Structured Weighted Low Rank Approximation and Structured Total Least Squares

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Structured Weighted Low Rank Approx.

How to solve the following equivalent double-minimization problem:

$$\min_{\substack{N\in\mathbb{R}^{ns\times(ns-r)}\\ N^TN=I}} \left(\min_{\substack{R\in\mathbb{R}^{m\times ns}\\ RN=0}} ||H-R||_W^2 \right)?$$

with

- $H\in\mathbb{R}^{m\times ns}$ a given block-row Hankel matrix with blocks of size $1\times s$
- $||H-R||_W^2 = vec_2(H-R)^T * W * vec_2(H-R)$
- W a positive definite symmetric weighting matrix
- $vec_2(A)$ a minimal vector representation of a block-row Hankel matrix A.

Different steps to solve the problem:

(1) find analytical an expression for $f(N)$:

$$f(N) = \min_{\substack{R\in\mathbb{R}^{m\times ns}\\ RN=0}} ||H-R||_W^2$$

(2) minimizing f on a Grassmann manifold $G_{(ns-r),ns}$.

Solution to (1)

To find the minimizing R, we use the Lagrange multipliers method: the Lagrangian is the following:

$$\psi(L,R) := vec_2(H-R)^T W vec_2(H-R) - tr(L^T RN).$$

If we set the partial derivatives of ψ w.r.t. L and R equal to zero, an expression for $vec_2(R)$ is found:

$$\begin{aligned} vec_2(R) = {} & (I_q - W^{-1}H_1^T(N\otimes I_m)[(N\otimes I_m)^T \\ & H_1W^{-1}H_1^T(N\otimes I_m)]^{-1}(N\otimes I_m)^T H_1)vec_2(H) \end{aligned}$$

As a result, the double minimization problem can be written as the following optimization problem:

$$\min_{\substack{N\in\mathbb{R}^{ns\times(ns-r)}\\ N^TN=I}} vec_2(H)^T H_2^T (H_2 W^{-1} H_2^T)^{-1} H_2 vec_2(H) \quad (*),$$

with $H_2 \equiv (N\otimes I_n)^T H_1$.Define $\Delta r = ns - r$.

Solution to (2)

The straightforward approach for solving $(*)$ would be by applying a non-linear least squares (NLLS) solver:

$*$ For $\Delta r = 1$: OK
$*$ For $\Delta r > 1$: $R=0$

Trivial solution NOT very surprising: The inner minimization $\equiv$ an orthogonal projection of $vec_2(H)$ on the orthogonal complement of the column space of $H_2^T \in \mathbb{R}^{s(n+m-1)\times m\Delta r}$.
To avoid this problem: rearranging the elements of H into a matrix $\tilde{H}^T$ with $r+1$ rows:

$$\tilde{H}^T = \begin{bmatrix} h_1 & h_2 & h_3 & \dots & h_n & \dots & h_{n+m-r-1} \\ h_2 & h_3 & \dots & & & & \\ h_3 & \dots & & & & & \\ \vdots & & & & & & \vdots \\ h_{r+1} & \dots & & & & \dots & h_{n+m-1} \end{bmatrix}$$

with h_i a row vector of length s for $i=1,\dots,n+m-1$ and applying the described method to $\tilde{H}$.

This time the optimization problem is the following ($\diamondsuit$):

$$\min_{\substack{\tilde{N}\in\mathbb{R}^{(r+1)\times 1}\\ \tilde{N}^T\tilde{N}=I}} vec_2(\tilde{H})^T \tilde{H}_2^T (\tilde{H}_2 W^{-1} \tilde{H}_2^T)^{-1} \tilde{H}_2 vec_2(\tilde{H}),$$

with $\tilde{H}_2 \equiv (\tilde{N}\otimes I)^T \tilde{H}_1 \in \mathbb{R}^{s(n+m-r-1)\times s(n+m-1)}$ and I the identity matrix of size $s(n+m-r-1)$.

