On solving mixed sparse-dense linear least-squares problems Part I: A Schur complement approach

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An aside ...

- With the exception of 2002 and 2014, I have attended all the *Sparse Days at CERFACS* meetings between 2001–2017 and, apart from 2006, I have given a talk each time.
- I also attended and presented at each of the wonderful St. Girons Conferences (1994, 2003, 2015).
- So 16 meetings ... not sure how many can equal or beat this (apart from Iain!)?
- HUGE thank you to Iain for all the great opportunities these meetings have offered.

Introduction

Least squares are used across a wide range of disciplines:

- simple curve fitting
- estimation of satellite image sensor characteristics
- powering internet mapping services
- exploration seismology
- NMR spectroscopy
- ultrasound for medical imaging
- aerospace systems
- neural networks
- data assimilation for weather forecasting and climate modelling

Introduction

Linear least squares (LS) arises on its own and as subproblem of nonlinear least squares problem.
Solve

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \|Ax - b\|_2,$$

where $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ is large and sparse and $b \in \mathbb{R}^m$.

Focus today on A having small number of "dense" rows.

The LS solution x satisfies the $n \times n$ *normal equations*

$$Cx = A^T b, \qquad C = A^T A.$$

If A is full rank, C is positive definite so use sparse Cholesky solver eg CHOLMOD (Davis), or `HSL_MA87` (Hogg, Reid and Scott) to compute factorization

$$C = LL^T,$$

where L is lower triangular.

Solve $Lz = A^T b$ then $L^T x = z$.

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Solve $Lz = A^T b$ then $L^T x = z$.

Or use sparse QR factorization eg SPQR (Davis) or qr_mumps (Buttari et al).

Now suppose

$$A = \begin{pmatrix} A_s \\ A_d \end{pmatrix}$$

where $A_s \in \mathbb{R}^{m_s \times n}$ is sparse but rows of $A_d \in \mathbb{R}^{m_d \times n}$ are dense ($m_s \gg m_d$). Then

$$C = \begin{pmatrix} A_s^T & A_d^T \end{pmatrix} \begin{pmatrix} A_s \\ A_d \end{pmatrix} = A_s^T A_s + A_d^T Ad$$

And so C is dense and sparse Cholesky or QR cannot be used.

This talk: A Schur complement approach

Next talk: A preconditioned conjugate gradient method

A Schur complement approach

$$\min_x \left\| \begin{pmatrix} A_s \\ A_d \end{pmatrix} x - \begin{pmatrix} b_s \\ b_d \end{pmatrix} \right\|_2 .$$

This is equivalent to solving the order $m + n$ augmented system

$$\begin{pmatrix} I & & A_s \\ & I & A_d \\ A_s^T & A_d^T & 0 \end{pmatrix} \begin{pmatrix} r_s \\ r_d \\ x \end{pmatrix} = \begin{pmatrix} b_s \\ b_d \\ 0 \end{pmatrix},$$

where r is the residual vector

$$r = \begin{pmatrix} r_s \\ r_d \end{pmatrix} = \begin{pmatrix} b_s \\ b_d \end{pmatrix} - \begin{pmatrix} A_s \\ A_d \end{pmatrix} x.$$

Important: We assume throughout that A has been scaled by normalising each column by its 2-norm so that $|a_{ii}| = 1$ and $|a_{ij}| \leq 1$.

Eliminate first m_s rows and columns to obtain the reduced augmented system of order $(m_d + n) \times (m_d + n)$

$$K \begin{pmatrix} x \\ r_d \end{pmatrix} = \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix}, \qquad K = \begin{pmatrix} -C_s & A_d^T \\ A_d & I \end{pmatrix}.$$

$C_s = A_s^T A_s$ is the reduced normal matrix.

