AMS230 – Homework #2

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April 30, 2018

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Course Name: AMS230
Assignment Name: Homework #2
Due Date: May 4, 2018
Student Discussions: I discussed the problems with the following students. All write-ups were prepared separately and independently.

- Ben Sherman

Exercise #1
Exercise 5.2 in Nocedal and Wright.

Show that if the nonzero vectors $p_0, p_1, \ldots, p_l$ satisfy Eq. (5.5) from Nocedal and Wright that

$$p_i^{\mathrm{T}} A p_j = 0, \text{ for all } i \neq j,$$

where A is symmetric and positive definite, then these vectors are linearly independent. (This result implies that A has at most n conjugate directions.)

Proof. By contradiction.

Assume vectors $\{p_0, p_1, \ldots, p_l\}$ are A-orthogonal but are not linearly independent. That means there is a set of non-zero constants $\{\alpha_0, \alpha_1, \ldots, \alpha_l\}$ such that:

$$\alpha_0 p_0 + \alpha_1 p_1 + \cdots + \alpha_l p_l = \vec{0}.$$

Multiply both sides by Ap_i where $0 \leq i \leq l$ yielding:

$$\alpha_0 p_0^{\mathrm{T}} A p_i + \alpha_1 p_1^{\mathrm{T}} A p_i + \cdots + \alpha_l p_l^{\mathrm{T}} A p_i = \vec{0}^{\mathrm{T}} A p_i.$$

Since p_i and p_j are A-orthogonal for $i \neq j$, this simplifies to:

$$\alpha_i p_i^{\mathrm{T}} A p_i = 0.$$

This is a contradiction since $\alpha_i \neq 0$ and A is symmetric, positive definite, i.e., $x^{\mathrm{T}} A x > 0$ for all non-zero x. □

Exercise #2
Exercise 5.6 in Nocedal and Wright.

Show that Eq. (5.24d)

$$\beta_{k+1} = \frac{r_{k+1}^{\mathrm{T}} r_{k+1}}{r_k^{\mathrm{T}} r_k}$$

is equivalent to Eq. (5.14d)

$$\beta_{k+1} = \frac{r_{k+1}^{\mathrm{T}} A p_k}{p_k^{\mathrm{T}} A p_k}.$$

Below is the extension of Eq. (5.24d) to Eq. (5.14d) using the equations and theorems in Nocedal and Wright.

Proof.

$$\begin{aligned}
\beta_{k+1} &= \frac{r_{k+1}^{\mathrm{T}} r_{k+1}}{r_k^{\mathrm{T}} r_k} && \text{Nocedal \& Wright (5.24d)} \\
&= \frac{r_{k+1}^{\mathrm{T}} r_{k+1}}{\alpha_k p_k^{\mathrm{T}} A p_k} && \text{By Nocedal \& Wright (5.24a)} \\
&= \frac{r_{k+1}^{\mathrm{T}} (r_k + \alpha_k p_k)}{\alpha_k p_k^{\mathrm{T}} A p_k} && \text{By Nocedal \& Wright (5.24c)} \\
&= \frac{r_{k+1}^{\mathrm{T}} \alpha_k A p_k}{\alpha_k p_k^{\mathrm{T}} A p_k} && \text{By Theorem 5.3 Eq. (5.16)} \\
&= \boxed{\frac{r_{k+1}^{\mathrm{T}} A p_k}{p_k^{\mathrm{T}} A p_k}} && \text{Cancelling } \alpha_k
\end{aligned}$$

□

Exercise #3

In this problem we will test the performance of linear conjugate gradient method for minimizing quadratic function $f(x) = \frac{1}{2}x^{\mathrm{T}}Ax - b^{\mathrm{T}}x$, where A is symmetric and positive definite.

- **Program CG Algorithm 5.2 in the textbook.**
- **Apply your program on a symmetric and positive definite matrix A of dimension $10^3 \times 10^3$ with eigenvalues uniformly distributed between 10 and 10^3. Test the convergence of the algorithm and compare your numerical findings with the theoretical result shown in formula (5.36) in the textbook.**
- **Change the distribution of eigenvalues of A so that some eigenvalues are distributed between 9 and 11, the rest of eigenvalues are distributed between 999 and 1001, i.e., two clusters around 10 and 1000 with radius 1. Test the convergence performance on such matrix. Extra points if you can explain your numerical findings using the theoretical convergence results discussed in the lecture.**

The Python implementation of the linear conjugate gradient method as detailed in Algorithm 5.2 is included at the end of this submission. The specific parameters used are enumerated in Table 1. $\mathcal{U}(a, b)$ represents a uniform random variable drawn from the range $[a, b)$. Note that for all experiments in this problem, the same random x_0 vector was used to ensure consistency of results.

