V-invariant methods for generalised least squares

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Abstract: The generalised least squares problem is

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

Computation of a solution can prove embarassing in many of its important applications:

- In data processing applications the dimension n of V is the size of the data set and can be extremely large. Structure in V needs to be exploited and, typically, explicit inversion avoided.

- The problem can be reformulated so that it may have a well defined solution in cases where V is illconditioned (even singular). An important instance is a reformulation to include equality constraints.

A class of V-invariant algorithms was introduced by Gulliksson and Wedin (SIAM J. Matrix Anal. Applic. 13(4)1298-1313,1992.) They have considerable potential for overcoming the indicated problems.

1. **Generalised least squares - the Gauss-Markov formulation.** Let

$$\varepsilon = A\mathbf{x}^* - \mathbf{b},\ \varepsilon \sim N(0, V).$$

Problem is given structure of model and a realization of $\mathbf{b}$ construct an estimate $\mathbf{x}$ of $\mathbf{x}^*$ by finding

$$\min_{\mathbf{x}} E\left\{\|\mathbf{x} - \mathbf{x}^*\|_2^2\right\}$$

Assume a class of estimators that are linear functions of the data

$$\begin{aligned} \mathbf{x} &= T\mathbf{b},\ T : R^n \to R^p. \\ E\left\{\|\mathbf{Tb} - \mathbf{x}^*\|_2^2\right\} &= \text{trace}\left\{TVT^T\right\} + \|(TA - I)\,\mathbf{x}^*\|_2^2. \end{aligned}$$

Assume estimator is unbiassed

$$TA = I \Rightarrow E\{\mathbf{x}\} = \mathbf{x}^*.$$

Removes unknown $\mathbf{x}^*$ from problem.

2. **Computation of T.** Have to solve problem

$$\min_T \text{trace}\left\{TVT^T\right\};\ TA = I.$$

Problem can be formulated

$$\begin{aligned}\min_{\mathbf{t}_i} \mathbf{t}_i^T V \mathbf{t}_i;\ \mathbf{t}_i^T A &= \mathbf{e}_i^T,\\ \text{where } \mathbf{t}_i &= T_{i*},\ i = 1, 2, \cdots, p.\end{aligned}$$

Necessary conditions give

$$\mathbf{t}_i^T V = \lambda_i^T A^T,\ i = 1, 2, \cdots, p,$$

or

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

Problem is well determined provided

$$\begin{bmatrix} V & -A \\ -A^T & 0 \end{bmatrix} \text{ well conditioned.}$$

Require V nonsingular on null space of A.

3. **Reprise - orthogonal factorization**. The prefered method for solving the linear least squares problem is based on the factorization

$$A \rightarrow \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} U \\ 0 \end{bmatrix}$$

where Q is orthogonal. Here $V = I$, and

$$Q^T I Q = I.$$

The algorithm builds up Q using elementary orthogonal matrices (eg Aitken-Householder reflectors)

$$Q_i = I - 2\mathbf{w}_i\mathbf{w}_i^T, \mathbf{w}_i^T I\ \mathbf{w}_i = 1.$$

Know the resulting algorithm has good properties. We will see that

- it is a special case of a V-invariant transformation corresponding to $V = I$, and
- it has optimally good properties within this class.

4. **V-invariance**. Motivating idea is that of simplifying A while preserving structure in V

$$\mathbf{r} = A\mathbf{x} - \mathbf{b} \rightarrow \mathbf{s} = JA\mathbf{x} - J\mathbf{b}.$$

How does Gauss-Markov operator transform? Require $\mathbf{x} = T\mathbf{b} = TJ^{-1}J\mathbf{b}$,
transformed V must be symmetric, right hand side must be preserved.

