Variable Projections for Separable Nonlinear Least Squares Problems Since 2002

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Abstract

In [3] we surveyed the applications of the Variable Projections (VARPRO) method for the numerical solution of separable nonlinear least squares problems [1973]. Since that date the interest in the method has not abated and therefore in this paper we update the survey.

The source of citations of [2] is Google Scholar. We have tried to complete these citations as much as possible. There is also a significant number of citations of VARPRO that do not refer to our papers and we have included some of those also in this survey. Since the list is fairly long, we do not include citations published before 2015 that have only a small number of citations.

We have chosen a new style of presentation: we put the different kinds of applications in classes and sub-classes. When there is a new field of application, not considered in earlier publications [2, 3, 1, 3], we start with a brief description. Instead of collecting alphabetically all the many references at the end, as is customary, we include the references in the classes. In that way practitioners will be able to find relevant information in a straightforward way.

We refer to the above papers for a description of the problem and method of solution, which is by now classic.

Contents

1. Separable Nonlinear Least Squares and the Variable Projection Method

Given a set of observations $\{y_i\}$, a separable nonlinear least squares problems is defined in [2] as one for which the model is a linear combination of nonlinear functions that can depend on multiple parameters, and for which the i component of the residual vector is written as

$$r_i(\mathbf{a}, \alpha) = y_i - \sum_{j=1}^{n} a_j \phi_j(\alpha; t_i).$$

Here the t_i are independent variables associated with the observations y_i, while the a_j, and the k-dimensional vector α are the parameters to be determined by minimizing the functional $||\mathbf{r}(\mathbf{a}, \alpha)||_2^2$, where $\mathbf{r}(\mathbf{a}, \alpha) = \sum_{i=1}^{m} r_i^2(\mathbf{a}, \alpha)$, and $||.||_2$ stands for the l_2 vector norm. We can write this functional using matrix notation as

$$||\mathbf{r}(\mathbf{a}, \alpha)||_2^2 = ||\mathbf{y} - \mathbf{\Phi}(\alpha)\mathbf{a}||_2^2,$$

where the columns of the matrix $\mathbf{\Phi}(\alpha)$ correspond to the nonlinear functions $\phi_j(\alpha;t_i)$ of the k parameters α evaluated at all the t_i values, and the vectors $\mathbf{a}$ and $\mathbf{y}$ represent the linear parameters and the observations respectively.

Now it is easy to see that if we knew the nonlinear parameters α, then the linear parameters $\mathbf{a}$ could be obtained by solving the linear least squares problem:

$$\mathbf{a} = \mathbf{\Phi}(\alpha)^{+}\mathbf{y}, \tag{1.1}$$

which stands for the minimum-norm solution of the linear least squares problem for fixed α, where $\mathbf{\Phi}(\alpha)^{+}$ is the Moore-Penrose generalized inverse of

$\mathbf{\Phi}(\alpha)$. By replacing this $\mathbf{a}$ in the original functional the minimization problem takes the form

$$\min_{\alpha} \frac{1}{2}||(\mathbf{I} - \mathbf{\Phi}(\alpha)\mathbf{\Phi}(\alpha)^{+})\mathbf{y}||_2^2, \tag{1.2}$$

where the linear parameters have been eliminated. Another way to see this is to observe that 1.1 is a nonlinear equality constraint. A joint method, where the two sets of variables are considered independent will not, in general, honor this constraint.

We define $\mathbf{r_2}(\alpha) = (\mathbf{I} - \mathbf{\Phi}(\alpha)\mathbf{\Phi}(\alpha)^{+})\mathbf{y}$, which will be called the Variable Projection (VP) of $\mathbf{y}$. Its name stems from the fact that the matrix in parentheses is the projector on the orthogonal complement of the column space of $\mathbf{\Phi}(\alpha)$, that we will denote in what follows by $P^{\perp}_{\mathbf{\Phi}(\alpha)}$. We will also refer to $\frac{1}{2}||\mathbf{r_2}(\alpha)||_2^2$ as the Variable Projection functional.

This is a more powerful paradigm than the simple idea of alternating between minimization of the two sets of variables (such as the NIPALS algorithm of Wold and Lyttkens [6]), which can be proven theoretically and practically not to result, in general, in the same enhanced performance.

In summary, the Variable Projection algorithm consists of first minimizing (1.2) and then using the optimal value obtained for α to solve for $\mathbf{a}$ in (1.1). One obvious advantage is that the iterative nonlinear algorithm used to solve the first minimization problem works in a reduced space and in particular, fewer initial guesses are necessary. However, the main payoff of this algorithm is the fact that it always converges in fewer iterations than the minimization of the full functional, including convergence when the same minimization algorithm for the full functional diverges (see for instance [4]), i.e., the minima for the reduced functional are better defined than those for the full one.

A different reason to use the reduced functional is to observe from the above results that the linear parameters are determined by the nonlinear ones, and therefore the full problem must be increasingly ill-conditioned as (and if) it converges to the optimal parameters. That is probably one of the reasons why the important and prevalent problem of real or complex exponential data fitting is so hard to solve directly.

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2. Electrical Engineering

Here we find applications to motor fault diagnostics, amplifiers, communications and wind energy systems. In separate categories we put power systems, signal identification (that includes location and antennas), VLSI design and signal processing. Gan and Li [7] consider the radial basis function network-based autoregressive with exogenous inputs. (RBF-ARX) models have much more linear parameters than nonlinear parameters. Taking advantage of this special structure, a variable projection algorithm is proposed to estimate the model parameters more efficiently by eliminating the linear parameters through the orthogonal projection. The proposed method not only substantially reduces the dimension of parameter space of the RBF-ARX model but also results in a better-conditioned problem. In this paper, both the full Jacobian matrix of Golub and Pereyra and the Kaufman's simplification are used to test the performance of the algorithm. An example of chaotic time series modeling is presented for the numerical comparison. It clearly demonstrates that the proposed approach is computationally more efficient than the previous structured nonlinear parameter optimization method and the conventional Levenberg–Marquardt algorithm without the parameters separated. Finally, the proposed method is also applied to a simulated nonlinear single-input single-output process, a time-varying nonlinear process and a real multi-input multi-output nonlinear industrial process to illustrate its usefulness.

In [8] Alamir considers the problem of sensitivity analysis of the simultaneous estimation of state and parameters for induction motors by writing it as a separable nonlinear least squares problem.

An interesting application is found in [13], for the adaptive sparse recovery of inverse synthetic aperture radar (ISAR) of uniformly rotating targets by parametric weighted L_1 minimization. One of the steps of this complicated algorithm requires solving a separable least squares problem and the authors apply the VARPRO idea successfully. The authors of [14] consider measurement-based load modeling, especially in the presence of new loads such as power electronics-interfaced loads and electric vehicles with fast dynamics, which require fast-converging algorithms that provide the model parameters with high reliability. In the current practice, all or only a subset of the parameters of an aggregated load model are estimated using iterative optimization algorithms. Thus, the identification problem either has a high dimension, which leads to a large variance for the estimated parameters, or does not include a subset of the parameters with low sensitivity. In this paper, an efficient approach for the estimation of the composite load model parameters is proposed that addresses these issues. This method partitions the parameters into two subsets; one that appears nonlinearly in the model output, and a second set that affects the outputs linearly. Then, the optimization is performed only with respect to the nonlinear set, with the linear parameters treated as explicit functions of the nonlinear ones. This approach effectively reduces the dimension of the search space since it only includes the nonlinear parameters in the optimization, and also includes the linear parameters by computing them using linear regression at each iteration. These features lead to a much faster convergence while all of the composite load model parameters are estimated reliably. Experimental and simulation data are presented to demonstrate the performance of the proposed method.

Bouleux [15] points out that an optimal prior-knowledge method for Direction Of Arrival (DOA) estimation has been proposed. This method solely estimates a subset of DOA's taking into account known ones. The global idea is to maximize the orthogonality between an estimated signal subspace and noise subspace by constraining the orthogonal noise-made projector to only project onto the desired unknown signal subspace. To understand how this is possible requires the derivation of the variance for the DOA estimates. During the derivation, oblique projection operators and their first order derivatives are required.

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2.1. Power Grid

The main objective of [6] is to estimate the voltage parameters, i.e. angular frequency and phasor, from the input three-phase signals, X. In this context, the author proposes the use of Maximum Likelihood estimator (MLE). MLE corresponds to a least square estimator when the noise is white Gaussian noise. This spectral estimation based parametric model can be decomposed into two steps: first, the estimation of angular frequency from X is the main difficult step. Then, the estimated phasor can be obtained once the angular frequency is estimated. This is, of course, a separable nonlinear LSQ problem.

Interesting comparisons between VARPRO, Prony, matrix pencil and ERA methods can be found in [7]. The conclusion, as in other studies, is that VARPRO is superior.

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[2] Maximum-likelihood frequency and phasor estimations for electric power grid monitoring. Z Oubrahim, V Choqueuse, Y Amirat, M. Benbouzid, IEEE Transactions on Industrial Informatics **14**:167-177 (2018).

[3] Disturbances classification based on a model order selection method for power quality monitoring. Z Oubrahim, V Choqueuse, Y Amirat, MEH Benbouzid, IEEE Transactions on Industrial Electronics **64**:9421-9432 (2017).

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[5] Power system modal analysis tool developed for industry use. A R Borden, B C Lesieutre, J Gronquist, North American Power Symposium (2013).

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[7] Variable projection method for power system modal identification. AR Borden, BC Lesieutre, IEEE Transactions on Power Systems **29**:2613-2620 (2014).

2.2. Signal Identification, Location, Antennas

Traditionally this has been a strong user of VARPRO, as we described in detail in our previous survey. The classical location algorithms MUSIC and SPRIT both owe inspiration from VARPRO. Current difficulties include interference cancellation, ghost signals. multi-path, noise, superimposed signal replicas, etc. This area includes many modern communication, radar and positioning systems.

In [5] the authors propose a two-stage estimation algorithm for global system positioning. At the first stage, they ignore the additional path error and obtain a relatively accurate initial position. Then, based on this result they include the additional path error in the estimation problem and estimate it by the variable projection method. Numerical results show that the proposed algorithm based on the VARPRO method can effectively mitigate multi-path interference.

[1] Maximum likelihood joint angle and delay estimation from multi-path and multi-carrier transmissions with application to indoor localization over IEEE 802.11ac radio. Faouzi Bellili, Souheib Ben Amor, Sofiéne Affes and Ali Ghrayeb, IEEE Transactions on Mobile Computing (2018).

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[8] Multi-path-assisted indoor positioning enabled by directional UWB sector antennas. M Rath, J Kulmer, MS Bakr, B Grosswindhager, K. Witrisal, IEEE 18th International Workshop on Signal Processing Advances in Wireless Communications 1-5 (2017).

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[15] A Bayesian approach to multi-path mitigation in GNSS receivers. P Closas, C Fernandez-Prades, JA Fernadez-Rubio, IEEE Journal of Selected Topics in Signal Processing **3**:695-706 (2009).

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[18] Bayesian nonlinear filters for direct position estimation. P Closas, C Fernández-Prades, IEEE Aerospace Conference 1-12 (2010).

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2.3. VLSI Design

This is an interesting new category that arose from a collaboration with R. Suaya of Mentor Graphics. In [1, 3] the authors models capacitance coupling and extraction of wires for timing and noise simulation of digital circuits. The model turns out to be separable and thus amenable to a successful application of VARPRO. This approach replaces the use of full field solvers in 3D, a daunting task. More elaborated use of similar ideas can be found in [6, 7, 8]

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2.4. Signal Processing

A number of different applications to identification and other problems in signal processing. For instance, [6] studies the reconstruction of a multichannel sampling scheme when both gains and offsets are unknown that appears in many practical signal processing applications.

In [16] the authors consider a very interesting and challenging problem: how to endow autonomous underwater vehicles with abilities akin to fish, in terms of sensing flows and nearby movements. To do this they add a lateral array of MEMS flow sensors. The calibration of this system leads to a SNLLS problem that is solved by VARPRO.

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[7] Fast and approximative estimation of continuous-time stochastic signals from discrete-time data. M Mossberg, EK Larsson, IEEE International Conference on Acoustics, Speech, and Signal Processing (2004).

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[16] Flow vision for autonomous underwater vehicles via an artificial lateral line. N Nguyen, DL Jones, Y Yang, C Liu, EURASIP Journal on Advances in Signal Processing **2011** (2011).

[17] Analysis of a nonlinear least squares procedure used in global positioning systems. GW Pulford, IEEE Transactions on Signal Processing **58**:4526-4534 (2010).

3. Numerical Analysis

These are application of VARPRO to general numerical analysis topics. Most papers are connected to polynomials, as in surrogates, interpolation, cubatures, conformal mappings and common divisors. For instance in [1] the authors observe that the problem of obtaining surrogates for expensive functions by using polynomials can be stated as a ridge approximation that turns out to be a separable problem and therefore amenable to variable projections. In [2, 5, 6] the formula for the derivative of the pseudo-inverse is used. In the sub-sections below we include more specific sub-fields. Hale [4, 10] considers the use of conformal mapping for polynomial approximation. In some cases this leads to a separable problem and VARPRO is used. In [7] the author applies VARPRO to the problem of computing cubature rules. Finally, in [8] the authors consider the problem of finding for a given N-tuple of polynomials (real or complex) the closest N -tuple that has a common divisor of degree at least d. They develop optimization methods based on the variable projection principle both for image and kernel representation.

[1] Data-driven polynomial ridge approximation using variable projection. JM Hokanson, PG Constantine, SIAM Journal on Scientific Computing **40**:A1566-A1589 (2018).

[2] Differentiating the pseudo determinant. A Holbrook, Linear Algebra and its Applications **548**:293-304 (2018).

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3.1. Variable Projection

This subsection includes work on Variable Projections itself: extensions and improvements. In [2, 3] the authors observe that separable nonlinear least-squares (SNLLS) problems arise frequently in many research fields, such as system identification and machine learning. They further indicate that the variable projection (VP) method is a very powerful tool for solving such problems. In this paper they consider the regularization of ill-conditioned SNLLS problems based on the VP method. Selecting an appropriate regularization parameter is difficult because of the nonlinear optimization procedure. They propose to determine the regularization parameter using the weighted generalized cross-validation method at every iteration. This makes the original objective function changing during the optimization procedure.

