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THE CONJUGATE GRADIENT METHOD FOR ITERATIVE SOLUTION OF LINEAR EQUATIONS

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Abstract.

1. The method

Solve Equations of form $b = Ax$ where A is positive definite. If A is invertible but not positive definite we apply the method to $A^\top Ax = A^\top b$.

Consider first

$$F(x) = \frac{1}{2}x^\top Ax$$

The method has the following form

$$x(t+1) = x(t) + \gamma(t)s(t)$$

$\gamma(t)$ are scalar step size parameter and $s(t)$ are search directions for $t = 0, 1, \dots$. Note that the gradient of F is given as

$$\nabla F(x) \mid_{x=x(t)} \equiv g(t) = Ax(t)$$

It would be informative to contrast conjugate gradients to a gradient descent algorithm. A gradient descent algorithm would look like

$$\begin{aligned} x(t+1) &= x(t) - \nu(t)g(t) \\ &= x(t) - \nu(t)Ax(t) = (I - \nu(t)A)x(t) \end{aligned}$$

In the conjugate gradient method, the search directions are chosen to be mutually conjugate meaning that

$$s(t)^\top As(r) = 0 \qquad \text{when} \;\; r \neq t$$

Once $s(t)$ is chosen, $\gamma(t)$ has a closed form solution.

In the sequel, we will show how to select $s(t)$ and $\gamma(t)$, but first provide an outline of the algorithm

1.1. Illustration of the algorithm.

At the first step, we select the search direction as the negative gradient

$$s(0) = -g(0)$$

The search direction will be found

$$\gamma(0) = \frac{s(0)^\top g(0)}{s(0)^\top As(0)} = -\frac{g(0)^\top g(0)}{g(0)^\top Ag(0)}$$

and let

$$x(1) = x(0) + \frac{s(0)^\top g(0)}{s(0)^\top As(0)}s(0)$$

At this stage, we can calculate the new gradient as

$$g(1) = Ax(1)$$

To execute the next step, we need to select $s(1)$ as a conjugate direction

$$s(0)^\top As(1) = 0$$

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We would select the gradient $s(1) = -g(1)$, but this choice won't be necessarily a conjugate direction. A reasonable choice is choosing the new direction $s(1)$ such that we can represent the gradient as

$$-g(1) = s(1) - c_0(1)s(0)$$

where $c_0(1)$ denotes a scalar coefficient for the first search direction in computation of the gradient $g(1)$ at time 1.

This leads to

$$\begin{aligned} s(0)^\top As(1) &= -s(0)^\top Ag(1) + c_0(1)s(0)^\top As(0) = 0 \\ c_0(1) &= \frac{s(0)^\top Ag(1)}{s(0)^\top As(0)} \end{aligned}$$

$$s(1) = -g(1) + c_0(1)s(0)$$

$$\begin{aligned} x(2) &= x(1) + \gamma(1)s(1) \\ g(2) &= Ax(2) \\ g(2) &= Ax(1) + \gamma(1)As(1) = g(1) + \gamma(1)As(1) \end{aligned}$$

Similarly we want now

$$-g(2) = s(2) - c_1(2)s(1) - c_0(2)s(0)$$

where $c_1(2)$ and $c_0(2)$ denote scalar coefficients for the search direction $s(2)$ in computation of the gradient $g(2)$ at time 2

This leads to two equations

$$\begin{aligned} s(2) &= -g(2) + c_1(2)s(1) + c_0(2)s(0) \\ s(0)^\top As(2) &= -s(0)^\top Ag(2) + c_1(2)s(0)^\top As(1) + c_0(2)s(0)^\top As(0) \\ s(1)^\top As(2) &= -s(1)^\top Ag(2) + c_1(2)s(1)^\top As(1) + c_0(2)s(1)^\top As(0) \end{aligned}$$

