V-invariant methods for generalised least squares problems

M.R.Osborne and Inge Söderkvist
School of Mathematical Sciences, ANU, and
Department of Mathematics, University of
Luleå

The generalised least squares problem is

$$\min_{\mathbf{x}} \mathbf{r}^T V^{-1} \mathbf{r};\ \mathbf{r} = A\mathbf{x} - \mathbf{b},$$

where $A : R^p \rightarrow R^n$, $V : R^n \rightarrow R^n$. It will be assumed that A has its full rank $p < n$, but only that V is positive semi-definite. Typically in data analytic situations V, which has the dimension of the data set, is large. An application is made to a class of Kalman Filter problems. This forces well defined sparse structures on both A and V.

A class of V-invariant algorithms has been introduced by Gulliksson and Wedin (SIAM J. Matrix Anal. Applic., 13(4)1298-1313,1992.) Their problem of particular interest was equality constrained least squares which can be formulated in generalised least squares form with singular (and diagonal) V. This is a particular example of the ability of these algorithms to support a form of multi-scaling. They point out the importance of column pivoting in this application.

Söderkvist (Proceedings of CTAC95,p.709-716, World Scientific) considered the Kalman Filter case with diagonal covariance matrix V and was able to demonstrate superior numerical performance of his V-invariant methods for problems in which V possessed several distinct scales. The restriction to diagonal V is important in developing algorithms, and he experimented with methods for reducing the problem to one having this form employing both Jacobi's method ($V = Q\Lambda Q^T$) and rank revealing Cholesky with diagonal pivoting ($PVP^T = LDL^T$). He was concerned about possible errors in small elements of D.

Osborne (Proceedings ICCS03,v.3,p.673-682, Springer) has argued that provided the number of small elements in D is $k \leq p$ then errors in these are benign so that errors due to the rank revealing factorization are insignificant. Our aim here is to present an application appropriate to a class of Kalman filter problems with distinctly illconditioned covariances and both stable and unstable dynamics.

V-invariant transformation J

$$JVJ^T = V$$

Let J_1 and J_2 be V-invariant. Then

- J_1^{-1}, J_2^{-1} $J_1 J_2$ and $J_2 J_1$ V-invariant,
- J_1^T, J_2^T V^{-1}-invariant (V nonsingular).

If

$$V = \begin{bmatrix} 0 & 0 \\ 0 & V_2 \end{bmatrix} \text{ (reduced form!)}$$

then J is V-invariant iff

$$J = \begin{bmatrix} J_{11} & 0 \\ J_{21} & J_{22} \end{bmatrix}, \; J_{22} V_2 J_{22}^T = V_2,$$

and J_{11}, J_{22} nonsingular.

Ordinary least squares.
Here V-invariance implies J orthogonal.

$$V = I \Rightarrow JIJ^T = I.$$

Analogue of Aitken-Householder elementary orthogonal transformation is

$$J = I - 2\frac{V\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T V\mathbf{v}},\ J^2 = I.$$

To use in matrix factorization need $\mathbf{v}$ such that

$$J\begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 \\ \gamma\mathbf{e}_1 \end{bmatrix}$$

Scale of $\mathbf{v}$ not important. Take

$$V\mathbf{v} = s\begin{bmatrix} 0 \\ \mathbf{u}_2 - \gamma\mathbf{e}_1 \end{bmatrix}$$

where s is a scale factor.

