Numerical Analysis Comprehensive Exam, Fall 2007

1 (a) $\phi(x) = \frac{1}{2}\|Ax-b\|_2^2 = \frac{1}{2}(Ax-b)^T(Ax-b)$

$$= \frac{1}{2}(x^TA^TAx - x^TA^Tb - b^TAx + b^Tb)$$

$$= \frac{1}{2}(x^TA^TAx - 2b^TAx + b^Tb) \qquad (\text{since } x^TA^Tb = b^TAx)$$

The necessary condition for a minimizer of $\phi(x)$ is $\nabla\phi(x) = 0$: Differentiating $\phi$,

$$0 = \nabla\phi(x) = \frac{1}{2}(2x^TA^TA - 2b^TA) \Rightarrow \boxed{A^TAx = A^Tb} \quad (*)$$

This linear system gives the normal equations for the least squares problem (1). Any solution of (1) must necessarily satisfy the normal equations. Conversely, a solution of $(*)$ satisfies (1).

The linear system $(*)$ is symmetric, positive semidefinite. For smaller systems, it could be efficiently solved using a Cholesky factorization and forward/backward substitution. For large, sparse systems, the method of conjugate gradients could be used. Note that (1) can also be solved without forming the normal equations.

1 (b) The solution of (1) is unique iff A has full column rank. If A is rank deficient, $\exists z \neq 0$ s.t. $Az = 0$, so that if $x$ is a solution of (1), $x+z$ is also a solution. If A has full column rank, the solution of $(*)$ is unique ($A^TA$ is non-singular), and since $(*)$ is a necessary condition, the solution of (1) is unique.

1 (c) (i) $\|Ax-b\|_2^2 = \|U\Sigma V^Tx - b\|_2^2 = \|\Sigma V^Tx - U^Tb\|_2^2$

where the last equality holds because $\|\cdot\|_2$ is invariant under orthogonal transformations. Next,

$$\|\Sigma V^Tx - U^Tb\|_2^2 = \sum_{i=1}^{n}(\sigma_i v_i^Tx - u_i^Tb)^2 + \sum_{i=n+1}^{m}(-u_i^Tb)^2$$

$$= \sum_{i=1}^{r}(\sigma_i v_i^Tx - u_i^Tb)^2 + \sum_{i=r+1}^{m}(-u_i^Tb)^2, \quad \text{using the fact that } \operatorname{rank}(A) = r$$

Thus, in order to minimize the 2-norm of the residual, we must choose $x$ s.t.

$$v_i^Tx = \frac{u_i^Tb}{\sigma_i}, \quad i = 1, \dots, r \quad (**)$$

Since $\{v_k\}_{k=1}^n$ form ~~an~~ orthonormal basis, we have $x = \sum_{k=1}^{n} v_k(v_k^Tx)$. $(**)$ gives the value of $v_k^Tx$ for $k=1,\dots,r$, and to minimize the 2-norm of, we thus choose $v_k^Tx = 0$ for $k = r+1,\dots,n$. Thus $x_{LS}$ is given by

$$x_{LS} = \sum_{k=1}^{n} v_k(v_k^Tx) = \sum_{k=1}^{r} v_k(v_k^Tx)$$

$$\boxed{x_{LS} = \sum_{k=1}^{r} \frac{v_k u_k^Tb}{\sigma_k}}$$

1 (c)(ii) From part (i), we have

$$\| Ax_{LS} - b\|_2^2 = \| \Sigma V^T x_{LS} - U^T b \|_2^2 = \sum_{i=1}^{r} (\sigma_i v_i^T x_{LS} - u_i^T b)^2 + \sum_{i=r+1}^{m} (-u_i^T b)^2$$

$x_{LS}$ is chosen so that the first term in the sum vanishes. The second term does not depend on $x$. Thus

$$\| r \|_2^2 = \| Ax_{LS} - b \|_2^2 = \sum_{i=r+1}^{m} (u_i^T b)^2$$

2 (a) backward Euler

$$\frac{y^{n+1} - y^n}{\Delta t} = \lambda y^{n+1}$$

$$\Rightarrow \quad (1 - \lambda \Delta t) y^{n+1} = y^n$$

$$\Rightarrow \quad y^{n+1} = (1 - \lambda \Delta t)^{-1} y^n$$

(b) trapezoidal rule

$$\frac{y^{n+1} - y^n}{\Delta t} = \frac{1}{2}\lambda y^n + \frac{1}{2}\lambda y^{n+1}$$

$$\Rightarrow \quad y^{n+1} = y^n + \frac{\Delta t}{2}\lambda y^n + \frac{\Delta t}{2}\lambda y^{n+1}$$

$$\Rightarrow \quad \left(1 - \frac{\Delta t}{2}\lambda\right) y^{n+1} = \left(1 + \frac{\Delta t}{2}\lambda\right) y^n$$

$$\Rightarrow \quad y^{n+1} = \left(1 - \frac{\Delta t}{2}\lambda\right)^{-1}\left(1 + \frac{\Delta t}{2}\lambda\right) y^n$$

(c) as $\Delta t \to \infty$, $(1 - \lambda\Delta t)^{-1} \to 0$, so the backward Euler update gives $y^{n+1} \to 0$, i.e., a steady state solution of $0$.
For trapezoidal rule, as $\Delta t \to \infty$, $y^{n+1} \to \dfrac{\Delta t \lambda / 2}{-\Delta t \lambda / 2} y^n = -y^n$, so the solution will oscillate, flipping sign in each iteration.

