

Electronic Supplementary Material to
Quantifying Adventitious Error in a Covariance Structure as a Random Effect
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This file contains the descriptions of the three MATLAB functions in the supplementary material.

1. File `MBLE.m`

This file involves a function `MBLE` that computes the maximum beta likelihood estimates of parameters from a given sample covariance matrix. It invokes another function `FgH` inside the same file that computes the value, gradient and Hessian matrix of the per-sample-size discrepancy function F . To be consistent with the symbol in the MATLAB file, we use s as the number of structural parameters instead of q .

1.1. *Input and output*

```
function [theta,v,err,Ohat,H]=...  
MBLE(S,df,nn,theta0,v0,funn,vfree,pr,bd,thrs,btol,maxiter,varargin)
```

Input arguments to the function `MBLE`

- `df` is the degrees of freedom. For unadjusted discrepancy function, use $p(p+1)/2$.
- `S` is the sample covariance matrix \mathbf{S} .
- `nn` is the df of the Wishart distribution $(\mathbf{S}|\boldsymbol{\Sigma}) \sim W_p(\boldsymbol{\Sigma}/n, n)$.

- **theta0** is the initial value of structure parameters ξ in the model.

- **v0** is the initial value of $v = 1/m$.

- **funn** is a function handle of the covariance structure of the form

`[O,err,R,d0dx,iRd0dx]=fun(theta,...)`

whose input and output arguments must be in the following format:

- **theta**: a row vector of parameters, ξ' .
- **O**: the model implied covariance matrix Ω .
- **[R,err]=chol(O)**; i.e. **R** is the upper triangular Cholesky factor \mathbf{R}_Ω of Ω and **err** is 0 if Ω is positive definite but greater than 0 if not.
- **d0dx**: the derivative of Ω , Δ , a p^2 by s matrix
- **iRd0dx**: $(\mathbf{R}'_\Omega \otimes \mathbf{R}'_\Omega)^{-1} \Delta$, an expression to be used frequently.

- **vfree** denotes whether $v = 1/m$ is treated as fixed or not:

- If **vfree=0**, v is fixed at **v0**;
- If it takes other values, v is estimated.

- **pr** prints iteration details:

- **0**: none;
- **1**: only **F**, **Res.Cos**, **cond.#.H**, **NPB** and **NEC**;
- **2**: only parameter values;
- **3**: both details in 1 and 2.

- **bd** is a matrix of size $s \times 2$, giving boundary conditions of the structural parameters.

Default value is $[-\infty, \infty]$ for all structural parameters. Boundaries of v $[0, 1/(p-1)]$ are automatically added.

- **thrs** is the threshold to stop the iterations. Default value is 10^{-7} .

- `btol` is matrix of boundary thresholds. It can be a scalar, a column vector or a 2-columned matrix.
 - a scalar: to be used for both the lower and upper boundaries of all structural parameters.
 - a column vector of length s : to be used for both the lower and upper boundaries.
 - a 2-columned matrix: specifies the threshold of each boundary of each structural parameter.

Default value is 10^{-8} . The boundary thresholds for v is 0 and 10^{-8} for the lower and upper bounds.

- `maxiter` is the maximum iterations allowed. Default value is 200.
- `varargin` passes arguments to `funn`, the function handle.

Output arguments from the function `MBLE`

- `theta` is the parameter estimate.
- `v` is the estimate \hat{v}_0 . It allows negative values.
- `err>0` means nonconvergence.
- `Ohat` is the estimated covariance matrix.
- `H` is the approximate Hessian for the covariance structure parameters.

Screen Outputs from the function `MBLE`

- `#`: iteration number
- `F`: discrepancy function value (per sample size)
- `Res.Cos`: residual cosine
- `cond.#.H`: (approximate) condition number of `H` (block for unconstrained parameters)

- NPB: number of parameters on boundary
- NEC: number of effective constraints
- `parameters`: parameter values, the first one is v , followed by structural parameters.