A formulation of the vectorized form of $\tilde{R}$ is equal to ($\star$):

$$\begin{aligned} vec_2(\tilde{R}) = {} & (I_q - W^{-1}\tilde{H}_1{}^T(\tilde{N}\otimes I)[(\tilde{N}\otimes I)^T \\ & \tilde{H}_1 W^{-1}\tilde{H}_1{}^T(\tilde{N}\otimes I)]^{-1}(\tilde{N}\otimes I)^T\tilde{H}_1)vec_2(\tilde{H}) \end{aligned}$$

Algorithm block-row SWLRA

Input: block-row Hankel matrix $H\in\mathbb{R}^{m\times ns}$ with blocks=row vectors $h_1, h_2, \dots, h_{n+m-1}$ of length s, rank r and weighting matrix W.
Output: block-row Hankel matrix R of rank $\le r$, such that R is as close as possible to H in $\|.\|_W$-sense.
Begin:

Step 1 Construct matrix $\tilde{H}$ by rearranging the elements of matrix H such that $\tilde{H}\in\mathbb{R}^{s(n+m-r-1)\times(r+1)}$ is a block Hankel matrix with blocks=column vectors $h_1^T,\dots,h_{n+m-1}^T$.
Step 2 Compute SVD of $\tilde{H}$: $\tilde{H} = U\Sigma V^T$.
Step 3 Take starting value p_0 equal to the $(r+1)$-right singular vector of $\tilde{H}$.
Step 4 Minimize the cost function in ($\star$).
Step 5 Compute $\tilde{R}$ using ($\diamondsuit$).
Step 6 Rearrange the elements of $\tilde{R}$ into a matrix R such that $R\in\mathbb{R}^{m\times ns}$ and R has the same structure as H.

Structured Total Least Squares

Problem formulation

Consider the multivariate linear errors-in-variables (EIV) model

$$AX\approx B, \qquad A=\bar{A}+\tilde{A}, \qquad B=\bar{B}+\tilde{B}, \qquad \bar{A}\bar{X}=\bar{B}.$$

$A\in\mathbb{R}^{m\times n}$, $B\in\mathbb{R}^{m\times d}$, $nd \ll m$, are observations, and $X\in\mathbb{R}^{n\times d}$ is a parameter of interest. $\bar{A}$, $\bar{B}$ are true values and $\tilde{A}$, $\tilde{B}$ are noises.
Assume that there is an a priori known affine function $\mathcal{S}:\mathbb{R}^{n_p}\to\mathbb{R}^{m\times(n+d)}$

$$\mathcal{S}(p) = S_0 + \textstyle\sum_{l=1}^{n_p} S_l p_l,$$

($\mathbb{R}^{n_p}$ is the parameter space and p the structure parameter) such that

$$C := \begin{bmatrix} A & B \end{bmatrix} = \mathcal{S}(p) \quad\text{and}\quad \bar{C} := \begin{bmatrix} \bar{A} & \bar{B} \end{bmatrix} = \mathcal{S}(\bar{p}).$$

The structured total least squares (STLS) problem is defined by the following optimization problem:

$$\min_{X,\Delta p} \left\| V_{\tilde{p}}^{-1/2}\Delta p \right\|_2^2 \quad \text{s.t.} \quad \mathcal{S}(p-\Delta p)\begin{bmatrix} X \\ -I_d \end{bmatrix} = 0,$$

We describe numerical algorithms with linear in the sample size m, computational complexity that can deal with a flexible structure specification $C=[C_1\cdots C_q]$, where the blocks C_i are Toeplitz, Hankel, unstructured, or noise free.

Equivalent optimization problem

First we derive an equivalent optimization problem $\min_X f_0(X)$ by eliminating the correction Δp

$$f_0(X) := \min_{\Delta p} ||V_{\tilde{p}}^{-1/2}\Delta p||^2 \quad \text{s.t.} \quad \mathcal{S}(p-\Delta p)\left[\begin{smallmatrix} X \\ -I \end{smallmatrix}\right] = 0. \tag{1}$$

Let $\mathbf{E}$ denotes expectation. Define $R(X) := AX - B = C\left[\begin{smallmatrix} X \\ -I \end{smallmatrix}\right]$,

$$r(X) := \operatorname{vec}\big(R^\top(X)\big) = \operatorname{vec}\big(\begin{bmatrix} r_1(X) & \cdots & r_m(X) \end{bmatrix} \big) = \begin{bmatrix} r_1(X) \\ \vdots \\ r_m(X) \end{bmatrix},$$

and the random part $\tilde{R} := R - \mathbf{E}R = \tilde{A}X - \tilde{B} = \tilde{C}X_{\text{ext}}$ of the residual.
$\mathcal{S}$ is affine, so that the constraint of (1) is linear in Δp

$$\mathcal{S}(p-\Delta p)X_{\text{ext}} = 0 \iff r(X) = G(X)\Delta p,$$

where

$$G(X) := \begin{bmatrix} \operatorname{vec}\big((S_1X_{\text{ext}})^\top\big) & \cdots & \operatorname{vec}\big((S_{n_p}X_{\text{ext}})^\top\big) \end{bmatrix}.$$

