數値分析

Chapter 6

Direct Methods for Solving Linear Systems

6.2 Gauss elimination

- Gauss elimination (forward elimination + backward substitution) P.238 Example 1.

- Gauss-Jordan elimination (forward elimination + backward substitution) P.243 Example 3.

- computational efficiency $O(n^3)$. P.245 Table 6.1

6.3 Pivoting Strategies

- P.249 Example 1

  The linear system

  E_1: $0.003000x_1 + 59.14x_2 = 59.17$

  E_2: $5.291x_1 - 6.13x_2 = 46.78$

  算出 $x_1 \approx -10$

  but x_1 真值爲 10

  (問題出在 0.003 相對於 59.14 太小)

  (Pivoting element 太小, 會放大 round off error)

- P.250 Example 2

  maximal column pivoting: 在第 i 個 column 中, 選最大的來當 pivot element.

- 但若將 $E_1 \times 10^4$

  $\Rightarrow$ E_1: $30.00x_1 + 591400x_2 = 591700$

  E_2: $5.291x_1 - 6.13x_2 = 46.78$

  則還是會選 30 當 pivot element, 依然會得到有誤差之解.

- P.252 Example 3 and 4

  scaled partial pivoting: 在第 k row (即第 k 個 equation) 中, 選係數最大的, 然後用此係數來 normalize 此 equation, normalize 後再從第 i 個 column 中, 選最大的來當 pivot element.

  (此法所增加之計算量 $O(n^2) <$ 原本之 $O(n^3)$ 之計算量 $\Rightarrow$ 並未增加 computational time)

- maximal (or full) pivoting: 由剩下的 square matrix 中, 選最大的 element 來當 pivoting element.

  (最強, 但會須 $O(n^3)$, 意即可能增加原來數倍之時間)

6.4 Linear Algebra and Matrix Inversion

- 矩陣之加減乘除

- If A^{-1} exists $\Rightarrow$ A is nonsingular or invertible.

- $A^{-1}A = I$ (Identity matrix)

- 解 $Ax = b$, 可以解 A^{-1}, 則 $x = A^{-1}b$. (但算 A^{-1}, 比解 $Ax = b$ 難)

- <u>Transpose Facts</u>

  (a) $(A^t)^t = A$

  (b) $(A + B)^t = A^t + B^t$

  (c) $(AB)^t = B^tA^t$

  (d) If A^{-1} exists, $(A^{-1})^t = (A^t)^{-1}$

- Determinant
  $\det A = \sum_{j=1}^{n} (-1)^{i+j} a_{ij} M_{ij}$ for $i = 1, 2, \ldots, n$ (by row)
  or
  $\det A = \sum_{i=1}^{n} (-1)^{i+j} a_{ij} M_{ij}$ for $j = 1, 2, \ldots, n$ (by column)

- Determinant Facts
  (a) 有一行 or 列爲 0, det = 0
  (b) 行 or 列互換, det 差一負號
  (c) 有二列 or 行相同, det = 0
  (d) 有一行 or 列 $\times\lambda \Rightarrow \det \rightarrow \det \lambda$
  (e) 作 linear system 之運算, det 不變
  (f) $\det A_{n\times n} B_{n\times n} = \det A_{n\times n} \det B_{n\times n}$
  (g) $\det A^t = \det A$
  (h) if A^{-1} exists, $\det A^{-1} = \frac{1}{\det A}$
  (i) if A 是 upper triangular, lower triangular, or diagonal matrix, $\det A = \Pi a_{ii}$

- <u>Equivalent Statements about $n \times n$ Matrix A</u>
  (a) The equation $Ax = 0$ has the unique solution $x = 0$
  (b) The system $Ax = b$ has a unique solution for any n-dimensional column vector b
  (c) The matrix A is nonsingular; that is, A^{-1} exists
  (d) $\det A \neq 0$
  (e) Gaussian elimination with row interchanges can be performed on the system $Ax = b$ for any n-dimensional column vector b

6.5 Matrix Factorization

$Ax = b$

如果 $A = LU$

$\Rightarrow LUx = b$

Let $y = Ux$

$\Rightarrow Ly = b$ (先解 y, 再解 x)

