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Wavelet and Multiscale Methods

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Abstract. Various scientific models demand finer and finer resolutions of relevant features. Paradoxically, increasing computational power serves to even heighten this demand. Namely, the wealth of available data itself becomes a major obstruction. Extracting essential information from complex structures and developing rigorous models to quantify the quality of information leads to tasks that are not tractable by standard numerical techniques. The last decade has seen the emergence of several new computational methodologies to address this situation. Their common features are the nonlinearity of the solution methods as well as the ability of separating solution characteristics living on different length scales. Perhaps the most prominent examples lie in multigrid methods and adaptive grid solvers. These have advanced the frontiers of computability for certain problem classes in numerical analysis. Other highly visible examples are: regression techniques in nonparametric statistical estimation, the design of universal estimators in the context of mathematical learning theory and machine learning; the investigation of greedy algorithms in complexity theory, compression techniques and encoding in signal and image processing; the solution of global operator equations through the compression of fully populated matrices arising from boundary integral equations with the aid of multipole expansions and hierarchical matrices; attacking problems in high spatial dimensions by sparse grid or hyperbolic wavelet concepts.

This workshop proposed to deepen the understanding of the underlying mathematical concepts that drive this new evolution of computation and to promote the exchange of ideas emerging in various disciplines. A special emphasis was placed on high dimensional problems since these amplify even further the need for novel theory and computation.

Mathematics Subject Classification (2000): 16xx (Numerical Analysis and Scientific Computing).

Introduction by the Organisers

Complex scientific models of turbulence, fluid structure interaction, nanosciences and reliability control, demand finer and finer resolution in order to increase reliability. This demand is not simply solved by increasing computational power. Indeed, higher computability even contributes to the problem by generating wealthy data sets for which efficient organization principles are not available. Extracting essential information from complex structures and developing rigorous models for quantifying the quality of information is an increasingly important issue. This manifests itself through recent developments in various areas. Examples include regression techniques such as projection pursuit in stochastic modeling, the investigation of greedy algorithms in complexity theory, or compression techniques and encoding in signal and image processing. Further representative examples are the compression of fully populated matrices arising from boundary integral equations through concepts like multipole expansions, panel clustering or, more generally, hierarchical matrices, and adaptive solution techniques in numerical simulation based on continuous models such as partial differential or integral equations.

The mathematical methods emerging to address these problems have several common features including the nonlinearity of the solution methods as well as the ability of separating solution characteristics living on different length scales. Having to deal with the appearance and interaction of local features at different levels of resolution has, for instance, brought about multigrid methods as a key methodology that has advanced the frontiers of computability for certain problem classes in numerical analysis. In fact, the separation of frequencies plays an important role in preconditioning linear systems arising from elliptic partial differential equations so that the corresponding large scale systems could be solved with discretization error accuracy optimally in linear time.

A related but different concept for managing the interaction of different length scales centers on wavelet bases and multilevel decompositions. In the very spirit of harmonic analysis they allow one to decompose complex objects into simple building blocks that again support analyzing multiscale features.

While this ability was exploited first primarily for treating *explicitly* given objects, like digital signals and images or data sets, the use of such concepts for recovering also *implicitly* given objects, like solutions of partial differential or boundary integral equations, has become a major recent focus of attention. The close marriage of discretization, analysis and the solution process based on *adaptive* wavelet methods has led to significant theoretical advances as well as new algorithmic paradigms for linear and nonlinear stationary variational problems. Through thresholding and best N-term approximation based on wavelet expansions, concepts from nonlinear approximation theory and harmonic analysis become practically manageable. In our opinion, these ideas open promising perspectives not only for signal and image processing but also for the numerical analysis of differential and integral equations covering, in particular, such operator equations with stochastic data.

These various concepts have developed relatively independently of one another. Our previous Oberwolfach Workshops 'Wavelet and Multiscale Methods' held in July 2004 and August 2007 sought to bring various disciplines utilizing multiscale techniques together by inviting leading experts and young emerging scientists in areas that rarely interact. Those workshops not only accelerated the advancement of nonlinear and multiscale methodologies but also provided beneficial cross–fertilizations to an array of diverse disciplines which participated in the workshop, see the Oberwolfach Reports 34/2004 and 36/2007. Among the several recognizable outcomes of the workshops were: (i) the emergence of compressed sensing as an exciting alternative to the traditional sensing-compression paradigm, (ii) fast online computational algorithms based on adaptive partition for mathematical learning, (iii) clarification of the role of coarsening in adaptive numerical methods for PDEs, (iv) injection of the notion of sparsity into stochastic models to identify computational paradigms that are more efficient than Monte Carlo techniques.

Compressed sensing, as developed by Candes, Donoho, Vershynin, Gilbert, Strauss, the organizers and others, advocates a fascinating alternative to the usual sensing and compression methodology. The classical model of limited bandwidth is replaced by sparsity models and the role of traditional sampling is played by sensing functionals that are typically based on random vectors. One can then prove that under certain circumstances the amount of observations which are needed to record all the information on general classes of signals is by far less than the amount required by the classical bandwidth mode.

Adaptive methods for numerically solving a wide range of partial differential equations with proven optimality (in terms of the number of computations needed to achieve a prescribed error tolerance) originally involved coarsening procedures. The necessity of such coarsening was brought into question at the previous workshop and subsequent work of Stevenson has shown that it is possible to avoid coarsening for scalar elliptic problems through cautious bulk chasing.

A new methodology for solving stochastic partial differential equations based on sparsity was advocated at the last workshop by Schwab. This has led to the interaction between experts in nonlinear approximation and numerical PDEs to quantify the possible gains of such an approach over the traditional Monte Carlo methods.

As in the previous workshops, the proposed participants are experts in areas like nonlinear approximation theory (e.g., DeVore, Temlyakov), statistics (e.g., Picard, Kerkyacharian), finite elements (e.g., Braess, Oswald), multigrid methods (e.g., Braess), spectral methods (e.g., Canuto), harmonic analysis and wavelets (e.g., Cohen, Petrushev, Schneider, Stevenson), numerical fluid mechanics (e.g., Süli), conservation laws (e.g., Tadmor), systems of stationary operator equations (e.g., Dahmen, Kunoth) or numerical methods for stochastic PDEs (e.g., Schwab).

One of the main objectives of this workshop was to foster synergies by the interaction of scientists from different disciplines resulting in more rapid developments of new methodologies in these various domains. It also served to bridge theoretical foundations with applications.

Examples of conceptual issues that were advanced by our workshop are:

- convergence theory for adaptive and nonlinear multilevel methods for high-dimensional PDEs;
- tensor methods for high dimensional problems;
- convergence theory for model reduction concepts for parameter dependent PDEs;
- extension of fast solution methods such as multigrid and multiscale methods to more complex models such as nonlinear elasticity and kinetic models of dilute polymers, or partial differential equations with stochastic data;
- adaptive multiscale methods for coupled systems involving partial differential and integral equations;
- multilevel meshless methods;
- incorporating anisotropy in analysis, estimation, compression and encoding;
- adaptive treatment of nonlinear and time–dependent variational problems;
- interaction of different scales under nonlinear mappings, e.g., for flow problems and for problems with stochastic data.

The proposed workshop has propelled further advancement of several emerging areas: the opening lecture by E. Süli reported on a recent breakthrough concerning the global existence of weak solutions to kinetic models of dilute polymers; the numerical aspects of compressed sensing including stability and optimality; deterministic methods for compressed sensing based on coding theory; the design and analysis of universal estimators in nonparametric statistical estimation and machine learning — nonlinear multiscale techniques may offer much more efficient alternatives to schemes based on complexity regularization; solution concepts for problems of high spatial dimension by utilizing anisotropy, for instance, in mathematical finance, in quantum chemistry and electronic structure calculations; quantifying the notion of sparsity in high space dimension — this leads to the development of more efficient high dimensional algorithms which avoid the curse of dimensionality.

In summary, the conceptual similarities that occur in these diverse application areas suggest a wealth of synergies and cross–fertilization. These concepts are in our opinion not only relevant for the development of efficient solution methods for large scale problems but also for the formulation of rigorous mathematical models for quantifying the extraction of essential information from complex objects.

Workshop: Wavelet and Multiscale Methods

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Abstracts

Hyperbolic Wavelet Discretization of the Electronic Schrödinger Equation: Explicit Correlation and Separable Approximation of Potentials

Markus Bachmayr

One of the major difficulties in discretizing the stationary electronic Schrödinger equation lies in the singular electron-electron Coulomb interaction, which causes cusps in the eigenfunctions that cannot be resolved efficiently by expansions into tensor products of single-electron basis functions.

The classical starting point for studying this issue is the two-electron case of the Helium atom, where the Schrödinger equation takes the form

$$-\frac{1}{2}\Delta u - \frac{2}{|x|}u - \frac{2}{|y|}u + \frac{1}{|x-y|}u = \lambda u\,, \tag{1}$$

with spatial electron coordinates $x, y \in \mathbb{R}^3$. Here the eigenfunction u_0 corresponding to the lowest eigenvalue λ_0, which is of most practical importance, has a diagonal electron-electron cusp at $\{x = y\}$.

A common approach for obtaining approximate solutions with improved convergence consists in incorporating factors with the correct first-order behavior of the electron-electron cusps into the equation. We consider a particular instance of such an explicitly correlated method in which an ansatz of the form $u = \exp(\frac{1}{2}|x-y|)w$ leads to the modified problem

$$-\frac{1}{2}\Delta w - \frac{2}{|x|}w - \frac{2}{|y|}w - \frac{1}{2}\frac{x-y}{|x-y|}\cdot(\nabla_x - \nabla_y)w - \frac{1}{4}w = \lambda w\,. \tag{2}$$

Different variants using bounded correlation factors or preserving symmetry are possible, but (2), known as the transcorrelated method in computational chemistry literature, is the most accessible approach for our purposes, and also has the advantage over self-adjoint formulations of avoiding integrals coupling four or more electrons in the many-particle case.

Adapting the basic strategy of [Ys1], it can be shown that in the weak formulation of (2), the factor w has higher regularity in terms of mixed weak derivatives than u: if $u_0 \in H^1(\mathbb{R}^6)$ is an eigenfunction of (1) with eigenvalue λ_0, then $w_0 = \exp(-\frac{1}{2}|x-y|)u_0$ is an eigenfunction of (2) with eigenvalue λ_0 and $\partial_{x_i}\partial_{y_j} w_0 \in H^1(\mathbb{R}^6)$ for $i, j \in \{1, 2, 3\}$. See [Ba] for a proof; this result is also contained as a special case in the recent work [Ys2].

On the basis of this regularity, one can obtain convergence rates for a hyperbolic wavelet discretization of (2), where the approximation error of w_0 in $H^1(\mathbb{R}^6)$ is guaranteed to decay like $N^{-1/3}$ up to logarithmic factors, see [Ba] and [Ze]. The approximation results are based on anisotropic tensor product basis functions

$$\Psi_{(\nu_x,\nu_y)}(x, y) := \gamma_{\nu_x}(x)\,\gamma_{\nu_y}(y)\,, \quad \nu_x, \nu_y \in \Lambda\,,$$

where $\{\gamma_\nu\}_{\nu\in\Lambda}$ is an isotropic tensor product wavelet basis on $\mathbb{R}^3$, which in turn is generated from wavelets and scaling functions on $\mathbb{R}$. Denoting by $|\nu| \in \mathbb{Z}$ the wavelet level, by $k(\nu) \in \mathbb{Z}^3$ the translation parameter, and by $s(\nu) \in \{0,1\}^3$ the combination of one-dimensional scaling functions and wavelets corresponding to γ_ν, a hyperbolic wavelet basis is obtained as a subset of the full tensor product by imposing a restriction of the type $|\nu_x| + |\nu_y| \le L$, which in the present case needs to be complemented by a condition on $k(\nu_x)$, $k(\nu_y)$ that takes the decay properties of the eigenfunctions into account.

For solving the accordingly discretized eigenvalue problem, orthonormal wavelets with sufficient smoothness, such as the Daubechies family, offer a number of important advantages. In particular, H^1-stability of the wavelet basis means that one obtains a well-conditioned system matrix by a simple diagonal scaling.

A crucial point for solving the eigenvalue problem by inverse iteration-type iterative methods is the efficient computation of matrix-vector products. This is particularly problematic for the two-electron operator in (2), and wavelet compression methods by themselves do not yield a tractable numerical cost.

However, due to their special structure the potential terms occurring in (2) admit a separable approximation based on best approximation of completely monotone functions by exponential sums. For instance, as shown in [BH], for $r > 0$ and for each $N \in \mathbb{N}$ there exist α_k, ω_k such that

$$\sup_{x\in\mathbb{R}^3,|x|\ge r}\left|\frac{1}{|x|} - \sum_{k=1}^{N}\frac{\omega_k}{r}\prod_{i=1}^{3}\exp\Big(-\frac{\alpha_k}{r^2}x_i^2\Big)\right| \le 8\sqrt{2}\,r^{-1}\exp(-\pi\sqrt{N/2})\,,$$

with slightly better estimates for bounded domains, and hence one obtains highly efficient approximations of the form

$$\frac{1}{|x|} \approx \sum_k \prod_{i=1}^{3} f_k(x_i)\,, \quad \frac{x-y}{|x-y|} \approx (x-y)\sum_k \prod_{i=1}^{3} g_k(x_i-y_i)\,. \tag{3}$$

Replacing the potential terms by such sums of separable functions, for each fixed combination of ν_x, ν_y, $s(\nu_x)$, $s(\nu_y)$ the corresponding block of the discretization matrix can be written as a sum of Kronecker products of lower-dimensional matrices. Given a suitable tensor product structure of active indices $k(\nu_x)$, $k(\nu_y)$ for each such block, these Kronecker products can be applied by successively operating along one or two tensor modes, respectively. The error in operator norm introduced by this further approximation can be estimated with the help of the Schur lemma, making use of H^1-stability of the wavelet basis, see [Ba].