1.2. Details of file `MBLE.m`

Global parameters

- `n=nn`.
- `vfr=vfree`
- `fun=funn`.
- `other=varargin`.
- `p`: The number of variables.
- `s`: The number of structural parameters.
- `CS`: The upper triangular Cholesky factor \mathbf{R}_S of \mathbf{S} .
- `detS`: The determinant of \mathbf{S} .
- `alpha`: The correction factor $\alpha = 2df/p(p+1)$.
- `coef`: A row vector of coefficients $(c_0, c_1, c_2, 2c_3)'$ in Lemma 5 of the paper.

Algorithm: Newton-Raphson with approximate Hessian.

- Target function `f` is in fact the per-sample-size discrepancy function F/n , where F is given by Equation 18 in the paper.
- The gradient of F w.r.t v and $\boldsymbol{\xi}$ are given in Section 5.2 of the paper. The actual gradient used is $(\frac{\partial(F/n)}{\partial(nv)}, \frac{\partial(F/n)}{\partial\boldsymbol{\xi}'})'$.

- The approximate Hessian matrix is $\text{diag} \left\{ \frac{\partial^2(F/n)}{\partial(nv)^2}, E \frac{\partial^2(F/n)}{\partial \boldsymbol{\xi} \partial \boldsymbol{\xi}'} \right\}$, where the elements are given in the Appendix B of the paper. Note the first element takes its (approximated) expected value if it is negative.
- Convergence criterion: $\min \left\{ f, \max_i \frac{g_i^2}{h_{ii}f} \right\}$, where the maximum only concerns the parameters not subject to an active boundary.
- If one move results in a higher, infinite or NA target function value, the step is halved until a value smaller than the current target function value is obtained.
- If one move results in one or more parameters outside their boundary, the move is shortened so that the resultant parameter value is on the boundary.
- When boundary parameters are present at one iteration, an unconstrained search is first attempted. If this search moves the iteration away from the boundary, it is executed; if not, the search is constrained on the boundary.

1.3. Sub-function FgH

`function [f,err,g,H]=FgH(theta,f0)`

Input arguments to the sub-function FgH

- **theta**: proposed next position of the full parameter vector, the first element being v .
- **f0**: the target function value at the current iteration.

Output arguments from the sub-function FgH

- **f**: target function value.
- **err**: whether the proposed move is admissible
 - > 0 : The new target function value is infinite, NA or higher than **f0**.
 - 0 : The new target function value is admissible.

- \mathbf{g} : the derivative of \mathbf{f} , or F/n , w.r.t. $(nv, \boldsymbol{\xi})$.
- \mathbf{H} : the approximate Hessian matrix.

Calculation of \mathbf{f} , \mathbf{g} and \mathbf{H} in the sub-function \mathbf{FgH} :

- Variables defined in the intermediate steps:
 - $\text{fac} = 1 + nv$.
 - \mathbf{R} : The upper triangular Cholesky factor \mathbf{R}_Ω of $\boldsymbol{\Omega}$.
 - $\mathbf{A} = \mathbf{R}_s \mathbf{R}_\Omega^{-1}$.
 - $\text{iOS} = \mathbf{A}' \mathbf{A} = \mathbf{R}_\Omega^{-1'} \mathbf{S} \mathbf{R}_\Omega^{-1}$.
 - $\text{iOaveOS} = (\mathbf{I} + nv \mathbf{R}_\Omega^{-1'} \mathbf{S} \mathbf{R}_\Omega^{-1}) / (1 + nv) = \mathbf{R}_\Omega^{-1'} \bar{\boldsymbol{\Sigma}} \mathbf{R}_\Omega^{-1}$.
 - $\text{dif} = \mathbf{R}_\Omega^{-1'} \mathbf{S} \mathbf{R}_\Omega^{-1} - \mathbf{I}$.
 - $\text{WLS} = \text{tr}(\boldsymbol{\Omega}^{-1} \mathbf{S} - \mathbf{I})^2$.
 - $\mathbf{B} = \frac{1}{1 + nv} \mathbf{R}_\Omega^{-1'} (\boldsymbol{\Omega} - \mathbf{S}) \bar{\boldsymbol{\Sigma}}^{-1} \mathbf{R}_\Omega = \frac{m}{n} \left\{ \mathbf{R}_\Omega \bar{\boldsymbol{\Sigma}}^{-1} \mathbf{R}_\Omega - \mathbf{I} \right\}$
- Gradient and Hessian w.r.t $\boldsymbol{\xi}$.
 - $\text{dFdx}: \partial f / \partial \boldsymbol{\xi} = m \boldsymbol{\Delta}' (\bar{\boldsymbol{\Sigma}} \otimes \boldsymbol{\Omega})^{-1} (\boldsymbol{\omega} - \mathbf{s}) / (m + n)$
 - $\text{d2Fdx dx}: \partial^2 f / \partial \boldsymbol{\xi} \partial \boldsymbol{\xi}' = m \boldsymbol{\Delta}' (\boldsymbol{\Omega} \otimes \boldsymbol{\Omega})^{-1} \boldsymbol{\Delta} / (m + n)$.
- Target function value $\mathbf{f} = F/n$.

