Solving \( Ax = b \), A spd, by gradient methods:

**Conjugate Gradients**

(1) Solution of \( Ax = b \) minimizes \( \phi(x) = \frac{1}{2} x^T A x - x^T b \) \( \overset{\text{Def}: \text{Residual (r(x)=b-AX)}}{\ Δ} \)

\[ r_k = b - A x_k \]

\[ \frac{\partial \phi}{\partial \alpha} \bigg|_{x_{k+1}} = 0 \]

This suggests an algorithm for successive approximation of the solution:

**Step k**: (given \( x_k \) (approx solution), \( P_{k+1} \) (search direction))

\[
\begin{bmatrix}
  r_k = b - A x_k \\
  \alpha_{k+1} = \frac{P_{k+1}^T r_k}{P_{k+1}^T A P_{k+1}} \\
  x_{k+1} = x_k + \alpha_{k+1} P_{k+1}
\end{bmatrix}
\]

[New search direction \( P_{k+1} \)?]

How do we choose \( P_k \)?
Two basic strategies for choosing $p_k$:

(i) Steepest descent, (ii) Conjugate directions

(i) Steepest descent: $p_{k+1} := -\nabla \phi |_{x_k} = b - Ax_k = r_k$

Algorithm:

\[ \begin{align*}
    x_{k+1} & = x_k + \alpha_{k+1} r_k \\
    r_{k+1} & = b - A x_{k+1} = r_k - \alpha_{k+1} A r_k
\end{align*} \]

This choice defines the method. It leads to steepest descent minimization which can be very slow if $A$ is ill-conditioned.

Convergence: Let $A Q = Q \Lambda$, write $r_k = Q s_k$. Then we have

\[ \sum_{i=1}^{n} (1 - \alpha_{k+1} \lambda_i) s_k^2 = 0 \]  \hspace{1cm} (4)

\[ \lambda_k = r_k^T r_k / r_k^T A r_k = s_k^T Q^T A Q s_k / s_k^T A Q s_k = S_k^T S_k / S_k^T A S_k \]

Corollary: $\frac{1}{\lambda_{\min}} \leq \alpha_{k+1} \leq \frac{1}{\lambda_{\max}}$ (say $\lambda_{\max} = \lambda_i$; $\lambda_{\min} = \lambda_n$).  \hspace{1cm} (5)

Substituting $r_k$ in expression for $r_{k+1}$:

\[ Q s_{k+1} = r_{k+1} = (I - \alpha_{k+1} A) Q s_k \Rightarrow s_{k+1} = (I - \alpha_{k+1} \Lambda) s_k \]

The $i$-th vector component of the residual, $s_{k, i}$, is multiplied by the factor $(1 - \lambda_i \alpha_{k+1})$ to produce $s_{k+1, i}$.

Since (5) $\lambda_i \leq \alpha_{k+1} \leq \lambda_n$, it follows that $s_{k, 1}$ and $s_{k, n}$ have largest negative or positive factors, respectively.

\[ \Rightarrow \text{Extreme eigenvector components govern convergence.} \]
(ii) **Conjugate direction**: choose \( p_k \) (linearly independent) so that \( x_k \) minimizes \( \phi(x) \) in \( [p_0, p_1, \ldots, p_k] \). If this is possible, then we will get solution at \( n \)-th step (if exact arithmetic). Thus, we want to choose set \( p_k \) so that solution to

\[
\min_{\alpha} \phi(x_k + \alpha p_{k+1})
\]

also gives \( \min_{x \in [p_0, \ldots, p_k]} \phi(x) \). Now let \( x = \sum_{i=0}^{k-1} [p_{i+1} y + \alpha p_k] \) \((P_{k+1}^{n \times (k-1)})\)

Then

\[
\phi(x) = \frac{1}{2} \left[ y^T P_{k-1}^T A P_{k-1} y + \alpha^2 P_k^T A p_k + 2 \alpha y^T P_{k-1}^T A p_k \right] - y^T P_{k-1}^T b - \alpha P_k^T b
\]

\[
= \phi(P_{k-1} y) + \alpha y^T \left\{ P_{k-1}^T A p_k \right\} + \frac{\alpha^2}{2} P_k^T A p_k - \alpha P_k^T b
\]

Hestenes \& Stiefel (1952): Let \( p_i^T A p_j = 0 \), \( i \neq j \). (7)

Then two separate minimizations!

(i) \( P_{k-1} y = x_{k-1} \), minimizer over \([p_0, \ldots, p_{k-1}]\)

(ii) \( \alpha = \alpha_k = \frac{p_k^T r_{k-1}}{p_k^T A p_k} \)

\( \Rightarrow \) Must ensure \( p_k^T A p_k = 0 \), \( k \neq l \); \( P_r p_k \neq 0 \).

