Computing the Rank and Nullspace of Rectangular Sparse Matrices

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To model biochemical networks, systems biologists are generating increasingly large *stoichiometric matrices* S, whose rows and columns correspond to chemical species and chemical reactions. An important step toward evaluating drug targets and analyzing transient behavior of the network is called *conservation analysis*, which reduces to finding the rank of S and the nullspace of S^T. SVD is not practical, but with care, sparse QR or sparse LU factors can serve both purposes.

On some large authentic examples, the sparse QR package of Davis [1, 2] has proved remarkably efficient (with Q stored in sparse product form). However, the QR factors are sometimes significantly less sparse than S.

As an alternative, we consider the threshold rook pivoting option in LUSOL [3, 4]. With suitable permutations, this finds factors $S = LDU$ in which L and U have unit diagonals and bounded off-diagonals and are likely to be well-conditioned, so that D should reliably indicate rank(S).

We find that LUSOL's LDU factors of S can be significantly more sparse than QR, but also significantly more expensive to compute. We therefore study two alternatives. Starting with conventional threshold partial pivoting factors $S = LU$ (with L well-conditioned),

- apply threshold rook pivoting to U,
- or apply threshold partial pivoting to U^T.

We evaluate the options using a new Matlab interface to LUSOL [5].

[1] T. A. Davis. SuiteSparseQR: multithreaded multifrontal sparse QR factorization, `http://www.cise.ufl.edu/research/sparse/SPQR/`

[2] T. A. Davis. SuiteSparseQR: Algorithm 9xx: SuiteSparseQR, a multifrontal multithreaded sparse QR factorization package, submitted to *ACM TOMS*

[3] P. E. Gill, W. Murray, M. A. Saunders. SNOPT: An SQP algorithm for large-scale constrained optimization, *SIAM Rev* 47(1), 99–131 (2005)

[4] P. E. Gill, W. Murray, M. A. Saunders, M. H. Wright. Maintaining LU factors of a general sparse matrix, *Linear Alg Appl* 88/89, 239–270 (1987)

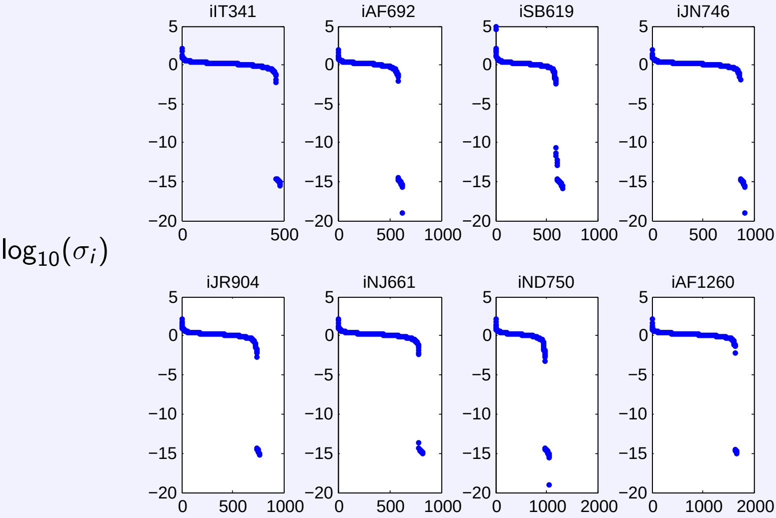
[5] N. W. Henderson. Matlab interface to LUSOL, `https://github.com/nwh/lusol`

rank(S) by SVD

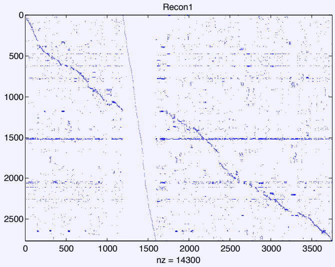
$$\boxed{\text{Singular value decomposition} \qquad S = UDV^T}$$

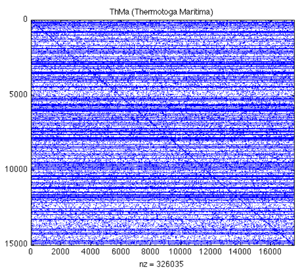
- $U^TU = I \qquad V^TV = I \qquad D$ diagonal $\qquad \text{rank}(S) = \text{rank}(D)$
- Ideal for rank-estimation but U, V are dense
- model 9 (Recon1) $\quad 2800 \times 3700 \quad$ 17 secs
  model 10 (ThMa) $\quad 15000 \times 18000 \quad$ 11 hours
  model 11 (GlcAer) $\quad 62000 \times 77000 \quad \infty$