$$F_1 = 2 \sum_i \left(\ln \Gamma \left[\frac{m - i + 1}{2} \right] - \ln \Gamma \left[\frac{m - i + n + 1}{2} \right] \right) - mp \ln \frac{m}{2} + (m + n)p \ln \frac{m + n}{2} - np$$

$$F_2/n = \ln(|\boldsymbol{\Omega}|/|\mathbf{S}|) + (1 + m/n) \ln |\bar{\boldsymbol{\Sigma}} \boldsymbol{\Omega}^{-1}|$$

$$F_{(\alpha)}/n = \alpha F_1/n + F_2/n$$

- If $v = 0$: $F/n = \ln(|\boldsymbol{\Omega}|/|\mathbf{S}|) + \text{tr}(\boldsymbol{\Omega}^{-1} \mathbf{S} - \mathbf{I})$
- If $(p = 1 \text{ and } v \leq 0.02)$ or $(p > 1 \text{ and } (p - 1)v < .02)$: F_1 is approximated by

$$F_1/n = \frac{c_0 \ln(1 + nv)}{n} + \frac{c_1}{m(m + n)} + \frac{c_2(2m + n)}{m^2(m + n)^2} + \frac{2c_3(3m(m + n) + n^2)}{m^3(m + n)^3}$$

where $c_0 - c_3$ are defined in Lemma 5 of the paper.

- Gradient w.r.t. v : $dFdv = \partial(F_{(\alpha)}/n)/\partial v$.

$$\begin{aligned}\frac{\partial F_1}{\partial m} &= \sum_i \left(\psi \left[\frac{m-i+1}{2} \right] - \psi \left[\frac{m-i+n+1}{2} \right] + \ln(1+nv) \right) \\ \frac{\partial F_2}{\partial m} &= \ln |\mathbf{R}_\Omega^{-1} \bar{\Sigma} \mathbf{R}_\Omega^{-1}| + \text{tr} \left\{ \mathbf{R}_\Omega \bar{\Sigma}^{-1} \mathbf{R}_\Omega - \mathbf{I} \right\} \\ \frac{\partial(F_{(\alpha)}/n)}{\partial v} &= -\frac{m^2}{n} \left(\alpha \frac{\partial F_1}{\partial m} + \frac{\partial F_2}{\partial m} \right)\end{aligned}$$

– If v is fixed in the optimization, $dFdv$ is set to 0.

– If $v = 0$: $\partial(F/n)/\partial v = \alpha p(p+1)/2 - n \text{tr}(\mathbf{\Omega}^{-1} \mathbf{S} - \mathbf{I})^2/2$.

– If $(p = 1 \text{ and } v \leq 0.02)$ or $(p > 1 \text{ and } (p-1)v < .02)$ we use the following approximation:

$$-\frac{m^2}{n} \frac{\partial F_1}{\partial m} = c_0 \frac{m}{m+n} + c_1 \frac{2m+n}{(m+n)^2} + c_2 \frac{2(3m(m+n) + n^2)}{m(m+n)^3} + 2c_3 \frac{3(m^2(4m+6n) + n^2(4m+n))}{m^2(m+n)^4}$$

where $c_0 - c_3$ are defined in Lemma 5 of the paper.