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Compute Cholesky factorization $C_s = L_s L_s^T$. Then

$$K = \begin{pmatrix} L_s & \\ B_d & I \end{pmatrix} \begin{pmatrix} -I & \\ & S_d \end{pmatrix} \begin{pmatrix} L_s^T & B_d^T \\ & I \end{pmatrix},$$

where B_d and the Schur complement S_d are given by

$$L_s B_d^T = -A_d^T \quad \text{and} \quad S_d = I + B_d B_d^T.$$

Solve $L_s B_d^T = -A_d^T$ by forward substitution.

Then compute $S_d = I + B_d B_d^T$ using dense linear algebra.

Then solve the reduced augmented system by solving

$$\begin{pmatrix} -L_s & \\ -B_d & S_d \end{pmatrix} \begin{pmatrix} y_s \\ y_d \end{pmatrix} = \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix},$$

followed by

$$\begin{pmatrix} L_s^T & B_d^T \\ & I \end{pmatrix} \begin{pmatrix} x \\ r_d \end{pmatrix} = \begin{pmatrix} y_s \\ y_d \end{pmatrix}.$$

This reduces to solving

$$\begin{aligned} L_s y_s &= A_s^T b_s, \\ S_d r_d &= b_d + B_d y_s, \\ L_s^T x &= y_s - B_d^T r_d. \end{aligned}$$

Thus dominant costs are

- sparse factorization of $m_s \times m_s$ matrix
- triangular solves
- (small) dense Cholesky factorization.

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Thus dominant costs are

- sparse factorization of $m_s \times m_s$ matrix
- triangular solves
- (small) dense Cholesky factorization.

What about using an iterative solver in place of a direct solver?

Preconditioning the Schur complement approach

Right-preconditioned reduced augmented system is

$$KM^{-1}\begin{pmatrix} w_s \\ w_d \end{pmatrix} = \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix}, \qquad M\begin{pmatrix} x \\ r_d \end{pmatrix} = \begin{pmatrix} w_s \\ w_d \end{pmatrix},$$

where M is the chosen preconditioner.

Let $C_s \approx \tilde{L}_s \tilde{L}_s^T$ be an incomplete Cholesky factorization.

Then set

$$M = \begin{pmatrix} \tilde{L}_s & \\ \tilde{B}_d & I \end{pmatrix} \begin{pmatrix} -I & \\ & \tilde{S}_d \end{pmatrix} \begin{pmatrix} \tilde{L}_s^T & \tilde{B}_d^T \\ & I \end{pmatrix},$$

where

$$\tilde{L}_s \tilde{B}_d^T = -A_d^T \quad \text{and} \quad \tilde{S}_d = I + \tilde{B}_d \tilde{B}_d^T.$$

We will refer to M as the block IC preconditioner.

Application of block IC preconditioner M

Input: $\tilde{L}_s$, $\tilde{B}_d$, the Cholesky factors of $\tilde{S}_d$, and $z = \begin{pmatrix} z_s \\ z_d \end{pmatrix}$.

Output: $y = \begin{pmatrix} y_s \\ y_d \end{pmatrix} = M^{-1} z$.

1. Solve $\tilde{L}_s u_s = -z_s$.
2. Compute $u_d = z_d + \tilde{B}_d u_s$.
3. Solve $\tilde{S}_d y_d = u_d$ using Cholesky factors of $\tilde{S}_d$.
4. Form $u_s \Leftarrow u_s - \tilde{B}_d^T y_d$.
5. Solve $\tilde{L}_s^T y_s = u_s$.

Problem of null columns

When A is partitioned into sparse and dense parts, A_s often contains some null columns.

In this case, $C_s = A_s^T A_s$ is rank deficient and Cholesky factorization breaks down.

How to deal with this?

$$A = \begin{pmatrix} A_1 & A_2 \end{pmatrix} \equiv \begin{pmatrix} A_{s_1} & 0 \\ A_{d_1} & A_{d_2} \end{pmatrix}$$

with $A_1 \in \mathbb{R}^{m \times n_1}$ and $A_2 \in \mathbb{R}^{m \times n_2}$ $(n = n_1 + n_2,\ n_2 \ll n_1)$.