One of the most interesting extensions of VP is to problems with constraints. Early on we contributed [8, 9] to this area by introducing so called separable equality constraints, which are of the form $H(\alpha)a = g(\alpha)$, where a, α are the linear and nonlinear parameters respectively. Extensions to other types of constraints have come from practitioners in different fields whose problems were constrained and they can be found in the appropriate sections. Some modern implementations in Matlab, Julia and C++ can be found in [5, 6**?**]. The paper [7] contains a very interesting discussion on the connection between VARPRO and the joint minimization approach, besides pointing to the excellent performance of VARPRO on some difficult affine bundle adjustment problems in computer vision that includes an scalable implementation for large problems.

Osborne [13], who has a long history of working on these problems, discusses in detail the rate of convergence of variable projections in conjunction with the Gauss-Newton algorithm and emphasizes its particular effectiveness for large data sets.

Bert Rust [14], an early champion of VARPRO at NIST, discusses linear and nonlinear least squares with strong emphasis on statistics in a four part series of papers. Part 4 is dedicated to VARPRO and diverse real life applications and models are used for illustration.

Shen and Ipma [15] present a method for solving separable nonlinear least squares problem. Their technique replaces this large problem by a much smaller problem in the nonlinear variables alone. They show how Newton's method can be used to solve the latter problem, obtaining quadratic convergence even in the nonzero residual case. While the method is in principle based on the use of one particular orthonormal basis for the null-space of A^T throughout the computation, they show that one can instead use any convenient orthonormal basis for this null-space at each successive iteration point without affecting the iteration.

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[2] Modified Gram-Schmidt method-based variable projection algorithm for separable nonlinear models. Guang-Yong Chen, Min Gan, Feng Ding and C. L. Philip Chen, IEEE Transactions on Neural Networks and Learning Systems 1-9 (2018).

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[10] A regularized Variable Projection algorithm for separable nonlinear least squares problems. GY Chen, M Gan, CLP Chen, H-X Li, IEEE Transactions on Automatic Control (2018).

[11] An efficient variable projection formulation for separable nonlinear least squares problems. M Gan, HX Li, IEEE Transactions on Cybernetics **44**:707-711 (2014).

[12] On some separated algorithms for separable nonlinear least squares problems. M Gan, CLP Chen, GY Chen, Long Chen, IEEE Transactions on Cybernetics 1-9 (2017).

[13] Separable least squares, variable projection, and the Gauss-Newton algorithm. MR Osborne, Electronic Transactions on Numerical Analysis (2007).

[14] Fitting nature's basic functions Part IV: the variable projection algorithm. BW Rust, Computing in Science & Engineering **5**:74-79 (2003).

[15] Solving separable nonlinear least squares problems using the QR factorization. Yunqiu Shen and Tjalling J Ypma, Journal of Computational and Applied Mathematics Volume 345:48-58 (2019).

[16] Variable projection for affinely structured low-rank approximation in weighted 2-norms. K Usevich, I Markovsky, Journal of Computational and Applied Mathematics **272**:430-448 (2014).

3.2. Exponential Fitting

This is a very classical application that is notoriously difficult. Even today one of the most used methods is that of Prony, dating to the eighteen century. The exponential fitting problem appears in diverse applications such as magnetic resonance spectroscopy, mechanical resonance, chemical reactions, system identification, and radioactive decay. In [3] we have collected the work of several authors that discuss these and other applications and they all agree that VARPRO and some modified and more stable versions of Prony's method are the algorithms of choice.

In his PhD Thesis, Hokanson [2] discusses and analyses stable algorithms, such as the classical method of Prony, its variants and variable projections. In [1] Halliday discusses the problem of determining the underlying parameters of general signal models through the application of maximum likelihood estimation theory for functions whose variables separate. He considers exponentials and Bessel basis functions. In [8], the authors consider the problem of time-resolved spectroscopy, microscopy and mass spectrometry, which are modeled by a sum of complex exponentials. Finally, in [10] the authors compare several methods for exponential data fitting, including modification of Prony's method, VARPRO and their own methods. Unfortunately this extensive comparison only considers models with up to 3 exponentials, but in any case provides valuable information about the relative performance of the methods, both in time, accuracy and stability.

[1] Maximum likelihood estimation of structural wave components from noisy data. PJ Halliday, K Grosh, The Journal of the Acoustical Society of America **111**:1709 (2002).

[2] Numerically Stable and Statistically Efficient Algorithms for Large Scale Exponential Fitting. JM Hokanson, PH D Thesis, Rice University (2013).

[3] Exponential Data Fitting and its Applications. V Pereyra, G Scherer, Bentham Science Publishers (2010).

[4] Fast minimum uncertainty estimates for the exponential fitting problem. JM Hokanson, arXiv preprint arXiv:1508.05890 (2015).

[5] Projected nonlinear least squares for exponential fitting. JM Hokanson, SIAM Journal on Scientific Computing **39**:A3107-A3128 (2017).

[6] A necessary and sufficient criteria for the existence of the least squares estimate for a 3-parametric exponential function. D Jukić, Applied Mathematics and Computation **147**:1-17 (2004).

[7] A genetic algorithms based technique for computing the nonlinear least squares estimates of the parameters of sum of exponentials model. S Mitra, A Mitra, Expert Systems with Applications **39**:6370-6379 (2012).

[8] Sum-of-exponentials models for time-resolved spectroscopy data. KM Mullen, IHM van Stokkum, Exponential Data Fitting and its Applications, Bentham Science Publishers 110-144 (2010).

[9] Estimation of parameters of impulse responses of mechanical systems by modified Prony method. V Slivinskas, V Šimonytė - Solid State Phenomena **113**:190-194 (2006).

[10] Optimal approximation with exponential sums by a maximum likelihood modification of Prony's method. Ran Zhang and Gerlind Plonka, Manuscript na.math.uni-goettingen.de (2018).

4. Optimization

An eclectic mixture of applications in optimization. The common thread is VARPRO. An interesting contribution is found in [1], where a modern implementation of VARPRO in MATLAB is offered. They include comments on constrained problems and also go against previous consensus by advising not to neglect the Kaufman term in the Jacobian since that may make the algorithm less robust, specially away from the solution. More extensive statistical calculations are also included. The authors of [2, 4] use the result about the smoothness of the pseudo-inverse in regions of constant rank.

[1] Variable projection for nonlinear least squares problems. DP O'Leary, BW Rust, Computational Optimization and Applications **54**:579-593 (2013).

[2] Deterministic guarantees for Burer-Monteiro factorizations of smooth semidefinite programs. N Boumal, V Voroninski, AS Bandeira, arXiv preprint arXiv:1804.02008 (2018).

[3] A stable primal–dual approach for linear programming under nondegeneracy assumptions. M Gonzalez-Lima, H Wei, H Wolkowicz, Computational Optimization and Applications **44**:213 (2009).

[4] Smoothed analysis of the low-rank approach for smooth semidefinite programs. Thomas Pumir, Samy Jelassi and Nicolas Boumal, arXiv:1806.03763 (2018).

[5] Solving semidefinite programs using preconditioned conjugate gradients. H Wolkowicz, Optimization Methods and Software **19**:653-672 (2004).

[6] Extended Gauss-Newton and Gauss-Newton-ADMM algorithms for low-rank matrix optimization. Q Tran-Dinh, Z Zhang - arXiv preprint arXiv:1606.03358 (2016).

4.1. Linear Algebra

This subsection collects mostly matrix applications, including pseudo-inverses, projectors, Hankel and lower rank approximations. The books [1, 3, 4, 5] describe different aspects of separable problems and variable projections.

[1] Generalized Inverses: Theory and Applications. A Ben-Israel, TNE Greville (2003).

[2] On one-sided (B, C)-inverses of arbitrary matrices. J Benitez, E Boasso, H Jin, arXiv preprint arXiv:1701.09054 (2017).

[3] Structured Matrix Nearness Problems: Theory and Algorithms. R Borsdorf, PH D Thesis, Univ. Manchester, England (2012).

[4] Generalized Inverses of Linear Transformations. SL Campbell, CD Meyer, SIAM Publications (2009).

[5] Projectors and Projection Methods. A Galántai, Springer (2013).

[6] Computing the nearest rank-deficient matrix polynomial. M Giesbrecht, J Haraldson, G Labahn, Proceedings of the 2017 ACM on International Symposium on Symbolic and Algebraic Computation 181-188 (2017).

[7] Computing lower rank approximations of matrix polynomials. M Giesbrecht, J Haraldson, G Labahn, arXiv preprint arXiv:1712.04007 (2017).

[8] Gene Howard Golub, 1932–2007. DP O'Leary, Linear Algebra and Its Applications **428**:2405-2409 (2008).

4.2. Nonlinear Equations

Here we consider a few applications to nonlinear problems, including Newton's method, robust estimators and bifurcation. Deuflhard in his book [1] discusses in detail separable problems and VARPRO and its variants. In [2] the authors use the formulas of differentiation of pseudo-inverses and projectors in the context of providing robust and accurate estimates for linear regression problems when both the measurement vector and the coefficient matrix are structured and subject to errors or uncertainty. In [4] the authors consider parametrized separable problems and study the bifurcation diagrams. In particular they handle the rank-one deficiency case at a bifurcation point, without loosing the properties of the general problem. The survey paper [5] discusses VARPRO applied to separable problems.

[1] Newton Methods for Nonlinear Problems: Affine Invariance and Adaptive Algorithms. P Deuflhard, Springer (2011).

[2] Structured least squares problems and robust estimators. M Pilanci, O Arikan, MC Pinar, IEEE Transactions on Signal Processing **58**:2453-2465 (2010).

[3] Solving separable nonlinear equations with Jacobians of rank deficiency one. YQ Shen, TJ Ypma, International Conference on Computational and Information Science CIS 99-104 (2004).

[4] Rank deficiencies and bifurcation into affine subspaces for separable parameterized equations. YQ Shen, T Ypma, Mathematics of Computation **85**:271-293 (2016).

[5] Recent advances in numerical methods for nonlinear equations and nonlinear least squares. YX Yuan, Numerical Algebra, Control & Optimization **1**:15-34 (2011).

4.3. Least Squares

Penalized, linear, total and alternating least squares are the problems considered in this section. Bates and DebRoy [1] consider the problem of linear mixed models via a penalized least squares method. They make good use of the formulas for the derivatives of projectors and pseudo-inverses to obtain analytical expressions for the profiled log-likelihood. In [4] the authors use the derivative of projectors that appear in a block Gauss-Seidel method that they study.

[1] Linear mixed models and penalized least squares. DM Bates, S DebRoy, Journal of Multivariate Analysis **91**:1-17 (2004).

[2] Linear Least Squares Problems. Å Björck - Numerical Methods in Matrix Computations, Springer (2015).

[3] Structured total least squares. P Lemmerling, S Van Huffel, Total Least Squares and Errors-in-Variables 79-91, Springer (2002).

[4] Alternating least squares as moving subspace correction. I Oseledets, M Rakhuba, A Uschmajew, arXiv preprint arXiv:1709.07286. SIAM Journal on NA **56**:3459-3479 (2018).

4.4. Splines

One of the original applications of Variable Projections was to splines with variable knots. Here we have some additional extensions. Dertimanis et al Molinari et al introduce a data-driven uncertainty quantification scheme relying on B-spline functions. Instead of predefining basis functions according to the statistics of the uncertain input, as in conventional polynomial chaos expansion (PCE)-based implementations, the method introduced herein takes advantage of the increased flexibility of B-splines, which is adaptable to a given input–output data set. Parameter estimation is effectively dealt through a Separable Non-linear Least Squares (SNLS) procedure that allows for simultaneous estimation of both the B-splines' free knots and the corresponding coefficients of projection.

In [3]the authors consider the bi-variate problem that leads to a separable problem with tensor product structure. Spiriti et al [5] consider penalized splines and the usual VARPRO reduction, but since the problem may have multiple minima they consider search methods and parallelization to solve the projected nonlinear system. The authors of [6]remark that a lack of accurate and fast reconstruction models hinders the development of intelligent sampling techniques for surface reconstruction. In this paper, a smart surrogate model based on free-knot B-splines and variable projections is used for intelligent surface sampling design with the aid of uncertainty modeling.

[1] Data-driven uncertainty quantification of structural systems via B-spline expansion. V K Dertimanis, M D Spiridonakos and E N Chatzi, Computers & Structures 207:245-257 (2018).

[2] Bounded optimal knots for regression splines. N Molinari, JF Durand, R Sabatier, Computational statistics & data analysis **45**:159-178 (2004).

[3] Bivariate free knot splines. T Schütze, H Schwetlick, BIT Numerical Mathematics **43**:153-178 (2003).

[4] Total least squares fitting of Bézier and B-spline curves to ordered data. CF Borges, T Pastva, Computer Aided Geometric Design **19**:275-289 (2002).

[5] Knot selection for least-squares and penalized splines. S Spiriti, R Eubank, PW Smith, D. Young, Journal of Statistical Computation and Simulation **83**:1020-1036 (2012).

[6] Uncertainty-guided intelligent sampling strategy for high-efficiency 2 surface measurement via free-knot B-spline regression modeling. Jian Wang, Luca Pagani, Liping Zhou, Xiaojun Liu, Wenlong Lu*, Richard Leach and Xiangqian (Jane) Jiang, Precision Engineering (2018).

5. Parameter Estimation, Approximation, Statistics

This is a large category that we have subdivided in appropriate subsections. It is interesting that here, as in other classes, there are included a number of PH D Thesis, showing active new research. Acosta and Vallejos [1] extended the known methodology for effective sample size computations for general spatial regression models. The approach, equipped with powerful computational machinery is appropriate for large spatial datasets and it provides formulas for a number of spatial processes. The methodology can easily be extended to more general models, such as a separable nonlinear model of the form

$$Y = X(\alpha)\beta + \epsilon.$$

In [2], Hokanson and Magruder develop a nonlinear least squares approach for constructing rational approximations with respect to the l_2 norm. They explore this approach using two parameterizations of rational functions: a ratio of two polynomials and a partial fraction expansion. In both cases, they show how one can use Variable Projection (VARPRO) to reduce the dimension of the optimization problem. Some of these references use the formula for the differentiation of the pseudo-inverse in various contexts [7, 6]. In [13] the authors present an interesting discussion of the large sample properties of separable problems in the complex valued case.

[1] Effective sample size for spatial regression models. Jonathan Acosta and Ronny Vallejos, Electronic Journal of Statistics 12:3147–3180 (2018).

[2] Least Squares Rational Approximation. Jeffrey M Hokanson and Caleb C Magruder, arXiv:1811.12590 [math.NA] (2018).