Then (1) is a least norm problem and its solution is

$$\Delta p_{\min}(X) = V_{\tilde{p}}G^\top(X)\big(G(X)V_{\tilde{p}}G^\top(X)\big)^{-1}r(X),$$

so that

$$\begin{aligned} f_0(X) &= \Delta p_{\min}^\top(X) V_{\tilde{p}}^{-1}\Delta p_{\min}(X) \\ &= r^\top(X)\big(G(X)V_{\tilde{p}}G^\top(X)\big)^{-1}r(X) \\ &=: r^\top(X)\Gamma^{-1}(X)r(X). \end{aligned} \tag{2}$$

The weight matrix Γ is the covariance matrix of $\tilde{r}$. Indeed, we have

$$G(X)V_{\tilde{p}}G^\top(X) = \mathbf{E}\big(G(X)\tilde{p}\big)\big(G(X)\tilde{p}\big)^\top,$$

but $\tilde{r}(X) = \operatorname{vec}\big(\tilde{R}^\top(X)\big) = G(X)\tilde{p}$, so that

$$\Gamma(X) = G(X)V_{\tilde{p}}G^\top(X) = \mathbf{E}\tilde{r}(X)\tilde{r}^\top(X) =: V_{\tilde{r}}(X). \tag{3}$$

Properties of the covariance matrix $V_{\tilde{r}}$

Only the assumption that $\mathcal{S}$ is an affine function was used in the derivation of the equivalent problem. Now we give the following additional assumptions:

(i). $\exists\ T\in\{0,1,\dots,n_p\}^{m\times(n+d)}$ s.t. $S_l(i,j) = \begin{cases} 1, & \text{if } T(i,j)=l \\ 0, & \text{otherwise} \end{cases}$

(ii). $T = \begin{bmatrix} T_1 & \cdots & T_q \end{bmatrix}$, where $T_i\in\{0,1,\dots,n_p\}^{m\times n_i}$ is:
`T` — Toeplitz, `H` — Hankel, `U` — unstructured, or `F` — noise free

(iii). $V_{\tilde{p}} = \operatorname{blk\,diag}\{V,\dots,V\}$, where $V\in\mathbb{R}^{(n+d)\times(n+d)}$, and $V>0$

The structure is specified by S_0 and $\mathcal{T}\in\{\{\mathtt{T},\mathtt{H},\mathtt{U},\mathtt{F}\}\times\mathbb{N}\}^q$, where $\mathcal{T}$ describes the structure of the blocks $\{T_k\}_{k=1}^q$. Assumptions (i)–(iii) are the basic assumptions for consistency.
Let $\tilde{c} := \operatorname{vec}(\tilde{C}^\top)$, $V_{\tilde{c}} := \mathbf{E}\tilde{c}\tilde{c}^\top$, and $V_{\tilde{c},ij}\in\mathbb{R}^{d\times d}$ be its (i,j)-th block.

$$V_{\tilde{r},ij}(X) = X_{\text{ext}}^\top V_{\tilde{c},ij}X_{\text{ext}} \in \mathbb{R}^{d\times d}$$

Due to our assumptions $V_{\tilde{c},ij} = V_{\tilde{c},i-j}$, $V_{\tilde{c},ij} = 0$ for $|i-j| \ge s+1$. Thus $V_{\tilde{r}}(X)$ has the block banded Toeplitz structure,

$$V_{\tilde{r}}(X) = \begin{bmatrix} V_{\tilde{r},0} & V_{\tilde{r},-1} & \cdots & V_{\tilde{r},-s} & & 0 \\ V_{\tilde{r},1} & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & V_{\tilde{r},-s} \\ V_{\tilde{r},s} & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & V_{\tilde{r},-1} \\ 0 & & V_{\tilde{r},s} & \cdots & V_{\tilde{r},1} & V_{\tilde{r},0} \end{bmatrix}, \quad \begin{aligned} V_{\tilde{r},k}(X) &= V_{\tilde{r},-k}^\top(X) \\ V_{\tilde{c},k} &= V_{\tilde{c},-k}^\top \end{aligned}. \tag{4}$$

Proposed numerical algorithm

We apply standard optimization methods to minimize f_0, *e.g.*, Gauss–Newton, Levenberg–Marquardt, or Quasi–Newton method. Since $n \ll m$, most expensive is the cost function evaluation.