First numerical experiments for determining the lowest eigenvalue of Helium from (2) show on the one hand that the rank of the exponential sums can be chosen fairly low in practice, but on the other hand that despite the explicit correlation factor, the hyperbolic wavelet approximation of w_0 still requires a very large number of degrees of freedom.

The structure of the approximations (3) used for the operator suggests a possible strategy for achieving further compression of w_0, keeping the advantages of the underlying hyperbolic wavelet approximation, by using a suitable structured tensor

representation for the wavelet coefficients. As a preliminary test, a rank reduction in the Tucker format is applied to the approximate solutions obtained for (2). This tensor decomposition is again done separately for each combination of ν_x, ν_y, $s(\nu_x)$, $s(\nu_y)$, where coordinate pairs (x_i, y_i), $i = 1, 2, 3$ are separated to obtain a tensor of order three. Making use of wavelet norm equivalences, by a simple weighting of errors on different levels one has explicit control over the truncation error in H^1-norm; truncating the ranks such that the error is balanced with the discretization error, a substantial reduction in the number of unknowns for representing w_0, with computationally tractable multilinear ranks, is observed. For computational purposes, this structure also matches very well the sums of Kronecker product matrices in the approximate operator.

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"Localized" Nonlocal Means with Application to Electron Microscopy

Peter G. Binev

(joint work with F. Blanco-Silva, D. A. Blom, W. Dahmen, P. Lamby, R. Sharpley, T. Vogt)

Many data gathering processes can be described using the observation model

$$y = Hx + n,$$

where x is the data we want to recover, y is the actual data we are receiving, H is an operator that depends upon the observation procedure and the instrument, and n is an additive noise component. Often the operator H is considered approximately known and it is approximated by a linear operator H_0 to define a linear observation model. In case the norm of the difference $\|H - H_0\|$ is small, the effect of approximating H by H_0 is not significant and (for bounded x) the error of this approximation can be considered as part of the additive noise.

In this presentation we target cases in which the error of approximating H is large and *cannot be treated by linear methods*. Usually, the ideal model of the instrument (identifying the operator H_0) is subject to significant distortions in its practical use. An important class of such problems is characterized by the fact that the position of the instrument and/or the observed object cannot be fixed and is subjected to unspecified motions.

Let P be the set of positions at which the observations are intended to be made. Thus, we mean to observe the signal x as a function f of $p \in P$ and based on our knowledge of the operator H_0 we want to recover f using the data y. However, we can only observe a function $\widetilde{f}$ of measurements y at some positions $\widetilde{p} \in \widetilde{P}$, which are not p but their distorted versions $\widetilde{p} := \mathcal{D}p$. Here $\mathcal{D}$ is an unknown distortion map projecting the set of intended positions P onto the set of actual positions $\widetilde{P} := \mathcal{D}P$. Thus, we have that $y = \widetilde{f}(\widetilde{p})$ instead of $y = \widetilde{f}(p)$. If the difference $p - \widetilde{p}$ is insignificant and both $\widetilde{f}$ and f are Lipschitz functions with well bounded Lipschitz constants, the problem can be solved by the usual methods. This is the case in standard video and photography but not in several other areas such as *scanning transmission electron microscopy* (STEM). For these other cases one has to find a way to obtain a good approximation of the distortion map $\mathcal{D}$ to use it in the recovery of $\widetilde{f}$ from its values at $\widetilde{p}$.

The basic idea is to design a data gathering process in which instead of using a dense set of positions P, say 1024×1024, we set a relatively coarse grid, say 256×256, and repeat sampling it several times, recording the results as different "frames" Y_t. This way we will have data subjected to different distortion mappings $\mathcal{D}_t$. A comparison of two different frames Y_t and $Y_{t'}$ could provide information about the mapping $\mathcal{D}_{t\to t'} := \mathcal{D}_t^{-1}\mathcal{D}_{t'}$. Thus, our goal is to collect the information about $\mathcal{D}_{t\to t'}$ for different pairs (t, t') and through a learning routine to extract good approximations of all mappings $\mathcal{D}_t$ and by this to resolve the problem of finding $\widetilde{p}$.

Since $\mathcal{D}_{t\to t'}$ is a very complex motion, its estimation is a serious issue. In addition, the images Y_t are usually very noisy and that makes a good identification of local features in them extremely difficult. Denoising based on time series requires processing of the same specimen portion appearing in different frames. It is therefore crucial to employ a technique that avoids an explicit registration and motion tracking. The concept of *nonlocal means* (NLM) has been developed by Buades, Coll and Morel in [BCM] as a denoising algorithm for a single image. The key idea is to define the result as a weighted average of the image portions whose intensity distributions are close to each other. This can be done as follows. We set $Y_t(p)$ to be the value received at the (intended) position p in the frame with time stamp t. Then, we associate the pair (p, t) with a set of descriptors $R(p, t)$ that reflects the behavior of the data at positions close to p in the same frame. Given the pairs (p, t) and (p', t'), we define the weight $w(p, t; p', t')$ based solely on the similarity of the sets of descriptors $R(p, t)$ and $R(p', t')$ in such a way that $w(p, t; p', t') = 1$, if $R(p, t) = R(p', t')$, and this weight is close to 0, if $R(p, t)$ and $R(p', t')$ differ significantly. In the standard formulation of NLM, $R(p, t)$ is a vector of the values $Y_t(q)$ taken at the intended positions q in a small rectangular patch centered at p. The similarity is then measured as the distance

$$\operatorname{dist}\big(R(p,t), R(p',t')\big) := \big\|R(p,t) - R(p',t')\big\|_{\ell_2}$$

and the weights are defined via

$$w(p,t;p',t') := \exp\left\{-\frac{\operatorname{dist}\big(R(p,t),R(p',t')\big)^2}{2\sigma^2}\right\},$$

where σ is a tuning parameter that is specific for the similarity notion. Finally, the updated value $z(p,t)$ associated with the pair (p,t) is produced by

$$z(p,t) = \frac{\sum_{p',t'} w(p,t;p',t')Y_{t'}(p')}{\sum_{p',t'} w(p,t;p',t')}$$

where the sum is usually running over all possible pairs (p',t'). In this classical formulation NLM has significant computational cost and tends to introduce blurring effects due to the averaging of too many elements. Thus, it is often suggested to restrict the sum over relevant neighborhood windows for both p' and t'. The result of such application of NLM is presented in Figure 1 (c).

The STEM images of crystallographic materials show a lot of symmetries and repetitions of similar patterns. However, the main goal is not to confirm the general structure but to *detect the anomalies* in it. One significant drawback of NLM in its standard application to STEM is the tendency to find the idealized pattern and to introduce it in the processed image.

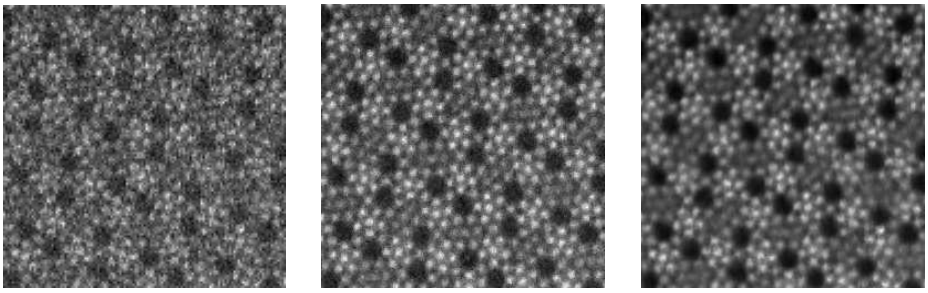
Our approach is to adopt the idea of NLM to the specifics of the problem by localizing the spatial window to a small area. Below, we briefly describe the three main steps in our approach in processing of high angle annular dark field STEM images.

In the *first step* we take advantage of the smoothing and denoising effects of the standard NLM to eventually define a better similarity distance by comparing the smoothed versions of the frames. In this step the time window for t' is usually restricted to one or few frames, while the spatial window N_p is as large as possible. The intent is not to modify the values $Y_t(p)$ but to use $z(p,t)$ in the definition of new descriptors $R(p,t)$ based on the better general structure provided by the smoothed version $z(p,t)$ of the frame $Y_t(p)$. Using the new descriptors and eventually smaller spatial windows N_p, we consider the recovery of $z(p,t)$ based on the values $Y_{t'}(p')$ *only* from the nearby frame at t'.

In the *second step* we analyze the concentration regions of the weights of this recovery, $w(p,t;p',t')$, to find an initial approximation of the mapping $\mathcal{D}_{t\to t'}$. Iterating the process, we can further reduce the size of the spatial neighborhood N_p. At the same time, we can exploit the fact that $\mathcal{D}_{t\to t'} = \mathcal{D}_{t\to t''}\mathcal{D}_{t''\to t'}$ and receive an approximation of $\mathcal{D}_{t\to t'}$ for more distant values of t and t', that is, increase the time window. Iterating further passes of NLM with improved descriptors and similarity criteria, one can gradually decrease the size of spatial neighborhoods while increasing time neighborhoods, so as to average eventually only image patches that correspond to each other. It is important to stress though that these iterative

passes will always apply to the original data, just using upgraded information concerning *local* registration extracted from the intermediate frames. In a way such an iterative procedure may be viewed as gradually refining the image formation in STEM and modeling the distortions encountered during the imaging process. Moreover, from the possible change of the weights over time one may be able to learn more about beam damage.

In the *third step* we map the values $Y_{t'}(p')$ from all the frames using the calculated mappings $\mathcal{D}_{t'\to t}$ onto one single frame and combine them (eventually discarding the outliers) with a simple learning routine to receive a single image based on all of the observations.



(a) (b) (c)

FIGURE 1. NLM processing $M1$ catalyst using a sequence of 11 frames: (a) original reference frame; (b) result by our routine; (c) result using nonlocal means.

In Figure 1 (b) we present the results of combining 11 frames aligned by the procedure described above. The resolution of the image is set to twice the one of the original single frames. Very low dose exposure (7 μs per pixel with a coarse raster) is used to receive the original frames. It is remarkable that our routine was able to depict a Te atom(s) in the central pore at the bottom (the standard NLM scheme displayed in Figure 1 (c) misses it completely). Using the conventional high resolution HAADF STEM requires much higher total doses to be able to identify such features in this material, but recall that Te is highly beam sensitive.

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Some Results about Adaptive Fourier Approximation of PDEs

Claudio Canuto
(joint work with Ricardo H. Nochetto, Marco Verani)

The design of adaptive spectral-element (or h-p) discretization algorithms for elliptic self-adjoint problems relies on the dynamic interplay between two fundamental stages: the refinement of the geometric decomposition into elements and the enrichment of the local basis within an element. While the former stage is by now well understood in terms of practical realization and optimality properties, less attention has been devoted to the latter one.

With the aim of shedding light on this topic, we focus on what happens in a single element of the decomposition. In order to reduce at a minimum the technical burdens, we actually assume periodic boundary conditions on the d-dimensional box $\Omega = (0, 2\pi)^d$, in order to exploit the orthogonality properties of the Fourier basis. Thus, we consider a fully adaptive Fourier method, in which at each iteration of the adaptive algorithm the Galerkin solution is spanned by a dynamically selected, finite subset of the whole set of Fourier basis functions. The active set is determined by looking at a fixed fraction of largest (scaled) Fourier coefficients of the residual, according to the bulk-chasing (or Dörfler marking) philosophy. The algorithm is proven to be convergent; in addition, exploiting the concentration properties of the inverse of the elliptic operator represented in the Fourier basis, one can show that the error reduction factor per iteration tends to 0 as the bulk-chasing fraction tends to 1.

After convergence has been established, one is faced with the issue of optimality. This leads to the comparison of the adaptive Galerkin solution spanned by, say, N Fourier modes, with the best N-term approximation of the exact solution. Consequently, we are led to introduce suitable classes of periodic H^1-functions for which the best N-term approximation error fulfils a prescribed decay as N tends to infinity. These classes can also be characterized in terms of behavior of the rearranged sequence of the (normalized) Fourier coefficients of the functions.

If the best N-term approximation error of the exact solution decays at an algebraic rate (this occurs if the solution belongs to a certain "oblique" scale of Besov spaces of periodic functions, corresponding to a finite regularity), then the arguments developed by Cohen, Dahmen and DeVore and by Stevenson in the framework of wavelet bases apply to our situation as well, and one can establish the optimality of the approximation without coarsening. The crucial ingredients in the analysis are the minimality property of the active set of degrees of freedom determined by bulk-chasing, and a geometric-series argument (essentially, the estimated number of degrees of freedom added at each iteration is comparable to the total number of degrees of freedom added in all previous iterations).

On the other hand, if the best N-term approximation error of the exact solution decays at an exponential (or even sub-exponential rate), the analysis is more delicate, as the previous argument fails to apply. Note that the case of a solution having (local) infinite-order regularity is quite significant in dealing with

spectral (spectral-element) methods. For the Navier-Stokes equations, regularity results in Gevrey classes have been first established by Foias and Temam; in these classes, the best N-term approximation error of a function decays precisely at a sub-exponential or exponential rate. In the present situation, optimality is guaranteed by the fact that at each iteration either the number of added degrees of freedom is bounded by a constant, or - if more degrees of freedom are added - a faster error decay is achieved. Numerical results, in the case of analytical solutions, confirm this kind of behavior.

