Below, HW indicates that the result is part of the next homework assignment.

We shall study the conjugate gradient algorithm applied to a SPD $n \times n$ matrix $A$ in this class. We start by introducing the so-called Krylov subspace, $K_m(K_m(A,r_0)) = \text{span}\{r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0\}$.

It is clear that the dimension of $K_m$ is at most $m$. Sometimes, $K_m$ has dimension less than $m$, for example, if $r_0$ was an eigenvector, then $\text{dim}(K_m)=1$, for $m = 1, 2, \ldots$ (why?).

A simple argument by mathematical induction (HW), shows that the search direction $p_i$ is in $K_{i+1}$, for $i = 0, 1, \ldots$. It follows that $x_i = x_0 + \theta$ for some $\theta \in K_i$ and $e_i = e_0 - \theta$ (for the same $\theta$).

We note that the dimension of the Krylov space keeps growing until $A^l r_0 \in K_l$ in which case $K_l = K_{l+1} = K_{l+2} \cdots$ (HW). Let $l_0$ be the minimal such value, i.e., $A^{l_0} r_0 \in K_{l_0}$ but $A^{l_0-1} r_0 \notin K_{l_0-1}$. Then there are coefficients, $c_0, \ldots, c_{l_0-1}$ satisfying

$$c_0 r_0 + c_1 Ar_0 + \ldots c_{l_0-1} A^{l_0-1} r_0 = A^{l_0} r_0.$$ 

Since $A^{l_0-1} r_0 \notin K_{l_0-1}$, $c_0 \neq 0$ (why?) and so

$$e_0 = A^{-1} r_0 = c_0^{-1} (A^{l_0-1} r_0 - c_1 r_0 - c_2 Ar_0 \cdots - c_{l_0-1} A^{l_0-2} r_0) \in K_{l_0}.$$ 

Similar arguments show that $l_0$ is, in fact, the smallest index such that $e_0 \in K_{l_0}$ (HW).

It is natural to consider the best approximation $\tilde{x}_i$ over vectors of the form $x_i = x_0 + \theta$ for $\theta \in K_i$ (best approximation with respect to the $A$-norm), i.e.,

$$(12.1) \quad \|x - \tilde{x}_i\|_A = \min_{\zeta \in K_i} \|x - (x_0 + \zeta)\|_A.$$

This can be rewritten

$$(12.2) \quad \|\tilde{e}_i\|_A = \min_{\zeta \in K_i} \|e_0 - \zeta\|_A$$

with $\tilde{e}_i = x - \tilde{x}_i$. As $e_0$ is in $K_{l_0}$, $\tilde{x}_{l_0} = x$, i.e., we have the solution at the $l_0$’th step (why?).
The minimization problem with respect to a finite dimensional space associated with a norm which comes from an inner product can always be reduced to a matrix problem. We illustrate this for the above minimization problem. This is contained in the following lemma:

**Lemma 1.** There is a unique solution $\tilde{x}_i = x_0 + \theta$ with $\theta \in K_i$ solving (12.1). It is characterized as the unique function of this form satisfying

$$ (x - \tilde{x}_i, \zeta)_A = 0 \quad \text{for all } \zeta \in K_i. $$

**Proof.** We first show that there is a unique function $\theta \in K_i$ for which (12.3) holds. Given a basis $\{v_1, \ldots, v_l\}$ for the Krylov space $K_i$, we expand

$$ \theta = \sum_{j=1}^l c_j v_j. $$

The condition (12.3) is equivalent to

$$ (x - x_0 - \sum_{j=1}^l c_j v_j, v_m)_A = 0 \quad \text{for } m = 1, \ldots, l $$

or

$$ \sum_{j=1}^l c_j (v_j, v_m)_A = (b - Ax_0, v_m) \quad \text{for } m = 1, \ldots, l. $$

This is the same as the matrix problem $Nc = F$ with

$$ N_{j,m} = (v_m, v_j)_A \quad \text{and} \quad F_m = (b - Ax_0, v_m), \quad j, m = 1, \ldots, l. $$

