Biostatistics 615/815 Lecture 15: Generating random numbers

Hyun Min Kang

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Annoucements

Homework #4

- Homework 4 due is Today

Midterm

- Midterm is on Thursday, March 10th.

Recap: Dealing with large data with `lm`

```
> y <- rnorm(5000000)
> x <- rnorm(5000000)
> system.time(print(summary(lm(y~x))))

Call:
lm(formula = y ~ x)

Residuals:
    Min      1Q  Median      3Q     Max
-5.1310 -0.6746  0.0004  0.6747  5.0860

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.0005130  0.0004473  -1.147    0.251
x            0.0002359  0.0004473   0.527    0.598

Residual standard error: 1 on 4999998 degrees of freedom
Multiple R-squared: 5.564e-08, Adjusted R-squared: -1.444e-07
F-statistic: 0.2782 on 1 and 4999998 DF,  p-value: 0.5979

   user  system elapsed
 57.434  14.229 100.607
```


Recap: A faster R implementation

```
# note that this is an R function, not C++
fastSimpleLinearRegression <- function(y, x) {
  y <- y - mean(y)
  x <- x - mean(x)
  n <- length(y)
  stopifnot(length(x) == n)        # for error handling
  s2y <- sum( y * y ) / ( n - 1 )  # \sigma_y^2
  s2x <- sum( x * x ) / ( n - 1 )  # \sigma_x^2
  sxy <- sum( x * y ) / ( n - 1 )  # \sigma_xy
  rxy <- sxy / sqrt( s2y * s2x )   # \rho_xy
  b <- rxy * sqrt( s2y / s2x )
  se.b <- sqrt( ( n - 1 ) * s2y * ( 1 - rxy * rxy ) / (n-2) )
  tstat <- rxy * sqrt( ( n - 2 ) / ( 1 - rxy * rxy ) )
  p <- pt( abs(t) , n - 2 , lower.tail=FALSE )*2
  return(list( beta = b , se.beta = se.b , t.stat = tstat, p.value = p ))
}
```

Recap: Streaming the inputs to extract sufficient statistics

Sufficient statistics for simple linear regression

1. n
2. $\sigma_x^2 = \hat{\text{Var}}(x) = (\mathbf{x} - \overline{x})^T(\mathbf{x} - \overline{x})/(n-1)$
3. $\sigma_y^2 = \hat{\text{Var}}(y) = (\mathbf{y} - \overline{y})^T(\mathbf{y} - \overline{y})/(n-1)$
4. $\sigma_{xy} = \hat{\text{Cov}}(x,y) = (\mathbf{x} - \overline{x})^T(\mathbf{y} - \overline{y})/(n-1)$

Extracting sufficient statistics from stream

- $\sum_{i=1}^n x = n\overline{x}$
- $\sum_{i=1}^n y = n\overline{y}$
- $\sum_{i=1}^n x^2 = \sigma_x^2(n-1) + n\overline{x}^2$
- $\sum_{i=1}^n y^2 = \sigma_y^2(n-1) + n\overline{y}^2$
- $\sum_{i=1}^n xy = \sigma_{xy}(n-1) + n\overline{x}\overline{y}$

Recap: Implementing multiple regression

```
JacobiSVD<MatrixXd> svd(X, ComputeThinU | ComputeThinV);     // compute SVD
MatrixXd betasSvd = svd.solve(y);  // solve linear model for computing beta
// calcuate VD^{-1}
MatrixXd ViD= svd.matrixV() * svd.singularValues().asDiagonal().inverse();
double sigmaSvd = (y - X * betasSvd).squaredNorm()/(n-p);  // compute \sigma^2
MatrixXd varBetasSvd = sigmaSvd * ViD * ViD.transpose();   // Cov(\hat{beta})
```


Today and Next Lectures

Generating random numbers from common distributions

- Why learn random number generation?
- 'Good' random number generators
- Sampling from uniform distribution
- Sampling from normal distribution
- Sampling from other common distributions

Generating random numbers from complex distributions

- Monte-Carlo Methods
- Importance Sampling

Random Numbers

True random numbers

- Truly random, non-determinstic numbers
- Easy to imagine conceptually
- Very hard to generate one or test its randomness
- For example, `http://www.random.org` generates randomness via atmospheric noise

Pseudo random numbers

- A deterministic sequence of random numbers (or bits) from a seed
- Good random numbers should be very hard to guess the next number just based on the observations.