$$\begin{bmatrix} T & \Lambda \end{bmatrix} \begin{bmatrix} J^{-1} & \\ & I \end{bmatrix} \begin{bmatrix} J & \\ & I \end{bmatrix} \begin{bmatrix} V & -A \\ -A^T & 0 \end{bmatrix} \begin{bmatrix} J^T & \\ & I \end{bmatrix}$$
$$= \begin{bmatrix} 0 & -I \end{bmatrix} \begin{bmatrix} J^T & \\ & I \end{bmatrix} = \begin{bmatrix} 0 & -I \end{bmatrix}$$

Obtain

$$\begin{bmatrix} TJ^{-1} & \Lambda \end{bmatrix} \begin{bmatrix} JVJ^T & -JA \\ -A^TJ^T & 0 \end{bmatrix} = \begin{bmatrix} 0 & -I \end{bmatrix}$$

If nonsingular matrix J satisfies

$$JVJ^T = V$$

say J is V-invariant.

5. **Properties**. 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.

6. **Elementary V-invariant transformations**.

$$\begin{aligned} J &= I - 2\mathbf{u}\mathbf{v}^T, \\ JVJ^T &= V - 2\left(\mathbf{u}\mathbf{v}^T V + V\mathbf{v}\mathbf{u}^T\right) + 4\mathbf{v}^T V\mathbf{v}\mathbf{u}\mathbf{u}^T \end{aligned}$$

If $\mathbf{v}$, $\mathbf{v}^T V\mathbf{v} \neq \mathbf{0}$ is given then the transformation defined by

$$\mathbf{u} = \frac{V\mathbf{v}}{\mathbf{v}^T V\mathbf{v}},\ J = I - 2\frac{V\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T V\mathbf{v}},\ J^2 = I,\ \det(J) = -1$$

is a V-invariant elementary reflector. If V is singular and $V\mathbf{v} = 0$, $\mathbf{u}$ arbitrary then J is V-invariant. If $\mathbf{v}^T\mathbf{u} = 1$ then J is an elementary reflector. If V is in reduced form then

$$J = I - 2\begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}\begin{bmatrix} \mathbf{v}_1^T & 0 \end{bmatrix}$$

is a V-invariant elementary reflector.

7. **Use of matrix factors**. Assume

$$JA = \begin{bmatrix} R \\ 0 \end{bmatrix},\ V_2 = \begin{bmatrix} V_{21} & 0 \\ 0 & V_{22} \end{bmatrix},\ V_{21} \in R^{p-k} \rightarrow R^{p-k}.$$

V_2 has become block diagonal. Transformed operator satisfies

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

where $W = \begin{bmatrix} 0 & I \end{bmatrix}$. Gives

$$\widetilde{T}_1 \begin{bmatrix} 0 & 0 \\ 0 & V_{21} \end{bmatrix} + \Lambda R^T = 0,\ \widetilde{T}_2 V_{22} = 0,\ \widetilde{T}_1 R = I$$

with solutions

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

Solution is well determined if R, V_{22} well determined.

8. **Factorization - first case**. Can factor A in desired form if we can solve the problem of constructing J giving

$$J\mathbf{v} = \gamma \mathbf{e}_{1.}$$

As J^T is V^{-1}-invariant we can calculate γ. Have

$$\begin{aligned} \gamma^2 \mathbf{e}_1^T V^{-1} \mathbf{e}_1 &= \mathbf{v}^T J^T V^{-1} J\mathbf{v} = \mathbf{v}^T V^{-1} \mathbf{v}, \\ \gamma &= \theta \surd \left\{ \mathbf{v}^T V^{-1} \mathbf{v} / \left(V^{-1} \right)_{11} \right\}. \end{aligned}$$

If first form of transformation applicable then

$$J\mathbf{v} = \mathbf{v} - \frac{2\mathbf{w}^T \mathbf{v}}{\mathbf{w}^T V \mathbf{w}} V\mathbf{w} = \gamma \mathbf{e}_{1.}$$

Note $\mathbf{w}$ scale invariant so take

$$V\mathbf{w} = \mathbf{v} - \gamma \mathbf{e}_{1.}$$

Standard argument suggests $\theta = -\mathrm{sgn}\,(\mathbf{v})_1$. Note γ independent of scale of V. $\mathbf{w}$ found most easily if V diagonal

$$V = \mathrm{diag}\,\{V_1, \cdots, V_n\}.$$

Form of γ suggests elements of V be sorted in increasing order!

