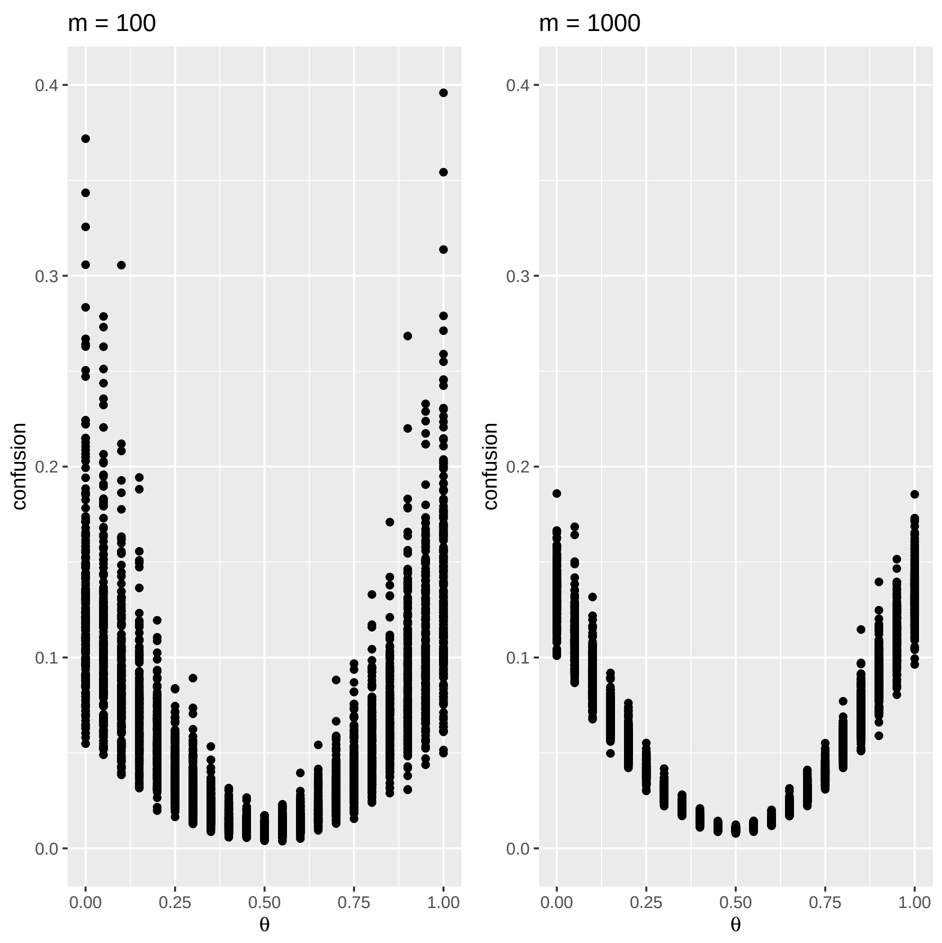
Multivariate Optimization 3

Exercise 1: Stochastic Gradient Descent

(a)
- $\mathbb{E}_{\mathbf{x},y}\nabla_{\boldsymbol{\theta}}\|\boldsymbol{\theta}^\top\mathbf{x}-y\|_2^2 = \mathbb{E}_{\mathbf{x}}\mathbb{E}_{y|\mathbf{x}}\nabla_{\boldsymbol{\theta}}\|\boldsymbol{\theta}^\top\mathbf{x}-y\|_2^2 = \mathbb{E}_{\mathbf{x}}\mathbb{E}_{y|\mathbf{x}}2\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta}-2\mathbf{x}y = \mathbb{E}_{\mathbf{x}}2\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta}-2\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta}^* = 2\boldsymbol{\Sigma}_{\mathbf{x}}(\boldsymbol{\theta}-\boldsymbol{\theta}^*)$
- $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x},y}\|\boldsymbol{\theta}^\top\mathbf{x}-y\|_2^2 = \nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x}}\mathbb{E}_{y|\mathbf{x}}\boldsymbol{\theta}^\top\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta} - 2\boldsymbol{\theta}^\top\mathbf{x}y + y^2 = \nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x}}\boldsymbol{\theta}^\top\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta} - 2\boldsymbol{\theta}^\top\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta}^* + \boldsymbol{\theta}^{*\top}\mathbf{x}\mathbf{x}^\top\boldsymbol{\theta}^*$
  $= \nabla_{\boldsymbol{\theta}}(\boldsymbol{\theta}^\top\boldsymbol{\Sigma}_{\mathbf{x}}\boldsymbol{\theta} - 2\boldsymbol{\theta}^\top\boldsymbol{\Sigma}_{\mathbf{x}}\boldsymbol{\theta}^* + \boldsymbol{\theta}^{*\top}\boldsymbol{\Sigma}_{\mathbf{x}}\boldsymbol{\theta}^*) = 2\boldsymbol{\Sigma}_{\mathbf{x}}(\boldsymbol{\theta}-\boldsymbol{\theta}^*)$

