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Solving Large Mixed-Effects Models in Spatial Regression with PDE Regularization

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Abstract

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Sommario

Traduzione dell'abstract in italiano.

1. Synopsis

Here goes the synopsis of your thesis. It consists of an introductory part followed by a description on the thesis content.

This thesis is organized as follows.

2. Introduction

2.1. Spatial regression with partial differential equation regularization

This work naturally stems from the studies in the research field called Spatial Regression with Partial Differential Equation regularization, abbreviated in the following as SR-PDE. SR-PDE constitutes a family of models which has been, and still is, under study beginning from 2013 in Sangalli, Ramsay, and Ramsay [SRR13].

SR-PDE effectively combines several branches of mathematics and statistics modeling. For a thorough analysis of its derivation and the enhancements it brings to the existing literature see [San21], I will limit myself to a brief introduction.

These models feature the minimization of a functional composed of two terms: a classical least-square term, with the goal of estimating a vector of unknown regression coefficients (in case of presence of covariates), and a regularization term, estimating an unknown deterministic spatial field.

The spatial field contributes to the functional by integration over the spatial domain of the square of a differential operator, most commonly the Laplacian operator. By properties of the Laplace operator, this choice induces an isotropic and stationary smoothing effect on the unknown spatial field, meaning equal in every direction and independent on the position. Other differential operators considered in this work are generic second order differential operators, that come from the physics of the problem or from some preexisting knowledge about the phenomenon under study. The inclusion of partial differential equations in the statistical model brings many advantages, like the aforementioned ability to include problem specific knowledge, dealing with boundary conditions, etc., but makes computations more cumbersome.

2.2. The mixed-effects model

In mixed At the i -th statistical unit, the observation j , for $j = 1 \dots n_i$, is modeled as

$$z_{ij} = \mathbf{w}_{ij}^T \boldsymbol{\beta} + \mathbf{v}_{ij}^T \mathbf{b}_i + f_i(\mathbf{p}_{ij}) + \epsilon_{ij} \quad (2.1)$$

ϵ_{ij} , for every i and j , are the random noise or errors, considered as the realizations of independent identically distributed (i.i.d.) random variables, with mean 0 and variance σ^2 .

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3.1. Functional

...by minimizing the following functional:

$$J_{\Omega_i, \lambda} (\beta', \mathbf{b}'_1, \dots, \mathbf{b}'_m, f_1, \dots, f_m) = \sum_{i=1}^m \left(\sum_{j=1}^{n_i} \left(z_{ij} - \mathbf{w}'_{ij} \beta' - \mathbf{v}'_{ij} \mathbf{b}'_i - f_i(\mathbf{p}_{ij}) \right)^2 + \lambda \int_{\Omega_i} \Delta f_i(\mathbf{p})^2 d\Omega_i \right) \quad (3.1)$$

3.2. Matrices

Assuming W'_i and V'_i for $i = 1, \dots, m$ full rank, define the following matrices:

$$X = \begin{bmatrix} W'_1 & V'_1 & 0 & \dots & 0 & 0 \\ W'_2 & 0 & V'_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ W'_{m-1} & 0 & 0 & \dots & V'_{m-1} & 0 \\ W'_m & 0 & 0 & \dots & 0 & V'_m \end{bmatrix} \quad (3.2)$$

with $X \in \mathbb{R}^{N \times (m-1)p+q}$, $H = X(X^T X)^{-1} X^T$ and $Q = I_N - H$, $\in \mathbb{R}^{N \times N}$, which are the matrices that project a vector, respectively, onto the subspace spanned by the columns of X and onto its orthogonal complement with respect to \mathbb{R}^N . Notice that despite the matrix $X^T X$ exhibits a pattern where only the first row, the first column and the diagonal are different from 0, the inverse of this type of matrix is usually dense.

Define also the vector of coefficients $\mathbf{v} = (\beta', \mathbf{b}'_1, \dots, \mathbf{b}'_m)$.