9. **Factorization - second case**. If $V = \mathrm{diag}\left\{0, \cdots, 0, V_{k+1}, \cdots, V_n\right\}$ has nontrivial reduced form then second form of transformation must be used. Consider

$$\begin{aligned}
V_\varepsilon &= \mathrm{diag}\left\{\varepsilon, \cdots, \varepsilon, V_{k+1}, \cdots, V_n\right\} \\
\lim_{\varepsilon \to 0} (V_\varepsilon)_1 V_\varepsilon^{-1} &= \begin{bmatrix} I_k & \\ & 0 \end{bmatrix}, \\
\lim_{\varepsilon \to 0} |\gamma_\varepsilon| &= \|\mathbf{v}_1\|_2 .
\end{aligned}$$

The resulting transformation gives the V-invariant reflector

$$J = I - 2 \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix} \begin{bmatrix} \mathbf{d}_1^T & 0 \end{bmatrix}$$

where

$$\begin{aligned}
\sqrt{2}\mathbf{c} &= \left(\mathbf{v} + \mathrm{sgn}\,(\mathbf{v})_1 \|\mathbf{v}_1\| \mathbf{e}_1\right) / \|\mathbf{v}_1\| , \\
\sqrt{2}\mathbf{d} &= \begin{bmatrix} \mathbf{v}_1 + \mathrm{sgn}\,(\mathbf{v})_1 \|\mathbf{v}_1\| \mathbf{e}_1 \\ 0 \end{bmatrix} / \left(\|\mathbf{v}_1\| + |(\mathbf{v})_1|\right) .
\end{aligned}$$

10. **Stability considerations** 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

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

(outline of proof) We require the largest eigenvalue of

$$J^T J\mathbf{w} = \mu\mathbf{w}$$

or, equivalently,

$$J\mathbf{w} = \mu J^T\mathbf{w}.$$

Further, it is easy to see that the maximizing eigenvector has form $\mathbf{w} = \alpha\mathbf{d} + \beta\mathbf{c}$. The determinantal condition for non-trivial α, β is

$$\begin{vmatrix} 1+\mu & 2\mu\|\mathbf{c}\|^2 \\ -2\|\mathbf{d}\|^2 & -(1+\mu) \end{vmatrix} = 0,$$

giving

$$\mu = 2\eta^2 - 1 + 2\eta\sqrt{\left\{\eta^2 - 1\right\}} = \|J\|_2^2 .$$

If $V = I$ then $\eta = 1$, otherwise $\eta > 1$.

11. **Application of Lemma**. Expect from general form for J in first class of transformations that stability requires that $\mathbf{w}^T V \mathbf{w} \neq \mathbf{0}$ is commensurate with $\|\mathbf{w}\| \, \|V\mathbf{w}\|$. Here

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

with V diagonal. Denominator is $2 |\gamma| \, |v_1 - \gamma| / V_1$. To estimate numerator

$$\begin{aligned} \left\| V^{-1} (\mathbf{v} - \gamma \mathbf{e}_1) \right\| &\geq |v_1 - \gamma| / V_1, \\ \|\mathbf{v} - \gamma \mathbf{e}_1\| &\geq \|\mathbf{v}\|. \end{aligned}$$

