$ should not have too large variance and too small variance, compared with $f(x)$.

See, for example, Smith and Roberts (1993), Bernardo and Smith (1994), O'Hagan (1994), Tierney (1994), Geweke (1996), Gamerman (1997), Robert and Casella (1999) and so on for the Metropolis-Hastings algorithm.

As an alternative justification, note that the Metropolis-Hastings algorithm is formulated as follows:

$$f_i(u) = \int f^*(u|v) f_{i-1}(v)\, \mathrm{d}v,$$

where $f^*(u|v)$ denotes the transition distribution, which is characterized by Step (iii).

x_{i-1} is generated from $f_{i-1}(\cdot)$ and x_i is from $f^*(\cdot|x_{i-1})$.

x_i depends only on x_{i-1}, which is called the **Markov property**.

The sequence $\{\cdots, x_{i-1}, x_i, x_{i+1}, \cdots\}$ is called the **Markov chain**.

The Monte Carlo statistical methods with the sequence $\{\cdots, x_{i-1}, x_i, x_{i+1}, \cdots\}$ is called the **Markov chain Monte Carlo (MCMC)**.

From Step (iii), $f^*(u|v)$ is given by:

$$f^*(u|v) = \omega(v,u)f_*(u|v) + \left(1 - \int \omega(v,u)f_*(u|v)\,\mathrm{d}u\right)p(u), \tag{20}$$

where $p(x)$ denotes the following probability function:

$$p(u) = \begin{cases} 1, & \text{if } u = v, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, x is generated from $f_*(u|v)$ with probability $\omega(v,u)$ and from $p(u)$ with probability $1-\int \omega(v,u)f_*(u|v)$ c

Now, we want to show $f_i(u) = f_{i-1}(u) = f(u)$ as i goes to infinity, which implies that both x_i and x_{i-1} are generated from the invariant distribution function $f(u)$ for sufficiently large i.

To do so, we need to consider the condition satisfying the following equation:

$$f(u) = \int f^*(u|v)f(v)\,\mathrm{d}v. \tag{21}$$

Equation (21) holds if we have the following equation:

$$f^*(v|u)f(u) = f^*(u|v)f(v), \tag{22}$$

which is called the **reversibility condition**.

By taking the integration with respect to v on both sides of equation (22), equation (21) is obtained.

Therefore, we have to check whether the $f^*(u|v)$ shown in equation (20) satisfies equation (22).

It is straightforward to verify that

$$\omega(v,u)f_*(u|v)f(v) = \omega(u,v)f_*(v|u)f(u),$$
$$\Big(1 - \int \omega(v,u)f_*(u|v)\,\mathrm{d}u\Big)p(u)f(v) = \Big(1 - \int \omega(u,v)f_*(v|u)\,\mathrm{d}v\Big)p(v)f(u).$$

Thus, as i goes to infinity, x_i is a random draw from the target density $f(\cdot)$.

If x_i is generated from $f(\cdot)$, then x_{i+1} is also generated from $f(\cdot)$.

Therefore, all the x_i, x_{i+1}, x_{i+2}, $\cdots$ are taken as random draws from the target density $f(\cdot)$.

The requirement for uniform convergence of the Markov chain is that the chain should be **irreducible** and **aperiodic**.

See, for example, Roberts and Smith (1993).

Let $C_i(x_0)$ be the set of possible values of x_i from starting point x_0.

If there exist two possible starting values, say x^* and x^{**}, such that $C_i(x^*) \cap C_i(x^{**}) = \emptyset$ (i.e., empty set) for all i, then the same limiting distribution cannot be reached from both starting points.

Thus, in the case of $C_i(x^*) \cap C_i(x^{**}) = \emptyset$, the convergence may fail.

A Markov chain is said to be **irreducible** if there exists an i such that $P(x_i \in C|x_0) > 0$ for any starting point x_0 and any set C such that $\int_C f(x)\,\mathrm{d}x > 0$.

The irreducible condition ensures that the chain can reach all possible x values from any starting point.

Moreover, as another case in which convergence may fail, if there are two disjoint set C^1 and C^2 such that $x_{i-1} \in C^1$ implies $x_i \in C^2$ and $x_{i-1} \in C^2$ implies $x_i \in C^1$, then the chain oscillates between C^1 and C^2 and we again have $C_i(x^*) \cap C_i(x^{**}) = \emptyset$ for all i when $x^* \in C^1$ and $x^{**} \in C^2$.

Accordingly, we cannot have the same limiting distribution in this case, either.

It is called **aperiodic** if the chain does not oscillate between two sets C^1 and C^2 or cycle around a partition $C^1, C^2, \cdots, C^r$ of r disjoint sets for $r > 2$.

See O'Hagan (1994) for the discussion above.

For the Metropolis-Hastings algorithm, x_1 is taken as a random draw of x from $f(x)$ for sufficiently large M.

To obtain N random draws, we need to generate $M + N$ random draws.

Moreover, clearly we have $\mathrm{Cov}(x_{i-1}, x_i) > 0$, because x_i is generated based on x_{i-1} in Step (iii).

Therefore, for precision of the random draws, the Metropolis-Hastings algorithm gives us the worst

random number of the three sampling methods. i.e., rejection sampling in Section 11.7.1, importance resampling in Section 11.7.2 and the Metropolis-Hastings algorithm in this section.

Based on Steps (i) – (iii) and (iv)', under some conditions the basic result of the Metropolis-Hastings algorithm is as follows:

$$\frac{1}{N}\sum_{i=1}^{N} g(x_i) \longrightarrow \mathrm{E}\Big(g(x)\Big) = \int g(x)f(x)\,\mathrm{d}x, \qquad \text{as } N \longrightarrow \infty,$$

where $g(\cdot)$ is a function, which is representatively taken as $g(x) = x$ for mean and $g(x) = (x - \overline{x})^2$ for variance.

$\overline{x}$ denotes $\overline{x} = (1/N)\sum_{i=1}^{N} x_i$.

Thus, it is shown that $(1/N)\sum_{i=1}^{N} g(x_i)$ is a consistent estimate of $\mathrm{E}\Big(g(x)\Big)$, even though $x_1, x_2, \cdots, x_N$ are mutually correlated.

As an alternative random number generation method to avoid the positive correlation, we can perform the case of $N = 1$ as in the above procedures (i) – (iv) N times in parallel, taking different initial values for x_{-M}.

In this case, we need to generate $M + 1$ random numbers to obtain one random draw from $f(x)$.

That is, N random draws from $f(x)$ are based on $N(1 + M)$ random draws from $f_*(x|x_{i-1})$.

Thus, we can obtain mutually independently distributed random draws.

For precision of the random draws, the alternative Metropolis-Hastings algorithm should be similar to rejection sampling.

However, this alternative method is too computer-intensive, compared with the above procedures (i) – (iii) and (iv)', which takes more time than rejection sampling in the case of $M > N_R$.

Furthermore, the sampling density has to satisfy the following conditions:

(i) we can quickly and easily generate random draws from the sampling density and

(ii) the sampling density should be distributed with the same range as the target density.

See, for example, Geweke (1992) and Mengersen, Robert and Guihenneuc-Jouyaux (1999) for the MCMC convergence diagnostics.

Since the random draws based on the Metropolis-Hastings algorithm heavily depend on choice of the sampling density, we can see that the Metropolis-Hastings algorithm has the problem of specifying the sampling density, which is the crucial criticism.

Several generic choices of the sampling density are discussed by Tierney (1994) and Chib and Greenberg (1995).

We can consider several candidates for the sampling density $f_*(x|x_{i-1})$, i.e., Sampling Densities I – III.

3.4.1.1 Sampling Density I (Independence Chain)

For the sampling density, we have started with $f_*(x)$ in this section.

Thus, one possibility of the sampling density is given by: $f_*(x|x_{i-1}) = f_*(x)$, where $f_*(\cdot)$ does not depend on x_{i-1}.

This sampling density is called the **independence chain**.

For example, it is possible to take $f_*(x) = N(\mu_*, \sigma_*^2)$, where μ_* and σ_*^2 are the hyper-parameters.

Or, when x lies on a certain interval, say (a, b), we can choose the uniform distribution $f_*(x) = 1/(b-a)$ for the sampling density.

3.4.1.2 Sampling Density II (Random Walk Chain)

We may take the sampling density called the **random walk chain**, i.e., $f_*(x|x_{i-1}) = f_*(x - x_{i-1})$.

Representatively, we can take the sampling density as $f_*(x|x_{i-1}) = N(x_{i-1}, \sigma_*^2)$, where σ_*^2 denotes the hyper-parameter.

Based on the random walk chain, we have a series of the random draws which follow the random walk

process.

3.4.1.3 Sampling Density III (Taylored Chain)

The alternative sampling distribution is based on approximation of the log-kernel (see Geweke and Tanizaki (1999, 2001, 2003)), which is a substantial extension of the **Taylored chain** discussed in Chib, Greenberg and Winkelmann (1998).

Let $p(x) = \log(f(x))$, where $f(x)$ may denote the kernel which corresponds to the target density.

Approximating the log-kernel $p(x)$ around x_{i-1} by the second order Taylor series expansion, $p(x)$ is represented as:

$$p(x) \approx p(x_{i-1}) + p'(x_{i-1})(x - x_{i-1}) + \frac{1}{2}p''(x_{i-1})(x - x_{i-1})^2, \tag{23}$$

where $p'(\cdot)$ and $p''(\cdot)$ denote the first- and second-derivatives.

Depending on the values of $p'(x)$ and $p''(x)$, we have the four cases, i.e., Cases 1 – 4, which are classified by (i) $p''(x) < -\epsilon$ in Case 1 or $p''(x) \geq -\epsilon$ in Cases 2 – 4 and (ii) $p'(x) < 0$ in Case 2, $p'(x) > 0$ in Case 3 or $p'(x) = 0$ in Case 4.

Geweke and Tanizaki (2003) suggested introducing ϵ into the Taylored chain discussed in Geweke and Tanizaki (1999, 2001).

Note that $\epsilon = 0$ is chosen in Geweke and Tanizaki (1999, 2001).

To improve precision of random draws, ϵ should be a positive value, which will be discussed later in detail (see Remark 1 for ϵ).

Case 1: $p''(x_{i-1}) < -\epsilon$: Equation (23) is rewritten by:

$$p(x) \approx p(x_{i-1}) - \frac{1}{2}\left(\frac{1}{-1/p''(x_{i-1})}\right)\left(x - (x_{i-1} - \frac{p'(x_{i-1})}{p''(x_{i-1})})\right)^2 + r(x_{i-1}),$$

where $r(x_{i-1})$ is an appropriate function of x_{i-1}.

Since $p''(x_{i-1})$ is negative, the second term in the right-hand side is equivalent to the exponential part of the normal density.

Therefore, $f_*(x|x_{i-1})$ is taken as $N(\mu_*, \sigma_*^2)$, where $\mu_* = x_{i-1} - p'(x_{i-1})/p''(x_{i-1})$ and $\sigma_*^2 = -1/p''(x_{i-1})$.

Case 2: $p''(x_{i-1}) \geq -\epsilon$ **and** $p'(x_{i-1}) < 0$: Perform linear approximation of $p(x)$.

Let x^+ be the nearest mode with $x^+ < x_{i-1}$.

Then, $p(x)$ is approximated by a line passing between x^+ and x_{i-1}, which is written as:

$$p(x) \approx p(x^+) + \frac{p(x^+) - p(x_{i-1})}{x^+ - x_{i-1}}(x - x^+).$$

From the second term in the right-hand side, the sampling density is represented as the exponential distribution with $x > x^+ - d$, i.e., $f_*(x|x_{i-1}) = \lambda \exp\Big(-\lambda\Big(x - (x^+ - d)\Big)\Big)$ if $x^+ - d < x$ and $f_*(x|x_{i-1}) = 0$ otherwise, where λ is defined as:

$$\lambda = \left|\frac{p(x^+) - p(x_{i-1})}{x^+ - x_{i-1}}\right|.$$

d is a positive value, which will be discussed later (see Remark 2 for d).

Thus, a random draw x^* from the sampling density is generated by $x^* = w + (x^+ - d)$, where w represents the exponential random variable with parameter λ.

Case 3: $p''(x_{i-1}) \geq -\epsilon$ and $p'(x_{i-1}) > 0$: Similarly, perform linear approximation of $p(x)$ in this case.

Let x^+ be the nearest mode with $x_{i-1} < x^+$.

Approximation of $p(x)$ is exactly equivalent to that of Case 2.

Taking into account $x < x^+ + d$, the sampling density is written as: $f_*(x|x_{i-1}) = \lambda \exp\Big(-\lambda\Big((x^+ + d) - x\Big)\Big)$ if $x < x^+ + d$ and $f_*(x|x_{i-1}) = 0$ otherwise.

Thus, a random draw x^* from the sampling density is generated by $x^* = (x^+ + d) - w$, where w is distributed as the exponential random variable with parameter λ.

Case 4: $p''(x_{i-1}) \geq -\epsilon$ and $p'(x_{i-1}) = 0$: In this case, $p(x)$ is approximated as a uniform distribution at the neighborhood of x_{i-1}.

As for the range of the uniform distribution, we utilize the two appropriate values x^+ and x^{++}, which satisfies $x^+ < x < x^{++}$.

When we have two modes, x^+ and x^{++} may be taken as the modes.

Thus, the sampling density $f_*(x|x_{i-1})$ is obtained by the uniform distribution on the interval between x^+ and x^{++}, i.e., $f_*(x|x_{i-1}) = 1/(x^{++} - x^+)$ if $x^+ < x < x^{++}$ and $f_*(x|x_{i-1}) = 0$ otherwise.

Thus, for approximation of the kernel, all the possible cases are given by Cases 1 – 4, depending on the values of $p'(\cdot)$ and $p''(\cdot)$.

Moreover, in the case where x is a vector, applying the procedure above to each element of x, Sampling III is easily extended to multivariate cases.

Finally, we discuss about ϵ and d in the following remarks.

Remark 1: ϵ in Cases 1 – 4 should be taken as an appropriate positive number.

It may seem more natural to take $\epsilon = 0$, rather than $\epsilon > 0$.

The reason why $\epsilon > 0$ is taken is as follows.

Consider the case of $\epsilon = 0$.

When $p''(x_{i-1})$ is negative and it is very close to zero, variance σ_*^2 in Case 1 becomes extremely large because of $\sigma_*^2 = -1/p''(x_{i-1})$.

In this case, the obtained random draws are too broadly distributed and accordingly they become unrealistic, which implies that we have a lot of outliers.

To avoid this situation, ϵ should be positive.

It might be appropriate that ϵ should depend on variance of the target density, because ϵ should be small if variance of the target density is large.

Thus, in order to reduce a number of outliers, $\epsilon > 0$ is recommended.

Remark 2: For d in Cases 2 and 3, note as follows.

As an example, consider the unimodal density in which we have Cases 2 and 3.

Let x^+ be the mode.

We have Case 2 in the right-hand side of x^+ and Case 3 in the left-hand side of x^+.

In the case of $d = 0$, we have the random draws generated from either Case 2 or 3.

In this situation, the generated random draw does not move from one case to another.

In the case of $d > 0$, however, the distribution in Case 2 can generate a random draw in Case 3.

That is, for positive d, the generated random draw may move from one case to another, which implies that the irreducibility condition of the MH algorithm is guaranteed.

Normal Distribution: $N(0, 1)$: As in Sections 11.7.1 and 11.7.2, we consider an example of generating standard normal random draws based on the half-normal distribution:

$$f(x) = \begin{cases} \dfrac{2}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}, & \text{for } 0 \le x < \infty, \\ 0, & \text{otherwise.} \end{cases}$$

As in Sections 11.7.1 and 11.7.2, we take the sampling density as the following exponential distribution:

$$f_*(x) = \begin{cases} e^{-x}, & \text{for } 0 \le x < \infty, \\ 0, & \text{otherwise,} \end{cases}$$

which is the independence chain, i.e., $f_*(x|x_{i-1}) = f_*(x)$.

Then, the acceptance probability $\omega(x_{i-1}, x^*)$ is given by:

$$\begin{aligned}\omega(x_{i-1}, x^*) &= \min\left(\frac{f(x^*)/f_*(x^*)}{f(x_{i-1})/f_*(x_{i-1})}, 1\right) \\ &= \min\left(\exp(-\frac{1}{2}x^{*2} + x^* + \frac{1}{2}x_{i-1}^2 - x_{i-1}), 1\right).\end{aligned}$$

Utilizing the Metropolis-Hastings algorithm, the standard normal random number generator is shown as follows:

(i) Take an appropriate initial value of x as x_{-M} (for example, $x_{-M} = 0$).

(ii) Set $y_{i-1} = |x_{i-1}|$.

(iii) Generate a uniform random draw u_1 from $U(0, 1)$ and compute $\omega(y_{i-1}, y^*)$ where $y^* = -\log(u_1)$.

(iv) Generate a uniform random draw u_2 from $U(0, 1)$, and set $y_i = y^*$ if $u_2 \leq \omega(y_{i-1}, y^*)$ and $y_i = y_{i-1}$ otherwise.

(v) Generate a uniform random draw u_3 from $U(0, 1)$, and set $x_i = y_i$ if $u_3 \leq 0.5$ and $x_i = -y_i$ otherwise.

(vi) Repeat Steps (ii) – (v) for $i = -M + 1, -M + 2, \cdots, 1$.

y_1 is taken as a random draw from $f(x)$. M denotes the burn-in period.

If a lot of random draws (say, N random draws) are required, we replace Step (vi) by Step (vi)' represented as follows:

(vi)' Repeat Steps (ii) – (v) for $i = -M+1, -M+2, \cdots, N$.

In Steps (ii) – (iv), a half-normal random draw is generated.

Note that the absolute value of x_{i-1} is taken in Step (ii) because the half-normal random draw is positive.

In Step (v), the positive or negative sign is randomly assigned to y_i.

Gamma Distribution: $G(\alpha, 1)$ for $0 < \alpha \leq 1$: When $X \sim G(\alpha, 1)$, the density function of X is given by:

$$f(x) = \begin{cases} \dfrac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}, & \text{for } 0 < x < \infty, \\ 0, & \text{otherwise.} \end{cases}$$

As in `gammarnd2` of Sections 11.7.1 and `gammarnd4` of 11.7.2, the sampling density is taken as:

$$f_*(x) = \frac{e}{\alpha + e} \alpha x^{\alpha-1} I_1(x) + \frac{\alpha}{\alpha + e} e^{-x+1} I_2(x),$$

where both $I_1(x)$ and $I_2(x)$ denote the indicator functions defined in Section 11.7.1.

Then, the acceptance probability is given by:

$$\omega(x_{i-1}, x^*) = \min\left(\frac{q(x^*)}{q(x_{i-1})}, 1\right) = \min\left(\frac{f(x^*)/f_*(x^*)}{f(x_{i-1})/f_*(x_{i-1})}, 1\right)$$

$$= \min\left(\frac{x^{*\alpha-1}e^{-x^*}/\left(x^{*\alpha-1}I_1(x^*) + e^{-x^*}I_2(x^*)\right)}{x_{i-1}^{\alpha-1}e^{-x_{i-1}}/\left(x_{i-1}^{\alpha-1}I_1(x_{i-1}) + e^{-x_{i-1}}I_2(x_{i-1})\right)}, 1\right).$$

As shown in Section 11.7.1, the cumulative distribution function of $f_*(x)$ is represented as:

$$F_*(x) = \begin{cases} \dfrac{e}{\alpha+e}x^\alpha, & \text{if } 0 < x \le 1, \\ \dfrac{e}{\alpha+e} + \dfrac{\alpha}{\alpha+e}(1 - e^{-x+1}), & \text{if } x > 1. \end{cases}$$

Therefore, a candidate of the random draw, i.e., x^*, can be generated from $f_*(x)$, by utilizing both the composition method and the inverse transform method.