Lemma (Scott and Tůma '17)

Let $z \in \mathbb{R}^{n_1}$ and $W \in \mathbb{R}^{n_1 \times n_2}$ be the solutions to

$$\min_z \|A_1 z - b\|_2 \quad \text{and} \quad \min_W \|A_1 W - A_2\|_F .$$

Then the solution of the original LS problem is

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} z - W x_2 \\ x_2 \end{pmatrix}$$

with

$$x_2 = (A_2^T (A_2 - A_1 W))^{-1} A_2^T (b - A_1 z).$$

Notes

Once we have solved $min_z \|A_1 z - b\|_2$, what is the extra work in solving $min_W \|A_1 W - A_2\|_F$?
Recall

$$\begin{aligned} L_{s1} y_s &= A_s^T b_s, \\ S_d r_d &= b_d + B_d y_s, \\ L_{s1}^T z &= y_s - B_d^T r_d. \end{aligned}$$

The columns of A_2 are $\begin{pmatrix} 0 \\ a_2 \end{pmatrix}$ and so, for each, solve

$$\begin{aligned} S_d r_d &= a_2, \\ L_{s1}^T w &= B_d^T r_d. \end{aligned}$$

Provided n_2 not large, this is cheap for a direct solver (solve simultaneously for all m_d cols).

With null columns removed, A_{s1} can still be rank deficient.

Propose employing a shift $\alpha > 0$

$$C_{s1}(\alpha) = A_{s1}^T A_{s1} + \alpha I = L_{s1}(\alpha) L_{s1}(\alpha)^T.$$

so that

$$C_{s1} \approx L_{s1}(\alpha) L_{s1}(\alpha)^T.$$

Employ the factor $L_{s1}(\alpha)$ to obtain a preconditioner to solve the original problem (hybrid method that combines a direct solver with an iterative one!).

Numerical experiments

- For sparse Cholesky, `HSL_MA87` (Hogg, Reid and Scott '10) (DAG-based code for multicore machines).
- For dense Cholesky, `dpotrf`.
- For incomplete Cholesky, `HSL_MI35` (Scott and Tuma '14).
- Use preconditioned GMRES as iterative solver.
- Experiments performed using 8× Intel i7-4790 (3.6 GHz) with 15.6 Gbytes memory.
- Timings are elapsed times in seconds.

Example 1: PDE1

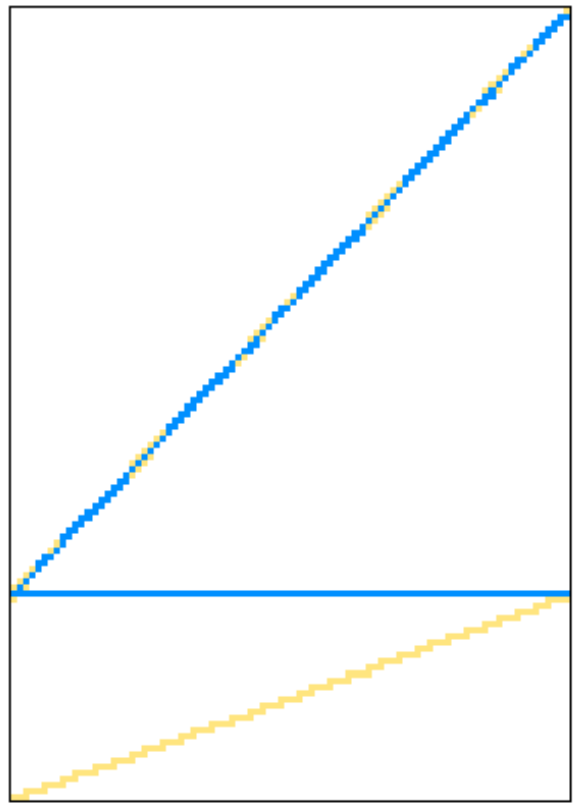
- $m = 271,792, n = 270,595$
- Single row with 66% density
- C is essentially dense. Not able to run direct solver.