Problem

$$V\mathbf{v} = s\left[\begin{array}{c} 0 \\ \mathbf{u}_2 - \gamma\mathbf{e}_1 \end{array}\right]$$

is as hard as original unless V readily invertible! Specialize to $V = D$ diagonal, $\dim(\mathbf{u}_1) = j-1$,

$$\begin{aligned} D &= \text{diag}\{d_1, d_2, \cdots, d_n\}, \\ &= \text{diag}\{\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_k, \nu_{k+1}, \cdots, \nu_n\}, \\ \varepsilon_1 \leq \varepsilon_2 &\leq \cdots \leq \varepsilon_k \ll \nu_{k+1} \leq \cdots \leq \nu_n, \\ \mathbf{v} &= \left[\begin{array}{c} 0 \\ \mathbf{v}_2 \end{array}\right] = d_j \left[\begin{array}{c} 0 \\ D_2^{-1}(\mathbf{u}_2 - \gamma\mathbf{e}_1) \end{array}\right]. \end{aligned}$$

Here $s = d_j$ and the effective diagonal matrix has elements ≤ 1. Importance of the ordering of the elements of D becomes clearer in the calculation of γ.

To calculate γ use V-invariance

$$\begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}^T J^T D^{-1} J \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 \\ \gamma \mathbf{e}_1 \end{bmatrix}^T D^{-1} \begin{bmatrix} \mathbf{u}_1 \\ \gamma \mathbf{e}_1 \end{bmatrix}$$

$$\Rightarrow \mathbf{u}_2^T D_2^{-1} \mathbf{u}_2 = \gamma^2 \mathbf{e}_1^T D_2^{-1} \mathbf{e}_1.$$

There are two cases depending on j and k.

$j \leq k$

$$\gamma^2 = (\mathbf{u}_2)_j^2 + \sum_{s=j+1}^{k} \frac{\varepsilon_j}{\varepsilon_s} (\mathbf{u}_2)_s^2 + \sum_{s=k+1}^{n} \frac{\varepsilon_j}{\nu_s} (\mathbf{u}_2)_s^2.$$

$j > k$

$$\gamma^2 = (\mathbf{u}_2)_j^2 + \sum_{s=j+1}^{n} \frac{\nu_j}{\nu_s} (\mathbf{u}_2)_s^2.$$

Note that there is multiple scale behavior when $j \leq k$ and that limit $\boldsymbol{\varepsilon} \to 0$ can be defined! Also γ is the column length in the re-scaled metric. Column pivoting can be required because of the multiple scaling.

If elements of J are large then this is an indicator of possible stability problems! Let

$$J = I - 2\mathbf{c}\mathbf{d}^T$$

be an elementary V-invariant reflector. Then

$$\|J\|_2 = \eta + \sqrt{\left\{\eta^2 - 1\right\}},\ \eta = \|\mathbf{c}\|_2 \|\mathbf{d}\|_2 .$$

Here

$$\eta = \frac{\left\|D_2^{-1}(\mathbf{u}_2 - \gamma\mathbf{e}_1)\right\| \|\mathbf{u}_2 - \gamma\mathbf{e}_1\|}{(\mathbf{u}_2 - \gamma\mathbf{e}_1)^T D_2^{-1} (\mathbf{u}_2 - \gamma\mathbf{e}_1)},$$

$$\Rightarrow \|J\| \geq \eta \geq \frac{\|\mathbf{u}_2\|}{2\gamma}$$

That is $\left\|J_j\right\|$ will be large if

$$\left|d_j \mathbf{u}_2^T D_2^{-1} \mathbf{u}_2\right| \ll \|\mathbf{u}_2\| .$$

the $\boldsymbol{\varepsilon} \to 0$ limit gives η large if

$$\|\mathbf{u}_\varepsilon\| \ll \|\mathbf{u}_2\| .$$

Here $\mathbf{u}_\varepsilon$ corresponds to $\{\varepsilon_j, \cdots, \varepsilon_k\}$ in D_2.