This problem has a unique solution if $N$ is nonsingular. To check this, we let $d \in \mathbb{R}^l$ be arbitrary and compute

$$ (Nd, d) = \sum_{j,k=1}^l (N_{j,k}d_k)d_j = \sum_{j,k=1}^l (v_k, v_j)_A d_kd_j $$

$$ = \sum_{k=1}^l d_k v_k, \sum_{j=1}^l d_j v_j)_A = (w, w)_A $$

where $w = \sum_{j=1}^l d_j v_j$. Since $\{v_1, \ldots, v_l\}$ is a basis, $w$ is nonzero whenever $d$ is nonzero. It follows from the definiteness property of the inner product that $0 \neq (w, w)_A = (Nd, d)$ whenever $d \neq 0$. Thus, $0$ is the only vector for which $Nd = 0$, i.e., the matrix $N$ is nonsingular and there is a unique $\theta \in K_i$ satisfying (12.3).
We next show that the unique solution of (12.3) solves the minimization problem. Indeed, if $\zeta$ is in $K_i$ then
\[
\|x - \tilde{x}_i\|_A^2 = (x - \tilde{x}_i, x - (x_0 + \zeta + (\theta - \zeta))}_A
= (x - \tilde{x}_i, x - (x_0 + \zeta))_A \leq \|x - \tilde{x}_i\|_A \|x - (x_0 + \zeta)\|_A
\]
It immediately follows that $\tilde{x}_i$ is the minimizer.

The proof will be complete once we show that anything which is a minimizer satisfies (12.3). Suppose that $\tilde{x}_i = x_0 + \theta$ solves the minimization problem. Given $\zeta \in K_i$, we consider for $t \in \mathbb{R}$,
\[
f(t) = \|x - \tilde{x}_i + t\zeta\|_A^2 = (x - \tilde{x}_i + t\zeta, x - \tilde{x}_i + t\zeta)_A.
\]
By using bilinearity of the inner product, we see that
\[
f(t) = (x - \tilde{x}_i, x - \tilde{x}_i)_A + 2t(x - \tilde{x}_i, \zeta)_A + t^2(\zeta, \zeta)_A.
\]
Since $\tilde{x}_i$ is the minimizer, $f'(0) = 2(x - \tilde{x}_i, \zeta)_A = 0$, i.e., (12.3) holds. \qed

**Theorem 1.** *(CG-equivalence)* Let $l_0$ be as above. Then for $i = 1, 2, \ldots, l_0$, $x_i$ defined by the conjugate gradient (CG) algorithm coincides with the best approximation from the Krylov space, $\tilde{x}_i$ satisfying (12.1).

The first step in the conjugate gradient method coincides with the steepest descent algorithm. It follows that the CG algorithm is not a linear iterative method.

The above theorem shows that the conjugate gradient algorithm provides a very efficient implementation of the Krylov minimization problem. As discussed above, at least mathematically, we get the exact solution on the $l_0$'th step ($x_{l_0} = x$). At this point the CG algorithm breaks down as $r_{l_0} = p_{l_0} = 0$ and so the denominators are zero.

Historically, when the conjugate gradient method was discovered, it was proposed as a direct solver. Since, $K_i \subseteq \mathbb{R}^n$, $l_0$ can at most be $n$. The above theorem shows that we get convergence in at most $n$ iterations. However, it was found that, because of round-off errors, implementations of the CG method sometimes failed to converge in $n$ iterations. Nevertheless, CG is very effective when used as an iterative method on problems with reasonable condition numbers. The following theorem gives a bound for its convergence rate.

**Theorem 2.** *(CG-error)* Let $A$ be a SPD $n \times n$ matrix and $e_i$ be the sequence of errors generated by the conjugate gradient algorithm. Then,
\[
\|e_i\|_A \leq 2 \left(\frac{\sqrt{K} - 1}{\sqrt{K} + 1}\right)^i \|e_0\|_A.
\]
Here $K$ is the spectral condition number of $A$. 
Proof. Since CG is an implementation of the Krylov minimization, \( \| e_0 + \theta \|_A \leq \| e_0 \|_A \) for any \( \theta \in K_i \). In particular, \( G_i \) of the multi-parameter theorem of an earlier class (with \( \tau_1, \ldots, \tau_i \) coming from \( \lambda_0 = \lambda_1 \) and \( \lambda_\infty = \lambda_n \)) satisfies

\[
\| G_i e_0 \|_A = \| \prod_{j=1}^{i} (I - \tau_j A) e_0 \|_A = \| e_0 + \theta \|_A
\]

for some \( \theta \in K_i \). The theorem follows immediately from the multi-parameter theorem.

