Computational Statistics - STAT 575 - HW #1

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Problem 1

Write your own code and find solution to the equation $x^3 + x - 4 = 0$ using Newton's method and the secant method. Compare the number of iterations needed for different starting values for the two methods.

Solution: Newton's method

If we have some function $f : \mathbb{R} \mapsto \mathbb{R}$ and we wish to find a root of f, i.e., an x such that $f(x) = 0$, we may use Newton's method.

We take an initial guess of the root as x_0 and try to refine it with a linear approximation of f given by

$$L(f|x_0) \coloneqq \lambda x . f(x_0) + f'(x_0)(x - x_0).$$

Now, we may approximate a root of f with a root of $L(f|x_0)$,

$$L(f|x_0)(x) = 0,$$

which may be rewritten as

$$f(x_0) + f'(x_0)(x - x_0) = 0.$$

Solving for a root x of $L(f|x_0)$ we get the result

$$x = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

Hoping that x results in a better approximation of the root of f than x_0, we approximate f with $L(f|x)$ and repeat the process.

Generalizing this result, we obtain the iterative procedure

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}.$$

We continue this process until we obtain some stopping condition, e.g., $|x_{i+1} - x_i| < \epsilon$.

Letting $f(x) \coloneqq x^3 + x - 4$ and $f'(x) = 3x^2 + 1$ and substituting into the above result, we get the result

$$x_{i+1} = x_i - \frac{x_i^3 + x_i - 4}{3x_i^2 + 1}.$$

We implement a general procedure for Newton's method:

```
newton_method <- function(f,dfdx,x0,eps)
{
  n <- 0
  repeat
  {
    x1 <- x0 - f(x0) / dfdx(x0)
    n <- n + 1
    if(abs(x1 - x0) < eps)
    {
      break
    }
    x0 <- x1
  }
  list(root=x0,iter=n)
}
```

We take an initial guess of $x_0 = 1$ and $\epsilon = 1 \times 10^{-6}$ and run the following R code to solve for a root of f using Newton's method:

```
f <- function(x) { x^3 + x - 4 }
dfdx <- function(x) { 3*x^2 + 1 }
eps <- 1e-6
x0 <- 1
result <- newton_method(f,dfdx,x0,eps)
```

We obtain $x \approx 1.3787967$ after 5 iterations. When we plug that approximate root into f we obtain the result $f(1.3787967) = 7.3825959 \times 10^{-9}$, which is approximately zero.

Solution: Secant method

In Newton's method, we linearize f using the derivative of f. If, instead, we use the secant of f with respect to two inputs x_i and x_{i+1}, as given by

$$\frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i},$$

we get the iterative procedure

$$x_{i+2} = x_{i+1} - f(x_{i+1}) \frac{x_{i+1} - x_i}{f(x_{i+1}) - f(x_i)},$$

which requires two initial values x_0 and x_1.

We define the secant method as a function given by:

```r
secant_method <- function(f,x0,x1,eps)
{
  n <- 0
  repeat
  {
    x2 <- x1 - f(x1) * (x1 - x0) / (f(x1) - f(x0))
    n <- n + 1
    if(abs(x2-x1) < eps)
    {
      break
    }
    x0 <- x1
    x1 <- x2
  }
  list(root=x1,iter=n)
}
```

We let $x_0 = 0$, $x_1 = 1$, and keep everything else the same and run the secant method with the following R code:

```r
x0 <- 0
x1 <- 1
result <- secant_method(f,x0,x1,eps)
```

We obtain $x \approx 1.3787965$ after 7 iterations. When we plug that approximate root into f we obtain the result $f(1.3787965) = -1.268648 \times 10^{-6}$, which is approximately zero.

Note that this is 2 more iterations than Newton's method.

Problem 2

Poisson regression. The Ache hunting data set has $n = 47$ observations recording is the number of monkeys killed over a period of days with each hunter along with hunter's age. It is of interest to estimate and quantify the monkey kill rate as a function of hunter's age. Hunting prowess confers elevated status among the group, so a natural question is whether hunting ability improves with age, and at which age hunting ability is best.

Hand-code Newton-Raphson in R to fit the Poisson regression model

$$monkeys_i \sim \text{Pois}\left(\exp(\log days_i + \theta_1 + \theta_2 age_i + \theta_3 age_i^2)\right).$$

Feel free to use jacobian and hessian in the numDeriv R package. You may need a sets of crude starting values.