Given these definitions, we can write the mixed-effect model in implementation version with this compact formula

$$\mathbf{z} = X\mathbf{v} + \mathbf{f}_N + \boldsymbol{\epsilon} \quad (3.3)$$

The discrete problem leads to the solution of the following linear system of equations:

$$\begin{bmatrix} \tilde{\Psi}^T Q \tilde{\Psi} & -\lambda \tilde{R}_1^T \\ -\lambda \tilde{R}_1 & -\lambda \tilde{R}_0 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{f}} \\ \hat{\mathbf{g}} \end{bmatrix} = \begin{bmatrix} \tilde{\Psi}^T Q \mathbf{z} \\ 0 \end{bmatrix} \quad (3.4)$$

We call it monolithic because the number of units might be big and so the number of nodes for each unit. Therefore, our aim is to avoid the solution of such high dimension linear system, in favor of splitting it into many systems of lower dimension. In case

3. My chapter

the dimensions of the monolithic system are treatable, the Woodbury decomposition formula, described in appendix A.1, can be used to speed up the computation of the solution for different values of λ . The decomposition is entirely analogous to the one described in the appendix, with

$$\begin{aligned} E &= \begin{bmatrix} \tilde{\Psi}^T \tilde{\Psi} & -\lambda \tilde{R}_1^T \\ -\lambda \tilde{R}_1 & -\lambda \tilde{R}_0 \end{bmatrix} & U &= \begin{bmatrix} \tilde{\Psi}^T X \\ 0 \end{bmatrix} \\ C &= - \left[(X^T X)^{-1} \right] & V &= U^T \end{aligned} \quad (3.5)$$

Once the unknown spatial field \hat{f} has been obtained, the vector of unknown coefficients $\hat{v} = (\hat{\beta}', \hat{b}'_1, \dots, \hat{b}'_m)$ can be computed solving a least-squares problem: the corresponding normal equations are written as

$$\hat{v} = (X^T X)^{-1} X^T (z - \hat{f}_N) \quad (3.6)$$

where I recall that $\hat{f}_N = \tilde{\Psi} \hat{f}$.

3.3. Iterative methods

Following the ideas stemmed from the spatio-temporal regression in Pollini and Ponti [PP13] and Massardi and Spaziani [MS21], we consider an iterative scheme. At each step i the scheme computes an approximate solution (\hat{f}^i, \hat{g}^i) of the monolithic system by solving a single-unit problem for each statistical unit. The algorithm stops with two possible criteria:

- A maximum number of iterations is reached;
- The following two conditions are true.
The first one is that the functional 3.1 evaluated in the estimated solution $J^i = J_{\Omega_i, \lambda}(\hat{\beta}^i, \hat{b}_1^i, \dots, \hat{b}_m^i, \hat{f}_1^i, \dots, \hat{f}_m^i)$ has reached stagnation, that is the relative increment $(J^i - J^{i-1}) / J^i$ is below a certain threshold (in the code such threshold is an input parameter, it was set to 10^{-8}). The term $\int_{\Omega_i} \Delta f_i(\mathbf{p})^2 d\Omega_i$ of the functional 3.1 is computed by exploiting the expansion into the finite element basis functions, leading to $\hat{g}_i^T R_0 \hat{g}_i$, where \hat{g}_i is the sub-vector of \hat{g} corresponding to unit i .
The second one is that the estimated solution is very close to the exact solution of the system 3.4, condition that is verified by checking that the residual, normalized by the Euclidean norm of the right-hand side, is below a certain threshold (this is another input parameter, 10^{-8} was used).

The details of a first possible implementation are described in the following section.

3.3.1. The block diagonal approach

Looking at the monolithic equation 3.4, the question of how to formulate an approximation of the term $\tilde{\Psi}^T Q \tilde{\Psi}$ naturally arises. In particular, a suitable block approximation allows to make the estimated field \hat{f}_i of statistical unit i independent of the observations in the other units, for every unit i ($i = 1 \dots m$).

To this purpose, the following approximation is first considered:

$$\tilde{\Psi}^T Q \tilde{\Psi} \simeq \Gamma := \begin{bmatrix} \Psi^T Q_1 \Psi & 0 & \dots & 0 \\ 0 & \Psi^T Q_2 \Psi & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \Psi^T Q_m \Psi \end{bmatrix} \quad (3.7)$$

Here Q_i indicates the i -th diagonal block of Q of dimension $n \times n$. By definition of Q , it is equal to $I_n - X_i (X^T X)^{-1} X_i^T$, with $X_i = X((i-1)n+1 : in, :)$, where the typical notation of the MATLAB language has been used to express a suitable submatrix.

Another possible way to express the blocks $\Psi^T Q_i \Psi$ of matrix 3.7 is through Woodbury decomposition (appendix A.1) with a use analogous to the one in 3.5.

