Numerical Linear Algebra

Preliminaries

Conditioning and Stability

- Some problems are inherently difficult: no algorithm involving rounding of inputs can be expected to work well. Such problems are called *ill-conditioned*.
- A numerical measure of conditioning, called a *condition number*, can sometimes be defined:
  - Suppose the objective is to compute $y = f(x)$.
  - If x is perturbed by Δx then the result is changed by
    $$\Delta y = f(x+\Delta x) - f(x).$$
  - If
    $$\frac{|\Delta y|}{|y|} \approx \kappa \frac{|\Delta x|}{|x|}$$
    for small perturbations Δx then κ is the *condition number* for the problem of computing $f(x)$.
- A particular algorithm for computing an approximation $\tilde{f}(x)$ to $f(x)$ is *numerically stable* if for small perturbations Δx of the input the result is close to $f(x)$.

Error Analysis

- Analyzing how errors accumulate and propagate through a computation, called *forward error analysis*, is sometimes possible but often very difficult.
- *Backward error analysis* tries to show that the computed result

  $$\tilde{y} = \tilde{f}(x)$$

  is the exact solution to a slightly perturbed problem, i.e.

  $$\tilde{y} = f(\tilde{x})$$

  for some $\tilde{x} \approx x$.
- If
  - the problem of computing $f(x)$ is well conditioned, and
  - the algorithm $\tilde{f}$ is stable,

  then

  $$\begin{aligned} \tilde{y} &= \tilde{f}(x) && \text{computed result} \\ &= f(\tilde{x}) && \text{exact result for some } \tilde{x} \approx x \\ &\approx f(x) && \text{since } f \text{ is well-conditioned} \end{aligned}$$

- Backward error analysis is used heavily in numerical linear algebra.

Solving Linear Systems

Many problems involve solving linear systems of the form

$$Ax = b$$

- least squares normal equations:

$$X^T X\beta = X^T y$$

- stationary distribution of a Markov chain:

$$\begin{aligned} \pi P &= \pi \\ \sum \pi_i &= 1 \end{aligned}$$

If A is $n \times n$ and non-singular then in principle the solution is

$$x = A^{-1}b$$

This is not usually a good numerical approach because

- it can be numerically inaccurate;
- it is inefficient except for very small n.

Triangular Systems

- Triangular systems are easy to solve.
- The upper triangular system

$$\begin{bmatrix} 5 & 3 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 16 \\ 4 \end{bmatrix}$$

  has solution

$$\begin{aligned} x_2 &= 4/2 = 2 \\ x_1 &= (16 - 3x_2)/5 = 10/5 = 2 \end{aligned}$$

- This is called *back substitution*
- Lower triangular systems are solved by *forward substitution*.
- If one of the diagonal elements in a triangular matrix is zero, then the matrix is singular.
- If one of the diagonal elements in a triangular matrix is close to zero, then the solution is very sensitive to other inputs:

$$\begin{bmatrix} 1 & a \\ 0 & \varepsilon \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

  has solution

$$\begin{aligned} x_2 &= \frac{b_2}{\varepsilon} \\ x_1 &= b_1 - a\frac{b_2}{\varepsilon} \end{aligned}$$

- This sensitivity for small ε is inherent in the problem: For small values of ε the problem of finding the solution x is ill-conditioned.

Gaussian Elimination

- The system
$$\begin{bmatrix} 5 & 3 \\ 10 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 16 \\ 36 \end{bmatrix}$$
can be reduced to triangular form by subtracting two times the first equation from the second.

- In matrix form:
$$\begin{bmatrix} 1 & 0 \\ -2 & 1 \end{bmatrix} \begin{bmatrix} 5 & 3 \\ 10 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -2 & 1 \end{bmatrix} \begin{bmatrix} 16 \\ 36 \end{bmatrix}$$
or
$$\begin{bmatrix} 5 & 3 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 16 \\ 4 \end{bmatrix}$$
which is the previous triangular system.

- For a general 2×2 matrix A the lower triangular matrix used for the reduction is
$$\begin{bmatrix} 1 & 0 \\ -\frac{a_{21}}{a_{11}} & 1 \end{bmatrix}$$

- The ratio $\frac{a_{21}}{a_{11}}$ is a called a *multiplier*.

- This strategy works as long as $a_{11} \neq 0$.

- If $a_{11} \approx 0$, say
$$A = \begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix}$$
for small ε, then the multiplier $1/\varepsilon$ is large and this does not work very well, even though A is very well behaved.

- Using this approach would result in a numerically unstable algorithm for a well-conditioned problem.

Partial Pivoting

- We can ensure that the multiplier is less than or equal to one in magnitude by switching rows before eliminating:

$$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}5 & 3\\10 & 8\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}16\\36\end{bmatrix}$$

or

$$\begin{bmatrix}10 & 8\\5 & 3\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=\begin{bmatrix}36\\16\end{bmatrix}$$

- The matrix to reduce this system to triangular form is now

$$\begin{bmatrix}1 & 0\\-0.5 & 1\end{bmatrix}$$

- So the final triangular system is constructed as

$$\begin{bmatrix}1 & 0\\-0.5 & 1\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}5 & 3\\10 & 8\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=\begin{bmatrix}1 & 0\\-0.5 & 1\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}16\\36\end{bmatrix}$$

or

$$\begin{bmatrix}10 & 8\\0 & -1\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=\begin{bmatrix}36\\-2\end{bmatrix}$$

- Equivalently, we can think of our original system as

$$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\0.5 & 1\end{bmatrix}\begin{bmatrix}10 & 8\\0 & -1\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=\begin{bmatrix}16\\36\end{bmatrix}$$

- The decomposition of A as

$$A = PLU$$

with P a permutation matrix, L lower trianbular with ones on the diagonal, and U upper triangular is called a *PLU decomposition*.