- Approximate Hessian w.r.t. v : $d^2Fdv^2 = \partial^2(F/n)/\partial v^2$.

$$\begin{aligned}\frac{\partial^2 F_1}{\partial m^2} &= \frac{1}{2} \sum \left(\left(\psi_1 \left[\frac{m-i+1}{2} \right] - 2v \right) - \left(\psi_1 \left[\frac{m-i+n+1}{2} \right] - \frac{2}{m+n} \right) \right) \\ \frac{\partial^2 F_2}{\partial m^2} &= -\frac{1}{m+n} \text{tr} \left\{ \mathbf{R}_\Omega \bar{\Sigma}^{-1} \mathbf{R}_\Omega - \mathbf{I} \right\}^2 \\ \frac{\partial^2(F_{(\alpha)}/n)}{\partial v^2} &= \frac{\alpha}{n} \left(m^4 \frac{\partial^2 F_1}{\partial m^2} + 2m^3 \frac{\partial F_1}{\partial m} \right) + \frac{m^4}{n} \frac{\partial^2 F_2}{\partial m^2} + 2 \frac{m^3}{n} \frac{\partial F_2}{\partial m}\end{aligned}$$

– If v is fixed in the optimization, d^2Fdv^2 is set to 1.

– If $v = 0$: $\partial^2(F/n)/\partial v^2 = n^2 \{ \text{tr}(\mathbf{\Omega}^{-1} \mathbf{S} - \mathbf{I})^2 - \frac{2}{3} \text{tr}(\mathbf{\Omega}^{-1} \mathbf{S} - \mathbf{I})^3 \} + \alpha \{ -c_0 n + 2c_1 \}$.

– If $(p = 1 \text{ and } v \leq 0.02)$ or $(p > 1 \text{ and } (p-1)v < .02)$ we use the following approximation:

$$\begin{aligned}\frac{m^4}{n} \frac{\partial^2 F_1}{\partial m^2} + \frac{2m^3}{n} \frac{\partial F_1}{\partial m} &= -\frac{c_0 n m^2}{(n+m)^2} + \frac{2c_1 m^3}{(n+m)^3} + \frac{2c_2(3m^3 + (m+n)(n^2 + 3m(m+n)))}{(m+n)^4} \\ &\quad + \frac{(2c_3)6[2m^4 + (n+m)(n^3 - 2m^2n + 4m(m+n)^2)]}{m(m+n)^5}\end{aligned}$$

– If the value obtained above is not positive, we use

$$\frac{\partial^2(F_{(\alpha)}/n)}{\partial v^2} = \alpha \left(-\frac{c_0 m^2 n^2}{(m+n)^2} + \frac{2c_1 m^3 n}{(m+n)^3} \right) + \frac{2m^2 n (c_0 n + c_1)}{(m+n)^2} + \frac{2c_1 m n}{m+n} + \frac{m^3 n p (p+3)}{(m+n)^3}$$

2. File MWLE.m

This file involves a function `MWLE` that computes the maximum Wishart likelihood estimates of parameters from a given sample covariance matrix. It is a simplified version of `MBLE.m` for the special case where v is set to 0. In this case, the algorithm becomes a Fisher scoring algorithm. We only list the input and output of this function. For details see notes to the file `MBLE.m`

```
function [theta,err,F,Ohat,H]=...  
MWLE(S,theta0,fun,pr,bd,thrs,btol,maxiter,varargin)
```

Input arguments to the function `MWLE`

- `S` is the sample covariance matrix \mathbf{S} .
- `theta0` is the initial value of structure parameters ξ in the model.
- `fun` is a function handle of the covariance structure of the form

```
[O,err,R,d0dx,iRd0dx]=fun(theta,...)
```

whose input and output arguments must be in the following format:

- `theta`: a row vector of parameters, ξ' .
 - `O`: the model implied covariance matrix Ω .
 - `[R,err]=chol(O)`; i.e. `R` is the upper triangular Cholesky factor \mathbf{R}_Ω of Ω and `err` is 0 if Ω is positive definite but greater than 0 if not.
 - `d0dx`: the derivative of Ω , Δ , a p^2 by s matrix
 - `iRd0dx`: $(\mathbf{R}'_\Omega \otimes \mathbf{R}'_\Omega)^{-1} \Delta$, an expression to be used frequently.
- `pr` prints iteration details:
 - 0: none;
 - 1: only `F`, `Res.Cos`, `cond.#.H`, `NPB` and `NEC`;
 - 2: only parameter values;

- 3: both details in 1 and 2.
- **bd** is a matrix of size $s \times 2$, giving boundary conditions of the structural parameters. Default value is $[-\infty, \infty]$ for all structural parameters.
- **thrs** is the threshold to stop the iterations. Default value is 10^{-7} .
- **btol** is matrix of boundary thresholds. It can be a scalar, a column vector or a 2-columned matrix.
 - a scalar: to be used for both the lower and upper boundaries of all structural parameters.
 - a column vector of length s : to be used for both the lower and upper boundaries.
 - a 2-columned matrix: specifies the threshold of each boundary of each structural parameter.