To show it, we notice that $\Psi^T Q_i \Psi$ is the i -th diagonal block of matrix $\tilde{\Psi}^T Q \tilde{\Psi}$. In fact $\tilde{\Psi}^T Q \tilde{\Psi}$ can be expressed as $\tilde{\Psi}^T \tilde{\Psi} - \tilde{\Psi}^T H \tilde{\Psi}$. Thus, defining $U = \tilde{\Psi}^T X$, $C = -(X^T X)^{-1}$, $V = U^T$, its i -th diagonal block is equal to $\Psi^T \Psi + U_i C V_i$, where

$$U_i = U((i-1)N_{\mathcal{T}} + 1 : iN_{\mathcal{T}}, :) = \tilde{\Psi}_i^T X = \begin{bmatrix} 0 & \dots & 0 & \Psi^T & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} X_1 \\ \vdots \\ X_i \\ \vdots \\ X_m \end{bmatrix} = \Psi^T X_i \quad (3.8)$$

$$V_i = U_i^T = X_i^T \Psi \quad (3.9)$$

In such a way we have

$$\Psi^T \Psi + U_i C V_i = \Psi^T \left(I_n - X_i (X^T X)^{-1} X_i^T \right) \Psi = \Psi^T Q_i \Psi \quad (3.10)$$

3.3.2. Initialization

The initialization consists in finding a good guess (\hat{f}^0, \hat{g}^0) to start the algorithm from; for this purpose, the following m problems are solved: for $i = 1, \dots, m$ solve

$$\begin{bmatrix} \Psi^T Q_i \Psi & -\lambda R_1^T \\ -\lambda R_1 & -\lambda R_0 \end{bmatrix} \begin{bmatrix} \hat{f}_i^0 \\ \hat{g}_i^0 \end{bmatrix} = \begin{bmatrix} \mathbf{u}_i \\ 0 \end{bmatrix} \quad (3.11)$$

where \mathbf{u}_i is the vector whose components are the first n components of $\tilde{\Psi}^T Q \mathbf{z}$ starting from the $n(i-1)+1$ -th component.

3.3.3. Iterations

The idea behind the iterative scheme is, having a guess of a solution $(\hat{\mathbf{f}}^{k-1}, \hat{\mathbf{g}}^{k-1})$, to compute a new guess $(\hat{\mathbf{f}}^k, \hat{\mathbf{g}}^k)$ by replacing the mutual interaction of the system variables corresponding to different units with their contribution given by their previous value. For example, the first n equations of the monolithic system 3.4 read

$$\begin{bmatrix} \Psi^T Q_{1,1} \Psi & \Psi^T Q_{1,2} \Psi & \dots & \Psi^T Q_{1,m} \Psi & -\lambda R_1^T \end{bmatrix} \begin{bmatrix} \hat{\mathbf{f}}_1 \\ \hat{\mathbf{f}}_2 \\ \vdots \\ \hat{\mathbf{f}}_m \\ \hat{\mathbf{g}}_1 \end{bmatrix} = [\mathbf{u}_1] \quad (3.12)$$

where $Q_{i,j}$ indicates block of row i and column j of matrix Q , which also coincides with $-H_{i,j}$ for $i \neq j$. Substituting $\hat{\mathbf{f}}_j$ for $j = 1, \dots, m$ with $\hat{\mathbf{f}}_j^{k-1}$, taking it to the right-hand side and generalizing, the iterative scheme reads: for $i = 1, \dots, m$ solve

$$\begin{bmatrix} \Psi^T Q_i \Psi & -\lambda R_1^T \\ -\lambda R_1 & -\lambda R_0 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{f}}_i^k \\ \hat{\mathbf{g}}_i^k \end{bmatrix} = \begin{bmatrix} \mathbf{r}_i \\ 0 \end{bmatrix} \quad (3.13)$$

where

$$\mathbf{r}_i = \mathbf{u}_i - \sum_{\substack{j=1 \\ j \neq i}}^m \Psi^T Q_{i,j} \Psi \hat{\mathbf{f}}_j^{k-1} \quad (3.14)$$

An estimate of \mathbf{v} , $\hat{\mathbf{v}}^i = (\hat{\beta}^i, \hat{\mathbf{b}}_1^i, \dots, \hat{\mathbf{b}}_m^i)$ has to be computed at each iteration for the estimation of the functional 3.1, according to equation 3.6.

3.3.4. The iterative method as a preconditioned Richardson method

Given a generic preconditioning matrix P , calling \mathbf{r}_k the residual of the linear system $A\mathbf{x} = \mathbf{b}$ (that is the vector $A\mathbf{x}_k - \mathbf{b}$) at step k , Richardson method (cf., for example, [Ger+14]) consists in solving (or rather trying to) the linear system iterating the following steps:

1. Solve $P\mathbf{z}_k = \mathbf{r}_k$
2. Compute the acceleration parameter α_k (for simplicity we use $\alpha_k = 1$)
3. Update the solution $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{z}_k$
4. Update the residual $\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A\mathbf{z}_k$

The iterative scheme described in the previous section is a Richardson scheme with the following preconditioning matrix:

$$P = \begin{bmatrix} \Gamma & -\lambda \tilde{R}_1^T \\ -\lambda \tilde{R}_1 & -\lambda \tilde{R}_0 \end{bmatrix} \quad (3.15)$$

Solving an awfully hard linear system involving this matrix is indeed like solving m linear systems of dimensions $2n \times 2n$.

