Numerical Mathematics:
Homework 4

Problem 1

Consider a continuous function $f(x)$ on $[0,1]$ and $P_n(x)$ of degree at most n:

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

Derive the normal equations:

$$Sa = d$$

which the coefficients $a = (a_0, a_1, \ldots, a_n)$ must satisy in order to minimize the quadratic cost:

$$E = \int_0^1 \left[f(x) - (a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n) \right] dx$$

Assuming that $f(x) = x^3$, write a matlab function called:

`[ a ] = leastsquares_monomial(n)`

which solves normal equations and obtains a. You may use the backslash operator here. What is the exact solution to this problem? What do you notice?

Solution. Shown below is the code.

```
function [ x ] = leastsquares_monomial(n)
%LEASTSQUARES_MONOMIAL Summary of this function goes here
%   Detailed explanation goes here


A = zeros(n,n);
for i = 1:n
   for j=1:n
       A(i,j)= 1 / (i+j-1);
   end
end

b = zeros(n,1);
for j=1:n
       b(j)= 1 / (3+j-1);
end

x = A \ b;

end
```

$\square$

Problem 2

Continuing from what we have discovered in problem 1, consider again the monomial basis $\phi_k(x) = x^k$ for $k = 0, 1, 2, 3, \ldots$ on $[-1, 1]$. The Gram-Schmidt process can be generalized to functions. The inner product and norms are replaced by:

$$\langle f(x), g(x) \rangle := \int_{-1}^1 f(x) g(x) dx, \qquad \|f(x)\|^2 := \langle f(x), f(x) \rangle$$

Let $l_k(x)$ for $k = 0, 1, 2, 3, \ldots$ denote the outputs (which are again polynomials) of this Gram-Schmidt process.

(a) Compute the first four $l_k(x)$ by applying the Gram-schmidt algorithm manually.

A general expression for the $l_k(x)$ is given by:

$$l_k(x) = \sqrt{\frac{2k+1}{2}}\frac{1}{2^k k!}\frac{d^k}{dx^k}\left[\left(x^2-1\right)^k\right] \tag{1}$$

(b) For the first four $l_k(x)$, verify that (1) coincides with what was previously established in question a.

We know that $l_k(x)$, by construction, must form an orthonormal sequence. This is of course not obvious from (1). To prove this, consider the following differential equation:

$$-\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_k(x)\right] = k(k+1)l_k(x)$$

(c) Verify that (1) satisfies the above differential equation. What interpretation can you give to $l_k(x)$? Think in terms of $Ax = \lambda x$. *Some guidelines and hints to help you:* Convince yourself that all that needs to be shown is:

$$\left[(x^2-1)\frac{d^{k+1}}{dx^{k+1}}\left[\left(x^2-1\right)^k\right]\right] = k(k+1)\frac{d^{k-1}}{dx^{k-1}}\left[\left(x^2-1\right)^k\right]$$

Then observe that:

$$\frac{d^{k+1}}{dx^{k+1}}\left[(x^2-1)^{k+1}\right] = \frac{d^{k+1}}{dx^{k+1}}\left[(x^2-1)^k(x^2-1)\right] = \frac{d^k}{dx^k}\left[(x^2-1)^k(2x)(k+1)\right]$$

Apply finally Leibnitz's product rule (for higher order derivatives) to the second and third expression above, i.e.

$$\frac{d^k}{dx^k}\left[u(x)v(x)\right] = \sum_{l=0}^{k}\binom{k}{l}\frac{d^{k-l}}{dx^{k-l}}\left[u(x)\right]\frac{d^l}{dx^l}\left[v(x)\right]$$

(d) Use the differenial equation as a means to show that $\langle l_m(x), l_n(x)\rangle = 0$ if $m \neq n$. *Hint:* start with:

$$\langle m(m+1)l_m(x), n(n+1)l_n(x)\rangle$$

and use integration by parts.

(e) It can be shown that $\langle l_n(x), l_n(x)\rangle = 1$. There is no need to prove this, but can you explain what the normal equations are now for the least squares problem? Specifally, what type of matrix is S now and what have we gained from this?

