Conjugate Gradient

Suppose we want to solve the system of linear equations

$$\mathbf{Ax} = \mathbf{b}$$

for the vector $\mathbf{x}$, where the known $n \times n$ matrix $\mathbf{A}$ is symmetric (i.e., $\mathbf{A}^T = \mathbf{A}$), positive-definite (i.e. $\mathbf{x}^T\mathbf{Ax} > 0$ for all non-zero vectors $\mathbf{x} \in \mathbb{R}^n$), and real, and $\mathbf{b}$ is known as well. We denote the unique solution of this system by $\mathbf{x}^*$.

Solution of the above system of equations is the same as $\operatorname{argmin}_{\mathbf{x}\in\mathbb{R}^n} \frac{1}{2}\mathbf{x}^T\mathbf{Ax} - \mathbf{b}^T\mathbf{x}$.

Definition 1 ($\mathbf{A}$-conjugate directions)**.** *Let $\mathbf{A}$ ($n \times n$) be a symmetric matrix. The vectors $\{\mathbf{d}_1, \ldots, \mathbf{d}_k\}$ (all $\in \mathbb{R}^n$) are called conjugate (or orthogonal) with respect to $\mathbf{A}$ if $\mathbf{d}_i^T\mathbf{A}\mathbf{d}_j = 0$ for all $i \neq j$.*

Lemma 1 (Linear independence)**.** *Let $\mathbf{A}$ ($n \times n$) be positive definite. If the vectors $\{\mathbf{d}_1, \ldots, \mathbf{d}_k\}$ (all $\in \mathbb{R}^n$) are conjugate (orthogonal) with respect to $\mathbf{A}$, then they are linearly independent.*

Proof. Let $\{\mathbf{d}_1, \ldots, \mathbf{d}_k\}$ are linearly dependent and let $\mathbf{d}_k = \sum_{j=1}^{k-1} \alpha_j \mathbf{d}_j$.

By definition of conjugacy, we have $\mathbf{d}_k^T\mathbf{A}\mathbf{d}_j = 0$ for all $j \neq k$. Since, $\mathbf{A}$ is pd, we have $\mathbf{d}_k^T\mathbf{A}\mathbf{d}_k > 0$. On the other hand, $\mathbf{d}_k^T\mathbf{A}\mathbf{d}_k = \sum_{j=1}^{k-1} \alpha_j \mathbf{d}_k^T\mathbf{A}\mathbf{d}_j = 0$ (Contradiction!) $\square$

If $\mathbf{x}^*$ is a solution of the above system of equation, we can represent it as a linear combination of $\{\mathbf{d}_1, \ldots, \mathbf{d}_n\}$, which are conjugate vectors with respect to $\mathbf{A}$.

Let $\mathbf{x}^* = \sum_{j=1}^{n} \alpha_j \mathbf{d}_j$. It is easy to check that $\mathbf{d}_j^T\mathbf{A}\mathbf{x}^* = \alpha_j \mathbf{d}_j^T\mathbf{A}\mathbf{d}_j$. Thus $\alpha_j = \frac{\mathbf{d}_j^T\mathbf{A}\mathbf{x}^*}{\mathbf{d}_j^T\mathbf{A}\mathbf{d}_j}$. But by assumption, $\mathbf{A}\mathbf{x}^* = \mathbf{b}$. Thus $\alpha_j = \frac{\mathbf{d}_j^T\mathbf{b}}{\mathbf{d}_j^T\mathbf{A}\mathbf{d}_j}$. Hence, to know α_j, we do not need to know $\mathbf{x}^*$.

Hence $\mathbf{x}^* = \sum_{j=1}^{n} \frac{\mathbf{d}_j^T\mathbf{b}}{\mathbf{d}_j^T\mathbf{A}\mathbf{d}_j}\mathbf{d}_j$, no matrix inversion or nothing.

In practice, we do not know the conjugate vectors. We thus may follow Gram–Schmidt type algorithm.