PLU Decomposition

- In general, we can write a square matrix A as

  $$A = PLU$$

  where

  - P is a *permutation matrix*, i.e.
    - it is an identity matrix with some rows switched
    - it satisfies $PP^T = P^T P = I$, i.e. it is an *orthogonal matrix*
  - L is a *unit lower triangular matrix*, i.e.
    - it is lower triangular
    - it has ones on the diagonal
  - U is upper triangular
- The permutation matrix P can be chosen so that the multipliers used in forming L all have magnitude at most one.
- A is non-singular if and only if the diagonal entries in U are all non-zero.
- If A is non-singular, then we can solve

  $$Ax = b$$

  in three steps:

  1. Solve $Pz = b$ for $z = P^T b$ (permute the right hand side)
  2. Solve $Ly = z$ for y (forward solve lower triangular system)
  3. Solve $Ux = y$ for x (back solve upper triangular system)
- Computational complexity:
  - Computing the PLU decomposition takes $O(n^3)$ operations.
  - Computing a solution from a PLU decomposition takes $O(n^2)$ operations.

Condition Number

- Linear systems $Ax = b$ have unique solutions if A is non-singular.
- Solutions are sensitive to small perturbations if A is close to singular.
- We need a useful measure of closeness to singularity
- The *condition number* is a useful measure:

$$\begin{aligned}\kappa(A) &= \frac{\max_{x\neq 0}\frac{\|Ax\|}{\|x\|}}{\min_{x\neq 0}\frac{\|Ax\|}{\|x\|}}\\ &= \left(\max_{x\neq 0}\frac{\|Ax\|}{\|x\|}\right)\left(\max_{x\neq 0}\frac{\|A^{-1}x\|}{\|x\|}\right)\\ &= \|A\|\|A^{-1}\|\end{aligned}$$

  where $\|y\|$ is a *vector norm* (i.e. a measure of length) of y and

$$\|B\| = \max_{x\neq 0}\frac{\|Bx\|}{\|x\|}$$

  is the corresponding *matrix norm* of B.

- Some common vector norms:

$$\|x\|_2 = \sqrt{\sum_{i=1}^n x_i^2} \qquad \text{Euclidean norm}$$

$$\|x\|_1 = \sum_{i=1}^n |x_i| \qquad L_1 \text{ norm, Manhattan norm}$$

$$\|x\|_\infty = \max_i |x_i| \qquad L_\infty \text{ norm}$$

Some Properties of Condition Numbers

- $\kappa(A) \geq 1$ for all A.
- $\kappa(A) = \infty$ if A is singular
- If A is diagonal, then
$$\kappa(A) = \frac{\max |a_{ii}|}{\min |a_{ii}|}$$
- Different norms produce different values; the values are usually qualitatively similar

Sensitivity of Linear Systems

Suppose x solves the original system and x^* solves a slightly perturbed system,

$$(A + \Delta A)x^* = b + \Delta b$$

and suppose that

$$\begin{aligned} \delta\kappa(A) &\leq \frac{1}{2} \\ \frac{\|\Delta A\|}{\|A\|} &\leq \delta \\ \frac{\|\Delta b\|}{\|b\|} &\leq \delta \end{aligned}$$

Then

$$\frac{\|x - x^*\|}{\|x\|} \leq 4\delta\kappa(A)$$

Stability of Gaussian Elimination with Partial Pivoting

Backward error analysis: The numerical solution $\hat{x}$ to the system

$$Ax = b$$

produced by Gaussian elimination with partial pivoting is the exact solution for a perturbed system

$$(A + \Delta A)\hat{x} = b$$

with

$$\frac{\|\Delta A\|_\infty}{\|A\|_\infty} \leq 8n^3 \rho \mathbf{u} + O(\mathbf{u}^2)$$

- The value of ρ is not *guaranteed* to be small, but is rarely larger than 10
- The algorithm would be considered numerically stable if ρ were guaranteed to be bounded.
- *Complete pivoting* is a bit more stable, but much more work.
- The algorithm is considered very good for practical purposes.

General Linear Systems in R

R provides

- `solve` for general systems, based on LAPACK's DGESV.
- DGESV uses the *PLU* decomposition.
- `forwardsolve`, `backsolve` for triangular systems.
- `kappa` computes an estimate of the condition number or the exact condition number based on the Euclidean norm.

Cholesky Factorization

Suppose A is symmetric and (strictly) positive definite, i.e.

$$x^T Ax > 0$$

for all $x \neq 0$. Examples:

- If X is the $n \times p$ design matrix for a linear model and X is of rank p, then $A = X^T X$ is strictly positive definite.

  If X is not of full rank then $A = X^T X$ is non-negative definite or positive semi-definite, i.e. $x^T Ax \geq 0$ for all x.

- If A is the covariance matrix of a random vector X then A is positive semidefinite:

  $$\begin{aligned} c^T Ac &= c^T E[(X-\mu)(X-\mu)^T]c \\ &= E[((X-\mu)^T c)^T (X-\mu)^T c] \\ &= \mathrm{Var}((X-\mu)^T c) \geq 0 \end{aligned}$$

  The covariance matrix is strictly positive definite unless $P(c^T X = c^T \mu) = 1$ for some $c \neq 0$, i.e. unless there is a perfect linear relation between some of the components of X.

Theorem

If A is strictly positive definite, then there exists a unique lower triangular matrix L with positive diagonal entries such that

$$A = LL^T$$

This is called the *Cholesky factorization*.

Properties of the Cholesky Factorization Algorithm

- It uses the symmetry to produce an efficient algorithm.
- The algorithm needs to take square roots to find the diagonal entries.
- An alternative that avoids square roots factors A as

  $$A = LDL^T$$

  with D diagonal and L unit lower triangular.
- The algorithm is numerically stable, and is guaranteed not to attempt square roots of negative numbers if

  $$q_n \mathbf{u} \kappa_2(A) \leq 1$$

  where q_n is a small constant depending on the dimension n.
- The algorithm will fail if the matrix is not (numerically) strictly positive definite.
- Modifications using pivoting are available that can be used for nonnegative definite matrices.
- Another option is to factor $A_\lambda = A + \lambda I$ with $\lambda > 0$ chosen large enough to make A_λ numerically strictly positive definite. This is often used in optimization.