Then, using the Metropolis-Hastings algorithm, the gamma random number generation method is shown as follows.

(i) Take an appropriate initial value as x_{-M}.

(ii) Generate a uniform random draw u_1 from $U(0,1)$, and set $x^* = \Big((\alpha/e+1)u_1\Big)^{1/\alpha}$ if $u_1 \le e/(\alpha+e)$ and $x^* = -\log\Big((1/e+1/\alpha)(1-u_1)\Big)$ if $u_1 > e/(\alpha+e)$.

(iii) Compute $\omega(x_{i-1}, x^*)$.

(iv) Generate a uniform random draw u_2 from $U(0,1)$, and set $x_i = x^*$ if $u_2 \le \omega(x_{i-1}, x^*)$ and $x_i = x_{i-1}$ otherwise.

(v) Repeat Steps (ii) – (iv) for $i = -M+1, -M+2, \cdots, 1$.

For sufficiently large M, x_1 is taken as a random draw from $f(x)$. u_1 and u_2 should be independently distributed.

M denotes the burn-in period. If we need a lot of random draws (say, N random draws), replace Step (v) by Step (v)', which is given by:

(v)' Repeat Steps (ii) – (iv) for $i = -M+1, -M+2, \cdots, N$.

Beta Distribution: The beta distribution with parameters α and β is of the form:

$$f(x) = \begin{cases} \dfrac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}, & \text{for } 0 < x < 1, \\ 0, & \text{otherwise.} \end{cases}$$

The sampling density is taken as:

$$f_*(x) = \begin{cases} 1, & \text{for } 0 < x < 1, \\ 0, & \text{otherwise,} \end{cases}$$

which represents the uniform distribution between zero and one.

The probability weights $\omega(x_i^*)$, $i = 1, 2, \cdots, n$, are given by:

$$\omega(x_{i-1}, x^*) = \min\left(\frac{f(x^*)/f_*(x^*)}{f(x_{i-1})/f_*(x_{i-1})}, 1\right) = \min\left(\left(\frac{x^*}{x_{i-1}}\right)^{\alpha-1}\left(\frac{1-x^*}{1-x_{i-1}}\right)^{\beta-1}, 1\right).$$

Then, utilizing the Metropolis-Hastings algorithm, the random draws are generated as follows.

(i) Take an appropriate initial value as x_{-M}.

(ii) Generate a uniform random draw x^* from $U(0, 1)$, and compute $\omega(x_{i-1}, x^*)$.

(iii) Generate a uniform random draw u from $U(0, 1)$, which is independent of x^*, and set $x_i = x^*$ if $u \leq \omega(x_{i-1}, x^*)$ and $x_i = x_{i-1}$ if $u > \omega(x_{i-1}, x^*)$.

(iv) Repeat Steps (ii) and (iii) for $i = -M + 1, -M + 2, \cdots, 1$.

For sufficiently large M, x_1 is taken as a random draw from $f(x)$.

M denotes the burn-in period.

If we want a lot of random draws (say, N random draws), replace Step (iv) by Step (iv)', which is represented as follows:

(iv)' Repeat Steps (ii) and (iii) for $i = -M + 1, -M + 2, \cdots, N$.

11.7.4 Ratio-of-Uniforms Method

As an alternative random number generation method, in this section we introduce the **ratio-of-uniforms method**.

This generation method does not require the sampling density utilized in rejection sampling (Section 11.7.1), importance resampling (Section 11.7.2) and the Metropolis-Hastings algorithm (Section 11.7.3).

Suppose that a bivariate random variable (U_1, U_2) is uniformly distributed, which satisfies the following inequality:

$$0 \leq U_1 \leq \sqrt{h(U_2/U_1)},$$

for any nonnegative function $h(x)$. Then, $X = U_2/U_1$ has a density function $f(x) = h(x)/\int h(x)\,\mathrm{d}x$.

Note that the domain of (U_1, U_2) will be discussed below.

The above random number generation method is justified in the following way.

The joint density of U_1 and U_2, denoted by $f_{12}(u_1, u_2)$, is given by:

$$f_{12}(u_1, u_2) = \begin{cases} k, & \text{if } 0 \le u_1 \le \sqrt{h(u_2/u_1)}, \\ 0, & \text{otherwise,} \end{cases}$$

where k is a constant value, because the bivariate random variable (U_1, U_2) is uniformly distributed.

Consider the following transformation from (u_1, u_2) to (x, y):

$$x = \frac{u_2}{u_1}, \qquad y = u_1,$$

i.e.,

$$u_1 = y, \qquad u_2 = xy.$$

The Jacobian for the transformation is:

$$J = \begin{vmatrix} \dfrac{\partial u_1}{\partial x} & \dfrac{\partial u_1}{\partial y} \\ \dfrac{\partial u_2}{\partial x} & \dfrac{\partial u_2}{\partial y} \end{vmatrix} = \begin{vmatrix} 0 & 1 \\ y & x \end{vmatrix} = -y.$$

Therefore, the joint density of X and Y, denoted by $f_{xy}(x, y)$, is written as:

$$f_{xy}(x, y) = |J| f_{12}(y, xy) = ky,$$

for $0 \leq y \leq \sqrt{h(x)}$.

The marginal density of X, denoted by $f_x(x)$, is obtained as follows:

$$f_x(x) = \int_0^{\sqrt{h(x)}} f_{xy}(x, y)\, \mathrm{d}y = \int_0^{\sqrt{h(x)}} ky\, \mathrm{d}y = k\left[\frac{y^2}{2}\right]_0^{\sqrt{h(x)}} = \frac{k}{2} h(x) = f(x),$$

where k is taken as: $k = 2/\int h(x)\, \mathrm{d}x$.

Thus, it is shown that $f_x(\cdot)$ is equivalent to $f(\cdot)$.

This result is due to Kinderman and Monahan (1977).

Also see Ripley (1987), O'Hagan (1994), Fishman (1996) and Gentle (1998).

Now, we take an example of choosing the domain of (U_1, U_2).

In practice, for the domain of (U_1, U_2), we may choose the rectangle which encloses the area $0 \leq U_1 \leq \sqrt{h(U_2/U_1)}$, generate a uniform point in the rectangle, and reject the point which does not satisfy $0 \leq u_1 \leq \sqrt{h(u_2/u_1)}$.

That is, generate two independent uniform random draws u_1 and u_2 from $U(0, b)$ and $U(c, d)$, respectively.

The rectangle is given by:

$$0 \le u_1 \le b, \qquad c \le u_2 \le d,$$

where b, c and d are given by:

$$b = \sup_x \sqrt{h(x)}, \qquad c = -\sup_x x\sqrt{h(x)}, \qquad d = \sup_x x\sqrt{h(x)},$$

because the rectangle has to enclose $0 \le u_1 \le \sqrt{h(u_2/u_1)}$, which is verified as follows:

$$\begin{aligned} &0 \le u_1 \le \sqrt{h(u_2/u_1)} \le \sup_x \sqrt{h(x)}, \\ &-\sup_x x\sqrt{h(x)} \le -x\sqrt{h(x)} \le u_2 \le x\sqrt{h(x)} \le \sup_x x\sqrt{h(x)}. \end{aligned}$$

The second line also comes from $0 \le u_1 \le \sqrt{h(u_2/u_1)}$ and $x = u_2/u_1$.

We can replace $c = -\sup_x x\sqrt{h(x)}$ by $c = \inf_x x\sqrt{h(x)}$, taking into account the case of $-\sup_x x\sqrt{h(x)} \le \inf_x x\sqrt{h(x)}$.

The discussion above is shown in Ripley (1987).

Thus, in order to apply the ratio-of-uniforms method with the domain $\{0 \le u_1 \le b,\ c \le u_2 \le d\}$, we need to have the condition that $h(x)$ and $x^2 h(x)$ are bounded.

The algorithm for the ratio-of-uniforms method is as follows:

(i) Generate u_1 and u_2 independently from $U(0, b)$ and $U(c, d)$.

(ii) Set $x = u_2/u_1$ if $u_1^2 \le h(u_2/u_1)$ and return to (i) otherwise.

As shown above, the x accepted in Step (ii) is taken as a random draw from $f(x) = h(x)/\int h(x)\,\mathrm{d}x$.

The acceptance probability in Step (ii) is $\int h(x)\,\mathrm{d}x/\Big(2b(d-c)\Big)$.

We have shown the rectangular domain of (U_1, U_2).

It may be possible that the domain of (U_1, U_2) is a parallelogram.

In Sections 11.7.4 and 11.7.4, we show two examples as applications of the ratio-of-uniforms method.

Especially, in Section 11.7.4, the parallelogram domain of (U_1, U_2) is taken as an example.

Normal Distribution: $N(0, 1)$: The kernel of the standard normal distribution is given by: $h(x) = \exp(-\frac{1}{2}x^2)$.

In this case, b, c and d are obtained as follows:

$$
\begin{aligned}
b &= \sup_x \sqrt{h(x)} = 1, \\
c &= \inf_x x\sqrt{h(x)} = -\sqrt{2e^{-1}}, \\
d &= \sup_x x\sqrt{h(x)} = \sqrt{2e^{-1}}.
\end{aligned}
$$

Accordingly, the standard normal random number based on the ratio-of-uniforms method is represented as follows.

(i) Generate two independent uniform random draws u_1 and v_2 from $U(0,1)$ and define $u_2 = (2v_2 - 1)\sqrt{2e^{-1}}$.

(ii) Set $x = u_2/u_1$ if $u_1^2 \leq \exp(-\frac{1}{2}u_2^2/u_1^2)$, i.e., $-4u_1^2 \log(u_1) \geq u_2^2$, and return to (i) otherwise.

The acceptance probability is given by:

$$
\frac{\int h(x)\,\mathrm{d}x}{2b(d-c)} = \frac{\sqrt{\pi e}}{4} \approx 0.7306,
$$

which is slightly smaller than the acceptance probability in the case of rejection sampling, i.e., $1/\sqrt{2e/\pi} \approx 0.7602$.

The Fortran source code for the standard normal random number generator based on the ratio-of-uniforms method is shown in snrnd9(ix,iy,rn).

snrnd9(ix,iy,rn)

```
      subroutine snrnd9(ix,iy,rn)
c
c  Use "snrnd9(ix,iy,rn)"
c  together with "urnd(ix,iy,rn)".
c
c  Input:
c    ix, iy:   Seeds
c  Output:
c    rn: Normal Random Draw N(0,1)
c
      e1=1./2.71828182845905
    1 call urnd(ix,iy,rn1)
      call urnd(ix,iy,rn2)
      rn2=(2.*rn2-1.)*sqrt(2.*e1)
      if(-4.*rn1*rn1*log(rn1).lt.rn2*rn2 ) go to 1
      rn=rn2/rn1
      return
      end
```

Gamma Distribution: $G(\alpha,\beta)$: When random variable X has a gamma distribution with parameters α and β, i.e., $X \sim G(\alpha,\beta)$, the density function of X is written as follows:

$$f(x) = \frac{1}{\beta^{\alpha}\Gamma(\alpha)} x^{\alpha-1} e^{-\frac{x}{\beta}},$$

for $0 < x < \infty$.

When $X \sim G(\alpha, 1)$, we have $Y = \beta X \sim G(\alpha,\beta)$.

Therefore, first we consider generating a random draw of $X \sim G(\alpha, 1)$.

Since we have discussed the case of $0 < \alpha \leq 1$ in Sections 11.7.1 – 11.7.3, now we consider the case of $\alpha > 1$.

Using the ratio-of-uniforms method, the gamma random number generator is introduced.

$h(x)$, b, c and d are set to be:

$$\begin{aligned}
h(x) &= x^{\alpha-1} e^{-x}, \\
b &= \sup_x \sqrt{h(x)} = \left(\frac{\alpha-1}{e}\right)^{(\alpha-1)/2}, \\
c &= \inf_x x\sqrt{h(x)} = 0,
\end{aligned}$$

$$d = \sup_x x\sqrt{h(x)} = \left(\frac{\alpha+1}{e}\right)^{(\alpha+1)/2}.$$

Note that $\alpha > 1$ guarantees the existence of the supremum of $h(x)$, which implies $b > 0$.

See Fishman (1996, pp.194 – 195) and Ripley (1987, pp.88 – 89).

By the ratio-of-uniforms method, the gamma random number with parameter $\alpha > 1$ and $\beta = 1$ is represented as follows:

(i) Generate two independent uniform random draws u_1 and u_2 from $U(0, b)$ and $U(c, d)$, respectively.

(ii) Set $x = u_2/u_1$ if $u_1 \leq \sqrt{(u_2/u_1)^{\alpha-1}e^{-u_2/u_1}}$ and go back to (i) otherwise.

Thus, the x obtained in Steps (i) and (ii) is taken as a random draw from $G(\alpha, 1)$ for $\alpha > 1$.

Based on the above algorithm represented by Steps (i) and (ii), the Fortran 77 program for the gamma random number generator with parameters $\alpha > 1$ and $\beta = 1$ is shown in `gammarnd6(ix,iy,alpha,rn)`.

`gammarnd6(ix,iy,alpha,rn)`

```
1:       subroutine gammarnd6(ix,iy,alpha,rn)
2: c
3: c  Use "gammarnd6(ix,iy,alpha,rn)"
4: c  together with "urnd(ix,iy,rn)".
5: c
6: c  Input:
7: c    ix, iy:   Seeds
8: c    alpha:  Shape Parameter (alpha>1)
9: c  Output:
10: c    rn: Gamma Random Draw
11: c        with Parameters alpha and beta=1
12: c
13:       e=2.71828182845905
14:       b=( (alpha-1.)/e )**(0.5*alpha-0.5)
15:       d=( (alpha+1.)/e )**(0.5*alpha+0.5)
16:     1 call urnd(ix,iy,rn0)
17:       call urnd(ix,iy,rn1)
18:       u=rn0*b
19:       v=rn1*d
20:       rn=v/u
21:       if( 2.*log(u).gt.(alpha-1.)*log(rn)-rn ) go to 1
22:       return
23:       end
```

`gammarnd6(ix,iy,alpha,rn)` should be used together with `urnd(ix,iy,rn)`.

b and d are obtained in Lines 14 and 15.

Lines 16 –19 gives us two uniform random draws `u` and `v`, which correspond to u_1 and u_2.

`rn` in Line 20 indicates a candidate of the gamma random draw.

Line 21 represents Step (ii).

To see efficiency or inefficiency of the generator above, we compute the acceptance probability in Step (ii) as follows:

$$\frac{\int h(x)\,\mathrm{d}x}{2b(d-c)} = \frac{e^{\alpha}\Gamma(\alpha)}{2(\alpha-1)^{(\alpha-1)/2}(\alpha+1)^{(\alpha+1)/2}}. \tag{24}$$

It is known that the acceptance probability decreases by the order of $O(\alpha^{-1/2})$, i.e., in other words, computational time for random number generation increases by the order of $O(\alpha^{1/2})$.

Therefore, as α is larger, the generator is less efficient.

See Fishman (1996) and Gentle (1998).

To improve inefficiency for large α, various methods have been proposed, for example, Cheng and Feast (1979, 1980), Schmeiser and Lal (1980), Sarkar (1996) and so on.

As mentioned above, the algorithm `gammarnd6` takes a long time computationally by the order of $O(\alpha^{1/2})$ as shape parameter α is large.

Chen and Feast (1979) suggested the algorithm which does not depend too much on shape parameter α.

As α increases the acceptance region shrinks toward $u_1 = u_2$.

Therefore, Chen and Feast (1979) suggested generating two uniform random draws within the parallelogram around $u_1 = u_2$, rather than the rectangle.

The source code is shown in `gammarnd7(ix,iy,alpha,rn)`.

gammarnd7(ix,iy,alpha,rn)

```
1:        subroutine gammarnd7(ix,iy,alpha,rn)
2:  C
3:  C  Use "gammarnd7(ix,iy,alpha,rn)"
4:  C  together with "urnd(ix,iy,rn)".
5:  C
6:  C  Input:
7:  C    ix, iy:   Seeds
8:  C    alpha:  Shape Parameter (alpha>1)
9:  C  Output:
10: C    rn: Gamma Random Draw
11: C        with Parameters alpha and beta=1
12: C
13:       e =2.71828182845905
```

```
14:       c0=1.857764
15:       c1=alpha-1.
16:       c2=( alpha-1./(6.*alpha) )/c1
17:       c3=2./c1
18:       c4=c3+2.
19:       c5=1./sqrt(alpha)
20:     1 call urnd(ix,iy,u1)
21:       call urnd(ix,iy,u2)
22:       if(alpha.gt.2.5) u1=u2+c5*(1.-c0*u1)
23:       if(0.ge.u1.or.u1.ge.1.) go to 1
24:       w=c2*u2/u1
25:       if(c3*u1+w+1./w.le.c4) go to 2
26:       if(c3*log(u1)-log(w)+w.ge.1.) go to 1
27:     2 rn=c1*w
28:       return
29:       end
```

See Fishman (1996, p.200) and Ripley (1987, p.90).

In Line 22, we use the rectangle for $1 < \alpha \leq 2.5$ and the parallelogram for $\alpha > 2.5$ to give a fairly constant speed as α is varied.

Line 25 gives us a fast acceptance to avoid evaluating the logarithm.

From computational efficiency, `gammarnd7(ix,iy,alpha,rn)` is better.

Gamma Distribution: $G(\alpha,\beta)$ for $\alpha > 0$ and $\beta > 0$: Combining gammarnd2 on p.339 and gammarnd7 on p.387, we introduce the gamma random number generator in the case of $\alpha > 0$. In addition, utilizing $Y = \beta X \sim G(\alpha,\beta)$ when $X \sim G(\alpha, 1)$, the random number generator for $G(\alpha,\beta)$ is introduced as in the source code gammarnd8(ix,iy,alpha,beta,rn).

gammarnd8(ix,iy,alpha,beta,rn)

```
1:        subroutine gammarnd8(ix,iy,alpha,beta,rn)
2: c
3: c  Use "gammarnd8(ix,iy,alpha,beta,rn)"
4: c  together with "gammarnd2(ix,iy,alpha,rn)",
5: c                "gammarnd7(ix,iy,alpha,rn)"
6: c           and  "urnd(ix,iy,rn)".
7: c
8: c  Input:
9: c    ix, iy:   Seeds
10: c   alpha:  Shape Parameter
11: c   beta:   Scale Parameter
12: c  Output:
13: c   rn: Gamma Random Draw
14: c       with Parameters alpha and beta
15: c
16:         if( alpha.le.1. ) then
17:       call gammarnd2(ix,iy,alpha,rn1)
```

```
18:         else
19:       call gammarnd7(ix,iy,alpha,rn1)
20:         endif
21:       rn=beta*rn1
22:       return
23:       end
```

Lines 16 – 20 show that we use `gammarnd2` for $\alpha \leq 1$ and `gammarnd7` for $\alpha > 1$.

In Line 21, $X \sim G(\alpha, 1)$ is transformed into $Y \sim G(\alpha, \beta)$ by $Y = \beta X$, where X and Y indicates `rn1` and `rn`, respectively.

Chi-Square Distribution: $\chi^2(k)$: The gamma distribution with $\alpha = k/2$ and $\beta = 2$ reduces to the chi-square distribution with k degrees of freedom.