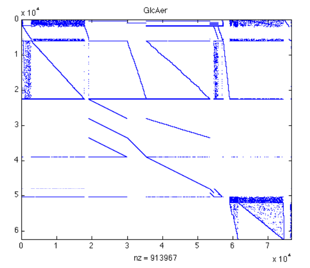
Singular values of models 1–8   Dense SVD of S^T



S for models 9, 10, 11







2800×3700 15000×18000 62000×77000

rank(S) by QR

$\boxed{\text{Householder QR factorization} \qquad SP = QR}$

- $P =$ col perm $\quad Q^TQ = I \quad R$ triangular
  rank(S) = rank(R)
- Nearly as reliable as SVD
- Dense QR used by Vallabhajosyula, Chickarmane, Sauro (2005)
- Sparse QR (SPQR) now available: Davis (2013)
- model 9 (Recon1) 2800×3700 0.1 secs
  model 10 (ThMa) 15000×18000 2.5 secs
  model 11 (GlcAer) 62000×77000 0.2 secs(!)

rank(S) by LUSOL with Threshold Rook Pivoting

$$\boxed{\text{Sparse LU with TRP} \qquad P_1 S P_2 = LDU}$$

- $P_1, P_2 =$ perms D diagonal $\text{rank}(S) \approx \text{rank}(D)$
  L, U well-conditioned
- $L_{ii} = U_{ii} = 1$
  $|L_{ij}|$ **and** $|U_{ij}| \le$ `factol` $= 4$ (or 2 or 1.2, 1.1, ...)
- LUSOL: Main engine in sparse linear/nonlinear optimizers
  MINOS, SQOPT, SNOPT
model 9 (Recon1)	2800×3700	0.1 secs
model 10 (ThMa)	15000×18000	4.0 secs
model 11 (GlcAer)	62000×77000	158 secs

rank(S) by LUSOL with Threshold Partial Pivoting

$$\boxed{\text{Sparse LU with TPP} \qquad P_1 S P_2 = LU}$$

- P_1, P_2 = perms U trapezoidal $\text{rank}(S) \approx \text{rank}(U)$
  L well-conditioned
- $L_{ii} = 1$
  $|L_{ij}| \le \texttt{factol} = 4$ (or 2 or 1.2, 1.1, ...)
- LUSOL: Main engine in sparse linear/nonlinear optimizers
  MINOS, SQOPT, SNOPT
- model 9 (Recon1) 2800×3700 0.1 secs
  model 10 (ThMa) 15000×18000 0.2 secs
  model 11 (GlcAer) 62000×77000 0.3 secs

SPQR vs LUSOL with Threshold Rook Pivoting

SPQR: $S = QR$

model	m	n	rank(S)	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	2766	3742	2674	14300	2750	21093	17.5	0.1
ThMa	15024	17582	14983	326035	844096	10595016	11hrs	2.5
GlcAer	62212	76664	62182	913967	1287	916600	infty	0.2

LUSOL: $S = LDU \qquad |L_{ij}|, |U_{ij}| \le 2.0$

model	nnz(L)	nnz(U)	time
Recon1	4280	16463	0.1
ThMa	30962	346122	4.1
GlcAer	635571	1810491	186.2

LUSOL: $S = LDU \qquad |L_{ij}|, |U_{ij}| \le 4.0$

model	nnz(L)	nnz(U)	time
Recon1	2701	12896	0.1
ThMa	36350	330485	4.0
GlcAer	427456	1584188	157.9

SPQR vs LUSOL with Threshold Rook Pivoting

SPQR: $S^T = QR$

model	m	n	rank(S')	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	3742	2766	2674	14300	107935	36929	17.2	0.1
ThMa	17582	15024	14983	326035	624640	605888	11hrs	0.7
GlcAer	76664	62212	62182	913967	3573696	4038988	infty	2.7

LUSOL: $S^T = LDU \qquad |L_{ij}|, |U_{ij}| \leq 2.0$

model	nnz(L)	nnz(U)	time
Recon1	12832	7421	0.3
ThMa	501198	358601	37.8
GlcAer	1996892	709448	586.0

LUSOL: $S^T = LDU \qquad |L_{ij}|, |U_{ij}| \leq 4.0$

model	nnz(L)	nnz(U)	time
Recon1	9811	6093	0.2
ThMa	410290	355475	14.8
GlcAer	1823067	711906	791.2

SPQR vs LUSOL with Threshold Partial Pivoting

SPQR: $S = QR$

model	m	n	rank(S)	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	2766	3742	2674	14300	2750	21093	17.5	0.1
ThMa	15024	17582	14983	326035	844096	10595016	11hrs	2.5
GlcAer	62212	76664	62182	913967	1287	916600	infty	0.2

