Computational Statistics - Suggested Solution for Exam

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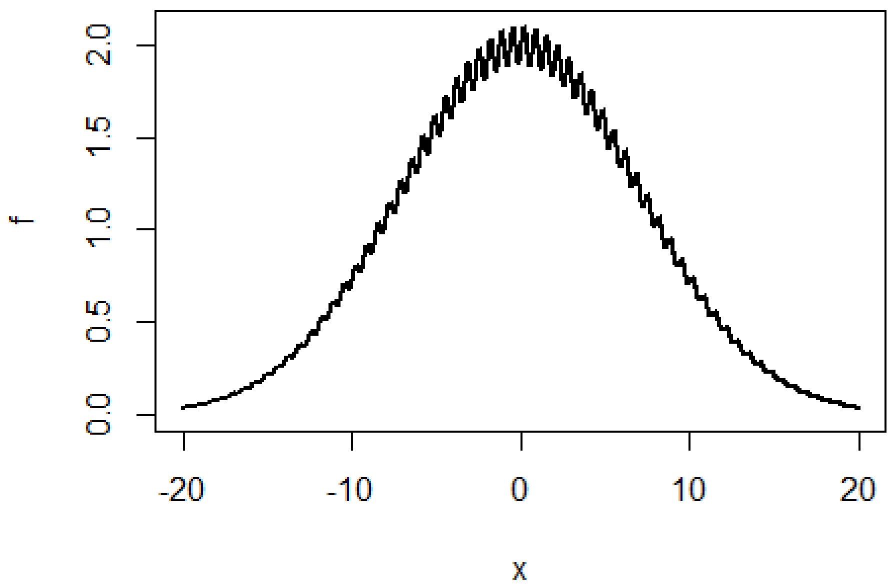
Assignment 1

Question 1.1

```
f <- function(x){
  exp(-x^2/100) * (2-0.1*cos(3*pi*(x+0.1)))
}
vf <- Vectorize(f)
xv <- -2000:2000/100
plot(c(min(xv), max(xv)), c(0, max(vf(xv))), type="n", xlab=expression(x),
ylab="f")
lines(xv, vf(xv), col=1, lwd=2)
```



Not requested:

```
optimize(f, c(-3, 3), maximum=TRUE)

## $maximum
## [1] 1.559289
##
```

```
## $objective
## [1] 2.049321
```

The main problem with Newton here is that it searches a local maximum usually close to the starting value. Here are a lot of local maxima. In generel the algorithm cannot find a global maximum. However, one could use a grid of many starting values and run Newton many times. The solution with the highest value of f can then be the approximation for the global maximum. An advantage of simulated annealing: It is build for searching a global maximum since it accepts also detoriations in the initial phase of the algorithm. By this, it can escape from local maxima. A disadvantage is that simulated annealing is much slower than Newton in converging.

Question 1.2

```r
simann <- function(xstart, taustart=10, maxiter=10000, taufac=0.95){
  tau   <- taustart           # current temperature
  x     <- xbest <- xstart    # current approximation
  fx    <- fxbest <- f(x)
  for (i in 1:maxiter){
    xcand  <- x + rnorm(1)
    fxcand <- f(xcand)
    if (fxcand>fx){
      x  <- xcand
      fx <- fxcand
      if (fxcand>fxbest){
        xbest  <- xcand
        fxbest <- fxcand
      }
    } else {
      if (runif(1) < exp((fxcand-fx)/tau)){
        x  <- xcand
        fx <- fxcand
      }
    }
    if (i/10-round(i/10)==0) tau <- tau/taufac
  }
  c(xbest, fxbest)
}
```

Question 1.3

A single run:

```r
set.seed(2024)
simann(5, taustart=0.01)

## [1] 0.2320901 2.0988623
```

The global maximum is at 0.23 with function value 2.0989 We count therefore, how many times we get a result x with f(x)>2.098 We use starttemperature 10 and 0.01 and run the algorithm 100 times

```r
succ <- 0
for (j in 1:100){
  xopt <- simann(5, taustart=10)
  succ <- succ + (xopt[2]>2.098)
}
succ/100

## [1] 0.77

succ <- 0
for (j in 1:100){
  xopt <- simann(5, taustart=0.01)
  succ <- succ + (xopt[2]>2.098)
}
succ/100

## [1] 1
```

The result is that starttemperature 10 is too high (around 70-75% success rate); better 0.01 with (almost) 100% success rate

Using optim, one can apply simulated anneling the following way (and below using the quasi-Newton BFGS (not required, here)

```r
optim(5, f, method="SANN", control=list(fnscale=-1, temp=10, maxit=10000,
tmax=10000))

## $par
## [1] 0.2295992
##
## $value
## [1] 2.098831
##
## $counts
## function gradient
##    10000       NA
##
## $convergence
## [1] 0
##
## $message
## NULL

optim(5, f, method="BFGS", control=list(fnscale=-1))

## $par
## [1] 4.213307
##
## $value
## [1] 1.756937
##
## $counts
```

```
## function gradient
##        8        4
##
## $convergence
## [1] 0
##
## $message
## NULL
```