Some Applications of the Cholesky Factorization

- Solving the normal equations in least squares. This requires that the predictors be linearly independent
- Generating multivariate normal random vectors.
- Parameterizing strictly positive definite matrices: Any lower triangular matrix L with arbitrary values below the diagonal and positive diagonal entries determines and is uniquely determined by the positive definite matrix $A = LL^T$

Cholesky Factorization in R

- The function `chol` computes the Cholesky factorization.
- The returned value is the upper triangular matrix $R = L^T$.
- LAPACK is used.

QR Factorization

An $m \times n$ matrix A with $m \geq n$ can be written as

$$A = QR$$

where

- Q is $m \times n$ with orthonormal columns, i.e. $Q^T Q = I_n$
- R is upper triangular
- Several algorithms are available for computing the QR decomposition:
  - Modified Gram-Schmidt
  - Householder transformations (reflections)
  - Givens transformations (rotations)

  Each has advantages and disadvantages.
- LINPACK `dqrdc` and LAPACK `DGEQP3` use Householder transformations.
- The QR decomposition exists regardless of the rank of A.
- The rank of A is n if and only if the diagonal elements of R are all nonzero.

Householder Transformations

- A Householder transformation is a matrix of the form

$$P = I - 2vv^T/v^Tv$$

  where v is a nonzero vector.

- Px is the reflection of x in the hyperplane orthogonal to v.

- Given a vector $x \neq 0$, choosing $v = x + \alpha e_1$ with

$$\alpha = \pm\|x\|_2$$

  and e_1 the first unit vector (first column of the identity) produces

$$Px = \mp\|x\|_2 e_1$$

  This can be used to zero all but the first element of the first column of a matrix:

$$P\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} = \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}$$

  This is the first step in computing the QR factorization.

- The denominator v^Tv can be written as

$$v^Tv = x^Tx + 2\alpha x_1 + \alpha^2$$

- Choosing $\alpha = \text{sign}(x_1)\|x\|_2$ ensures that all terms are non-negative and avoids cancellation.

- With the right choice of sign Householder transformations are very stable.

Givens Rotations

- A Givens rotation is a matrix G that is equal to the identity except for elements $G_{ii}, G_{ij}, G_{ji}, G_{jj}$, which are

  $$\begin{bmatrix} G_{ii} & G_{ij} \\ G_{ji} & G_{jj} \end{bmatrix} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$$

  with $c = \cos(\theta)$ and $s = \sin(\theta)$ for some θ.

- Premultiplication by G^T is a clockwise rotation by θ radians in the (i, j) coordinate plane.

- Given scalars a, b one can compute c, s so that

  $$\begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

  This allows G to zero one element while changing only one other element.

- A stable way to choose c, s:

```
if $b = 0$
    $c = 1$; $s = 0$
else
    if $|b| > |a|$
        $\tau = -a/b$; $s = 1/\sqrt{1+\tau^2}$; $c = s\tau$
    else
        $\tau = -b/a$; $c = 1/\sqrt{1+\tau^2}$; $s = c\tau$
    end
end
```

- A sequence of Givens rotations can be used to compute the QR factorization.
  - The zeroing can be done working down columns or across rows.
  - Working across rows is useful for incrementally adding more observations.

Applications

- The QR decomposition can be used for solving $n \times n$ systems of equations
$$Ax = b$$
since $Q^{-1} = Q^T$ and so
$$Ax = QRx = b$$
is equivalent to the upper triangular system
$$Rx = Q^T b$$
- The QR decomposition can also be used to solve the normal equations in linear regression: If X is the $n \times p$ design matrix then the normal equations are
$$X^T Xb = X^T y$$
If $X = QR$ is the QR decomposition of X, then
$$\begin{aligned} X^T X &= R^T Q^T QR = R^T R \\ X^T y &= R^T Q^T y \end{aligned}$$
If X is of full rank then R^T is invertible, and the normal equations are equivalent to the upper triangular system
$$Rb = Q^T y$$
This approach avoids computing $X^T X$.
- If X is of full rank then $R^T R$ is the Cholesky factorization of $X^T X$ (up to multiplications of rows of R by ± 1).

QR with Column Pivoting

Sometimes the columns of X are linearly dependent or nearly so.

By permuting columns we can produce a factorization
$$A = QRP$$
where

- P is a permutation matrix
- R is upper triangular and the diagonal elements of R have non-increasing magnitudes, i.e.

  $$|r_{ii}| \geq |r_{jj}|$$

  if $i \leq j$
- If some of the diagonal entries of R are zero, then R will be of the form

  $$R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix}$$

  where R_{11} is upper triangular with non-zero diagonal elements non-increasing in magnitude.
- The rank of the matrix is the number of non-zero rows in R.
- The *numerical rank* of a matrix can be determined by
  - computing its QR factorization with column pivoting
  - specifying a tolerance level ε such that all diagonal entries $|r_{ii}| < \varepsilon$ are considered numerically zero.
  - Modifying the computed QR factorization to zero all rows corresponding to numerically zero r_{ii} values.

Some Regression Diagnostics

The projection matrix, or hat matrix, is

$$H = X(X^T X)^{-1} X^T = QR(R^T R)^{-1} R^T Q^T = QQ^T$$

The diagonal elements of the hat matrix are therefore

$$h_i = \sum_{j=1}^{p} q_{ij}^2$$

If $\hat{e}_i = y_i - \hat{y}_i$ is the residual, then

$$\begin{aligned}
s_{-i}^2 &= \frac{\text{SSE} - \hat{e}_i^2/(1-h_i)}{n-p-1} = \text{ estimate of variance without obs. } i \\
t_i &= \frac{\hat{e}_i}{s_{-i}\sqrt{1-h_i}} = \text{externally studentized residual} \\
D_i &= \frac{\hat{e}_i^2 h_i}{(1-h_i)^2 s^2 p} = \text{Cook's distance}
\end{aligned}$$

QR Decomposition and Least Squares in R

- The R function `qr` uses either LINPACK or LAPACK to compute QR factorizations.
- LINPACK is the default.
- The core linear model fitting function `lm.fit` uses QR factorization with column pivoting.

