Computer Lab 4 Computational Statistics

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Contents

Question 1: Computations with Metropolis - Hastings

Consider the following probability density function:

$$f(x) \propto x^5 e^{-x}, \ x > 0$$

You can see that the distribution is known up to some constant of proportionality. If you are interested (NOT part of the Lab) this constant can be found by applying integration by parts multiple times and equals 120.

1. Use Metropolis-Hastings algorithm

to generate samples from this distribution by using proposal distribution as log-normal $\text{LN}(\text{X}_\text{t}, 1)$, take some starting point. Plot the chain you obtained as a time series plot. What can you guess about the convergence of the chain? If there is a burn-in period, what can be the size of this period?

```
rm(list=ls())
set.seed(123456)
#pdf -  probability density function
pdf_target = function(x){
  if(x<= 0){
    stop("x needs to be bigger than 0")
  }
  # stopifnot(x>0) # check - x >0
  return(x^5 * exp(-x))
}
```

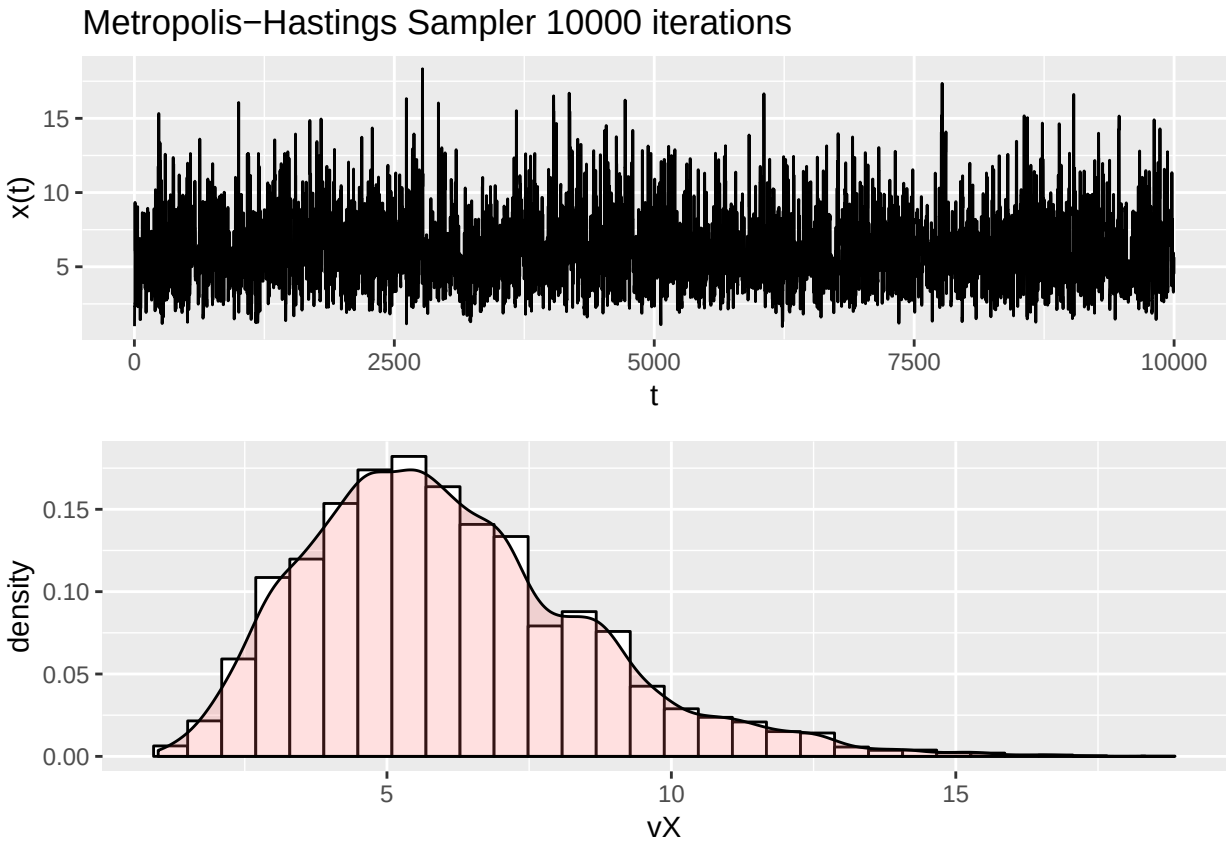
Below you can see the code for the Metropolis-Hastings algorithm. We decided to initialize the starting point (X_0) with 1 and use 10000 for t, as max iterations.