Proof of Theorem (CG-equivalence). The proof is by induction. We shall prove that for \( i = 1, \ldots, l_0 \),

1. \( \{ p_0, p_1, \ldots, p_{i-1} \} \) forms an \( A \)-orthogonal basis for \( K_i \).
2. \( (e_i, \theta)_A = 0 \) for all \( \theta \in K_i \).

By definition, \( p_0 = r_0 \) and forms a basis for \( K_1 \). Moreover, \( (e_1, r_0)_A = 0 \) by the definition of \( \alpha_0 \) so (I.1) and (I.2) hold for \( i = 1 \).

We inductively assume that (I.1) and (I.2) hold for \( i = k \) with \( k < l_0 \). By the definition of \( \beta_{k-1}, p_k \) is \( A \)-orthogonal to \( p_{k-1} \). For \( j < k - 1 \),

\[
(p_k, p_j)_A = (r_k - \beta_{k-1} p_{k-1}, p_j)_A = (e_k, Ap_j)_A - \beta_{k-1} (p_{k-1}, p_j)_A.
\]

Of the two terms on the right, the first vanishes by Assumption (I.2) with \( k \) since \( Ap_j \in K_k \) while the second vanishes by assumption (I.1) with \( k \). Thus, \( p_k \) satisfies the desired orthogonality properties.

The validity of (I.1) for \( k + 1 \) will follow if we show that \( p_k \neq 0 \). If \( p_k = 0 \) then \( r_k = \beta_{k-1} p_{k-1} \in K_k \) and by (I.1) at \( k \),

\[
0 = (e_k, p_{k-1})_A = (r_k, p_{k-1}) = -\beta_{k-1} (p_{k-1}, p_{k-1}).
\]

This implies that \( r_k = 0 \) and hence \( e_k = 0 \). This means that \( e_0 \in K_k \) contradicting the assumption that \( k < l_0 \).

We next verify (I.2) at \( k + 1 \). As observed in the previous class, \( p_k \) and \( \alpha_k \) are constructed so that \( e_{k+1} \) is \( A \)-orthogonal to both \( p_k \) and \( p_{k-1} \). To complete the proof, we need only check its orthogonality to \( p_j \) for \( j < k - 1 \). In this case,

\[
(e_{k+1}, p_j)_A = (e_k - \alpha_k p_k, p_j)_A = (e_k, p_j)_A - \alpha_k (p_k, p_j)_A.
\]

The first term is handled by the induction assumption (I.2) while the second follows from (I.1) for \( k + 1 \) (which we proved above).

Thus, (I.1) and (I.2) hold for \( i = 1, 2, \ldots, l_0 \). We already observed that \( e_i = e_0 + \theta \) for some \( \theta \in K_i \). Thus, (I.2) and Lemma 1 implies that \( x_i = \bar{x}_i \). ☐
Preconditioned conjugate gradient iteration. In the development and analysis of the conjugate gradient algorithm, we see the interaction of the matrix $A$ and the inner product. In fact, if you look carefully, you see that the entire development goes through replacing the $\ell^2$ inner product $(\cdot, \cdot)$ by any other inner product provided that the matrix $A$ is positive definite and self adjoint with respect to new inner product. This observation immediately leads to a preconditioned conjugate gradient algorithm. Specifically, we assume that we are given two SPD matrices $A$ and $B$ (with $B$ a preconditioner). As usual, we consider the preconditioned system

$$BAx = Bb$$

and use the $B^{-1}$-inner product as our base inner product (which replaces the $\ell^2$ inner product). We now apply CG to the preconditioned system (12.6) with the $B^{-1}$-inner product to obtain:

**Algorithm 1.** (Preconditioned Conjugate Gradient, Version 1). Let $A$ and $B$ be SPD $n \times n$ matrices and $x_0 \in \mathbb{R}^n$ (the initial iterate) and $b \in \mathbb{R}^n$ (the right hand side) be given. Start by setting $p_0 = r_0 = Bb - BAx_0$. Then for $i = 0, 1, \ldots$, define

$$x_{i+1} = x_i + \alpha_i p_i, \quad \text{where} \quad \alpha_i = \frac{(r_i, p_i)_{B^{-1}}}{(BAp_i, p_i)_{B^{-1}}},$$

$$r_{i+1} = r_i - \alpha_i BAp_i,$$

$$p_{i+1} = r_{i+1} - \beta_i p_i, \quad \text{where} \quad \beta_i = \frac{(r_{i+1}, BAp_i)_{B^{-1}}}{(BAp_i, p_i)_{B^{-1}}}.$$