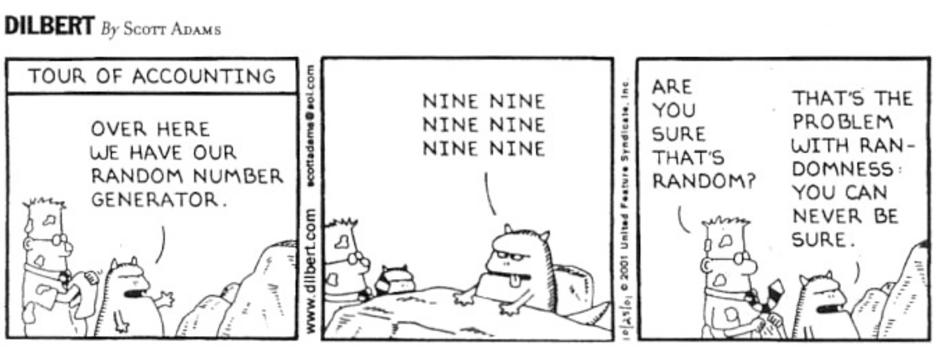
Usage of random numbers in statistical methods

- Resampling procedure
  - Permutation
  - Boostrapping
- Simulation of data for evaluating a statistical procedure (e.g. HMM).
- Stochastic processes
  - Markov-Chain Monte-Carlo (MCMC) methods

Usage of random numbers in other areas

- Hashing
  - Good hash function uniformly distribute the keys to the hash spcae
  - Good pseudo-random number generators can replace a good hash function
- Cryptography
  - Generating pseudo-random numbers given a seed is equivalent to encrypting the seed to a sequence of random bits
  - If the pattern of pseudo-random numbers can be predicted, the original seed can also be deciphered.

True random numbers



- Generate on throough physical process
- Hard to generate automatically
- Very hard to provde true randomness

Pseudo-random numbers : Example code

```
#include <iostream>
#include <cstdlib>
int main(int argc, char** argv) {
  int n = (argc > 1) ? atoi(argv[1]) : 1;
  int seed = (argc > 2 ) ? atoi(argv[2]) : 0;

  srand(seed); // set seed -- same seed, same pseudo-random numbers

  for(int i=0; i < n; ++i) {
    std::cout << (double)rand()/RAND_MAX << std::endl;
    // generate value between 0 and 1
  }

  return 0;
}
```

Pseudo-random numbers : Example run

```
user@host:~/$ src/randExample 3 0
0.242578
0.0134696
0.383139
user@host:~/$ src/randExample 3 0 (same seed should generate same pseudo-random numbers)
0.242578
0.0134696
0.383139
user@host:~/$ src/randExample 3 10
7.82637e-05
0.315378
0.556053
```


Properties of pseudo-random numbers

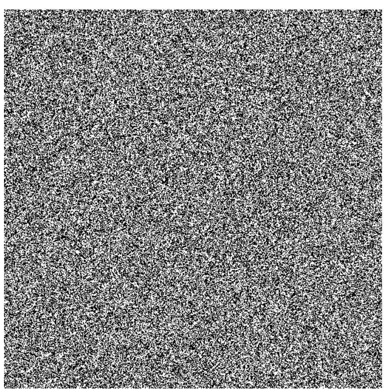
Deterministic

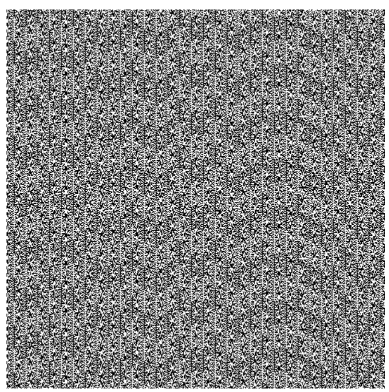
- Given a fixed random seed, the pseudo-random numbers should generate identical sequence of random numbers
- Deterministic feature is useful for debugging a code

Irregularity and Unpredictablility

- Without knowning the seed, the random numbers should be hard to guess
- If you can guess it better than random, it is possible to exploit the weakness to generate random numbers with a skewed distribution.

