23MAT204 – Mathematics for Intelligent Systems - 3

Practise Sheet-5

(Conjugate Gradient Method)

Conjugate Directions:

$Let\ A$ be a real symmetric $n \times n$ matrix with rank n.

The directions $d_0, d_1, \ldots, d_{n-1}$ are A−Conjugate if,
for all $i \neq j$, we have $d_i^T A d_j = 0$

$$d_i^T A d_j = d_j^T A d_i = 0, \forall i \neq j$$

A new type of orthogonality.
It is defined w.r.t. a symmetric matrix A

Creation of A-conjugate Directions

Example w.r.t a 3 by 3 matrix A:

Generating Conjugate directions for 3x3 symmetric matrix.
We can find 3 independent conjugate directions.
We will use this as paths along which we descend to minima point
(These directions are not unique)

$Let\ A = \begin{pmatrix} x & y & z \\ y & p & r \\ z & r & q \end{pmatrix}$

$Let\ \ d_1^T = [1\ 0\ 0]$.

$d_1^T A = [x, y, z]$, or $\mathrm{Ad}_1 = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

d_2 such that $d_1^T A d_2 = 0 \Rightarrow d_2 \perp Ad_1 \Rightarrow d_2 \perp \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow$ one $d_2 = \begin{pmatrix} yz \\ -2xz \\ xy \end{pmatrix}$

$d_2^T = [yz\ \ -2xz\ xy]$

Find d_3 such that
$\mathrm{d}_1^T \mathrm{Ad}_3 = 0 \in \mathrm{R}$
$\mathrm{d}_2^T \mathrm{Ad}_3 = 0 \in \mathrm{R}$
or
$\mathrm{d}_3^T \mathrm{Ad}_1 = 0 \in \mathrm{R}$
$\mathrm{d}_3^T \mathrm{Ad}_2 = 0 \in \mathrm{R}$

$$\left.\begin{matrix} \mathrm{d}_1^T \mathrm{Ad}_3 = 0 \in \mathrm{R} \\ \mathrm{d}_2^T \mathrm{Ad}_3 = 0 \in \mathrm{R} \end{matrix}\right\} \Rightarrow d_3 \text{ is orthogonal to vectors } \mathrm{Ad}_1 \text{ and } \mathrm{Ad}_2$$

So, d_3 can be easily obtained by cross producting Ad_1 and Ad_2

Conjugate Gradient Method is used to solve –

(i) Linear System Ax=b, where A is symmetric positive definite
or the equivalent optimization problem

(ii) Minimize f(x), where f(x) is a quadratic optimization problem:

Algorithm for Conjugate Gradient Method:

Algorithm:- Step 1:- Input → A, b, $x^{(0)}$

Step 2:- Compute $\bar{r}_0 = b - Ax^{(0)}$ $\left(\bar{r}_0 = -g(x^{(0)})\right)$

Set $\bar{d}_0 = \bar{r}_0$

Step 3:- For $k = 0, 1, 2, ----$ until convergence

Calculate $\alpha_k = \dfrac{\langle r_k, r_k \rangle}{\langle d_k, Ad_k \rangle}$ $\left(\alpha_k = \dfrac{r_k^T r_k}{d_k^T A d_k}\right)$

Step 4:- $x^{(k+1)} = x^{(k)} + \alpha_k d_k$

Step 5:- $r_{k+1} = r_k - \alpha_k A d_k$ ⟶ $\left(\begin{aligned} r_{k+1} &= b - Ax^{(k+1)} \\ &= b - A\left(x^{(k)} + \alpha_k d_k\right) \\ &= \underbrace{b - Ax^{(k)}} - \alpha_k A d_k \\ &= r_k - \alpha_k A d_k \end{aligned}\right)$

Step 6:- If $r_{k+1} = 0$, then stop

Else, calculate $\beta_k = \dfrac{\langle r_{k+1}, r_{k+1} \rangle}{\langle r_k, r_k \rangle}$

Step 7:- Find $d_{k+1} = r_{k+1} + \beta_k d_k$ (d_{k+1} which will be A conjugate with $d_1, d_2, \dots d_k$)

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In Conjugate gradient method to solve a system AX=B with n unknowns, we get the solution in exactly n iterations.