Example Let

$$D = \begin{bmatrix} \varepsilon & & \\ & \varepsilon & \\ & & 1 \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} \alpha \\ \beta \\ \nu \end{bmatrix}.$$

The transformation taking $\mathbf{w}$ to $\gamma\mathbf{e}_1$ in limit $\varepsilon \longrightarrow 0$ is

$$I - \pi \left(\begin{bmatrix} \alpha \\ \beta \\ \nu \end{bmatrix} + \theta(\pi 1)\mathbf{e}_1 \right) \left(\begin{bmatrix} \alpha \\ \beta \\ 0 \end{bmatrix} + \theta(\pi 1)\mathbf{e}_1 \right)^T,$$

where

$$\pi = \frac{1}{\pi 1 \pi 2}, \ \theta = \mathrm{sgn}(\alpha),$$
$$\pi 1 = (\alpha^2 + \beta^2)^{1/2},$$
$$\pi 2 = |\alpha| + (\alpha^2 + \beta^2)^{1/2}.$$

Note that $\pi\nu$ would be large if $\alpha, \ \beta \ll \nu$ violating the stability condition.

Solution of GLSQ problem is $\mathbf{x} = T\mathbf{b}$ where T solves

$$\begin{bmatrix} T & \Lambda \end{bmatrix} \begin{bmatrix} D & A \\ A^T & 0 \end{bmatrix} = \begin{bmatrix} 0 & I \end{bmatrix}.$$

Let $JA = \begin{bmatrix} R \\ 0 \end{bmatrix}$. Transformed operator satisfies

$$\begin{bmatrix} \begin{bmatrix} \widetilde{T}_1 & \widetilde{T}_2 \end{bmatrix} & \Lambda \end{bmatrix} \begin{bmatrix} \begin{bmatrix} \begin{bmatrix} D_\varepsilon & 0 \\ 0 & D_{21} \end{bmatrix} & 0 \\ 0 & D_{22} \end{bmatrix} & \begin{bmatrix} R \\ 0 \end{bmatrix} \\ \begin{bmatrix} R^T & 0 \end{bmatrix} & 0 \end{bmatrix} = \begin{bmatrix} 0 & I \end{bmatrix}.$$

Gives

$$\begin{aligned} \widetilde{T}_1 &= R^{-1}, \ \widetilde{T}_2 = 0, \\ \Lambda &= R^{-1} \begin{bmatrix} D_\varepsilon & 0 \\ 0 & D_{21} \end{bmatrix} R^{-T}, \\ \mathbf{x} &= \begin{bmatrix} R^{-1} & 0 \end{bmatrix} J\mathbf{b}. \end{aligned}$$

When V is not diagonal start with an LDL^T factorization of V and rewrite problem by setting $L^{-1}\mathbf{r} = \widetilde{\mathbf{r}} = D^{1/2}\mathbf{s}$ to obtain

$$\min_{\mathbf{x}} \mathbf{s}^T\mathbf{s};\ D^{1/2}\mathbf{s} = L^{-1}A\mathbf{x} - L^{-1}\mathbf{b}.$$

Implement by making a rank-revealing Cholesky:

$$PVP^T \rightarrow L\text{diag}\left\{d_n, d_{n-1}, \cdots, d_1\right\} L^T$$

where the diagonal pivoting ensures

$$d_n \geq d_{n-1} \geq \cdots \geq d_1$$

and process stops if a very small or negative d_i encountered. Key point is that illconditioning in V is largely forced into D. Conditions for success (eg Higham) correspond to the assumptions made already on D but need further step to reverse order of computed D to construct V-invariant transformation. Would expect that small d_i could have high relative error. Does this matter?

The case

$$D = \text{diag}\left\{0, \cdots, 0, d_{k+1}, \cdots, d_n\right\},\ k < p,$$

gives the equality constrained problem

$$\min_{\mathbf{x}} \mathbf{s}^T\mathbf{s};\ \begin{bmatrix} 0 & \\ & D_2^{1/2} \end{bmatrix} \mathbf{s} = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}.$$

This is the limiting problem associated with the penalised objective

$$\min_{\mathbf{x}} \left\{\mathbf{r}_2^T D_2^{-1} \mathbf{r}_2 + \lambda \mathbf{r}_1^T \mathbf{r}_1\right\};\ \mathbf{r} = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}$$

which has the alternative form

$$\min_{\mathbf{x}} \mathbf{s}^T\mathbf{s};\ \begin{bmatrix} \lambda^{-1/2} I & \\ & D_2^{1/2} \end{bmatrix} \mathbf{s} = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}.$$