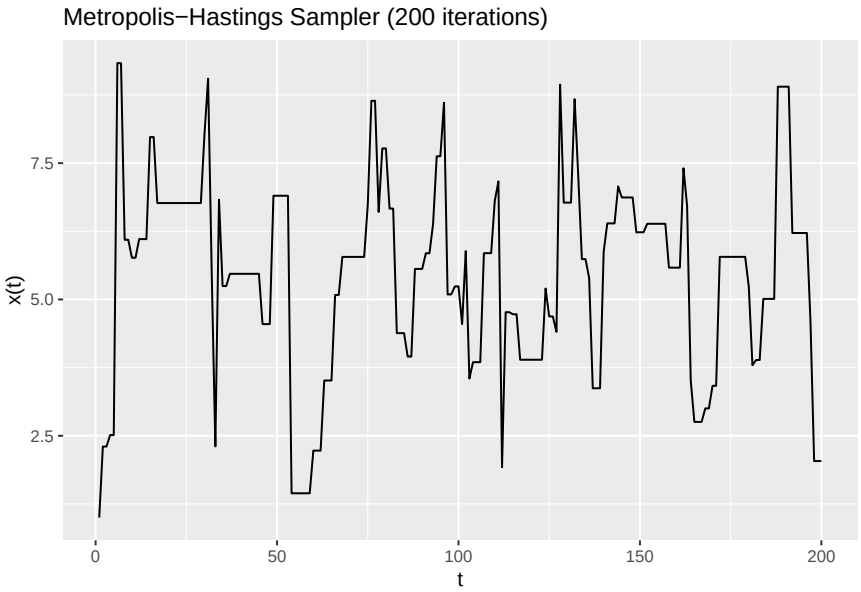
```
# Metropolis-Hastings Sampler

# Initilize chain to X_0, t=0
t_max = 10000
x_0 = 1 # starting point

# algorithm from the slide
MCMC <- function(t_max, x_0){
  rej = 0
  # browser()
  x_t = rep(x_0, t_max) # vector to save y or x_t
  for (t in 2: t_max){
    X = x_t[t-1]
    Y = rlnorm(n = 1, meanlog = log(X), sdlog = 1)
    u = runif(1,0,1)
    num = pdf_target(Y) * dlnorm(X, meanlog = log(Y), sdlog = 1)
    den  = pdf_target(X) * dlnorm(Y, meanlog = log(X), sdlog = 1)
    alpha = min(1, num/den)
    if(u < alpha){
      x_t[t] = Y
    } else{
      # reject the Y when is FALSE
      # then we keep x_{t-1} as x_{t}
      x_t[t] = X
      rej = rej+1
```

```
    }
  }
  cat("Reject rate: ",rej/t_max,"\n")
  return(data.frame(vN=1:t_max, vX=x_t))
}

data_1_1 = MCMC(t_max, x_0)
```

```
## Reject rate:  0.5611
```

Plot of the chain obtained as a time series plot:





The sample points seem to be convergent around 2.5 and 15. We also draw another plot with 200 iterations to find the burn-in period, but it seems that burn-in period is so short (from 0 to 10).

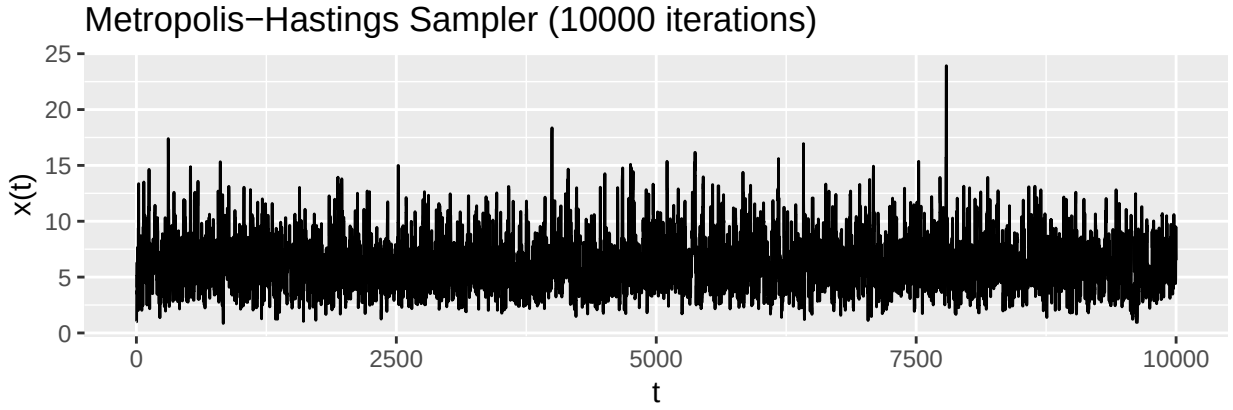
2. Perform Step 1 by using the chi-square distribution