Singular Value Decomposition

An $m \times n$ matrix A with $m \geq n$ can be factored as

$$A = UDV^T$$

where

- U is $m \times n$ with orthonormal columns, i.e. $U^TU = I_n$.
- V is $n \times n$ orthogonal, i.e. $VV^T = V^TV = I_n$.
- $D = \text{diag}(d_1, \ldots, d_n)$ is $n \times n$ diagonal with $d_1 \geq d_2 \geq \cdots \geq d_n \geq 0$.

This is the *singular value decomposition*, or *SVD* of A.

- The values $d_1, \ldots, d_n$ are the *singular values* of A.
- The columns of U are the *right singular vectors* of A.
- The columns of V are the *left singular vectors* of A.
- If the columns of A have been centered so the column sums of A are zero, then the columns of UD are the *principal components* of A.
- Excellent algorithms are available for computing the SVD.
- These algorithms are usually several times slower than the QR algorithms.

Some Properties of the SVD

- The Euclidean matrix norm of A is defined as
$$\|A\|_2 = \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}$$
with $\|x\|_2 = \sqrt{x^T x}$ the Euclidean vector norm.
- If A has SVD $A = UDV^T$, then
$$\|A\|_2 = d_1$$
- If $k < \text{rank}(A)$ and
$$A_k = \sum_{i=1}^{k} d_i u_i v_i^T$$
then
$$\min_{B:\text{rank}(B) \leq k} \|A - B\|_2 = \|A - A_k\| = d_{k+1}$$
In particular,
  - $d_1 u_1 v_1^T$ is the best rank one approximation to A (in the Euclidean matrix norm).
  - A_k is the best rank k approximation to A.
  - If $m = n$ then $d_n = \min\{d_1, \ldots . d_n\}$ is the distance between A and the set of singular matrices.
- If A is square then the condition number based on the Euclidean norm is
$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|_2 = \frac{d_1}{d_n}$$
- For an $n \times p$ matrix with $n > p$ we also have
$$\kappa_2(A) = \frac{\max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}}{\min_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}} = \frac{d_1}{d_n}$$
  - This can be used to relate $\kappa_2(A^T A)$ to $\kappa_2(A)$.
  - This has implications for regression computations.
- The singular values are the non-negative square roots of the eigenvalues of $A^T A$ and the columns of V are the corresponding eigenvectors.

Moore-Penrose Generalized Inverse

Suppose A has rank $r \leq n$ and SVD $A = UDV^T$. Then

$$d_{r+1} = \cdots = d_n = 0$$

Let

$$D^+ = \text{diag}\left(\frac{1}{d_1}, \ldots, \frac{1}{d_r}, 0, \ldots, 0\right)$$

and

$$A^+ = VD^+U^T$$

Then A^+ satisfies

$$\begin{aligned} AA^+A &= A \\ A^+AA^+ &= A^+ \\ (AA^+)^T &= AA^+ \\ (A^+A)^T &= A^+A \end{aligned}$$

A^+ is the unique matrix with these properties and is called the Moore-Penrose *generalized inverse* or *pseudo-inverse*.

SVD and Least Squares

If X is an $n \times p$ design matrix of less than full rank, then there are infinitely many values of b that minimize

$$\|y - Xb\|_2^2$$

Among these solutions,

$$b = (X^T X)^+ X^T y$$

minimizes $\|b\|_2$.

This is related to *penalized regression* where one might choose b to minimize

$$\|y - Xb\|_2^2 + \lambda \|b\|_2^2$$

for some choice of $\lambda > 0$.

SVD and Principal Components Analysis

- Let X be an $n \times p$ matrix of n observations on p variables.
- Principal components analysis involves estimating the eigenvectors and eigenvalues of the covariance matrix.
- Let $\widetilde{X}$ be the data matrix with columns centered at zero by subtracting the column means.
- The sample covariance matrix is

$$S = \frac{1}{n-1}\widetilde{X}^T\widetilde{X}$$

- Let $\widetilde{X} = UDV^T$ be the SVD of the centered data matrix $\widetilde{X}$.
- Then

$$S = \frac{1}{n-1}VDU^TUDV^T = \frac{1}{n-1}VD^2V^T$$

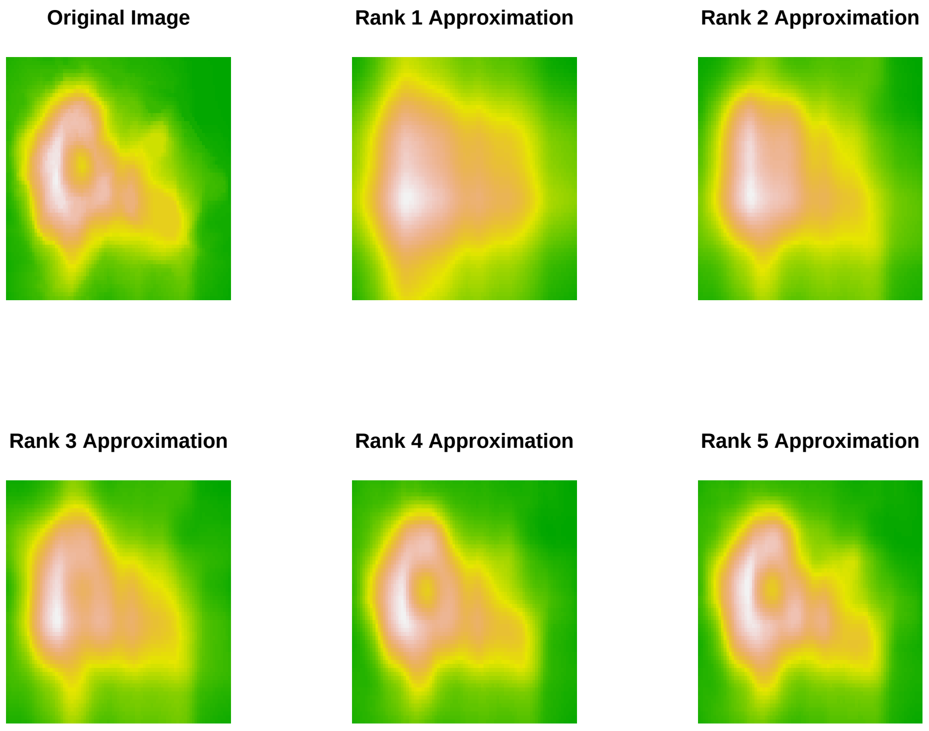
- So
  - The diagonal elements of $\frac{1}{n-1}D^2$ are the eigenvalues of S.
  - The columns of V are the eigenvectors of S.
- Using the SVD of $\widetilde{X}$ is more numerically stable than
  - forming $\widetilde{X}^T\widetilde{X}$
  - computing the eigenvalues and eigenvectors.