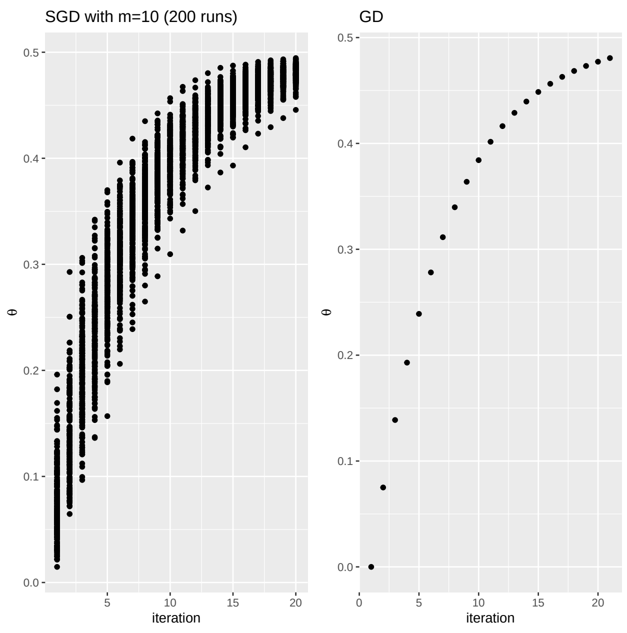
(b) We can estimate $\mathbb{E}_{\mathbf{x},y}\nabla_{\boldsymbol{\theta}}\|\boldsymbol{\theta}^\top\mathbf{x}-y\|_2^2$ without bias via SGD since we have access to realizations of $\nabla_{\boldsymbol{\theta}}\|\boldsymbol{\theta}^\top\mathbf{x}-y\|_2^2$. From a) it follows that this estimate is also an unbiased estimate of the gradient of our objective $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x},y}\|\boldsymbol{\theta}^\top\mathbf{x}-y\|_2^2$. Hence, SGD can be successfully applied in this situation.

(c)
```r
library(ggplot2)
library(gridExtra)

set.seed(123)

sigma_x = 0.5
sigma_y = 0.1

n = 10000
x = sort(rnorm(n, sd = sigma_x))
theta_star = 0.5
y = theta_star * x + rnorm(n, sd = sigma_y)

theta = 0.9
mean(2*(x*x*theta - y*x))

## [1] 0.2015163

compute_conf <- function(theta, n){
  x = rnorm(n, sd = sigma_x)
  y = theta_star * x + rnorm(n, sd = sigma_y)
  # mean of squared differences between the sampled gradients and
  # the gradient of the objective
  return(mean((2*(x*x*theta - y*x) - 2*sigma_x^2*(theta - theta_star))^2))
}

# compute confusions for m = 100

confs = c()
m = 100
reps = 200
thetas = seq(from=0, to=1, length.out = 21)
for(i in 1:reps){
  for(theta in thetas){
    confs = c(confs, compute_conf(theta, m))
  }
}

p_batch100 = ggplot(data.frame(thetas = rep(thetas, reps), confs = confs),
                                   aes(x = thetas, y = confs)) +
  geom_point() + xlab(expression(theta)) + ylim(0, 0.4) + ggtitle("m = 100") +
  ylab("confusion")

# compute confusions for m = 1000

confs = c()
m = 1000
reps = 200
thetas = seq(from=0, to=1, length.out = 21)
for(i in 1:reps){
  for(theta in thetas){
    confs = c(confs, compute_conf(theta, m))
  }
}

p_batch1000 = ggplot(data.frame(thetas = rep(thetas, reps), confs = confs),
                                     aes(x = thetas, y = confs)) +
  geom_point() + xlab(expression(theta)) + ylim(0, 0.4) + ggtitle("m = 1000")  +
  ylab("confusion")

# plot all
grid.arrange(p_batch100, p_batch1000, ncol = 2)
```



(d) Qualitatively, we observe for both settings that the mean and the variance of the confusion rise symmetrically around $\boldsymbol{\theta}^*$. As expected, the mean and the variance of the confusion is smaller for the larger batch size $m = 1000$ than for $m = 100$.

(e)
```r
set.seed(123)

# SGD
thetas = NULL
alpha = 0.3
m = 10
for(j in 1:200){
  theta = 0
  for(i in 1:20){
    x = rnorm(m, sd = sigma_x)
    y = theta_star * x + rnorm(n, sd = sigma_y)

    theta = theta  - alpha * mean(2*(x*x*theta - y*x))
    thetas = rbind(thetas, theta)
  }
}

plot_sgd = ggplot(data.frame(thetas = thetas, it = rep(1:20, 200)),
       aes(x = it, y = thetas)) +
  geom_point() + ylab(expression(theta)) + xlab("iteration") +
  ggtitle("SGD with m=10 (200 runs)")

# GD
theta = 0
thetas = theta
alpha = 0.3

for(i in 1:20){
  theta = theta  - alpha *  2*sigma_x^2*(theta - theta_star)
  thetas = rbind(thetas, theta)
}

plot_gd = ggplot(data.frame(thetas = thetas, it = 1:21),
                 aes(x = it, y = thetas)) +
  geom_point() + ylab(expression(theta)) + xlab("iteration") + ggtitle("GD")

# plot all
grid.arrange(plot_sgd, plot_gd, ncol=2)
```


SGD with m=10 (200 runs)
GD
θ
iteration