I run a linear regression for the "empirical log-rates" and get starting values $(5.99, 0.167, 0.001)$. Feel free to use those. Compare your result with glm() function in R using

```r
glm(monkeys~age+I(age^2), family="poisson", offset=log(day
```

Solution

We are given the following data:

```r
d <- read.table("ache.txt", header=T)
n <- length(d$age)
X <- cbind(rep(1,n), d$age, d$age^2)

loglike <- function(theta)
{
  sum(dpois(d$monkeys,exp(log(d$days)+X%*%theta),log=T))
}
```

Observe that the design matrix is defined as

$$X = \begin{pmatrix} 1 & a_1 & a_1^2 \\ 1 & a_2 & a_2^2 \\ \vdots & \vdots & \vdots \\ 1 & a_n & a_n^2 \end{pmatrix},$$

the parameter vector is defined as

$$\vec{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix},$$

and the response variables are defined as

$$\vec{m} = \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_n \end{pmatrix}.$$

In poisson regression, we find the best fit for

$$M_i \sim \text{POI}(\exp(\log \mathrm{d_i} + \mathrm{X}\,)).$$

where M_i is the random response variable for $i = 1, \ldots, n$.

The log-likelihood is defined as

$$\ell(\vec{\theta}|data) = \sum_{i=1}^{n} \log f_{M_i}(m_i|g(\vec{\theta}))$$

where

$$g(\vec{\theta}) = \exp(\log d_i + X\vec{\theta}).$$

We generalize the univariate Newton's method in Problem 1 to the multivariate case. We implement the multivariate Newton-Raphson method with numerical hessian and jacobian with the following R code:

```r
library(numDeriv)
newton_raphson_method <- function(x0,f,eps)
{
  n <- 0
  x1 <- x0
  repeat
  {
      x1 <- x0 - solve(hessian(f,x0))%*%t(jacobian(f,x0))
      n <- n + 1
      if (max(abs(x1 - x0)) < eps) { break }
      x0 <- x1
  }
  list(root=x1,iter=n)
}
```

We use the multivariate Newton-Raphson method to find the MLE of θ in the poisson regression model:

```r
eps <- 1e-6
theta0 <- c(5.99, 0.167, 0.001) # starting values
theta_mle <- newton_raphson_method(theta0,loglike,eps)$root
```

The MLE of θ is given by:

```
##               [,1]
## [1,] -5.484245905
## [2,]  0.124647667
## [3,] -0.001203418
```

We compare the results with the builtin method:

```r
glm(monkeys~age+I(age^2),family="poisson", offset=log(days),data=d)$coefficients
```

```
##  (Intercept)          age     I(age^2)
## -5.484245904  0.124647667 -0.001203418
```

The hand-coded approach and the builtin approach obtain the same point estimate $\hat{\theta} = (-5.4842, 0.1246, -0.0012)'$.

Problem 3

Logistic and Cauchy distributions are well-suited to the inverse transform method. For each of the following, generate 10,000 random variables using the inverse transform. Compare your program with the built-in R functions rlogis() and rcauchy(), respectively:

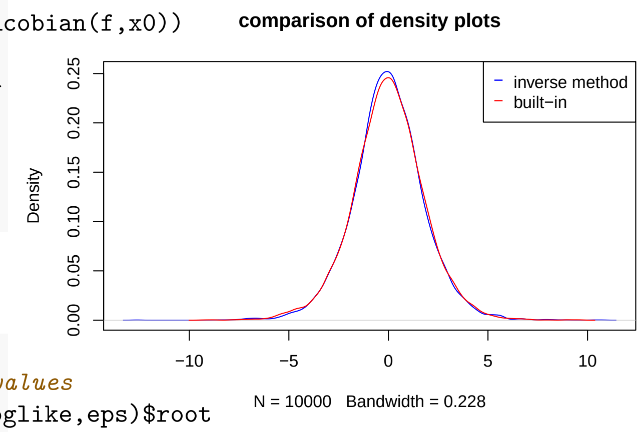
Solution: part (a)

Standard logistic distribution

$$F(x) = \frac{1}{1+e^{-x}}$$

Solve for x in

$$u = F(x)$$
$$u = \frac{1}{1+e^{-x}}$$
$$x = \log(u/(1-u)).$$



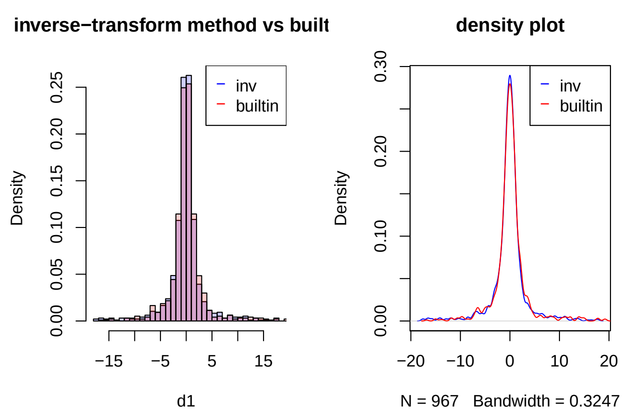
Solution: part (b)

Standard Cauchy distribution

$$F(x) = \frac{1}{2} + \frac{1}{\pi}\arctan(\mathrm{x})$$

Solve for x in

$$u = F(x)$$
$$u = \frac{1}{2} + \frac{1}{\pi}\arctan(\mathrm{x})$$
$$x = \tan(\pi(u - 1/2)).$$



Problem 4

Generating 10,000 random variables from Geometric(p) distribution based off Bernoulli trials.

