Note Title 9/3/2010

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Conjugate Gradient Methods

Popular for solving sparse systems of linear eqns.

We want to solve the linear system

$$Ax = b$$

where $A \in \mathbb{R}^{n \times n}$ is symmetric and positive definite.

Definition

let $u = (u_1, u_2, \ldots, u_n)$ and $v = (v_1, v_2, \ldots, v_n)$.

The <u>inner product</u> of u and v can be written as

$$\langle u, v \rangle = u^T v = \sum_{i=1}^{n} u_i v_i \quad \text{(scalar sum)}$$

Clearly

$$\langle u, v \rangle = \langle v, u \rangle$$

<u>Example</u>

$u = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$, $v = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$ then $\langle u, v \rangle = u^T v = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$

$= (1)(4) + (2)5 + 3(6)$

If u and v are mutually orthogonal,

then $\langle u, v \rangle = 0$

Definition

$$(AB)^T = B^T A^T$$

An A-inner product of two vector u and v is defined as

$$\langle u, v \rangle_A = \langle Au, v \rangle$$

$$= (AU)^T v \quad \text{by definition of inner product}$$

$$= U^T A^T v$$

Two non zero vectors u and v are said to be .

A-Conjugate if $\langle u, v \rangle_A = 0$

i.e.

$$U^T A^T v = 0$$

An $n \times n$ matrix A is positive definite if

$$\langle x, x \rangle_A > 0 \qquad [x^T A^T x > 0]$$

for all non zero vectors $x \in \mathbb{R}^n$.

Note that generally, expressions such as $\langle u, v \rangle$ and $\langle u, v \rangle_A$ reduce to 1×1 matrices which are just scalar values.

Definition

A quadratic form is a scalar quadratic function of a vector of the form

$$f(x) = \frac{1}{2}\langle x, x\rangle_A - \langle b, x\rangle + c$$

where

x and b are vectors

A is a matrix

c is a scalar constant.

$$f(x,y) = x^2 + y^3 + xy$$

$$\frac{\partial f}{\partial x} = 2x + 0 + y$$

$$\frac{\partial f}{\partial y} = 0 + 3y^2 + x$$

The <u>gradient</u> of the quadratic form is

$$f'(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} & \frac{\partial f(x)}{\partial x_2} & \cdots & \frac{\partial f(x)}{\partial x_n} \end{bmatrix}^T$$

Note that

$$f(x) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j - \sum_{i=1}^{n} b_i x_i + c$$

So

$$\frac{\partial f(x)}{\partial x_k} = \frac{1}{2}\left[\sum_{\substack{j=1 \\ j \neq k}}^{n} a_{kj} x_j + 2 a_{kk} x_k + \sum_{\substack{i=1 \\ i \neq k}}^{n} a_{ik} x_i \right] - b_k$$

$$= \frac{1}{2}\left[\sum_{j=1}^{n} a_{kj} x_j + \sum_{i=1}^{n} a_{ik} x_i\right] - b_k \quad \text{True for } k = 1, 2, \ldots n$$

Ax $\quad$ $A^T x$

Hence

$$f'(x) = \frac{1}{2} A^T x + \frac{1}{2} A x - b$$

If A is symmetric then $A^T = A$. So

$$f'(x) = Ax - b$$

Setting the gradient equal to zero, we get

$$0 = Ax - b$$

i.e.

$Ax = b$ which is the linear system to be solved?

Conclusion

The solution of $Ax = b$ is a critical point of $f(x)$

We observe that if A is symmetric and positive definite then $f(x)$ is minimized by the solution of $Ax = b$.

So an alternative way of solving the linear

System $Ax = b$ is to find an x that minimizes $f(x)$.

Example

Let $A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$. Is A positive definite?

Question:

$$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} > 0 \ ?$$

for all non zero $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$.