SVD and Numerical Rank

- The rank of a matrix A is equal to the number of non-zero singular values.
- Exact zeros may not occur in the SVD due to rounding.
- Numerical rank determination can be based on the SVD. All $d_i \leq \delta$ can be set to zero for some choice of δ. Golub and van Loan recommend using
$$\delta = \mathbf{u}\|A\|_\infty$$
- If the entries of A are only accurate to d decimal digits, then Golub and van Loan recommend
$$\delta = 10^{-d}\|A\|_\infty$$
- If the numerical rank of A is $\hat{r}$ and $d_{\hat{r}} \gg \delta$ then $\hat{r}$ can be used with some confidence; otherwise caution is needed.

Other Applications

- The SVD is used in many areas of numerical analysis.
- It is also often useful as a theoretical tool.
- Some approaches to compressing $m \times n$ images are based on the SVD.
- A simple example using the `volcano` data:



```
s$d
 [1] 9644.2878216  488.6099163  341.1835791  298.7660207  141.8336254
 [6]   72.1244275   43.5569839   33.5231852   27.3837593   19.9762196
 ...
[61]    0.9545092
```

SVD in R

- R provides the function `svd` to compute the SVD.
- Implementation used to use LINPACK but now can use LINPACK or LAPACK, with LAPACK the default.
- You can ask for the singular values only—this is will be faster for larger problems.

Eigenvalues and Eigenvectors

Let A be an $n \times n$ matrix. λ is an *eigenvalue* of A if

$$Av = \lambda v$$

for some $v \neq 0$; v is an *eigenvector* or A.

- If A is a real $n \times n$ matrix then it has n eigenvalues.
  - Several eigenvalues may be identical
  - Some eigenvalues may be complex; if so, then they come in conjugate pairs.
  - The set of eigenvalues is called the *spectrum*
- If A is symmetric then the eigenvalues are real
- If A is symmetric then
  - A is strictly positive definite if and only if all eigenvalues are positive.
  - A is positive semi-definite if and only if all eigenvalues are non-negative.
  - There exists an orthogonal matrix V such that
    $$A = V \Lambda V^T$$
    with $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$; the columns of V are the corresponding normalized eigenvectors.
  - This is called the *spectral decomposition* of A.
- Some problems require only the largest eigenvalue or the largest few, sometimes the corresponding eigenvectors are also needed.
  - The stationary distribution of an irreducible finite state-space Markov chain is the unique eigenvector, normalized to sum to one, corresponding to the largest eigenvalue $\lambda = 1$.
  - The speed of convergence to the stationary distribution depends on the magnitude of the second largest eigenvalue.
- The R function `eigen` can be used to compute eigenvalues and, optionally, eigenvectors.

Determinants

- Theoretically the determinant can be computed as the product of
  - the diagonals of U in the PLU decomposition
  - the squares of the diagonals of L in the Cholesky factorization
  - the diagonals of R in the QR decomposition
  - the eigenvalues
- Numerically these are almost always bad ideas.
- It is almost always better to work out the sign and compute the sum of the logarithms of the magnitudes of the factors.
- The R functions `det` and `determinant` compute the determinant.
  - `determinant` is more complicated to use, but has a `logarithm` option.
- Likelihood and Bayesian analyses often involve a determinant;
  - usually the log likelihood and log determinant should be used.
  - usually the log determinant can be computed from a decomposition needed elsewhere in the log likelihood calculation, e.g. a Cholesky factorization

Non-Negative Matrix Factorization

A number of problems lead to the desire to approximate a non-negative matrix X by a product

$$X \approx WH$$

where W, H are non-negative matricies of low rank, i.e. with few columns.

There are a number of algorithms available, most of the form

$$\min_{W,H}[D(X,WH)+R(W,H)]$$

where D is a loss function and R is a possible penalty for encouraging desirable characteristics of W, H, such as smoothness or sparseness.

The R package `NMF` provides one approach, and a vignette in the package provides some background and references.