Solution

A random variable $X \sim$ Geometric(p) is given by the number of i.i.d. trials needed to have a success where success occurs with probability p.

Thus, we may simulate this distribution with the following R code:

```
# simulate n realizes of geometric(p)
rgeo <- function(n,p)
{
  outcomes <- vector(length=n)
  for (i in 1:n)
  {
    trials <- 0
    while (T)
    {
      trials <- trials + 1
      if (rbinom(1,1,p) == 1) { break }
    }
    outcomes[i] <- trials
  }
  outcomes
}
```

Problem 5

Generate random values from a Standard Half Normal distribution with pdf,

$$f(x) = \frac{2}{\sqrt{2\pi}} e^{-x^2/2}, x > 0.$$

For the candidate pdf, choose the exponential density with rate 1. Verify that your method works via a plot of the true density, and a histogram of the generated values.

Solution

We are given the density of the standard half-normal distribution,

$$\text{dhalfnormal}(x) = \frac{2}{\sqrt{2\pi}} e^{-x^2/2}, x > 0.$$

We model this density with the following R code:

```
# density for standard half-normal
dhalfnormal <- function(x) { 2/sqrt(2*pi)*exp(-x^2/2) }
```

We sample from the exponential distribution $\text{EXP}(\lambda = 1)$, with density g and thus we first find the c satisfying

$$c = \max\left\{\frac{\text{dhalfnormal}(x)}{\text{dexp}(x|\lambda = 1)} | x \in \mathbb{R}\right\},$$

which is found to be approximately $c = 1.315489247$.

We implement the standard half-normal sampler, rhalfnormal, using the acceptance-rejection sampling technique with the following R code:

```
# accept-rejection sampling for standard half-normal
# using exp(rate=1)
rhalfnormal <- function(N)
{
  c <- 1.315489247
  xs <- vector(length=N)
  k <- 1
  while (T)
  {
    x <- rexp(n=1)
    if (runif(n=1) < dhalfnormal(x)/(c*dexp(x)))
    {
      xs[k] <- x
      k <- k + 1
      if (k == N) { break }
    }
  }
  xs
}
```

Problem 6

Use accept-reject to sample from this bimodal density:

$$f(x) \propto 3e^{-0.5(x+2)^2} + 7e^{-0.5(x-2)^2}$$

The normalizing constant is 25.066. For your proposal $g(\cdot)$, use a $N(0, 2^2)$ distribution. Verify that your method works via a plot of the true normalized density, and a histogram of the generated values.

Solution

We are given the kernel of the bimodal distribution of interest,

$$\text{ker-bimodal}(x) = 3e^{-0.5(x+2)^2} + 7e^{-0.5(x-2)^2},$$

with the normalizing constant $C = 25.0663$ and thus the pdf for the bimodal is given by

$$\text{dbimodal}(x) = \frac{\text{ker}(x)}{C}.$$

We model these two functions with the following R code:

```
# density for biomodal density
kerbimodal <- function(x) { 3*exp(-0.5*(x+2)^2) + 7*exp(-(
kerbimodal.C <- 25.0663
dbimodal <- function(x) { kerbimodal(x) / kerbimodal.C }
```

We sample from the normal distribution $N(\mu = 0, \sigma^2 = 2^2)$, with density g and thus we first find the c satisfying

$$c = \max \left\{ \frac{\text{ker-bimodal}(x)}{g(x|\mu = 0, \sigma^2 = 2^2)} | x \in \mathbb{R} \right\},$$

which is found to be approximately $c = 68.35212$.

We implement the bimodal sampler, rbimodal, using the acceptance-rejection sampling technique with the following R code:

```r
# accept-rejection sampling for bimodal distribution
# with density dbimodal using normal(0,2^2).
rbimodal <- function(N)
{
  c <- 68.35212
  xs <- vector(length=N)
  k <- 1
  while (T)
  {
    x <- rnorm(n=1,mean=0,sd=2)
    y <- kerbimodal(x)/(c*dnorm(x,mean=0,sd=2))
    if (runif(n=1) < y)
    {
      xs[k] <- x
      if (k == N) { break }
      k <- k + 1
    }
  }
  xs
}
```