3.In chemical kinetics the Michaelis-Menten model...

(a) A quick way for finding rough estimates...

Using lm function in R, we can easily get the β_0 and β_1 with least squares

```
## [1] "beta0 is 0.00510718164158581 beta1 is 0.000247220961099642"
```

so that we can get $\hat{\theta}_1 = 1/\beta_0$ and $\hat{\theta}_2 = \beta_1/\beta_0$ as follows:

```
## [1] "theta1_hat is 195.80270884775 theta2_hat is 0.0484065338672541"
```

(b)

$$
\begin{aligned}
g(\theta_1, \theta_2) &= \sum_{i=1}^{n}(y_i - \frac{\theta_1 x_i}{x_i + \theta_2})^2 \\
\frac{\partial g}{\partial \theta_1} &= 2\sum_{i=1}^{n}(y_i - \frac{\theta_1 x_i}{x_i + \theta_2})(-\frac{x_i}{x_i + \theta_2}) \\
\frac{\partial g}{\partial \theta_2} &= 2\sum_{i=1}^{n}(y_i - \frac{\theta_1 x_i}{x_i + \theta_2})(\frac{\theta_1 x_i}{(x_i + \theta_2)^2}) \\
\frac{\partial^2 g}{(\partial \theta_1)^2} &= 2\sum_{i=1}^{n}(\frac{x_i}{x_i + \theta_2})^2 \\
\frac{\partial^2 g}{\partial \theta_1 \partial \theta_2} &= 2\sum_{i=1}^{n}(\frac{y_i x_i}{(x_i + \theta_2)^2} - \frac{2\theta_1 x_i^2}{(x_i + \theta_2)^3}) \\
\frac{\partial^2 g}{(\partial \theta_2)^2} &= 2\sum_{i=1}^{n}(\frac{-2y_i\theta_1 x_i}{(x_i + \theta_2)^3} + \frac{3\theta_1^2 x_i^2}{(x_i + \theta_2)^4})
\end{aligned}
$$

and then we can get the first derivative vector and the hessian matrix and do a Newton-Raphson algorithm. The code is in the code file, here is the results.

```
##        theta1     theta2
## [1,] 212.6837 0.06412128
```

(c) Repeat (b) with the steepest descent algorithm.

change the update rule to

$$X_{t+1} = X_t - \alpha_t g'(X_t)$$

if $g(X_{t+1}) > g(X_t)$ then half α

I firstly use $\alpha = 1$, but it seems the magnitude of θ_1 and θ_2 is so different so that the algorithm will not converage to the ideal point. I try to set the $\alpha = diag(\theta_0)$ which will solve the magnitude problem, and the result is shown as below.

```
##        theta1     theta2
## [1,] 212.6504 0.06409098
```

(d) Repeat (b) with the Gauss-Newton algorithm.

Consider

$$g(\theta) = -\sum_{i=1}^{n}(y_i - f_i(\theta))^2$$

where

$$f_i(\theta) = \frac{\theta_1 x_i}{x_i + \theta_2}$$
$$f_i'(\theta) = [\frac{x_i}{x_i + \theta_2}, -\frac{\theta_1 x_i}{(x_i + \theta_2)^2}]^T$$

then we get

$$A = A(\theta) = [f_1'(\theta)^T, ..., f_n'(\theta)^T]^T$$
$$Z = Z(\theta) = [y_1 - f_1(\theta), ..., y_n - f_n(\theta)]^T$$

The updating formula is

$$\theta_{t+1} = \theta_t + (A_t^T A_t)^{-1} A_t^T Z_t$$

here is the results

```
##         theta1     theta2
## [1,] 212.6837 0.06412128
```