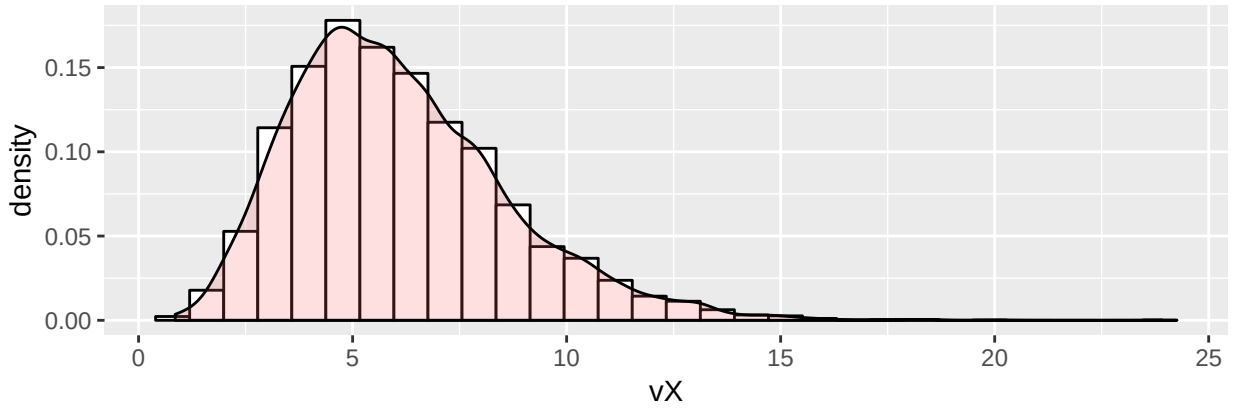
χ^2 ($\lfloor X_t + 1 \rfloor$) as a proposal distribution, where$\lfloor x \rfloor$ is the floor function, meaning the integer part of x for positive x, i.e.$\lfloor 2.95 \rfloor = 2$

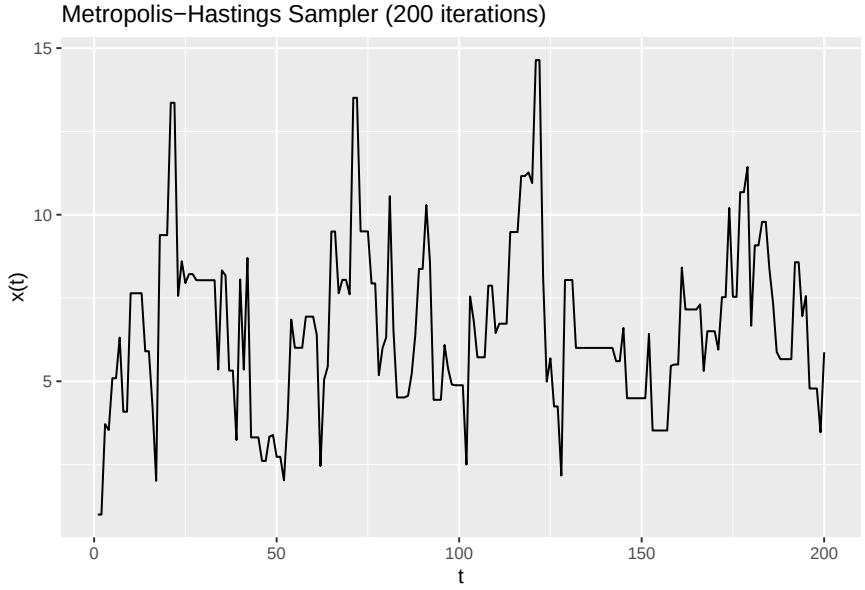
Metropolis-Hastings algorithm with chi-square as proposal distribution

```
MCMC2 <- function(t_max, x_0){
  rej = 0
  x_t = rep(x_0, t_max) # vector to save y or x_t
  for (t in 2: t_max){
    X = x_t[t-1]
    Y = rchisq(1,df=floor(X+1))
    u = runif(1,0,1)
    num = pdf_target(Y)*dchisq(X,floor(Y+1))
    den = pdf_target(X)*dchisq(Y,floor(X+1))

    alpha = min(1, num/den)
    if(u < alpha){
      x_t[t] = Y
    } else{
      # reject the Y when is FALSE
      # then we keep x_{t-1} as x_{t}
      x_t[t] = X
      rej = rej+1
    }
  }
  cat("Reject rate: ",rej/t_max,"\n")
  return(data.frame(vN=1:t_max, vX=x_t))
}

data_1_2 = MCMC2(t_max, x_0)
```

```
## Reject rate:  0.4005
```







3. Compare the results of Steps 1 and 2 and make conclusions.

In step 2, the MH method based on chi-square distribution has similar burn-in period (0~10) and convergent interval (2.5~15). However, the rejection rate of the method in step 2 is around 0.4, but in step 1 is more than 0.5, which means that chi-square distribution might be a better proposal distribution than log-normal

distribution to generate the samples of our target distribution.