- input data: $C := \mathcal{S}(p)$, structure description $\mathcal{T}$, and cov. matrix V
- construct T from $\mathcal{T}$

example: with $\mathcal{T} = \{\begin{bmatrix}\mathtt{T} & 3\end{bmatrix}, \begin{bmatrix}\mathtt{H} & 2\end{bmatrix}, \begin{bmatrix}\mathtt{U} & 2\end{bmatrix}, \begin{bmatrix}\mathtt{F} & 1\end{bmatrix}\}$, $s=2$ and we have

$$T(1{:}s+1,:) = \left[\begin{array}{ccc|cc|cc|c} 3 & 2 & 1 & 6 & 7 & 10 & 13 & 0 \\ 4 & 3 & 2 & 7 & 8 & 11 & 14 & 0 \\ 5 & 4 & 3 & 8 & 9 & 12 & 15 & 0 \end{array}\right]$$

- construct $\{V_{\tilde{c},k}\}_{k=0}^s$ from V and $T(1{:}s+1,:)$

$$V_{\tilde{c},k}(i,j) = \mathbf{E}\tilde{c}_{1i}\tilde{c}_{kj} = \mathbf{E}\tilde{p}\big(T(1,i)\big)\tilde{p}\big(T(k,j)\big) = V\big(T(1,i),T(k,j)\big)$$

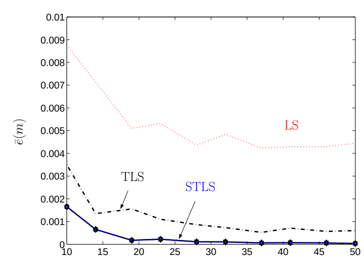
We can evaluate the cost function $f_0(X) := r^\top(X)V_{\tilde{r}}^{-1}(X)r(X)$ by solving the system $V_{\tilde{r}}(X)y_r(X) = r(X)$, $f_0(X) = r^\top(X)y_r(X)$. The SLICOT subroutine `MB02GD.f` performs Cholesky factorization by exploiting both the bandedness and the Toeplitz structure. The resulting computational complexity of the optimization algorithm is $O(m)$ per iteration.

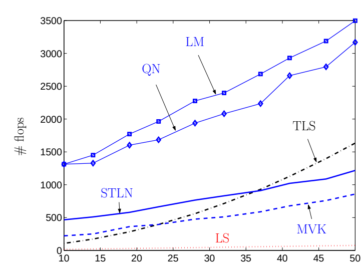
Matlab implementation

```
% Hankel low rank approximation

n = 2;  m = 20;  np = m+n;                       % constants
struct = [2 n+1 1 1];                             % C is Hankel m x (n+1)

sys = drss(n);                                    % n-th order random system
p0  = impulse(sys,np+1); p0  = p0(2:end); % = [CB CAB ... ]
p   = p0 + 0.01*randn(np,1);                      % noisy measurement
c0  = hankel(p0(1:m),p0(m:np));                   % true data
c   = hankel(p(1:m),p(m:np));                     % noisy data

a = c(:,1:n);  b = c(:,n+1);
[xh,ch] = stls(a,b,struct);                       % find structured approx.

format long, sv_ch = svd(ch), format      % check rank deficiency
error_data     = norm(c0-c ,'fro')
error_estimate = norm(c0-ch,'fro')
```

Numerical example

Define the average relative error of estimation $\bar{e} = ||\bar{x}-\hat{x}||/||\bar{x}||$. We plot $\bar{e}$ and the average flop counts as a function of m. C is a Hankel matrix.





LM=Levenberg–Marquardt, QN=Quasi–Newton, MVK=proposed iterative method, STLN—structured total least norm