3.4. Generalized cross validation

As we mentioned before, the system is solved multiple times on a grid of λ s. The best λ is then chosen according to a generalized cross-validation criterion. In particular, as in [San21], the minimum of the generalized cross-validation (GCV) parameter is used as a model selection criterion. The generalization of this parameter to the mixed-effect model reads as follows:

$$\text{GCV}(\lambda) = \frac{1}{N(1 - (q - p + mp + \text{tr}(S))/N)^2} \|z - \hat{z}\|^2 \quad (3.16)$$

where for q, m, p we follow the notation of section 3.1, and S indicates the smoothing matrix, which is the matrix that maps the observations vector z into the estimated spatial field \hat{f} evaluated at the location of the observations ($\hat{f}_N = \tilde{\Psi}\hat{f} = Sz$). Its value is

$$S = \tilde{\Psi} \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \tilde{\Psi}^T Q \quad (3.17)$$

and it stems as a Schur complement for system 3.4 with respect to the estimated field \hat{f} . The computation of the GCV parameter 3.16 involves the expensive computation of the trace of the smoothing matrix S . Since for any two matrices A and B such that the product AB is defined, it holds that $\text{tr}(AB) = \text{tr}(BA)$, the trace of S can be computed as the trace of

$$\tilde{S} = \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \tilde{\Psi}^T Q \tilde{\Psi} \quad (3.18)$$

4. Statistical inference

4.1. Properties of the estimators

4.1.1. Spatial field component

To study the statistical properties of the estimated spatial field that is obtained by solving the monolithic system 3.4, we write it in the following equivalent manner

$$\begin{cases} \tilde{\Psi}^T Q \tilde{\Psi} \hat{f} - \lambda \tilde{R}_1^T \hat{g} = \tilde{\Psi}^T Q z \\ \hat{g} = -\tilde{R}_0^{-1} \tilde{R}_1 \hat{f} \end{cases} \quad (4.1)$$

By recalling the mixed-effect model in the implementative form 3.3, that is $z = Xv + f_N + \epsilon$, and substituting the second equation inside the first we get

$$\tilde{\Psi}^T Q \tilde{\Psi} \hat{f} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \hat{f} = \tilde{\Psi}^T Q (Xv + f_N + \epsilon) \quad (4.2)$$

Recalling that Q projects on the orthogonal space of the columns of X , implying $QX = 0$,

$$\left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right) \hat{f} = \tilde{\Psi}^T Q f_N + \tilde{\Psi}^T Q \epsilon \quad (4.3)$$

That can be rearranged as follows

$$\left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right) (\hat{f} - f) + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 f = \tilde{\Psi}^T Q \epsilon \quad (4.4)$$

where we have defined f as the coefficients of the finite element expansion of the true vector field $f(\cdot)$. Deriving now the term $\hat{f} - f$

$$\hat{f} - f = - \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 f + \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \tilde{\Psi}^T Q \epsilon \quad (4.5)$$

The first term above is not random, thus we can derive the following:

1. Thanks to the property that, for generic suitably dimensioned matrices and vectors, $\mathbb{E}[Mx] = M\mathbb{E}[x]$, we get that $\mathbb{E}[\hat{f} - f] = - \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 f$;

2. Thanks to the property that again, for generic suitably dimensioned matrices and vectors, $\text{Var}[Mx] = M\text{Var}[x]M^T$, we get this result for $\text{Var}[\hat{f} - f] = \text{Var}[\hat{f}]$

$$\text{Var}[\hat{f} - f] = \sigma^2 \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \tilde{\Psi}^T Q \tilde{\Psi} \left(\tilde{\Psi}^T Q \tilde{\Psi} + \lambda \tilde{R}_1^T \tilde{R}_0^{-1} \tilde{R}_1 \right)^{-1} \quad (4.6)$$

where we have exploited symmetric matrices and the fact that $Q^2 = Q$.