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Adaptive Sparse Methods for High Dimensional Parametric PDE's

Albert Cohen
(joint work with Ronald DeVore and Christoph Schwab)

We are interested in the model elliptic equation

$$-\mathrm{div}(a\nabla u) = f,$$

on a domain $D \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conditions, and parameter dependent coefficients

$$a = a(x,y) = \bar{a}(x) + \sum_{j>0} y_j \psi_j(x), \quad x \in D, \quad y = (y_j) \in U = [-1,1]^{\mathbb{N}},$$

where the functions $\overline{a}$ and ψ_j are in $L^\infty(D)$. The y_j may be either thought as deterministic parameters that should be tuned in control or optimization problems for the solution $u(y) = u(\cdot, y)$, or as random variables which is the typical situation in stochastic modelling.

We work under the uniform ellipticity assumption (UEA)

$$0 < r \leq a(x,y) \leq R < \infty, \quad x \in D, \quad y \in U,$$

so that for all $y \in U$, the solution $u(y)$ is well defined as an element of $V = H^1_0(D)$ with a-priori estimate

$$\|u(y)\|_V = \|\nabla u(y)\|_{L^2(D)} \leq C_0 := \frac{\|f\|_{V^*}}{r}.$$

Numerical approximation of the map $y \mapsto u(y)$ is a challenging task since it depends on infinitely many variable y_j, and in addition it takes its values in an infinite dimensional Hilbert space. We study its Taylor expansion

$$u(y) = \sum_{\nu \in \mathcal{F}} t_\nu y^\nu,$$

where $y^\nu := \prod_{j>0} y_j^{\nu_j}$ for $\nu = (\nu_j) \in \mathcal{F}$ the set of finitely supported sequences of positive integers, and where

$$t_\nu := \frac{1}{\nu!}\partial^\nu u(0) \in V, \;\; \nu! := \prod_{j>0} \nu_j!,$$

with the convention that $0! = 1$. Our main result, which is proved in [CDS2] is the following.

Theorem 1. *If (UEA) holds and if* $(\|\psi_j\|_{L^\infty})_{j>0} \in \ell^p(\mathbb{N})$ *for some* $p < 1$, *then* $(\|t_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F})$.

A similar result holds when Taylor coefficients are replaced by Legendre coefficients. This result reveals that the sequence $(\|t_\nu\|_V)_{\nu\in\mathcal{F}}$ inherits the same amount of sparsity as the coefficient expansion reflected by the sequence $(\|\psi_j\|_{L^\infty})_{j>0}$. An immediate consequence is the existence of sets $\Lambda_N^* \subset \mathcal{F}$ with $\#(\Lambda_N^*) = N$ and such that

$$\sup_{y\in U} \|u(y) - \sum_{\nu\in\Lambda_N^*} t_\nu y^\nu\|_V \leq \sum_{\nu\notin\Lambda_N^*} \|t_\nu\|_V \leq CN^{-s}, \;\; s := \frac{1}{p} - 1.$$

In particular, this holds with $C = \|(\|t_\nu\|_V)\|_{\ell^p}$ if we choose for Λ_N^* the indices corresponding to the N largest $\|t_\nu\|_V$. The fact that we may get an algebraic rate in the approximation of a function that depends of infinitely many variable is quite remarkable. The proof of this theorem is based on the analytic dependence of u with respect to the variable y_j. We believe that the method of proof can be extended to other parameter dependent PDE's for which such analyticity properties hold.

Another consequence of this theorem is that the solutions $u(y)$ are simultaneously approximated at rate N^{-s} by the N-dimensional space

$$E_N := \mathrm{Span}\{t_\nu \; ; \; \nu \in \Lambda_n^*\}.$$

Consequently, the set $\mathcal{K} := \{u(y) \; ; \; y \in U\}$ is compact in V with Kolmogorov width

$$\begin{aligned} d_N(\mathcal{K}) &:= \inf_{\dim(E)=N} \max_{v\in\mathcal{K}} \min_{w\in E} \|v - w\|_V \\ &\leq \max_{v\in\mathcal{K}} \min_{w\in E_N} \|v - w\|_V \\ &\leq \sup_{y\in U} \|u(y) - \sum_{\nu\in\Lambda_N^*} t_\nu y^\nu\|_V \\ &\leq CN^{-s}. \end{aligned}$$

This suggest the possibility of *reduced modeling* for approximately the parametric problem. Recent results on the so-called reduced basis method in [BCDDPW] have shown that one may select particular solutions $\{u_1, \cdots, u_N\} \in \mathcal{K}$ by a greedy procedure and obtain that

$$\max_{v\in\mathcal{K}} \min_{w\in F_N} \|v - w\|_V \leq \tilde{C}N^{-s},$$

where $F_N := \mathrm{Span}\{u_1, \cdots, u_N\}$, therefore reducing the work to the accurate computation of N particular solutions. The greedy procedure being difficult to apply in high parameter dimension, one may prefer to search for a direct approximation of $u(y)$ by its partial Taylor series. One of the main difficulty is that the optimal

sets Λ_N^* are unknown to us. We propose a strategy - based on a bulk chasing procedure - that adaptively builds a sequence of sets

$$\Lambda_0 \subset \Lambda_1 \subset \cdots \subset \Lambda_n \subset \cdots,$$

and computing the corresponding coefficient t_ν for $\nu \in \Lambda_n$. We show that this strategy has the optimal convergence rate

$$\sup_{y\in U} \|u(y) - \sum_{\nu\in\Lambda_n} t_\nu y^\nu\|_V \leq \sum_{\nu\notin\Lambda_n} \|t_\nu\|_V \lesssim \#(\Lambda_n)^{-s}, \quad s := \frac{1}{p} - 1,$$

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Convergence Rates for Greedy Algorithms in Reduced Basis Methods

Wolfgang Dahmen

(joint work with Peter Binev, Albert Cohen, Ronald DeVore, Guergana Petrova, and Przemyslaw Wojtaszczyk)

The reduced basis method was introduced for the accurate online evaluation of solutions to a parameter dependent family of elliptic partial differential equations. The idea is to determine offline for any given target accuracy a suitable problem dependent space of possibly small dimension so that the Galerkin projection onto that subspace provides for any parameter value an approximation to the corresponding exact solution within the desired target accuracy tolerance. Frequent online parameter queries, e.g. in an optimization context, are then reduced to solving the low dimensional Galerkin problems where again offline computations facilitate rapidly assembling the corresponding stiffness matrices.

Abstractly, the core task can be viewed as determining a "good" n dimensional space $\mathcal{H}_n$ to be used in approximating the elements of a compact set $\mathcal{F}$ in a Hilbert space $\mathcal{H}$. One by now popular computational approach is to find $\mathcal{H}_n$ through a *greedy* strategy, see e.g. [3, 4]. In idealized form this greedy strategy can be described as follows. Having computed a basis $\{f_0, \ldots, f_{n-1}\}$ for $\mathcal{H}_n$, the next basis function f_n is obtained as

$$f_n = \mathrm{argmax}_{f\in\mathcal{F}} \|f - P_n\|_{\mathcal{H}}. \tag{1}$$

However, the actual computation of such a maximizer would not be feasible. Instead, one tries to find a surrogate $r_n(f)$ which, on one hand, satisfies

$$cr_n(f) \leq \|f - P_n f\|_{\mathcal{H}} \leq Cr_n(f), \quad f \in \mathcal{F}, \tag{2}$$

and, on the other hand, can be evaluated much more efficiently, see [4]. For families of uniformly $\mathcal{H}$-elliptic variational problems such computable surrogates

can indeed be formulated in terms of *residuals* of Galerkin projections. It is then readily seen that

$$f_n := \operatorname{argmax}_{f\in\mathcal{F}} r_n(f) \tag{3}$$

satisfies

$$\|f_n - P_n f_n\|_{\mathcal{H}} \geq \gamma \max_{f\in\mathcal{F}} =: \gamma\sigma_n(\mathcal{F}), \tag{4}$$

where $\gamma := c/C$ and c, C are the constants from (2). The *weak greedy* algorithm consists then in replacing the solutions to (1) by elements satisfying (4).

It is now natural to compare the approximation performance $\sigma_n(\mathcal{F})$ of the "(weak) greedy spaces" $\mathcal{H}_n$ generated by this strategy with that of the Kolmogorov widths $d_n(\mathcal{F})$ since the latter gives the smallest error that can be achieved by subspaces of fixed dimension n. The first such comparisons, given in [1], show that the greedy approximation error, $\sigma_n(\mathcal{F}) = \operatorname{dist}(\mathcal{F}, \mathcal{H}_n)$, obtained by the exact greedy strategy with $\gamma = 1$ satisfies

$$\sigma_n(\mathcal{F}) \leq Cn2^n d_n(\mathcal{F}). \tag{5}$$

In this talk, various improvements and extensions of this result are presented. First, up to the factor n, (5) can be shown to be in general best possible. However, when dispensing with direct comparisons between the greedy errors $\sigma_n(\mathcal{F})$ and the Kolmogorov widths $d_N(\mathcal{F})$, and this is the main point of this talk, one can still obtain meaningful convergence rates for $\sigma_n(\mathcal{F})$ when $2^n d_n(\mathcal{F}) \not\to 0$. Specifically, it is shown for the general case $\gamma \leq 1$ that, whenever $d_n(\mathcal{F}) \leq Mn^{-\alpha}$, for all $n > 0$, and some $M, \alpha > 0$, we also have

$$\sigma_n(\mathcal{F}) \leq C_\alpha M n^{-\alpha}, \quad n \in \mathbb{N}, \tag{6}$$

where C_α depends only on α. Similar results are derived for generalized exponential rates of the form Me^{-an^α}. In this case, however, the greedy error $\sigma_n(\mathcal{F})$ is only shown to decay like CMe^{-cn^β} with $\beta = \alpha/(\alpha+1)$. Of course, this guarantees a faster convergence than (6) in a range where $d_n(\mathcal{F})$ decays faster than $n^{-\alpha}$ for any $\alpha > 0$ but not faster than 2^{-n}. Moreover, such convergence rates are shown to be robust under perturbations which arise, for instance, due to discretizations for the offline computation of the greedy basis functions.

The talk concludes with some remarks on the main conceptual ingredients of the proofs. In particular, a key tool for proving the above convergence rates is the following "delayed comparison" when the decay of the greedy errors is "flat" in the following sense: if for some $\theta \in (0,1), m \in \mathbb{N}$ and $q = \lceil 2(\gamma\theta)^{-1}\rceil^2$ one has $\sigma_{n+qm}(\mathcal{F}) \geq \theta\sigma_n(\mathcal{F})$, then $\sigma_n(\mathcal{F}) \leq q^{1/2} d_m(\mathcal{F})$.

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Anisotropic Representations And Function Spaces In R^n

Shai Dekel

(joint work with Pencho Petrushev and Tal Weissblat)

We investigate representation systems and function spaces over multi-level ellipsoid covers of R^n which may change rapidly from point to point and in depth, from level to level (see previous papers [DHP, DDP]). At this time we are focused on Triebel-Lizorkin spaces and in particular the Hardy spaces. We generalize previous work [B] and classic elements of the Hardy space theory in this setting such as the various maximal function definition, atomic decompositions, the dual BMO spaces, etc.

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Sparsity in Learning Theory

Christine De Mol

(joint work with Ernesto De Vito, Sofia Mosci, Lorenzo Rosasco, Magali Traskine and Alessandro Verri)

In contemporary science, we are more and more often faced with the problem of extracting meaningful information or inferring models from a data-rich environment. For example, in bioinformatics, one measures by means of microarrays, for each patient (or experiment) i, a high-dimensional vector of expression levels x_i of p genes. In a supervised learning setting, besides these "input" data, one is given, for each patient i, a response or "output" y_i which can be a real-valued index (survival time or gravity of an illness) or else, in classification problems, a discrete label discriminating between e.g. two different pathological states. A first approach consists in assuming a linear relationship between output and input, i.e. that y_i is just the scalar product of x_i with a p-dimensional vector β. Two distinct problems are of interest: (i) the prediction or "generalization" problem consisting in predicting the response y for new patients to come on the basis of their

gene expression data and (ii) the identification of the vector β defining the model. This latter problem is also referred to as "variable selection" when the vector β is assumed to be sparse, i.e. to contain many zeroes corresponding to irrelevant predictors/variables. To cope with the fact that there are generically many more variables (genes) than patients or experiments, i.e. to address the so-called "large p, small n paradigm", the problem can be reformulated as a multivariate least-squares regression with a regularizing penalty whose aim is to provide the dimension reduction necessary to get stable estimates of β. In so-called "ridge" regression, one uses a quadratic penalty, namely the square of the euclidean norm of the vector β (L_2-norm), whereas in "lasso" regression [Ti], one uses instead a L_1-norm penalty which enforces sparsity and allows for variable selection. In the presence of correlation among the variables, however, the lasso presents some drawbacks which can be overcome by the use of an additional L_2-norm penalty. This allows to select sparse groups of correlated variables without knowing in advance the composition of the groups (for known groups one could use instead the so-called "group lasso" or "joint sparsity" strategies). This "elastic-net" strategy was proposed by Zou and Hastie [ZH] for fixed-design linear regression. In the paper [DDR], we extend this setting to the framework of supervised learning theory, i.e. of random-design nonlinear regression. The regression function f_β is assumed to have a sparse expansion, with coefficients β_γ, on the elements (atoms or features) φ_γ of a possibly infinite dictionary: $f_\beta(x) = \sum_\gamma \beta_\gamma \varphi_\gamma(x)$. For example, one could consider frames of wavelets or of some of their relatives. On the basis of a collection of examples (training set) made of n independent input-output random pairs (X_i, Y_i), $i = 1, \ldots, n$ (the inputs belong to a separable metric space and the outputs to $\mathbb{R}$ or to a separable Hilbert-space), distributed according to an unknown probability distribution, we define the following elastic-net estimator for the regression function

$$\beta_\lambda^n = \mathrm{argmin}_\beta \left[\frac{1}{n} \sum_{i=1}^{n} |Y_i - f_\beta(X_i)|^2 + \lambda \sum_\gamma (u_\gamma |\beta_\gamma| + \varepsilon v_\gamma |\beta_\gamma|^2) \right]$$

where λ is a tunable positive regularization parameter, whereas $\varepsilon > 0$ is considered as fixed, and where u_γ and v_γ are two sets of weights (positive and bounded from below) encoding the regularity of the regression function through the assumptions $\sum_\gamma u_\gamma |\beta_\gamma| < \infty$ and $\sum_\gamma v_\gamma |\beta_\gamma|^2 < \infty$. In [DDR], by means of appropriate concentration inequalities, we derive consistency results for this estimator as $n \to \infty$, both for prediction and for variable/feature selection. Our results include finite-sample bounds and an adaptive scheme to select the regularization parameter λ. Thanks to the additional quadratic penalty, stability is guaranteed with respect to the fluctuations arising from random design and no assumptions have to be made to restrict the possible correlations between the features as usually done in the literature dealing with pure lasso strategies.