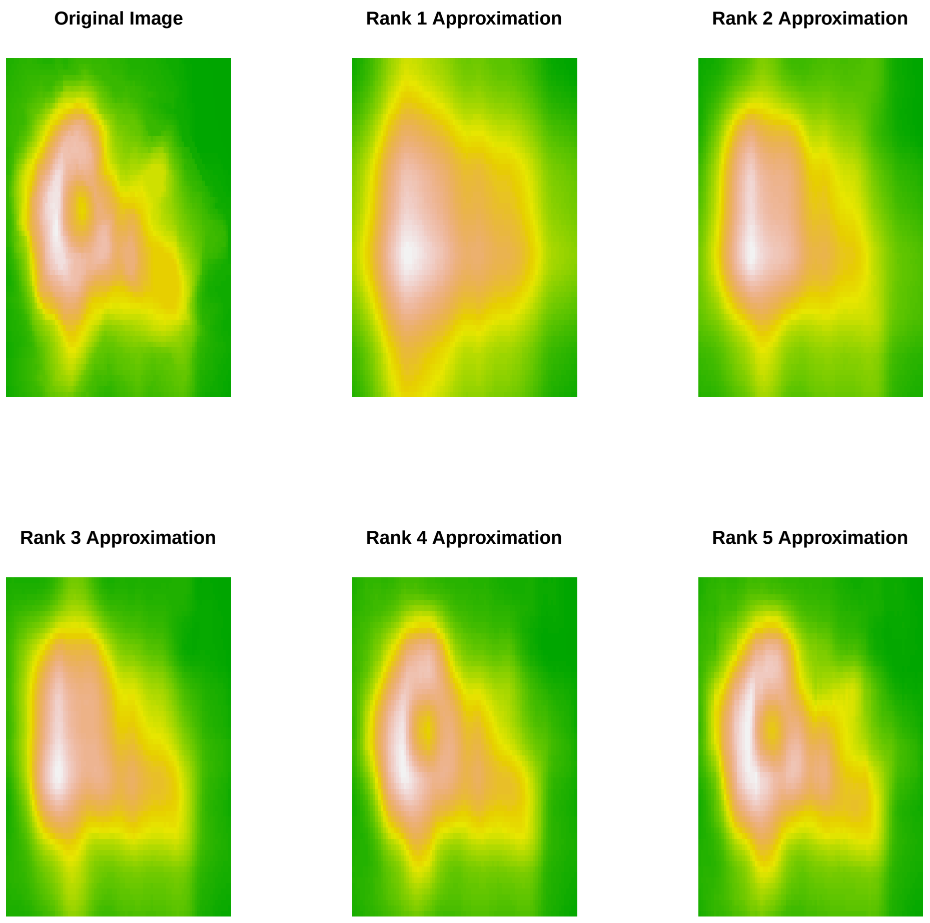
As an example, using default settings in the NMF package the `volcano` image can be approximated with factorizations of rank $1,\dots,5$ by

```
library(NMF)
nmf1 = nmf(volcano, 1); V1 <- nmf1@fit@W %*% nmf1@fit@H
nmf2 = nmf(volcano, 2); V2 <- nmf2@fit@W %*% nmf2@fit@H
nmf3 = nmf(volcano, 3); V3 <- nmf3@fit@W %*% nmf3@fit@H
nmf4 = nmf(volcano, 4); V4 <- nmf4@fit@W %*% nmf4@fit@H
nmf5 = nmf(volcano, 5); V5 <- nmf5@fit@W %*% nmf5@fit@H
```

The relative error for the final image is

```
> max(abs(volcano - V5)) / max(abs(volcano))
[1] 0.03273659
```

The images:



Another application is *recommender systems*.

- For example, X might be ratings of movies (columns) by viewers (rows).
- The set of actual values would be very sparse as each viewer will typically rate only a small subset of all movies.
- W would be a user preference matrix, H a corresponding movie feature matrix.
- The product WH would provide predicted ratings for movies the users have not yet seen.

Other Factorizations

Many other factorizations of matrices are available and being developed. Some examples are

- Robust variants of the SVD
- Sparse variants, e.g. Dan Yang, Zongming Ma, and Andreas Buja (2014), "A Sparse Singular Value Decomposition Method for High-Dimensional Data," Journal of Computational and Graphical Statistics 23(4), 923–942.
- Constrained factorizations, e.g. C. Ding, T. Li, and M. I. Jordan (2010), "Convex and Semi-Nonnegative Matrix Factorizations," IEEE Transactions on Pattern Analysis and Machine Intelligence, 32(1), 45–55.

Exploiting Special Structure

Specialized algorithms can sometimes be used for matrices with special structure.

Toeplitz Systems

- Stationary time series have covariance matrices that look like

$$\begin{bmatrix} \sigma_0 & \sigma_1 & \sigma_2 & \sigma_3 & \dots \\ \sigma_1 & \sigma_0 & \sigma_1 & \sigma_2 & \dots \\ \sigma_2 & \sigma_1 & \sigma_0 & \sigma_1 & \dots \\ \sigma_3 & \sigma_2 & \sigma_1 & \sigma_0 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

- This is a *Toeplitz* matrix.
- This matrix is also symmetric — this is not required for a Toeplitz matrix.
- Special algorithms requiring $O(n^2)$ operations are available for Toeplitz systems.
- General Cholesky factorization requires $O(n^3)$ operations.
- The R function `toeplitz` creates Toeplitz matrices.

Circulant Systems

- Some problems give rise to matrices that look like

$$C_n = \begin{bmatrix} a_1 & a_2 & a_3 & \dots & a_n \\ a_n & a_1 & a_2 & \dots & a_{n-1} \\ a_{n-1} & a_n & a_1 & \dots & a_{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_2 & a_3 & a_4 & \dots & a_1 \end{bmatrix}$$

- This is a *circulant* matrix, a subclass of Toeplitz matrices.
- Circulant matrices satisfy

$$C_n = F_n^* \operatorname{diag}(\sqrt{n} F_n a) F_n$$

where F_n is the *Fourier matrix* with

$$F_n(j,k) = \frac{1}{\sqrt{n}} e^{-(j-1)(k-1)2\pi\sqrt{-1}/n}$$

and F_n^* is the *conjugate transpose*, *Hermitian transpose*, or *adjoint matrix* of F_n.

- The eigen values are the elements of $\sqrt{n} F_n a$.
- Products $F_n x$ and $F_n^* x$ can be computed with the *fast Fourier transform (FFT).*
- In R

$$\begin{aligned} \sqrt{n} F_n x &= \texttt{fft(x)} \\ \sqrt{n} F_n^* x &= \texttt{fft(x, inverse = TRUE)} \end{aligned}$$

- These computations are generally $O(n \log n)$ in complexity.
- Circulant systems can be used to approximate other systems.
- Multi-dimensional analogs exist as well.
- A simple example is available on line.

Sparse Systems

- Many problems lead to large systems in which only a small fraction of coefficients are non-zero.
- Some methods are available for general sparse systems.
- Specialized methods are available for structured sparse systems such as
  - tri-diagonal systems
  - block diagonal systems
  - banded systems
- Careful choice of row and column permutations can often turn general sparse systems into banded ones.

Sparse and Structured Systems in R

- Sparse matrix support in R is improving.
- Some packages, like `nlme`, provide utilities they need.
- One basic package available on CRAN is `sparseM`
- A more extensive package is `Matrix`
- `Matrix` is the engine for mixed effects/multi-level model fitting in `lme4`

Update Formulas

- Update formulas are available for most decompositions that allow for efficient adding or dropping of rows or columns.
- These can be useful for example in cross-validation and variable selection computations.
- They can also be useful for fitting linear models to very large data sets; the package `biglm` uses this approach.
- I am not aware of any convenient implementations in R at this point but they may exist.