Remove dense row:

- A_s is full rank.
- $density(C_s) = 4.5 \times 10^{-5}$
- $nnz(L) = 2 \times 10^7$
- Schur complement direct solver solution time 1.21 seconds.

Example 2: scagr7-2b

$m = 13,247, n = 9,743$



A row of A is defined to be dense if its density is at least ρ.

m_d is the number of dense rows.

n_2 is the number of null cols in A_s.

ρ	0	0.1	0.01	0.001
m_d	0	1	7	263
n_2	0	1	1	257
$density(C_s)$	$4.15\times^{-2}$	1.45×10^{-2}	1.73×10^{-4}	5.74×10^{-4}
$nfactor$	8.64×10^6	5.11×10^6	1.62×10^5	1.45×10^5
$nflops$	1.08×10^{10}	3.55×10^9	3.81×10^6	3.21×10^6
Time	1.19	0.29	0.08	0.49 (0.33*)

* Time for the solves needed to deal with the 257 null cols.

Note: C does not have to be very dense for it to be advantageous to use the Schur complement approach.

Same example: Schur complement with GMRES + block IC

ρ	0	0.1	0.01	0.001
m_d	0	1	7	263
n_2	0	1	1	257
$density(C_s)$	$4.15\times^{-2}$	1.45×10^{-2}	1.73×10^{-4}	5.74×10^{-4}
Times:				
Compute IC	0.34	0.39	0.02	0.05
GMRES (Iters)	0.31 (370*)	0.08 (99)	0.001 (3)	0.012 (2)
		0.05 (73)	0.001 (2)	2.94 (2)
Total	0.65	0.47	0.019	3.00

* For $\rho = 0$ use IC preconditioned LSMR (dense rows ignored).

If n_2 large, better to ignore these null columns and use shift.
For $\rho = 0.001$ this reduces total time to 0.07.

Appending single "dense" row: LSMR with IC preconditioner

Problem	m	n	Its	T_p	T_s	T_{total}
$\rho = 0.01$						
GL7d20	1,911,124	1,437,546	40	166	19	185
LargeRegFile	2,111,154	801,374	70	127	7.7	134
relat9	9,746,232	274,667	90	20	29	49
$\rho = 0.1$						
GL7d20			–	>600	–	>600
LargeRegFile			–	>600	–	>600
relat9			90	64	29	92
$\rho = 0.5$						
GL7d20			–	>600	–	>600
LargeRegFile			–	>600	–	>600
relat9			–	>600	–	>600

ρ is the density of the added row.

Appending single dense row ($\rho = 1.0$)

Cannot solve these examples using LSMR + IC as IC is prohibitively expensive (in time) to compute.

Results for Schur complement using GMRES + block IC:

	Its	T_p	T_s	T_{total}
GL7d20	32	187	39	226
LargeRegFile	11	1.61	0.53	2.14
CONT11_L	142	9.23	22.8	32.0

Appending $m_d \geq 1$ dense rows ($\rho = 1.0$)

Results for Schur complement using GMRES + block IC:

Problem	$m_d = 1$		$m_d = 50$		$m_d = 100$	
	Its	T_{total}	Its	T_{total}	Its	T_{total}
`GL7d20`	32	226	22	222	22	231
`LargeRegFile`	11	2.14	9	3.28	9	4.83
`CONT11_L`	142	32.0	12	13.0	13	15.9

Increase in time with m_d is because the dense factorization of S_d becomes more expensive (it is trivial with $m_d = 1$).

Merci de votre attention!

Paper/reports on solving LS problems available from
http://www.numerical.rl.ac.uk/people/j_scott/

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Finally, at RAL we have two vacancies at post doc level: one to join Iain in the NLAFET project and the other as a numerical analysis researcher to work in part on sparse (non)linear least squares. **Please ask if you or someone you know might be interested!**