The paper [DMTV] deals with an application to bioinformatics and proposes a new method, based on linear regression with an elastic-net penalty, to select

relevant groups of correlated genes from microarray data. Using a two-stage approach and an appropriate tuning of the regularization parameters, we are able to demonstrate the good performances of the method on benchmark microarray data sets and to produce expanding gene lists which are almost perfectly nested when increasing the parameter ε. The proposed methodology could also be applied to other practical problems where the goal is to select relevant variables or features in the presence of high correlation among certain groups of these variables.

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Hard Thresholding Pursuit: An Algorithm for Compressive Sensing

Simon Foucart

We introduce a new iterative algorithm to find s-sparse solutions $\mathbf{x} \in \mathbb{C}^N$ of underdetermined linear systems $A\mathbf{z} = \mathbf{y}$, $A \in \mathbb{C}^{m\times N}$, $\mathbf{y} \in \mathbb{C}^m$. The algorithm, called Hard Thresholding Pursuit, is a simple combination of the Iterative Hard Thresholding [BD1, BD2] algorithm and of the Compressive Sampling Matching Pursuit [NT] or Subspace Pursuit [DM] algorithms. It reads:
Start with an s-sparse $\mathbf{x}^0 \in \mathbb{C}^N$, typically $\mathbf{x}^0 = 0$, and iterate the scheme

$$(\mathrm{HTP}_1) \qquad S^{n+1} = \big\{\text{indices of } s \text{ largest entries of } \mathbf{x}^n + A^*(\mathbf{y} - A\mathbf{x}^n)\big\},$$

$$(\mathrm{HTP}_2) \qquad \mathbf{x}^{n+1} = \operatorname{argmin}\big\{\|\mathbf{y} - A\mathbf{z}\|_2, \operatorname{supp}(\mathbf{z}) \subseteq S^{n+1}\big\},$$

until the stopping criterion $S^{n+1} = S^n$ is met.
We first notice that the sequence $(\mathbf{x}^n)$ is eventually periodic, so that, assuming convergence of the algorithm, its limit is exactly achieved after a finite number of iterations. Next, we give a short and elegant proof of the following theorem:
Suppose that the $3s$th order restricted isometry constant of the matrix $A \in \mathbb{C}^{m\times N}$ satisfies $\delta_{3s} < 1/\sqrt{3}$. Then, for any s-sparse $\mathbf{x} \in \mathbb{C}^N$, the sequence $(\mathbf{x}^n)$ defined by the Hard Thresholding Pursuit algorithm with $\mathbf{y} = A\mathbf{x}$ converges towards $\mathbf{x}$ at a geometric rate given by

$$\|\mathbf{x}^n - \mathbf{x}\|_2 \le \rho^n \, \|\mathbf{x}^0 - \mathbf{x}\|_2, \qquad \rho := \sqrt{\frac{2\delta_{3s}^2}{1-\delta_{2s}^2}} < 1.$$

We remark that the same result (with a different ρ) holds for fast versions of the algorithm, where the projection step (HTP_2) is replaced by any number of gradient descent iterations. We also remark that the result extends to the case of non-sparse

$\mathbf{x} \in \mathbb{C}^N$ acquired with an inaccurate vector $\mathbf{y} = A\mathbf{x} + \mathbf{e}$, $\mathbf{e} \in \mathbb{C}^m$. It is worth pointing out that the sufficient condition $\delta_{3s} < 1/\sqrt{3}$ is heuristically better than the sufficient conditions $\delta_t < \delta_*$ currently available for other Compressive Sensing algorithms [F], in the sense that it has the smallest ratio t/δ_*^2. We conclude with some numerical experiments to demonstrate the good empirical performances and the low complexity of the Hard Thresholding Pursuit algorithm.

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A New Multiscale Finite Element Method for High-Contrast Elliptic Interface Problems

Ivan G. Graham

(joint work with C.-C. Chu, T.Y. Hou and R.R. Millward)

We introduce a new multiscale finite element method which is able to accurately capture solutions of elliptic interface problems with high contrast coefficients by using only coarse quasiuniform meshes, and without resolving the interfaces. A typical application would be the modelling of flow in a porous medium containing a number of inclusions of low (or high) permeability embedded in a matrix of high (respectively low) permeability. Our method is H^1- conforming, with degrees of freedom at the nodes of a triangular mesh and requires the solution of subgrid problems for the basis functions on elements which straddle the coefficient interface, but uses standard linear approximation otherwise. A key point is the introduction of novel coefficient-dependent boundary conditions for the subgrid problems. Under some assumptions, we prove that our methods have (optimal) convergence rate of $O(h)$ in the energy norm and $O(h^2)$ in the L_2 norm where h is the (coarse) mesh diameter and the hidden constants in these estimates are independent of the "contrast" (i.e. ratio of largest to smallest value) of the PDE coefficient. For standard elements the best estimate in the energy norm would be $\mathcal{O}(h^{1/2-\epsilon})$ with a hidden constant which in general depends on the contrast. The new interior boundary conditions depend not only on the contrast of the coefficients, but also on the angles of intersection of the interface with the element edges.

Since the new boundary conditions are somewhat technical to implement, we also present an adaptive method which formulates appropriate interior boundary

conditions (on a fine local subgrid) automatically in a few iterations and yields accuracy which is comparable to that of the a priori multiscale method. The adaptive method is closely related to the adaptive local-global iterative method of Durlovsky, Efendiev and Ginting [2]. Numerical examples showing the performance of the adaptive method in the case of high contrast coefficients with non-quasimonotone cross points were given, and these show optimal convergence on uniform meshes independent of the contrast, despite the strong singularity at the cross point.

The results have recently appeared [1]. Some of the arguments used are also used in the analysis of geometric and algebraic domain decomposition methods, e.g. [3, 4].

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Tensorization and Multiscale Methods

Lars Grasedyck

In this report we review the construction of tensors

$$A \in \mathbb{R}^{n_1 \times \cdots \times n_d}, \qquad n_1, \ldots, n_d \in \mathbb{N},$$

from vectors

$$x \in \mathbb{R}^N, \qquad N := n_1 \cdots n_d.$$

The aim for such a "tensorization" is to find a data-sparse representation of the tensor A and thus reduce, among others, the storage complexity.

This idea was first formulated by Oseledets [OS09] in the context of matrix tensorization. In numerical experiments he found out that the TT-rank of a tensorization of the 1d and 2d Laplacian as well as the Hilbert matrix has its rank bounded by a small constant. In [GR10] we prove that the rank is indeed bounded. Khoromskij [KH09] was able to prove that vectors of the exponential form

$$x_i = c \cdot d^i, \qquad i = 1, \ldots, N,$$

allow for a canonical rank one representation after tensorization. Thus, exponential sums and trigonometric sums have tensorizations of small canonical and hierarchical rank proportional to the number of addends. Khoromskij and Oseledets [OSKH09] have then successfully applied the tensorization for the solution of PDEs in high dimension and with very large mode sizes.

Here, we will address the question for which vectors (respectively matrices and tensors) such a tensorization is possible with low (hierarchical) rank. We prove that

the tensorization of vectors that stem from the evaluation of polynomials of degree at most p on an equispaced grid has a hierarchical rank of at most $p+1$. Then, we prove that any asymptotically smooth, i.e., piecewise analytic, function with m singularities or discontinuities can be discretized and tensorized such that the rank for an ε-approximation in the $\|\cdot\|_\infty$-norm is bounded by $C + \log_2(1/\varepsilon) + 2m$.

The important point is that the existence can be proven independently of the construction of an approximation. Thus, considering high-order polynomials and additional locally singular functions is reasonable. The strongest requirement is the structure of the underlying grid (typically equispaced).

Vector-Tensorization: For vectors $x \in \mathbb{R}^{n_1 \cdots n_d}$ we define the tensorization

$$\mathcal{F} : \mathbb{R}^{n_1 \cdots n_d} \to \mathbb{R}^{n_1 \times \cdots \times n_d}$$

for all indices $i_\mu \in \{1, \dots, n_\mu\}, \mu = 1, \dots, d$, by

$$\mathcal{F}(x)_{i_1,\dots,i_d} := x_\ell, \qquad \ell := i_1 + \sum_{\mu=2}^{d} (i_\mu - 1) \prod_{\nu=1}^{\mu-1} n_\nu.$$

The idea why one could be interested in a tensorization of vectors is that the tensor might allow for a low rank representation and correspondingly for a low rank arithmetic. For dimension $d > 2$ there exist several notions of rank.

Matricization: For a tensor $A \in \mathbb{R}^I$, $I = I_1 \times \cdots \times I_d$, a collection of dimension indices $t \subset \{1, \dots, d\}$ and the complement $s := \{1, \dots, d\} \setminus t$ the matricization

$$A^{(t)} \in \mathbb{R}^{I_t \times I_s}, \qquad I_t := \times_{\mu \in t} I_\mu, \quad I_s := \times_{\mu \in s} I_\mu,$$

is defined by its entries

$$\left(A^{(t)}\right)_{(i_\mu)_{\mu \in t}, (i_\mu)_{\mu \in s}} := A_{i_1,\dots,i_d}.$$

Based on the matricization of a tensor A with respect to several sets $t \subset \{1, \dots, d\}$ one can define the hierarchical rank and the hierarchical Tucker format. In order to be able to perform efficient arithmetics, we require the sets t to be organized in a tree, for details see [GR09].

Hierarchical rank, $\mathcal{H}$-Tucker(k): The *hierarchical rank* k_t for a node $t \subset \{1, \dots, d\}$ of a so-called dimension tree [GR09] and a tensor $A \in \mathbb{R}^I$ is defined by

$$k_t := \operatorname{rank}(A^{(t)}).$$

Tensors with hierarchical rank at most k are called $\mathcal{H}$-Tucker(k) tensors.

In the hierarchical format only some of the possible subsets t of all modes appear. The storage complexity for an $\mathcal{H}$-Tucker(k) tensor is

$$\text{Storage} \;\le\; \mathit{Const} \left((d-1)k^3 + k \sum_{\mu=1}^{d} n_\mu \right) \tag{1}$$

i.e. linear in the order d.

Basic arithmetic operations like linear combinations of tensors of hierarchical rank k can be performed exact (efficiently), but the representation rank k will be proportional to the sum of the representation ranks. It is therefore necessary to reduce (truncate) the rank of a tensor A by finding (almost) best approximations with prescribed rank, or (almost) minimal rank approximations with prescribed truncation accuracy ε. Such a truncation is possible with complexity $\mathcal{O}(dk^3 + dnk^2)$. [GR09, Theorem 3.11, Remark 3.12, Lemma 4.9]. Let A^{best} denote a best approximation of A with hierarchical rank k and $\mathcal{T}_{\tilde{k}}(A)$ the truncation of A to rank $\tilde{k}$. Then the truncation is quasi-optimal:

$$\|A - \mathcal{T}_{\tilde{k}}(A)\| \leq \sqrt{2d-3}\|A - A^{\text{best}}\|$$

Polynomial Approximation: Let $(x_i)_{i=1}^{n_1 \cdots n_d}$, $d \geq 1$, be the discrete evaluation of a polynomial $f(y)$ of degree p on a regular (equispaced) grid of points $\xi_i = (i-1)h, h := 1/(N-1)$, $N := \prod_{\mu=1}^{d} n_\mu$, i.e.

$$x_i = f(\xi_i).$$

Then for every $t = \{r+1, \ldots, s\} \subset \{1, \ldots, d\}$ the tensorization $\mathcal{F}(x)^{(t)}$ fulfills

$$\operatorname{rank}(\mathcal{F}(x)^{(t)}) \leq p + 1.$$

Let $f : J = [a, b] \to \mathbb{R}$ be a function and let $S := \{s_1, \ldots, s_m\} \subset J$. The function f is said to be asymptotically smooth with singular points S, if for all points $y \in J \setminus S$ holds

$$|\partial^i f(y)| \leq C_1 \gamma^\sigma \gamma^i i!, \quad \gamma \leq C_2 \operatorname{dist}(y, S)^{-1},$$

where σ is the degree of singularity.

Rank of tensorizations of asymptotically smooth functions: Let $(x_i)_{i=1}^{N}$, $d \geq 1$, be the discrete evaluation of an asymptotically smooth function f with singular points $S = \{s_1, \ldots, s_m\}$ on a regular (equispaced) grid of points $\xi_i = (i-1)h, h := 1/(N-1)$, $N = \prod_{\mu=1}^{d} n_\mu$, i.e.

$$x_i = f(\xi_i).$$

Then there exists a tensor $Z \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ that approximates the tensorization $\mathcal{F}(x)$ point-wise with accuracy ε and that has its hierarchical rank bounded by

$$\operatorname{rank}(Z^{(t)}) \leq C + \log_2(1/\varepsilon) + 2m, \qquad t = \{1, \ldots, q\}.$$

The constant C depends on the degree of singularity σ.