Solution. (a) Straightforward verification.

(b) Straightforward verification.

(c) From:

$$\begin{aligned}
-\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_k(x)\right] &= k(k+1)l_k(x) \\
\frac{d}{dx}\left[(x^2-1)\frac{d}{dx}l_k(x)\right] &= k(k+1)l_k(x)
\end{aligned}$$

Observe that the coefficient $\sqrt{\frac{2k+1}{2}}\frac{1}{2^k k!}$ appears on both the left and right side, and therefore cancels and does not play a role. All we need to verify now is:

$$\begin{aligned}
\frac{d}{dx}\left[(x^2-1)\frac{d^{k+1}}{dx^{k+1}}\left[\left(x^2-1\right)^k\right]\right] &= k(k+1)\frac{d^k}{dx^k}\left[\left(x^2-1\right)^k\right] \\
\left[(x^2-1)\frac{d^{k+1}}{dx^{k+1}}\left[\left(x^2-1\right)^k\right]\right] &= k(k+1)\frac{d^{k-1}}{dx^{k-1}}\left[\left(x^2-1\right)^k\right]
\end{aligned}$$

Let us proceed and do this. Consider:

$$\frac{d^{k+1}}{dx^{k+1}}\left[(x^2-1)^{k+1}\right] = \frac{d^{k+1}}{dx^{k+1}}\left[(x^2-1)^k(x^2-1)\right] = \frac{d^k}{dx^k}\left[(x^2-1)^k(2x)(k+1)\right]$$

Apply Leibnitz rule on the second and third expression above:

$$\begin{aligned}
\frac{d^{k+1}}{dx^{k+1}}\left[(x^2-1)^k(x^2-1)\right] &= \frac{d^{k+1}}{dx^{k+1}}\left[(x^2-1)^k\right](x^2-1) + \frac{d^k}{dx^k}\left[(x^2-1)^k\right](2x)(k+1) + \frac{d^{k-1}}{dx^{k-1}}\left[(x^2-1)^k\right](k+1)k \\
\frac{d^k}{dx^k}\left[(x^2-1)^k(2x)(k+1)\right] &= \frac{d^k}{dx^k}\left[(x^2-1)^k\right](2x)(k+1) + \frac{d^{k-1}}{dx^{k-1}}\left[(x^2-1)^k\right]2(k+1)k
\end{aligned}$$

Equating the above two expression should yield the desired result.

(d)

First of all:

$$\begin{aligned}
\langle m(m+1)l_m(x), n(n+1)l_n(x)\rangle &= -\left\langle \frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_m(x)\right], n(n+1)l_n(x)\right\rangle \\
\langle m(m+1)l_m(x), n(n+1)l_n(x)\rangle &= -\left\langle m(m+1)l_m(x), \frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_n(x)\right]\right\rangle
\end{aligned}$$

Subtract the two:

$$\begin{aligned}
\left\langle \frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_m(x)\right], n(n+1)l_n(x)\right\rangle - \left\langle m(m+1)l_m(x), \frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_n(x)\right]\right\rangle &= 0 \\
\int_{-1}^{1}\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_m(x)\right]n(n+1)l_n(x)dx - \int_{-1}^{1}m(m+1)l_m(x)\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}l_n(x)\right]dx &= 0
\end{aligned}$$

Now apply integration by parts to obtain:

$$(n(n+1)-m(m+1))\langle l_n(x), l_m(x)\rangle = 0 \tag{2}$$

Since $n(n+1)-m(m+1)\neq 0$, it must be that $\langle l_n(x), l_m(x)\rangle = 0$.

(e) The matrix S is the identity matrix, we no longer need to do an inversion!

□

Problem 3

Consider the simple problem of multiplying a vector $x\in\mathbb{R}^n$ with a Householder transform:

$$Q(v) = I - 2vv^T, \quad \|v\| = 1$$

Discuss the complexity (i.e. using big-O notation) doing it the right way and wrong way. There is no need to code things up, becuase you will be doing it anyway implicitly in the next problem!