[3] Geometric Bayes. A Holbrook, UC Irvine Electronic Theses and Dissertations (2018).

[4] A novel joint diagonalization approach for linear stochastic systems and reliability analysis. F Wang, C Li, J Feng, S Cen, DRJ Owen, Engineering Computations **29** (2012).

[5] Structured Higher-Order Algorithmic Differentiation in the Forward and Reverse Mode with Application in Optimum Experimental Design. S Walter, PH D Thesis, Humboldt University, Berlin (2012).

[6] Chaos, Observability and Symplectic Structure in Optimal Estimation. D Rey, PH D Thesis, UC San Diego, CA (2017).

[7] Communication-efficient algorithms for distributed stochastic principal component analysis. D Garber, O Shamir, N Srebro, arXiv preprint arXiv:1702.08169 (2017).

[8] Maximum Likelihood Estimation and Inference: with Examples in R, SAS and ADMB. RB Millar, Wiley (2011).

[9] Statistical models. TJ Hastie, JM Chambers, Statistical Models in S, Chapter 2 (2017).

[10] Modified F tests for assessing the multiple correlation between one spatial process and several others. P Dutilleul, B Pelletier, G Alpargu, Journal of Statistical Planning and Inference **138**:1402-1415 (2008).

[11] Improved multivariate normal mean estimation with unknown covariance when p is greater than n. D Chételat, MT Wells, The Annals of Statistics **6**:3137-3160 (2012).

[12] Spectral Analysis of Non-uniformly Sampled Data and Applications. P Babu, PH D Thesis, Uppsala University, Sweden (2012).

[13] Large sample properties of separable nonlinear least squares estimators. K Mahata and T Soderstrom, IEEE Transactions on Signal Processing **52**:1650-1658 (2004).

5.1. Modeling, Identification

A large number of applications involving modeling and system identification by linear combinations of parametrized basis functions. In [3] the authors consider B-spline models with free knots, a classical application of VARPRO, for data driven uncertainty quantification, while in [17] they consider radial function basis, another classical application.

The practical application of FS–TARMA identification requires expertise on part of the user, in particular because model structure (including functional subspace) estimation is a rather complicated problem (Spiridonakos and Fassois 2009). The aim of [5] is to develop a novel complete approach that largely circumvents this drawback. The approach uses regression type methods for the simultaneous – for the first time – estimation of the necessary functional subspaces and model coefficients of projection. This is accomplished through proper parametrization and a Variable Projection scheme. The effectiveness of the proposed approach is assessed via its application to the identification of the time–varying dynamics of a laboratory pick–and–place mechanism from a vibration response data record.

The Generalized Instrumental Variable Estimator (GIVE) has been introduced in So¨derstro¨m [7] as a class of estimators based on the bias–eliminating principle containing many previously known methods as special cases. In its most general form, one uses a θ-dependent weighting matrix $W(\theta)$, and the problem is then indeed a separable nonlinear least squares problem. See also [11].

In [13] the authors consider a nonlinear optimization-based identification procedure for fully parameterized multivariable state-space models. The method can be used to identify linear time-invariant, linear parameter-varying, composite local linear, bilinear, Hammerstein and Wiener systems. On the other hand, Xu et al [24] consider a time-partitioned piecewise affine output error (PWA-OE) model for batch processes, in which the time index is used to simplify the partition of regression domain by utilizing the repetitive nature of batch processes. The identification problem involves both continuous and discrete variables, and the derivative information on discrete variables is unavailable. Thus, an identification algorithm based on separable nonlinear least-squares is developed to reduce the complexity of nonlinear minimization.

[1] Small Dispersion Asymptotics in Stratified Models. X Mei, PH D Thesis, Northwestern University, Evanston, Ill (2017).

[2] Identification of systems with slowly sampled outputs using LPV model. W Yan, Y Zhu, L Zhu, X Liu, Computers & Chemical Engineering **112**:316-330 (2018).

[3] Data-driven uncertainty quantification of structural systems via B-spline expansion. VK Dertimanis, MD Spiridonakos, EN Chatzi, Computers & Structures (2017).

[4] Identificação de Sistemas Utilizando a Parametrização MOLI. Patrícia Gomes Saraiva, Master Thesis, U. Porto, Portugal (2018).

[5] Output–only identification of time–varying structures via a complete FS–TARMA model approach. MD Spiridonakos, SD Fassois, Proceedings of the 4th International Operational Modal Analysis Conference (IOMAC 2011) Istanbul, Turkey (2011).

[6] Optimal design of experiments with mixtures. R H H Khashab, PHD Thesis, U. of Southhampton (2018).

[7] A generalized instrumental variable method for errors-in-variables. T So¨derstro¨m, Automatica, **47**:1656–1666, (2011).

[8] A unified framework for EIV identification methods when the measurement noises are mutually correlated. T Söderström, R Diversi, U Soverini, Automatica **50**:3216-3223 (2014).

[9] Fitting linear mixed-effects models using lme4. D Bates, M Mächler, B Bolker, S Walker, arXiv preprint arXiv:1406.5823 (2014).

[10] Filtering and System Identification: a Least Squares Approach. M Verhaegen, V Verdult, Cambridge University Press (2007).

[11] A unified framework for EIV identification methods in the presence of mutually correlated noises. T Söderström, R Diversi, U Soverini, 19th World Congress IFAC Proceedings (2014).

[12] Modeling and Identification of Linear Parameter-Varying Systems. R Tóth, Lecture Notes in Control and Information Sciences **403** (2010).

[13] Identification of fully parameterized linear and nonlinear state-space systems by projected gradient search. V Verdult, N Bergboer, M Verhaegen, IFAC Proceedings (2003).

[14] On new parametrization methods for the estimation of linear state–space models. T Ribarits, M Deistler, B Hanzon, International Journal of Adaptive Control and Signal Processing **18** (2004).

[15] Statistical Methods for Constructing Mathematical Models. DV Ivanov, EP Melisheva, Science Book Publishing House (2014).

[16] Estimation of nonlinear ARX models. Y Zhu, Decision and Control, 2002, Proceedings of the 41st IEEE Conference on Decision and Control **4** (2002).

[17] Structured parameter optimization method for the radial basis function-based state-dependent autoregressive model. H Peng, T Ozaki, V Haggan-Ozaki, Y Toyoda, International Journal of Systems Science **33**:1087-1098 (2002).

[18] Approximation of a multidimensional dependency based on linear expansion in a dictionary of parametric functions. MG Belyaev, EV Burnaev, Informatics and its Applications **7**:114-125 (2013).

[19] Maximum likelihood estimation of linear SISO models subject to missing output data and missing input data. R Wallin, A Hansson, International Journal of Control **87**:2354-2364 (2014).

[20] Hierarchical-likelihood approach for nonlinear mixed-effects models. M Noh, Y Lee, Computational Statistics & Data Analysis **52**:3517-3527 (2008).

[21] Identification of spatially distributed discrete-time state-space models. A Haber, M Verhaegen, IFAC Proceedings **45**:410-415 (2012).

[22] An iterative Kalman smoother/least-squares algorithm for the identification of delta-ARX models. MA Chadwick, SR Anderson, V. Kadirkamanathan, International Journal of Systems Science **41**:839-851 (2010).

[23] Adaptive post-processing internal models design for MIMO minimum-phase nonlinear systems. M Bin, L Marconi, arXiv preprint arXiv:1805.05629 (2018).

[24] Time-partitioned piecewise affine output error model for batch processes. Zuhua Xu, Yaobo Huang, Jun Zhao, Chunyue Song and Zhijiang Shao, Ind. Eng. Chem. Res. 57:1560–1568 (2018).

5.2. Hammerstein Models

This subsection refers to the use of nonlinear models that originate from Volterra series methods. Since those are problematic to identify, block structured systems are introduced as simplified alternatives, whose structures could be exploited to improve the identification. Among these we find the Hammerstein and Wiener models and their combinations. It turns out that since these models combine linear and nonlinear parts, they are amenable to a Variable Projection treatment.

In [3] the authors discuss a Kautz-basis-expansion based Hammerstein system identification method and separable least squares is adopted to estimate linear and nonlinear parameters. Elden and Ahmadi-Asl [4] consider bilinear tensor least squares problems that occur in applications such as Hammerstein system identification and social network analysis. A linearly constrained problem of medium size is considered, and nonlinear least squares solvers of Gauss–Newton-type are applied to numerically solve it. The problem is separable, and the variable projection method can be used. Perturbation theory is presented and used to motivate the choice of constraint. Numerical experiments with Hammerstein models and random tensors are performed, comparing the different methods and showing that a variable projection method performs best.

In [?] the authors focus on the digital predistortion for the linearization of power amplifiers (PAs) with intrinsic hard nonlinearities, such as Doherty PAs, envelope tracking (ET) PAs, widely explored in third generation (3G) communication systems. Conventional Volterra-series-based predistortion with high degree nonlinearities suffers from the difficulty of real-time implementation and numerical instability. Accordingly, a block-oriented Hammerstein predistortion with cubic-spline static nonlinearity is proposed, and the separable nonlinear least squares (SNLS) method is used to identify the Hammerstein coefficients, which significantly reduces the dimension of search space. A similar application can be found in [7], where a Hammerstein predistorter modeling for power amplifier (PA) linearization is proposed. The key feature of the model is that the cubic splines, instead of conventional high-order polynomials, are utilized as the static nonlinearities, due to the fact that the splines are able to represent hard nonlinearities accurately and circumvent the numerical instability problem simultaneously. The predistorter is implemented on the indirect learning architecture, and the separable nonlinear least squares (SNLS) Levenberg-Marquardt algorithm is adopted given that the separation method reduces the dimension of the nonlinear search space and thus greatly simplifies the identification procedure.

In [1, 8] Ase and Katayama deal with identification of Hammerstein-Wiener systems, or NLN systems, in which a linear subsystem is sandwiched by two nonlinearities. Then, initializing by an estimated linear model, they apply separable least-squares to optimize the mean square error of the OE model, where a version of the DDLC-based gradient search is employed.

[1] A subspace-based identification of Wiener–Hammerstein benchmark model. H Ase, T Katayama, Control Engineering Practice **44**:126-137 (2015).

[2] Identification of Hammerstein-Wiener systems in closed-loop. Hajime Ase and Tohru Katayama, Proceedings of the 49th ISCIE International Symposium on Stochastic Systems Theory and Its Applications Hiroshima (2017).

[3] Kautz basis expansion-based Hammerstein system identification through separable least squares method. C M Cheng, X J Dong, Z K Peng, W M Zhang and G Meng, Mechanical Systems and Signal Processing 121:929-941 (2019).

[4] Solving bilinear tensor least squares problems and application to Hammerstein identification. Lars Eldén and Salman Ahmadi-Asl

[5] On the identification of Hammerstein systems with time-varying parameters. BI Ikharia, DT Westwick, Engineering in Medicine and Biology Society, 29th Annual International Conference of the IEEE 6475-6478 (2007).

[6] Global identification of wind turbines using a Hammerstein identification method. G van der Veen, JW van Wingerden, M. Verhaegen, IEEE Transactions on Control Systems Technology **21**:1471-1478 (2013).

[7] Adaptive predistortion using cubic spline nonlinearity based Hammerstein modeling. X Wu, J Shi, IEICE TRANSACTIONS on Fundamentals of Electronics, Communications and Computer Sciences **E95-A**:542-549 (2012).

[8] Identification of Hammerstein-Wiener systems using subspace method and separable least-squares. H Ase, T Katayama, Proceedings of the ISCIE International Symposium on Stochastic Systems Theory and its Applications 40-47 (2017).

[9] Estimation of an N–L–N Hammerstein–Wiener model.Y Zhu, Automatica **38**:1607-1614 (2002).

[10] Linear approximation and identification of MIMO Wiener–Hammerstein systems. T Katayama, H Ase, Automatica **71**:118-124 (2016).

[11] Identification of time-varying Hammerstein systems using a basis expansion approach. BI Ikharia, DT Westwick, Canadian Conference on Electrical and Computer Engineering (2006).

[12] Quasiconvexity analysis of the Hammerstein model. M Rasouli, D Westwick, W Rosehart, Automatica **50**:277-281 (2014).

[13] Identification of IIR Wiener systems with spline nonlinearities that have variable knots. MC Hughes, DT Westwick, IEEE Transactions on Automatic Control **50**:1617-1622 (2005).

5.3. Error in Variables

The least-squares method generally gives biased parameter estimates when the observed input-output data are corrupted with noise. If the noise acting on both the input and output is white, and if the noise variances are known, or if estimates of the noise variances are available, then the principle of biased-compensated least squares (CLS) can be used to obtain consistent estimates. An extended version of CLS is shown to be a separable nonlinear least squares problem. The errors-in-variables (EIV) framework concerns static or dynamic systems whose input and output variables are affected by noise that is mostly assumed to be additive. These models play an important role in several engineering applications, such as, time series modeling, direction-of-arrival estimation, blind channel equalization and many other signal and image processing problems.

In [4] the authors consider the problem of dynamic errors-in-variables identification. In order to avoid possible divergence of the iteration-type bias-eliminating algorithms in the case of high noise, the bias-eliminating problem is re-formulated as a minimization problem associated with a concentrated loss function. A variable projection algorithm is proposed to efficiently solve the resulting minimization problem. See also [6].

[1] Algorithms for recursive/semi-recursive bias-compensating least squares system identification within the errors-in-variables framework. JG Linden, T Larkowski, KJ Burnham, International Journal of Control **85**:1625-1643 (2012).

[2] System identification for the errors-in-variables problem. T Söderstrom, UKACC International Conference on Control 19-32 (2010).

[3] Convergence properties of bias-eliminating algorithms for errors-in-variables identification. T Söderström, M Hong, WX Zheng, International Journal of Adaptive Control and Signal Processing **19** (2005).

[4] [**?**]A covariance matching approach for identifying errors-in-variables systems. T Söderström, M Mossberg, M Hong, Automatica **45**:2018-2031 (2009).

[5] A separable nonlinear least-squares approach for identification of linear systems with errors in variables. M Ekman, M Hong, T Söderström, IFAC Proceedings **39**:178-183 (2006).

[6] Errors-in-variables system identification using structural equation modeling. D Kreiberg, T Söderström, F Yang-Wallentin, Automatica **66**:218-230 (2016).

[7] Novel algorithms based on conjunction of the Frisch scheme and extended compensated least squares. T Larkowski, JG Linden, B Vinsonneau, KJ Burnham, Conference on Control (2008).