Default value is 10^{-8} . The boundary thresholds for v is 0 and 10^{-8} for the lower and upper bounds.

- **maxiter** is the maximum iterations allowed. Default value is 200.
- **varargin** passes arguments to **funn**, the function handle.

Output arguments from the function **MWLE**

- **theta** is the parameter estimate.
- **err>0** means nonconvergence.
- **F** is the MWL discrepancy function value.
- **Ohat** is the estimated covariance matrix.
- **H** is the approximate Hessian for the covariance structure parameters.

Screen outputs (first stage) from the function **MWLE**

- #: iteration number
- F: inverse Wishart discrepancy function value
- Res.Cos: residual cosine
- cond.#.H: (approximate) condition number of H (block for unconstrained parameters)
- NPB: number of parameters on boundary
- NEC: number of effective constraints
- parameters: values of the structural parameters.

Screen outputs (second stage) from the function MWLE

- #: iteration number
- F: inverse Wishart -2 log-likelihood value (less a constant)
- Res.Cos: residual cosine
- H: value of h_{vv} , the second derivative.
- v: value of v

3. File MIWLE.m

This file involves a function MIWL that computes the maximum inverse Wishart likelihood estimates of parameters from a given population covariance matrix. It involves two sub-functions: FgHtheta computes the value, gradient and Hessian of the MIWL discrepancy function; FgHv computes the gradient and Hessian used in the second stage of optimization.

3.1. Input and Output

```
function [theta,v,err,F0,Ohat,H0]=...
MIWLE(SS,df,theta0,v0,funn,vfr,pr,bd,thrs,btol,maxiter,varargin)
```

Input arguments to the function MIWL.m

- **df** is the degrees of freedom. For unadjusted discrepancy function, use $p(p + 1)/2$.
- **SS** is the input covariance matrix Σ .
- **theta0** is the initial value of structure parameters ξ in the model.
- **v0** is the initial value of $v = 1/m$.

- **funn** is a function handle of the covariance structure of the form

`[0,err,R,d0dx,iRd0dx]=fun(theta,...)`

whose input and output arguments must be in the following format:

- **theta**: a row vector of parameters, ξ' .
- **0**: the model implied covariance matrix Ω .
- **[R,err]=chol(0)**; i.e. **R** is the upper triangular Cholesky factor \mathbf{R}_Ω of Ω and **err** is 0 if Ω is positive definite but greater than 0 if not.
- **d0dx**: the derivative of Ω , Δ , a p^2 by s matrix
- **iRd0dx**: $(\mathbf{R}'_\Omega \otimes \mathbf{R}'_\Omega)^{-1} \Delta$, an expression to be used frequently.
- **vfr** denotes whether $v = 1/m$ is treated as fixed or not:
 - If **vfr=0**, v is fixed at **v0**;
 - If it takes other values, v is estimated.
- **pr** prints iteration details:
 - 0: none;
 - 1: only **F**, **Res.Cos**, **cond.#.H**, **NPB** and **NEC**;
 - 2: only parameter values;
 - 3: both details in 1 and 2.
- **bd** is a matrix of size $s \times 2$, giving boundary conditions of the structural parameters. Default value is $[-\infty, \infty]$ for all structural parameters.

- `thrs` is the threshold to stop the iterations. Default value is 10^{-7} .
- `btol` is matrix of boundary thresholds. It can be a scalar, a column vector or a 2-columned matrix.
 - a scalar: to be used for both the lower and upper boundaries of all structural parameters.
 - a column vector of length s : to be used for both the lower and upper boundaries.
 - a 2-columned matrix: specifies the threshold of each boundary of each structural parameter.