11.7.5 Gibbs Sampling

The sampling methods introduced in Sections 11.7.1 – 11.7.3 can be applied to the cases of both univariate and multivariate distributions.

The Gibbs sampler in this section is the random number generation method in the multivariate cases.

The Gibbs sampler shows how to generate random draws from the unconditional densities under the situation that we can generate random draws from two conditional densities.

Geman and Geman (1984), Tanner and Wong (1987), Gelfand, Hills, Racine-Poon and Smith (1990), Gelfand and Smith (1990), Carlin and Polson (1991), Zeger and Karim (1991), Casella and George (1992), Gamerman (1997) and so on developed the Gibbs sampling theory.

Carlin, Polson and Stoffer (1992), Carter and Kohn (1994, 1996) and Geweke and Tanizaki (1999, 2001) applied the Gibbs sampler to the nonlinear and/or non-Gaussian state-space models.

There are numerous other applications of the Gibbs sampler.

The Gibbs sampling theory is concisely described as follows.

We can deal with more than two random variables, but we consider two random variables X and Y in order to make things easier.

Two conditional density functions, $f_{x|y}(x|y)$ and $f_{y|x}(y|x)$, are assumed to be known, which denote the conditional distribution function of X given Y and that of Y given X, respectively.

Suppose that we can easily generate random draws of X from $f_{x|y}(x|y)$ and those of Y from $f_{y|x}(y|x)$. However, consider the case where it is not easy to generate random draws from the joint density of X and Y, denoted by $f_{xy}(x, y)$.

In order to have the random draws of (X, Y) from the joint density $f_{xy}(x, y)$, we take the following procedure:

(i) Take the initial value of X as x_{-M}.

(ii) Given x_{i-1}, generate a random draw of Y, i.e., y_i, from $f(y|x_{i-1})$.

(iii) Given y_i, generate a random draw of X, i.e., x_i, from $f(x|y_i)$.

(iv) Repeat the procedure for $i = -M + 1, -M + 2, \cdots, 1$.

From the convergence theory of the Gibbs sampler, as M goes to infinity, we can regard x_1 and y_1 as random draws from $f_{xy}(x, y)$, which is a joint density function of X and Y.
M denotes the **burn-in period**, and the first M random draws, (x_i, y_i) for $i = -M + 1, -M + 2, \cdots, 0$, are excluded from further consideration.
When we want N random draws from $f_{xy}(x, y)$, Step (iv) should be replaced by Step (iv)', which is as follows.

(iv)' Repeat the procedure for $i = -M + 1, -M + 2, \cdots, N$.

As in the Metropolis-Hastings algorithm, the algorithm shown in Steps (i) – (iii) and (iv)' is formulated

as follows:

$$f_i(u) = \int f^*(u|v) f_{i-1}(v)\, \mathrm{d}v.$$

For convergence of the Gibbs sampler, we need to have the invariant distribution $f(u)$ which satisfies $f_i(u) = f_{i-1}(u) = f(u)$. If we have the reversibility condition shown in equation (22), i.e.,

$$f^*(v|u) f(u) = f^*(u|v) f(v),$$

the random draws based on the Gibbs sampler converge to those from the invariant distribution, which implies that there exists the invariant distribution $f(u)$.

Therefore, in the Gibbs sampling algorithm, we have to find the transition distribution, i.e., $f^*(u|v)$. Here, we consider that both u and v are bivariate vectors.

That is, $f^*(u|v)$ and $f_i(u)$ denote the bivariate distributions. x_i and y_i are generated from $f_i(u)$ through $f^*(u|v)$, given $f_{i-1}(v)$.

Note that $u = (u_1, u_2) = (x_i, y_i)$ is taken while $v = (v_1, v_2) = (x_{i-1}, y_{i-1})$ is set.

The transition distribution in the Gibbs sampler is taken as:

$$f^*(u|v) = f_{y|x}(u_2|u_1) f_{x|y}(u_1|v_2)$$

Thus, we can choose $f^*(u|v)$ as shown above.

Then, as i goes to infinity, (x_i, y_i) tends in distribution to a random vector whose joint density is $f_{xy}(x, y)$.

See, for example, Geman and Geman (1984) and Smith and Roberts (1993).

Furthermore, under the condition that there exists the invariant distribution, the basic result of the Gibbs sampler is as follows:

$$\frac{1}{N}\sum_{i=1}^{N} g(x_i, y_i) \longrightarrow \mathrm{E}\Big(g(x, y)\Big) = \iint g(x, y) f_{xy}(x, y)\, \mathrm{d}x\, \mathrm{d}y, \quad \text{as } N \longrightarrow \infty,$$

where $g(\cdot, \cdot)$ is a function.

The Gibbs sampler is a powerful tool in a Bayesian framework.

Based on the conditional densities, we can generate random draws from the joint density.

Remark 1: We have considered the bivariate case, but it is easily extended to the multivariate cases.

That is, it is possible to take multi-dimensional vectors for x and y.

Taking an example, as for the tri-variate random vector (X, Y, Z), if we generate the ith random draws from $f_{x|yz}(x|y_{i-1}, z_{i-1})$, $f_{y|xz}(y|x_i, z_{i-1})$ and $f_{z|xy}(z|x_i, y_i)$, sequentially, we can obtain the random draws from $f_{xyz}(x, y, z)$.

Remark 2: Let X, Y and Z be the random variables.

Take an example of the case where X is highly correlated with Y.

If we generate random draws from $f_{x|yz}(x|y, z)$, $f_{y|xz}(y|x, z)$ and $f_{z|xy}(z|x, y)$, it is known that convergence of the Gibbs sampler is slow.

In this case, without separating X and Y, random number generation from $f(x, y|z)$ and $f(z|x, y)$ yields better random draws from the joint density $f(x, y, z)$.

Rejection Sampling, Importance Resampling and the Metropolis-Hastings Algorithm: We compare rejection sampling, importance resampling and the Metropolis-Hastings algorithm from precision of the estimated moments and CPU time.

All the three sampling methods utilize the sampling density and they are useful when it is not easy to generate random draws directly from the target density.

When the sampling density is too far from the target density, it is known that rejection sampling takes a lot of time computationally while importance resampling and the Metropolis-Hastings algorithm yields unrealistic random draws.

In this section, therefore, we investigate how the sampling density depends on the three sampling methods.

For simplicity of discussion, consider the case where both the target and sampling densities are normal. That is, the target density $f(x)$ is given by $N(0, 1)$ and the sampling density $f_*(x)$ is $N(\mu_*, \sigma_*^2)$.

$\mu_* = 0, 1, 2, 3$ and $\sigma_* = 0.5, 1.0, 1.5, 2.0, 3.0, 4.0$ are taken.

For each of the cases, the first three moments $\mathrm{E}(X^j)$, $j = 1, 2, 3$, are estimated, generating 10^7 random draws.

For importance resampling, $n = 10^4$ is taken, which is the number of candidate random draws.

The Metropolis-Hastings algorithm takes $M = 1000$ as the burn-in period and the initial value is $x_{-M} = \mu_*$.

As for the Metropolis-Hastings algorithm, note that is the independence chain is taken for $f_*(x)$ because of $f_*(x|z) = f_*(x)$.

Comparison of Three Sampling Methods

E(X)	μ_* \ σ_*	0.5	1.0	1.5	2.0	3.0	4.0
	0	RS — IR — MH —0.000	RS — IR — MH —0.000	RS — IR — MH —0.000	RS — IR — MH —0.000	RS — IR — MH —0.000	RS — IR — MH —0.001
	1	RS — IR — MH 0.558	RS — IR — MH 0.559	RS — IR — MH 0.559	RS — IR — MH 0.559	RS — IR — MH 0.559	RS — IR — MH 0.559
	2	RS — IR — MH 1.118	RS — IR — MH 1.118	RS — IR — MH 1.118	RS — IR — MH 1.118	RS — IR — MH 1.118	RS — IR — MH 1.118
	3	RS — IR — MH 1.677	RS — IR — MH 1.677	RS — IR — MH 1.677	RS — IR — MH 1.677	RS — IR — MH 1.677	RS — IR — MH 1.677

Comparison of Three Sampling Methods

E(X^2)	μ_* \ σ_*	0.5	1.0	1.5	2.0	3.0	4.0
	0	RS 0.828 IR 0.828 MH 0.828	RS 0.972 IR 0.972 MH 0.972	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000
	1	RS 1.309 IR 1.309 MH 1.309	RS 1.080 IR 1.080 MH 1.080	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000
	2	RS 2.677 IR 2.677 MH 2.677	RS 1.382 IR 1.382 MH 1.382	RS 1.044 IR 1.044 MH 1.044	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000
	3	RS 4.746 IR 4.746 MH 4.746	RS 1.896 IR 1.896 MH 1.896	RS 1.095 IR 1.095 MH 1.095	RS 1.008 IR 1.008 MH 1.008	RS 1.000 IR 1.000 MH 1.000	RS 1.000 IR 1.000 MH 1.000

Comparison of Three Sampling Methods

E(X^3)	μ_* \ σ_*	0.5	1.0	1.5	2.0	3.0	4.0
	0	RS — IR — MH −0.217	RS — IR — MH 0.094	RS — IR — MH −0.001	RS — IR — MH −0.008	RS — IR — MH −0.008	RS — IR — MH −0.004
	1	RS — IR — MH 0.517	RS — IR — MH −0.093	RS — IR — MH 0.069	RS — IR — MH −0.069	RS — IR — MH 0.027	RS — IR — MH −0.021
	2	RS — IR — MH 1.230	RS — IR — MH 0.435	RS — IR — MH −0.081	RS — IR — MH 0.005	RS — IR — MH 0.000	RS — IR — MH 0.004
	3	RS — IR — MH 3.030	RS — IR — MH 0.936	RS — IR — MH −0.004	RS — IR — MH 0.001	RS — IR — MH 0.008	RS — IR — MH −0.000

Comparison of Three Sampling Methods: CPU Time (Seconds)

μ_* \ σ_*	0.5	1.0	1.5	2.0	3.0	4.0
0	RS 439.89 IR 439.20 MH 439.55	RS 439.40 IR 439.20 MH 439.36	RS 439.36 IR 439.20 MH 439.55	RS 439.36 IR 439.20 MH 439.55	RS 439.82 IR 439.20 MH 439.77	RS 439.77 IR 439.20 MH 439.77
1	RS 439.73 IR 439.20 MH 439.55	RS 439.56 IR 439.20 MH 439.81	RS 439.81 IR 439.20 MH 439.55	RS 439.76 IR 439.20 MH 439.55	RS 439.86 IR 439.20 MH 439.55	RS 440.09 IR 439.20 MH 439.55
2	RS 439.90 IR 439.20 MH 439.55	RS 439.23 IR 439.20 MH 439.74	RS 439.84 IR 439.20 MH 439.55	RS 439.78 IR 439.20 MH 439.55	RS 439.46 IR 439.20 MH 439.55	RS 439.18 IR 439.20 MH 439.55
3	RS 439.32 IR 439.20 MH 439.55	RS 439.48 IR 439.20 MH 439.99	RS 439.99 IR 439.20 MH 439.55	RS 439.75 IR 439.20 MH 439.55	RS 439.61 IR 439.20 MH 439.55	RS 439.76 IR 439.20 MH 439.55

RS, IR and MH denotes rejection sampling, importance resampling and the Metropolis-Hastings algorithm, respectively.

In each table, "—" in RS implies the case where rejection sampling cannot be applied because the supremum of $q(x)$, $\sup_x q(x)$, does not exist.

As for MH in the case of $\mathrm{E}(X) = 0$, the values in the parentheses represent the acceptance rate (percent) in the Metropolis-Hastings algorithm.

The results obtained from each table are as follows.

$\mathrm{E}(X)$ should be close to zero because we have $\mathrm{E}(X) = 0$ from $X \sim N(0, 1)$.

When $\mu_* = 0.0$, all of RS, IR and MH are very close to zero and show a good performance.

When $\mu_* = 1, 2, 3$, for $\sigma_* = 1.5, 2.0, 3.0, 4.0$, all of RS, IR and MH perform well, but IR and MH in the case of $\sigma_* = 0.5, 1.0$ have the case where the estimated mean is too different from zero.

For IR and MH, we can see that given σ_* the estimated mean is far from the true mean as μ_* is far from mean of the target density.

Also, it might be concluded that given μ_* the estimated mean approaches the true value as σ_* is large.

$\mathrm{E}(X^2)$ should be close to one because we have $\mathrm{E}(X^2) = \mathrm{V}(X) = 1$ from $X \sim N(0, 1)$.

The cases of $\sigma_* = 1.5, 2.0, 3.0, 4.0$ and the cases of $\mu_* = 0, 1$ and $\sigma_* = 1.0$ are very close to one, but the other cases are different from one.

These are the same results as the case of $\mathrm{E}(X)$.

$\mathrm{E}(X^3)$ should be close to zero because $\mathrm{E}(X^3)$ represents skewness.

For skewness, we obtain the similar results, i.e., the cases of $\sigma_* = 1.5, 2.0, 3.0, 4.0$ and the cases of $\mu_* = 0, 1$ and $\sigma_* = 0.5, 1.0$ perform well for all of RS, IR and MH.

In the case where we compare RS, IR and MH, RS shows the best performance of the three, and IR

and MH is quite good when σ_* is relatively large.

We can conclude that IR is slightly worse than RS and MH.

As for the acceptance rates of MH in $\mathrm{E}(X) = 0$, from the table a higher acceptance rate generally shows a better performance.

The high acceptance rate implies high randomness of the generated random draws.

For variance of the sampling density, both too small variance and too large variance give us the relatively low acceptance rate, which result is consistent with the discussion in Chib and Greenberg (1995).

MH has the advantage over RS and IR from computational point of view.

IR takes a lot of time because all the acceptance probabilities have to be computed in advance (see Section 11.7.2 for IR).

That is, 10^4 candidate random draws are generated from the sampling density $f_*(x)$ and therefore 10^4 acceptance probabilities have to be computed.

For MH and IR, computational CPU time does not depend on μ_* and σ_*.

However, for RS, given σ_* computational time increases as μ_* is large.

In other words, as the sampling density is far from the target density the number of rejections increases.

When σ_* increases given μ_*, the acceptance rate does not necessarily increase.

However, from the table a large σ_* is better than a small σ_* in general.

Accordingly, as for RS, under the condition that mean of $f(x)$ is unknown, we can conclude that relatively large variance of $f_*(x)$ should be taken.

Finally, the results are summarized as follows.

(1) For IR and MH, depending on choice of the sampling density $f_*(x)$, we have the cases where the estimates of mean, variance and skewness are biased.

For RS, we can always obtain the unbiased estimates without depending on choice of the sampling density.

(2) In order to avoid the biased estimates, it is safe for IR and MH to choose the sampling density with relatively large variance.

Furthermore, for RS we should take the sampling density with relatively large variance to reduce computational burden.

But, note that too large variance leads to an increase in computational disadvantages.

(3) MH is the least computational sampling method of the three.

For IR, all the acceptance probabilities have to be computed in advance and therefore

IR takes a lot of time to generate random draws.

In the case of RS, the amount of computation increases as $f_*(x)$ is far from $f(x)$.

(4) For the sampling density in MH, it is known that both too large variance and too small variance yield slow convergence of the obtained random draws.

The slow convergence implies that a great amount of random draws have to be generated from the sampling density for evaluation of the expectations such as $\mathrm{E}(X)$ and $\mathrm{V}(X)$.

Therefore, choice of the sampling density has to be careful,

Thus, RS gives us the best estimates in the sense of unbiasedness, but RS sometimes has the case where the supremum of $q(x)$ does not exist and in this case it is impossible to implement RS.
As the sampling method which can be applied to any case, MH might be preferred to IR and RS in a sense of less risk.
However, we should keep in mind that MH also has the problem which choice of the sampling density is very important.

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– 86.

12 Bayesian Estimation — Examples

12.1 Heteroscedasticity Model

In Section 12.1, Tanizaki and Zhang (2001) is re-computed using the random number generators.

Here, we show how to use Bayesian approach in the multiplicative heteroscedasticity model discussed by Harvey (1976).

The Gibbs sampler and the Metropolis-Hastings (MH) algorithm are applied to the multiplicative heteroscedasticity model, where some sampling densities are considered in the MH algorithm.

We carry out Monte Carlo study to examine the properties of the estimates via Bayesian approach and the traditional counterparts such as the modified two-step estimator (M2SE) and the maximum likelihood estimator (MLE).

The results of Monte Carlo study show that the sampling density chosen here is suitable, and Bayesian approach shows better performance than the traditional counterparts in the criterion of the root mean square error (RMSE) and the interquartile range (IR).

12.1.1 Introduction

For the heteroscedasticity model, we have to estimate both the regression coefficients and the heteroscedasticity parameters.

In the literature of heteroscedasticity, traditional estimation techniques include the two-step estimator (2SE) and the maximum likelihood estimator (MLE).

Harvey (1976) showed that the 2SE has an inconsistent element in the heteroscedasticity parameters and furthermore derived the consistent estimator based on the 2SE, which is called the modified two-step estimator (M2SE).

These traditional estimators are also examined in Amemiya (1985), Judge, Hill, Griffiths and Lee (1980) and Greene (1997).

Ohtani (1982) derived the Bayesian estimator (BE) for a heteroscedasticity linear model.

Using a Monte Carlo experiment, Ohtani (1982) found that among the Bayesian estimator (BE) and some traditional estimators, the Bayesian estimator (BE) shows the best properties in the mean square error (MSE) criterion.

Because Ohtani (1982) obtained the Bayesian estimator by numerical integration, it is not easy to

extend to the multi-dimensional cases of both the regression coefficient and the heteroscedasticity parameter.

Recently, Boscardin and Gelman (1996) developed a Bayesian approach in which a Gibbs sampler and the Metropolis-Hastings (MH) algorithm are used to estimate the parameters of heteroscedasticity in the linear model.

They argued that through this kind of Bayesian approach, we can average over our uncertainty in the model parameters instead of using a point estimate via the traditional estimation techniques.

Their modeling for the heteroscedasticity, however, is very simple and limited. Their choice of the heteroscedasticity is $V(y_i) = \sigma^2 w_i^{-\theta}$, where w_i are known "weights" for the problem and θ is an unknown parameter.

In addition, they took only one candidate for the sampling density used in the MH algorithm and compared it with 2SE.

In Section 12.1, we also consider Harvey's (1976) model of multiplicative heteroscedasticity.

This modeling is very flexible, general, and includes most of the useful formulations for heteroscedasticity as special cases.

The Bayesian approach discussed by Ohtani (1982) and Boscardin and Gelman (1996) can be extended

to the multi-dimensional and more complicated cases, using the model introduced here.

The Bayesian approach discussed here includes the MH within Gibbs algorithm, where through Monte Carlo studies we examine two kinds of candidates for the sampling density in the MH algorithm and compare the Bayesian approach with the two traditional estimators, i.e., M2SE and MLE, in the criterion of the root mean square error (RMSE) and the interquartile range (IR).

We obtain the results that the Bayesian estimator significantly has smaller RMSE and IR than M2SE and MLE at least for the heteroscedasticity parameters.

Thus, the results of the Monte Carlo study show that the Bayesian approach performs better than the traditional estimators.

12.1.2 Multiplicative Heteroscedasticity Regression Model

The multiplicative heteroscedasticity model discussed by Harvey (1976) can be shown as follows:

$$y_t = X_t\beta + u_t, \qquad u_t \sim N(0, \sigma_t^2), \tag{25}$$

$$\sigma_t^2 = \sigma^2 \exp(q_t\alpha), \tag{26}$$

for $t = 1, 2, \cdots, n$, where y_t is the tth observation, X_t and q_t are the tth $1 \times k$ and $1 \times (J-1)$ vectors of explanatory variables, respectively.