This implies

$$\|J\| \geq \eta \geq \frac{\|\mathbf{v}\|}{2\gamma}.$$

That is $\|J\|$ will be large if

$$\left| V_1 \mathbf{v}^T V^{-1} \mathbf{v} \right| \ll \|\mathbf{v}\|.$$

For the second class of transformations the $\varepsilon \to 0$ limit gives η large if

$$\|\mathbf{v}_1\| \ll \|\mathbf{v}\|.$$

12. **When V is not diagonal** . Start with the problem

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

Given an LDL^T factorization of V can rewrite problem by setting $L^{-1}\mathbf{r} = \widetilde{\mathbf{r}} = D^{1/2}\mathbf{s}$ to obtain

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

The necessary conditions give

$$M \begin{bmatrix} \mathbf{r} \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} -\mathbf{b} \\ 0 \end{bmatrix}$$

where M is the matrix of the equations determining the Gauss-Markov operator

$$\begin{bmatrix} T & \Lambda \end{bmatrix} M = \begin{bmatrix} 0 & -I \end{bmatrix}.$$

Postmultiplying by $\begin{bmatrix} \mathbf{r} \\ \mathbf{x} \end{bmatrix}$ gives

$$\begin{bmatrix} T & \Lambda \end{bmatrix} \begin{bmatrix} -\mathbf{b} \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & -I \end{bmatrix} \begin{bmatrix} \mathbf{r} \\ \mathbf{x} \end{bmatrix} = -\mathbf{x}$$

demonstrating the equivalence of the two approaches.

13. **Is LDL^T practicable**? One problem for which there is considerable amount of software in sparse and structured cases.
A rank-revealing Choleski has the form

$$V \rightarrow L\text{diag}\{D_n, D_{n-1}, \cdots, D_1\} L^T$$

where pivoting ensures

$$D_n \geq D_{n-1} \geq \cdots \geq D_1.$$

Need to reverse order to construct V-invariant transformation. Condition for success (eg Higham) is

$$\begin{aligned}
&\{D_1, D_2, \cdots, D_k\} \text{ commensurate, small,}\\
&D_k \ll D_{k+1},\\
&\left\{D_{k+1}, \cdots, D_n\right\} \text{ commensurate,}\\
&k \leq p
\end{aligned}$$

Would expect that $\{D_1, D_2, \cdots, D_k\}$ could have high relative error. Does that matter?

14. **A stable problem**. Case $D = \text{diag}\left\{0, \cdots, 0, D_{k+1}, \cdots, D_n\right\}$ 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

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

15. **Perturbation behaviour**. Necessary conditions for the penalty problem are

$$\mathbf{r}_2^T D_2^{-1} A_2 + \lambda \mathbf{r}_1^T A_1 = 0.$$

Set $\tau = 1/\lambda$ and define

$$\tau \mathbf{u} = A_1 \mathbf{x} - \mathbf{b}_1 \ (= \mathbf{r}_1).$$

Can find equations defining a trajectory satisfied by $\mathbf{x}(\tau), \mathbf{u}(\tau)$ by differentiating these relations.

$$\begin{aligned} A_2^T D_2^{-1} A_2 \frac{d\mathbf{x}}{d\tau} + A_1^T \frac{d\mathbf{u}}{d\tau} &= 0, \\ A_1 \frac{d\mathbf{x}}{d\tau} - \tau \frac{d\mathbf{u}}{d\tau} &= \mathbf{u}. \end{aligned}$$

Matrix of this system is nonsingular for τ small enough provided A_1, A_2 are of full rank. Thus can integrate back to $\tau = 0$ and Taylor series expansion is well defined.

Conclusion - Let $D = \text{diag}\{D_1, D_2\}$. The equality constrained problem obtained by setting $D_1 = 0$ has a well defined solution which differs from that of the original problem by $O(\|D_1\|)$.