By conjugacy of $s(0), s(1)$ and $s(2)$ we have

$$\begin{aligned} 0 &= -s(0)^\top Ag(2) + c_0(2)s(0)^\top As(0) \\ 0 &= -s(1)^\top Ag(2) + c_1(2)s(1)^\top As(1) \end{aligned}$$

$$\begin{aligned} c_0(2) &= \frac{s(0)^\top Ag(2)}{s(0)^\top As(0)} = \frac{s(0)^\top Ag(2)}{s(0)^\top As(0)} \\ c_1(2) &= \frac{s(1)^\top Ag(2)}{s(1)^\top As(1)} \end{aligned}$$

In the general case, we will need to find scalar coefficients $c_i(t)$ for the i'th search direction in computation of the gradient $g(t)$ at time t $i = 0 \dots t-1$. In general we will have

$$\begin{aligned} -g(t) &= s(t) - c_{t-1}(t)s(t-1) - c_{t-2}(t)s(t-2) - \cdots - c_0(t)s(0) \\ &= s(t) - \sum_{i=0}^{t-1} c_i(t)s(i) \end{aligned}$$

In other words, we require that the gradient lives in the subspace spanned by $S_t = \{s(0), \dots, s(t)\}$, a set of mutually conjugate vectors where $s(i)^\top As(t) =$ for $i \neq t$ We will later show that most $c_i(t)$ are in fact 0.

1.2. Finding the line search minimizer $\gamma(t)$. For given $x(t)$, $s(t)$ and A, we define $\gamma(t)$ as the line search minimizer

$$\gamma(t) = \operatorname*{argmin}_{\gamma} F(x(t) + \gamma s(t))$$

This problem has the following solution

$$\begin{aligned} U(\gamma) &= F(x(t) + \gamma s(t)) \\ &= \frac{1}{2}(x(t) + \gamma s(t))^\top A(x(t) + \gamma s(t)) \\ &= \frac{1}{2}(x(t)^\top + \gamma s(t)^\top)(Ax(t) + \gamma As(t)) \\ &= \frac{1}{2}x(t)^\top Ax(t) + \gamma s(t)^\top Ax(t) + \gamma^2 \frac{1}{2}s(t)^\top As(t) \end{aligned}$$

$$\frac{dU}{d\gamma} = s(t)^\top Ax(t) + \gamma s(t)^\top As(t) = 0$$

$$\begin{aligned} \gamma(t) &= -s(t)^\top Ax(t)/s(t)^\top As(t) \\ &= -s(t)^\top g(t)/s(t)^\top As(t) \end{aligned}$$

1.3. Selection of the conjugate directions $s(t)$. The search directions have the following form

$$s(t) = -g(t) + \sum_{i=0}^{t-1} c_i(t)s(i)$$

In a sense, we use the current gradient and a linear combination of past search directions. Before we derive how the coefficients $c_i(t)$ are found, we need some results.

The update has the form

$$x(t+1) = x(t) + \gamma(t)s(t)$$

This leads to the identity about the difference of two consecutive gradients

$$\begin{aligned} Ax(t+1) &= Ax(t) + \gamma(t)As(t) \\ g(t+1) - g(t) &= \gamma(t)As(t) \qquad (1.3.1) \end{aligned}$$

1.3.1. *Orthogonality of $s(t)$ and $g(t+1)$.*

$$\begin{aligned} Ax(t+1) &= Ax(t) + \gamma(t)As(t) \\ g(t+1) &= g(t) - \frac{s(t)^\top g(t)}{s(t)^\top As(t)}As(t) \\ s(t)^\top g(t+1) &= s(t)^\top g(t) - \frac{s(t)^\top g(t)}{s(t)^\top As(t)}s(t)^\top As(t) = 0 \qquad (1.3.2) \end{aligned}$$

1.3.2. *Orthogonality of $s(i)$ and $g(t+1)$ for $i < t$.* For $i < t$, if we proceed similarly,

$$\begin{aligned} Ax(t+1) &= Ax(t) + \gamma(t)As(t) \\ s(i)^\top g(t+1) &= s(i)^\top g(t) + \gamma(t)s(i)^\top As(t) \\ s(i)^\top g(t+1) &= s(i)^\top g(t) \\ 0 &= s(i)^\top(g(t+1) - g(t)) \end{aligned}$$

