CSE383C: Assignment 3

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Exercise 1. Show the modified Gram-Schmidt algorithm is equivalent to the classical algorithm.

Show

1.
$$w_m = \left[\prod_{j=1}^{i-1} (I - P_j)\right] a_j, \ P_j = q_j^* q_j, \ q_i = \frac{w_m}{\|w_m\|_2}$$

2. $w_c = a_j - \sum_{j=1}^{i-1} \lambda_j q_j, \ \lambda_j = q_j^* a_i, \ q_i = \frac{w_c}{\|w_c\|_2}$
yield equivalent $q_i \ \forall 1 \leq i \leq n$.

Proof. 1 and 2 are equivalent.

It is sufficient to show that $w_m = w_c$.

Consider w_c . (\star)

$$\begin{split} w_c &= a_j - \sum_{j=1}^{i-1} \lambda_j q_j, \ \lambda_j = q_j^* a_i \\ &= a_j - \sum_{j=1}^{i-1} (q_j^* a_i) q_j \\ &= a_j - \sum_{j=1}^{i-1} q_j (q_j^* a_i) \text{ Since } q_j^* a_i \text{ is a scalar.} \\ &= a_j - \sum_{j=1}^{i-1} (q_j q_j^*) a_i \text{ Associativity matrix vector multiplication.} \\ &= (I - \sum_{j=1}^{i-1} (q_j q_j^*)) a_i \text{ Distributivity over matrix vector.} \end{split}$$

Lemma. Show that $\prod_{j=1}^{i-1} (I - q_j q_j^*) = (I - \sum_{j=1}^{i-1} (q_j q_j^*))$. Proof by induction.

Let i = 3;

$$\prod_{j=1}^{2} (I - q_{j}q_{j}^{*}) = (I - q_{1}q_{1}^{*})(I - q_{2}q_{2}^{*})$$

$$= I^{2} - q_{2}q_{2}^{*} - q_{1}q_{1}^{*} + (q_{1}q_{1}^{*})(q_{2}q_{2}^{*})$$

$$= I - q_{2}q_{2}^{*} - q_{1}q_{1}^{*} + (q_{1}q_{1}^{*})(q_{2}q_{2}^{*})$$

$$= I - q_{2}q_{2}^{*} - q_{1}q_{1}^{*} + q_{1}(q_{1}^{*}q_{2})q_{2}^{*} \text{ Associativity of matrix vector multiplication.}$$

$$= I - q_{2}q_{2}^{*} - q_{1}q_{1}^{*} + q_{1}(0)q_{2}^{*} \text{ Inner product of orthogonal vectors is 0.}$$

$$= I - q_{2}q_{2}^{*} - q_{1}q_{1}^{*}$$

$$= I - \sum_{j=1}^{2} q_{j}q_{j}^{*}$$

Assume for some i = k, that $\prod_{j=1}^{k-1} (I - q_j q_j^*) = (I - \sum_{j=1}^{k-1} (q_j q_j^*))$.

Let i = k + 1.

$$\begin{split} \prod_{j=1}^k (I-q_jq_j^*) &= \Big(\prod_{j=1}^{k-1} (I-q_jq_j^*)\Big)(I-q_kq_k^*) \\ &= \Big(I-\sum_{j=1}^{k-1} (q_jq_j^*)\Big)(I-q_kq_k^*) \text{ By induction hypothesis.} \\ &= I^2-q_kq_k^*-\sum_{j=1}^{k-1} (q_jq_j^*)+\sum_{j=1}^{k-1} (q_jq_j^*)(q_kq_k^*) \\ &= I-q_kq_k^*-\sum_{j=1}^{k-1} (q_jq_j^*)+\sum_{j=1}^{k-1} (q_jq_j^*)(q_kq_k^*) \\ &= I-q_kq_k^*-\sum_{j=1}^{k-1} (q_jq_j^*)+\sum_{j=1}^{k-1} q_j(q_j^*q_k)q_k^* \text{ Associativity of matrix vector multiplication.} \\ &= I-q_kq_k^*-\sum_{j=1}^{k-1} (q_jq_j^*)+\sum_{j=1}^{k-1} q_j(0)q_k^* \text{ Inner product of orthogonal vectors is 0.} \\ &= I-q_kq_k^*-\sum_{j=1}^{k-1} (q_jq_j^*) \text{ Inner product of orthogonal vectors is 0.} \\ &= I-\sum_{j=1}^{k-1} (q_jq_j^*)-q_kq_k^* \text{ Commutatitivity of matrix vector addition.} \\ &= I-\sum_{j=1}^{k} (q_jq_j^*) \end{split}$$

We see that $\prod_{j=1}^{i-1} (I - q_j q_j^*) = (I - \sum_{j=1}^{i-1} (q_j q_j^*)) \ \forall 1 \le i \le n.$

Consider w_m . $(\star\star)$

$$w_m = \left[\prod_{j=1}^{i-1} (I - q_j^* q_j)\right] a_j$$
$$= \left(I - \sum_{j=1}^{i-1} (q_j q_j^*)\right) a_j \text{ By Lemma.}$$

By (\star) and $(\star\star)$, we have shown equality and can see the two algorithms yield the same Q.

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Exercise 2. Implement the classical and modified Gram-Schmidt Orthogonalization.

```
function [Q, R] = gramschmidt(A, flag)
% Decomposes a matrix A into Q, orthogonal and R, upper triangular.
%
% Params:
    A: m x n matrix, full rank.
%
    flag: [0, 1], 0 for classical, 1 for modified.
%
% Returns:
   Q: m x n matrix, orthogonal, spans A.
   r: n x n matrix, upper triangular.
[m, n] = size(A);
Q = zeros(m, n);
R = zeros(n, n);
for j = 1:n
    V(:, j) = A(:, j);
    for i = 1:j-1
        if flag == 1
            R(i, j) = Q(:, i)' * A(:, j);
        else
            R(i, j) = Q(:, i)' * V(:, j);
        V(:, j) = V(:, j) - R(i, j) * Q(:, i);
    end
    R(j, j) = norm(V(:, j));
    Q(:, j) = V(:, j) / R(j, j);
end
```

Exercise 3. Suggest tests to judge the numerical accuracy of the algorithms.

The main problem that can arise from this algorithm is rounding errors from the normalization step. To test the accuracy of this algorithm, I checked the 'orthogonality' of the column vectors of Q. I found the maximum inner product value for every pair of column vectors and that was the score. The 'better' the orthogonality, the lower the value.

```
function epsilon = gramschmidt_verification(Q)
% Finds the greatest inner product between the column vectors.
%
% Params:
% Q: m x n matrix, the Q from a QR decomposition.
%
% Returns:
% epsilon: a scalar.

[m, n] = size(Q);
epsilon = 0;

for i = 1:n
    for j = i+1: n
        epsilon = max(epsilon, Q(:, i)' * Q(:, j));
    end
end
```

The results from the tests are as follows.

Kappa: 1

Classical: 1.110223e-16 Modified: 1.110223e-16 Matlab: 4.718448e-16

Kappa: 1000

Classical: 1.789457e-12 Modified: 2.171874e-14 Matlab: 4.302114e-16

Kappa: 1000000

Classical: 4.655908e-06 Modified: 9.193776e-12 Matlab: 4.857226e-16

Kappa: 1000000000

Classical: 9.381781e-01

Modified: 7.949187e-09 Matlab: 4.996004e-16

We can see as the condition number increases, the numerical error of the classical algorithm increases. This makes sense, since the condition number tells the limit of error given a small perturbation of the function. The classical algorithm error then compounds on itself, and the higher the condition number the more noticable the numerical accuracy.