From theory of penalty functions expect

$$\|\mathbf{x}(\lambda) - \mathbf{x}(\infty)\| = O(1/\lambda),\ \lambda \to \infty.$$

Generalised spline objects having the general form $\mathcal{E}\{\mathbf{h}^T\mathbf{x}(t)|y_1,\cdots,y_n\}$ can be obtained by considering the stochastic differential equation

$$d\mathbf{x} = M\mathbf{x}dt + \sigma\sqrt{\lambda}\mathbf{b}dw,$$

where $M : R^m \to R^m$, in conjunction with the observation process

$$\mathbf{h}^T\mathbf{x}(t_i) + \varepsilon_i = y_i,\ \mathcal{V}\{\varepsilon_i\} = \sigma^2.$$

Let

$$\frac{dX}{dt} = MX,\ X(\xi,\xi) = I.$$

Variation of parameters gives the dynamics equation

$$\mathbf{x}_{i+1} = X_i\mathbf{x}_i + \sigma\sqrt{\lambda}\mathbf{u}_i$$

where

$$\mathbf{u}_i = \int_{t_i}^{t_{i+1}} X(t_{i+1},s)\mathbf{b}\frac{dw}{ds}ds,$$
$$\mathbf{u}_i \sim N(0,\sigma^2\lambda R_i)).$$

This leads, via the Kalman filter subject to a diffuse prior, to the generalised least squares problem

$$\min_{\mathbf{x}} \left\{ \mathbf{r}_1^T R^{-1} \mathbf{r}_1 + \mathbf{r}_2^T V^{-1} \mathbf{r}_2 \right\},$$

where

$$\begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{bmatrix} = \begin{bmatrix} -X_1 & I & & & \\ & -X_2 & I & & \\ & & \cdots & & \\ & & & -X_{n-1} & I \\ \mathbf{h}^T & & & & \\ & \mathbf{h}^T & & & \\ & & \cdots & & \\ & & & & \mathbf{h}^T \end{bmatrix} \mathbf{x} - \begin{bmatrix} 0 \\ \mathbf{y} \end{bmatrix},$$

$$R = \sigma^2 \lambda \text{diag}\{R_1, R_2, \cdots, R_{n-1}\},\ V = \sigma^2 I$$

and

$$R_i = \int_{t_i}^{t_{i+1}} X(t_{i+1}, s) \mathbf{b}\mathbf{b}^T X(t_{i+1}, s)^T ds$$

V-invariant factorization applied to successive column blocks requires rank-revealing factorization of the corresponding R_j and within column block sorting. Straight forward application under the given ordering results in accumulating fill. The first few steps are:

$$\begin{bmatrix} -X_1 & I & \\ & -X_2 & I \\ \vdots & \vdots & \vdots \\ \mathbf{h}^T & & \\ & \mathbf{h}^T & \\ & & \mathbf{h}^T \end{bmatrix} \rightarrow \begin{bmatrix} U_1 & W_1 & \\ & -X_2 & I \\ \vdots & \vdots & \vdots \\ & \mathbf{z}_{11}^T & \\ & \mathbf{h}^T & \\ & & \mathbf{h}^T \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} U_1 & W_1 & \\ & U_2 & W_2 \\ \vdots & \vdots & \vdots \\ & & \mathbf{z}_{21}^T \\ & & \mathbf{z}_{22}^T \\ & & \mathbf{h}^T \end{bmatrix}$$

The ordering used in Paige and Saunders information filter generates less direct fill.