Solution. When you compute the matrix vector product, notice that:

$$Q(v)x = (I-2vv^T)x = x - 2(v^Tx)v$$

We only need to evaluate one inner product v^Tx and then subtract two vectors. This is an $\mathcal{O}(n)$ operation. □

Problem 4

In this problem you are going to write your own general purpose regression (or data fitting) code based on what you have learned in class. Consider the discrete least-squares problem:

$$E = \sum_{k=1}^{m} \left(f(x_k) - \sum_{l=0}^{d} c_l T_l(x_k) \right)^2$$

where $x_k \in [-1, 1]$ and $f(x_k)$ are samples of some unknown function. The terms $T_l(x)$ refer to the Chebyshev polynomials.

Write a function called:

`[ c ] = chebfit( x, y, d )`

that returns the coefficients c_l in a column vector denoted by `c`. The arguments `x` and `y` are column vectors whose entries contain the data points x_1, x_2,...x_m and $f(x_1)$, $f(x_2)$,...$f(x_m)$. In addition to returning estimates, you are expected display a plot showing the data points and the least-squares fit.

You are not allowed use the backslash operator to solve the least squares problem. Instead, you have to write your own Householder algorithm. As discussed in class, please consider a careful implementation of the householder reflections to keep the algorithm numerically stable. I advise you to use sub functions to keep your code clean and organized. Getting practice with this will be helpful for later in the course.

Tip: Matlab has a built in function called `chebyshevT`, which may be useful to you.

Solution. Shown below is the code.

```
function [ c ] = chebfit( x, y, d )

% construct chebyshev matrix
A = zeros(length(x),d+1);
for k = 0:d
A(:,k+1) = chebyshevT(k,x);
end

% compute R and modified b
[ R, bhat ] = QRhouseholder( A, y );

% Back substition (it is okay to use backlash here...)
c = R \ bhat;


% plotting
xplot = (-1:0.01:1)';
A = zeros(length(xplot),d+1);
for k = 0:d
A(:,k+1) = chebyshevT(k,xplot);
end
yplot = A*c;


%plot figure
plot(x,y,'x')
hold on
plot(xplot,yplot)
```

```
xlabel('x')
ylabel('y')


end



function [ R, bhat ] = QRhouseholder( A, b )
%UNTITLED Summary of this function goes here
%   Detailed explanation goes here

for k=1:size(A,2)

    %construct v
    x = A(k:end , k);
    v = [sign(x(1))*norm(x);  zeros(size(A,1)-k,1)]-x;
    v = v/norm(v);

    % Update A
    A(k:end,k) = [sign(x(1))*norm(x);  zeros(size(A,1)-k,1)];
    A((k):end,(k+1):end) = A((k):end,(k+1):end) - 2*v * v'*A((k):end,(k+1):end);

    %update b
    b(k:end) = b(k:end)  - 2*v * v'* b(k:end);
end

R = A(1:size(A,2),1:size(A,2));
bhat = b(1:size(A,2));

end
```

□

(extra) Problem 5

Show that the Chebyshev polynomials $T_n(x) = \cos(n \arccos(x))$ are orthogonal with respect to the inner product:

$$\langle T_l(x), T_m(x) \rangle := \int_{-1}^{1} \frac{T_l(x) T_m(x)}{\sqrt{1-x^2}} dx = 0$$

whenever $m \neq 0$ Hint!: Use change of variables!

Solution.

$$\begin{aligned} \int_{-1}^{1} \frac{\cos(n \arccos(x)) \cos(m \arccos(x))}{\sqrt{1-x^2}} dx &= -\int_{-\pi}^{0} \cos(nu)\cos(mu) du \\ &= -\int_{-\pi}^{0} \cos(nu)\cos(mu) du \\ &= \int_{0}^{\pi} \cos(nu)\cos(mu) du \\ &= 0 \end{aligned}$$

□