Example 1:

Solve Ax=b using conjugate gradient method with initial point as $\overset{x^{(0)}}{(0,0,0)^T}$ if $A = \begin{pmatrix} 3 & 0 & 1 \\ 0 & 4 & 2 \\ 1 & 2 & 3 \end{pmatrix}$, $b = \begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix}$

$r_0 = b - Ax^{(0)} = \begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix}$; $d_0 = r_0 = \begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix}$

$\alpha_0 = \dfrac{r_0' r_0}{d_0' A d_0} = \dfrac{5}{18} = 0.2778$;

$x^{(1)} = x^{(0)} + \alpha_0 d_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} + \dfrac{5}{18}\begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 5/6 \\ 0 \\ 5/18 \end{pmatrix} = \begin{pmatrix} 0.8333 \\ 0 \\ 0.2778 \end{pmatrix}$

$r_1 = r_0 - \alpha_0 A d_0 = \begin{pmatrix} 2/9 \\ -5/9 \\ -2/3 \end{pmatrix} = \begin{pmatrix} 0.2222 \\ -0.5556 \\ -0.6667 \end{pmatrix} \rightarrow \|r_1\| \neq 0$

$\beta_0 = \dfrac{\langle r_1, r_1 \rangle}{\langle r_0, r_0 \rangle} = 0.0802$

$d_1 = r_1 + \beta_0 d_0 = \begin{pmatrix} 0.4630 \\ -0.5556 \\ -0.5864 \end{pmatrix}$

$\alpha_1 = \dfrac{r_1' r_1}{d_1' A d_1} = 0.2187$

$x^{(2)} = x^{(1)} + \alpha_1 d_1 = \begin{pmatrix} 0.9346 \\ -0.1215 \\ 0.1495 \end{pmatrix}$

$r_2 = r_1 - \alpha_1 A d_1 = \begin{pmatrix} 0.0467 \\ 0.1869 \\ -0.1402 \end{pmatrix} \rightarrow \|r_2\| \neq 0$

$\beta_1 = \dfrac{\langle r_2, r_2 \rangle}{\langle r_1, r_1 \rangle} = 0.0707$

$d_2 = r_2 + \beta_1 d_1 = \begin{pmatrix} 0.0795 \\ 0.1476 \\ -0.1817 \end{pmatrix}$

$\alpha_2 = \dfrac{\langle r_2, r_2 \rangle}{d_2' A d_2} = 0.8231$

$x^{(3)} = x^{(2)} + \alpha_2 d_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

$r_3 = r_2 - \alpha_2 A d_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$

```
A=[3,0,1;0,4,2;1,2,3];
b=[3;0;1];
x0=[0;0;0];
r0=b-A*x0;
d0=r0;
alpha0=(r0'*r0)/((A*d0)'*d0);
x1=x0+alpha0*d0;
r1=r0-alpha0*A*d0;
beta0=(r1'*r1)/(r0'*r0);
d1=r1+beta0*d0;
alpha1=(r1'*r1)/((A*d1)'*d1);
x2=x1+alpha1*d1;
r2=r1-alpha1*A*d1;
beta1=(r2'*r2)/(r1'*r1);
d2=r2+beta1*d1;
alpha2=(r2'*r2)/((A*d2)'*d2)
x3=x2+alpha2*d2
r3=r2-alpha2*A*d2
```

OR

```
A=[3,0,1;0,4,2;1,2,3];
b=[3;0;1];
x=randi([-9, 9],length(b),1);
r = b - A * x;
d = r;
rsold = r' * r;
for i = 1:length(b)
Ad = A * d;
alpha = rsold / (d' * Ad);
x = x + alpha * d;
r = r - alpha * Ad;
rsnew = r' * r;
if sqrt(rsnew) < 1e-10
break;
end
d = r + (rsnew / rsold) * d;
rsold = rsnew;
end
x
residue=b-A*x
```

```
x = 3×1
     1.0000
    -0.0000
     0.0000

residue = 3×1
10^-15 ×
     0.4441
     0.5017
     0.1110
```

Example 2:

Solve the system AX=B, where $A = \begin{bmatrix} 5 & 1 & 2 & -1 \\ 1 & 9 & 1 & 3 \\ 2 & 1 & 4 & 0 \\ -1 & 3 & 0 & 6 \end{bmatrix}$ and $b = \begin{bmatrix} 7 \\ 14 \\ 7 \\ 8 \end{bmatrix}$ using conjugate gradient method with any initial vector

```
A=[5,1,2,-1;1,9,1,3;2,1,4,0;-1,3,0,6];
b=[7;14;7;8];
x=randi([-9, 9],length(b),1)
r = b - A * x;
d = r;
rsold = r' * r;
for i = 1:length(b)
Ad = A * d;
alpha = rsold / (d' * Ad);
x = x + alpha * d;
r = r - alpha * Ad;
rsnew = r' * r;
if sqrt(rsnew) < 1e-10
break;
end
d = r + (rsnew / rsold) * d;
rsold = rsnew;
end
x
residue=b-A*x
```