β and α are vectors of unknown parameters.

The model given by equations (25) and (26) includes several special cases such as the model in Boscardin and Gelman (1996), in which $q_t = \log w_t$ and $\theta = -\alpha$.

As shown in Greene (1997), there is a useful simplification of the formulation.

Let $z_t = (1, q_t)$ and $\gamma = (\log \sigma^2, \alpha')'$, where z_t and γ denote $1 \times J$ and $J \times 1$ vectors.

Then, we can simply rewrite equation (26) as:

$$\sigma_t^2 = \exp(z_t \gamma). \tag{27}$$

Note that $\exp(\gamma_1)$ provides σ^2, where γ_1 denotes the first element of γ.

As for the variance of u_t, hereafter we use (27), rather than (26).

The generalized least squares (GLS) estimator of β, denoted by $\hat{\beta}_{GLS}$, is given by:

$$\hat{\beta}_{GLS} = \left(\sum_{t=1}^{n} \exp(-z_t \gamma) X_t' X_t \right)^{-1} \sum_{t=1}^{n} \exp(-z_t \gamma) X_t' y_t, \tag{28}$$

where $\hat{\beta}_{GLS}$ depends on γ, which is the unknown parameter vector.

To obtain the feasible GLS estimator, we need to replace γ by its consistent estimate.

We have two traditional consistent estimators of γ, i.e., M2SE and MLE, which are briefly described as follows.

Modified Two-Step Estimator (M2SE): First, define the ordinary least squares (OLS) residual by $e_t = y_t - X_t\hat{\beta}_{OLS}$, where $\hat{\beta}_{OLS}$ represents the OLS estimator, i.e., $\hat{\beta}_{OLS} = (\sum_{t=1}^{n} X_t' X_t)^{-1} \sum_{t=1}^{n} X_t' y_t$. For 2SE of γ, we may form the following regression:

$$\log e_t^2 = z_t\gamma + v_t.$$

The OLS estimator of γ applied to the above equation leads to the 2SE of γ, because e_t is obtained by OLS in the first step.

Thus, the OLS estimator of γ gives us 2SE, denoted by $\hat{\gamma}_{2SE}$, which is given by:

$$\hat{\gamma}_{2SE} = (\sum_{t=1}^{n} z_t' z_t)^{-1} \sum_{t=1}^{n} z_t' \log e_t^2.$$

A problem with this estimator is that v_t, $t = 1, 2, \cdots, n$, have non-zero means and are heteroscedastic. If e_t converges in distribution to u_t, the v_t will be asymptotically independent with mean $\mathrm{E}(v_t) = -1.2704$ and variance $\mathrm{V}(v_t) = 4.9348$, which are shown in Harvey (1976).

Then, we have the following mean and variance of $\hat{\gamma}_{2SE}$:

$$\mathrm{E}(\hat{\gamma}_{2SE}) = \gamma - 1.2704(\sum_{t=1}^{n} z_t' z_t)^{-1} \sum_{t=1}^{n} z_t', \tag{29}$$

$$\mathrm{V}(\hat{\gamma}_{2SE}) = 4.9348(\sum_{t=1}^{n} z_t' z_t)^{-1}.$$

For the second term in equation (29), the first element is equal to -1.2704 and the remaining elements are zero, which can be obtained by simple calculation.

Therefore, the first element of $\hat{\gamma}_{2SE}$ is biased but the remaining elements are still unbiased.

To obtain a consistent estimator of γ_1, we consider M2SE of γ, denoted by $\hat{\gamma}_{M2SE}$, which is given by:

$$\hat{\gamma}_{M2SE} = \hat{\gamma}_{2SE} + 1.2704(\sum_{t=1}^{n} z_t' z_t)^{-1} \sum_{t=1}^{n} z_t'.$$

Let Σ_{M2SE} be the variance of $\hat{\gamma}_{M2SE}$.

Then, Σ_{M2SE} is represented by:

$$\Sigma_{M2SE} \equiv \mathrm{V}(\hat{\gamma}_{M2SE}) = \mathrm{V}(\hat{\gamma}_{2SE}) = 4.9348(\sum_{t=1}^{n} z_t' z_t)^{-1}.$$

The first element of $\hat{\gamma}_{2SE}$ and $\hat{\gamma}_{M2SE}$ corresponds to the estimate of σ^2, which value does not influence $\hat{\beta}_{GLS}$.

Since the remaining elements of $\hat{\gamma}_{2SE}$ are equal to those of $\hat{\gamma}_{M2SE}$, $\hat{\beta}_{2SE}$ is equivalent to $\hat{\beta}_{M2SE}$, where $\hat{\beta}_{2SE}$ and $\hat{\beta}_{M2SE}$ denote 2SE and M2SE of β, respectively.

Note that $\hat{\beta}_{2SE}$ and $\hat{\beta}_{M2SE}$ can be obtained by substituting $\hat{\gamma}_{2SE}$ and $\hat{\gamma}_{M2SE}$ into γ in (28).

Maximum Likelihood Estimator (MLE): The density of $Y_n = (y_1, y_2, \cdots, y_n)$ based on (25) and (27) is:

$$f(Y_n|\beta,\gamma) \propto \exp\left(-\frac{1}{2}\sum_{t=1}^{n}\Big(\exp(-z_t\gamma)(y_t - X_t\beta)^2 + z_t\gamma\Big)\right), \tag{30}$$

which is maximized with respect to β and γ, using the method of scoring.

That is, given values for $\beta^{(j)}$ and $\gamma^{(j)}$, the method of scoring is implemented by the following iterative procedure:

$$\beta^{(j)} = \Big(\sum_{t=1}^{n}\exp(-z_t\gamma^{(j-1)})X_t'X_t\Big)^{-1}\sum_{t=1}^{n}\exp(-z_t\gamma^{(j-1)})X_t'y_t,$$

$$\gamma^{(j)} = \gamma^{(j-1)} + 2(\sum_{t=1}^{n}z_t'z_t)^{-1}\frac{1}{2}\sum_{t=1}^{n}z_t'\Big(\exp(-z_t\gamma^{(j-1)})e_t^2 - 1\Big),$$

for $j = 1, 2, \cdots$, where $e_t = y_t - X_t\beta^{(j-1)}$.

The starting value for the above iteration may be taken as $(\beta^{(0)}, \gamma^{(0)}) = (\hat{\beta}_{OLS}, \hat{\gamma}_{2SE})$, $(\hat{\beta}_{2SE}, \hat{\gamma}_{2SE})$ or $(\hat{\beta}_{M2SE}, \hat{\gamma}_{M2SE})$.

Let $\theta = (\beta, \gamma)$.

The limit of $\theta^{(j)} = (\beta^{(j)}, \gamma^{(j)})$ gives us the MLE of θ, which is denoted by $\hat{\theta}_{MLE} = (\hat{\beta}_{MLE}, \hat{\gamma}_{MLE})$.

Based on the information matrix, the asymptotic covariance matrix of $\hat{\theta}_{MLE}$ is represented by:

$$\begin{aligned} \mathrm{V}(\hat{\theta}_{MLE}) &= \left(- \mathrm{E}\left(\frac{\partial^2 \log f(Y_n|\theta)}{\partial\theta\partial\theta'} \right) \right)^{-1} \\ &= \begin{pmatrix} \left(\sum_{t=1}^{n} \exp(-z_t\gamma) X_t' X_t \right)^{-1} & 0 \\ 0 & 2(\sum_{t=1}^{n} z_t' z_t)^{-1} \end{pmatrix}. \end{aligned} \tag{31}$$

Thus, from (31), asymptotically there is no correlation between $\hat{\beta}_{MLE}$ and $\hat{\gamma}_{MLE}$, and furthermore the asymptotic variance of $\hat{\gamma}_{MLE}$ is represented by: $\Sigma_{MLE} \equiv \mathrm{V}(\hat{\gamma}_{MLE}) = 2(\sum_{t=1}^{n} z_t' z_t)^{-1}$, which implies that $\hat{\gamma}_{M2SE}$ is asymptotically inefficient because $\Sigma_{M2SE} - \Sigma_{MLE}$ is positive definite.

Remember that the variance of $\hat{\gamma}_{M2SE}$ is given by: $\mathrm{V}(\hat{\gamma}_{M2SE}) = 4.9348(\sum_{t=1}^{n} z_t' z_t)^{-1}$.

12.1.3 Bayesian Estimation

We assume that the prior distributions of the parameters β and γ are noninformative, which are represented by:

$$f_\beta(\beta) = \text{constant}, \qquad f_\gamma(\gamma) = \text{constant}. \tag{32}$$

Combining the prior distributions (32) and the likelihood function (30), the posterior distribution $f_{\beta\gamma}(\beta, \gamma|y)$ is obtained as follows:

$$f_{\beta\gamma}(\beta, \gamma|Y_n) \propto \exp\left\{-\frac{1}{2}\sum_{t=1}^{n}\Big(\exp(-z_t\gamma)(y_t - X_t\beta)^2 + z_t\gamma\Big)\right\}.$$

The posterior means of β and γ are not operationally obtained.

Therefore, by generating random draws of β and γ from the posterior density $f_{\beta\gamma}(\beta, \gamma|Y_n)$, we consider evaluating the mathematical expectations as the arithmetic averages based on the random draws.

Now we utilize the Gibbs sampler, which has been introduced in Section 11.7.5, to sample random draws of β and γ from the posterior distribution.

Then, from the posterior density $f_{\beta\gamma}(\beta, \gamma|Y_n)$, we can derive the following two conditional densities:

$$f_{\gamma|\beta}(\gamma|\beta, Y_n) \propto \exp\left\{-\frac{1}{2}\sum_{t=1}^{n}\left(\exp(-z_t\gamma)(y_t - X_t\beta)^2 + z_t\gamma\right)\right\}, \tag{33}$$

$$f_{\beta|\gamma}(\beta|\gamma, Y_n) = N(B_1, H_1), \tag{34}$$

where

$$H_1^{-1} = \sum_{t=1}^{n}\exp(-z_t\gamma)X_t'X_t, \qquad B_1 = H_1\sum_{t=1}^{n}\exp(-z_t\gamma)X_t'y_t.$$

Sampling from (34) is simple since it is a k-variate normal distribution with mean B_1 and variance H_1. However, since the J-variate distribution (33) does not take the form of any standard density, it is not easy to sample from (33).

In this case, the MH algorithm discussed in Section 11.7.3 can be used within the Gibbs sampler. See Tierney (1994) and Chib and Greeberg (1995) for a general discussion.

Let γ_{i-1} be the $(i-1)$th random draw of γ and γ^* be a candidate of the ith random draw of γ.

The MH algorithm utilizes another appropriate distribution function $f_*(\gamma|\gamma_i)$, which is called the sampling density or the proposal density.

Let us define the acceptance rate $\omega(\gamma_{i-1}, \gamma^*)$ as:

$$\omega(\gamma_{i-1}, \gamma^*) = \min\left(\frac{f_{\gamma|\beta}(\gamma^*|\beta_{i-1}, Y_n)/f_*(\gamma^*|\gamma_{i-1})}{f_{\gamma|\beta}(\gamma_{i-1}|\beta_{i-1}, Y_n)/f_*(\gamma_{i-1}|\gamma^*)},\ 1\right).$$

The sampling procedure based on the MH algorithm within Gibbs sampling is as follows:

(i) Set the initial value β_{-M}, which may be taken as $\hat{\beta}_{M2SE}$ or $\hat{\beta}_{MLE}$.

(ii) Given β_{i-1}, generate a random draw of γ, denoted by γ_i, from the conditional density $f_{\gamma|\beta}(\gamma|\beta_{i-1}, Y_n)$, where the MH algorithm is utilized for random number generation because it is not easy to generate random draws of γ from (33).

The Metropolis-Hastings algorithm is implemented as follows:

(a) Given γ_{i-1}, generate a random draw γ^* from $f_*(\cdot|\gamma_{i-1})$ and compute the acceptance rate $\omega(\gamma_{i-1}, \gamma^*)$.

We will discuss later about the sampling density $f_*(\gamma|\gamma_{i-1})$.

(b) Set $\gamma_i = \gamma^*$ with probability $\omega(\gamma_{i-1}, \gamma^*)$ and $\gamma_i = \gamma_{i-1}$ otherwise,

(iii) Given γ_i, generate a random draw of β, denoted by β_i, from the conditional density $f_{\beta|\gamma}(\beta|\gamma_i, Y_n)$, which is $\beta|\gamma_i, Y_n \sim N(B_1, H_1)$ as shown in (34).

(iv) Repeat (ii) and (iii) for $i = -M+1, -M+2, \cdots, N$.

Note that the iteration of Steps (ii) and (iii) corresponds to the Gibbs sampler, which iteration yields random draws of β and γ from the joint density $f_{\beta\gamma}(\beta, \gamma|Y_n)$ when i is large enough.

It is well known that convergence of the Gibbs sampler is slow when β is highly correlated with γ.

That is, a large number of random draws have to be generated in this case.

Therefore, depending on the underlying joint density, we have the case where the Gibbs sampler does not work at all.

For example, see Chib and Greenberg (1995) for convergence of the Gibbs sampler.

In the model represented by (25) and (26), however, there is asymptotically no correlation between $\hat{\beta}_{MLE}$ and $\hat{\gamma}_{MLE}$, as shown in (31).

It might be expected that correlation between $\hat{\beta}_{MLE}$ and $\hat{\gamma}_{MLE}$ is not too high even in the small sample.

Therefore, it might be appropriate to consider that the Gibbs sampler works well in this model.

In Step (ii), the sampling density $f_*(\gamma|\gamma_{i-1})$ is utilized.

We consider the multivariate normal density function for the sampling distribution, which is discussed as follows.

Choice of the Sampling Density in Step (ii): Several generic choices of the sampling density are discussed by Tierney (1994) and Chib and Greenberg (1995).

Here, we take $f_*(\gamma|\gamma_{i-1}) = f_*(\gamma)$ as the sampling density, which is called the independence chain because the sampling density is not a function of γ_{i-1}.

We consider taking the multivariate normal sampling density in the independence MH algorithm, because of its simplicity.

Therefore, $f_*(\gamma)$ is taken as follows:

$$f_*(\gamma) = N(\gamma^+, c^2\Sigma^+), \tag{35}$$

which represents the J-variate normal distribution with mean γ^+ and variance $c^2\Sigma^+$.

The tuning parameter c is introduced into the sampling density (35).

We have mentioned that for the independence chain (Sampling Density I) the sampling density with the variance which gives us the maximum acceptance probability is not necessarily the best choice.

From some Monte Carlo experiments, we have obtained the result that the sampling density with the 1.5 – 2.5 times larger standard error is better than that with the standard error which maximizes the acceptance probability.

Therefore, $c = 2$ is taken in the next section, and it is the larger value than the c which gives us the maximum acceptance probability.

This detail discussion is given in Section 12.1.4.

Thus, the sampling density of γ is normally distributed with mean γ^+ and variance $c^2\Sigma^+$.

As for (γ^+, Σ^+), in the next section we choose one of $(\hat{\gamma}_{M2SE}, \Sigma_{M2SE})$ and $(\hat{\gamma}_{MLE}, \Sigma_{MLE})$ from the criterion of the acceptance rate.

As shown in Section 2, both of the two estimators $\hat{\gamma}_{M2SE}$ and $\hat{\gamma}_{MLE}$ are consistent estimates of γ.

Therefore, it might be very plausible to consider that the sampling density is distributed around the consistent estimates.

Bayesian Estimator: From the convergence theory of the Gibbs sampler and the MH algorithm, as i goes to infinity we can regard γ_i and β_i as random draws from the target density $f_{\beta\gamma}(\beta, \gamma|Y_n)$.

Let M be a sufficiently large number. γ_i and β_i for $i = 1, 2, \cdots, N$ are taken as the random draws from the posterior density $f_{\beta\gamma}(\beta, \gamma|Y_n)$.

Therefore, the Bayesian estimators $\hat{\gamma}_{BZZ}$ and $\hat{\beta}_{BZZ}$ are given by:

$$\hat{\gamma}_{BZZ} = \frac{1}{N}\sum_{i=1}^{N}\gamma_i, \qquad \hat{\beta}_{BZZ} = \frac{1}{N}\sum_{i=1}^{N}\beta_i,$$

where we read the subscript BZZ as the Bayesian estimator which uses the multivariate normal sampling density with mean $\hat{\gamma}_{ZZ}$ and variance Σ_{ZZ}. ZZ takes M2SE or MLE.

We consider two kinds of candidates of the sampling density for the Bayesian estimator, which are denoted by BM2SE and BMLE.

Thus, in Section 12.1.4, we compare the two Bayesian estimators (i.e, BM2SE and BMLE) with the two traditional estimators (i.e., M2SE and MLE).

12.1.4 Monte Carlo Study

Setup of the Model: In the Monte Carlo study, we consider using the artificially simulated data, in which the true data generating process (DGP) is presented in Judge, Hill, Griffiths and Lee (1980, p.156).

The DGP is defined as:

$$y_t = \beta_1 + \beta_2 x_{2,t} + \beta_3 x_{3,t} + u_t, \tag{36}$$

where u_t, $t = 1, 2, \cdots, n$, are normally and independently distributed with $\mathrm{E}(u_t) = 0$, $\mathrm{E}(u_t^2) = \sigma_t^2$ and,

$$\sigma_t^2 = \exp(\gamma_1 + \gamma_2 x_{2,t}), \qquad \text{for } t = 1, 2, \cdots, n. \tag{37}$$

As it is discussed in Judge, Hill, Griffiths and Lee (1980), the parameter values are set to be $(\beta_1, \beta_2, \beta_3, \gamma_1, \gamma_2) = (10, 1, 1, -2, 0.25)$.

From (36) and (37), Judge, Hill, Griffiths and Lee (1980, pp.160 – 165) generated one hundred samples of y with $n = 20$.

In the Monte Carlo study, we utilize $x_{2,t}$ and $x_{3,t}$ given in Judge, Hill, Griffiths and Lee (1980, pp.156), which is shown in Table 2, and generate G samples of y_t given the X_t for $t = 1, 2, \cdots, n$.

That is, we perform G simulation runs for each estimator, where $G = 10^4$ is taken.

The simulation procedure is as follows:

(i) Given γ and $x_{2,t}$ for $t = 1, 2, \cdots, n$, generate random numbers of u_t for $t = 1, 2, \cdots, n$, based on the assumptions: $u_t \sim N(0, \sigma_t^2)$, where $(\gamma_1, \gamma_2) = (-2, 0.25)$ and $\sigma_t^2 = \exp(\gamma_1 + \gamma_2 x_{2,t})$ are taken.

(ii) Given β, $(x_{2,t}, x_{3,t})$ and u_t for $t = 1, 2, \cdots, n$, we obtain a set of data y_t, $t = 1, 2, \cdots, n$, from equation (36), where $(\beta_1, \beta_2, \beta_3) = (10, 1, 1)$ is assumed.