[8] Errors-in-variables identification using a generalized instrumental variable estimation method. T Söderström, 49th IEEE Conference on Decision and Control (CDC) (2010).

6. Medical and Biological

Many applications to imaging and spectroscopy in biological and medical systems. Again, identification problems are common. A software tool which appears in several articles is the open source package, TIMP [3]. TIMP is a problem solving environment for fitting separable nonlinear models to measurements arising in Physics and Chemistry. It has been extensively tested for time-resolved spectroscopy and FLIM-FRET data (FLIM: Fluorescent Lifetime Imaging Microscopy, FRET: Förster resonance energy transfer).

In [1], a tool for the processing and automatic quality grading in the fish industry is developed based on diffuse reflectance imaging and the subsequent unmixing of the absorption spectra using a constrained least squares model to detect hemoglobin concentration. It is common for the absorption lines to have a Gaussian or Lorentzian distribution shape, so VARPRO is used in the decomposition of the spectra.

In [6], a dynamic model, described by the equations of motion of a spring-mass-damper system, was set up to estimate the impedance (force-position) for the human elbow. Then, a system identification technique based on prediction-error minimization (PEM) was developed of this non-parametric time-domain model augmented with a parametric noise model. VARPRO is used in the approximation.

The paper [8] describes a methodology to determine the Förster resonance energy transfer in live cells as measured using fluorescence imaging microscopy. The parameters of the nonlinear quantitative model can be computed using a variable projection type of algorithm. The software used is part of the open source package TIMP.

In [11] VARPRO is used to fit NMR spectra to depict small and highly oblique nerves of the lumbosacral plexus. The aim is to use the methodology for diagnostics of pathologies.

The following articles [4, 5, 9, 7] are all about compartmental analysis, a mathematical modeling tool that originated in pharmacokinetics and is now used widely in medical and biological applications. The compartment model is formed by separate homogeneous compounds, compartments. These may represent a certain space (blood, brain, etc) or a compound in a specific form (for example in a different chemical binding). The important point is that each compartment is assumed to be homogeneous. They interact with each other by exchanging material and for most medical and biological systems this exchange is assumed to obey a linear differential equation with constant transfer coefficients, so that the system behavior in time is modeled by a linear system of differential equations. Although the equations are linear the solution is not. It can be fitted by a linear combination of nonlinear functions (basis functions), and the parameters can then obtained through a variable projection algorithm.

For medical imaging applications, a radioligand (a radioactive biochemical substance, in particular a radiolabelled substance) or tracer is introduced, usually intravenously. The transport and the binding rate of the tracer are assumed to depend linearly of the difference of the tracer concentration between two compartments, so defining the system of ODE in the tracer concentrations. Often the data measured are sums of the concentrations.

[1] Detection of blood in fish muscle by constrained spectral unmixing of

hyper-spectral images. MH Skjelvareid, K Heia, SH Olsen, S. Kristian, Journal of Food Engineering **212**:252-261 (2017).

[2] Parameter estimation and Cramér-Rao lower bounds in non-contact temperature measurement. Dominik Exel, Bernhard Zagar, Stefan Schuster, Vera Ganglberger and Johann Reisinger, Technisches Messen 86 (2018).

[3] TIMP: An R package for modeling multi-way spectroscopic measurements. Katharine M. Mullen, Ivo H. M. van Stokkum, Journal of Statistical Software **18**:1-46 (2007).

[4] Generalized separable parameter space techniques for fitting 1K-5K serial compartment models. DJ Kadrmas, MB Oktay, Medical Physics **40** (2013).

[5] Separable parameter estimation method for nonlinear biological systems. FX Wu, L Mu, 3rd International Conference on Bioinformatics and Biomedical Engineering 1-4 (2009).

[6] Closed-loop identification: application to the estimation of limb impedance in a compliant environment. DT Westwick, EJ Perreault, IEEE Transactions on Biomedical Engineering **58**:521-530 (2011).

[7] Blind identification of the kinetic parameters in three-compartment models. DY Riabkov, EVR Di Bella, Physics in Medicine & Biology **49** (2004).

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6.1. Spectroscopy

After obtaining expressions for the identification of relaxation times associated with kinetic fluorescence decay and those associated with the dynamic evolution of fluorophores (chemical compounds that can re-emit light upon light excitation), the author [1] suggests the use of variable projection algorithms in the evaluation of photochemical bioimaging when the fluorophores are used as the probe molecules. In these studies a multi-exponential decay surface can be ascribed to each pixel, where the fluorescence decay times and the corresponding emission or excitation wavelength dependent amplitudes can be recovered by the VARPRO algorithm.

The first part of [4] is a survey of the adaptation of the variable projection algorithm to the case of matrix data and of constraints on the linear parameters. This form of least squares approximation to fit linear combination of nonlinear functions is common in the applications considered in the paper, spectroscopy, microscopy and mass spectrometry. The authors emphasize the importance of forming the residual vector in a particular manner to avoid storing and operating with tensor products, and describe a way to compute the covariance for the linear parameters using less memory resources.

The application to spectroscopy involves determining the kinetics of a compartmental model of a photo-system for conversion of photons into chemical energy, using the time-resolved fluorescence measurements. This is a separable nonlinear least squares problem with matrix data Ψ , unknown kinetic model $C\left(z\right)E^{T}$, where z are the non-linear parameters and the spectra is represented by the (non-negative) linear coefficient matrix E^{T}: $\Psi \simeq C\left(z\right)E^{T}$. It was solved using the software package TIMP.

In the application to microscopy they consider the detection of a protein-protein interaction by the simultaneous analysis of multiple FLIM images. FLIM counts the photons detected at several time intervals and over many locations. The data analysis gives rise to a separable nonlinear problem with the same nonlinear parameters but different linear ones, and multiple right hand sides (also termed global analysis problem) and with a matrix data:

$$min_{z\in\mathbb{R}^{n}}\left\|\Psi - C\left(z\right)E^{T}\right\|_{2}$$

The kinetic processes of the fluorescence decays are exponential and are represented in the columns of $C\left(z\right)$ convolved with an instrumental response function (IRF). The rows of E are the amplitudes corresponding to each kinetic process.

An additional point to consider here is the distribution of errors in the FLIM data, a count of number of photons detected at a given position and time. If the count is large, then to assume that the data errors have a Gaussian distribution with mean 0 and variance σ^2 is valid and the least squares criteria acceptable. For smaller counts, the errors have a Poisson distribution and the least squares estimates are not very good. One possible correction is to weight the data points $\Psi[i,j]$ with the factor $1/\sqrt{\Psi[i,j]}$.

The third area of application considered is mass spectrometry (MS), in conjunction with gas (GC/MS) or liquid (LC/MS) chromatography. These are analytical chemistry techniques that combine the physical separation of the different molecules in the chromatography column with the separation of the ions according to their mass-to-charge ratio in the MS step. In the GC or LC step the sample molecules passing through a column, elute or come off at different times according to their affinity with the chemical in the column. In the MS step the sample is ionized and the resulting ions separated according to mass-to-charge ratio by deflection due to a electric or magnetic field.

The GC/MS or LC/MS measurements of a sample can be modeled by $\Psi \approx CE^T$. Here $C$are the elution profiles and E the mass spectra resolved with respect to the mass-to-charge ratio. When several samples of the same compound are considered, the elution profiles are different but the mass spectra is considered the same. Often C can be well represented by choosing columns of exponentially modified Gaussian with 4 parameters, width, location, decay rate and amplitude. The problems can be solved with variable projections algorithms.

The performance of three gradient type algorithms: alternating least squares, Golub-Pereyra VARPRO and the Kaufman simplification is compared in the case of a multi-exponential model of a photo-physical system [5]. Corroborating results of other authors, alternating least squares where the linear and nonlinear parameters are alternatively fixed and the problem minimized over the complementary set, is found the least efficient. The Fisher information matrix computation enables the authors to determine a lower bound for the covariance estimate of the precision of the nonlinear parameters, and conclude that in the present case the Kaufman simplification is the most cost efficient.

MEG or magnetoencephalogram is an imaging tool that can measure changes in the neural activity on a very small time scale (of the order of milliseconds). In this paper [6] the authors compare several algorithms that solve the inverse problem: given magnetic field values at a number of measurement points, reconstruct the sources, i.e., compute the location and moment parameters of the set of dipoles whose fields best approximates the data in the least squares sense.

This is a large nonlinear optimization problem with a complex objective function and many local minima. However, the model is a separable function, i.e., a linear combination, with coefficients depending on the dipole moment parameters, of nonlinear functions of the location parameters, amenable to variable projection. They compare several gradient-free algorithms for the reduced nonlinear problem: simulated annealing, genetic algorithms and a tabu search, and conclude that for the given problem, the best algorithm is a local genetic algorithm.

In 2D spectroscopy, contrary to conventional 1D, the third order optic signal at given population times is a function of two frequencies. In [8] the authors propose a method to analyze the 2D signals using a global analysis method based on the variable projection algorithm.

To reduce the dimensionality, the 3D complex valued data arrays containing the signal as a function of the excitation and emission frequency and time, are reorganized into a matrix Y, each of its columns representing the evolution in time of a specific pair of frequencies. A multi-exponential model is then defines by $M = E\,A$, where each column of E contains a complex exponential function $E_{nk} = e^{b_n t_k}$ and the amplitudes are found in the matrix A.

The data analysis can also be extended to fit rephasing and non-rephasing data simultaneously by building appending blocks of data to form the matrix Y. As this problem is computationally challenging due to the size, they suggest using in the minimization step a subsample of the data in the frequency dimensions, reporting that even using only 5% of the data gives satisfactory results.

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6.2. Tomography

The next articles concern tomography: the imaging by sectioning of objects, or more general, 2 and 3D imaging of the inside of objects using different signals and the reconstruction techniques employed to recover the information about these objects from the imaging data. For some of the medical imaging methods, a radiation source is used and the data acquired are multiple 2D images or projections taken from different angles. In transmission tomography, like the computerized tomography (CT), the radiation source is outside the object: a rotating X-ray tube generates X-rays that travel through the object. The detector measures the line integral of the beam intensity and the quantity to be reconstructed is the attenuation coefficient of the medium. In emission tomography (ECT), like PET and SPECT, the radiation source is inside; a radioactive tracer is introduced into the body. In the case of SPECT, the tracers emit gamma radiation that is measured. PET tracers emit positrons that when colliding with nearby electrons produce two gamma photons. The gamma radiation is detected by a rotating gamma camera that acquires multiple 2D images from different angles. The quantity to be reconstructed in both cases is the distribution and concentration of the radioactive tracer in the different parts of the body. Finally, photo-acoustic tomography is based on the PA effect, the formation of sound waves following light absorption. The PA signals are acquired at several locations around the object using a transducer array, the goal of the photo-acoustic imaging reconstruction being to retrieve the local pressure rise inside the tissue.

The next article [2] evaluates reconstruction techniques applied to data obtained from CT scans. Incidentally they could also be applied to data for other applications, for example seismic tomography. For medical tomography, there are two different reconstruction ways: the direct inversion methods that reverse the Radon transform, that is the line integral of the beam intensity, by for example filtered back projection, and the algebraic reconstruction methods, more adequate when the data have not been regularly sampled.

The data produced by a CT scan of an unknown object $\mathbf{u} \in \mathbb{R}^3$ are a finite number of samples $p_i\,(s_i,\,\eta_i)_1^m$ of the intensity integral of a X-ray defined by its so called acquisition parameters, origin $\mathbf{s}$ and direction $\boldsymbol{\eta}$:

$$p\,(\mathbf{s},\,\boldsymbol{\eta}) = \int_{\mathbb{R}} \mathbf{u}\,(\mathbf{s} + t\,\boldsymbol{\eta})\,dt.$$

The reconstruction problem is then reduced to solving the linear rectangular system $W\,\mathbf{u} = \mathbf{p}$, where W is the $m \times n$ projection matrix, depending on the parameters $(s_i,\, t_i)$. This can be computed by least squares methods. But in practice often the geometry of the imaging system, i,e., the acquisition parameters $(\mathbf{s},\, \boldsymbol{\eta})$ are not known accurately, for example due to faulty calibration, and this produces alignment errors. One option would be to consider the problem as a Total Least Squares problem, i.e., a linear problem where the errors are not only restricted to the observations $\mathbf{p}$ but also the matrix W is not known exactly.

Instead the authors suggest a method belonging to the class of projection matching methods. Basically they solve the nonlinear model,

$$W\,(\mathbf{a})\;\mathbf{u} = \mathbf{p},$$

where the unknown $\mathbf{a} \in \mathbb{R}^l$ contains the parametrization of possible rigid motions, three shifts and three rotations, for each projection image. The authors note that this is a possible severely ill-conditioned problem and since its parameters "separate", into the nonlinear $\mathbf{a}$ and the linear $\mathbf{u}$, they suggest an alternating optimization procedure. After solving "analytically" for the linear parameters $\mathbf{u}$, i.e., "eliminating" the reconstruction part of the problem, they describe several gradient-descent algorithms to solve the resulting nonlinear optimization problem, and state their convergence behavior, considering when approximate derivatives are used and in case of constraints on the alignment parameters.

The articles [1, 2, 3] consider the case of SPECT tomography. ECT imaging methods are governed by the photon transport equation and the reconstruction involves the attenuated Radon transform. Two unknown quantities must be estimated simultaneously, the radioactive emission source (the distribution of the radionuclides) $f\,(x, E)$ and the photon attenuation coefficient of the tissue $\mu\,(x)$, from the acquired data $p\,(s, \theta)$ on the line defined by (s, θ). The variables x and E are position and energy. The attenuated Radon transform is:

$$R_\mu f\,(s,\theta) = \int_{-\infty}^{\infty} f\left(s\theta + t\theta^\perp\right) exp\left(-\int_t^{\infty} \mu\left(s\theta + \tau\theta^\perp\right) d\tau\right) dt\; = p\,(s,\theta)\,.$$

Under the assumption that the emission data follow a Gaussian distribution, a nonlinear least squares problem can be defined including a regularization term to avoid irregular distributions of (f, μ),

$$\min_{f,\mu} \left\|R_\mu f - p\right\|_2^2 + \alpha I\,[f, \mu]\,.$$

Bronnikov exploits the fact that the variables f and μ are respectively linear and nonlinear to design a variable projection algorithm along the lines of VARPRO, which works well. On the other hand, Gourion et al. use nonlinear optimization methods directly. They also consider that a Poisson distribution is more appropriate for the data.