Table 1: Parameters for the linear conjugate gradient experiments of problem #3

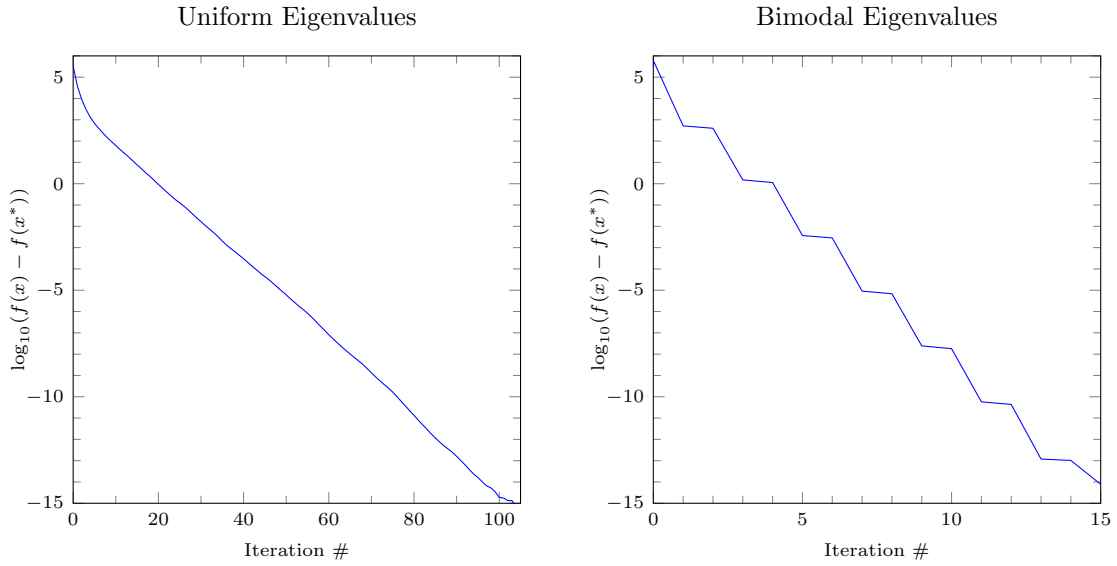
Parameter	**Value**
n	1,000
b	$\mathrm{rand}(n, 1)$
x_0	$2 \cdot \mathrm{rand}(n, 1)$
Uniform	$\mathcal{U}(10, 1000)$
Bimodal	10% from $\mathcal{U}(9, 10)$ and 90% from $\mathcal{U}(999, 1001)$

Figures 1a and 1b show the performance of the linear conjugate gradient method with n uniform and n bimodal eigenvalues respectively. For matrix A with bimodal eigenvalues, it took about 15 steps to fully converge. Similar to the results shown in Figure 5.4 of Nocedal and Wright, matrix A with uniform eigenvalues takes longer to converge.

Figures 2a and 2b show the corresponding A-weighted error versus the calculated upper bound for the uniform and bimodal eigenvalues respectively. These results use Nocedal and Wright Eq. (5.36) which states that:

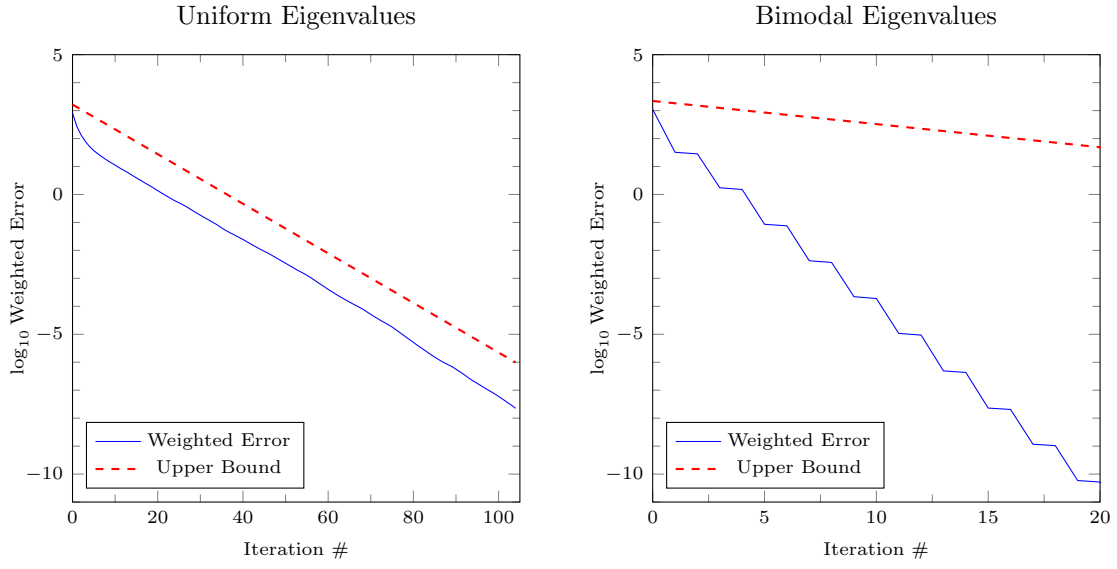
$$\|x_k - x^*\|_A \leq 2\left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}\right)^k \|x_0 - x^*\|_A$$

where $\kappa(A) = \lambda_n/\lambda_1$. For both sets of eigenvalues (i.e., uniform and bimodal), the condition number $\kappa(A) \approx \frac{1000}{10} = 100$. This means that the upper bound estimate will be approximately the same for both experiments. Observe that the upper bound tracks well for the uniform eigenvalues. In contrast, the upper bound is quite loose when the eigenvalues are clustered bimodally. This is expected given an approximately equivalent upper bound and the large difference in Figures 1a and 1b.



(a) 1,000 λ from the distribution $\mathcal{U}(10, 10^3)$ (b) 1,000 λ from distributions $\mathcal{U}(9, 11)$ and $\mathcal{U}(999, 1001)$

Figure 1: Log of cost function f error for problem #3



(a) Weighted error for 1,000 uniform eigenvalues (b) Weighted error for 1,000 bimodal eigenvalues

Figure 2: WA-weighted error results for problem #3

Exercise #4
Consider the problem of minimizing

$$f(x_1, x_2, \cdots, x_n) = \sum_{i=1}^{n-1} [100(x_i^2 - x_{i+1})^2 + (x_i - 1)^2].$$

The global minimum is at $x = [1, 1, \cdots, 1]^{\mathrm{T}}$. Numerically solve this problem using nonlinear conjugate gradient algorithms:

1. **FR (Algorithm 5.4)**
2. **FR with restart based on (5.52)**
3. **PR based on (5.44)**

and compare their performance. (In the numerical experiments you can set $n = 100$ or any number that is not too small. The initial condition can be chosen as a random vector, for example, $2\mathbf{rand}(n, 1)$.)

The gradient of f is:

$$\nabla f = \begin{cases} 400x_i(x_i^2 - x_{i+1}) + 2(x_i - 1), & i = 1 \\ 400x_i(x_i^2 - x_{i+1}) + 2(x_i - 1) - 200(x_{i-1}^2 - x_i), & 1 < i < n \\ -200(x_{i-1}^2 - x_i), & i = n \end{cases}.$$

Define $\psi_i = x_i + \alpha p_i$. Therefore, the derivative of ϕ is

$$\phi' = \sum_{i=1}^{n-1} 200(2p_i\psi_i - p_{i+1})(\psi_i^2 - \psi_{i+1}) + 2p_i(\psi_i - 1).$$

The parameters used for this experiment are specified in Table 2.