The above algorithm is not completely satisfactory. The reason being is that the preconditioner may be defined by a fairly complicated process and so its inverse may not be computationally available. Except for the numerator in the definition of $\alpha_i$, the $B^{-1}$ cancels with an application of $B$. We can deal with this troublesome term by introducing an intermediate variable, $\tilde{r}_i$ satisfying $\tilde{r}_i = b - Ax_i$. Then $r_i = B\tilde{r}_i$ and the algorithm becomes:

**Algorithm 2.** (Preconditioned Conjugate Gradient). Let $A$ and $B$ be SPD $n \times n$ matrices and $x_0 \in \mathbb{R}^n$ (the initial iterate) and $b \in \mathbb{R}^n$ (the right hand side) be given. Start by setting $\tilde{r}_0 = b - Ax_0$, $p_0 = r_0 = B\tilde{r}_0$. Then for $i = 0, 1, \ldots$, define

$$x_{i+1} = x_i + \alpha_i p_i, \quad \text{where} \quad \alpha_i = \frac{(\tilde{r}_i, p_i)}{(Ap_i, p_i)},$$

$$\tilde{r}_{i+1} = \tilde{r}_i - \alpha_i Ap_i,$$

$$r_{i+1} = B\tilde{r}_{i+1},$$

$$p_{i+1} = r_{i+1} - \beta_i p_i, \quad \text{where} \quad \beta_i = \frac{(r_{i+1}, Ap_i)}{(Ap_i, p_i)}.$$
We note that in the above algorithm, there is exactly one evaluation of \(B\) and one evaluation of \(A\) per iterative step after startup. The original CG method minimized the error in the \(A\)-norm which was defined using the base inner product, \((\cdot, \cdot)\), i.e. \((\cdot, \cdot)_A = (A, \cdot)\). The preconditioned conjugate gradient method minimizes the error in the operator inner product defined in terms of the base inner product \((\cdot, \cdot)_{B^{-1}}\) and leads to
\[
((v, w))_{BA} = (BAv, w)_{B^{-1}} = (Av, w) = (v, w)_A.
\]
In fact, the use of the \(B^{-1}\)-inner product was motivated by this observation, i.e., we get the best approximation in the Krylov space in the usual \(A\)-inner product (See the remark below).

The analysis of the preconditioned version is identical to the original CG algorithm except the minimization is over the preconditioned Krylov space,

\[
K_i = K_i(BA, r_0).
\]

We again prove (I.1) and (I.2) by induction. The critical property which makes everything work is that \(BA\) is self adjoint with respect to the \(A\)-inner product so (12.4) is replaced by
\[
(p_k, p_j)_A = (r_k - \beta_{k-1}p_{k-1}, p_j)_A = (e_k, BAp_j)_A - \beta_{k-1}(p_{k-1}, p_j)_A.
\]
This shows that for the preconditioned algorithm,
\[
\|x - x_i\|_A = \min_{\zeta \in K_i(BA, r_0)} \|x - (x_0 - \zeta)\|_A.
\]
Applying the multi-parameter preconditioned theorem of last class then gives the following theorem.

**Theorem 3.** (PCG-error) Let \(A\) and \(B\) be SPD \(n \times n\) matrices and \(e_i\) be the sequence of errors generated by the preconditioned conjugate gradient algorithm. Then,
\[
\|e_i\|_A \leq 2 \left( \frac{\sqrt{K} - 1}{\sqrt{K} + 1} \right)^i \|e_0\|_A.
\]
Here \(K\) is the spectral condition number of \(BA\).

**Remark 1.** Alternative preconditioned conjugate gradient algorithms can be defined. For example, one can use the \(A\)-inner product as a base. The Krylov space remains the same, i.e., \(K_i(BA, r_0)\). The only difference is that the error minimization is with respect to the \(ABA\)-inner product, i.e.
\[
\|x - x_i\|_{ABA} = \min_{\zeta \in K_i(BA, r_0)} \|x - (x_0 - \zeta)\|_{ABA}.
\]
This results in the corresponding error bound
\[
\|e_i\|_{ABA} \leq 2 \left( \frac{\sqrt{K} - 1}{\sqrt{K} + 1} \right)^i \|e_0\|_{ABA}.
\]