Iterative Methods

- Iterative methods can be useful in large, sparse problems.
- Iterative methods for sparse problems can also often be parallelized effectively.
- Iterative methods are also useful when
  - Ax can be computed efficiently for any given x
  - It is expensive or impossible to compute A explicitly

Gauss-Seidel Iteration

Choose an initial solution $x^{(0)}$ to

$$Ax = b$$

and then update from $x^{(k)}$ to $x^{(k+1)}$ by

$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k)}\right)$$

for $i = 1, \ldots, n$.

This is similar in spirit to Gibbs sampling.

This can be written in matrix form as

$$x^{(k+1)} = (D+L)^{-1}(-Ux^{(k)}+b)$$

with

$$\begin{aligned}
L &= \begin{bmatrix} 0 & 0 & \dots & \dots & 0 \\ a_{21} & 0 & \dots & & \vdots \\ a_{31} & a_{32} & \ddots & & 0 \\ \vdots & & & 0 & 0 \\ a_{n1} & a_{n2} & \dots & a_{n,n-1} & 0 \end{bmatrix} \\
D &= \operatorname{diag}(a_{11},\dots,a_{nn}) \\
U &= \begin{bmatrix} 0 & a_{12} & \dots & \dots & a_{1n} \\ 0 & 0 & \dots & & \vdots \\ 0 & 0 & \ddots & & a_{n-2,n} \\ \vdots & & & & a_{n-1,n} \\ 0 & 0 & \dots & 0 & 0 \end{bmatrix}
\end{aligned}$$

Splitting Methods

The Gauss-Seidel method is a member of a class of *splitting methods* where

$$Mx^{(k+1)} = Nx^{(k)} + b$$

with $A = M - N$.

For the Gauss-Seidel method

$$\begin{aligned} M &= D + L \\ N &= -U. \end{aligned}$$

Other members include Jacobi iterations with

$$\begin{aligned} M_J &= D \\ N_J &= -(L + U) \end{aligned}$$

Splitting methods are practical if solving linear systems with matrix M is easy.

Convergence

A splitting method for a non-singular matrix A will converge to the unique solution of $Ax = b$ if

$$\rho(M^{-1}N) < 1$$

where

$$\rho(G) = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } G\}$$

is the *spectral radius* of G.

This is true, for example, for the Gauss-Seidel method if A is strictly positive definite.

Convergence can be very slow if $\rho(M^{-1}N)$ is close to one.

Successive Over-Relaxation

A variation is to define

$$x_i^{(k+1)} = \frac{\omega}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k)}\right) + (1-\omega)x_i^{(k)}$$

or, in matrix form,

$$M_\omega x^{(k+1)} = N_\omega x^{(k)} + \omega b$$

with

$$\begin{aligned} M_\omega &= D + \omega L \\ N_\omega &= (1-\omega)D - \omega U \end{aligned}$$

for some ω, usually with $0 < \omega < 1$.

- This is called *successive over-relaxation (SOR)*, from its first application in a structural engineering problem.
- For some choices of ω we can have

  $$\rho(M_\omega^{-1}N_\omega) \ll \rho(M^{-1}N)$$

  and thus faster convergence.
- For some special but important problems the value of ω that minimizes $\rho(M_\omega^{-1}N_\omega)$ is known or can be computed.

Conjugate Gradient Method

If A is symmetric and strictly positive definite then the unique solution to $Ax = b$ is the unique minimizer of the quadratic function

$$f(x) = \frac{1}{2}x^T Ax - x^T b$$

Any nonlinear or quadratic optimization method can be used to find the minimum; the most common one used in this context is the conjugate gradient method.

Choose an initial x_0, set $d_0 = -g_0 = b - Ax_0$, and then, while $g_k \neq 0$, for $k = 0, 1, \ldots$ compute

$$\begin{aligned}
\alpha_k &= -\frac{g_k^T d_k}{d_k^T A d_k}\\
x_{k+1} &= x_k + \alpha_k d_k\\
g_{k+1} &= Ax_{k+1} - b\\
\beta_{k+1} &= \frac{g_{k+1}^T A d_k}{d_k^T A d_k}\\
d_{k+1} &= -g_{k+1} + \beta_{k+1} d_k
\end{aligned}$$

Some properties:

- An alternate form of g_{k+1} is

  $$g_{k+1} = g_k + \alpha_k A d_k$$

  This means only one matrix-vector multiplication is needed per iteration.
- The vector g_k is the gradient of f at x_k.
- The initial direction $d_0 = -g_0$ is the *direction of steepest descent* from x_0
- The directions $d_0, d_1, \ldots$ are A-*conjugate*, i.e. $d_i^T A d_j = 0$ for $i \neq j$.
- The directions $d_0, d_1, \ldots, d_{n-1}$ are linearly independent.

Convergence

- With exact arithmetic,
$$Ax_n = b$$
That is, the conjugate gradient algorithm terminates with the exact solution in n steps.
- Numerically this does not happen.
- Numerically, the directions will not be exactly A-conjugate.
- A convergence tolerance is used for termination; this can be based on the relative change in the solution
$$\frac{\|x_{k+1} - x_k\|}{\|x_k\|}$$
or the residual or gradient
$$g_k = Ax_k - b$$
or some combination; an iteration count limit is also a good idea.
- If the algorithm does not terminate within n steps it is a good idea to restart it with a steepest descent step from the current x_k.
- In many sparse and structured problems the algorithm will terminate in far fewer than n steps for reasonable tolerances.
- Convergence is faster if the condition number of A is closer to one. The error can be bounded as
$$\|x - x_k\|_A \le 2\|x - x_0\|_A \left(\frac{\sqrt{\kappa_2(A)} - 1}{\sqrt{\kappa_2(A)} + 1}\right)^k$$
with $\|x\|_A = \sqrt{x^T Ax}$.
- *Preconditioning* strategies can improve convergence; these transform the original problem to one with $\tilde{A} = C^{-1}AC^{-1}$ for some symmetric strictly positive definite C, and then use the conjugate gradient method for $\tilde{A}$
- Simple choices of C are most useful; sometimes a diagonal matrix will do.
- Good preconditioners can sometimes be designed for specific problems.