Table 2: Experiment parameters for problem #4

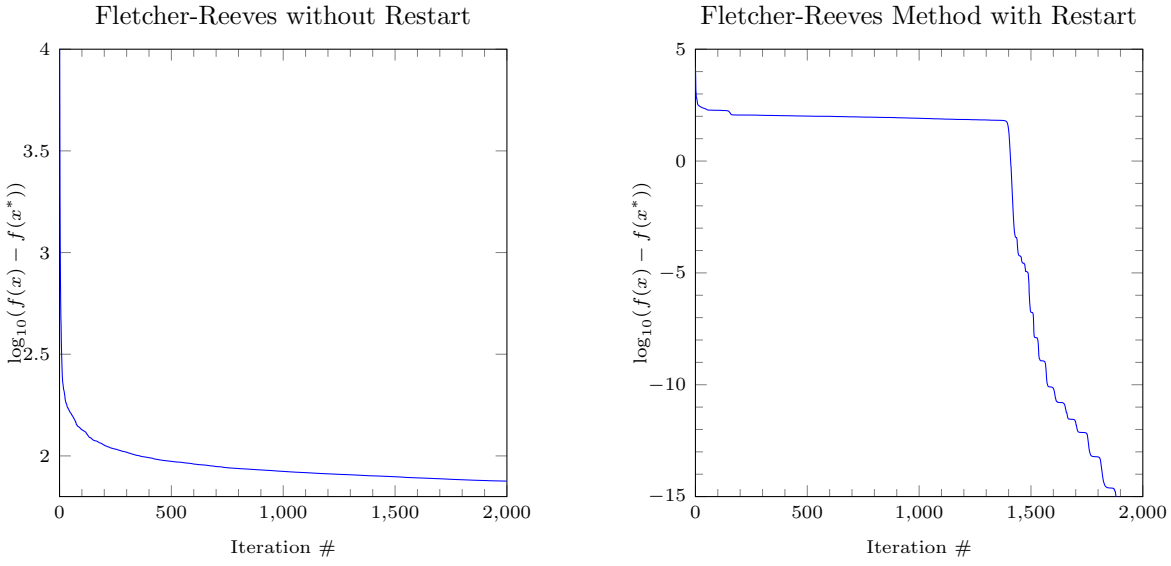
Parameter	**Value**
n	100
c_1	0.1
c_2	0.9
v	0.1
x_0	$2 \cdot \mathrm{rand}(n, 1)$

To calculate α_k, I reused most of my implementation of inexact line search from homework #1.

Figures 3a, 3b, and 4 show the performance of Fletcher-Reeves, Fletcher-Reeves with Restart, and Polak-Ribière respectively. In all experiments, the same random x_0 was used to ensure consistency. As expected, standard Fletcher-Reeves had the worst performance. Between 500 and 2,000 iterations, the algorithm made

barely any progress and never came close to converging to the optimal solution. In Fletcher-Reeves with restart, the algorithm behaves similar to Fletcher-Reeves without restart for ˜1,400 iterations. Similar to what is explained in Nocedal and Wright, the algorithm then enters a region where the error decreases rapidly. Across multiple trials with different random x_0, this avalanche point shifted anywhere within the range of 50 to over 2,000 iterations.

Generally, across different random x_0, the Polak-Ribière method converged the fastest. It was however only marginal better than Fletcher-Reeves with restart and exhibited the same avalanche behavior.



(a) (b)

Figure 3: Problem #4 performance for Fletcher-Reeves without and with restart

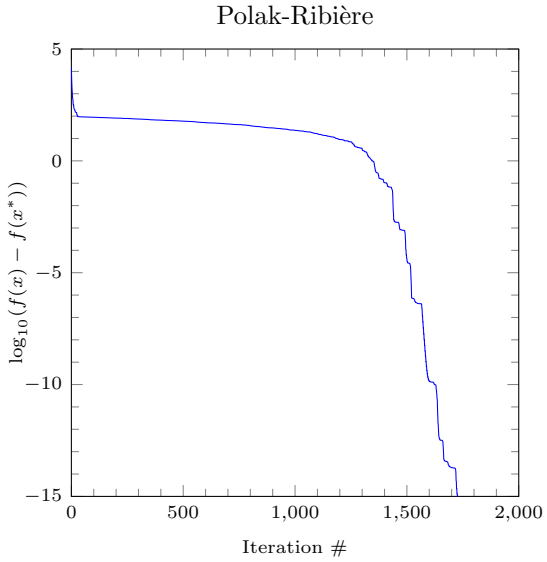


Figure 4: Problem #4 performance for the Polak-Ribière Method