Multivariate Optimization 3

Solution 1: Stochastic Gradient Descent

(a) We compute both expressions and compare the results.

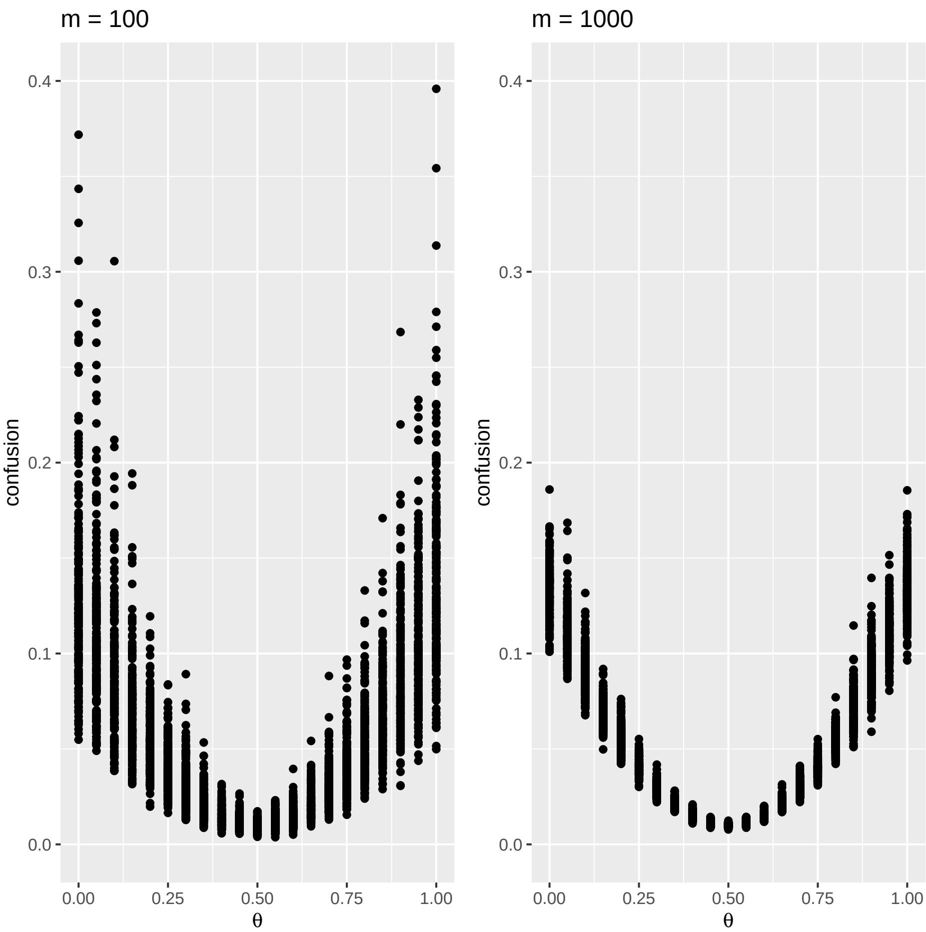
$$\begin{aligned}\mathbb{E}_{\mathbf{x},y}[\nabla_{\boldsymbol{\theta}}[(\boldsymbol{\theta}^\top \mathbf{x} - y)^2]] &= \mathbb{E}_{\mathbf{x},y}[2\mathbf{x}\mathbf{x}^\top \boldsymbol{\theta} - 2\mathbf{x}y] \\ &= \mathbb{E}_{\mathbf{x}}\mathbb{E}_{y|\mathbf{x}}[2\mathbf{x}\mathbf{x}^\top \boldsymbol{\theta} - 2\mathbf{x}y] \\ &= \mathbb{E}_{\mathbf{x}}[2\mathbf{x}\mathbf{x}^\top \boldsymbol{\theta} - 2\mathbf{x}\mathbf{x}^\top \boldsymbol{\theta}^*] \\ &= 2\boldsymbol{\Sigma}_{\mathbf{x}}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)\end{aligned}$$

$$\begin{aligned}\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x},y}[(\boldsymbol{\theta}^\top \mathbf{x} - y)^2] &= \nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x},y}[\boldsymbol{\theta}^\top \mathbf{x}\mathbf{x}^\top \boldsymbol{\theta} - 2\boldsymbol{\theta}^\top \mathbf{x}y + y^2] \\ &= \nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x}}[\boldsymbol{\theta}^\top \mathbf{x}\mathbf{x}^\top \boldsymbol{\theta}] - \nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x},y}[2\boldsymbol{\theta}^\top \mathbf{x}y] + \nabla_{\boldsymbol{\theta}}\mathbb{E}_{y}[y^2] \\ &= 2\Sigma_{\mathbf{x}}\boldsymbol{\theta} - 2\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x}}\mathbb{E}_{y|\mathbf{x}}[\boldsymbol{\theta}^\top \mathbf{x}y] \\ &= 2\Sigma_{\mathbf{x}}\boldsymbol{\theta} - 2\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x}}\mathbb{E}_{y|\mathbf{x}}[\boldsymbol{\theta}^\top \mathbf{x}\mathbf{x}^\top \boldsymbol{\theta}^*] \\ &= 2\Sigma_{\mathbf{x}}\boldsymbol{\theta} - 2\nabla_{\boldsymbol{\theta}}(\boldsymbol{\theta}^\top \Sigma_{\mathbf{x}}\boldsymbol{\theta}^*) \\ &= 2\Sigma_{\mathbf{x}}\boldsymbol{\theta} - 2\Sigma_{\mathbf{x}}\boldsymbol{\theta}^* \\ &= 2\boldsymbol{\Sigma}_{\mathbf{x}}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)\end{aligned}$$

(b) We can estimate $\mathbb{E}_{\mathbf{x},y}[\nabla_{\boldsymbol{\theta}}[(\boldsymbol{\theta}^\top \mathbf{x} - y)^2]]$ without bias via SGD, since we have access to realizations of gradients $\nabla_{\boldsymbol{\theta}}[(\boldsymbol{\theta}^\top \mathbf{x} - y)^2]$. From a), it follows that this estimate is also an unbiased estimate of the gradient of our objective function $\nabla_{\boldsymbol{\theta}}\mathbb{E}_{\mathbf{x},y}[(\boldsymbol{\theta}^\top \mathbf{x} - y)^2]$. 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
```

```r
  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)
```
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
```

```r
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)
```