We conclude that a large class of vectors that stem from the evaluation of a polynomial or asymptotically smooth function on an equispaced grid, allows for a tensorization with small hierarchical rank k. A truncated arithmetic for such tensorized vectors is possible in $O(k^4 \log N)$, where N is the length of the vector. This holds independently of the number N, i.e., whether N can be factorized or not is not relevant.

The tensorization of vectors (resp. functions) might be interesting in the context of multiscale methods. There, in each subdomain Ω_i of the domain Ω a fine-scale

problem has to be solved in order to find a specialized basis by which the global problem in Ω can be discretized. The reason for this is twofold. First, there are features on the small scale that have to be resolved. Second, the global problem can be discretized with fewer basis functions that are adapted to the problem. By use of the tensorization one can decouple the number of global basis functions (number of domains) from the local degrees of freedom in each subdomain. Thus, the total complexity scales as the sum of the two as opposed to the product.

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The Range of Localization Operators and Lifting Properties of Modulation Spaces

Karlheinz Gröchenig

(joint work with Joachim Toft)

Time-frequency localization operators arise in various applications and in mathematical theory: time-frequency masking in signal processing, phase-space localization (Daubechies [3]), Toeplitz operators on Bargmann-Fock space (Berger-Coburn [1]), quantization (Berezin), the approximation of pseudodifferential operators for proofs of the Garding and Fefferman-Phong inequalities (Lerner).

We address the question of how to understand the range of a time-frequency localization operator. Precisely, a localization operator is defined as follows: for a point $z = (x, \xi)$ in phase-space $\mathbb{R}^{2d}$ define the phase-space shift $\pi(z)$ acting on a function f as

$$\pi(z)f(t) = e^{2\pi i \xi \cdot t} f(t - x) \qquad x, \xi, t \in \mathbb{R}^d .$$

Next fix a suitable "window function" g in $\mathcal{S}(\mathbb{R}^d)$, say, and a "symbol" $m(z)$ on $\mathbb{R}^{2d}$. Then the localization operator A_m^g is defined formally by

$$A_m^g f = \int_{\mathbb{R}^{2d}} m(z)\langle f, \pi(z)g\rangle \pi(z)g \, dz$$

The definition resembles the definition of Fourier multipliers, except that in the case of localization operators it is the short-time Fourier transform $\langle f, \pi(z)g\rangle$ that is multiplied by the symbol m before the inverse transform is applied.

The relevant function spaces for the study of mapping properties of localization operators are the modulation spaces (as always in time-frequency analysis). For a non-zero test function g, usually the Gaussian, the modulation space $M_\mu^{p,q}$ is defined by the norm

$$\|f\|_{M_\mu^{p,q}} = \Big(\int_{\mathbb{R}^d} \Big(\int_{\mathbb{R}^d} |\langle f, \pi(x,\xi)g\rangle|^p \mu(x,\xi)^p \, dx \Big)^{q/p} \, d\xi \Big)^{1/q}$$

for $1 \le p, q \le \infty$ and moderate weight functions μ, quite in analogy to the classical Besov spaces.

We will discuss results of the following type, so-called isomorphism theorems.

Theorem 1. *If m is a moderate weight function, then A_m^g is an isomorphism from $M_\mu^{p,q}$ **onto** $M_{\mu/m}^{p,q}$ for every $1 \le p, q \le \infty$ and moderate weight μ.*

The isomorphism theorem resembles the lifting theorems for Besov spaces, where the operator of fractional differentiation establishes an isomorphism between Besov spaces of different smoothness. Modulation spaces can be interpreted as function spaces that describe the smoothness through the phase space distribution. In this sense the isomorphism theorem for localization operators is a lifting theorem for modulation spaces.

Of course, the precise formulation of the isomorphism theorem requires precise conditions on the window g and on the symbol m. For weights of polynomial growth or decay the isomorphism theorem has been established recently with J. Toft [5]. The techniques used pseudodifferential calculus and a deep result of Bony and Chemin [2].

These methods fail for super-algebraic weights, for instance when $m(z) = e^{a|z|^b}$ for $a \in \mathbb{R} \setminus \{0\}$ and $0 < b < 1$ or $m(z) = e^{\frac{|z|}{\log(e+|z|)}}$. To treat symbols with a growth or decay faster than polynomial, we develop a new technique based on pure time-frequency methods. The main ingredients of the proof are
(a) the spectral invariance of pseudodifferential operators in the generalized Sjöstrand class $M_v^{\infty,1}(\mathbb{R}^{2d})$ [4], and
(b) the explicit construction of canonical isomorphisms between the Hilbert spaces $L^2(\mathbb{R}^d)$ and the modulation space $M_m^2(\mathbb{R}^d)$. Whereas for weights of polynomial growth such isomorphisms were constructed by Bony and Chemin [2], for radial weights of superalgebraic growth we develop a new technique.

It is a bizarre fact that the surjectivity of certain localization operators follows from a new class of inequalities about generalized Gamma functions labeled by

moderate weight function θ. As a example we mention the inequality

$$C^{-1} \leq \int_0^\infty m(\sqrt{x/\pi})\frac{x^n}{n!}e^{-x}dx \int_0^\infty \frac{1}{\theta(\sqrt{x/\pi})}\frac{x^n}{n!}e^{-x}dx \leq C \qquad \text{for all } n \geq 0\,.$$

The obtained results yield also new insights into Toeplitz operators on the Bargmann-Fock space of entire functions on $\mathbb{C}^d$ and on Gabor multipliers (earlier considered by Feichtinger).

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On Error Estimation in FEM without Having Galerkin Orthogonality

Helmut Harbrecht

(joint work with Reinhold Schneider)

Let $\Omega \subset \mathbb{R}^2$ denote a two-dimensional bounded polygonal domain with boundary $\partial\Omega$. In the present talk we intend to solve the Poisson equation

$$-\Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega \tag{1}$$

by adaptive finite element methods. To do so, we need an error estimator, which estimates the residual $r = \Delta u_h + f$ in the $H^{-1}(\Omega)$-norm. In general, to derive such error estimators, Galerkin orthogonality is employed.

Consider a shape regular triangulation $\mathcal{K}_h$ of the domain Ω by triangular or quadrilateral elements $\mathcal{K}_h$. The set of edges is indicated by $\mathcal{E}_h$. The space of continuous piecewise (bi-) linear elements will be denoted by V_h. For a given function $u_h \in V_h$, we define the element residual

$$q := \Delta u_h + f \quad \text{for all elements } K \in \mathcal{K}_h$$

and the jumps at the edges

$$\delta := \left[\frac{\partial u_h}{\partial \mathbf{n}}\right] \quad \text{for all edges } E \in \mathcal{E}_h.$$

Then, the standard local lower error bound (cf. [4]), related with the element $K \in \mathcal{K}_h$, is given by

$$h_K^2\|q\|_{L^2(K)}^2 + \sum_{E\in\partial K} h_E\|\delta\|_{L^2(E)}^2 \lesssim \|r\|_{H^{-1}(\Omega)}^2 + \sum_{\substack{K'\in\mathcal{K}:\ K=K' \\ \text{or } K \text{ and } K' \text{ have} \\ \text{a common edge}}} h_K^2\|f - f_h\|_{L^2(K')}^2$$

where the last term reflects the so-called data oscillation. Moreover, $h_K := \operatorname{diam}(K)$ for all $K \in \mathcal{K}_h$ and $h_E := \operatorname{diam}(E)$ for all $E \in \mathcal{E}_h$ are the related local mesh sizes. We emphasize that the proof of this local lower bound does not require Galerkin orthogonality, i.e., it holds for any given finite element function $u_h \in V_h$.

The upper error bound is nonlocal and given by

$$\|r\|^2_{H^{-1}(\Omega)} \sim \|u-u_h\|^2_{H^1(\Omega)} \lesssim \sum_{K\in\mathcal{K}} h_K^2 \|q\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}} h_E \|\delta\|^2_{L^2(E)}, \tag{2}$$

see [1, 7]. The standard trick to obtain this estimate of the error is to rewrite

$$\|u-u_h\|^2_{H^1(\Omega)} \sim \sup_{v\in H^1_0(\Omega)} \frac{\langle \nabla(u-u_h), \nabla v\rangle_{L^2(\Omega)}}{\|v\|_{H^1(\Omega)}}$$

and to employ Galerkin orthogonality by introducing the local Clemónt interpolant v_h of v

$$\|u-u_h\|^2_{H^1(\Omega)} \sim \sup_{v\in H^1_0(\Omega)} \frac{\langle \nabla(u-u_h), \nabla(v-v_h)\rangle_{L^2(\Omega)}}{\|v\|_{H^1(\Omega)}}.$$

Duality together with an approximation property provides the desired estimate.

To our knowledge, all this kind of a-posteriori error analysis requires that the actually discretized finite element problem is solved exactly, or nearly exactly like in [6] where a perturbation argument is applied. This means in the Galerkin framework that the residual is perpendicular to the actual trial space. However, an exact solution of the corresponding discrete equations can be very costly, even though a linearly scaling iterative scheme like a multigrid method is used. Especially in case of eigenvalue problems one has in general no Galerkin orthogonality.

The crucial problem in constructing a-posteriori error estimators is that the residual has to be measured in the dual space $H^{-1}(\Omega)$. Here, we will compute the error directly by using the fact that the infinite BPX scheme enables us to measure the residual's norm in $H^{-1}(\Omega)$.

The construction starts with a coarse triangulation or quadrangulation $\mathcal{T}_0 = \{\tau_{0,k}\}$ of the given domain Ω. Dyadic refinement of each element on level $j-1$ into 4 elements on level j recursively yields for any $j > 0$ the triangulation or quadrangulation $\mathcal{T}_j = \{\tau_{j,k}\}$. On the mesh $\mathcal{T}_j$ we consider standard Lagrangian piecewise linear or bilinear continuous finite elements $\Phi_j = \{\varphi_{j,k} : k \in \triangle_j\}$. This yields a nested sequence of finite dimensional trial spaces

$$V_0 \subset V_1 \subset \cdots \subset V_j \subset \cdots \subset H^1_0(\Omega),$$

where

$$V_j = \operatorname{span}\{\varphi_{j,k} : k \in \triangle_j\} = \{u \in C(\Omega) : u|_\tau \in \Pi_1 \text{ for all } \tau \in \mathcal{T}_j\}$$

($\triangle_j$ denotes an appropriate index set) and $\dim V_j \sim 4^j$. Assuming that the Lagrangian finite elements are normalized with respect to the energy space, i.e.,

$$\|\varphi_{j,k}\|_{H^1(\Omega)} \sim 1,$$

the infinite collection

$$\Phi = \{\varphi_{j,k} : k \in \Delta_j, j \in \mathbb{N}_0\}$$

defines a frame for $H_0^1(\Omega)$, i.e., there holds

$$\|r\|^2_{H^{-1}(\Omega)} \sim \sum_{j\in\mathbb{N}_0} \sum_{k\in\Delta_j} \langle r, \varphi_{j,k}\rangle^2_{L^2(\Omega)}. \tag{3}$$

This frame underlies the construction of the so-called BPX preconditioner, see [3].

On the given sequence of uniform meshes we can introduce an adaptive finite element space V_h by means of one-irregularity [2]. That is, we consider (adaptive) triangular or quadrilateral meshes with at most one hanging node per edge. Then, there exists an index set Σ such that the collection

$$\Phi_\Sigma = \{\varphi_{j,k} : (k,j) \in \Sigma\} \subset \Phi$$

forms a finite element basis which represents a function $u_h \in V_h$ exactly, i.e., $u_h = \Phi_\Sigma \mathbf{u}_\Sigma$. In particular, the Galerkin discretization of the Poisson equation (1) relative to the given triangulation yields the linear system of equations

$$\mathbf{A}_\Sigma \mathbf{u}_\Sigma = \mathbf{f}_\Sigma$$

where

$$\mathbf{A}_\Sigma = [\langle \nabla\varphi_{j',k'}, \nabla\varphi_{j,k}\rangle_{L^2(\Omega)}]_{(j,k),(j',k')\in\Sigma}, \quad \mathbf{f}_\Sigma = [\langle f, \varphi_{j,k}\rangle_{L^2(\Omega)}]_{(j,k)\in\Sigma}.$$

We will prove that, except for the data oscillation, the residual error is equivalent to the sum of the discrete residual $\mathbf{r}_\Sigma = \mathbf{f}_\Sigma - \mathbf{A}_\Sigma \mathbf{u}_\Sigma$ plus the interior residual q and the jump δ across the edges, that is

$$\|r\|^2_{H^{-1}(\Omega)} \sim \mathrm{BPX}(\mathbf{r}_\Sigma)^2 + \sum_{K\in\mathcal{K}} h_K^2 \|q\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}} h_E \|\delta\|^2_{L^2(E)}$$

(modulo data oscillation).

In other words, the upper bound (2) needs just to be corrected by the discrete residual $\mathbf{r}_\Sigma$, measured in the $H^{-1}(\Omega)$-norm via the BPX scheme. Additionally this bound is not only reliable but also efficient. Notice that, due to the nonlocal nature of the BPX multilevel scheme, this error estimator is non-local.

As a consequence of our analysis, we can finally verify the hierarchical error estimation. If one incorporates the data oscillation in the right hand side of (3), it is reasonable that the $H^{-1}(\Omega)$-norm of the remaining residual can be recovered, up to an equivalent measure, by using a BPX scheme applied on an appropriately refined grid. Appropriate means here that we have to uniformly refine the actual mesh three times in case of quadrilateral and two times in case of triangular meshes. In this talk we will show how this can be achieved rigorously.