3 (a) We can rewrite this as a first order system, $\dot{u} = Au$, where

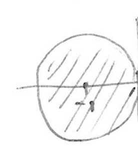
$$u = \begin{pmatrix} x \\ \dot{x} \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{pmatrix}.$$

The eigenvalues of the matrix $A$ are the roots of the characteristic polynomial

$$|A - \lambda I| = \begin{vmatrix} -\lambda & 1 \\ -\frac{k}{m} & -\frac{c}{m} - \lambda \end{vmatrix} = \lambda\left(\lambda + \frac{c}{m}\right) + \frac{k}{m} = \lambda^2 + \frac{c}{m}\lambda + \frac{k}{m}.$$

Using the quadratic formula, these are $\lambda = -\frac{c}{m} \pm \sqrt{\left(\frac{c}{m}\right)^2 - 4\frac{k}{m}}$.

(b) The update rule for forward Euler is $y^{n+1} = (1 + \Delta t \lambda) y^n$, so for absolute stability we require $|1 + \Delta t \lambda| \le 1 \;\; \forall \lambda$, or $|\Delta t \lambda - (-1)| \le 1$, so that $\Delta t \lambda$ lies in the unit circle in the complex plane centered at $-1$.
Thus $\Delta t$ must be chosen so that this holds for all eigenvalues of $A$. Note that $\lambda$ above has nonpositive real part.



(c). For trapezoidal rule to be absolutely stable, we need

$$\frac{\left|1 + \frac{\Delta t}{2}\lambda\right|}{\left|1 - \frac{\Delta t}{2}\lambda\right|} \le 1.$$

Since $\lambda$ has nonpositive real part, this inequality is satisfied. (This can be easily seen as the numerator is the distance of $\frac{\Delta t}{2}\lambda$ to $-1$, and the denominator is the distance of $\frac{\Delta t}{2}\lambda$ to $1$.) Thus trapez. rule is absolutely stable for any choice of $\Delta t$.

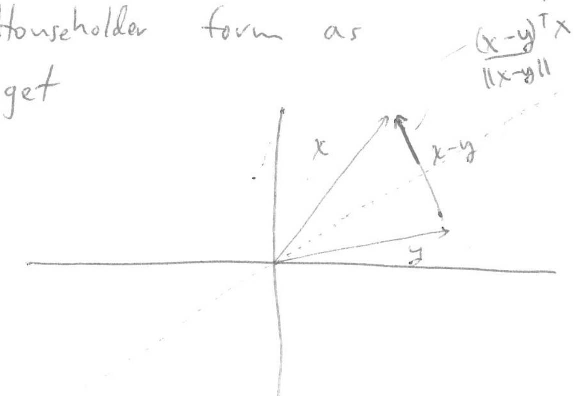
$\boxed{4}$ We require $\sum_{j=1}^{n} u_{ij} z_j = \sum_{j=i}^{n} u_{ij} z_j = 0$ for each $i \in$ ~~0,~~ $1 \cdots n$.

This is satisfied unconditionally for $i = n$ since $u_{nn} = 0$, so set $z_n = 1$. The other components of $z$ can be computed in reverse order via

$$z_i = \frac{-1}{u_{ii}} \sum_{j=i+1}^{n} u_{ij} z_j$$

since $u_{ii} \neq 0$ for $i < n$ and $z_j$, $j > i$ are known when $z_i$ is computed.

$\boxed{5}$ (a) Writing the unknown reflection in Householder form as $A = I - 2uu^T$ for $|u| = 1$, we get




$$Ax = y$$

$$x - 2u(u^T x) = y$$

$$u = \frac{x - y}{2u^T x} \quad (*)$$

Since $|u| = 1$, it suffices to set $u = \frac{x - y}{\|x - y\|}$ unless $x = y$, in which case $u$ can be any vector orthogonal to $x = y$. $(*)$ holds since ~~$2u^T x$~~

$$2u^T x = 2\frac{x^T x - y^T x}{(x^T x - 2y^T x + y^T y)^{1/2}} \overset{\#}{=} \frac{x^T x - 2y^T x + y^T y}{(x^T x - 2y^T x + y^T y)^{1/2}} = \|x - y\|$$

if $\|x\| = \|y\|$.

(b) It suffices to compute $Az$ as

$$Az = (I - 2uu^T)z = z - 2u(u^T z)$$

$$= z - (2u^T z)u$$