But actually we have a more powerful result where $s(i)^\top g(t+1) = s(i)^\top g(t) = 0$. To see this, consider the solution $x(t+1)$ at time $t+1$ as a function of a past solution at $i+1$

$$x(t+1) = x(i+1) + \sum_{k=i+1}^{t} \gamma(k)s(k)$$

$$\begin{aligned} s(i)^\top Ax(t+1) &= s(i)^\top Ax(i+1) + s(i)^\top A \sum_{k=i+1}^{t} \gamma(k)s(k) \\ s(i)^\top g(t+1) &= s(i)^\top g(i+1) = 0 \end{aligned} \tag{1.3.3}$$

Here, 1.3.3 follows from 1.3.2

1.3.3. *Orthogonality of $g(i)$ and $g(t)$ for $i < t$.* We have the identity

$$-g(i) = s(i) - \sum_{j=0}^{i-1} c_j(i)s(j)$$

Multiply both sides by $g(t)^\top$ for some $i < t$

$$\begin{aligned} -g(t)^\top g(i) &= g(t)^\top s(i) - \sum_{j=0}^{i-1} c_j(i)g(t)^\top s(j) \\ &= 0 \end{aligned}$$

1.4. **Calculation of $c_i(t)$.** In general, the gradient at time t is given

$$-g(t) = s(t) - \sum_{j=0}^{t-1} c_j(t)s(j)$$

Multiplying both sides with $s(i)^\top A$ for some $i < t$ results in

$$\begin{aligned} -s(i)^\top Ag(t) &= s(i)^\top As(t) - \sum_{j=0}^{t-1} c_j(t)s(i)^\top As(j) \\ -s(i)^\top Ag(t) &= 0 - c_i(t)s(i)^\top As(i) \end{aligned}$$

This implies that

$$c_i(t) = \frac{s(i)^\top Ag(t)}{s(i)^\top As(i)}$$

But this coefficients can be further simplified. From (1.3.1) we have $g(i+1) - g(i) = \gamma(i)As(i)$ we obtain

$$c_i(t) = \frac{(g(i+1) - g(i))^\top g(t)}{(g(i+1) - g(i))^\top s(i)}$$

This implies that for $i < t - 1$ we have

$$c_i(t) = \frac{g(i+1)^\top g(t) - g(i)^\top g(t)}{(g(i+1) - g(i))^\top s(i)} = 0$$

For $i = t - 1$ we have

$$\begin{aligned} c_{t-1}(t) &= \frac{(g(t) - g(t-1))^\top g(t)}{(g(t) - g(t-1))^\top s(t-1)} \\ &= \frac{g(t)^\top g(t)}{g(t)^\top s(t-1) - g(t-1)^\top s(t-1)} \\ &= \frac{g(t)^\top g(t)}{-g(t-1)^\top s(t-1)} \end{aligned}$$

This leads to the following update:

$$\begin{aligned} s(t) &= -g(t) + c_{t-1}(t)s(t-1) \\ &= -g(t) + \frac{g(t)^\top g(t)}{-g(t-1)^\top s(t-1)} s(t-1) \end{aligned}$$

This udate can be further simplified. Consider, the update for the previous time step

$$s(t-1) \quad = \quad -g(t-1) + c_{t-2}(t-1)s(t-2)$$

We have

$$\begin{aligned} -g(t-1)^\top s(t-1) &= g(t-1)^\top g(t-1) - c_{t-2}(t-1)g(t-1)^\top s(t-2) \\ &= g(t-1)^\top g(t-1) \\ c_{t-1}(t) &= \frac{g(t)^\top g(t)}{g(t-1)^\top g(t-1)} \end{aligned}$$