Question 2

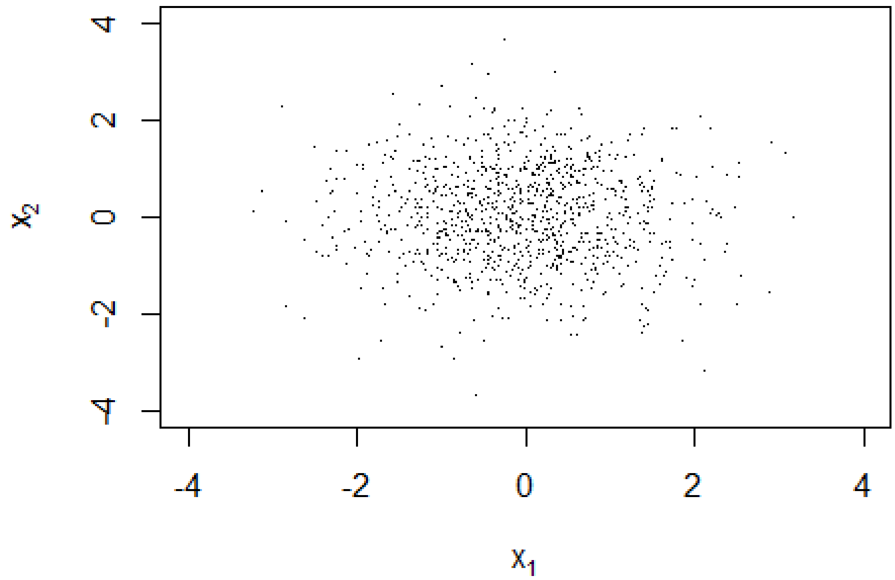
Question 2.1

A function for Gibbs sampling; we include here already plotting the generated sample since this is needed in 2.2

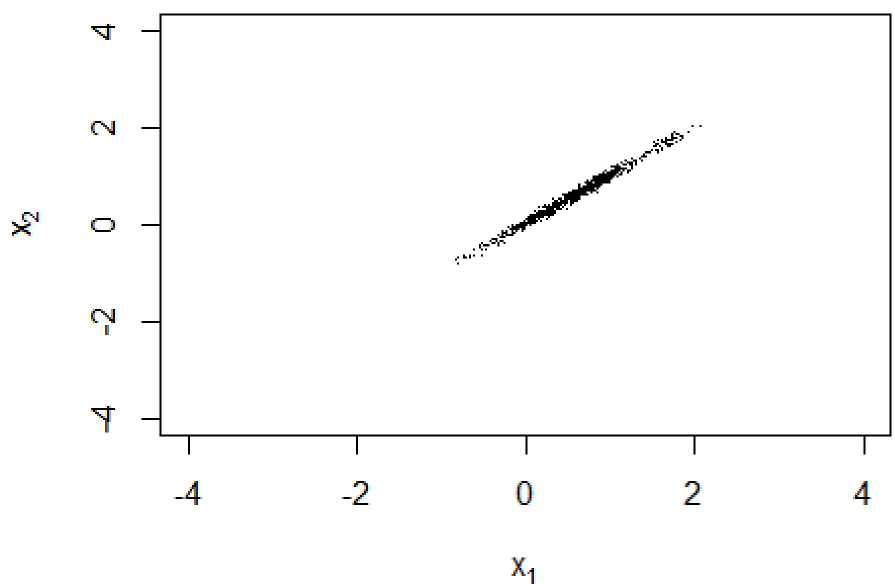
```
gibbs <- function(xstart=c(0, 0), n=1000, rho=0){
  x   <- xstart
  x2n <- x[2]
  plot(c(-4, 4), c(-4, 4), type="n", xlab=expression(x[1]),
ylab=expression(x[2]))
  for (i in 1:1000){
    x1n  <- rnorm(1, mean=rho*x2n, sd=sqrt(1-rho^2))
    x2n  <- rnorm(1, mean=rho*x1n, sd=sqrt(1-rho^2))
    newx <- c(x1n, x2n)
    x <- cbind(x, newx)
    points(x1n, x2n, pch=".")
  }
  x
}
```

Question 2.2

```
set.seed(240319)
res0 <- gibbs(rho=0)
```




```r
res9 <- gibbs(rho=0.998)
```



The first case works well and the sample seems to represent the bivariate normal well. For high correlation, Gibbs can only make small steps in each iteration and does not manage to explore the whole distribution when n=1000 samples are generated. Therefore, the distribution is not well represented by the sample (with very high n, this problem disappears).

Question 2.3

```r
sum(colSums(res0)>0)/1000
```

```
## [1] 0.486
```

```r
sum(colSums(res9)>0)/1000
```

```
## [1] 0.894
```

The second result shows that the generated sample does not represent the distribution well.

Question 2.4

We can generate two independent standard normal variables y_1 and y_2. Set $x_1 = y_1$ and $x_2 =$ an appropriate linear combination (=weighted sum) of y_1 and y_2 such that x1 and x2 have correlation rho ($x_2 = \rho x_1 + \sqrt{1-\rho^2} x_2$). (x_1, x_2) is then a two-dimensional sample. Advantage of this alternative: One does not need to derive the conditional distributions in general (here however, they are already given). Problems like seen here with high correlation are avoided. Disadvantage of this alternative: When generalizing this method to higher dimensions, it becomes necessary to compute the root of a symmetric matrix which might slow down the simulation process.