4. Generate 10 MCMC sequences

using the generator from Step 2 and starting points 1, 2, . . . , or 10. Use the Gelman-Rubin method to analyze convergence of these sequences.

```
# Generation 10 MCMC sequences with start points 1~10
set.seed(123456)
df <- data.frame(vN=1:t_max)
for (i in 1:10) {
  df <- cbind(df,MCMC2(t_max,i)$vX)
}
```

```
## Reject rate:  0.3988
## Reject rate:  0.4042
## Reject rate:  0.3955
## Reject rate:  0.3852
## Reject rate:  0.3997
## Reject rate:  0.4016
## Reject rate:  0.407
## Reject rate:  0.4011
## Reject rate:  0.4001
## Reject rate:  0.3959
```

```
mcmc_list = list()

for (i in 1:10){
  mcmc_list[[i]] = as.mcmc(df[,i+1], start = i)
}

# Gelman-Rubin method:
gelman.diag(mcmc_list)
```

```
## Potential scale reduction factors:
##
##      Point est. Upper C.I.
## [1,]          1          1
```

Since both potential scale reduction factor and their upper confidence limits are 1's, we can ensure that our samples are convergent.

5. Estimate

$$\int_0^\infty x f(x) dx$$

using the samples from Steps 1 and 2.

Down here follows the rule on how to calculate a definite integral based on lecture slide.

To estimate a θ which is

$$\theta = \int_D f(x) dx,$$

we can decompse such $f(x)$ into:

$$f(x) = g(x)p(x),$$

where

$$\int_D p(x)dx = 1.$$

- Thus, if $X \sim p(.)$ and

$$\theta = E[g(X)] = \int_D g(x)p(x)dx,$$

we can conclude that

$$\hat{\theta} = \frac{1}{n}\sum_i^n g(x_i),\ \forall_i \sim p(.)$$

Our target function is a probability density function, whose integral must be 1. Since we already have the samples from the target distribution by Metropolis-Hastings algorithm, the final integral of $xf(x)$ can be estimated as the mean of such samples.

Mean of sample 1:

```
## [1] 6.061493
```

Mean of sample 2:

```
## [1] 6.085729
```

6. In fact

The distribution generated is a gamma distribution. Look in the literature and define the actual value of the integral. Compare it with the one you obtained.

PDF of gamma distribution $X \approx \Gamma(\alpha, \beta)$:

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

for $x > 0$, and $\alpha, \beta > 0$.

Based on the standard formula, we know that $\alpha = 6$ and $\beta = 1$ in our target PDF. Thus, we can calculate the mean of our target PDF as

$$E[X] = \frac{\alpha}{\beta} = \frac{6}{1} = 6,$$

which closes to our estimated results.

Question 2: Gibbs sampling

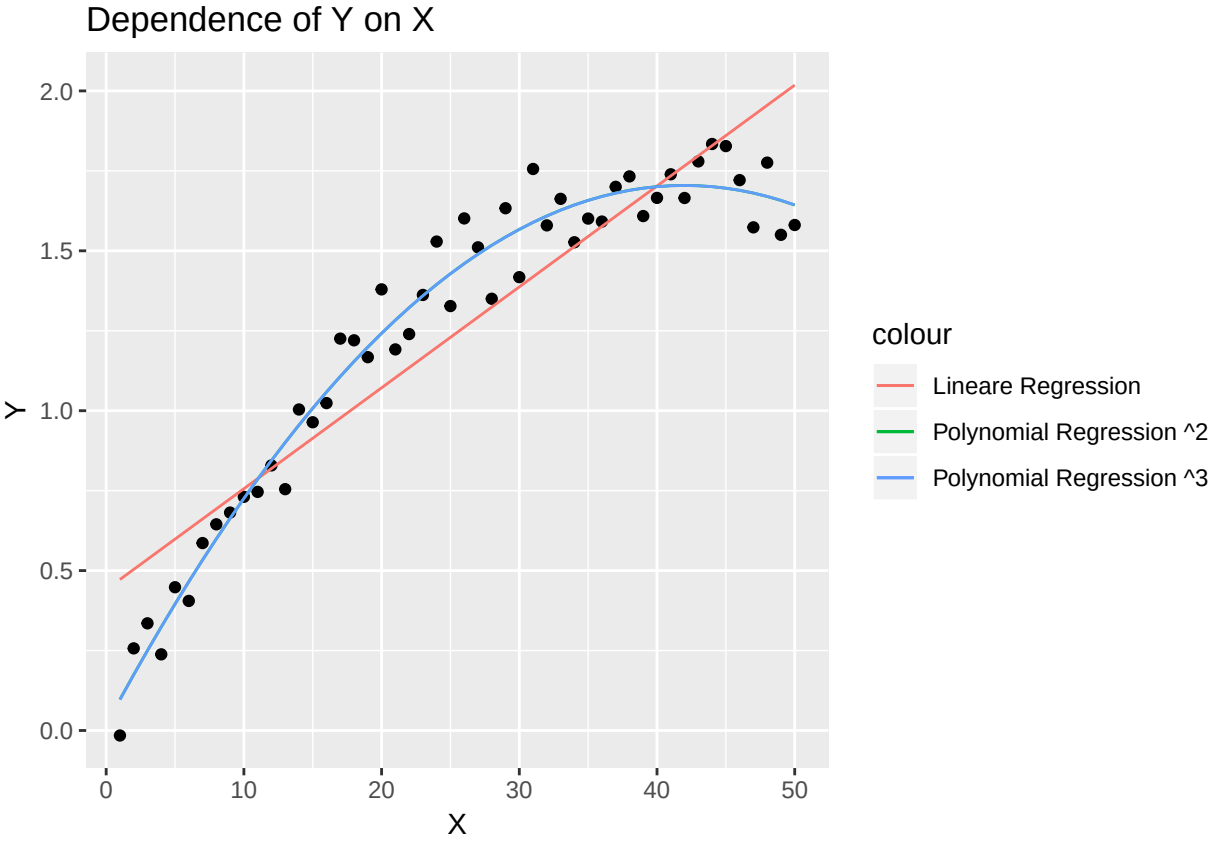
A concentration of a certain chemical was measured in a water sample, and the result was stored in the data *chemical.RData* having the following variables:

- X: day of the measurement
- Y: measured concentration of the chemical.

The instrument used to measure the concentration had certain accuracy; this is why the measurements can be treated as noisy. Your purpose is to restore the expected concentration values.

1. Import the data to R and plot the dependence of Y on X.

What kind of model is reasonable to use here?



It could already be seen that a linear regression does not describe the data too much. However, a second degree polynomial regression is well consistent with the course of the data. As expected can be seen that the progression of polynomials 2 and 3 overlap, so a second grade is sufficient.

2. Present the formula showing the likelihood $p(\vec{Y} \mid \vec{\mu})$ and the prior $p(\vec{\mu})$

A researcher has decided to use the following (random-walk) Bayesian model (n=number of observations, $\vec{\mu} = (\mu_1, ..., \mu_n)$ are unknown parameters):

$$Y_i = \mathcal{N}(\mu, \sigma = 0.2), \quad i = 1, ..., n$$

where the prior is

$$p(\mu_1) = 1$$

$$p(\mu_{i+1} \mid \mu_i) = \mathcal{N}(\mu_i, 0.2) \quad i = 1, ..., n-1$$

Present the formulae showing the likelihood and the prior: $p(\vec{Y} \mid \vec{\mu})$ and $p(\vec{\mu})$.

Likelihood:

$$\begin{aligned}\mathcal{L}[p(\vec{Y}|\vec{\mu}, 0.2)] =& \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi \cdot 0.2}} \exp(-\frac{(y_i - \mu_i)^2}{2 \cdot 0.2}) \\ =& \Big(\frac{1}{\sqrt{0.4\pi}}\Big)^n \exp\Big(-\frac{\sum_{i=1}^{n}(y_i - \mu_i)^2}{0.4}\Big)\end{aligned}$$

Prior:

$$\begin{aligned}p(\vec{\mu}) &= p(\mu_1) \cdot p(\mu_2|\mu_1) \cdot p(\mu_3|\mu_2) \cdot \cdots \cdot p(\mu_n|\mu_{n-1}) \\ &= 1 \cdot \prod_{i=2}^{n} p(\mu_n|\mu_{n-1}) \\ &= \frac{1}{\sqrt{0.4\pi}} \exp(-\frac{(\mu_2 - \mu_1)^2}{0.4}) \cdots \exp(-\frac{(\mu_n - \mu_{n-1})^2}{0.4}) \\ &= \Big(\frac{1}{\sqrt{0.4\pi}}\Big)^{n-1} \exp(-\frac{\sum_{i=2}^{n}(\mu_i - \mu_{i-1})^2}{0.4})\end{aligned}$$

3. Use Bayes' Theorem

to get the posterior up to a constant proportionality, and then fnd out the distributions of $(\mu_i|\vec{\mu}_{-i}, \vec{Y})$, where μ_{-i} is a vector containing all μ values except of μ_i.

Firstly, we calculate

$$\begin{aligned}p(\vec{\mu}, \vec{Y}) =& \ p(\vec{Y}|\vec{\mu}) \cdot p(\vec{\mu}) \\ \propto& \ \exp\Big(-\frac{\sum_{i=1}^{n}(y_i - \mu_i)^2}{0.4}\Big) \cdot \exp(-\frac{\sum_{i=2}^{n}(\mu_i - \mu_{i-1})^2}{0.4}) \\ =& \ \exp(-\frac{\sum_{i=1}^{n}(y_i - \mu_i)^2 + \sum_{i=2}^{n}(\mu_i - \mu_{i-1})^2}{0.4}) \quad .\end{aligned}$$