So the search direction has the simple expression in terms of the gradients

$$s(t) \quad = \quad -g(t) + \frac{g(t)^\top g(t)}{g(t-1)^\top g(t-1)} s(t-1)$$

2. The Algorithm

In general, we wish to solve $Ax = b$
Select x_0
For $t = 0, 1, \dots$

$$g(t) \quad = \quad Ax(t) - b$$

$$\begin{aligned} c_{t-1}(t) &= \frac{g(t)^\top g(t)}{g(t-1)^\top g(t-1)} \\ s(t) &= -g(t) + c_{t-1}(t)s(t-1) \end{aligned}$$

$$\gamma(t) \quad = \quad -s(t)^\top g(t)/s(t)^\top As(t)$$

$$x(t+1) \quad = \quad x(t) + \gamma(t)s(t)$$

3. Implementation

```
%% Generate a random problem
N = 20;
randn('seed', 1);

A = randn(N,5);
A = A*A'+0.01*eye(N);
b = randn(N,1);
x_true = A\b;


%% Conjugate Gradients
x = randn(N,1);
s_past = zeros(N,1);
gt_g_past = 1; % avoid NaN

for t=1:N-1,
    % Gradient
    g = A*x - b;

    % Search direction
    gt_g = g'*g;
    c = gt_g/gt_g_past;
    s = -g + c*s_past;

    % Stepsize
```

```
    gam = - s'*g/(s'*A*s);

    % Update
    x = x + gam*s;

    [x x_true]'
    pause
    s_past = s;
    gt_g_past = gt_g;
end
```

4. Modified Gram Schmidt

Suppose we are given a set of vectors $a_1, a_2, \dots, a_n$ and wish to find a basis for the space they span, moreover

$$
\begin{aligned}
\langle a_1 \rangle &= \langle q_1 \rangle \\
\langle a_1, a_2 \rangle &= \langle q_1, q_2 \rangle \\
\langle a_1, a_2, a_3 \rangle &= \langle q_1, q_2, q_3 \rangle
\end{aligned}
$$

This asks for the following decomposition:

$$
\left[\begin{array}{c|c|c|c} a_1 & a_2 & \dots & a_n \end{array}\right] = \left[\begin{array}{c|c|c|c} q_1 & q_2 & \dots & q_n \end{array}\right] \left[\begin{array}{c|c|c|c} r_{1,1} & r_{1,2} & \dots & r_{1,n} \\ & r_{2,2} & \dots & r_{2,n} \\ & & \ddots & \vdots \\ & & & r_n \end{array}\right]
$$

A numerically unstable method to compute q_j is as follows:

$$
\begin{aligned}
z_1 &= a_1 \\
r_{1,1} &= \|z_1\| \\
q_1 &= a_1 / r_{1,1}
\end{aligned}
$$

$$
\begin{aligned}
r_{1,2} &= q_1^* a_2 \\
z_2 &= a_2 - q_1 q_1^* a_2 = a_2 - q_1 r_{1,2} \\
r_{2,2} &= \|z_2\| \\
q_2 &= z_2 / r_{2,2}
\end{aligned}
$$

$$
\begin{aligned}
r_{1,3} &= q_1^* a_3 \\
r_{2,3} &= q_2^* a_3 \\
z_3 &= a_3 - q_1 r_{1,3} - q_2 r_{1,3} \\
r_{3,3} &= \|z_3\| \\
q_3 &= z_3 / r_{3,3}
\end{aligned}
$$

5. Alternative Derivation (Trefethen and Bau)

Define the $A - norm$

$$
\|x\|_A \equiv \sqrt{x^\top A x}
$$

Define a system of nested Krylov subspaces for $n = 1, 2 \dots$

$$
\mathcal{K}_n = \left\langle b, Ab, A^2 b, \dots, A^{n-1} b \right\rangle
$$

We wish to solve when A is positive definite

$$Ax = b$$

The solution is

$$x^* = A^{-1}b$$

We define the error $\epsilon = x - x^*$ and a quadratic cost function

$$\begin{aligned}
\phi(x) &= \frac{1}{2}\|\epsilon\|_A^2 = \frac{1}{2}\|x - x^*\|_A^2 \\
&= \frac{1}{2}(x - x^*)^\top A(x - x^*) \\
&= \frac{1}{2}(x - A^{-1}b)^\top (Ax - b) \\
&= \frac{1}{2}x^\top Ax - b^\top x + \frac{1}{2}b^\top A^{-1}b \\
&= F(x) + \text{const} \\
F(x) &= \frac{1}{2}x^\top Ax - b^\top x
\end{aligned}$$

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