Good vs. bad random numbers





- Images using true random numbers from `random.org` vs. `rand()` function in PHP
- Visible patterns suggest that `rand()` gives predictable sequence of pseudo-random numbers

Generating uniform random numbers - example in R

```
> x <- runif(10)       # x is size 10 vector uniformly distributed from 0 to 1
> x <- runif(10,0,10)       # x ranges 0 to 0
> x <- as.integer(10,0,10)  # integers from 0 to 9
> set.seed(3429248)         # set an arbitrary seed
> x <- as.integer(runif(10,0,10))
> x
 [1] 7 6 3 4 6 7 4 9 2 1
> set.seed(3429248)         # setting the same seed
> x <- as.integer(runif(10,0,10))  # reproduce the same random variables
> x
 [1] 7 6 3 4 6 7 4 9 2 1
```

Generating uniform random numbers in C++

```
#include <iostream>
#include <boost/random/uniform_int.hpp>
#include <boost/random/uniform_real.hpp>
#include <boost/random/variate_generator.hpp>
#include <boost/random/mersenne_twister.hpp>
int main(int argc, char** argv) {
  typedef boost::mt19937 prgType; // Mersenne-twister : a widely used
  prgType rng;       //    lightweight pseudo-random-number-generator
  boost::uniform_int<> six(1,6);  // uniform distribution from 1 to 6
  boost::variate_generator<prgType&, boost::uniform_int<> > die(rng,six);
  // die maps random numbers from rng to uniform distribution 1..6

  int x = die();     // generate a random integer between 1 and 6
  std::cout << "Rolled die : " << x << std::endl;

  boost::uniform_real<> uni_dist(0,1);
  boost::variate_generator<prgType&, boost::uniform_real<> > uni(rng,uni_dist);
  double y = uni();  // generate a random number between 0 and 1
  std::cout << "Uniform real : " << y << std::endl;
  return 0;
}
```


Running Example

```
user@host:~/$ ./randExample
Rolled die : 5
Uniform real : 0.135477

user@host:~/$ ./randExample
Rolled die : 5
Uniform real : 0.135477
```

The random number does not vary (unlike R)

Specifying the seed

```
int main(int argc, char** argv) {
  typedef boost::mt19937 prgType;
  prgType rng;
  if ( argc > 1 )
    rng.seed(atoi(argv[1]));  // set seed if argument is specified

  boost::uniform_int<> six(1,6);
  // ... same as before
}
```


Running Example

```
user@host:~/$ ./randExample
Rolled die : 5
Uniform real : 0.135477

user@host:~/$ ./randExample 1
Rolled die : 3
Uniform real : 0.997185

user@host:~/$ ./randExample 3
Rolled die : 4
Uniform real : 0.0707249

user@host:~/$ ./randExample 3
Rolled die : 4
Uniform real : 0.0707249
```

If we don't want the reproducibility

```
// include other headers as before
#include <ctime>
int main(int argc, char** argv) {
  typedef boost::mt19937 prgType;
  prgType rng;
  if ( argc > 1 )
    rng.seed(atoi(argv[1]));  // set seed if argument is specified
  else
    rng.seed(std::time(0));   // otherwise, use current time to pick arbitrary seed to start

  boost::uniform_int<> six(1,6);
  // ... same as before
}
```


Running Example

```
user@host:~/$ ./randExample
Rolled die : 4
Uniform real : 0.367588

user@host:~/$ ./randExample
Rolled die : 5
Uniform real : 0.0984682

user@host:~/$ ./randExample 3
Rolled die : 4
Uniform real : 0.0707249

user@host:~/$ ./randExample 3
Rolled die : 4
Uniform real : 0.0707249
```


Generating random numbers from non-uniform distribution

Sampling from known distribution using R

```
> x <- rnorm(1)       # x is a random number sampled from N(0,1)
> y <- rnorm(1,3,2)   # y is a random number sampled from N(3,2^2)
> z <- rbinom(1,1,0.3) # z is a Bernolli random number with p=0.3
```

What if `runif()` was the only random number generator we have?

If we know the inverse CDF, it is easy to implement

```
> x <- qnorm(runif(1))        # x follows N(0,1)
> y <- qnorm(runif(1),3,2)    # equivalent to y <- qnorm(runif(1))*2+3
> z <- qbinom(runif(1),1,0.3) # z is a Bernolli random number with p=0.3
```


Random number generation in C++

```
#include <iostream>
#include <ctime>
#include <boost/random/normal_distribution.hpp>
#include <boost/random/variate_generator.hpp>
#include <boost/random/mersenne_twister.hpp>
int main(int argc, char** argv) {
  typedef boost::mt19937 prgType;
  prgType rng;

  if ( argc > 1 )
    rng.seed(atoi(argv[1]));
  else
    rng.seed(std::time(0));

  boost::normal_distribution<> norm_dist(0,1);  // standard normal distribution
  // PRG sampled from standard normal distribution
  boost::variate_generator<prgType&, boost::normal_distribution<> > norm(rng,norm_dist);

  double x = norm();  // Generate a random number from the PRG
  std::cout << "Sampled from standard normal distribution : " << x << std::endl;
  return 0;
}
```