Since

$$p(\mu_i|\vec{\mu}_{-i}, \vec{Y}) \cdot p(\vec{\mu}_{-i}, \vec{Y}) = p(\mu_i, \vec{\mu}_{-i}, \vec{Y}) = p(\vec{\mu}, \vec{Y}) \quad ,$$

we can conclude that

$$\begin{aligned}p(\mu_1|\vec{\mu}_{-1}, \vec{Y}) =& \ \frac{p(\vec{\mu}, \vec{Y})}{p(\vec{\mu}_{-1}, \vec{Y})} \\ \propto& \ \exp\Big(-\frac{(y_1 - \mu_1)^2 + (\mu_2 - \mu_1)^2}{2\sigma^2}) \\ \propto& \ \exp(-\frac{(\mu_1 - (y_1 + \mu_2)/2)^2}{2\sigma^2/2}) \quad ,\end{aligned}$$

and

$$\begin{aligned}p(\mu_n|\vec{\mu}_{-n}, \vec{Y}) =& \ \frac{p(\vec{\mu}, \vec{Y})}{p(\vec{\mu}_{-n}, \vec{Y})} \\ \propto& \ \exp\Big(-\frac{(y_n - \mu_n)^2 + (\mu_n - \mu_{n-1})^2}{2\sigma^2}) \\ \propto& \ \exp(-\frac{(\mu_n - (y_n + \mu_{n-1})/2)^2}{2\sigma^2/2}) \quad ,\end{aligned}$$

and

$$\begin{aligned} p(\mu_i|\vec{\mu}_{-i},\vec{Y}) = & \frac{p(\vec{\mu},\vec{Y})}{p(\vec{\mu}_{-i},\vec{Y})} \\ \propto & \exp\Big(-\frac{(y_i-\mu_i)^2+(\mu_{i+1}-\mu_i)^2+(\mu_i-\mu_{i-1})^2}{2\sigma^2}\Big) \\ \propto & \exp(-\frac{(\mu_i-(y_i+\mu_{i-1}+\mu_{i+1})/3)^2}{2\sigma^2/3}), \quad i\in(1,n). \end{aligned}$$

Thus, the results of our deduction can be shown as

$$(\mu_i|\vec{\mu}_{-i},\vec{Y}) \sim \begin{cases} N(\frac{y_1+\mu_2}{2},0.1) & i=1 \\ N(\frac{y_i+\mu_{i-1}+\mu_{i+1}}{3},\frac{0.2}{3}) & Otherwise \\ N(\frac{y_n+\mu_{n-1}}{2},0.1) & i=n \end{cases}$$

4.Use the distributions derived in Step 3 to implement a Gibbs sampler

that uses $\vec{\mu}^0=(0,...,0)$ as a starting point. Run the Gibbs sampler to obtain 1000 values of $\vec{\mu}$ and then compute the expected value of $\vec{\mu}$ by using a Monte Carlo approach. Plot the expected value of $\vec{\mu}$ versus X and Y versus X in the same graph. Does it seem that you have managed to remove the noise? Does it seem that the expected value of $\vec{\mu}$ can catch the true underlying dependence between Y and X?

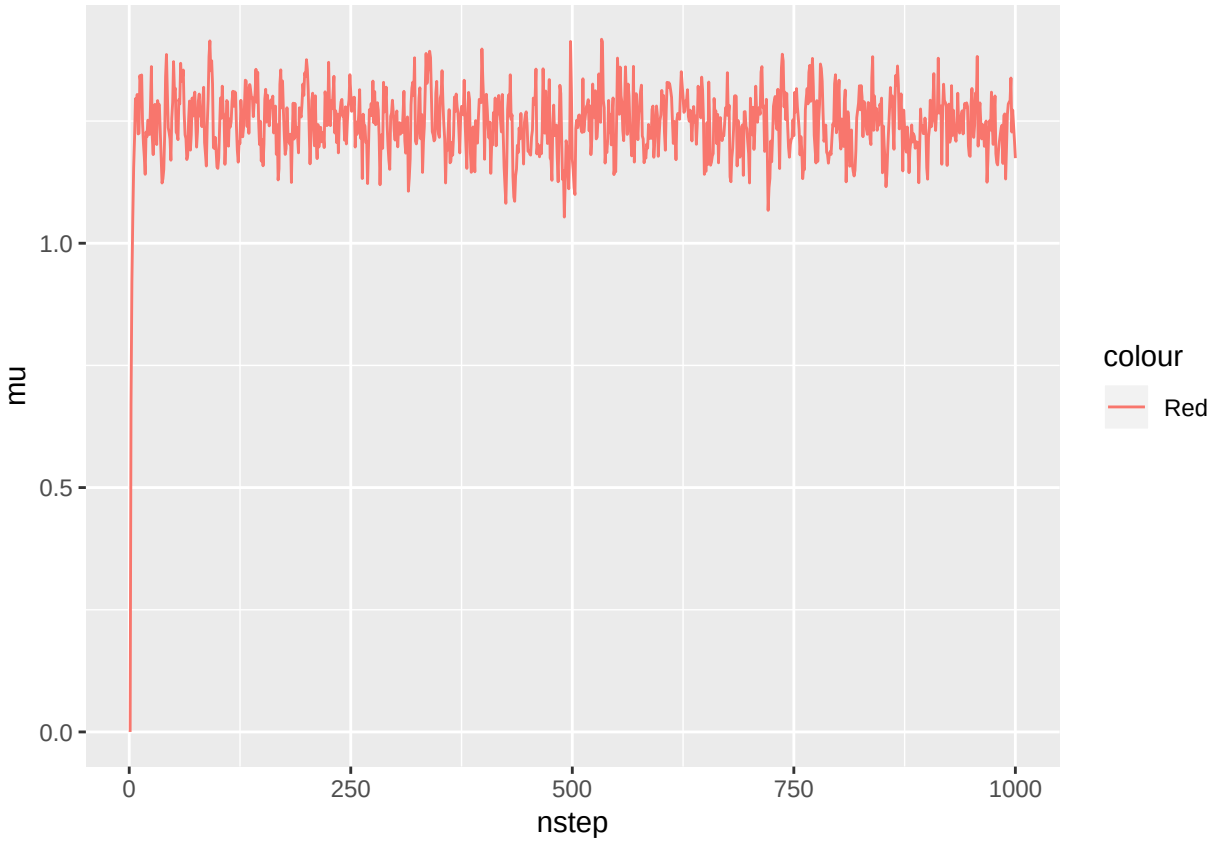
```
nstep = 1000
d = length(Y)
mu0 = rep(0,d)

gibbs = function(nstep, mu0, y){
    d <- length(mu0)
    mat_mu <- matrix(0, nrow=nstep, ncol=d)
    mat_mu[1,] <- mu0

    for (t in 2:nstep) {
      mat_mu[t,1] = rnorm(1,(y[1]+mat_mu[t-1,2])/2,sqrt(0.1))
      for (i in 2:(d-1)) {
        mat_mu[t,i] = rnorm(1,(y[i]+mat_mu[t,i-1]+mat_mu[t-1,i+1])/3,sqrt(0.2/3))
      }
      mat_mu[t,d] = rnorm(1,(y[d]+mat_mu[t,d-1])/2,sqrt(0.1))
    }
    mat_mu
}

re = gibbs(nstep, mu0, Y)
```