16. **Kalman Filter**. Let $\mathbf{x}_k = \mathbf{x}(t_k) \in R^p$ be an unobserved state variable describing the state of a system at time t_k. System evolves in accordance with dynamics equation

$$\mathbf{x}_{k+1} = X_k \mathbf{x}_k + \mathbf{u}_k, \; k = 1, 2, \cdots, n-1,$$

and information on state is available through observations

$$\begin{aligned}
&\mathbf{y}_k \in R^m, \; \mathbf{y}_k = H_k \mathbf{x}_k + \varepsilon_k, \; k = 1, 2, \cdots, n-1 \\
&\mathcal{C}\left\{\varepsilon_i, \varepsilon_j\right\} = V_i \delta_{ij}, \; \mathcal{C}\left\{\mathbf{u}_i, \mathbf{u}_j\right\} = R_i \delta_{ij}, \; \mathcal{C}\left\{\varepsilon_i, \mathbf{u}_j\right\} = 0, \\
&\quad \Rightarrow \mathcal{C}\left\{\mathbf{x}_i, \mathbf{u}_k\right\} = \mathcal{C}\left\{\mathbf{x}_i, \varepsilon_k\right\} = 0, \; j \le k.
\end{aligned}$$

Let $\mathcal{Y}_k = \left\{\mathbf{x}_{1|0}, \mathbf{y}_1, \cdots, \mathbf{y}_n\right\}$. The Kalman filter produces the linear, minimum variance prediction $\mathbf{x}_{k|k} = E\left\{\mathbf{x}_k | \mathcal{Y}_k\right\}$ can be formulated as the generalised least squares problem

$$\min_{\mathbf{x}} \mathbf{s}^T \mathbf{s}; \; \text{diag}\left\{S_{i-1|i-1}^{1/2}, R_{i-1}^{1/2}, V_i^{1/2}\right\} \mathbf{s} = X\mathbf{x} - \mathbf{y},$$

$$X = \begin{bmatrix} I & 0 \\ -X_{i-1} & I \\ 0 & H_i \end{bmatrix}, \; \mathbf{y} = \begin{bmatrix} \mathbf{x}_{i-1|i-1} \\ 0 \\ \mathbf{y}_i \end{bmatrix}, \; \mathbf{x} = \begin{bmatrix} \mathbf{x}_{i-1} \\ \mathbf{x}_i \end{bmatrix},$$

with output $\mathbf{x}_{i-1|i}, \mathbf{x}_{i|i}$.

17. **V-invariant filter example**. Example due to Inge Söderkvist (CTAC 1995)

$$
\begin{aligned}
X_i &= I_2,\ R_i = I_2,\ i \neq 3,\ I_3 = \begin{bmatrix} k^2 & \\ & 1/k^2 \end{bmatrix}, \\
H_i &= \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix},\ V_i = I_2, \\
\mathbf{y}_i &= \begin{bmatrix} 15 \\ 5 \end{bmatrix},\ i = 1, 2, \cdots, 5, \\
\mathbf{x}_{1|0} &= \begin{bmatrix} 10 \\ 5 \end{bmatrix} = \mathbf{x}_i,\ \text{independent of covariances}, \\
S_{1|0} &= I_2.
\end{aligned}
$$

18. **Sorting of D_i.** An analogue of the sorting of the D_i has occurred before. Consider the penalised formulation of the constrained least squares problem

$$\min_{\mathbf{x}} \left\{ \|\mathbf{r}_2\|^2 + \left\| \lambda^{1/2} \mathbf{r}_1 \right\|^2 \right\}.$$

This can be solved by an orthogonal factorization of the matrix

$$\begin{bmatrix} \lambda^{1/2} A_1 \\ A_2 \end{bmatrix}.$$

Easy to see there is trouble if system not ordered so large rows are first (or row interchanges used). Result due to Powell and Reid, IFIP 1968. Consider

$$\begin{bmatrix} 0 & 2 & 1 \\ 10^6 & 10^6 & 0 \\ 10^6 & 0 & 10^6 \\ 0 & 1 & 1 \end{bmatrix}.$$

If row interchanges are not used in first step of orthogonal factorization then all information on first row is lost in five decimal arithmetic.