Finally, articles [3] and [5] study the newest field in biomedical imaging, photo-acoustic computed tomography (PACT). In this imaging technique, short laser pulses are directed at the object. The absorption of the optical energy produces local heating causing expansion of the tissue and consequent photo-acoustic wave-fields that can be measured outside the body using piezoelectric ultrasonic transducers. The signals that they receive are convolved with their acoustic-electric impulse response (EIR). In [4] the authors choose to incorporate the effect of EIR into the reconstruction. This results in an inverse model with separable linear and nonlinear parameters:

$$\mathbf{u} = \mathbf{H}\,(\mathbf{h})\boldsymbol{\theta}.$$

Here, the matrix $\mathbf{H}$ contains the approximations to the function $\mathbf{A}\,(\mathbf{r}) = \sum \theta_j \phi_j\,(\mathbf{r})$ which represents the absorbed optical density of the object under study. $\mathbf{H}$ also depends on the sampled EIR values represented by $\mathbf{h}$. The image reconstruction is now formulated as an optimization problem in $\mathbf{h}$ and $\boldsymbol{\theta}$ with regularization terms:

$$\min \left\|\mathbf{u} - \mathbf{H}\,(\mathbf{h})\,\boldsymbol{\theta}\right\|^2 + \lambda R_1\,(\boldsymbol{\theta}) + \alpha R_2\,(\mathbf{h})\,.$$

To estimate the parameters, the authors alternate the minimization between the linear and the nonlinear parameters.

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6.3. Nuclear Magnetic Resonance Spectroscopy (NMR) and Imaging

This is one of the most important applications of VARPRO as explained in [3] and we keep seen strong use as many more specific and new results come out for practical applications.

The physical phenomenon associated with NMR involves a sample that is placed in a magnetic field and irradiated with a radiofrequency (RF) pulse of a determined resonant frequency. The nuclei in the sample emit a signal that can be recorded and interpreted. NMR can be used to identify what molecules are present because the resonant frequency (Larmor frequency) depends among other factors, on the molecules. In imaging applications, typically hydrogen is the molecule of interest.

In more detail, the $\frac{1}{2}$-protons in the hydrogen nuclei have two eigenstates ($m = +\frac{1}{2}$ and $m = -\frac{1}{2}$), which in the absence of a magnetic field have the same energy. After a strong external static magnetic field is applied most of the protons fall into the lower of the two states (for most isotopes used in NMR: $m = +1/2$). When the RF pulse is applied some protons are excited back into higher energy state ($m = -1/2$), and when they decay back to the lower state an electromagnetic radiation is emitted that can be measured. In the literature, T_1 or relaxation time defines the equilibrium recovery time needed by the sample after the RF excitations. To produce images of the interior of the sample, i.e., to localize the NMR signals, spatial variations in the magnetic field strenght accross the sample are generated, the gradient fields.

Already in our 2003 review article we listed a number of articles with applications in which the data obtained through NMR was evaluated using the variable projection algorithm. An important area of application is still in vivo MR spectroscopy.

In [4] contrast enhanced MR imaging is used to obtain a time-series of the contrast concentration in the blood plasma and the extra-vascula, extra-cellular space (EES) of prostate tissue, both cancerous and non-cancerous. The perfusion model, i.e. the pharmacokinetic model of the passage of fluid between the capillaries and the capillary bed (EES) used is a two-compartment model (Tofts) with the contrast concentration in each voxel given (after discretization) by $\mathbf{p}_i = \mathbf{a}_i v_p + \mathbf{A}\mathbf{h}_i(k_{ep})\, K^{trans}$. Here, the linear parameters are the transfer constant K^{trans} and the vascular fraction v_p and the nonlinear parameter is the rate constant k_{ep}. The arterial input function $\mathbf{a}$ is a known function of time. This model can be fitted voxel-wise to the MR image data in the least squares sense.

The authors have compared two different algorithms to obtain the perfusion parameters: using Levenberg-Marquardt to estimate all the parameters, and applying the variable projection separation of variables idea to define a nonlinear LSQ problem in the parameter k_p, followed by the solution of the linear LSQ problem in the two linear parameters. To solve the nonlinear optimization problem in one variable they use Golden Section Search. Their accuracy and noise sensitivity comparisons included numerical simulations using parameter values in the range reported both for normal and malignant tissue to generate simulated MR signals that where later converted back into concentration functions after the determination of the parameters by the two optimization algorithms mentioned above. The results were comparable, but the VP based technique was three times as fast as LM for all the variables. More important for the medical application were the clinical trials with 20 patients. Here the LM failed to converge in approximately 15% of the tissues, including normal and cancerous, whereas the VP technique converged in 100% of cases.

In article [10], global and target analysis of the time-resolved spectra obtained in bioenergetic applications are reviewed. Spectroscopy is used here as a tool to investigate the dynamic properties of complex biological systems through the application of a short pulse of high energy that produces reactions like absorption or fluorescence. Often the data collected are two-way (2D), one variable is the wave length and the second is the time after excitation.

To analyse the measurements and estimate the physico-chemical parameters, both the kinetics (the compartmental model determined by transitions between the states) and the spectra must be modelled. One assumption is that the system is separable, meaning that the spectroscopic data of a complex compound are the superposition of the spectroscopic properties of the components weighted by their concentration. The simplest unidirectional kinetic model is used in global analysis, when the response is considered to be a sum of a few (2-4) exponential decays convolved with the instrument response function (IRF), i.e., the data at different wavelenghts are all approximated with a single set of exponentials. Target analysis is used when the problem requires a more complicated kinetic model involving for example forward and reversible reactions, independent decays, etc.

In both cases the parameters in the final model (both the kinetic and the spectra) must be fitted. Assuming normally distributed noise, a nonlinear least squares fit gives the maximum likelihood estimator. The nonlinear least squares approximation leads to a separable nonlinear problem that is solved using the variable projection algorithm. Results for the application to the study of ultrafast dinamics of the photoactive yellow protein are presented.

In [6] a complementary approach to global analysis is described, the so called lifetime density analysis (LDA). It is a technique used in ultrafast (femto- and pico-second) spectroscopy, when investigating energy and charge transfer in complex photosystems. Instead of using a small set of exponential decays to fit the data, one assumes that they are better represented by the integral of a continuous distribution of decays. This integral is discretised using a sum of a large ($\sim$ 100) lifetimes distributed along the time of the experiment. The resulting approximation problem in matrix notation is:

$$min_{x,\tau} \left\| D\left(\tau\right) x - A_n \right\|_2^2 .$$

Here, A_n is the (mxn) measurement matrix at the m time delays and n wavelengths, D is the matrix of the IRF convoluted with the exponential delays and x contains the amplitudes associated with the lifetimes. Again, it is a separable nonlinear least squares problem and is solved by the variable projection algorithm.

Contrary to the global analysis strategy, the LDA approach has a large number of parameters and overfitting must be considered. The authors suggest the use of the wellknown regularization techniques, truncated SVD and Tikhonov regularization. They also discuss briefly several other methods which they have included into the software, an open source Python package with GUI, that can be downloaded from the web.

Article [9] describes a technique to obtain more accurate estimates of spectral parameters when evaluating MR spectroscopic imaging (MRSI). One of the difficulties in spectral quantification is that the problem is not well conditioned. A way to avoid the large uncertainties is to incorporate the spatial smoothness information contained in the tissue properties. So, instead of computing the spectral parameters for each voxel independently, the idea is to work with a joint formulation:

$$\left(\hat{\mathbf{a}},\, \hat{\boldsymbol{\theta}}\right) = \arg\min_{\mathbf{a},\, \boldsymbol{\theta}} \left\| \mathbf{d} - \mathbf{K}\left(\boldsymbol{\theta}\right) \mathbf{a} \right\|_2^2 + \mathbf{R}\left(\mathbf{a},\, \boldsymbol{\theta}\right). \tag{6.1}$$

$\mathbf{a}$, $\boldsymbol{\theta}$ are the linear and nonlinear parameters, $\mathbf{d}$ the data, and $\mathbf{R}\left(\mathbf{a},\, \boldsymbol{\theta}\right)$ is a two-term penalty function added for regularization:

$$\mathbf{R}\left(\mathbf{a},\, \boldsymbol{\theta}\right) = \lambda \left\| \mathbf{W}_{\boldsymbol{\theta}} \right\|_2^2 + \eta \left\| \mathscr{W}_{\mathbf{a}} \right\|_1 .$$

The terms in $\mathbf{W}_{\boldsymbol{\theta}}$ and $\mathscr{W}_{\mathbf{a}}$ are designed to impose smoothness of the nonlinear $\boldsymbol{\theta}$ and linear $\mathbf{a}$ parameters respectively across the voxels.

The proposed algorithm reformulates the optimization problem (6.1) as two consecutive subproblems, the first is the nonlinear least squares problem (6.1) but only with the l_2 penalty term of $\mathbf{R}$, the second subproblem is again equation (6.1) now only with the l_1 penalty term of $\mathbf{R}$. The first subproblem is solved using the variable projection strategy to compute an updated value for the nonlinear parameters $\boldsymbol{\theta}$, which is then fed into the second subproblem. This is then a linear least squares problem in the parameters $\mathbf{a}$ with an l_1-norm regularization tem and is solved by an alternating direction method of multipliers.

The technique was tested using several data sets, both from simulated and from *in vivo* experiments, and its performance was compared with QUEST, another method. The conclusion is that the accuracy is considerably improved, which was also confirmed by a Cramer-Rao bound analysis. The drawback is the cost of the computations, $\mathcal{O}\left(P^2N^2\right)$, with P the number of voxels and N the parameters for each voxel. This compares unfavorably with a voxel by voxel approach, where the cost is $\mathcal{O}\left(PN^2\right)$.

For long *echo-time* MRS signal modeling, VARPRO is used to fit a sum of complex damped exponentials. In articles [15] and [13] data quantification of metabolites in the case of *short echo-time* is considered. The *in vivo* short *echo-time* MRS are richer and therefore a more efficient solution is to create first a database of *in vitro* spectra measurements v_k of the individual metabolites. The *in vivo* signals $y(t)$ are then fitted with a combination of these v_k, corrected by parameters α_k, ς_k, and η_k to be determined in order to allow for specific scans. A baseline term $b(t)$ that globally represents the signals of other non-dominant, non-specified metabolites possible present may also be added. This term is approximated by splines. The approximation problem considered is a non-linear least squares problem with some regularizing term:

$$\min_{\boldsymbol{\alpha},\mathbf{c},\boldsymbol{\varsigma},\boldsymbol{\eta}} \sum_{t=t_0}^{t_m} \left| y(t) - \sum_{k=1}^{K} \alpha_k \left(\varsigma_k\right)^t \left(\eta_k\right)^{t^2} v_k(t) - \left(\mathscr{A}\mathbf{c}\right)(t) \right|^2 + \lambda^2 \mathbf{c}^H D^H D \mathbf{c}.$$

Here, the matrix D is a discrete differential operator acting as a regularization matrix. The parameters α_k have the form $\alpha_k = a_k \exp(i\phi_k)$ with a_k the real amplitudes and ϕ_k the phase shifts. The ς_k and η_k are nonlinear in the damping correction parameters. The coefficients of the spline approximation of the baseline $\mathbf{c}$ are always linear. If the amplitude parameters α_k are linear the problem can be computed with VARPRO for complex problems. This is also the case even when constrains on the nonlinear parameters are imposed.

However, if there are constraints on the linear parameters α_k there is a difficulty because it is not possible, as is done in the variable projection technique, to write a closed-form solution to the linear problem part. One common occurrence for the approximation in MRS data quantification is that it requires equal phase corrections ϕ_k and non-negative real amplitudes a_k.

The algorithm described in the articles approaches this case by optimizing the nonlinear problem with the nonlinear parameters augmented by a common phase correction ϕ_0. At each iteration of the nonlinear optimization an approximate value for the linear parameters is computed from the constrained linear least squares problem with the fixed nonlinear parameters of the last iteration step.

It is shown in [15], by numerical tests, that this algorithm is more efficient and more accurate than a "full" LS solution, where the linear and nonlinear parameters are optimized together.

An open source software package AQSES based on the above techniques is described and tested. See [13].

In article [26] this software is further improved by taking into account the effect of inhomogeneities in the applied magnetic field and heterogeneities of the tissue. These cause distortions of the NMR signals, for example a broadening of the frequency-domain line with a consequent possible spectral overlap, thereby impeding a correct metabolite quantification.

The components of an NMR signal in the time-domain are the resonance frequencies multiplied by the natural damping function (Lorentzian, Gaußian or Voigt), in turn multiplied by an instrumental broadening function and all with an added noise. The lineshape (actually damping function because it is done in the time-domain) correction algorithm described in this article is an iterative procedure:

A first step is a nonlinear least squares approximation via VARPRO of the signals $\mathbf{y}(t)$ with a model $\bar{y}(t)$ where lineshape distortions and baseline are ignored:

$$\bar{y}(t) = \sum_{k=1}^{K} \alpha_k . \exp(-d_k t - g_k t^2 + 2\pi i f_k t)\, v_k\,(t)\,.$$

Using the spectral parameters thus obtained, an undisturbed signal $\hat{\mathbf{y}}(t)$ without the damping part is constructed. From the quotient ${}^{y(t)}/_{\hat{y}(t)}$ a correction of the damping function $g(t)$ is constructed. After smoothing $g(t)$, eliminating any numerical instability and noise, a nonlinear least squares approximations step via VARPRO is again performed of $[\hat{y}(t)\,\cdot\, g(t)]_{denoised}$. This process is continued until convergence of the spectral parameters or the damping function.The authors have validated the efficiency of this technique in improving the quantitation results using Monte Carlo simulations.

The next three articles [7, 16, 28] consider how to estimate the T_1 relaxation time parameter using the variable projection technique. The T_1 parameter is an intrinsic magnetic property of tissue and of importance in many clinical applications. For *in vivo* determination of T_1, multiple datasets of signal intensity at different timings are obtained. The signal intensity can be modelled by the rational function:

$$S(t_i,\, A,\, B,\, C,\, T_1) = \frac{A + B\, \exp(-{}^{t_i}/_{T_1})}{1 - C\, \exp(-{}^{t_i}/_{T_1})},\ i = 1, ...N.$$

If the radio-frequency pulse flip angles are almost perfect (Ernst angle), then the parameter C in the above rational model is close to zero and the model is a very simple one where the linear parameters can easily be separated from the nonlinear one. This model is solved in [16] and [28]. The rational model is considered in [7] and the parameters are again determined using VARPRO.

