Conjugate gradient ideas

An iterative method for solving a linear system $Au = b$ that begins with an initial guess $u_0$ for $u$ and tries to improve that guess by getting a sequence of guesses $u_0, u_1, u_2, \ldots$.

Often one can think of $u_{k+1}$ as $u_k$ plus a correction, say $u_{k+1} = u_k + \lambda_k p_k$, where $\lambda_k p_k$ is a correction vector ($\lambda_k$ a scalar, $p_k$ a vector).

To choose $\lambda_k$ we note that the solution to $Au = b$ is also the solution to $\min F(u) = \frac{1}{2} u^T A u - b^T u$ for a symmetric positive definite (spd) matrix. (Calculus can be used to prove this!)

Given $p_k$ and $u_k$ we can choose $\lambda_k$ to minimize $F(u_k + \lambda p_k)$ over all $\lambda$ to minimize $F(u_k + \lambda p_k)$ over all $\lambda$. (1)

and choose $p_k$ so that $r_k = b - Au_k$ is perpendicular to $r_k - 1, r_k - 2, \ldots, r_0$. (2)

By (1), $F(u_{k+1}) \leq F(u_k)$, so at each iteration the method improves (or gets no worse) in the sense that $F(u)$ decreases (or won’t increase).

By (2) the method is guaranteed to converge in $n$ iterations or less: $r_0, r_1, \ldots, r_n$ are all perpendicular to each other and the only way that $n + 1$ vectors can be perpendicular in $n$ dimensional space is if one of the vectors is zero. Therefore for some $k \leq n$, $r_k = b - A x_k = 0$.

Terminology

**conjugate:** one can show that the $p$ vectors satisfy $p_i^T A p_j = 0$, for $i \neq j$. Vectors satisfying this relation are said to be conjugate.

**gradient:** $p_k$ is related to the “gradient” of $F(u)$.