- $A = LU$ (並非唯一決定)

  (i) $l_{11}u_{11} = a_{11}$ (決定 l_{11} 與 u_{11})

  (ii) $l_{j1} = \frac{a_{j1}}{u_{11}}$ and $u_{1j} = \frac{a_{1j}}{l_{11}}$ (決定 L 之第一列, U 之第一行)

  (iii) $l_{ii}u_{ii} = a_{ii} - \sum_{k=1}^{i-1} l_{ik}u_{ki}$ (決定 l_{ii} 與 u_{ii})

  (iv) $l_{ji} = \frac{1}{u_{ii}}[a_{ji} - \sum_{k=1}^{i-1} l_{jk}u_{ki}]$ and $u_{ij} = \frac{1}{l_{ii}}[a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj}]$

  (決定 L 之第 i 列, U 之第 i 行)

  (v) $l_{nn}u_{nn} = a_{nn} - \sum_{k=1}^{n-1} l_{nk}u_{kn}$

  P.272 Example 3

  If $LU = LL^t = A$

  $\Rightarrow$ Cholesky's decomposition P.277, P.278 Example 2.

  Permutation Matrix: precisely one entry whose valus is 1 in each column and row and all of whose other entries are 0

  (前乘是 row 互換, 後乘是 column 互換)

  P.272 Example 2.

- 矩陣微分

  $\frac{\partial Ax}{\partial x} = A$

  $\frac{\partial x'Ax}{\partial x} = (A + A')x$

  $\frac{\partial x'Ax}{\partial A} = x'x$ (if all elements of A is different)

$\frac{\partial ln|A|}{\partial A} = (A^{-1})'$
$Y = X\beta + \varepsilon$
$\frac{\partial (Y-X\beta)'(Y-X\beta)}{\partial \beta} = \frac{\partial (Y'Y-Y'X\beta-\beta'X'Y+\beta'X'X\beta)}{\partial \beta}$
$0 = 0 - X'Y - X'Y + 2X'X\beta \Rightarrow 2X'Y = 2X'X\beta$
$\Rightarrow \beta = (X'X)^{-1}X'Y$

- multi-variable function (用矩陣表達微分)
  $f(x_1, \ldots, x_n)$
  $\Rightarrow \frac{\partial f}{\partial X} = [\ ]_{n\times 1}$
  $\frac{\partial f}{\partial X \partial X'} = [\ ]_{n\times n}$

  $f_1(x_1, ..., x_n)$
  $f_2(x_1, ..., x_n)$
  $\vdots$
  $f_m(x_1, ..., x_n)$
  $\Rightarrow \frac{\partial f}{\partial X} = [\ ]_{n\times m}$

  $f([A]_{n\times k})$, 亦即 $f(a_{11}, a_{12}, \ldots, a_{nk})$
  $\Rightarrow \frac{\partial f}{\partial A} = [\ ]_{n\times k}$

6.6 Techniques for Special Matrices

- A matrix A is positive definite matrix if it's symmetric and if $x'Ax > 0$ for any $x \neq 0$

- If A is positive definite matrix $\Rightarrow$
  (a) A is nonsigular
  (b) $a_{ii} > 0$
  (c) 最大的 element 一定出現在 diagonal elements 之中

(d) $(a_{ij})^2 < a_{ii}a_{jj}$

- Positive Definite matrix equivalence

  (a) A is positive definite

  (b) 因 $a_{ii} > 0$, 所以 Gaussian elimination 可不用作 row interchange

  (c) A can be factored in the form LL', where L is lower triangular with posive diagonal entries

  (d) A can be factored in the form LDL', where L is lower triangular with 1s on its diagonal and D is a diagonal matrix with diagonal entries

  (e) 所有 submatrix 之 determinant > 0

- Tridiagonal Matrix (Cubic Spline)

  先做 LU, 再解 linear system, 速度快很多.

  P.279 $\sim$ P.281

  P.281 Example 3

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	Advantages	Disadvantages
Gauss elimination	最基本	
Gauss-Jordan elimination	可用來算 inverse	比 Gauss elimination 稍微沒效率
LU decomposition	efficient if 只換常數項 b	如果只用一次 此法顯得比較笨
singular value decomposition		