The two articles [12] and [24] describe a software for the quantification of brain metabolites using data obtained from 2D J-resolved magnetic resonance spectroscopy, a technique developed to reduce the spectral overlap common when using clinical strength 3T NMR.

The ProFit tool described in the articles implements a variable projection algorithm that also takes into account possible linear relations between parameters of different metabolites, differences between parametesr of different spins in the same metabolite and fixing specific parameters.

The Dixon technique is a chemical shift imaging method that allows to create fat only or water only images, and can therefore be used when fat or water conceal the signal of interest. In [17], in order to reconstruct the images from a dual-echo Dixon, a voxel-wise cost function is defined in the linear parameters, water and fat magnitudes W_ν, F_ν, and the nonlinear ones, initial phase shared by water and fat Φ_{0_ν} and ω_ν, the phase induced by the inhomogeneity of the static magnetic field.

To determine the maximum likelihood estimates of these parameters a variable projection technique is used to solve a simplified nonlinear least squares problem. The method is applied to *in vivo* studies of foot/ankle and CE-MRA of thighs.

The following [5] study on the effect of intra-or-extracellular water accumulation and intracellular acidification in muscles on the rate of tranverse relaxation was performed using spectroscopy before and after exercise. The resulting imaging data was modelled by a sum of exponentials and the maximum likelihood fit, a nonlinear least squares approximation, was solved using VARPRO.

The subject of article [20], diffusion MRI (dMRI) uses the diffusion of water molecules in the generation of MRI tissue images. Molecular diffusion in tissues is constrained by interactions with obstacles such as macromolecules, fibers or membranes. In this paper, MIX, a method to characterize the tissue microstructure of white matter fibers is developed.

It uses a multicompartmental model (intra-axonal, extra-axonal, isotropic) and allows for multiple fiber orientations. The data are fitted in the least squares sense to a combination of exponentials with constraints on the linear coefficients. In a first step, the algorithm constructs good initial values both of the linear and the nonlinear parameters. This is accomplished by applying the variable projection technique to separate linear from nonlinear parameters disregarding for the time being the fact that there are constraints on the linear parameters. The reduced nonlinear problem is solved using a stochastic method, a genetic algorithm, and the linear problem with constrainted parameters by CVX (Convex programming Matlab program designed by S. Boyd) . In a second step, a trust region method is used to estimate all the parameters. The method was tested on synthetic and *ex-vivo* and *in-vivo* brain data.

Data-acquisition time length is a factor in the applicability of $in - vivo$ spectroscopic imaging. Short data-acquisition time is possible when applying echo-planar spectroscopy imaging (EPSI) but with the disadvantage of a poor signal-to-noise ratio. The approach taken in [4] to obtain a high spatio-temporal resolution is to use a hybrid technique using a first step of double-echo chemical shift imaging (CSI) followed by an EPSI step.

In the CSI step, the data sets $\mathscr{D}_{1s}$ and $\mathscr{D}_{1L}$ with a limited number of spatial values but with high temporal resolution are acquired. In the second EPSI stage, a data set $\mathscr{D}_2$ with extended space coverage but limited temporal sampling is obtained. The algorithm uses the union-of-spaces idea, namely that the measured signals are a sum of nuisance, baseline (macromolecules) and metabolite signals. It also assumes partial separability of each subsignal, i.e., that it can then be modeled by a linear combination of temporal basis functions $\varphi_l(t)$ with spatial components $c_l(\mathbf{k})$. In a first preliminary step of the data processing, the nuisance signals are removed from the measured data. In a second step, the temporal basis functions of the baseline and the metabolite signals are determined from the information in the data sets obtained from CSI. Finally, the spatial components are obtained from the signals measured with EPSI. The two last steps involve the solutions of a nonlinear least squares problems and are computed using VARPRO.

An interesting technique for quantitative MRI inspired by Compressed Sensing and developed recently, Magnetic Resonance Fingerprinting (MRF), is the subject of the article [25]. The aim is to acquire enough magnetic resonance signal information in a reasonable short time to be able to deduce multiple tissue-specific parameters such as T_1 and T_2 times and spin density $\rho(\mathbf{x})$. Given the time restriction, and based on the assumption that the image can be approximated by a low-dimensional model, MRF opts for an undersampled $\mathbf{k}-$space using incoherent data acquisition schemes.

The data model has the form: $\mathbf{d} = \mathbf{F}\,\mathbf{S}\,\boldsymbol{\Phi}(\mathbf{T_1},\, \mathbf{T_2})\,\boldsymbol{\rho}$, with $\boldsymbol{\Phi}$ and $\boldsymbol{\rho}$ enclosing the parameters that are of interest, $\mathbf{S}$ containing data-acquisition information (coil sensitivities) and $\mathbf{F}$ the Fourier encoding matrix. If the noise is Gaussian a maximum likelihood estimation leads to a nonlinear least squares problem to determine the optimum times $\mathbf{T_1}$, $\mathbf{T_2}$ and spin density $\boldsymbol{\rho}$. One of the complications while using optimization methods to solve the problem is the fact that, since there is no analytic expression for the elements of $\mathbf{\Phi}$, then Bloch equation simulations would have to be performed at each iteration. The algorithm proposed by the authors is an iterative method of a reformulated problem obtained by the introduction of auxiliary variables and the subsequent splitting into three subproblems, two of them linear least squares problems. The third is a nonlinear separable variables least squares problem solved using variable projection techniques. The time consuming Bloch equation solutions needed here are substituted by dictionary values computed in advance.

In the Ph.D thesis [1] the author models the quantitative T_2 maps obtained exploring the microstructural parcellation of the cortex using multi-contrast MRI with a two-compartment model one for the contribution from cerebrospinal fluid and one where none is present. The signal at a given echo-time is represented by a sum of two exponentials with exponents involving the T_2. The parameters are computed using VARPRO.

Wilson [29] considers a new method for spectral registration. In contrast to previous approaches, the registration problem is formulated as variable-projection (VARPRO) in the frequency domain. The use of VARPRO allows the incorporation of baseline modeling, whilst also reducing the iterative optimization complexity from two parameters (phase and frequency) to one (frequency). The approach is compared with TDSR (time-domain spectral registration), and found to be more robust to large frequency shifts ($>$7Hz), baseline distortions and edited-MRS frequency misalignment. In his PhD Thesis Zhou [30] discusses and compares various methods for exponential fitting associated with NMRI, including VARPRO. In [27] the authors consider an interesting application to the assessment of myofascial trigger point via MRI for patients with migraine.

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This is an interesting area with great future potential as more brain research with electro-magnetic methods is performed.

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7. Image Processing, Vision, Video

7.1. Blind Deconvolution

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7.3. Vision

In [5] the authors observe that VarPro applies a second order optimizer such as the Gauss- Newton on a reduced objective, after optimally eliminating one set of the unknowns. It is especially applicable to factorization problems, since in these problem instances one of the involved unknown factors can be eliminated in closed form. It has been shown repeatedly that VarPro applied to geometric vision problems has much higher probability of reaching a global optimum (termed success rate in this paper) than using a second order method on the full problem (joint optimization, i.e. without eliminating one set of unknowns). VarPro, which also turns out to be closely connected to joint optimization, has generally no trouble improving the current solution.

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A surprising number of different applications to robotics, with identification a predominant one, as in other fields.

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8. Geophysics, Petroleum Engineering

This is an area of particular interest to one the authors, who has worked many years in the area of exploration geophysics, mainly on geological modeling, seismic ray tracing and inverse problems [6, 10, 11]. In the past few years VARPRO has been discovered as one of the keys for solving the fundamental earth imaging problem using full waveform inversion [22]. This is a notoriously expensive procedure (requires many solutions of the wave equation in 3D) and it leads also to multimodal optimization problems, where local optimization algorithms have difficulties in avoiding sub-optimal minima. It turns out that several different applications within this area can be stated as separable problems, making them amenable to the use of VARPRO, which as we have seen, tends to deliver much better behaved optimization problems in the reduced space of the nonlinear variables. It turns out that Bill Symes had foreseen this early with his related method of differential semblance [8].

For instance, in [1] the authors tackle the well-known global convergence issue associated to any full waveform inversion (FWI) approach by solving an extended-image space least-squares migration problem to remove any local minima present in the FWI objective function. They discuss the connection between the reflectivity and migration velocity inversion and show the importance of combining the two problems using one objective function. Moreover, they show the full separability of the two inverse problems by using the variable projection method. Furthermore, in [2] the same authors indicate that the main issue inherent to full waveform inversion (FWI) is its inability to correctly recover the Earth's subsurface seismic parameters from inaccurate starting models. This behavior is due to the presence of local minima in the FWI objective function. To overcome this problem, they propose a new objective function in which they modify the nonlinear modeling operator of the FWI problem by adding a correcting term that ensures phase matching between predicted and observed data. This additional term is computed by demigrating an extended model variable, and its contribution is gradually removed during the optimization process while ensuring convergence to the true solution. Since the proposed objective function is quadratic with respect to the extended model variable, they make use of the variable projection method. They refer to this technique as full waveform inversion by model extension (FWIME) and illustrate its potential on two synthetic examples for which FWI fails to retrieve the correct solution.

In [38] the authors consider planar waves events recorded in a seismic array that can be represented as lines in the Fourier domain. However, in the real world, seismic events usually have curvature or amplitude variability, which means that their Fourier transforms are no longer strictly linear but rather occupy conic regions of the Fourier domain that are narrow at low frequencies but broaden at high frequencies where the effect of curvature becomes more pronounced. One can consider these regions as localised "signal cones". In this work, the authors consider a space–time variable signal cone to model the seismic data. The variability of the signal cone is obtained through scaling, slanting, and translation of the kernel for cone-limited (C-limited) functions (functions whose Fourier transform lives within a cone) or C-Gaussian function (a multivariate function whose Fourier transform decays exponentially with respect to slowness and frequency), which constitutes our dictionary. The authors find a discrete number of scaling, slanting, and translation parameters from a continuum by optimally matching the data. This is a non-linear optimization problem, which is ed by a fixed-point method that utilizes a variable projection method with $\ell 1$ constraints on the linear parameters and bound constraints on the non-linear parameters.

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9. Mechanical Systems

A large number of applications involving mechanical systems. We include some sub-classes. In the Master Thesis [2] the authors consider a new method to estimate the unknown pitch actuator gain for a wind turbine system. The wind speed is included in an augmented system state. Earlier was shown that a Kalman filter can be rewritten over a moving time window both as a linear and a nonlinear LMS algorithm. A nonlinear LMS problem with a particular structure can be defined over a moving time window w, which can be solved as a so-called separable least squares (SLS) problem. The authors of [5] are motivated by the idea of turbo-machinery active subspace performance maps. In this paper they study dimension reduction in turbo-machinery 3D CFD simulations. First, they show that these subspaces exist across different blades—under the same parametrization—largely independent of their Mach number or Reynolds number. This is demonstrated via a numerical study on three different blades. Then, in an attempt to reduce the computational cost of identifying a suitable dimension reducing subspace, they examine statistical sufficient dimension reduction methods, including sliced inverse regression, sliced average variance estimation, principal Hessian directions and contour regression. Unsatisfied by these results, they evaluate a new idea based on polynomial variable projection—a non-linear least squares problem. Their results using polynomial variable projection clearly demonstrate that one can accurately identify dimension reducing subspaces for turbo-machinery functionals at a fraction of the cost associated with prior methods. They apply these subspaces to the problem of comparing design configurations across different flight points on a working line of a fan blade. They demonstrate how designs that offer a healthy compromise between performance at cruise and sea-level conditions can be easily found by visually inspecting their subspaces.

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[4] Unbalanced estimation using linear and nonlinear regression. P Nauclér, T Söderström, Automatica **46**:1752-1761 (2010).

[5] Supporting Multi-point Turbo-machinery Dimension Reduction via Polynomial-based Variable Projection S Yuchi, P Seshadri, G Parks and S Shahpar, Manuscript, Rolls-Royce (2018).

9.1. Vibrations

In [1] the authors consider the modeling and identification of non-stationary random vibration signals in various applications. A recent development in this area is the postulation of FS–TARMA models with complex exponential or spline basis functions, accompanied by the development of a Separable Nonlinear Least Squares (SNLS) method which achieves simultaneous estimation of the model coefficients of projection and the basis functions themselves

[2]. This method drastically simplifies the identification procedure; results from application case studies are very promising.

In [3], the authors investigate the nonparametric estimation of the frequency dependent complex modulus of a viscoelastic material. The strains due to flexural wave propagation in a bar specimen are registered at different cross sections. The time domain data is transformed into frequency domain using discrete Fourier transform and a separable nonlinear least squares algorithm is then employed to estimate the complex modulus at each frequency. Inherent numerical problems due to associated ill-conditioned matrices are treated with special care. An analysis of the quality of the nonlinear least squares estimate is also carried out.

Functional Series Time-dependent Autoregressive Moving Average (FS-TARMA) models are characterized by time varying parameters which are projected onto selected functional subspaces. They offer parsimonious and effective representations for a wide range of non-stationary random signals where the evolution in the dynamics is of deterministic nature. Yet, their identification remains challenging, with a main difficulty pertaining to the determination of the functional subspaces. In [4] the authors overcome this challenge via the introduction of the novel class of Adaptable FS-TARMA (AFS-TARMA) models, that is models with basis functions properly parametrized and directly estimated based on the modelled signal. Model identification is effectively dealt with through a Separable Non-linear Least Squares (SNLS) based estimation procedure that decomposes the problem into two simpler subproblems: a quadratic one and a reduced-dimensionality non-quadratic constrained optimization one.

A discrete-time Linear Parameter-Varying (LPV) model can be seen as the combination of local LTI (Linear Time Invariant) models together with a scheduling signal dependent function set, that selects one of the models to describe the continuation of the signal trajectories at every time instant. An identification strategy of LPV models is proposed that consists of the separate approximation of the local model set and the scheduling functions. The local model set is represented as a linear combination (series expansion) of Orthonormal Basis Functions (OBFs). First the OBFs, that guarantee the least asymptotic worst-case modeling error for the local models are selected through the Fuzzy Kolmogorov c-Max approach. With the resulting OBFs, the weighting functions are identified through a separable least- squares algorithm.