Table 2: The Exogenous Variables $x_{1,t}$ and $x_{2,t}$

t	1	2	3	4	5	6	7	8	9	10
$x_{2,t}$	14.53	15.30	15.92	17.41	18.37	18.83	18.84	19.71	20.01	20.26
$x_{3,t}$	16.74	16.81	19.50	22.12	22.34	17.47	20.24	20.37	12.71	22.98
t	11	12	13	14	15	16	17	18	19	20
$x_{2,t}$	20.77	21.17	21.34	22.91	22.96	23.69	24.82	25.54	25.63	28.73
$x_{3,t}$	19.33	17.04	16.74	19.81	31.92	26.31	25.93	21.96	24.05	25.66

(iii) Given (y_t, X_t) for $t = 1, 2, \cdots, n$, perform M2SE, MLE, BM2SE and BMLE discussed in Sections 12.1.2 and 12.1.3 in order to obtain the estimates of $\theta = (\beta, \gamma)$, denoted by $\hat{\theta}$.

Note that $\hat{\theta}$ takes $\hat{\theta}_{M2SE}$, $\hat{\theta}_{MLE}$, $\hat{\theta}_{BM2SE}$ and $\hat{\theta}_{BMLE}$.

(iv) Repeat (i) – (iii) G times, where $G = 10^4$ is taken as mentioned above.

(v) From G estimates of θ, compute the arithmetic average (AVE), the root mean square error (RMSE), the first quartile (25%), the median (50%), the third quartile (75%) and the interquartile range (IR) for each estimator.

AVE and RMSE are obtained as follows:

$$\text{AVE} = \frac{1}{G}\sum_{g=1}^{G}\hat{\theta}_j^{(g)}, \qquad \text{RMSE} = \left(\frac{1}{G}\sum_{g=1}^{G}(\hat{\theta}_j^{(g)} - \theta_j)^2\right)^{1/2},$$

for $j = 1, 2, \cdots, 5$, where θ_j denotes the jth element of θ and $\hat{\theta}_j^{(g)}$ represents the j-element of $\hat{\theta}$ in the gth simulation run.

As mentioned above, $\hat{\theta}$ denotes the estimate of θ, where $\hat{\theta}$ takes $\hat{\theta}_{M2SE}$, $\hat{\theta}_{MLE}$, $\hat{\theta}_{BM2SE}$ and $\hat{\theta}_{BMLE}$.

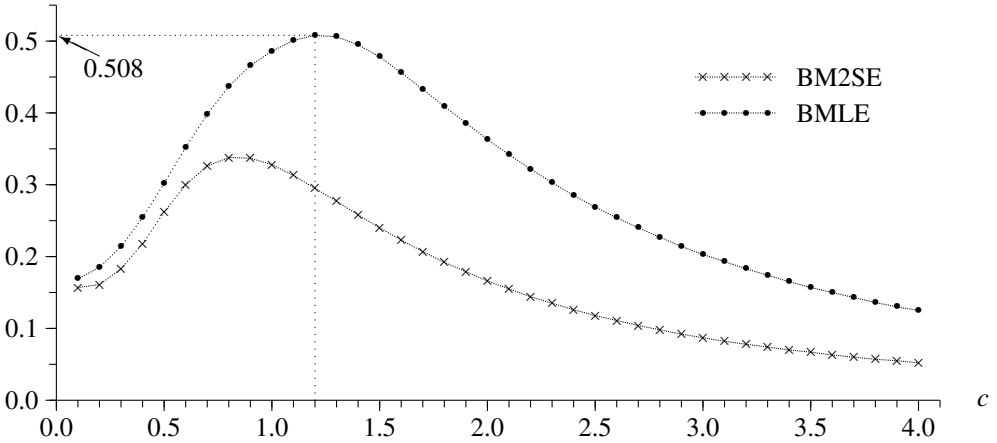
Choice of (γ^+, Σ^+) and c: For the Bayesian approach, depending on (γ^+, Σ^+) we have BM2SE and BMLE, which denote the Bayesian estimators using the multivariate normal sampling density whose mean and covariance matrix are calibrated on the basis of M2SE or MLE.

We consider the following sampling density: $f_*(\gamma) = N(\gamma^+, c^2\Sigma^+)$, where c denotes the tuning parameter and (γ^+, Σ^+) takes $(\gamma_{M2SE}, \Sigma_{M2SE})$ or $(\gamma_{MLE}, \Sigma_{MLE})$.

Generally, for choice of the sampling density, the sampling density should not have too large variance and too small variance.

Chib and Greenberg (1995) pointed out that if standard deviation of the sampling density is too low,

Figure 2: Acceptance Rates in Average: $M = 5000$ and $N = 10^4$



the Metropolis steps are too short and move too slowly within the target distribution; if it is too high, the algorithm almost always rejects and stays in the same place.

The sampling density should be chosen so that the chain travels over the support of the target density. First, we consider choosing (γ^+, Σ^+) and c which maximizes the arithmetic average of the acceptance rates obtained from G simulation runs.

The results are in Figure 2, where $n = 20$, $M = 5000$, $N = 10^4$, $G = 10^4$ and $c = 0.1, 0.2, \cdots, 4.0$ are taken (choice of N and M is discussed in Appendix of Section 12.1.6).

In the case of $(\gamma^+, \Sigma^+) = (\gamma_{MLE}, \Sigma_{MLE})$ and $c = 1.2$, the acceptance rate in average is 0.5078, which gives us the largest one.

It is important to reduce positive correlation between γ_i and γ_{i-1} and keep randomness.

Therefore, $(\gamma^+, \Sigma^+) = (\gamma_{MLE}, \Sigma_{MLE})$ is adopted, rather than $(\gamma^+, \Sigma^+) = (\gamma_{M2SE}, \Sigma_{M2SE})$, because BMLE has a larger acceptance probability than BM2SE for all c (see Figure 2).

However, the sampling density with the largest acceptance probability is not necessarily the best choice.

We have the result that the optimal standard error should be 1.5 – 2.5 times larger than the standard error which gives us the largest acceptance probability.

Here, $(\gamma^+, \Sigma^+) = (\gamma_{MLE}, \Sigma_{MLE})$ and $c = 2$ are taken.

When c is larger than 2, both the estimates and their standard errors become stable although here we do not show these facts.

Therefore, in this Monte Carlo study, $f_*(\gamma) = N(\gamma_{MLE}, 2^2\Sigma_{MLE})$ is chosen for the sampling density.

Hereafter, we compare BMLE with M2SE and MLE (i.e., we do not consider BM2SE anymore).

As for computational CPU time, the case of $n = 20$, $M = 5000$, $N = 10^4$ and $G = 10^4$ takes about 76 minutes for each of $c = 0.1, 0.2, \cdots, 4.0$ and each of BM2SE and BMLE, where Dual Pentium III 1GHz CPU, Microsoft Windows 2000 Professional Operating System and Open Watcom FORTRAN 77/32 Optimizing Compiler (Version 1.0) are utilized.

Note that WATCOM Fortran 77 Compiler is downloaded from

`http://www.openwatcom.org/`.

Results and Discussion: Through Monte Carlo simulation studies, the Bayesian estimator (i.e., BMLE) is compared with the traditional estimators (i.e., M2SE and MLE).

The arithmetic mean (AVE) and the root mean square error (RMSE) have been usually used in Monte Carlo study.

Moreover, for comparison with the standard normal distribution, Skewness and Kurtosis are also computed.

Moments of the parameters are needed in the calculation of AVE, RMSE, Skewness and Kurtosis.

However, we cannot assure that these moments actually exist.

Therefore, in addition to AVE and RMSE, we also present values for quartiles, i.e., the first quartile (25%), median (50%), the third quartile (75%) and the interquartile range (IR).

Thus, for each estimator, AVE, RMSE, Skewness, Kurtosis, 25%, 50%, 75% and IR are computed from G simulation runs.

The results are given in Table 3, where BMLE is compared with M2SE and MLE.

The case of $n = 20$, $M = 5000$ and $N = 10^4$ is examined in Table 3.

A discussion on choice of M and N is given in Appendix 12.1.6, where we examine whether $M = 5000$ and $N = 10^4$ are sufficient.

Table 3: The AVE, RMSE and Quartiles: $n = 20$

		β_1	β_2	β_3	γ_1	γ_2
	True Value	10	1	1	−2	0.25
M2SE	AVE	10.064	0.995	1.002	−0.988	0.199
	RMSE	7.537	0.418	0.333	3.059	0.146
	Skewness	0.062	−0.013	−0.010	−0.101	−0.086
	Kurtosis	4.005	3.941	2.988	3.519	3.572
	25%	5.208	0.728	0.778	−2.807	0.113
	50%	10.044	0.995	1.003	−0.934	0.200
	75%	14.958	1.261	1.227	0.889	0.287
	IR	9.751	0.534	0.449	3.697	0.175

Table 3: The AVE, RMSE and Quartiles: $n = 20$ — Cont.

		β_1	β_2	β_3	γ_1	γ_2
	True Value	10	1	1	−2	0.25
MLE	AVE	10.029	0.997	1.002	−2.753	0.272
	RMSE	7.044	0.386	0.332	2.999	0.139
	Skewness	0.081	−0.023	−0.014	0.006	−0.160
	Kurtosis	4.062	3.621	2.965	4.620	4.801
	25%	5.323	0.741	0.775	−4.514	0.189
	50%	10.056	0.998	1.002	−2.710	0.273
	75%	14.641	1.249	1.229	−0.958	0.355
	IR	9.318	0.509	0.454	3.556	0.165
	True Value	10	1	1	−2	0.25
BMLE	AVE	10.034	0.996	1.002	−2.011	0.250
	RMSE	6.799	0.380	0.328	2.492	0.117
	Skewness	0.055	−0.016	−0.013	−0.016	−0.155
	Kurtosis	3.451	3.340	2.962	3.805	3.897
	25%	5.413	0.745	0.778	−3.584	0.176
	50%	10.041	0.996	1.002	−1.993	0.252
	75%	14.538	1.246	1.226	−0.407	0.325
	IR	9.125	0.501	0.448	3.177	0.150

$c = 2.0$, $M = 5000$ and $N = 10^4$ are chosen for BMLE

First, we compare the two traditional estimators, i.e., M2SE and MLE.

Judge, Hill, Griffiths and Lee (1980, pp.141–142) indicated that 2SE of γ_1 is inconsistent although 2SE of the other parameters is consistent but asymptotically inefficient.

For M2SE, the estimate of γ_1 is modified to be consistent.

But M2SE is still asymptotically inefficient while MLE is consistent and asymptotically efficient.

Therefore, for γ, MLE should have better performance than M2SE in the sense of efficiency.

In Table 3, for all the parameters except for IR of β_3, RMSE and IR of MLE are smaller than those of M2SE.

For both M2SE and MLE, AVEs of β are close to the true parameter values.

Therefore, it might be concluded that M2SE and MLE are unbiased for β even in the case of small sample.

However, the estimates of γ are different from the true values for both M2SE and MLE.

That is, AVE and 50% of γ_1 are -0.988 and -0.934 for M2SE, and -2.753 and -2.710 for MLE, which are far from the true value -2.0.

Similarly, AVE and 50% of γ_2 are 0.199 and 0.200 for M2SE, which are different from the true value 0.25.

But 0.272 and 0.273 for MLE are slightly larger than 0.25 and they are close to 0.25.

Thus, the traditional estimators work well for the regression coefficients β but not for the heteroscedasticity parameters γ.

Next, the Bayesian estimator (i.e., BMLE) is compared with the traditional ones (i.e., M2SE and MLE).

For all the parameters of β, we can find from Table 3 that BMLE shows better performance in RMSE and IR than the traditional estimators, because RMSE and IR of BMLE are smaller than those of M2SE and MLE.

Furthermore, from AVEs of BMLE, we can see that the heteroscedasticity parameters as well as the regression coefficients are unbiased in the small sample.

Thus, Table 3 also shows the evidence that for both β and γ, AVE and 50% of BMLE are very close to the true parameter values.

The values of RMSE and IR also indicate that the estimates are concentrated around the AVE and 50%, which are vary close to the true parameter values.

For the regression coefficient β, all of the three estimators are very close to the true parameter values. However, for the heteroscedasticity parameter γ, BMLE shows a good performance but M2SE and

MLE are poor.

The larger values of RMSE for the traditional counterparts may be due to "outliers" encountered with the Monte Carlo experiments.

This problem is also indicated in Zellner (1971, pp.281).

Compared with the traditional counterparts, the Bayesian approach is not characterized by extreme values for posterior modal values.

Now we compare empirical distributions for M2SE, MLE and BMLE in Figures 3 – 7.

For the posterior densities of β_1 (Figure 3), β_2 (Figure 4), β_3 (Figure 5) and γ_1 (Figure 6), all of M2SE, MLE and BMLE are almost symmetric (also, see Skewness in Table 3).

For the posterior density of γ_2 (Figure 7), both MLE and BMLE are slightly skewed to the left because Skewness of γ_2 in Table 3 is negative, while M2SE is almost symmetric.

As for Kurtosis, all the empirical distributions except for β_3 have a sharp kurtosis and fat tails, compared with the normal distribution.

Especially, for the heteroscedasticity parameters γ_1 and γ_2, MLE has the largest kurtosis of the three.

For all figures, location of the empirical distributions indicates whether the estimators are unbiased or not.

Figure 3: Empirical Distributions of β_1

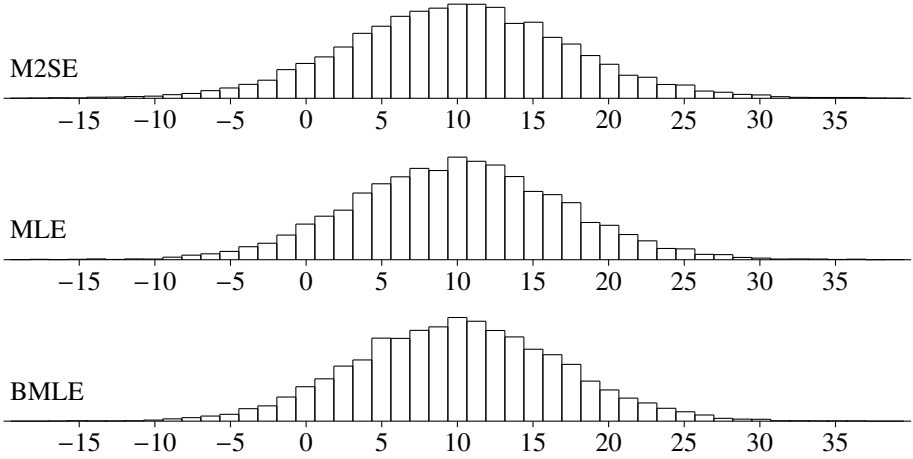


Figure 4: Empirical Distributions of β_2

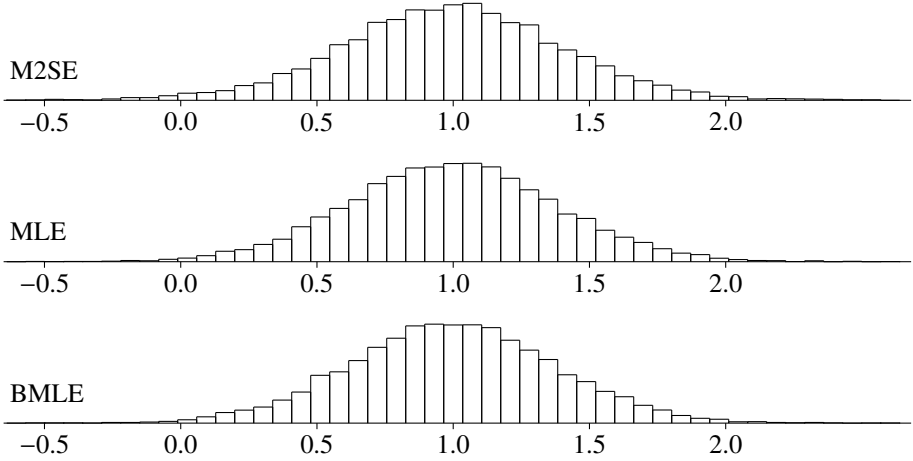


Figure 5: Empirical Distributions of β_3

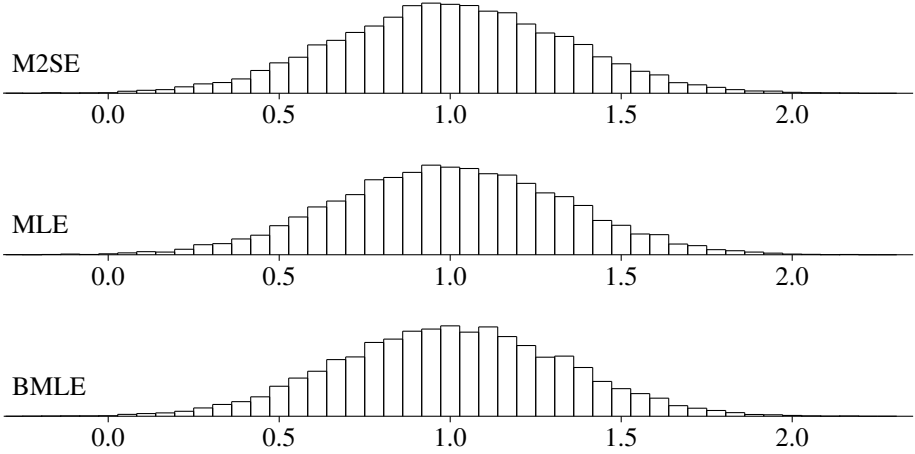


Figure 6: Empirical Distributions of γ_1

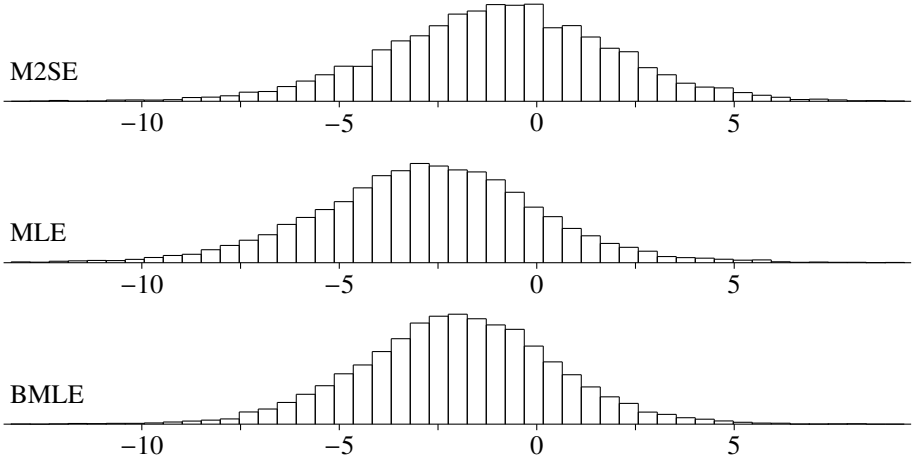
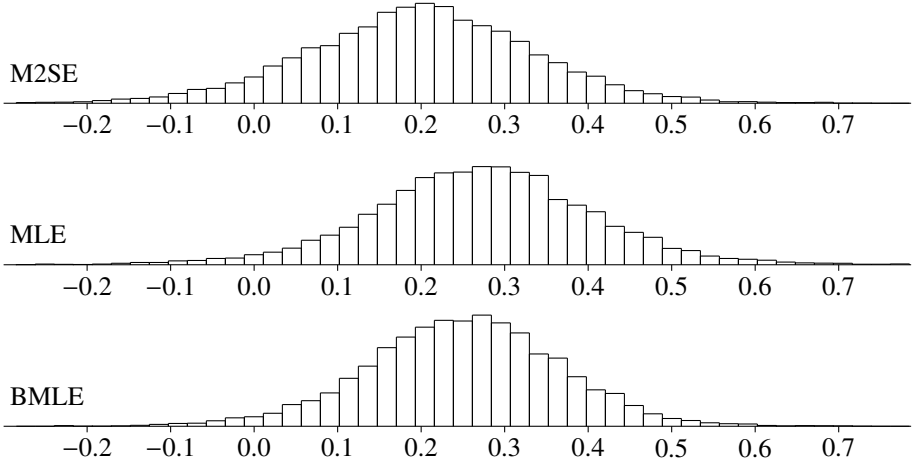


Figure 7: Empirical Distributions of γ_2



For β_1 in Figure 3, β_2 in Figure 4 and β_3 in Figure 5, M2SE is biased while MLE and BMLE are distributed around the true value.