Expected value of $\vec{\mu}$ versus X and Y versus X:

In the generated visualization a very similar course of Y and mu can be seen. This means that the noise could be removed well. In the area the variance is greatest. It can also be said that the expected value of $\vec{\mu}$ can catch the true underlying dependence between Y and X well.

5.Trace plot

Make a trace plot for μ_n and comment on the burn-in period and convergence.



In the visualization can we see an early burn-in, already after some interactions does it converges.

Appendix

```r
knitr::opts_chunk$set(echo = TRUE, out.width = "480px")
# libraries used in this lab
library(ggplot2)
# install.packages("coda")
library(coda)
library(gridExtra)
# infromation & marterial
# vey nice blog - MCMC and the Metropolis-Hastings algorithm
#https://blog.stata.com/2016/11/15/introduction-to-bayesian-statistics-part-2-mcmc-and-the-metropolis-h
rm(list=ls())
set.seed(123456)
#pdf -  probability density function
pdf_target = function(x){
  if(x<= 0){
    stop("x needs to be bigger than 0")
  }
  # stopifnot(x>0) # check - x >0
  return(x^5 * exp(-x))
}
# Metropolis-Hastings Sampler

# Initilize chain to X_0, t=0
t_max = 10000
x_0 = 1 # starting point

# algorithm from the slide
MCMC <- function(t_max, x_0){
  rej = 0
  # browser()
  x_t = rep(x_0, t_max) # vector to save y or x_t
  for (t in 2: t_max){
    X = x_t[t-1]
    Y = rlnorm(n = 1, meanlog = log(X), sdlog = 1)
    u = runif(1,0,1)
    num = pdf_target(Y) * dlnorm(X, meanlog = log(Y), sdlog = 1)
    den  = pdf_target(X) * dlnorm(Y, meanlog = log(X), sdlog = 1)
    alpha = min(1, num/den)
    if(u < alpha){
      x_t[t] = Y
    } else{
      # reject the Y when is FALSE
      # then we keep x_{t-1} as x_{t}
      x_t[t] = X
      rej = rej+1
    }
  }
  cat("Reject rate: ",rej/t_max,"\n")
  return(data.frame(vN=1:t_max, vX=x_t))
}

data_1_1 = MCMC(t_max, x_0)
```

```r
# create time series plot

# create the plot object
points11= ggplot(data = data_1_1, aes(x= vN, y= vX)) +
  geom_line()+
  ggtitle("Metropolis-Hastings Sampler 10000 iterations")+
  ylab("x(t)")+
  xlab("t")

density11= ggplot(data_1_1,aes(x=vX))+
  geom_histogram(aes(y=..density..),
                 colour="black",
                 fill="white",
                 bins=30)+
  geom_density(alpha=.2, fill="#FF6666")

grid.arrange(points11,density11,nrow=2)
ggplot(data = data_1_1[1:200,], aes(x= vN, y= vX)) +
  geom_line()+
  ggtitle("Metropolis-Hastings Sampler (200 iterations)")+
  ylab("x(t)")+
  xlab("t")

MCMC2 <- function(t_max, x_0){
  rej = 0
  x_t = rep(x_0, t_max) # vector to save y or x_t
  for (t in 2: t_max){
    X = x_t[t-1]
    Y = rchisq(1,df=floor(X+1))
    u = runif(1,0,1)
    num = pdf_target(Y)*dchisq(X,floor(Y+1))
    den = pdf_target(X)*dchisq(Y,floor(X+1))

    alpha = min(1, num/den)
    if(u < alpha){
      x_t[t] = Y
    } else{
      # reject the Y when is FALSE
      # then we keep x_{t-1} as x_{t}
      x_t[t] = X
      rej = rej+1
    }
  }