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Well Localized Frames, Representation of Function Spaces, and Heat Kernel Estimates

Gerard Kerkyacharian
(joint work with T. Coulhon, P.Petrushev,D. Picard)

Since during the last twenty years, wavelet theory has proved to be a very useful tool for theorical purposes as well as for applications, in this talk, we will revisit and provide an extension of this theory in a general geometric framework.

This extension has already been performed for different cases: the interval [PX], the ball [PX2], the sphere [NPW1] and [NPW2], and has been extensively used in statistical applications (see for instance [KKLPP]).

Our object here, will be a metric space (M, ρ) equipped with a positive Radon measure, such that (M, ρ, μ) is a homogeneous space in the sense of Harmonic Analysis (there exists $d > 0$,which plays the role of a dimension, such that for all $x \in M$, and $r > 0$, $\mu(B(x, 2r)) \leq 2^d \mu(B(x, r))$.
Moreover, the geometry of the space is related to a positive self-adjoint operator L and to the associated semi-group e^{-tL}. We suppose in addition that e^{-tL} is markovian.

Here is the main hypothesis : e^{-tL} is a kernel operator, and this kernel $P_t(x, y)$ has the following Gaussian estimate : for all x, y in M, $t > 0$,

$$\frac{C_1 e^{-c\frac{\rho^2(x,y)}{t}}}{\sqrt{\mu(B(x,\sqrt{t}))\mu(B(y,\sqrt{t}))}} \leq P_t(x,y) \leq \frac{C_2 e^{-c\frac{\rho^2(x,y)}{t}}}{\sqrt{\mu(B(x,\sqrt{t}))\mu(B(y,\sqrt{t}))}}.$$

It is well known that this property is equivalent to some Poincare inequalities, or to a parabolic Harnack inequality, and is verified for the Laplacian of a Riemannian manifold with non negative Ricci curvature, for Nilpotent Lie Groups, compact Lie Groups and their homogeneous spaces (see [G], [CS], [O], [S], ...) and many other examples.

From the spectral decomposition $\sqrt{L} = \int_0^\infty \lambda dE_\lambda$, we consider the spectral spaces $\Sigma_\lambda = \{f \in L^2, E_\lambda f = f\}$ and more generally one can define Σ_λ^p the L^p- analogues.

The Besov spaces $B^s_{p,q},\ 0 < s,\ 1 \le p \le \infty,\ 0 < q \le \infty$ are naturally defined as the spaces of approximation :

$$\|f\|_{B^s_{p,q}} = \|f\|_p + \Big(\int_0^\infty (t^s \sigma(t,f,p))^q\Big), \quad \text{(usual modification for } \ q=\infty)$$

$$\sigma(t,f,p) = \inf\{\|f-g\|_p,\ g \in \Sigma^p_\lambda\}$$

The main results are the following :

(1) One can build an efficient Littlewood-Paley decomposition and give a charaterization of the Besov spaces.

(2) It is possible to build localized frames in duality : $\psi_{j,\xi},\ \tilde{\psi}_{j,\xi}, j \in \mathbb{N}, \xi \in A_j$ where A_j is a maximal γb^j-net, ($\gamma > 0$ and $b > 1$ suitably chosen) such that :

(a)

$$\forall f \in L^p, 1 \le p \le \infty, \quad f(x) = \sum_j \sum_{\xi \in A_j} \langle f, \psi_{j,\xi}\rangle \tilde{\psi}_{j,\xi}(x)$$

(b)

$$\exists\, C, \quad \forall j \in \mathbb{N}, \quad \Big(\sum_{\xi\in A_j} |\langle f,\psi_{j,\xi}\rangle|^p \|\tilde{\psi}_{j,\xi}\|_p\Big)^{1/p} \le C\|f\|_p$$

$$\Big\|\sum_{\xi\in A_j} \lambda_\xi \tilde{\psi}_{j,\xi}\Big\|_p \le C\Big(\sum_{\xi\in A_j} |\lambda_\xi|^p \|\tilde{\psi}_{j,\xi}\|_p\Big)^{1/p}$$

(c)

$$\exists\, c > 0,\ \forall j \in \mathbb{N}, \xi \in A_j, \quad \psi_{j,\xi} \text{ and } \tilde{\psi}_{j,\xi} \in \Sigma_{cb^j}$$

(d) and we have the following characterization :

$$f \in B^s_{p,q} \Longleftrightarrow \forall j \in \mathbb{N}, \Big(\sum_{\xi\in A_j} |\langle f,\psi_{j,\xi}\rangle|^p \|\tilde{\psi}_{j,\xi}\|_p\Big)^{1/p} = \alpha_j b^{-js}, \quad \alpha_\cdot \in l_q$$

(with the usual modification for $p = \infty$.)

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High-Dimensional Scattered Data Approximation with Sparse Occupancy Trees

Philipp Lamby

(joint work with Peter Binev, Wolfgang Dahmen and Ronald A. DeVore)

In this work we consider the following problem: Given a data set $X \subset \Omega \subset \mathbb{R}^d$ of N data points along with values $y^i \in \mathbb{R}^{d'}$, $i = 1, \dots, N$, and viewing the y^i as values $y^i = f(x^i)$ of some unknown function f, we wish to return for any query point $x \in \Omega$ an approximation $\tilde{f}(x)$ to $y = f(x)$. Hereby we assume that d is large, say $4 < d < 500$. We wish to emphasize that we do not seek a representation of $\tilde{f}$ in terms of a fixed set of trial functions but define $\tilde{f}$ through recovery schemes which, in the first place, are designed to be fast and to deal efficiently with large data sets. A typical example for such a recovery strategy is to determine for any given query point its k *nearest neighbors* in the given data site and to use their average value as the approximate function value. Unfortunately, exact nearest neighbor search requires either a preprocessing time which is exponential in d or a single query time which is linear in N, the latter characterizing the brute force algorithm where the distance $\|x^i - x\|$ is computed for each training point. Actually, for function recovery purposes one would also be satisfied with an approximate solution which can be achieved much more efficiently, see for instance [In, LMGY]. However, none of the currently available methods seems to perform very well if d goes into the hundreds and N into the millions. For this reason we propose new methods based on what we call *sparse occupancy trees* and piecewise linear schemes based on *simplex subdivisions.*

To start with, let us assume that

$$\{\Omega\} = \mathcal{P}_0 \prec \mathcal{P}_1 \prec \dots \prec \mathcal{P}_j \prec \dots$$

is a hierarchy of nested partitions of the (bounded) input space Ω. This means that for all $l \geq 0$ the sets $\mathcal{P}_l = \{\Omega_{l,k}, k \in \mathcal{I}_l\}$ are partitions of Ω and each cell $\Omega_{l,k} \in \mathcal{P}_l$ is the disjunct union of cells on the next finer level $l + 1$:

$$\Omega_{l,k} = \bigcup_{r \in \mathcal{I}_{l,k}} \Omega_{l+1,r} \ .$$

In the following we assume that the partitions consist of cubes or simplices and that the cardinality of the index sets $\mathcal{I}_{l,k} \subset \mathcal{I}_{l+1}$ is 2^d, i.e., refinement is dyadic. The hierarchy of partitions induces an infinite *master tree* $\mathcal{T}^*$ whose root is Ω and whose other nodes are the cells $\Omega_{l,k}$. Each node $\Omega_{l,k}$ of this tree is connected by

an edge to its children $\Omega_{l+1,r}$ where $r \in \mathcal{I}_{l,k}$. An appropriate simplex subdivision hierarchy can be realized using the subdivision rule provided in [Ma].

A sparse occupancy tree $\mathcal{T}(X)$ is a finite subtree of $\mathcal{T}^*$ which consists only of cells that are occupied, i.e., contain at least one element from the set X. The most basic algorithm based on this data structure provides a piecewise constant approximation. For a given point $x \in \mathbb{R}^d$ it finds the finest cell $K(x)$ from $\mathcal{T}(X)$ it falls into. Then $\tilde{f}(x)$ is set to the average value of all the points in $X \cap K(x)$. As shown in [BDL] a special indexing and ordering scheme generalizing the so-called *linear octree*, which is sometimes used to store voxel information in computer graphics (see [SSB],[BWG]), allows us to store all the information about the tree using only $\mathcal{O}(LdN)$ bits where L is a chosen upper limit for the number of dyadic levels in the tree. The construction of this data structure can be performed in $\mathcal{O}(LdN \log N)$ time and a query can be answered in $\mathcal{O}(Ld \log N)$ time. However, the quality of this approximation depends significantly on the size of the cell $K(x)$ which can be large even if there are points from X close to x.

This disadvantage can be overcome if one constructs piecewise linear approximations on *simplex subdivisions*. Let $\mathcal{T}$ be an occupancy tree based on a hierarchy of simplices. Then let us denote with $\mathcal{S}_l(\mathcal{T}, v)$ the set of all level-l simplices in $\mathcal{T}$ which have the vertex v as a corner point. Vice versa, let $\mathcal{V}_l(\mathcal{T})$ be the set of all vertices which are corner points of a level-l cell in $\mathcal{T}$.

In the training stage of our new algorithm we prescribe values for every level l and every vertex $v \in \mathcal{V}_l(\mathcal{T})$ as averages of the points in the surrounding level-l simplices:

$$y_l(v) = \mathcal{A}(\{y^i \,|\, x^i \in \bigcup_{S \in \mathcal{S}_l(\mathcal{T},v)} S\}).$$

The simplex subdivision rule in [Ma] employs edge subdivision. Hence every level $l+1$ vertex arises as average of two level l vertices $p_1(v)$ and $p_2(v)$. Therefore, if $v \notin \mathcal{V}_l(T)$, we can define the vertex value recursively by averaging the values of its parents:

$$y_l(v) = \frac{1}{2}(y_{l-1}(p_1(v)) + y_{l-1}(p_2(v))).$$

This recursion terminates, because the level-0 values of the initial simplex are defined, if the training data set is not empty. One has to note that this training stage is actually executed as follows: for each vertex one stores the sum of all the training points in the adjacent simplices and the number of contributors. If one reads a new training point x^i, one computes its path through the master tree, adds its value to every vertex connected to the cells it belongs to, and increases the number of contributors for these vertices by one. Hence, this algorithm is suited for streaming data acquisition and online learning.

In the evaluation stage the level-l value of a query point x is then determined by piecewise linear interpolation of the vertex values of the level-l cell $S_l(x)$ *in the master tree* the query falls into. Note that this cell need not to be occupied. Concretely, for any simplex S let $\mathcal{V}(S)$ be the set of its vertices and $\tau(S, v, x)$ be the barycentric coordinate of x with respect to v. Then for each refinement level

l a response to the query is defined by

$$\tilde{f}_l(x) = \sum_{v \in \mathcal{V}(S_l(x))} \tau(S_l(x), v, x)\; y_l(v).$$

This description provides a general framework for the construction of piecewise linear approximations to the given data. To define a concrete scheme, one has still to specify, how deep the tree $\mathcal{T}$ is to be refined, and what evaluation level l is to be chosen. If, for example, one chooses the same evaluation level l for all queries, one effectively defines a globally continuous approximation. Here we aim at another property: we want the approximation to be *interpolatory*, i.e., if x coincides with one of the data points x^i we want to return its value y^i. This can be achieved by choosing the occupancy tree such that no two leafs of $\mathcal{T}$ have a vertex in common, and the evaluation level l maximal, such that $S_l(x)$ is still connected to at least one vertex connected to the occupancy tree.

Another technical issue is, that in order to initialize the algorithm one has to assume that all the data is contained in one initial simplex. If one originally has data in the unit cube $[0,1]^d$ this can be achieved by mapping all training data and query points into the standard simplex $\{x \in \mathbb{R}^d : 0 \le x_1 \le x_2 \le \ldots \le x_d \le 1\}$ using the so-called *root transformation*

$$x = (x_i)_{i=1}^d \longmapsto T(x) = \left(\prod_{j=i}^{d} x_j^{1/j} \right)_{i=1}^{d},$$

see [FW].

Numerical experiments show that, concerning accuracy, the above described algorithm can compete with or even improve on the approximate nearest neighbor method and its computational costs scale favorably if d and N become large.

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Optimal Mesh Adaptation for Finite Element Approximation

Jean-Marie Mirebeau
(joint work with Albert Cohen)

Mesh adaption procedures for finite element approximation allows one to adapt the resolution, by local refinement in the regions of strong variation of the function of interest. The use of anisotropic triangles allows to improve the efficiency of the procedure by introducing long and thin triangles that fit in particular the directions of the possible curves of discontinuity. In our work, we study the optimal mesh for the interpolation error measured in the L^p norm or the Sobolev $W^{1,p}$ semi norm. More precisely, given a function f defined on a closed bounded and polygonal domain $\Omega \subset \mathbb{R}^2$, and an integer $N > 0$, we look for the mesh $\mathcal{T}_N$ of Ω consisting of N triangles such that the interpolation error $\|f - f_N\|_p$, or $\|\nabla(f - f_N)\|_p$, between f and its interpolation f_N by $\mathbb{P}_m$ finite elements on $\mathcal{T}_N$ is minimal.

A known result, see [CSX, Mi1], bounds this error in the case of a function $f \in C^2(\Omega)$ and of piecewise linear $\mathbb{P}_1$ finite elements:

$$\limsup_{N\to\infty} N\|f - f_N\|_p \leq C\|\sqrt{|\det d^2 f|}\|_\tau, \tag{1}$$

where $\tau := p/(p+1)$ and where C is a universal constant (independent of f, Ω and p). In comparison, if one restricts to triangulations consisting of "isotropic" (close to equilateral) triangles, this estimate becomes $\limsup N\|f - f_N\| \leq C\|d^2 f\|_\tau$, for the same value of τ. The introduction of anisotropy hence allows to replace in the L^τ-norm the spectral norm of the hessian $\|d^2 f\|$ by the smaller quantity $\sqrt{|\det d^2 f|}$ which depends non linearly on the derivatives of f. The presence of the lim sup operator reflects the fact that a sufficiently fine resolution is needed to adapt the triangulation $\mathcal{T}_N$ to the local features of the function f. Under reasonnable hypotheses, one can establish that the estimate (1) is optimal.