For γ_1 in Figure 6 and γ_2 in Figure 7, the empirical distributions of M2SE, MLE and BMLE are quite different.

For γ_1 in Figure 6, M2SE is located in the right-hand side of the true parameter value, MLE is in the left-hand side, and BMLE is also slightly in the left-hand side.

Moreover, for γ_2 in Figure 7, M2SE is downward-biased, MLE is overestimated, and BMLE is distributed around the true parameter value.

On the Sample Size *n*: Finally, we examine how the sample size n influences precision of the parameter estimates.

Since we utilize the exogenous variable X shown in Judge, Hill, Griffiths and Lee (1980), we cannot examine the case where n is greater than 20.

In order to see the effect of the sample size n, here the case of $n = 15$ is compared with that of $n = 20$.

The case $n = 15$ of BMLE is shown in Table 4, which should be compared with BMLE in Table 3.

As a result, all the AVEs are very close to the corresponding true parameter values.

Therefore, we can conclude from Tables 3 and 4 that the Bayesian estimator is unbiased even in the small sample such as $n = 15, 20$.

However, RMSE and IR become large as n decreases.

That is, for example, RMSEs of $\beta_1, \beta_2, \beta_3, \gamma_1$ and γ_2 are given by 6.799, 0.380, 0.328, 2.492 and 0.117 in Table 3, and 8.715, 0.455, 0.350, 4.449 and 0.228 in Table 4.

Thus, we can see that RMSE and IR decrease as n is large.

Table 4: BMLE: $n = 15$, $c = 2.0$, $M = 5000$ and $N = 10^4$

	β_1	β_2	β_3	γ_1	γ_2
True Value	10	1	1	−2	0.25
AVE	10.060	0.995	1.002	−2.086	0.252
RMSE	8.715	0.455	0.350	4.449	0.228
Skewness	0.014	0.033	−0.064	−0.460	0.308
Kurtosis	3.960	3.667	3.140	4.714	4.604
25%	4.420	0.702	0.772	−4.725	0.107
50%	10.053	0.995	1.004	−1.832	0.245
75%	15.505	1.284	1.237	0.821	0.391
IR	11.085	0.581	0.465	5.547	0.284

12.1.5 Summary

In Section 12.1, we have examined the multiplicative heteroscedasticity model discussed by Harvey (1976), where the two traditional estimators are compared with the Bayesian estimator.

For the Bayesian approach, we have evaluated the posterior mean by generating random draws from the posterior density, where the Markov chain Monte Carlo methods (i.e., the MH within Gibbs algorithm) are utilized.

In the MH algorithm, the sampling density has to be specified.

We examine the multivariate normal sampling density, which is the independence chain in the MH algorithm.

For mean and variance in the sampling density, we consider using the mean and variance estimated by the two traditional estimators (i.e., M2SE and MLE).

The Bayesian estimators with M2SE and MLE are called BM2SE and BMLE in Section 12.1.

Through the Monte Carlo studies, the results are summarized as follows:

(i) We compare BM2SE and BMLE with respect to the acceptance rates in the MH algorithm.

In this case, BMLE shows higher acceptance rates than BM2SE for all c, which is shown in Figure 2.

For the sampling density, we utilize the independence chain through Section 12.1.

The high acceptance rate implies that the chain travels over the support of the target density.

For the Bayesian estimator, therefore, BMLE is preferred to BM2SE.

However, note as follows.

The sampling density which yields the highest acceptance rate is not necessarily the best choice and the tuning parameter c should be larger than the value which gives us the maximum acceptance rate.

Therefore, we have focused on BMLE with $c = 2$ (remember that BMLE with $c = 1.2$ yields the maximum acceptance rate).

(ii) For the traditional estimators (i.e., M2SE and MLE), we have obtained the result that MLE has smaller RMSE than M2SE for all the parameters, because for one reason the M2SE is asymptotically less efficient than the MLE.

Furthermore, for M2SE, the estimates of β are unbiased but those of γ are different from the true parameter values (see Table 3).

(iii) From Table 3, BMLE performs better than the two traditional estimators in the sense of RMSE and IR, because RMSE and IR of BMLE are smaller than those of the traditional ones for all the cases.

(iv) Each empirical distribution is displayed in Figures 3 – 7.

The posterior densities of almost all the estimates are distributed to be symmetric (γ_2 is slightly skewed to the left), but the posterior densities of both the regression coefficients (except for β_3) and the heteroscedasticity parameters have fat tails.

Also, see Table 3 for skewness and kurtosis.

(v) As for BMLE, the case of $n = 15$ is compared with $n = 20$.

The case $n = 20$ has smaller RMSE and IR than $n = 15$, while AVE and 50% are close to the true parameter values for β and γ.

Therefore, it might be expected that the estimates of BMLE go to the true parameter values as n is large.

12.1.6 Appendix: Are $M = 5000$ and $N = 10^4$ Sufficient?

Table 5: BMLE: $n = 20$ and $c = 2.0$

	True Value	β_1 10	β_2 1	β_3 1	γ_1 −2	γ_2 0.25
$M = 1000$ $N = 10^4$	AVE	10.028	0.997	1.002	−2.008	0.250
	RMSE	6.807	0.380	0.328	2.495	0.117
	Skewness	0.041	−0.007	−0.012	0.017	−0.186
	Kurtosis	3.542	3.358	2.963	3.950	4.042
	25%	5.413	0.745	0.778	−3.592	0.176
	50%	10.027	0.996	1.002	−1.998	0.252
	75%	14.539	1.245	1.226	−0.405	0.326
	IR	9.127	0.500	0.448	3.187	0.150

Table 5: BMLE: $n = 20$ and $c = 2.0$ — Cont.

	True Value	β_1 10	β_2 1	β_3 1	γ_1 −2	γ_2 0.25
$M = 5000$ $N = 5000$	AVE	10.033	0.996	1.002	−2.010	0.250
	RMSE	6.799	0.380	0.328	2.491	0.117
	Skewness	0.059	−0.016	−0.011	−0.024	−0.146
	Kurtosis	3.498	3.347	2.961	3.764	3.840
	25%	5.431	0.747	0.778	−3.586	0.176
	50%	10.044	0.995	1.002	−1.997	0.252
	75%	14.532	1.246	1.225	−0.406	0.326
	IR	9.101	0.499	0.447	3.180	0.149

In Section 12.1.4, only the case of $(M, N) = (5000, 10^4)$ is examined.

In this appendix, we check whether $M = 5000$ and $N = 10^4$ are sufficient.

For the burn-in period M, there are some diagnostic tests, which are discussed in Geweke (1992) and

Mengersen, Robert and Guihenneuc-Jouyaux (1999).

However, since their tests are applicable in the case of one sample path, we cannot utilize them.

Because G simulation runs are implemented in Section 12.1.4 (see p.425 for the simulation procedure), we have G test statistics if we apply the tests.

It is difficult to evaluate G testing results at the same time.

Therefore, we consider using the alternative approach to see if $M = 5000$ and $N = 10^4$ are sufficient.

For choice of M and N, we consider the following two issues.

(i) Given fixed $M = 5000$, compare $N = 5000$ and $N = 10^4$.

(ii) Given fixed $N = 10^4$, compare $M = 1000$ and $M = 5000$.

(i) examines whether $N = 5000$ is sufficiently large, while (ii) checks whether $M = 1000$ is large enough. If the case of $(M, N) = (5000, 5000)$ is close to that of $(M, N) = (5000, 10^4)$, we can conclude that $N = 5000$ is sufficiently large.

Similarly, if the case of $(M, N) = (1000, 10^4)$ is not too different from that of $(M, N) = (5000, 10^4)$, it might be concluded that $M = 1000$ is also sufficient.

The results are in Table 5, where AVE, RMSE, Skewness, Kurtosis, 25%, 50%, 75% and IR are shown

for each of the regression coefficients and the heteroscedasticity parameters.

BMLE in Table 3 should be compared with Table 5.

From Tables 3 and 5, the three cases, i.e., $(M, N) = (5000, 10^4)$, $(1000, 10^4)$, $(5000, 5000)$, are very close to each other.

Therefore, we can conclude that both $M = 1000$ and $N = 5000$ are large enough in the simulation study shown in Section 12.1.4.

We take the case of $M = 5000$ and $N = 10^4$ for safety in Section 12.1.4, although we obtain the results that both $M = 1000$ and $N = 5000$ are large enough.

12.2 Autocorrelation Model

In the previous section, we have considered estimating the regression model with the heteroscedastic error term, where the traditional estimators such as MLE and M2SE are compared with the Bayesian estimators.

In this section, using both the maximum likelihood estimator and the Bayes estimator, we consider the regression model with the first order autocorrelated error term, where the initial distribution of the autocorrelated error is taken into account.

As for the autocorrelated error term, the stationary case is assumed, i.e., the autocorrelation coefficient is assumed to be less than one in absolute value.

The traditional estimator (i.e., MLE) is compared with the Bayesian estimator. Utilizing the Gibbs sampler, Chib (1993) discussed the regression model with the autocorrelated error term in a Bayesian framework, where the initial condition of the autoregressive process is not taken into account.

In this section, taking into account the initial density, we compare the maximum likelihood estimator and the Bayesian estimator.

For the Bayes estimator, the Gibbs sampler and the Metropolis-Hastings algorithm are utilized to obtain random draws of the parameters.

As a result, the Bayes estimator is less biased and more efficient than the maximum likelihood estimator. Especially, for the autocorrelation coefficient, the Bayes estimate is much less biased than the maximum likelihood estimate.

Accordingly, for the standard error of the estimated regression coefficient, the Bayes estimate is more plausible than the maximum likelihood estimate.

12.2.1 Introduction

In Section 12.2, we consider the regression model with the first order autocorrelated error term, where the error term is assumed to be stationary, i.e., the autocorrelation coefficient is assumed to be less than one in absolute value.

The traditional estimator, i.e., the maximum likelihood estimator (MLE), is compared with the Bayes estimator (BE).

Utilizing the Gibbs sampler, Chib (1993) and Chib and Greenberg (1994) discussed the regression model with the autocorrelated error term in a Bayesian framework, where the initial condition of the autoregressive process is ignored.

Here, taking into account the initial density, we compare MLE and BE, where the Gibbs sampler and the Metropolis-Hastings (MH) algorithm are utilized in BE.

As for MLE, it is well known that the autocorrelation coefficient is underestimated in small sample and therefore that variance of the estimated regression coefficient is also biased.

See, for example, Andrews (1993) and Tanizaki (2000, 2001).

Under this situation, inference on the regression coefficient is not appropriate, because variance of the

estimated regression coefficient depends on the estimated autocorrelation coefficient.

We show in Section 12.2 that BE is superior to MLE because BEs of both the autocorrelation coefficient and the variance of the error term are closer to the true values, compared with MLEs.

12.2.2 Setup of the Model

Let X_t be a $1 \times k$ vector of exogenous variables and β be a $k \times 1$ parameter vector.

Consider the following regression model:

$$y_t = X_t\beta + u_t, \qquad u_t = \rho u_{t-1} + \epsilon_t, \qquad \epsilon_t \sim N(0, \sigma_\epsilon^2),$$

for $t = 1, 2, \cdots, n$, where $\epsilon_1, \epsilon_2, \cdots, \epsilon_n$ are assumed to be mutually independently distributed.

In this model, the parameter to be estimated is given by $\theta = (\beta, \rho, \sigma_\epsilon^2)$.

The unconditional density of y_t is:

$$f(y_t|\beta, \rho, \sigma_\epsilon^2) = \frac{1}{\sqrt{2\pi\sigma_\epsilon^2/(1-\rho^2)}} \exp\Big(-\frac{1}{2\sigma_\epsilon^2/(1-\rho^2)}(y_t - X_t\beta)^2\Big).$$

Let Y_t be the information set up to time t, i.e., $Y_t = \{y_t, y_{t-1}, \cdots, y_1\}$.

The conditional density of y_t given Y_{t-1} is:

$$\begin{aligned} f(y_t|Y_{t-1},\beta,\rho,\sigma_\epsilon^2) &= f(y_t|y_{t-1},\beta,\rho,\sigma_\epsilon^2) \\ &= \frac{1}{\sqrt{2\pi\sigma_\epsilon^2}}\exp\Big(-\frac{1}{2\sigma_\epsilon^2}\big((y_t-\rho y_{t-1})-(X_t-\rho X_{t-1})\beta\big)^2\Big). \end{aligned}$$

Therefore, the joint density of Y_n, i.e., the likelihood function, is given by :

$$\begin{aligned} f(Y_n|\beta,\rho,\sigma_\epsilon^2) &= f(y_1|\beta,\rho,\sigma_\epsilon^2)\prod_{t=2}^{n} f(y_t|Y_{t-1},\beta,\rho,\sigma_\epsilon^2) \\ &= (2\pi\sigma_\epsilon^2)^{-n/2}(1-\rho^2)^{1/2}\exp\Big(-\frac{1}{2\sigma_\epsilon^2}\sum_{t=1}^{n}(y_t^*-X_t^*\beta)^2\Big), \end{aligned} \tag{38}$$

where y_t^* and X_t^* represent the following transformed variables:

$$y_t^* = y_t^*(\rho) = \begin{cases} \sqrt{1-\rho^2}\,y_t, & \text{for } t=1, \\ y_t-\rho y_{t-1}, & \text{for } t=2,3,\cdots,n, \end{cases}$$

$$X_t^* = X_t^*(\rho) = \begin{cases} \sqrt{1-\rho^2}\,X_t, & \text{for } t=1, \\ X_t-\rho X_{t-1}, & \text{for } t=2,3,\cdots,n, \end{cases}$$

which depend on the autocorrelation coefficient ρ.

Maximum Likelihood Estimator: We have shown above that the likelihood function is given by equation (38).

Maximizing equation (38) with respect to β and σ_ϵ^2, we obtain the following expressions:

$$\hat{\beta} \equiv \hat{\beta}(\rho) = (\sum_{t=1}^{n} X_t^{*\prime} X_t^*)^{-1} \sum_{t=1}^{n} X_t^{*\prime} y_t^*,$$
$$\hat{\sigma}_\epsilon^2 \equiv \hat{\sigma}_\epsilon^2(\rho) = \frac{1}{n} \sum_{t=1}^{n} (y_t^* - X_t^* \hat{\beta})^2. \tag{39}$$

By substituting $\hat{\beta}$ and $\hat{\sigma}_\epsilon^2$ into β and σ_ϵ^2 in equation (38), we have the concentrated likelihood function:

$$f(Y_n|\hat{\beta}, \rho, \hat{\sigma}_\epsilon^2) = \Big(2\pi\hat{\sigma}_\epsilon^2(\rho)\Big)^{-n/2} (1-\rho^2)^{1/2} \exp\Big(-\frac{n}{2}\Big), \tag{40}$$

which is a function of ρ.

Equation (40) has to be maximized with respect to ρ.

In the next section, we obtain the maximum likelihood estimate of ρ by a simple grid search, in which the concentrated likelihood function (40) is maximized by changing the parameter value of ρ by 0.0001 in the interval between -0.9999 and 0.9999.

Once the solution of ρ, denoted by $\hat{\rho}$, is obtained, $\hat{\beta}(\hat{\rho})$ and $\hat{\sigma}_\epsilon^2(\hat{\rho})$ lead to the maximum likelihood estimates of β and σ_ϵ^2.

Hereafter, $\hat{\beta}$, $\hat{\sigma}_\epsilon^2$ and $\hat{\rho}$ are taken as the maximum likelihood estimates of β, σ_ϵ^2 and ρ, i.e., $\hat{\beta}(\hat{\rho})$ and $\hat{\sigma}_\epsilon^2(\hat{\rho})$ are simply written as $\hat{\beta}$ and $\hat{\sigma}_\epsilon^2$.

Variance of the estimate of $\theta = (\beta', \sigma^2, \rho)'$ is asymptotically given by: $\mathrm{V}(\hat{\theta}) = I^{-1}(\theta)$, where $I(\theta)$ denotes the information matrix, which is represented as:

$$I(\theta) = -\mathrm{E}\left(\frac{\partial^2 \log f(Y_n|\theta)}{\partial\theta\partial\theta'}\right).$$

Therefore, variance of $\hat{\beta}$ is given by $\mathrm{V}(\hat{\beta}) = \sigma^2(\sum_{t=1}^n X_t^{*\prime} X_t^*)^{-1}$ in large sample, where ρ in X_t^* is replaced by $\hat{\rho}$, i.e., $X_t^* = X_t^*(\hat{\rho})$.

For example, suppose that X_t^* has a tendency to rise over time t and that we have $\rho > 0$.

If ρ is underestimated, then $\mathrm{V}(\hat{\beta})$ is also underestimated, which yields incorrect inference on the regression coefficient β.

Thus, unless ρ is properly estimated, the estimate of $\mathrm{V}(\hat{\beta})$ is also biased.

In large sample, $\hat{\rho}$ is a consistent estimator of ρ and therefore $\mathrm{V}(\hat{\beta})$ is not biased.

However, in small sample, since it is known that $\hat{\rho}$ is underestimated (see, for example, Andrews

(1993), Tanizaki (2000, 2001)), clearly $V(\hat{\beta})$ is also underestimated.

In addition to $\hat{\rho}$, the estimate of σ^2 also influences inference of β, because we have $V(\hat{\beta}) = \sigma^2(\sum_{t=1}^{n} X_t^{*\prime} X_t^*)^{-1}$ as mentioned above.

If σ^2 is underestimated, the estimated variance of β is also underestimated.

$\hat{\sigma}^2$ is a consistent estimator of σ^2 in large sample, but it is appropriate to consider that $\hat{\sigma}^2$ is biased in small sample, because $\hat{\sigma}^2$ is a function of $\hat{\rho}$ as in (39).

Therefore, the biased estimate of ρ gives us the serious problem on inference of β.

Bayesian Estimator: We assume that the prior density functions of β, ρ and σ_ϵ^2 are the following noninformative priors:

$$f_\beta(\beta) \propto \text{constant}, \qquad \text{for } -\infty < \beta < \infty, \tag{41}$$

$$f_\rho(\rho) \propto \text{constant}, \qquad \text{for } -1 < \rho < 1, \tag{42}$$

$$f_{\sigma_\epsilon}(\sigma_\epsilon^2) \propto \frac{1}{\sigma_\epsilon^2}, \qquad \text{for } 0 < \sigma_\epsilon^2 < \infty. \tag{43}$$

In equation (42), theoretically we should have $-1 < \rho < 1$.

As for the prior density of σ_ϵ^2, since we consider that $\log \sigma_\epsilon^2$ has the flat prior for $-\infty < \log \sigma_\epsilon^2 < \infty$, we obtain $f_{\sigma_\epsilon}(\sigma_\epsilon^2) \propto 1/\sigma_\epsilon^2$.

Note that in Section 12.1 the first element of the heteroscedasticity parameter γ is also assumed to be diffuse, where it is formulated as the logarithm of variance of the error term, i.e., $\log \sigma_\epsilon^2$.