  cat("Reject rate: ",rej/t_max,"\n")
  return(data.frame(vN=1:t_max, vX=x_t))
}

data_1_2 = MCMC2(t_max, x_0)
# create the plot - t_max = 10.000

# create the plot object
points12= ggplot(data = data_1_2, aes(x= vN, y= vX)) +
  geom_line()+
```

```
  ggtitle("Metropolis-Hastings Sampler (10000 iterations)")+
  ylab("x(t)")+
  xlab("t")

density12= ggplot(data_1_2,aes(x=vX))+
  geom_histogram(aes(y=..density..),
                 colour="black",
                 fill="white",
                 bins=30)+
  geom_density(alpha=.2, fill="#FF6666")

grid.arrange(points12,density12,nrow=2)

# create the plot object
ggplot(data = data_1_2[1:200,], aes(x= vN, y= vX)) +
  geom_line()+
  ggtitle("Metropolis-Hastings Sampler (200 iterations)")+
  ylab("x(t)")+
  xlab("t")
# Generation 10 MCMC sequences with start points 1~10
set.seed(123456)
df <- data.frame(vN=1:t_max)
for (i in 1:10) {
  df <- cbind(df,MCMC2(t_max,i)$vX)
}
mcmc_list = list()

for (i in 1:10){
  mcmc_list[[i]] = as.mcmc(df[,i+1], start = i)
}

# Gelman-Rubin method:
gelman.diag(mcmc_list)
mean_set1 = mean(data_1_1$vX)
mean_set1
mean_set2 = mean(data_1_2$vX)
mean_set2
rm(list=ls())
set.seed(123456)
# set working directory
# import the data
load("chemical.RData")
# create table for plot
data = data.frame("X" = X,
                  "Y" = Y)
# plot dependence of Y on X
X_Y_dependence = ggplot(data, aes(x = X, y = Y)) +
  geom_point()+
  ggtitle("Dependence of Y on X") +
  geom_smooth()
# which model would fit the data
# lookes like a polinomial regression -> test until poly 3
model1 = lm(Y ~  X,
```

```
            data = data)
model2 = lm(Y ~  X + I(X^2),
            data = data)
model3 = lm(Y ~  X + I(X^2)+ I(X^3),
            data = data)

cols <- c("Lineare Regression"="#62c76b",
          "Polynomial Regression ^2"="#3591d1",
          "Polynomial Regression ^3"="#f04546")

X_Y_dependence_fit = ggplot(data, aes(x = X, y = Y)) +
  geom_point()+
  ggtitle("Dependence of Y on X") +
  geom_line(aes(x = X, y = predict(model1), colour = "Lineare Regression")) +
  geom_line(aes(x = X, y = predict(model2), colour = "Polynomial Regression ^2")) +
  geom_line(aes(x = X, y = predict(model3), colour = "Polynomial Regression ^3"))
X_Y_dependence_fit
nstep = 1000
d = length(Y)
mu0 = rep(0,d)

gibbs = function(nstep, mu0, y){
    d <- length(mu0)
    mat_mu <- matrix(0, nrow=nstep, ncol=d)
    mat_mu[1,] <- mu0

    for (t in 2:nstep) {
      mat_mu[t,1] = rnorm(1,(y[1]+mat_mu[t-1,2])/2,sqrt(0.1))
      for (i in 2:(d-1)) {
        mat_mu[t,i] = rnorm(1,(y[i]+mat_mu[t,i-1]+mat_mu[t-1,i+1])/3,sqrt(0.2/3))
      }
      mat_mu[t,d] = rnorm(1,(y[d]+mat_mu[t,d-1])/2,sqrt(0.1))
    }
    mat_mu
}

re = gibbs(nstep, mu0, Y)
data_2_4 = data.frame(cbind(X=X,Y=Y, mu=colMeans(re)))
data_melt  <- reshape2::melt(data_2_4, id="X")
ggplot(data_melt, aes(x=X,y=value,color=variable))+
  geom_line()+
  geom_point()

data_gribbs = data.frame(nstep=1:1000,mu=rowMeans(re))
ggplot(data_gribbs, aes(x=nstep, y=mu, color = "Red"))+
  geom_line()
```