Algorithm 1: Conjugate gradient

(i) Start setting $\mathbf{r}_1 = \mathbf{b} - \mathbf{A}\mathbf{x}_1$ with some starting value $\mathbf{x}_1$.
(ii) If $\mathbf{r}_0$ is small enough, return $\mathbf{x} = \mathbf{x}_1$ as solution.
(iii) Otherwise, set $\mathbf{d}_1 = \mathbf{r}_1$ and $k = 1$.
(iv) Start loop

- $\alpha_k = \frac{\mathbf{r}_k^T \mathbf{r}_k}{\mathbf{d}_k^T \mathbf{A} \mathbf{d}_k}$
- $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
- $\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{d}_k$
- If $\mathbf{r}_{k+1}$ is small enough, return $\mathbf{x} = \mathbf{x}_{k+1}$ as solution.
- Otherwise, $\beta_k = \frac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k}$, $\mathbf{d}_{k+1} = \mathbf{r}_{k+1} + \beta_k \mathbf{d}_k$, move $k = k + 1$ and Repeat

In the above algorithm, how the term ‘gradient’ fits in? Say $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{A}\mathbf{x} - \mathbf{b}^T \mathbf{x}$ and we are trying to solve $\min_{\mathbf{x}} f(\mathbf{x})$. Following the steps in gradient descent, the updates should look like $\mathbf{x}_{k+1} = \mathbf{x}_k - t_k \bigtriangledown f(\mathbf{x}_k)$. For our function, we have $\bigtriangledown f(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$. Thus, we need to move towards $\mathbf{b} - \mathbf{A}\mathbf{x}$. The other vectors in the basis will be made conjugate to this gradient vector. Thus, the term ‘conjugate gradient’ comes in.

To see above, note that $\beta_k = \frac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k} = -\frac{\mathbf{r}_{k+1} \mathbf{A} \mathbf{d}_k}{\mathbf{d}_k^T \mathbf{A} \mathbf{d}_k}$. Then, $\mathbf{d}_{k+1}^T \mathbf{A} \mathbf{d}_k = 0$

If the condition number of $\mathbf{A}$ is large, the convergence is slow as it leads to slower improvement. Hence, to ensure faster convergence in this case, **Preconditioning conjugate gradient** is used. [Condition number of a matrix $\mathbf{A}$ is $\kappa(\mathbf{A}) = \dfrac{\sigma_{\max}(\mathbf{A})}{\sigma_{\min}(\mathbf{A})}$, where $\sigma_{\max}(\mathbf{A})$ and $\sigma_{\min}(\mathbf{A})$ are maximal and minimal singular values of $\mathbf{A}$ respectively. In our case, the singular values and eigenvalues are the same as $\mathbf{A}$ is symmetric]

Algorithm 2: Pre-conditioned conjugate gradient

$$\begin{aligned}
\mathbf{r}_0 &= \mathbf{b} - \mathbf{A}\mathbf{x}_0 \\
\mathbf{z}_0 &= \mathbf{M}^{-1}\mathbf{r}_0 \\
\mathbf{p}_0 &= \mathbf{z}_0 \\
k &= 0
\end{aligned}$$

repeat

$$\begin{aligned}
\alpha_k &= \frac{\mathbf{r}_k^{\mathsf{T}}\mathbf{z}_k}{\mathbf{p}_k^{\mathsf{T}}\mathbf{A}\mathbf{p}_k} \\
\mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha_k\mathbf{p}_k \\
\mathbf{r}_{k+1} &= \mathbf{r}_k - \alpha_k\mathbf{A}\mathbf{p}_k
\end{aligned}$$

if r_{k+1} is sufficiently small, then exit loop end if

$$\begin{aligned}
\mathbf{z}_{k+1} &= \mathbf{M}^{-1}\mathbf{r}_{k+1} \\
\beta_k &= \frac{\mathbf{r}_{k+1}^T\mathbf{z}_{k+1}}{\mathbf{r}_k^T\mathbf{z}_k} \\
\mathbf{p}_{k+1} &= \mathbf{z}_{k+1} + \beta_k\mathbf{p}_k \\
k &= k+1,
\end{aligned}$$

end repeat;
The result is x_{k+1}

In the above algorithm $\mathbf{M}$ is fixed. We often set $\mathbf{M}$ as $\mathbf{L}\mathbf{L}^T$ where $\mathbf{L}$ is an incomplete Cholesky decomposition of $\mathbf{A}$ or sometimes the diagonal entries in $\mathbf{A}$ (Jacobi preconditioner). Or, we often set $\mathbf{M}^{-1}$= some approximate inverse of $\mathbf{A}$. The approximate inverse computation would depend on the shape and structure of $\mathbf{A}$.