Combining the four densities (38) and (41) – (43), the posterior density function of β, ρ and σ_ϵ^2, denoted by $f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n)$, is represented as follows:

$$
\begin{aligned}
& f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n) \\
& \quad \propto f(Y_n|\beta, \rho, \sigma_\epsilon^2) f_\beta(\beta) f_\rho(\rho) f_{\sigma_\epsilon}(\sigma_\epsilon^2) \\
& \quad \propto (\sigma_\epsilon^2)^{-(n/2+1)} (1-\rho^2)^{1/2} \exp\Big(-\frac{1}{2\sigma_\epsilon^2} \sum_{t=1}^{n} (y_t^* - X_t^*\beta)^2\Big). \qquad (44)
\end{aligned}
$$

We want to have random draws of β, ρ and σ_ϵ^2 given Y_n.

However, it is not easy to generate random draws of β, ρ and σ_ϵ^2 from $f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n)$.

Therefore, we perform the Gibbs sampler in this problem.

According to the Gibbs sampler, we can sample from the posterior density function (44), using the three conditional distributions $f_{\beta|\rho\sigma_\epsilon}(\beta|\rho, \sigma_\epsilon^2, Y_n)$, $f_{\rho|\beta\sigma_\epsilon}(\rho|\beta, \sigma_\epsilon^2, Y_n)$ and $f_{\sigma_\epsilon|\beta\rho}(\sigma_\epsilon^2|\beta, \rho, Y_n)$, which are

proportional to $f_{\beta\rho\sigma}(\beta, \rho, \sigma^2|Y_n)$ and are obtained as follows:

- $f_{\beta|\rho\sigma_\epsilon}(\beta|\rho, \sigma_\epsilon^2, Y_n)$ is given by:

$$
\begin{aligned}
& f_{\beta|\rho\sigma_\epsilon}(\beta|\rho, \sigma_\epsilon^2, Y_n) \\
& \quad \propto f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n) \propto \exp\Big(-\frac{1}{2\sigma_\epsilon^2}\sum_{t=1}^{n}(y_t^* - X_t^*\beta)^2\Big) \\
& \quad = \exp\Big(-\frac{1}{2\sigma_\epsilon^2}\sum_{t=1}^{n}\Big((y_t^* - X_t^*\hat{\beta}) - X_t(\beta - \hat{\beta})\Big)^2\Big) \\
& \quad = \exp\Big(-\frac{1}{2\sigma_\epsilon^2}\sum_{t=1}^{n}(y_t^* - X_t^*\hat{\beta})^2 - \frac{1}{2\sigma_\epsilon^2}(\beta - \hat{\beta})'(\sum_{t=1}^{n}X_t^{*\prime}X_t^*)(\beta - \hat{\beta})\Big) \\
& \quad \propto \exp\Big(-\frac{1}{2}(\beta - \hat{\beta})'(\frac{1}{\sigma_\epsilon^2}\sum_{t=1}^{n}X_t^{*\prime}X_t^*)(\beta - \hat{\beta})\Big), \qquad (45)
\end{aligned}
$$

which indicates that $\beta \sim N\Big(\hat{\beta}, \sigma_\epsilon^2(\sum_{t=1}^{n}X_t^{*\prime}X_t^*)^{-1}\Big)$, where $\hat{\beta}$ represents the OLS estimate, i.e., $\hat{\beta} = (\sum_{t=1}^{n}X_t^{*\prime}X_t^*)^{-1}(\sum_{t=1}^{n}X_t^{*\prime}y_t^*)$.

Thus, (45) implies that β can be sampled from the multivariate normal distribution with mean $\hat{\beta}$ and variance $\sigma_\epsilon^2(\sum_{t=1}^{n}X_t^{*\prime}X_t^*)^{-1}$.

• $f_{\rho|\beta\sigma_\epsilon}(\rho|\beta, \sigma_\epsilon^2, Y_n)$ is obtained as:

$$f_{\rho|\beta\sigma_\epsilon}(\rho|\beta, \sigma_\epsilon^2, Y_n) \propto f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n)$$
$$\propto (1-\rho^2)^{1/2} \exp\Big(-\frac{1}{2\sigma_\epsilon^2} \sum_{t=1}^{n} \Big(y_t^* - X_t^*\beta\Big)^2\Big), \tag{46}$$

for $-1 < \rho < 1$, which cannot be represented in a known distribution.

Note that $y_t^* = y_t^*(\rho)$ and $X_t^* = X_t^*(\rho)$.

Sampling from (46) is implemented by the MH algorithm.

A detail discussion on sampling will be given later.

• $f_{\sigma_\epsilon|\beta\rho}(\sigma_\epsilon^2|\beta, \rho, Y_n)$ is represented as:

$$f_{\sigma_\epsilon|\beta\rho}(\sigma_\epsilon^2|\beta, \rho, Y_n) \propto f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n)$$
$$\propto \frac{1}{(\sigma_\epsilon^2)^{n/2+1}} \exp\Big(-\frac{1}{2\sigma_\epsilon^2} \sum_{t=1}^{n} (y_t^* - X_t^*\beta)^2\Big), \tag{47}$$

which is written as follows: $\sigma_\epsilon^2 \sim IG(n/2,\ 2/\sum_{t=1}^{n} \epsilon_t^2)$, or equivalently, $1/\sigma_\epsilon^2 \sim G(n/2,\ 2/\sum_{t=1}^{n} \epsilon_t^2)$, where $\epsilon_t = y_t^* - X_t^*\beta$.

Thus, in order to generate random draws of β, ρ and σ_ϵ^2 from the posterior density $f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n)$, the following procedures have to be taken:

(i) Let β_i, ρ_i and $\sigma_{\epsilon,i}^2$ be the ith random draws of β, ρ and σ_ϵ^2.

Take the initial values of $(\beta, \rho, \sigma_\epsilon^2)$ as $(\beta_{-M}, \rho_{-M}, \sigma_{\epsilon,-M}^2)$.

(ii) From equation (45), generate β_i given ρ_{i-1}, $\sigma_{\epsilon,i-1}^2$ and Y_n, using $\beta \sim N\left(\hat{\beta}, \sigma_{\epsilon,i-1}^2(\sum_{t=1}^n X_t^{*\prime} X_t^*)^{-1}\right)$, where $\hat{\beta} = (\sum_{t=1}^n X_t^{*\prime} X_t^*)^{-1}(\sum_{t=1}^n X_t^{*\prime} y_t^*)$, $y_t^* = y_t^*(\rho_{i-1})$ and $X_t^* = X_t^*(\rho_{i-1})$.

(iii) From equation (46), generate ρ_i given β_i, $\sigma_{\epsilon,i-1}^2$ and Y_n.

Since it is not easy to generate random draws from (45), the Metropolis-Hastings algorithm is utilized, which is implemented as follows:

(a) Generate ρ^* from the uniform distribution between -1 and 1, which implies that the sampling density of ρ is given by $f_*(\rho|\rho_{i-1}) = 1/2$ for $-1 < \rho < 1$.

Compute the acceptance probability $\omega(\rho_{i-1}, \rho^*)$, which is defined as:

$$\omega(\rho_{i-1}, \rho^*) = \min\left\{\frac{f_{\rho|\beta\sigma_\epsilon}(\rho^*|\beta_i, \sigma_{\epsilon,i-1}^2, Y_n)/f_*(\rho^*|\rho_{i-1})}{f_{\rho|\beta\sigma_\epsilon}(\rho_{i-1}|\beta_i, \sigma_{\epsilon,i-1}^2, Y_n)/f_*(\rho_{i-1}|\rho^*)},\ 1\right\}$$

$$= \min\left\{ \frac{f_{\rho|\beta\sigma_\epsilon}(\rho^*|\beta_i, \sigma^2_{\epsilon,i-1}, Y_n)}{f_{\rho|\beta\sigma_\epsilon}(\rho_{i-1}|\beta_i, \sigma^2_{\epsilon,i-1}, Y_n)},\ 1 \right\}.$$

(b) Set $\rho_i = \rho^*$ with probability $\omega(\rho_{i-1}, \rho^*)$ and $\rho_i = \rho_{i-1}$ otherwise.

(iv) From equation (47), generate $\sigma^2_{\epsilon,i}$ given β_i, ρ_i and Y_n, using $1/\sigma^2_\epsilon \sim G(n/2,\ 2/\sum_{t=1}^n u_t^2)$, where $u_t = y_t^* - X_t^*\beta$, $y_t^* = y_t^*(\rho_i)$ and $X_t^* = X_t^*(\rho_i)$.

(v) Repeat Steps (ii) – (iv) for $i = -M+1, -M+2, \cdots, N$, where M indicates the burn-in period.

Repetition of Steps (ii) – (iv) corresponds to the Gibbs sampler.

For sufficiently large M, we have the following results:

$$\frac{1}{N}\sum_{i=1}^{N} g(\beta_i) \longrightarrow \mathrm{E}\Big(g(\beta)\Big),$$

$$\frac{1}{N}\sum_{i=1}^{N} g(\rho_i) \longrightarrow \mathrm{E}\Big(g(\rho)\Big),$$

$$\frac{1}{N}\sum_{i=1}^{N} g(\sigma^2_{\epsilon,i}) \longrightarrow \mathrm{E}\Big(g(\sigma^2_\epsilon)\Big),$$

where $g(\cdot)$ is a function, typically $g(x) = x$ or $g(x) = x^2$.

We define the Bayesian estimates of β, ρ and σ_ϵ^2 as $\widetilde{\beta} \equiv (1/N)\sum_{i=1}^N \beta_i$, $\widetilde{\rho} \equiv (1/N)\sum_{i=1}^N \rho_i$ and $\widetilde{\sigma}_\epsilon^2 \equiv (1/N)\sum_{i=1}^N \sigma_{\epsilon,i}^2$, respectively.

Thus, using both the Gibbs sampler and the MH algorithm, we have shown that we can sample from $f_{\beta\rho\sigma_\epsilon}(\beta, \rho, \sigma_\epsilon^2|Y_n)$.

See, for example, Bernardo and Smith (1994), Carlin and Louis (1996), Chen, Shao and Ibrahim (2000), Gamerman (1997), Robert and Casella (1999) and Smith and Roberts (1993) for the Gibbs sampler and the MH algorithm.

12.2.3 Monte Carlo Experiments

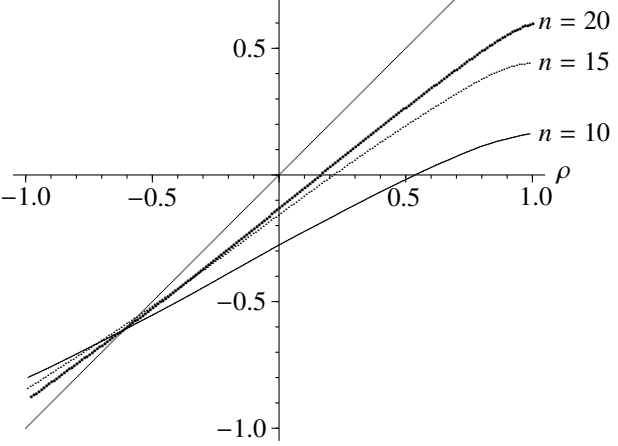
For the exogenous variables, again we take the data used in Section 12.1, in which the true data generating process (DGP) is presented in Judge, Hill, Griffiths and Lee (1980, p.156).

As in equation (36), the DGP is defined as:

$$y_t = \beta_1 + \beta_2 x_{2,t} + \beta_3 x_{3,t} + u_t, \qquad u_t = \rho u_{t-1} + \epsilon_t, \tag{48}$$

where ϵ_t, $t = 1, 2, \cdots, n$, are normally and independently distributed with $\mathrm{E}(\epsilon_t) = 0$ and $\mathrm{E}(\epsilon_t^2) = \sigma_\epsilon^2$.

As in Judge, Hill, Griffiths and Lee (1980), the parameter values are set to be $(\beta_1, \beta_2, \beta_3) = (10, 1, 1)$.



We utilize $x_{2,t}$ and $x_{3,t}$ given in Judge, Hill, Griffiths and Lee (1980, pp.156), which is shown in Table 2, and generate G samples of y_t given the X_t for $t = 1, 2, \cdots, n$.

That is, we perform G simulation runs for each estimator, where $G = 10^4$ is taken.

The simulation procedure is as follows:

(i) Given ρ, generate random numbers of u_t for $t = 1, 2, \cdots, n$, based on the assumptions: $u_t =$

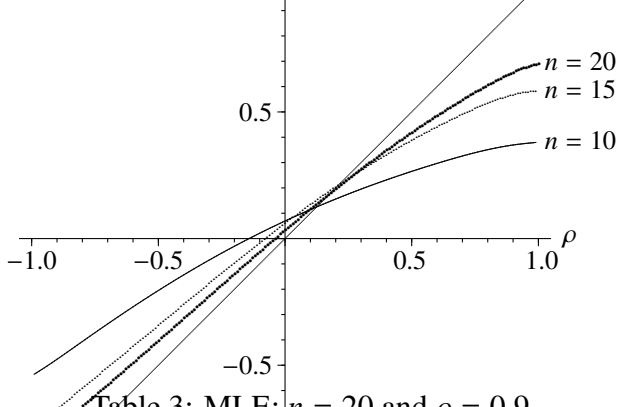


Table 3: MLE: $n = 20$ and $\rho = 0.9$

Parameter	β_1	β_2	β_3	ρ	σ_ϵ^2
True Value	10	1	1	0.9	1
AVE	10.012	−1.000	1.000	0.559	0.752
SER	3.025	0.171	0.053	0.240	0.276
RMSE	3.025	0.171	0.053	0.417	0.372
Skewness	0.034	−0.045	−0.008	−1.002	0.736
Kurtosis	2.979	3.093	3.046	4.013	3.812
5%	5.096	0.718	0.914	0.095	0.363
10%	6.120	0.785	0.933	0.227	0.426
25%	7.935	0.883	0.965	0.426	0.550
50%	10.004	0.999	1.001	0.604	0.723
75%	12.051	1.115	1.036	0.740	0.913
90%	13.913	1.217	1.068	0.825	1.120
95%	15.036	1.274	1.087	0.863	1.255

RMSE	2.782	0.160	0.051	0.304	0.384
Skewness	0.008	−0.029	−0.022	−1.389	0.725
Kurtosis	3.018	3.049	2.942	5.391	3.783
5%	5.498	0.736	0.915	0.285	0.515
10%	6.411	0.798	0.934	0.405	0.601
25%	8.108	0.891	0.966	0.572	0.776
50%	10.013	1.000	1.000	0.707	1.011
75%	11.888	1.107	1.036	0.799	1.275
90%	13.578	1.205	1.067	0.852	1.555
95%	14.588	1.258	1.085	0.875	1.750
Parameter	β_0	β_1	β_2	β_3	β_4
True Value	10	1	1	0.9	1

Table 59: BE with $W = 5000$ and $N = 5000$: $n = 20$ and $\rho = 0.9$

AVE	10.011	0.999	1.000	0.661	1.051
SER	2.785	0.160	0.051	0.189	0.380
RMSE	2.785	0.160	0.052	0.305	0.384
Skewness	0.004	−0.027	−0.022	−1.390	0.723
Kurtosis	3.028	3.056	2.938	5.403	3.776
5%	5.500	0.736	0.915	0.285	0.514
10%	6.402	0.797	0.934	0.405	0.603
25%	8.117	0.891	0.966	0.572	0.775
50%	10.015	1.000	1.001	0.707	1.011
75%	11.898	1.107	1.036	0.799	1.277
90%	13.612	1.205	1.066	0.852	1.559
95%	14.600	1.257	1.085	0.876	1.747
Parameter	β_0	β_1	β_2	β_3	β_4
True Value	10	1	1	0.9	1

Table 60: BE with $W = 1000$ and $N = 1000$: $n = 20$ and $\rho = 0.9$

AVE	10.010	0.999	1.000	0.661	1.051
SER	2.783	0.160	0.051	0.188	0.380
RMSE	2.783	0.160	0.051	0.304	0.384
Skewness	0.008	−0.029	−0.021	−1.391	0.723
Kurtosis	3.031	3.055	2.938	5.404	3.774
5%	5.495	0.736	0.915	0.284	0.514
10%	6.412	0.797	0.935	0.404	0.602
25%	8.116	0.891	0.966	0.573	0.774
50%	10.014	1.000	1.001	0.706	1.011
75%	11.897	1.107	1.036	0.799	1.275
90%	13.587	1.204	1.067	0.852	1.558
95%	14.588	1.257	1.085	0.876	1.746

$\rho u_{t-1} + \epsilon_t$ and $\epsilon_t \sim N(0, 1)$.

(ii) Given β, $(x_{2,t}, x_{3,t})$ and u_t for $t = 1, 2, \cdots, n$, we obtain a set of data y_t, $t = 1, 2, \cdots, n$, from equation (48), where $(\beta_1, \beta_2, \beta_3) = (10, 1, 1)$ is assumed.

(iii) Given (y_t, X_t) for $t = 1, 2, \cdots, n$, obtain the estimates of $\theta = (\beta, \rho, \sigma_\epsilon^2)$ by the maximum likelihood estimation (MLE) and the Bayesian estimation (BE) discussed in Sections 12.2.2, which are denoted by $\hat{\theta}$ and $\widetilde{\theta}$, respectively.

(iv) Repeat (i) – (iii) G times, where $G = 10^4$ is taken.

(v) From G estimates of θ, compute the arithmetic average (AVE), the standard error (SER), the root mean square error (RMSE), the skewness (Skewness), the kurtosis (Kurtosis), and the 5, 10, 25, 50, 75, 90 and 95 percent points (5%, 10%, 25%, 50%, 75%, 90% and 95%) for each estimator.

For the maximum likelihood estimator (MLE), we compute:

$$\text{AVE} = \frac{1}{G}\sum_{g=1}^{G} \hat{\theta}_j^{(g)}, \qquad \text{RMSE} = \left(\frac{1}{G}\sum_{g=1}^{G} (\hat{\theta}_j^{(g)} - \theta_j)^2\right)^{1/2},$$

for $j = 1, 2, \cdots, 5$, where θ_j denotes the jth element of θ and $\hat{\theta}_j^{(g)}$ represents the jth element of

$\hat{\theta}$ in the gth simulation run.

For the Bayesian estimator (BE), $\hat{\theta}$ in the above equations is replaced by $\widetilde{\theta}$, and AVE and RMSE are obtained.

(vi) Repeat (i) – (v) for $\rho = -0.99, -0.98, \cdots, 0.99$.

Thus, in Section 12.2.3, we compare the Bayesian estimator (BE) with the maximum likelihood estimator (MLE) through Monte Carlo studies.

In Figures 8 and 9, we focus on the estimates of the autocorrelation coefficient ρ.

In Figure 8 we draw the relationship between ρ and $\hat{\rho}$, where $\hat{\rho}$ denotes the arithmetic average of the 10^4 MLEs, while in Figure 9 we display the relationship between ρ and $\widetilde{\rho}$, where $\widetilde{\rho}$ indicates the arithmetic average of the 10^4 BEs.

In the two figures the cases of $n = 10, 15, 20$ are shown, and $(M, N) = (5000, 10^4)$ is taken in Figure 9 (we will discuss later about M and N).

If the relationship between ρ and $\hat{\rho}$ (or $\widetilde{\rho}$) lies on the 45° degree line, we can conclude that MLE (or BE) of ρ is unbiased.

However, from the two figures, both estimators are biased.

Take an example of $\rho = 0.9$ in Figures 8 and 9.