[1] Non-stationary random vibration modeling and analysis via functional series time-dependent ARMA (FS-TARMA) models: a critical survey. MD Spiridonakos, SD Fassois, Mechanical Systems and Signal Processing **47**:175-224 (2014).

[2] FS–TARMA models for non–stationary vibration analysis: an overview and recent advances. Spiridonakos M.D. and Fassois S.D. Proceedings

of the 17th International Congress on Sound and Vibration (ICSV 17) (2010),

[3] On the use of flexural wave propagation experiments for identification of complex modulus. K Mahata, S Mousavi, T Söderstrom, M. Mossberg, U. Valdek, L. Hillstron, IEEE Transactions on Control Systems Technology **11**:863-874 (2003).

[4] Adaptable functional series TARMA models for non-stationary signal representation and their application to mechanical random vibration modeling. MD Spiridonakos, SD Fassois, Signal Processing **96**:63-79 (2014).

[5] Flexible model structures for LPV identification with static scheduling dependency. R Tóth, PSC Heuberger, P.M.J. Van den Hof, Proceedings of the 47th IEEE Conference on Decision and Control ThB03.6 (2008).

[6] Maximum likelihood estimation of flexural wave-numbers in lightly damped plates. CR Halkyard, Journal of Sound and Vibration **300**:217-240 (2007).

9.2. Control

Several contributions to system control and identification. Some only use the formulas for derivatives of projectors, but others concern themselves with separable models. Papers [1, 2, 6] use the formulas of differentiation of the pseudo-inverse in various contests.

In [3] a novel identification algorithm for a class of non-linear, possibly parameter varying models is proposed. The algorithm is based on separable least squares ideas. These models are given in the form of a linear fractional transformation (LIFT) where the 'forward' part is represented by a conventional linear regression and the 'feedback' part is given by a nonlinear map which can take into account scheduling variables available for measurement. The non-linear part of the model can be parameterized according to various paradigms, such as neural network (NN) or general nonlinear autoregressive exogenous (NARX) models. The estimation algorithm exploits the separability of the criterion used to estimate the parameters. When using a NN, the results in the Golub-Pereyra paper facilitates de calculation of the Frechet derivative needed to implement a separable least squares algorithm.

The Thesis [5] considers the problem of identifying nonlinear systems with errors-in-variables by using separable NLLS. A bias-eliminating approach, based on a compensated least- squares (CLS) solution of an overdetermined system of equations and separable nonlinear LS is used. On the other hand, the Thesis [7] considers the identification of parameters in a Hammerstein-Wiener separable model for control valves.

[1] Optimal Nonlinear Control and Estimation Using Global Domain Linearization. LA Wendt, PH D Thesis, University of Illinois, Urbana-Champaign (2017).

[2] Elements of Robustness and Optimal Control for Infrastructure Networks. Q Ba, PH D Thesis, University of Southern California (2018).

[3] Identification of non-linear parametrically varying models using separable least squares. F Previdi, M Lovera, International Journal of Control **77**:1382-1392 (2004).

[4] Regularized data-driven construction of fuzzy controllers. M Burger, J Haslinger, U Bodenhofer, HW Engl, Journal of Inverse and Ill-Posed Problems **10** (2002).

[5] Modeling and Control of Bilinear Systems: Application to the Activated Sludge Process. M Ekman, PH D Thesis, University of Uppsala (2005).

[6] Algebraic invariance conditions in the study of approximate (null-) controllability of Markov switch processes. D Goreac, M Martinez, Mathematics of Control, Signals, and Systems **27**:551-558 (2015).

[7] Identificação de Processos Não-Lineares e Quantificação de Atrito em Válvulas de Controle. RA Romano, PH D Thesis, Escola Politécnica, San Pablo, Brazil (2010).

[8] On decentralized robust weight control for DC power networks. Q Ba, K Savla, American Control Conference (ACC) (2016).

[9] Switching strategy based on homotopy continuation for non-regular affine systems with application in induction motor control. A Borisevich, G Schullerus, arXiv preprint arXiv:1203.5919 (2012).

10. Machine Learning

A very current field where Variable Projections has diverse applications to classification, Markov decision processes, computer vision, discriminant analysis, clustering and image super-resolution.

Molinari [1, 3] uses splines with variable knots to represent functional data curves. This is one the classical applications of VARPRO and the author takes good advantage of it. Chatterjee and Milanfar [4] consider separable models for patch denoising by learning a best basis for each cluster of similar patches and apply VARPRO for optimization.

In [5] the authors propose a novel computationally efficient single image super-resolution method that learns multiple linear mappings (MLM), to directly transform low-resolution feature subspaces into high-resolution subspaces. The problem is separable with multiple right-hand sides and VARPRO is used successfully.

[1] Free knot splines for supervised classification. N Molinari, Journal of Classification **24**:221-234 (2007).

[2] Invariant Representations and Learning for Computer Vision. A Vedaldi, PH D Thesis UCLA (2008).

[3] Choice of B-splines with free parameters in the flexible discriminant analysis context. C Reynès, R Sabatier, N Molinari, Computational Statistics & Data Analysis **51**:1765-1778 (2006).

[4] Clustering-based denoising with locally learned dictionaries. P Chatterjee, P Milanfar, IEEE Transactions on Image Processing **18**:1438-1451 (2009).

[5] Learning multiple linear mappings for efficient single image super-resolution. K Zhang, D Tao, X Gao, X Li, Z. Xiong, IEEE Transactions on Image Processing **24**:846-861 (2015).

10.1. Neural Networks

This is an area of renovated interest in Machine Learning. In [1] the authors rediscovers the fact that single layer perceptrons are separable non-linear models and thus amenable to training via VARPRO [2]. Given the current rage about multilayer networks (DNN), it might be of interest to extend these results to that case. In [12] there is a first attempt to do just that.

Mizutani and Demmel [4] describe in detail an economical trust-region implementation of VARPRO in the framework of a so-called block-arrow least squares (BA) algorithm for a general multiple-response nonlinear model. They then present numerical results using an exponential-mixture benchmark, seven-bit parity, and color reproduction problems; in some situations, VARPRO enjoys quick convergence and attains high classification rates, while in some others VARPRO works poorly. This observation motivates them to investigate original VARPRO's strengths and weaknesses compared with other (full-functional) approaches. To overcome the limitation of VARPRO they suggests how VARPRO can be modified as a Hessian matrix-based approach that exploits negative curvature when it arises. For this purpose, an economical BA algorithm is very useful in implementing such a modified VARPRO especially when a given model is expressed in a multi-layer (neural) network for efficient Hessian evaluation by the so-called second-order stage-wise backpropagation.

One of the most interesting contributions is [7], which proves that the reduced VARPRO functional is always better conditioned than the original one for the full problem and that the Levenberg-Marquardt version for separable problems usually converges orders of magnitude faster for notoriously ill-conditioned single hidden layer NN. Early reference to this application are [15, 18, 19]. We have also pointed out the usefulness of VARPRO in training single hidden layer networks in [2], which is re-enforced later on by [5, 6]. It is worth insisting on this fact: it is not only the reduction in the number of variables that makes VARPRO powerful, but rather its regularization effect. Highly non-convex multi-modal problems become much better defined in the reduced form for the nonlinear parameters.

Several authors discuss B-splines NN and their training by VARPRO [8, 9]. In [13] the authors consider representation discovery in reinforcement learning (RL) posing basis adaptation as a nonlinear separable least-squares value function approximation solvable by VARPRO.

[1] Learning algorithms for neural networks and neuro-fuzzy systems with separable structures. BA Skorohod, Cybernetics and Systems Analysis **51**:173-186 (2015).

[2] Variable projection neural network training. V Pereyra, G Scherer and F Wong, Applied Mathematics and Computers in Simulation **73**:231-243 (2006).

[3] Multi-illuminant color reproduction for electronic cameras via CANFIS neuro-fuzzy modular network device characterization. E Mizutani, K Nishio, IEEE Transactions on Neural Networks **13**:1009-1022 (2002).

[4] On improving trust-region variable projection algorithms for separable nonlinear least squares learning. E Mizutani, J Demmel. The 2011 International Joint Conference on Neural Networks (2011).

[5] Variable projection method and Levenberg-Marquardt algorithm for neural network training. CT Kim, JJ Lee, H Kim, 32nd Annual Conference on IEEE Industrial Electronics, IECON (2006).

[6] Training two-layered feedforward networks with variable projection method. CT Kim, JJ Lee, IEEE Transactions on Neural Networks **71**:3640-3643 (2008).

[7] Separable non-linear least-squares minimization - possible improvements for neural net fitting. J Sjoberg, M Viberg, Neural Networks for Signal Processing VII (1997).

[8] Extending the functional training approach for B-splines. CL Cabrita, AE Ruano, PM Ferreira, LT Koczy. The 2012 International Joint Conference on Neural Networks (IJCNN) (2012).

[9] Supervised training algorithms for B-spline neural networks and neuro-fuzzy systems. AE Ruano, C Cabrita, JV Oliveira, International Journal of Systems Science **33**:689-711 (2002).

[10] On the optimal structure design of multilayer feedforward neural networks for pattern recognition. D Chen, P Burrell, International Journal of Pattern Recognition and Artificial Intelligence **16**:375-398 (2002).

[11] Training neural networks and neuro-fuzzy systems: A unified view. AE Ruano, PM Ferreira, C Cabrita, S Matos, IFAC Proceedings (2002).

[12] A generalized learning paradigm exploiting the structure of feedforward neural networks. R Parisi, ED Di Claudio, G Orlandi, BD Rao, IEEE Transactions on Neural Networks **7**:1450-1460 (1996).

[13] Basis adaptation for sparse nonlinear reinforcement learning. S Mahadevan, S Giguere, N Jacek, Proceedings of the Twenty-Seventh AAAI Conference on Artificial Intelligence (2013).

[14] Reduction of adjusting weights space dimension in feedforward artificial neural networks training. SL Blyumin, PV Saraev, Proceedings 2002 IEEE International Conference on Artificial Intelligence Systems (2002).

[15] A new formulation of the learning problem of a neural network controller. AE Ruano, DI Jones, P.J Fleming, Proceedings of the 30th IEEE Conference on Decision and Control (1991).

[16] Towards a more analytical training of neural networks and neuro-fuzzy systems. AE Ruano, CL Cabrita, PM Ferreira, Signal Processing (WISP) (2011).

[17] Fuzzy mixtures of complementary local experts: towards neuro-fuzzy modular networks. E Mizutani, K Nishio, 2002 IEEE International Conference on Fuzzy Systems FUZZ-IEEE '02 (2002).

[18] Application of projection learning to the detection of urban areas in SPOT. K Weigl, G Giraudon, M Berthod, Report 2143, INRIA , France (1993).

[19] Projection learning: alternative approach to the computation of the projection. K Weigl, M Berthod, Proc European Symp on Artificial Neural Networks 19-24, Brussels, Belgium (1994).

11. Mathematics

In [1] the authors describe and analyze an algorithm for computing the homology (Betti numbers and torsion coefficients) of basic semi-algebraic sets which works in weak exponential time. For this purpose they use the formulas of differentiation of the pseudo-inverse.

[1] Computing the homology of basic semi-algebraic sets in weak exponential time. P Bürgisser, F Cucker and P Lairez - Journal of the ACM 66:1-30 (2018).

[2] A Riemannian trust-region method for low-rank tensor completion. Gennadij Heidel and Volker Schulz, Numerical Linear Algebra with Applications 25 (2018).

11.1. Differential Equations and Dynamical Systems

Applications to direct and inverse problems involving differential equations are presented here, including several on model order reduction. The dynamic mode decomposition (DMD) has become a leading tool for data-driven modeling of dynamical systems, providing a regression framework for fitting linear dynamical models to time- series measurement data. The method is akin to POD for model order reduction. In [1] the authors present an algorithm for computing an optimized version of the DMD for data that may be collected at unevenly spaced sample times. The primary computational tool at the heart of these algorithms is the variable projection method. To apply variable projection, the DMD is rephrased as a problem in exponential data fitting (specifically, inverse differential equations), an area of research which has been extensively developed and has many applications. A careful discussion and some impressive numerical examples are included.

In [4] the authors consider a set of response observations for a parametrized dynamical system. This an interesting application that combines separable least squares with model order reduction. The authors seek a parametrized dynamical model that will yield uniformly small response error over a range of parameter values yet has low order. Frequently, access to internal system dynamics or equivalently, to realizations of the original system is either not possible or not practical; only response observations over a range of parameter settings might be known. Respecting these typical operational constraints, they propose a two phase approach that first encodes the response data into a high fidelity intermediate model of modest order, followed then by a compression stage that serves to eliminate redundancy in the intermediate model. For the first phase, they extend non-parametric least-squares fitting approaches so as to accommodate parameterized systems. This results in a (discrete) separable least-squares problem formulated with respect to both frequency and parameter that identifies “local” system response features. The second phase uses an H2-optimal model reduction strategy accommodating the specialized parametric structure of the intermediate model obtained in the first phase. The final compressed model inherits the parametric dependence of the intermediate model and maintains the high fidelity of the intermediate model, while generally having dramatically smaller system order. We provide a variety of numerical examples demonstrating our approach. Also [6] considers model order reduction, this time through projected nonlinear least squares that leads to a separable complex NLLSQ problem.

Harker and Rath [3] describe a new method for identifying the system parameters of a dynamic system in state-space form by minimizing the least-squares error of the measured system output. The variable projection method is used to eliminate the necessity of estimating the system states, and reduce the system identification cost function to a function of only the system parameters. In [14] the authors consider the mesh-less solution of PDE's in irregular domains by using radial functions and Galerkin collocation. They investigate the problem of the adaptive calculation of the basis function centers, which will not be coinciding with the collocation points. This leads to a SNLLSQ problem that is solved with VARPRO.

[1] Variable projection methods for an optimized dynamic mode decomposition. T Askham, JN Kutz, SIAM Journal on Applied Dynamical Systems **17**:380-416 (2018).

[2] Scientific Computing with Ordinary Differential Equations. P Deuflhard, F Bornemann, Springer (2012).

[3] An ODE-based method for computing the approximate greatest common divisor of polynomials. Antonio Fazzi, Nicola Guglielmi and Ivan Markovsky, Numerical Algorithms (2018).

[4] Empirical least-squares fitting of parametrized dynamical systems. Alexander Grimm, Christopher Beattie, Zlatko Drmaˇc and Serkan Gugercin, arXiv.org > math > arXiv:1808.05716 (2018).