Fill can be controlled to a total of $m+1$ rows in the next to pivotal block column by orthogonal transformations which are in the context used V-invariant.First applied at step m

$$\begin{bmatrix} \cdots & \cdots & \cdots \\ U_m & W_m & \\ & -X_{m+1} & I \\ \cdots & \cdots & \cdots \\ & \mathbf{z}_{m1}^T & \\ & \mathbf{z}_{m2}^T & \\ & \vdots & \\ & \mathbf{z}_{mm}^T & \\ & \mathbf{h}^T & \end{bmatrix} \rightarrow \begin{bmatrix} \cdots & \cdots & \cdots \\ U_m & W_m & \\ & -X_{m+1} & I \\ \cdots & \cdots & \cdots \\ & Z_m & \\ & 0 & \end{bmatrix}$$

where $Z_m : R^m \rightarrow R^m$. It is convenient to carry out the transformation in two steps in order to compute auxiliary quantities.

$$\begin{bmatrix} \mathbf{z}_{i1}^T \\ \vdots \\ \mathbf{z}_{im}^T \\ \mathbf{h}^T \end{bmatrix} \rightarrow \begin{bmatrix} Z_i^1 \\ \mathbf{h}^T \end{bmatrix} \rightarrow \begin{bmatrix} Z_i \\ 0 \end{bmatrix}.$$

Example: Quintic spline. This corresponds to the case

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \ \mathbf{h} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \ \mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix},$$

with $\mathbf{h}$ and $\mathbf{b}$ chosen for maximum smoothness. The covariance matrix blocks are readily computed:

$$R_i = \delta \begin{bmatrix} \frac{\delta^4}{20} & \frac{\delta^3}{8} & \frac{\delta^3}{6} \\ \frac{\delta^3}{8} & \frac{\delta^2}{3} & \frac{\delta}{2} \\ \frac{\delta^3}{6} & \frac{\delta}{2} & 1 \end{bmatrix}.$$

The rank revealing Cholesky gives

$$PR_iP^T = \delta \begin{bmatrix} 1 & & \\ \frac{\delta}{2} & 1 & \\ \frac{\delta^2}{6} & -\frac{\delta}{2} & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & \frac{\delta^2}{12} & \\ & & \frac{\delta^4}{720} \end{bmatrix} \begin{bmatrix} 1 & \frac{\delta}{2} & \frac{\delta^2}{6} \\ & 1 & -\frac{\delta}{2} \\ & & 1 \end{bmatrix}.$$

Note the small elements in D_i. However, there are $(n-1)(m-1)$ of these all told while the design is $R^{nm} \rightarrow R^{nm+n}$ so the conditions for the solubility of the generalised least squares problem can be satisfied.

Example: Tension splines. This corresponds to an example with unstable dynamics. For one and two parameter splines we have

$$M = \begin{bmatrix} 0 & 1 \\ \alpha^2 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 & 0 \\ \alpha^2 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \beta^2 & 0 \end{bmatrix}$$

Smoothness is maximized by choice $\mathbf{h} = \mathbf{e}_1$, $\mathbf{b} = \mathbf{e}_m$. Again covariances have small elements.The examples are not very unstable.

$\alpha = 1$	
$n = 11$	$D_i = \{8.3-5, 1.0-1\}$
$n = 51$	$D_i = \{6.7-7, 2.0-2\}$
$\alpha = 1, \beta = 2$	
$n = 11$	$D_i = \{9.9-13, 1.4-8, 8.3-5, 1.0-1\}$
$n = 51$	$D_i = \{0.0, 4.4-12, 6.7-7, 2.0-2\}$

Example: A stable example is provided by the simple chemical reaction $A \rightarrow B \rightarrow C$ with rates k_1 and k_2. Here

$$\frac{d}{dt}\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix}\begin{bmatrix} A \\ B \\ C \end{bmatrix}$$

Well posedness of the estimation problem requires $(\mathbf{h})_3 \neq 0$. Maximum smoothness of the g-spline is achieved with $\mathbf{b} = \mathbf{e}_1$, $\mathbf{h} = \mathbf{e}_3$.

$k_1 = 1,\ k_2 = 2$	
$n = 11$	$D_i = \{5.5-8, 6.8-5, 9.1-2\}$
$n = 51$	$D_i = \{1.8-11, 6.4-7, 2.0-2\}$