Default value is 10^{-8} . The boundary threshold for v is 10^{-7} for both the lower and upper bounds.

- `maxiter` is the maximum iterations allowed. Default value is 200.
- `varargin` passes arguments to `funn`, the function handle.

Output arguments from the function `MIWLE`

- `theta` is the parameter estimate.
- `v` is the estimate of v_0 . It allows negative values.
- `err>0` means nonconvergence.
- `F0` is the inverse Wishart discrepancy function value.
- `Ohat` is the estimated covariance matrix.
- `H0` is the approximate Hessian for the covariance structure parameters.

Screen Outputs from the function `MIWLE`

- `#`: iteration number
- `F`: discrepancy function value (per sample size)

- `Res.Cos`: residual cosine
- `cond.#.H`: (approximate) condition number of \mathbf{H} (block for unconstrained parameters)
- `NPB`: number of parameters on boundary
- `NEC`: number of effective constraints
- `parameters`: structural parameter values

3.2. Details of file *MIWLE.m*

Global parameters

- `S=SS`.
- `fun=funn`.
- `other=varargin`.
- `p`: The number of variables.
- `CS`: The upper triangular Cholesky factor \mathbf{R}_S of \mathbf{S} .
- `detS`: The determinant of \mathbf{S} .
- `alpha`: The correction factor $\alpha = 2df/p(p+1)$.
- `coef`: A row vector of coefficients $(c_0, c_1, c_2, 2c_3)'$ in Lemma 5 of the paper.

Algorithm Stage I: Estimating the structural parameters through Fisher-scoring

- Target function \mathbf{f} is the MIWL discrepancy function given by Equation 12 in Section 4.3.1 of the paper.
- The gradient and Fisher information matrix of F w.r.t $\boldsymbol{\xi}$ are given in Section 4.3.1 of the paper.
- Convergence criterion: $\min \left\{ f, \max_i \frac{g_i^2}{h_{ii}f} \right\}$, where the maximum only concerns the parameters not subject to an active boundary.

- If one move results in a higher, infinite or NA target function value, the step is halved until a value smaller than the current target function value is obtained.
- If one move results in one or more parameters outside their boundary, the move is shortened so that the resultant parameter value is on the boundary.
- When boundary parameters are present at one iteration, an unconstrained search is first attempted. If this search moves the iteration away from the boundary, it is executed; if not, the search is constrained on the boundary.

Algorithm Stage II: Estimating parameter v

- The target function $\alpha f(m) + m\hat{F}^{IW}$ minimized by Newton's method, where \hat{F}^{IW} has been obtained through Stage I.
- The derivative is $g = -m^2(\alpha f'(m) + \hat{F}^{IW})$.
- The second derivative is $H = m^4\alpha f''(m) + 2m^3(\alpha f'(m) + \hat{F}^{IW})$. Note $H > 0$ because $f'(m)$ is monotonically increasing.
- Convergence criterion: g^2/H .
- Other details similar to Stage I.

3.3. Sub-function *FgHtheta*

function [f,err,g,H]=FgHtheta(theta,f0)

Input arguments to the sub-function *FgHtheta*

- **theta**: proposed next position of ξ .
- **f0**: the MIWL discrepancy function value at the current iteration.

Output arguments from the sub-function *FgHtheta*

- **f**: MIWL discrepancy function value.

- **err**: whether the proposed move is admissible
 - > 0 : The new target function value is infinite, NA or higher than f_0 .
 - 0 : The new target function value is admissible.
- **g**: the derivative of F^{IW} .
- **H**: the Fisher information matrix.

3.4. Sub-function $FgHv$

`function [f,errv,dfdvd,d2fdv2]=FgHv(v,F0,f0)`

Input arguments to the sub-function $FgHv$

- **v**: proposed next position of v .
- **f0**: the stage II target function value at the current iteration.
- **F0**: the inverted Wishart discrepancy function value obtained in stage I.

Output arguments from the sub-function $FgHv$

- **f**: the target function.
- **err**: whether the proposed move is admissible
 - > 0 : The new target function value is infinite, NA or higher than f_0 .
 - 0 : The new target function value is admissible.
- **g**: the derivative of the target function.
- **H**: the second derivative of the target function.