[5] Global least squares for time-domain system identification of state-space models. M Harker and G Rath, 2018 7th Mediterranean Conference on Embedded Computing 2018

[6] Optimal model reduction using projected nonlinear least squares. J M Hokanson and C C Magruder, arXiv t arXiv:1811.11962 (2018).

[7] Identification of fractional linear dynamical systems with autocorrelated errors in variables by generalized instrumental variables. D V Ivanov, I L Sandler, E V Kozlov, IFAC-PapersOnLine, 51:580-584 (2018).

[8] Numerical Computation 1: Methods, Software and Analysis. CW Ueberhuber, Springer (2012).

[9] Gewöhnliche Differentialgleichungen. P Deuflhard, F Bornemann. de Gruyter Studium (2013).

[10] Conformal maps to multiply slit domains and applications. N Hale, TW Tee, SIAM Journal on Scientific Computing **31**:3195-3215 (2009).

[11] Improved estimation performance using known linear constraints. K Mahata, T Söderström, Automatica **40**:1307-1318 (2004).

[12] An analysis of separable least squares data driven local coordinates for maximum likelihood estimation of linear systems. T Ribarits, M Deistler, B Hanzon, Automatica **41**:531-544 (2005).

[13] Data-driven operator inference for nonintrusive projection-based model reduction. B Peherstorfer, K Willcox, Computer Methods in Applied Mechanics and Engineering **306**:196-215 (2016).

[14] Radial function collocation solution of partial differential equations in irregular domains. V Pereyra, G Scherer, Journal of Computing Science and Mathematics **1:28-41** (2007).

11.2. Inverse Problems

The interesting paper [3] proposes an alternative to VARPRO for separable inverse problems: first linearize the whole problem and then project. This approach gives more flexibility and it turns out to be more efficient as shown in several nontrivial examples.

[1] Generalization of the solution of the inverse Richards' problem. M Vocciante, AP Reverberi, VG Dovì, Chemical Engineering Transactions **52**:1285-1290 (2016).

[2] Large-scale inverse problems in imaging. J Chung, S Knepper, J G Nagy, Handbook of Mathematical Methods in Imaging 43-86 (2011).

[3] LAP: a linearize and project method for solving inverse problems with coupled variables. James L Herring, James G Nagy and Lars Ruthotto, arXiv preprint arXiv:1705.09992 (2017).

[4] A Unified Framework for Identifiability Analysis in Bilinear Inverse Problems. Y Li, PH D Thesis, University of Illinois (2015).

[5] Discrete spectrum reconstruction using integral approximation algorithm. V Sizikov, D Sidorov, Applied Spectroscopy **71**:1640-1651 (2017).

[6] A general method for the solution of inverse problems in transport phenomena. M Vocciante, AP Reverberi, VG Dovì, Chemical Engineering Transactions **43**:1615-1620 (2015).

[7] Estimating nuisance parameters in inverse problems. AY Aravkin, T Van Leeuwen, Inverse Problems **28** (2012).

[8] An efficient iterative approach for large-scale separable nonlinear inverse problems. J Chung, JG Nagy, SIAM Journal on Scientific Computing **31**:4654-4674 (2010).

[9] Use of inverse modeling techniques for the estimation of heat transfer coefficients to fluids in cylindrical conduits. AP Reverberi, B Fabiano, VG Dovì, International Communications in Heat and Mass Transfer **42**:25-31 (2013).

[10] The inverse problem of bioelectricity: an evaluation. A van Oosterom, Medical & Biological Engineering & Computing **50**:891-902 (2012).

12. Physics

The work in [4] shows an interesting connection between NMR spectroscopy (a bestseller of VARPRO) and lattice quantum chromodynamics. From this connection and somewhat fortuitously surged a collaboration [5, 6].

[1] Deconfinement, gradient, and cooling scales for pure SU (2) lattice gauge theory. BA Berg, DA Clarke, Physical Review D **95**:094508 (2017).

[2] An artificial photosynthetic model based on a molecular triad of boron dipyrromethene and phthalocyanine. EA Ermilov, JY Liu, R Menting, YS Huang, B Roder, DKP Ng, Physical Chemistry Chemical Physics **18**:10964-10975 (2016).

[3] Dark nuclei. II. Nuclear spectroscopy in two-color QCD/ FW Detmold, M McCullough, A Pochinsky, Physical Review D **90**:114506 (2014).

[4] What can Lattice QCD theorists learn from NMR spectroscopists?. GT Fleming, QCD and Numerical Analysis **III**:143-152 (2005).

[5] Excited state effective masses. George T. Fleming, Saul D. Cohen, Huey-Wen Lin,Victor Pereyra, Proceedings XXV International Symposium on Lattice Field Theory (2007)

[6] Excited-state effective masses in Lattice QCD. GT Fleming, SD Cohen, H-W Lin, V Pereyra, Physical Reviews D **80**:074506 (2009).

[7] Convolution-based one and two component FRAP analysis: theory and application. A Tannert, S Tannert, S Burgold, M Schaefer, European Biophysics Journal **38**:649-661 (2009).

[8] Evolutionary fitting methods for the extraction of mass spectra in lattice field theory. GM von Hippel, R Lewis, RG Petry, Computer Physics Communications **178**:713-723 (2008).

[9] Least squares fitting with one explicit parameter less. BA Berg, Computer Physics Communications **200**:254-258 (2016).

[10] Geometry of nonlinear least squares with applications to sloppy models and optimization. MK Transtrum, BB Machta, JP Sethna, Physical Review E **83** (2011).

13. Optics

[1] Improved approximation of spatial light distribution. D Kaljun, T Novak, J Žerovnik, PLOS one (2017).

[2] Exploiting the spatiotemporal correlation in adaptive optics using data-driven H2-optimal control. K Hinnen, M Verhaegen, N Doelman, JOSA A **24**:1714-1725 (2007).

[3] Optimum selection of input polarization states in determining the sample Mueller matrix: a dual photo-elastic polarimeter approach. D Layden, MFG Wood, IA Vitkin, Optics Express **20**:20466-20481 (2012).

[4] Towards unsupervised fluorescence lifetime imaging using low dimensional variable projection. Y Zhang, A Cuyt, W Lee, GL Bianco, G Wu, Y Chen, DD Li, Optics Express **24**:26777-26791 (2016).

14. Chemistry

These are applications to various topics in chemistry, including gas chromatography, spectroscopy, photo-induced processes and sequential energy and charge transfer. Several of these applications are trying to fit parameters in separable modeling problems. In [1] the authors use the formula for differentiation of the pseudo-inverse. The talk [4] uses separation of variables for models of permeation of gases in polymers.

A notable contribution is [8], where the author considers in detail the application of Variable Projections to a number of important problems in Physics and Chemistry. She also is the implementor of a version of VARPRO in the R language, including the problem of multiple right hand sides.

An application of separation of variables combined with a genetic algorithm for multi-exponential fluorescence decay surface calculation can be found in [9].

[1] Path optimization by a variational reaction coordinate method. II. Improved computational efficiency through internal coordinates and surface interpolation. AB Birkholz, HB Schlegel, The Journal of Chemical Physics **144**:184101 (2016).

[2] The influence of solvent polarity and metalation on energy and electron transfer in porphyrin– phthalocyanine heterotrimers. S Tannert, EA Ermilov, JO Vogel, M.T.M. Choi, D.K.P. Ng, The Journal of Physical Chemistry **111**:8053-8062 (2007).

[3] Spectroscopic study of electron and energy transfer in novel silicon phthalocyanine—boron dipyrromethene triads. EA Ermilov, JY Liu, DKP Ng, B Röder, Physical Chemistry Chemical Physics **11**:6230-6440 (2009).

[4] Permeation of gases in polymers: parameter identification and nonlinear regression analysis. R Scheichl, MH Klopffer, Z Benjelloun-Dabaghi, B. Flaconneche, Journal of Membrane Science **254**:275-293 (2005).

[5] Switching the photo-induced processes in host–guest complexes of β-cyclodextrin-substituted silicon (iv) phthalocyanines and a tetrasulfonated porphyrin. EA Ermilov, R Menting, JTF Lau, X Leng, B. Roder, D. Ng, Physical Chemistry Chemical Physics (2011).

[6] Sequential energy and charge transfer processes in mixed host–guest complexes of subphthalocyanine, porphyrin and phthalocyanine chromophores. R Menting, DKP Ng, B Röder, E.A. Ermilov, Physical Chemistry Chemical Physics (2012).

[7] Signal amplification between Gβγ release and PI3Kγ-mediated PI(3,4,5)P3 formation monitored by a fluorescent Gβγ biosensor protein and repetitive two component total internal reflection/fluorescence redistribution after photobleaching analysis. A Tannert, P Voigt, S Burgold, S Tannert, M. Schaefer, Biochemistry **47**:11239-11250 (2008).

[8] Separable Nonlinear Models: Theory, Implementation and Applications in Physics and Chemistry. KM Mullen, PH D Thesis, Vrije University (2008).

[9] Combined genetic algorithm and multiple linear regression (GA-MLR) optimizer: application to multi-exponential fluorescence decay surface. JJ Fisz, The Journal of Physical Chemistry A **110**:12977-12985 (2006).

14.1. Gas Chromatography

These are inverse problems using reversed flow gas chromatography that are amenable to Variable Projections. Many of these chemistry papers are behind a paying wall and thus they are inaccessible to us and we cannot comment in more detail.

[1] New approach to the acidity characterization of pristine zeolite crystals by ethylene using reversed-flow inverse gas chromatography (RF-IGC). MA Benghalem, A Astafan, L Pinard, T. Jean Daou, Thomas Belin, The Journal of Physical Chemistry **121**:2738-2747 (2017).

[2] Interactions of H2 on the isobutane adsorption over bifunctional catalyst PtHBEA revealed by reversed-flow inverse gas chromatography. T Belin, N Batalha, L Pinard, F Lemos, Y. Pouilloux, The Journal of Physical Chemistry **119**:1791-1799 (2015).

[3] Impact of the BEA zeolite morphology on isobutane adsorption followed by reversed-flow inverse gas chromatography. N Batalha, A Soualah, L Pinard, Y Pouilloux, F. Lemos, T. Belin, Journal of Chromatography A **1260**:206-214 (2012).

15. Environmental Sciences

[1] Improved remediation processes through cost-effective estimation of soil properties from surface measurements. M Vocciante, AP Reverberi, L Pietrelli, VG Dovi, Journal of Cleaner Production **167**:680-686 (2017).

[2] Spatio-Temporal Heterogeneity: Concepts and Analyses. P Dutilleul, Cambridge University Press (2011).

[3] Forecasting seasonal time series using weighted gradient RBF network based autoregressive model. W Ruan, QZ Sheng, P Xu, NK Tran, NJG Falkner, X. Li, WE Zhang, Proceedings of the 25th ACM International on Conference on Information and Knowledge Management (2016).

[4] Generalized exponential autoregressive models for nonlinear time series: stationarity, estimation and applications. G Chen, M Gan, G Chen, Information Sciences **438**:46-57 (2018).

[5] Discriminative non-negative matrix factorization for multiple pitch estimation.. N Boulanger-Lewandowski, Y Bengio, P Vincent, 13th International Society for Music Information Retrieval Conference 205-210 (2012).

[6] Multiple Gaussian process models for direct time series forecasting. T Hachino, V Kadirkamanathan, IEEJ Transactions on Electrical and Electronic Engineering **6**:245-252 (2011).

[7] Time series forecasting using multiple Gaussian process prior model. T Hachino, V Kadirkamanathan, Symposium on Computational Intelligence and Data Mining 604-609 (2007).

16. Astronomy

Stellar winds are flows ejected from the upper atmosphere of a star. With their moments and energies they affect the physics of stellar atmospheres and influence the evolution of stars and galaxies. They allow spectroscopic studies of the most luminous stellar objects, even of distant galaxies, thereby enabling the observer to obtain quantitative information of their host galaxies. The determination of the wind properties such as velocities, moments, energy and mass-loss rates in first stars driven by Carbon-Nitrogen-Oxygen cycles is an important problem in astronomy [2]. These winds can only be simulated numerically since there are no available observations. A first test is to check if the winds are possible on first stars, by comparing a calculated radiative force against the gravitational force. For those stars for which it is shown that the winds exist, the hydrodynamic equations are solved to predict the wind-mass loss rate. The mass-loss rate M can be fitted in the least squares sense by the following non-linear function in variables, luminosity L, mass fraction of heavier elements (heavier than Helium and Hydrogen) Z, and effective temperature Teff:

$$M = \alpha_0 L^{\alpha_1} 10^{\frac{\alpha_2 (logZ + \alpha_3 logL)}{logZ(\alpha_4 + \alpha_5 logL) + 1} + \alpha_6 logT_{eff}}.$$

The values of the parameters α_i can be obtained using VARPRO.

Another application refers to gravitational lenses. A gravitational lens is a distribution of matter (a cluster of galaxies, for example) between a distant light source and an observer that bends the electromagnetic radiation passing through its gravitational field. This deformation leads to a folding of the wave-front, and thus the observer is hit several times by the wave-front seeing multiple images at different times, i.e., there is a time delay between the pulses. A measurement of the time delay leads to a scaling of the model of the gravitational lens system.

The article [1] compares three estimator techniques to measure time delays based on the data from optical light curves of lensed quasars. All three rely on iterative non-linear optimization algorithms. The estimators functions take n light curves, (n=2 or 4) as input and return n corresponding time shifts τ, one for each curve. These time shifts directly translate into time delay estimations between each pair of curves. The first estimator technique chooses a free-knot splines function to fit a single continuous model to all data points of the light curves, simultaneously adjusting time and magnitude shifts between these curves so as to minimize a $\chi 2$ fitting statistic between the data and the model. As usual, VARPRO allows to separate the linear from the non-linear part of the free-knot spline approximation problem.

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21. Neurosciences

An important problem in motor neurosciences is the accurate description of movements [1]. This would allow, for example, to characterize developmental coordination or to diagnose disorders like stages in Parkinson's disease, or autism spectrum disorder, etc. One technique used to describe an action is the SB-ST method. Here, a set of key postures of the movement (for example joint rotations) are represented by vectors thereby forming the spatial basis, SB. Then their ST profiles, representing the trajectories in time of these postures are defined. A nonlinear Gaussian model is then fitted to the spatio-temporal ST profiles, with the parameters in it representing how much (control) and when (coordination) the postures are being recruited. The parameters in the nonlinear model are computed via VARPRO.

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