Our work [Mi1, Mi2] extends these results to finite elements of arbitrary degree, both for L^p norms or $W^{1,p}$ semi-norms. For example, in the case of interpolation by piecewise quadratic $\mathbb{P}_2$ elements, the corresponding estimates involve nonlinear quantities that depend on the derivatives of order three of f. At all points of Ω one can associate to $d^3 f$ an homogeneous polynomial of degree 3 in x and y, in the same way that one associates an homogeneous quadratic polynomial to $d^2 f$. On the other hand we define

$$D\big(ax^3 + 3bx^2y + 3cxy^2 + dy^3\big)^4 := (a^2 + 2b^2 + c^2)(b^2 + 2c^2 + d^2) - (ab + 2bc + cd)^2.$$

If $f \in C^3(\Omega)$, and if $\tilde{f}_N$ is its $\mathbb{P}_2$ interpolation on the optimal mesh $\tilde{\mathcal{T}}_N$, we have shown that

$$\limsup_{N\to\infty} N\|\nabla(f - \tilde{f}_N)\|_p \leq C\|D(d^3 f)\|_\tau, \tag{2}$$

where again $\tau := p/(p+1)$ and C is a universal constant. An optimality result completes this estimate, and similar expressions are given for arbitrary degrees of interpolation $\mathbb{P}_m$. The nonlinear quantities which appear in these estimates, such

as $\det(d^2 f)$ or $D(d^3 f)$, are particular cases of the theory of invariant polynomials which allows to generalize such estimates to finite elements of arbitrary order.

Several algorithms allow to produce triangulations satisfying these optimal inequalities. In order to achieve the estimate (1), the area, aspect ratio and orientation of the triangles $T \in \mathcal{T}_N$ should obey some local prescriptions. We have studied in [CoMi2] an algorithm that produces (nonconforming) triangulations satisfying these requirements under certain assumptions, and also satisfies an additional property : the triangulations form a hierarchical family, in other words $\mathcal{T}_{N+1}$ is a refinement of $\mathcal{T}_N$. In the case (2) of Sobolev norms the triangulation $\tilde{\mathcal{T}}_N$ needs to be conforming and the maximal angle of any triangle $T \in \tilde{\mathcal{T}}_N$ needs to be uniformly bounded away from π, in addition to the requirements of area, aspect ratio and orientation of T. Our current research involves the construction of a practical mesh generation algorithm that combines in such a way arbitrary anisotropy with a maximal angle condition.

The extension of the approximation results (1) and (2) to non smooth functions requires as a first step a well posed extension of the non-linear quantities appearing on the right hand side of these inequalities. We have studied in [CoMi1] the case of functions featuring discontinuities along regular curves. For instance, consider a function f which is C^2 on Ω, except along a curve Γ which is also C^2. Consider a family $\varphi_\delta(z) := \frac{1}{\delta^2}\varphi(\frac{z}{\delta})$ of mollifiers and denote $f_\delta := f * \varphi_\delta$. We obtain

$$\lim_{\delta \to 0} \|\sqrt{|\det d^2 f_\delta|}\|_{2/3}^{2/3} = \int_{\Omega \setminus \Gamma} |\det d^2 f(z)|^{\frac{1}{3}} dz + C(\varphi) \int_\Gamma |\kappa(s)|^{1/3} |\gamma(s)|^{2/3} ds$$

where κ denotes the curvature of Γ, and γ the jump of f at a point of this interface. A parallel is established and discussed between this quantity and the total variation $TV(f) := |f|_{BV}$, which counts the length of the curves of discontinuity but does not penalise their curvature.

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"Compactly" Supported Frames for Spaces of Distributions on the Ball

Pencho Petrushev
(joint work with George Kyriazis)

Bases and frames for spaces of functions or distributions are valuable for various theoretical and practical reasons. In this talk we focus on the problem for construction of multiscale frames on the unit ball B^d in $\mathbb{R}^d$ consisting of C^∞ functions with small supports which shrink at higher scales. More precisely, we discuss the construction of a frame in [2] of the form $\{\theta_\xi\}_{\xi\in\mathcal{X}}$, where $\mathcal{X}=\cup_j\mathcal{X}_j$ is a multilevel index set ($\mathcal{X}_j\subset B^d$), and each jth level frame element θ_ξ ($\xi\in\mathcal{X}_j$) is supported on $B(\xi,c2^{-j})$ the ball centered at $\xi\in B^d$ of radius $c2^{-j}$ with respect to the distance

$$d(x,y):=\arccos\left\{\langle x,y\rangle+\sqrt{1-|x|^2}\sqrt{1-|y|^2}\right\}\quad\text{on } B^d.$$

Here $\langle\cdot,\cdot\rangle$ and $|\cdot|$ are the Euclidean inner product and norm on $\mathbb{R}^d$, and hence this is just the geodesic distance between the lifted images of $x,y\in B^d$ to the upper unit hemisphere in $\mathbb{R}^{d+1}$. In fact, the set $\mathcal{X}_j$ consisting of the "centers" of the jth level frame elements is a $c2^{-j}$-net on B^d. The frame $\{\theta_\xi\}_{\xi\in\mathcal{X}}$ is reminiscent of compactly supported wavelets on $\mathbb{R}$.

The quality of this tool is guaranteed by the fact that, as shown in [2], $\{\theta_\xi\}_{\xi\in\mathcal{X}}$ can be used for decomposition of weighted Triebel-Lizorkin and Besov spaces on B^d with weight

$$w_\mu(x):=(1-|x|^2)^{\mu-1/2},$$

where $\mu\geq 0$ is a half integer.

The construction of $\{\theta_\xi\}_{\xi\in\mathcal{X}}$ relies on the general scheme for construction of frames from [1] and the frames (called needlets) for weighted Triebel-Lizorkin and Besov spaces on B^d developed in [3, 4].

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Entropy Viscosity

Bojan Popov
(joint work with Jean-Luc Guermond and Richard Pasquetti)

We introduce a new shock-capturing technique for solving nonlinear conservation laws. The method is an extension of the work in [GP] and consists of adding a nonlinear viscosity to the Galerkin formulation of the nonlinear equation or system of equations. The key idea is that the added viscosity is proportional to the residual of the entropy equation and it is always limited from above by first order dissipation. The treatment of the nonlinear viscous term is explicit in time which makes the method very simple to implement for various discretizations: finite elements, spectral elements, and Fourier approximations. We prove that the method is convergent in some simple scalar cases and verify its performance numerically on various one and two dimensional benchmarks including scalar equations and nonlinear systems of conservation laws. The general formulation of the method and many numerical tests are given in our paper [GPP].

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Compressive Sensing, Structured Random Matrices and Recovery of Functions in High Dimensions

Holger Rauhut

Compressive sensing predicts that sparse vectors can be recovered efficiently from highly undersampled measurements. While it is well-understood by now that Gaussian random matrices provide optimal measurement matrices in this context, such "highly" random matrices suffer from certain drawbacks: applications require more structure arising from physical or other constraints, and recovery algorithms such as greedy methods or algorithms for ℓ_1-minimization demand fast matrix vector multiplies in order to make them feasible for large scale problems. In order to meet such desiderata, we study two types of structured random measurement matrices: partial random circulant matrices, and random sampling matrices associated to bounded orthonormal systems (e.g. random Fourier type matrices). The latter maybe used to study reconstruction problems in high spatial dimensions.

Compressive Sensing. A vector $x \in \mathbb{C}^N$ is called s-sparse if $\|x\|_0 := \#\{\ell, x_\ell \neq 0\} \leq s$. The ℓ_p-norm is defined as usual, $\|x\|_p := (\sum_{\ell=1}^N |x_\ell|^p)^{1/p}$, $0 < p < \infty$. The best s-term approximation error of an arbitrary vector in ℓ_p is defined as

$$\sigma_s(x)_p = \inf_{\|z\|_0 \leq s} \|x - z\|_p.$$

Informally, x is called compressible if $\sigma_s(x)_p$ decays quickly in s. An estimate originally due to Stechkin states that $\sigma_s(x)_p \leq s^{1/p-1/q}\|x\|_q$ for $q < p$ so that $B_q^N = \{x \in \mathbb{C}^N, \|x\|_q \leq 1\}$ is a good model for compressible vectors if $q \in (0,1]$ is chosen small.

The task of compressive sensing is to recover a sparse or compressible vector $x \in \mathbb{C}^N$ from undersampled measurements

$$y = Ax \ \in \mathbb{C}^m,$$

where $A \in \mathbb{C}^{m\times N}$ is a suitable measurement matrix and $m \ll N$. The first approach for recovering x that probably comes to mind consists in solving the ℓ_0-minimization problem

$$\min_{z\in\mathbb{C}^N} \|z\|_0 \quad \text{subject to } Az = y.$$

Unfortunately, this combinatorial optimization problem is NP hard in general. For this reason, several tractable alternatives have been introduced, most notably ℓ_1-minimization, which consists in solving the convex optimization problem

$$\min_{z\in\mathbb{C}^N} \|z\|_1 \quad \text{subject to } Az = y.$$

A very useful concept for analyzing ℓ_1-minimization are the restricted isometry constants. For $s < N$ they are defined as the smallest constant δ_s such that

$$(1-\delta_s)\|x\|_2^2 \leq \|Ax\|_2^2 \leq (1+\delta_s)\|x\|_2^2 \quad \text{for all } x \in \mathbb{C}^N, \|x\|_0 \leq s.$$

If $\delta_{2s} < 0.46$ then ℓ_1-minimization reconstructs all s-sparse vectors x exactly from $y = Ax$, and compressible vectors approximately, see [1, 4] for precise statements.

It is an open problem to construct deterministic (explicit) measurement matrices that have small restricted isometry constants for small m (or large s, respectively). So far, all good constructions use randomness. A matrix with independent standard normal distributed entries is called a Gaussian random matrix. It is by now well-known [2] that a rescaled Gaussian matrix $\frac{1}{\sqrt{m}}A \in \mathbb{R}^{m\times N}$ satisfies $\delta_s \leq \delta$ with probability at least $1-\varepsilon$ provided

$$m \geq C\delta^{-2}(s\log(N/s) + \log(\varepsilon^{-1})),$$

where $C > 0$ is a universal constant. In particular, exact recovery of s-sparse vectors via ℓ_1-minimization is possible if $m \asymp s\log(N/s)$. This estimate for the minimal number m of measurements is optimal as follows from lower bounds of Gelfand widths of B_q^N [5].

Partial random circulant matrices. While Gaussian random matrices are optimal for compressive sensing, they are not structured at all, which poses severe limitations for practical applications as mentioned above. Therefore, we consider instead the following structured random matrix. For a vector $b \in \mathbb{C}^N$ we define its associated circulant matrix $\Phi = \Phi(b) \in \mathbb{C}^{N\times N}$ with entries

$$\Phi_{k,j} = b_{j-k \mod N}, \quad k,j = 1,\dots,N.$$

For an abritrary subset $\Theta \subset \{1,\dots,N\}$ we define the restriction operator $R_\Theta : \mathbb{C}^N \to \mathbb{C}^\Theta$ as $(R_\Theta x)_\ell = x_\ell$, $\ell \in \Theta$. Then the partial circulant matrix $\Phi^\Theta =$

$\Phi^\Theta(b) = R_\Theta \Phi(b)$ consists of the rows of $\Phi = \Phi(b)$ indexed by the set Θ. An application of Φ^Θ to a vector x corresponds to convolution with b followed by subsampling on Θ. Since a circulant matrix can be diagonalized by the Fourier matrix, the FFT can be used for fast matrix vector multiplies. For the purpose of compressive sensing, the vector b is chosen at random, more precisely, as Rademacher sequence, that is, all entries are independent, and take the value $+1$ or -1 with equal probability. This turns the matrix $\Phi^\Theta = \Phi^\Theta(b)$ into a partial random circulant matrix. In [6] the following nonuniform recovery result for Φ^Θ has been shown.

Theorem. *Let $\Theta \subset \{1, \dots, N\}$ be an arbitrary (deterministic) set of cardinality m. Let $x \in \mathbb{C}^N$ be s-sparse such that the signs of its non-zero entries form a Rademacher or Steinhaus sequence. Choose $b \in \{-1, +1\}^N$ to be a Rademacher sequence. Let $y = \Phi^\Theta(b)x \in \mathbb{C}^m$. If*

$$m \geq 57 s \ln^2(17N^2/\varepsilon)$$

then x can be recovered from y via ℓ_1-minimization with probability at least $1 - \varepsilon$.

Unfortunately, this result does not imply the existence of a single matrix $\Phi^\Theta(b)$ that guarantees recovery of all s-sparse vectors simultaneously. Such type of statement is implied by the next theorem on the restricted isometry constants shown in [7].

Theorem. *Let $\Theta \subset \{1, \dots, N\}$ be an arbitrary (deterministic) set of cardinality m. Choose $b \in \mathbb{R}^N$ to be a Rademacher sequence. Assume that*

$$m \geq C\delta^{-1} s^{3/2} \log^{3/2}(N), \tag{1}$$

and, for $\varepsilon \in (0, 1)$, $m \geq C\delta^{-2} s \log^2(s) \log^2(N) \log(\varepsilon^{-1})$. Then with probability at least $1 - \varepsilon$ the restricted isometry constants of $\frac{1}{\sqrt{m}} \Phi^\Theta(b)$ satisfy $\delta_s \leq \delta$.