(*) **Condition (7)** is the \( A \)-conjugacy condition that defines the method (still needs a unique specification!)

Since we are building the \( p_j \) "from scratch," we need to specify the space they are chosen from. Once that is fixed, the \( p_j \) are an \( A \)-orthogonal basis.

It turns out that \([r_0, \ldots, r_{k-1}]\) is a reasonable choice. Then, selecting \( p_{k+1} = r_k + \beta p_k \), turns that space into a Krylov space, \( K_n = [r_0, \ldots, r_{k-1}] \). Here, \( \beta \) is:
Theorem: A spd, $r_k \neq 0$; let $p_0 = 0$. Then the recurrence
\[ P_{k+1} = r_k + \beta_k p_k, \quad k \geq 0 \] (8)
with $\beta = \beta_{k+1}$ chosen so that $P_{k+1}^T A P_k = 0$
gives sequences \{\(r_0, \ldots, r_k, r_{k+1}, \ldots\)\}, \{\(p_0, \ldots, p_k, p_{k+1}, \ldots\)\} \{\(x_0, \ldots, x_k, x_{k+1}\}\} that satisfy
(i) $p_k \in K_k$ and $r_k \in K_{k+1}$
where $K_k = \{r_0, \ldots, r_k\}$ is the Krylov space of $r_0$.
(ii) $P_{k+1}^T A x = 0$, $\forall x \in K_k$ ($p_{k+1} \perp K_k$)
(iii) $x_k^T x = 0$, $\forall x \in K_k$ ($r_k \perp K_k$)

We have the following defining equation for the sequences \{\(P_k\)\}, \{\(r_k\)\}:
\[
\begin{align*}
\{P_0 = 0; x_0 \text{ arbitrary} \\
n_k = b - A x_0 \\
n_k = p_k + \beta_k p_{k+1} \quad (\beta_k \text{ chosen to impose } P_{k+1}^T A P_k = 0) \\
r_{k+1} = r_k - \alpha_{k+1} A p_{k+1} \\
\end{align*}
\]
\[\alpha_{k+1} = P_{k+1}^T r_k / P_{k+1}^T A p_{k+1} \]

(i) induction assumption: $p_{k-1} \in K_{k-1}$; $r_{k-1} \in K_{k-1} \subset K_k$
Then $P_{k-1} = r_k + \beta_k p_k \in K_{k+1}$, while, since $K_k$ is the $k$-th order
Krylov space of $r_0$, $x \in K_k$ is the $k$-th order
Krylov space of $r_0$, $x \in K_k$, and if
\[ P_{k+1} e_{K_{k+1}} \Rightarrow A p_{k+1} \in K_{k+2} \]
(iii) Now the induction assumption is that
\[ \beta_{k+1} \neq 0, \forall e_{K_{k+1}} \quad \text{for } l = 1, \ldots, k-1 \]
(iii) $r_k^T x = 0$, $\forall x \in K_{k+1}$ true for $l = k$
To show $P_{k+1}^TA \mathbf{f} = 0$, $\mathbf{f} \in \mathbb{F}_k$ we can show that

$$P_{k+1}^TA \mathbf{r}_l = 0, \ l = 0, \ldots, k-1$$

(since by assumption the $\mathbf{r}_l$ are mutually orthogonal and, so, independent)

that is $\mathbb{F}_k = [\mathbf{r}_0, \ldots, \mathbf{r}_{k-1}]$ (9)

Now

$$P_{k+1}^TA \mathbf{r}_l = P_l^TA \mathbf{r}_l + \beta_{k+1} P_{k+1}^TA \mathbf{r}_l$$

(a) For $l \leq k-2$: $\mathbf{r}_l \in \mathbb{F}_{l+1} \subset \mathbb{F}_{k-1}$

But $P_k \perp \mathbb{F}_{k-1} = [\mathbf{r}_0, \ldots, \mathbf{r}_{k-2}] \Rightarrow P_k^TA \mathbf{r}_l = 0$

and $\mathbf{r}_l \in \mathbb{F}_{k-1} \Rightarrow A \mathbf{r}_l \in \mathbb{F}_k \perp \mathbf{r}_k \Rightarrow r_l(A \mathbf{r}_l) = 0$

$$\Rightarrow P_{k+1}^TA \mathbf{r}_l = 0, \ l \leq k-2$$

(b) We may choose $\beta_{k+1}$ to make $P_{k+1}^TA \mathbf{r}_{k-1} = 0$; this gives

$$0 = r_{k-1}^T A \mathbf{r}_{k-1} + \beta_{k+1} P_{k+1}^T A \mathbf{r}_{k-1} \Rightarrow \beta_{k+1} = -\frac{r_{k-1}^T A \mathbf{r}_{k-1}}{P_{k+1}^T A \mathbf{r}_{k-1}}$$