4. Statistical inference

4.1.2. Parametric component

For what concerns the estimation of the parameter \mathbf{v} , we recall that $\hat{\mathbf{v}}$ solves the normal equations

$$\mathbf{X}^\top \mathbf{X} \hat{\mathbf{v}} = \mathbf{X}^\top (\mathbf{z} - \tilde{\Psi} \hat{\mathbf{f}}) \quad (4.7)$$

that with model 3.3 can be written as

$$\mathbf{X}^\top \mathbf{X} \hat{\mathbf{v}} = \mathbf{X}^\top (\mathbf{X} \mathbf{v} + \tilde{\Psi} \mathbf{f} + \boldsymbol{\epsilon} - \tilde{\Psi} \hat{\mathbf{f}}) \quad (4.8)$$

or

$$\mathbf{X}^\top \mathbf{X} (\hat{\mathbf{v}} - \mathbf{v}) = -\mathbf{X}^\top \tilde{\Psi} (\hat{\mathbf{f}} - \mathbf{f}) + \mathbf{X}^\top \boldsymbol{\epsilon} \quad (4.9)$$

From this we can derive:

$$\mathbb{E} [\hat{\mathbf{v}} - \mathbf{v}] = \left(\mathbf{X}^\top \mathbf{X} \right)^{-1} \mathbf{X}^\top \tilde{\Psi} \left(\tilde{\Psi}^\top \mathbf{Q} \tilde{\Psi} + \lambda \tilde{\mathbf{R}}_1^\top \tilde{\mathbf{R}}_0^{-1} \tilde{\mathbf{R}}_1 \right)^{-1} \lambda \tilde{\mathbf{R}}_1^\top \tilde{\mathbf{R}}_0^{-1} \tilde{\mathbf{R}}_1 \mathbf{f} \quad (4.10)$$

and the expression of $\text{Var} [\hat{\mathbf{v}} - \mathbf{v}]$ that is not reported for brevity.

4.1.3. Asymptotic properties

We study the limiting properties of the estimators in the setting where the number of basis $N_{\mathcal{T}}$ and the triangulation \mathcal{T} are fixed. The number of observation n_i for each statistical unit increases to infinity.

In a similar fashion as in [SFF21], where the simple spatial problem is considered, we make some assumptions for studying the asymptotic properties of the considered estimators.

5. Simulation studies

In this chapter we see some examples...

6. Applications

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7. Conclusions

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Appendices

A. Formulae

A.1. Woodbury decomposition

The following matrix identity holds.

Proposition A.1 (Woodbury matrix identity). *Let M be a square $m \times m$ matrix which can be written as the sum $E + UCV$, with E being $m \times m$, U being $m \times n$, C being a square $n \times n$ matrix, and V $n \times m$. Then*

$$M^{-1} = (E + UCV)^{-1} = E^{-1} - E^{-1}U \left(C^{-1} + VE^{-1}U \right)^{-1} VE^{-1} \quad (\text{A.1})$$

In particular, in the case where inverting matrix E can be considered cheap or useful, on the right-hand side solving the system involves solving an $n \times n$ system (the one characterized by matrix $C^{-1} + VE^{-1}U$), whilst on the left the dimensions are $m \times m$. This equation is exploited for faster system solving in the `fdaPDE` library. As an example, consider the space-only problem, described *e.g.* in [sangalli]: the presence of covariates leads to a linear system involving the following matrix M :

$$M = \begin{bmatrix} \Psi^T Q \Psi & -\lambda R_1^T \\ -\lambda R_1 & -\lambda R_0 \end{bmatrix}$$

Remembering that the projection matrix Q is defined as $I - H$, M can be split into the following two components, one independent from λ :

$$M = \begin{bmatrix} \Psi^T \Psi & -\lambda R_1^T \\ -\lambda R_1 & -\lambda R_0 \end{bmatrix} + \begin{bmatrix} -\Psi^T H \Psi & 0 \\ 0 & 0 \end{bmatrix}$$

By defining E the left matrix of the two above (which is also the matrix corresponding to the problem without covariates), and remembering that $H = W(W^T W)^{-1} W^T$, Woodbury decomposition can be exploited defining the following matrices U, C, V :

$$\begin{bmatrix} -\Psi^T W (W^T W)^{-1} W^T \Psi & 0 \\ 0 & 0 \end{bmatrix} = UCV$$

$$U = \begin{bmatrix} \Psi^T W \\ 0 \end{bmatrix}$$

$$C = - \left[(W^T W)^{-1} \right]$$

A. Formulae

$$V = U^T = \begin{bmatrix} W^T \Psi & 0 \end{bmatrix}$$

where the 0s indicate matrices of zeros of suitable dimensions.

Since matrices U, C, V do not depend on λ , computing the solution of the system for different values of λ involves only the factorization of the matrix E (and the cheaper $C^{-1} + VE^{-1}U$).

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