A Simple Implementation

```
cg <- function(A, b, x, done) {
    dot <- function(x, y) crossprod(x, y)[1]

    n <- 0
    g <- A(x) - b
    d <- -g

    repeat {
        h <- A(d)
        u <- dot(d, h)
        a <- -dot(g, d) / u

        n <- n + 1
        x.old <- x
        x <- x + a * d
        g <- g + a * h

        b <- dot(h, g) / u
        d <- -g + b * d
        if (done(g, x, x.old, n))
            return(list(x = as.vector(x),
                        g = as.vector(g),
                        n = n))
    }
}
```

- The linear transformation and the termination condition are specified as functions.
- The termination condition can use a combination of the gradient, current solution, previous solution, or iteration count.
- A simple example:

```
> X <- crossprod(matrix(rnorm(25), 5))
> y <- rnorm(5)
> cg(function(x) X %*% x, y, rep(0, 5), function(g, x, x.old, n) n >= 5)
$x
[1] 11.461061 -7.774344  1.067511 87.276967 -8.151556

$g
[1] -9.219292e-13  2.566836e-13 -1.104117e-12  1.690870e-13  1.150191e-13

$n
[1] 5

> solve(X, y)
[1] 11.461061 -7.774344  1.067511 87.276967 -8.151556
```

Linear Algebra Software

Some Standard Packages

Open source packages developed at national laboratories:

- LINPACK for linear equations and least squares
- EISPACK for eigenvalue problems
- LAPACK newer package for linear equations and eigenvalues

Designed for high performance. Available from Netlib at

```
http://www.netlib.org/
```

Commercial packages:

- IMSL used more in US
- NAG used more in UK
- ...

BLAS: Basic Linear Algebra Subroutines

Modern BLAS has three levels:

Level 1: Vector and vector/vector operations such as

- dot product $x^T y$
- scalar multiply and add (axpy): $\alpha x + y$
- Givens rotations

Level 2: Matrix/vector operations, such as Ax

Level 3: Matrix/matrix operations, such as AB

- LINPACK uses only Level 1; LAPACK uses all three levels.
- BLAS defines the interface.
- Standard reference implementations are available from Netlib.
- Highly optimized versions are available from hardware vendors and research organizations.

Cholesky Factorization in LAPACK

The core of the DPOTRF routine:

```
*
*        Compute the Cholesky factorization A = L*L'.
*
         DO 20 J = 1, N
*
*           Compute L(J,J) and test for non-positive-definiteness.
*
            AJJ = A( J, J ) - DDOT( J-1, A( J, 1 ), LDA, A( J, 1 ),
     $            LDA )
            IF( AJJ.LE.ZERO ) THEN
               A( J, J ) = AJJ
               GO TO 30
            END IF
            AJJ = SQRT( AJJ )
            A( J, J ) = AJJ
*
*           Compute elements J+1:N of column J.
*
            IF( J.LT.N ) THEN
               CALL DGEMV( 'No transpose', N-J, J-1, -ONE, A( J+1, 1 ),
     $                     LDA, A( J, 1 ), LDA, ONE, A( J+1, J ), 1 )
               CALL DSCAL( N-J, ONE / AJJ, A( J+1, J ), 1 )
            END IF
   20    CONTINUE
```

- DDOT and DSCAL are Level 1 BLAS routines
- DGEMV is a Level 2 BLAS routine

ATLAS: Automatically Tuned Linear Algebra Software

Available at

`http://math-atlas.sourceforge.net/`

- Analyzes machine for properties such as cache characteristics.
- Runs extensive tests to determine performance trade-offs.
- Creates Fortran and C versions of BLAS and some LAPACK routines tailored to the particular machine.
- Provides some routines that take advantage of multiple processors using *worker threads*.

OpenBLAS

- Another high-performance BLAS library was developed and maintained by Kazushige Goto.
- This is now being developed and maintained as the OpenBLAS project, available from

  `http://xianyi.github.com/OpenBLAS/`

- Also provides versions that take advantage of multiple processors.

Vendor Libraries

- Intel provides the Math Kernel Libraries (MKL)
- AMD has a similar library.

Using a High-Performance BLAS with R

- R comes with a basic default BLAS.
- R can be built to use a specified BLAS.
- Once built one can change the BLAS R uses by replacing the shared library R uses.
- Some simple computations using the default and MKL vendor BLAS for the data

  ```
  N <- 1000
  X <- matrix(rnorm(N^2), N)
  XX <- crossprod(X)
  ```

  Results:

Timing Expression	Default/ Reference	MKL SEQ	MKL THR
`system.time(for (i in 1:5) crossprod(X))`	2.107	0.405	0.145
`system.time(for (i in 1:5) X %*% X)`	3.401	0.742	0.237
`system.time(svd(X))`	3.273	0.990	0.542
`system.time(for (i in 1:5) qr(X))`	2.290	1.094	1.107
`system.time(for (i in 1:5) qr(X, LAPACK=TRUE))`	2.629	0.834	0.689
`system.time(for (i in 1:20) chol(XX))`	2.824	0.556	0.186

- These results are based on the non-threaded and threaded Intel Math Kernel Library (MKL) using the development version of R.
- Versions of the current R using MKL for BLAS are available as

  ```
  /group/statsoft/R-patched/build-MKL-seq/bin/R
  /group/statsoft/R-patched/build-MKL-thr/bin/R
  ```

- Currently the standard version of R on our Linux systems seems to be using OpenBLAS with multi-threading disabled.

Final Notes

- Most reasonable approaches will be accurate for reasonable problems.
- Choosing good scaling and centering can make problems more reasonable (both numerically and statistically)
- Most methods are efficient enough for our purposes.
- In some problems worrying about efficiency is important if reasonable problem sizes are to be handled.
- Making sure you are using the right approach to the right problem is much more important than efficiency.
- Some quotes:
  - D. E. Knuth, restating a comment by C. A. R. Hoare:

    > We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil.

  - W. A. Wulf:

    > More computing sins are committed in the name of efficiency (without necessarily achieving it) than for any other single reason — including blind stupidity.