(10)

This establishes: $P_{k+1}^TA \mathbf{f} = 0$, $\mathbf{f} \in \mathbb{F}_k$

In particular, then: $P_{k+1}^T A \mathbf{p}_k = 0$ since $\mathbf{p}_k \in \mathbb{F}_k$

(as well as $P_{k+1}^T A \mathbf{r}_l = 0$, $l = 0, \ldots, k$)

Similarly, for the residual

$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_{k+1} A \mathbf{p}_{k+1}$$

(a) $r_{k+1}^T \mathbf{r}_l = r_k^T \mathbf{r}_l - \alpha_{k+1} P_{k+1}^T A \mathbf{r}_l \quad l = 0, \ldots, k-1$

But $r_k^T \mathbf{r}_l = 0$ by assumption

$$r_{k+1}^T \mathbf{r}_l = 0 \quad l = 0, \ldots, k-1$$

(12)

$p_{k+1}^T A \mathbf{r}_l = 0$ by above discussion

Since $\mathbb{F}_k = \text{span} [\mathbf{r}_0, \ldots, \mathbf{r}_{k-1}]$, see above (9), i.e. $r_{k+1}^T \mathbf{f} = 0$ $\forall \mathbf{f} \in \mathbb{F}_k$.
Efficient Formulation: (minimize computation)

Lemma: $r_k \neq 0$, A spd. Then
\[
\alpha_{k+1} = \frac{||r_k||_2^2}{||P_k||_A^2} \quad \implies \quad \varrho_{k+1} = \frac{||r_k||_2^2}{||r_{k-1}||_2^2}
\]

Use: $P_{k+1} = r_k + \varrho_{k+1} P_k$ ; $r_{k+1} = r_k - \alpha_{k+1} A P_{k+1}$

So: $P_k^T A P_k = P_k^T A (P_{k-1} + \varrho_k P_k)$

\[
P_k^T r_k = (r_{k-1}^T + \varrho_k P_k^T) r_k = r_{k-1}^T r_k + \varrho_k P_k^T r_k = 0 \quad (\text{A-conjugacy})
\]

\[
P_{k+1} = (r_k^T + \varrho_k P_k) r_k = r_k^T r_k + \varrho_k P_k^T r_k = 0
\]

\[
= \frac{||r_k||_2^2}{||P_k^T r_k||_2}
\]

Then $\alpha_{k+1} = \frac{P_{k+1}^T r_k}{P_k^T A P_{k+1}} = \frac{||r_k||_2^2}{||P_{k+1}||_A^2}$

Also $r_k^T A r_{k-1} = r_k^T A (P_k - \varrho_k P_{k-1}) = r_k^T A P_k = P_k^T A r_k \; (17)$

\[
(13) \quad P_k^T A r_{k-1} = P_k^T A P_k = ||P_k||_A^2 = \frac{||r_{k-1}||_2^2}{\alpha_k}
\]

\[
(17) \quad r_k^T A r_{k-1} = r_k^T A P_k
\]

\[
||r_k||_2 = r_k^T (r_{k-1} - \alpha_k P_k) = -\alpha_k r_k^T A P_k
\]

So: $\varrho_{k+1} = -\frac{r_k^T A r_{k-1}}{P_k^T A r_{k-1}} = \frac{||r_k||_2^2}{||r_{k-1}||_2^2} \; (18)$

---

\[
x_0 \text{ arbitrary} \quad \begin{align*}
  x_1 &= x_0 + \alpha_1 P_1 \\
  r_1 &= b - A x_1 \\
  \alpha_1 &= \frac{||r_0||_2^2}{||P_0||_A^2}
\end{align*}
\]

\[
\begin{array}{c|c|c|c|}
  k = 0, 2, \ldots & \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \varrho_{k+1} = \frac{||r_k||_2^2}{||P_k||_A^2} \\
  \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \varrho_{k+1} = \frac{||r_k||_2^2}{||P_k||_A^2} \\
  \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \varrho_{k+1} = \frac{||r_k||_2^2}{||P_k||_A^2} \\
  \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \varrho_{k+1} = \frac{||r_k||_2^2}{||P_k||_A^2} \\
  \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \beta_{k+1} = \frac{||r_k||_2^2}{||r_{k+1}||_2^2} & \varrho_{k+1} = \frac{||r_k||_2^2}{||P_k||_A^2} \\

\end{array}
\]

\[
r_k = P_k r_k \quad \text{or} \quad r_{k+1} = b - A x_{k+1}
\]