Solution of this is $(1,1,1,1)^T$

Example 3:

Solve the optimization problem:

$$f(x_1,x_2)=2x_1^2+1x_2^2+2x_1x_2+x_1-x_2$$
$$=\frac{1}{2}\begin{pmatrix}x_1 & x_2\end{pmatrix}\begin{pmatrix}4 & 2\\ 2 & 2\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}-\begin{pmatrix}-1 & 1\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}$$
$$=\frac{1}{2}x^TAx-b^Tx$$

```
A=[4,2;2,2];
b=[-1;1];
x=randi([-9, 9],length(b),1)
r = b - A * x;
d = r;
rsold = r' * r;
for i = 1:length(b)
Ad = A * d;
alpha = rsold / (d' * Ad);
x = x + alpha * d;
r = r - alpha * Ad;
rsnew = r' * r;
if sqrt(rsnew) < 1e-10
break;
end
d = r + (rsnew / rsold) * d;
rsold = rsnew;
end
x
residue=b-A*x
```

```
x = 2×1
   -1.0000
    1.5000

residue = 2×1
10^-14 ×
   -0.3553
    0.0888
```

Practice questions:

1. Find a set of A conjugate directions for the matrix: $A=\begin{bmatrix}9 & 2\\ 2 & 9\end{bmatrix}$.
2. Find a set of A conjugate directions for the matrix: $A=\begin{bmatrix}8 & 2 & 1\\ 2 & 7 & 2\\ 1 & 2 & 5\end{bmatrix}$.
3. Solve the given linear systems using conjugate gradient method by taking different starting points.
   (a) 2x+y-z=1, x+2y-z = 2, -x-y+4z=9
   (b) Ax=b, where $A=\begin{bmatrix}11 & 2 & 1\\ 2 & 4 & -1\\ 1 & -1 & 6\end{bmatrix}$ and $b=\begin{bmatrix}12\\ 1\\ 7\end{bmatrix}$
   (c) Ax=b, where $A=\begin{pmatrix}3 & 0 & 1\\ 0 & 4 & 2\\ 1 & 2 & 3\end{pmatrix}$, $b=\begin{pmatrix}3\\ 0\\ 1\end{pmatrix}$
4. Consider the optimization problem:
   Minimize $f(x,y)=4x^2+3y^2-16x-36y+25$
   (a) Solve the problem analytically and obtain the solution.
   (b) Starting from (0,0), perform conjugate gradient method and obtain the solution. Also plot the path taken to reach the final solution.

(c) Starting from (50,0), perform conjugate gradient method and obtain the solution. Also plot the path taken to reach the final solution.

(d) Starting from (0,-25), perform conjugate gradient method and obtain the solution. Also plot the path taken to reach the final solution.

(e) Starting from (-21,35), perform conjugate gradient method and obtain the solution. Also plot the path taken to reach the final solution.

5. Solve the given quadratic optimization problems using conjugate gradient method by taking different starting points.
   (a) Minimize $f(x, y, z) = 6x^2 + 8y^2 + z^2 + 2xz + 4yz - 3x - 3z$
   (b) Minimize $f(x, y, z) = 9x^2 + 5y^2 + 3z^2 - 36x + 30y - 8z$

6. Solve the system AX=B, where $A = \begin{bmatrix} 9 & 1 & 1 & 0 & 0 \\ 1 & 5 & 0 & 0 & 2 \\ 1 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 4 & 2 \\ 0 & 2 & 0 & 2 & 6 \end{bmatrix}$ and $B = \begin{bmatrix} 11 \\ 8 \\ 4 \\ 6 \\ 10 \end{bmatrix}$ using conjugate gradient method with initial vector as x=[a,b,c,b,a]T, where: a is the last two digits of your registration number, b is your date of birth, c is your month of birth.

7. Generate a random integer symmetric matrix A of order 9. Obtain a vector b, such that Ax=b, with $x=[1,2,3,4,5,6,7,8,9]^T$. Now, Solve the system AX=b using conjugate gradient method and verify the solution is $X=[1,2,3,4,5,6,7,8,9]^T$. In how many iterations you could get the solution?