Generating random numbers from complex distributions

Problem

- When the distribution is complex, the inverse CDF may not be easily obtainable
- Need to implement your own function to generate the random numbers

A simple example - mixture of two normal distributions

$$f(x; \mu_1, \sigma_1^2, \mu_2, \sigma_2^2, \alpha) = \alpha f_{\mathcal{N}}(x; \mu_1, \sigma_1^2) + (1-\alpha) f_{\mathcal{N}}(x; \mu_2, \sigma_2^2)$$

How to generate random numbers from this distribution?

Sample from Gaussian mixture

Key idea

- Introduce a Bernoulli random variable $w \sim \text{Bernoulli}(\alpha)$
- Sample $y \sim \mathcal{N}(\mu_1, \sigma_1^2)$ and $z \sim \mathcal{N}(\mu_2, \sigma_2^2)$
- Let $x = wy + (1-w)z$.

An R implementation

```
w <- rbinom(1,1,alpha)
y <- rnorm(1,mu1,sigma1)
z <- rnorm(1,mu2,sigma2)
x <- w*y + (1-w)*z
```


A C++ implementation

Will be included the next homework!

Sampling from bivariate normal distribution

Bivariate normal distribution

$$\begin{pmatrix} x \\ y \end{pmatrix} \sim \mathcal{N}\left(\begin{matrix} \mu_x \\ \mu_y \end{matrix}, \begin{bmatrix} \sigma_x^2 & \sigma_{xy} \\ \sigma_{xy} & \sigma_y^2 \end{bmatrix} \right)$$

Sampling from bivariate normal distribution

```
x <- rnorm(1,mu.x,sigma.x)
y <- rnorm(1,mu.y,sigma.x)  # WRONG. Valid only when sigma.xy = 0
```

How can we sample from a joint distribution?

Possible approaches

Use known packages

- `mvtnorm()` package provides `rmvnorm()` function for sampling from a multivariate-normal distribution
- If we use this, we would never learn how to implement it

Use conditional distribution

$$y|x \sim \mathcal{N}\left(\mu_y + \frac{\sigma_{xy}}{\sigma_x^2}(x-\mu_x), \sigma_y^2\left(1 - \frac{\sigma_{xy}^2}{\sigma_x^2\sigma_y^2}\right)\right)$$

```
x <- rnorm(1, mu.x, sigma.x)
y <- rnorm(1, mu.y + sigma.xy/sigma.x^2*(x-mu.x),
        sigma.y^2 - sigma.xy^2/sigma.x^2)
```


Sampling from multivariate normal distribution

Problem

- Randomly sample from $\mathbf{x} \sim \mathcal{N}(\mathbf{m}, V)$
- The covariance matrix V is positive definite

Using conditional distribution

- Sample $x_1 \sim \mathcal{N}(m_1, V_{11})$
- Sample $x_2 \sim \mathcal{N}(m_2 + V_{12}V_{22}^{-1}(x_1 - m_1), V_{22} - V_{12}^T V_{11}^{-1} V_{12})$
- Repetitively sample x_i from subsequent conditional distributions.

This approach would require excessive amount of computational time

Using Cholesky decomposition for sampling from MVN

Key idea

- If $\mathbf{x} \sim \mathcal{N}(\mathbf{m}, V)$, $A\mathbf{x} \sim \mathcal{N}(A\mathbf{m}, AVA^T)$.
- Sample $\mathbf{z} \sim \mathcal{N}(0, I_n)$ from standard normal distribution
- Find A such that

$$\mathbf{x} = A\mathbf{z} + \mathbf{m} \sim \mathcal{N}(\mathbf{m}, AA^T) = \mathcal{N}(\mathbf{m}, V)$$

- Choleskey decomposition $V = U^T U$ generates an example $A = U^T$.

An example R code

```
z <- rnorm(length(m))
U <- chol(V)
x <- m + t(U) %*% z
```


Summary

Today

- True random numbers and pseudo-random numbers
- Sampling from a uniform distribution
- Sampling from a normal distribution
- Sampling from multivariate nomal distribution

More complex distributions

- Monte-Carlo Methods
- Importance Sampling