When the true value is $\rho = 0.9$, the arithmetic averages of 10^4 MLEs are given by 0.142 for $n = 10$, 0.422 for $n = 15$ and 0.559 for $n = 20$ (see Figure 8), while those of 10^4 BEs are 0.369 for $n = 10$, 0.568 for $n = 15$ and 0.661 for $n = 20$ (see Figure 9).

As n increases the estimators are less biased, because it is shown that MLE gives us the consistent estimators.

Comparing BE and MLE, BE is less biased than MLE in the small sample, because BE is closer to the 45° degree line than MLE.

Especially, as ρ goes to one, the difference between BE and MLE becomes quite large.

Tables 3 – 6 represent the basic statistics such as arithmetic average, standard error, root mean square error, skewness, kurtosis and percent points, which are computed from $G = 10^4$ simulation runs, where the case of $n = 20$ and $\rho = 0.9$ is examined.

Table 3 is based on the MLEs while Tables 4 – 6 are obtained from the BEs.

To check whether M and N are enough large, Tables 4 – 6 are shown for BE.

Comparison between Tables 4 and 5 shows whether $N = 5000$ is large enough and we can see from Tables 4 and 6 whether the burn-in period $M = 1000$ is large enough.

Figure 10: Empirical Distributions of β_1

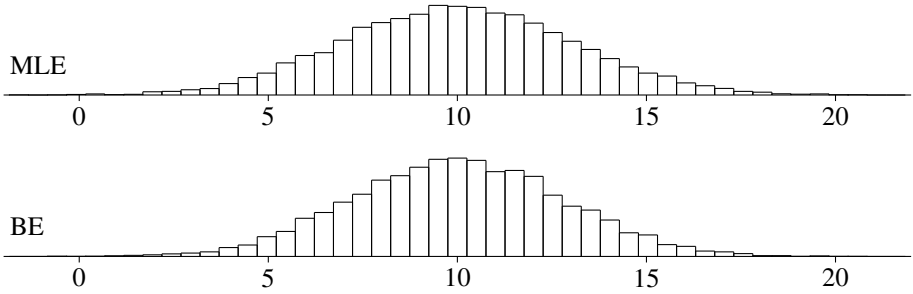


Figure 11: Empirical Distributions of β_2

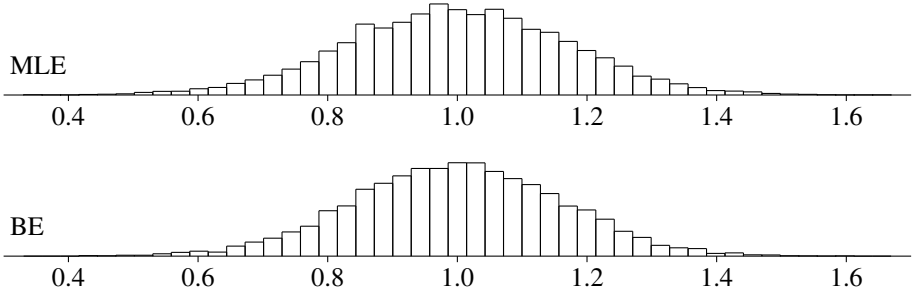


Figure 12: Empirical Distributions of β_3

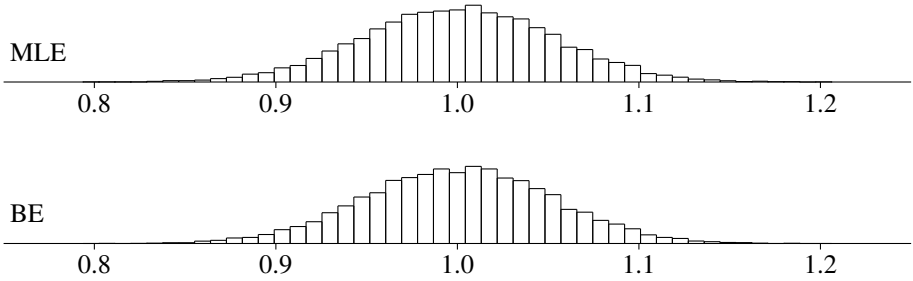


Figure 13: Empirical Distributions of ρ

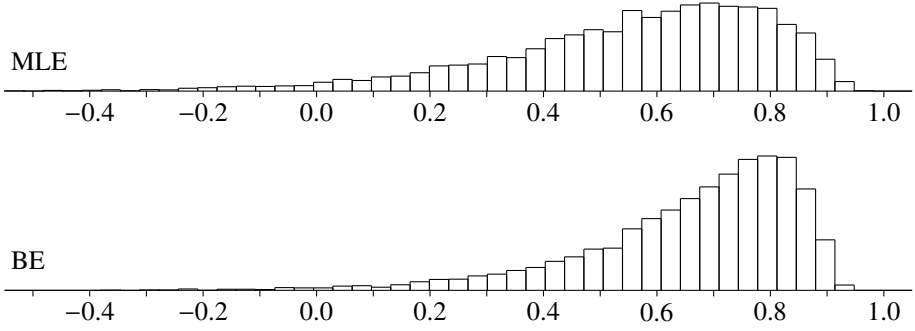
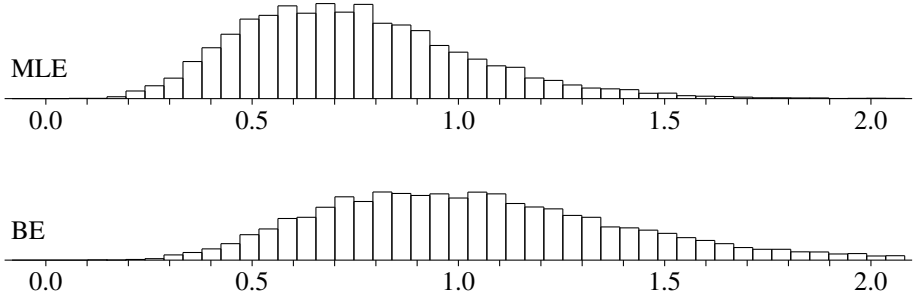


Figure 14: Empirical Distributions of σ_ϵ^2



We can conclude that $N = 5000$ is enough if Table 4 is very close to Table 5 and that $M = 1000$ is enough if Table 4 is close to Table 6.

The difference between Tables 4 and 5 is at most 0.034 (see 90% in β_1) and that between Tables 4 and 6 is less than or equal to 0.013 (see Kurtosis in β_1).

Thus, all the three tables are very close to each other.

Therefore, we can conclude that $(M, N) = (1000, 5000)$ is enough.

For safety, hereafter we focus on the case of $(M, N) = (5000, 10^4)$.

We compare Tables 3 and 4.

Both MLE and BE give us the unbiased estimators of regression coefficients β_1, β_2 and β_3, because the arithmetic averages from the 10^4 estimates of β_1, β_2 and β_3, (i.e., AVE in the tables) are very close to the true parameter values, which are set to be $(\beta_1, \beta_2, \beta_3) = (10, 1, 1)$.

However, in the SER and RMSE criteria, BE is better than MLE, because SER and RMSE of BE are smaller than those of MLE. From Skewness and Kurtosis in the two tables, we can see that the empirical distributions of MLE and BE of $(\beta_1, \beta_2, \beta_3)$ are very close to the normal distribution. Remember that the skewness and kurtosis of the normal distribution are given by zero and three, respectively.

As for σ_ϵ^2, AVE of BE is closer to the true value than that of MLE, because AVE of MLE is 0.752 (see

Table 3) and that of BE is 1.051 (see Table 4).

However, in the SER and RMSE criteria, MLE is superior to BE, since SER and RMSE of MLE are given by 0.276 and 0.372 (see Table 3) while those of BE are 0.380 and 0.384 (see Table 4).

The empirical distribution obtained from 10^4 estimates of σ_ϵ^2 is skewed to the right (Skewness is positive for both MLE and BE) and has a larger kurtosis than the normal distribution because Kurtosis is greater than three for both tables.

For ρ, AVE of MLE is 0.559 (Table 3) and that of BE is given by 0.661 (Table 4).

As it is also seen in Figures 8 and 9, BE is less biased than MLE from the AVE criterion.

Moreover, SER and RMSE of MLE are 0.240 and 0.417, while those of BE are 0.188 and 0.304.

Therefore, BE is more efficient than MLE.

Thus, in the AVE, SER and RMSE criteria, BE is superior to MLE with respect to ρ.

The empirical distributions of MLE and BE of ρ are skewed to the left because Skewness is negative, which value is given by -1.002 in Table 3 and -1.389 in Table 4.

We can see that MLE is less skewed than BE.

For Kurtosis, both MLE and BE of ρ are greater than three and therefore the empirical distributions of the estimates of ρ have fat tails, compared with the normal distribution.

Since Kurtosis in Table 4 is 5.391 and that in Table 3 is 4.013, the empirical distribution of BE has more kurtosis than that of MLE.

Figures 10 – 14 correspond to the empirical distributions for each parameter, which are constructed from the G estimates used in Tables 3 and 4.

As we can see from Skewness and Kurtosis in Tables 3 and 4, $\hat{\beta}_i$ and $\widetilde{\beta}_i$, $i = 1, 2, 3$, are very similar to normal distributions in Figures 10 – 12.

For β_i, $i = 1, 2, 3$, the empirical distributions of MLE have the almost same centers as those of BE, but the empirical distributions of MLE are more widely distributed than those of BE.

We can also observe these facts from AVEs and SERs in Tables 3 and 4.

In Figure 13, the empirical distribution of $\hat{\rho}$ is quite different from that of $\widetilde{\rho}$.

$\widetilde{\rho}$ is more skewed to the left than $\hat{\rho}$ and $\widetilde{\rho}$ has a larger kurtosis than $\hat{\rho}$.

Since the true value of ρ is 0.9, BE is distributed at the nearer place to the true value than MLE.

Figure 14 displays the empirical distributions of σ_ϵ^2. MLE $\hat{\sigma}_\epsilon^2$ is biased and underestimated, but it has a smaller variance than BE $\widetilde{\sigma}_\epsilon^2$.

In addition, we can see that BE $\widetilde{\sigma}_\epsilon^2$ is distributed around the true value.

12.2.4 Summary

In Section 12.2, we have compared MLE with BE, using the regression model with the autocorrelated error term.

Chib (1993) applied the Gibbs sampler to the autocorrelation model, where the initial density of the error term is ignored.

Under this setup, the posterior distribution of ρ reduces to the normal distribution.

Therefore, random draws of ρ given β, σ_ϵ^2 and (y_t, X_t) can be easily generated.

However, when the initial density of the error term is taken into account, the posterior distribution of ρ is not normal and it cannot be represented in an explicit functional form.

Accordingly, in Section 12.2, the Metropolis-Hastings algorithm have been applied to generate random draws of ρ from its posterior density.

The obtained results are summarized as follows.

Given $\beta' = (10, 1, 1)$ and $\sigma^2 = 1$, in Figure 8 we have the relationship between ρ and $\hat{\rho}$, and $\widetilde{\rho}$ corresponding to ρ is drawn in Figure 9.

In the two figures, we can observe:

(i) both MLE and BE approach the true parameter value as n is large, and

(ii) BE is closer to the 45° degree line than MLE and accordingly BE is superior to MLE.

Moreover, we have compared MLE with BE in Tables 3 and 4, where $\beta' = (10, 1, 1)$, $\rho = 0.9$ and $\sigma^2 = 1$ are taken as the true values.

As for the regression coefficient β, both MLE and BE gives us the unbiased estimators.

However, we have obtained the result that BE of β is more efficient than MLE. For estimation of σ^2, BE is less biased than MLE.

In addition, BE of the autocorrelation coefficient ρ is also less biased than MLE.

Therefore, as for inference on β, BE is superior to MLE, because it is plausible to consider that the estimated variance of $\hat{\beta}$ is biased much more than that of $\widetilde{\beta}$.

Remember that variance of $\hat{\beta}$ depends on both ρ and σ^2.

Thus, from the simulation studies, we can conclude that BE performs much better than MLE.

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12.3 Marginal Likelihood, Convergence Diagnostic and so on

12.3.1 Marginal Likelihood (周辺尤度)

Model Selection $\Longrightarrow$ Marginal Likelihood

$$f_y(y) = \int f_{y|\theta}(y|\theta) f_\theta(\theta) \mathrm{d}\theta$$

Evaluation of Marginal Likelihood $\Longrightarrow$ Proper Prior

(i) Importance Sampling: Use of Prior Distribution

$$f_y(y) = \mathrm{E}_\theta(f_{y|\theta}(y|\theta)) \approx \frac{1}{N}\sum_{i=1}^{N} f_{y|\theta}(y|\theta_i),$$

where θ_i is the ith random draw generated from the prior distribution $f_\theta(\theta)$.

(ii) Importance Sampling: Use of the Appropriate Importance Distribution

$$f_y(y) = \int \frac{f_{y|\theta}(y|\theta) f_\theta(\theta)}{g(\theta)} g(\theta) \mathrm{d}\theta = \mathrm{E}\left(\frac{f_{y|\theta}(y|\theta) f_\theta(\theta)}{g(\theta)} \right)$$
$$\approx \frac{1}{N} \sum_{i=1}^{N} \frac{f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)}{g(\theta_i)},$$

where θ_i is the ith random draw generated from the appropriately chosen importance distribution $g(\theta)$.

(iii) Harmonic Mean $\Longrightarrow$ Gelfand and Dey (1994) and Newton and Raftery (1994)

$$\begin{aligned}\frac{1}{f_y(y)} &= \int \frac{g(\theta)}{f_y(y)}\mathrm{d}\theta = \int \frac{g(\theta)}{f_y(y) f_{\theta|y}(\theta|y)} f_{\theta|y}(\theta|y)\mathrm{d}\theta \\ &= \int \frac{g(\theta)}{f_{y|\theta}(y|\theta) f_\theta(\theta)} f_{\theta|y}(\theta|y)\mathrm{d}\theta \approx \frac{1}{N}\sum_{i=1}^{N} \frac{g(\theta_i)}{f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)},\end{aligned}$$

where θ_i is the ith random draw generated from the posterir distribution $f_{\theta|y}(\theta|y)$.

Thus, the marginal distribution is evaluated by:

$$f_y(y) \approx \left(\frac{1}{N}\sum_{i=1}^{N} \frac{g(\theta_i)}{f_{y|\theta}(y|\theta_i) f_\theta(\theta_i)}\right)^{-1}, \qquad \Longrightarrow \qquad \text{Gelfand and Dey (1994).}$$

When $g(\theta) = f_\theta(\theta)$ is taken, the marginal distribution is given by:

$$f_y(y) \approx \left(\frac{1}{N}\sum_{i=1}^{N} \frac{1}{f_{y|\theta}(y|\theta_i)}\right)^{-1}, \qquad \Longrightarrow \qquad \text{Newton and Raftery (1994).}$$

(iv) Chib (1995) and Chib and Jeliazkov (2001)

$$f_y(y) = \frac{f_{y|\theta}(y|\theta) f_\theta(\theta)}{f_{\theta|y}(\theta|y)}$$

$$\log f_y(y) = \log f_{y|\theta}(y|\hat{\theta}) + \log f_\theta(\hat{\theta}) - \log f_{\theta|y}(\hat{\theta}|y),$$

where $\hat{\theta}$ denotes the Bayes estimates.

We need to evaluate $\log f_{\theta|y}(\hat{\theta}|y)$, using the Gibbs sampler or the MH algorithm.

12.3.2 Convergence Diagnostic (収束判定)

We need to check whether the **burn-in period** is enough and whether MCMC converges to the **invariant distribution** (不変分布).

Geweke (1992)

Divide the sample path into three periods, excluding the burn-in period..

Test whether the first period is different from the third period.

Suppose that we have the MCMC sequence, i.e., $\theta_{-M+1}, \cdots, \theta_0, \theta_1, \cdots, \theta_N$.

The burn-in period is denoted by $\theta_{-M+1}, \cdots, \theta_0$.

$\theta_1, \cdots, \theta_N$ are divided by three periods.

The first period is given by $\theta_1, \cdots, \theta_{N_1}$.

The second period is given by $\theta_{N_1+1}, \cdots, \theta_{N_2}$.

The third period is given by $\theta_{N_2+1}, \cdots, \theta_N$.

Consider a function $g(\cdot)$.

Define $\quad \overline{g}_1 = \dfrac{1}{N_1} \displaystyle\sum_{i=1}^{N_1} g(\theta_i) \quad$ and $\quad \overline{g}_3 = \dfrac{1}{N_3} \displaystyle\sum_{i=N_1+N_2+1}^{N} g(\theta_i) \quad$ for $N_3 = N - N_2 - N_1$.

Estimate $\quad \dfrac{1}{N_1} \mathrm{V}(\displaystyle\sum_{i=1}^{N_1} g(\theta_i)) \quad$ and $\quad \dfrac{1}{N_3} \mathrm{V}(\displaystyle\sum_{i=N_1+N_2+1}^{N} g(\theta_i)),$

which are denoted by s_1^2 and s_3^2, respectively.

By the central limit theorem,

$$\frac{\overline{g}_1 - \mathrm{E}(\overline{g}_1)}{s_1/\sqrt{N_1}} \longrightarrow N(0,1) \qquad \text{and} \qquad \frac{\overline{g}_3 - \mathrm{E}(\overline{g}_3)}{s_3/\sqrt{N_3}} \longrightarrow N(0,1).$$

Therefore, under the null hypothesis $H_0 : \mathrm{E}(\overline{g}_1) = \mathrm{E}(\overline{g}_3)$,

$$\frac{\overline{g}_1 - \overline{g}_3}{\sqrt{s_1^2/N_1 + s_3^2/N_3}} \longrightarrow N(0,1).$$

The case of $g(\theta_i) = \theta_i \implies$ Testing whether the two means (i.e., first-moments) are equal.

The case of $g(\theta_i) = \theta_i^2 \implies$ Testing whether the two second-moments are equal.

Computation of s_1^2 and s_3^2 has to be careful, because $g(\theta_1), \cdots, g(\theta_N)$ are serially correlated.

$\implies$ Long-run variance.

Take an example of s_1^2, which is an estimate of $\frac{1}{N_1}\mathrm{V}(\sum_{i=1}^{N_1} g(\theta_i))$.

$$\begin{aligned}\frac{1}{N_1}\mathrm{V}(\sum_{i=1}^{N_1} g(\theta_i)) &= \frac{1}{N_1}\sum_{i=1}^{N_1}\sum_{j=1}^{N_1}\mathrm{Cov}(g(\theta_i), g(\theta_j)) \\ &= \frac{1}{N_1}(N_1\gamma(0) + 2(N_1-1)\gamma(1) + 2(N_1-2)\gamma(2) + \cdots + 2\gamma(N_1-1)) \\ &= \gamma(0) + 2\sum_{\tau=1}^{N_1-1} k(\frac{\tau}{N_1})\gamma(\tau), \quad \Longrightarrow \quad \text{Bartlett Kernel (Newy-West Est.)}\end{aligned}$$

where $\gamma(\tau) = \mathrm{Cov}(g(\theta_i), g(\theta_{i+\tau}))$.

We may choose the other kernels (for example, Parzen kernel or second-order spectrum kernel; see p.166-167) for $k(x)$.

Thus, s_1^2 is estimated by:

$$s_1^2 = \hat{\gamma}(0) + 2\sum_{\tau=1}^{q} k(\frac{\tau}{q+1})\hat{\gamma}(\tau),$$

for $q \leq N_1 - 1$. $\Longrightarrow$ Choice of q and $k(\cdot)$.