LUSOL: $S = LU \qquad |L_{ij}|, |U_{ij}| \leq 2.0$

model	nnz(L)	nnz(U)	time
Recon1	721	13585	0.1
ThMa	7779	324483	0.2
GlcAer	533	913781	0.4

LUSOL: $S = LU \qquad |L_{ij}|, |U_{ij}| \leq 4.0$

model	nnz(L)	nnz(U)	time
Recon1	764	13577	0.1
ThMa	7782	323929	0.2
GlcAer	533	913781	0.4

SPQR vs LUSOL with Threshold Partial Pivoting

SPQR: $S^T = QR$

model	m	n	rank(S')	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	3742	2766	2674	14300	107935	36929	17.2	0.1
ThMa	17582	15024	14983	326035	624640	605888	11hrs	0.7
GlcAer	76664	62212	62182	913967	3573696	4038988	infty	2.7

LUSOL: $S^T = LU$ $|L_{ij}| \le 2.0$

model	nnz(L)	nnz(U)	time
Recon1	9304	7813	0.2
ThMa	81506	268938	2.7
GlcAer	337433	703619	126.7

LUSOL: $S^T = LU$ $|L_{ij}| \le 4.0$

model	nnz(L)	nnz(U)	time
Recon1	9030	6259	0.1
ThMa	77274	268424	2.0
GlcAer	316889	701139	176.5

Rank of Rectangular Sparse A

Matrix color code: well-conditioned ill-conditioned

SVD	$A = UDV^T$	too dense
QR with col perms	$A = QR$	SuiteSparseQR
QR + QR on R^T	$A = QR = QLP$	insurance
partial pivoting? beware	$A = \begin{pmatrix} \delta & x & x & x \\ & \delta & x & x \\ & & \delta & x \\ & & & \delta \end{pmatrix} = LU$	
rook pivoting	$A = LDU$	LUSOL
partial pivoting	$A = LU$	often ok
pp + rp on U	$A = LU = L\bar{L}\bar{D}\bar{U}$	safer
pp + pp on U^T	$A = LU = L\bar{U}^T\bar{L}^T$	safer + cheaper

LUSOL with TPP then TRP on U

model	m	n	rank(S)	nnz(S)	nnz(Q)	nnz(R)	SVD	SPQR
Recon1	2766	3742	2674	14300	2750	21093	17.5	0.1
ThMa	15024	17582	14983	326035	844096	10595016	11hrs	2.5
GlcAer	62212	76664	62182	913967	1287	916600	infty	0.2

Scaled $S = LU \quad |L_{ij}| \le 2.0$ then $U = \bar{L}\bar{D}\bar{U} \quad |\bar{L}_{ij}|, |\bar{U}_{ij}| \le 2.0$

	nnz(L)	nnz(U)	time
Recon1	712	13598	0.0
	89	13550	0.0
ThMa	4043	327461	1.2
	36298	355276	6.8
GlcAer	534	913883	2.6
	404044	1414563	152.5

The same for scaled S^T

	nnz(L)	nnz(U)	time
Recon1	9797	4612	0.1
	53	4562	0.0
ThMa	130976	218256	1.8
	218144	67419	2.2
GlcAer	820879	307625	39.8
	121717	342990	25.6

LUSOL with TPP then TPP on U^T

model	m	n	rank(S)	nnz(S)	nnz(Q)	nnz(R)	SVD	SPQR
Recon1	2766	3742	2674	14300	2750	21093	17.5	0.1
ThMa	15024	17582	14983	326035	844096	10595016	11hrs	2.5
GlcAer	62212	76664	62182	913967	1287	916600	infty	0.2

Scaled $S = LU$ $\quad |L_{ij}| \le 2.0$ $\quad$ then $\quad U^T = \bar{L}\bar{U}$ $\quad |\bar{L}_{ij}| \le 2.0$

	nnz(L)	nnz(U)	time
Recon1	712	13598	0.0
	9789	3885	0.0
ThMa	4043	327461	1.2
	132658	218914	1.8
GlcAer	534	913883	2.6
	809860	341586	41.8

The same for scaled S^T

Recon1	9797	4612	0.1
	686	3908	0.0
ThMa	130976	218256	1.8
	15746	213081	0.6
GlcAer	820879	307625	39.7
	1630	306306	1.0

Conclusions

Sparse rank-revealing factorizations:

- SuiteSparseQR on A or A^T often best
- LUSOL usually more sparse
  Important if used as null space operator
- Threshold rook pivoting reliable (LU version of SVD)
  but can be slow
- Threshold partial pivoting reliable for stoichiometric S or S^T
- General A might needs safeguards:
  - $A = LU = L\bar{L}\bar{D}\bar{U}$
  - $A = LU = L\bar{U}^T\bar{L}^T$