The exponent $3/2$ in (1) does not seem to be optimal. Unfortunately, the proof technique in [7] is likely not powerful enough in order to obtain the expected exponent 1.

Random Sampling in Bounded Orthonormal Systems. Let $\Omega \subset \mathbb{R}^d$ be endowed with a probability measure ν, and $\phi_1, \dots, \phi_N$ be a system of orthonormal functions, i.e., $\int_\Omega \phi_j(t)\overline{\phi_k(t)} d\nu(t) = \delta_{j,k}$. We further assume that the function system is bounded in the sense that

$$\sup_{j=1,\dots,N} \|\phi_j\|_\infty \leq K$$

for some constant $K \geq 1$. A function of the form

$$f(t) = \sum_{j=1}^N x_j \phi_j(t)$$

is called s-sparse if $\|x\|_0 \leq s$. Our goal is to reconstruct sparse (or compressible) functions from sample values $f(t_1), \dots, f(t_m)$ with $t_1, \dots, t_m \in \Omega$. Introducing the sampling matrix $A \in \mathbb{C}^{m \times N}$ with entries $A_{k,j} = \phi_j(t_k)$ yields $y = (f(t_1), \dots, f(t_m))^T = Ax$. Therefore, we are interested in the restricted isometry constants of the sampling matrix. We choose the points $t_1, \dots, t_m$ independent

and distributed according to ν. This makes A a structured random matrix. The most important example consists in choosing $\phi_j(t) = e^{2\pi i t\cdot j}, j \in \mathbb{Z}^d, t \in [0,1]^d$, $\Omega = [0,1]^d$ and ν to be the Lebesgue measure. The resulting sampling matrix is then a non-equispaced Fourier matrix for which fast (approximate) matrix vector multiplies are available. In [6] the following estimate for the restricted isometry constants has been derived, generalizing and improving slightly on [2, 9].

Theorem. *Let $A \in \mathbb{C}^{m\times N}$ be the random sampling matrix associated to a bounded orthonormal system with constant $K \geq 1$. If*

$$\frac{m}{\ln(m)} \geq CK^2\delta^{-2}s\ln^2(s)\ln(N).$$

then with probability at least $1 - N^{-\gamma\ln^2(s)\ln(m)}$ the restricted isometry constant of $\frac{1}{\sqrt{m}}A$ satisfies $\delta_s \leq \delta$. The constants $C, \gamma > 0$ are universal.

This result can be used to extend reconstruction from sample values via compressive sensing to infinite dimensional function spaces, and in particular, to suitable spaces of functions of many variables. We refer to [3, 8] for details.

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Collaborative Hierarchical Structured Sparse Modeling

Guillermo Sapiro

(joint work with P. Sprechmann, I. Ramirez, Y. Eldar, G. Yu, and S. Mallat)

In addition to being very attractive at the theoretical level, sparse signal modeling has been shown to lead to numerous state-of-the-art results in signal processing. The standard model assumes that a signal can be efficiently represented by a sparse linear combination of atoms from a given or learned dictionary. The selected atoms form what is usually referred to as the *active set*, whose cardinality is significantly smaller than the size of the dictionary. In recent years, it has been

shown that adding structural constraints to this active set has value both at the level of representation robustness and at the level of signal interpretation (in particular where the active set indicates some physical properties of the signal). This leads to *group* or *structured* sparse coding, where instead of considering the atoms as singletons, the atoms are grouped, and a few groups are active at a time. An alternative way to add structure (and robustness) to the problem is to consider the simultaneous encoding of multiple signals, requesting that they all share the same active set. This is a natural collaborative filtering approach to sparse coding.

In this work we extend these models in a number of directions. First, we present a hierarchical sparse model, where not only a few (sparse) groups of atoms are active at a time, but also each group enjoys internal sparsity.[1] At the conceptual level, this means that the signal is represented by a few groups (models), and inside each group only a few members are active at a time. A simple example of this is a piece of music (numerous applications in genomics exist as well), where only a few instruments are active at a time (each instrument is a group), and the actual music played by the instrument is efficiently represented by a few atoms of the sub-dictionary/group corresponding to it. Thereby, this proposed hierarchical sparse coding framework permits to efficiently perform source identification and separation, where the individual sources (models) that generated the signal are identified at the same time as their efficient representation (the sparse code inside the group) is reconstructed. An efficient optimization procedure is proposed to solve this hierarchical sparse coding framework.

Then, we go a step beyond this. Imagine now that we have multiple recordings of the same two instruments, each time playing different songs. Then, if we collaboratively apply this new hierarchical sparse coding approach, we expect that the different recordings will share the same groups (since they are of the same instruments), but each will have its unique sparsity pattern inside the group (since each recording is a different melody). We propose a collaborative hierarchical sparse coding framework addressing exactly this, a powerful new framework for collaborative source separation.[2] An efficient optimization procedure for this case is derived as well.

During the talk we introduce these new models and their corresponding optimization, theoretical bounds for the new models, present numerous examples illustrating them (both in audio and image processing), and provide possible directions of research opened by these new frameworks, including some theoretical ones.

We conclude the talk with a brief presentation of a different model on structure sparsity, tuned to image analysis, that relates sparse modeling with Gaussian

[1] While we here consider only 2 levels of sparsity, the proposed framework is easily extended to multiple levels

[2] Note that different recordings can also have different instruments, so some of them will share the same groups while not necessarily all of them will be exactly the same.

Mixture Models, and via very simple and computational efficient linear operations, achieves state-of-the-art performance in a number of image enhancement application.

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Adaptive Multiresolution Discontinuous Galerkin Schemes for Conservation Laws

Roland Schäfer

(joint work with N. Hovhannisyan, S. Müller)

We consider a scalar conservation law with source term

$$u_t + f(u)_x = s(u) \quad \text{on } \mathbb{R}$$

subject to the initial conditions $u(0,x) = u_0(x)$ for $x \in \mathbb{R}$. We are interested in approximating the entropy solution $u \in L^\infty(0,T,L^1_{loc}(\mathbb{R}))$, see [O63, TT95]. For that purpose we introduce an adaptive scheme with the following features:

- The data is evolved on a locally coarsened grid where we never use the fully refined grid.
- The error compared to the fully refined grid increases only by a constant factor, therefore we retain the accuracy of the uniform grid without computing on it.
- Limiting is performed only on cells next to a discontinuity. In regions where the solution is smooth, no limiting is used at all.
- The adaptive grid does not have to be graded, in contrast to the Multiresolution Finite Volume (MR-FV) schemes [M03, CKMP03].
- Higher polynomial degrees and therefore better compression rations and coarser grids can easily be used due to the locality of the DG scheme, whereas in the case of MR-FV schemes the grading of the grid increases.

The analysis is based on a reference scheme acting on the uniformly refined grid. In this work we chose the Discontinuous Galerkin scheme by Cockburn and Shu [CS89]. To obtain the adaptive scheme, we employ a multiscale transformation using the biorthogonal multiwavelets of Alpert et. al. [ABGV02], and then use hard thresholding to compress the data. This corresponds to a grid coarsening. The time evolution is then performed on the coarsened grid, while never using the uniformly refined grid. Between time levels we have to adapt the grid to resolve non-stationary features of the solution. Therefore, a prediction strategy is needed that indicates, which detail coefficients can become significant.

Our goal will be to present a prediction strategy that allows to control the final error introduced by the thresholding by the thresholding parameter. For a given reference discretization, we then chose this parameter to balance the thresholding error with the discretization error, leading to an increase in error only by a constant factor. At the same time, the adaptive scheme significantly reduces the number of degrees of freedom and therefore accelerates the computation. We present numerical experiments that validate the analysis, see [HMS10] for further reference.

Using the basis expansion of $u_h(t,\cdot) = \sum_{k\in\mathcal{I}_h, 0\le i<p} v_{k,i}(t)\phi_{k,i} \in S^p$, the space of piecewise polynomial of degree less than p with spacial index k, the semi-discrete Discontinuous Galerkin scheme reads

$$\frac{d}{dt}v_{k,i}(t) = -F(u_h(t,x^-), u_h(t,x^+))\tilde{\phi}_{k,i}(x)\Big|_{x_k}^{x_{k+1}} + \langle f(u_h(t)), \tilde{\phi}'_{k,i}\rangle + \langle s(u_h(t)), \tilde{\phi}_{k,i}\rangle$$

where $F(v,w)$ is a monotone, consistent and Lipschitz continuous numerical flux function, $\tilde{\phi}_{k,i}$ a biorthogonal test function, $x_k = x_0 + kh$ and $\langle g,h\rangle = \int g(x)h(x)dx$.

We then apply the explicit Euler scheme for time discretization with time step size τ and obtain the fully discrete **single scale scheme**

$$v_{k,i}^{n+1} = v_{k,i}^n - \tau(B_{i,k}^n - G_{i,k}^n - S_{i,k}^n)$$

where $B_{i,k}^n$ denotes the flux balance, $G_{i,k}^n$ the flux quadrature and $S_{i,k}^n$ the source quadrature. This scheme will be denoted as *reference scheme* on the uniform *reference mesh*.

Assuming that the grid stems from L dyadic grid refinements of a coarse scale grid, we perform a multiresolution analysis on the data using biorthogonal multiwavelets. Let $\{\phi_{0,k,i}, \psi_{l,k,i}\}_{l,k,i}$ denote the primal and $\{\tilde{\phi}_{0,k,i}, \tilde{\psi}_{l,k,i}\}_{l,k,i}$ the dual multiscale basis with the biorthogonal wavelets $\psi_{l,k,i}$ and $\tilde{\psi}_{l,k,i}$. We note that the scaling functions and wavelets are compactly supported on a single grid cell. Then we can expand $u_h \in S^p$ in the multiscale basis

$$u_h = \sum_{l=0}^{L} \sum_{k\in\mathcal{I}_l, 0\le i<p} d_{l,k,i}\,\psi_{l,k,i} + \sum_{k\in\mathcal{I}_0, 0\le i<p} v_{0,k,i}\,\phi_{0,k,i}$$

with the detail $d_{l,k,i} = \langle u_h, \tilde{\psi}_{l,k,i}\rangle$ and coarse scale coefficients $v_{0,k,i} = \langle u_h, \tilde{\phi}_{0,k,i}\rangle$.

If we perform a multiscale transformation of the single scale scheme, we obtain the equivalent **multiscale scheme**

$$\begin{aligned} d_{l,k,i}^{n+1} &= d_{l,k,i}^n - \tau(\bar{B}_{l,k,i}^n - \bar{G}_{l,k,i}^n - \bar{S}_{l,k,i}^n) \\ v_{0,k,i}^{n+1} &= v_{0,k,i}^n - \tau(B_{0,i,k}^n - G_{0,i,k}^n - S_{0,i,k}^n). \end{aligned}$$

The **adaptive scheme** is then obtained from the multiscale scheme by hard thresholding on the coefficients of the initial conditions. Starting from the thresholded initial conditions, we adapt the grid and then use the equations of the multiscale scheme to evolve the coefficients corresponding to that grid. All other coefficients remain zero. Limiting is performed only on cells on the highest level. Therefore in smooth regions where the grid is coarser, no limiting is used.

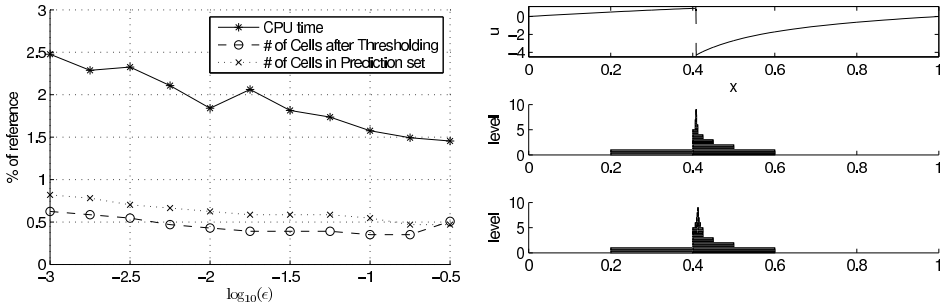

FIGURE 1. Left: Computational savings compared to reference scheme; Right: Solution and detail coefficient trees for optimal value of ε

We do not know the set of detail coefficients that can become significant on the next time level. The goal of this work is to construct, from data on the current time level, a prediction set $\tilde{\mathcal{D}}$ that contains the indices of significant details on the current and on the next time level. This corresponds to the grid adaptation. Under some assumptions on the reference scheme, the following holds true.

Theorem: (Reliability of the adaptive scheme) If the prediction set $\tilde{\mathcal{D}}$ is constructed such that $(l,k,i) \notin \tilde{\mathcal{D}}$ implies $|d_{l,k,i}^{n+1}| \leq \varepsilon_l$, then the error of the adaptive scheme with respect to the reference scheme at the final time is bounded by ε.

In [HMS10] we give a construction of the prediction set that ensures the reliability of the scheme, accounting for both nonlinearities, the limiting and the evolution step.

To validate this analysis, we consider the Burgers equation with a source term

$$u_t + uu_x = u(u-1)(u-0.5) \quad \text{on } [0,1]$$

with initial conditions $u_0(x) = \sin(2\pi x)$. For a sequence of threshold values $\varepsilon = 10^{-0.5}, \ldots, 10^{-3}$ we compute the adaptive solution and then compare it to the reference solution on the uniform grid and the exact solution. For $\varepsilon = 10^{-1.75}$ we find that the discretization error of the reference solution compared to the exact solution and the thresholding error of the adaptive solution compared to the reference solution are balanced. For smaller values of ε the discretization error dominates the total error, for bigger values the thresholding error is dominant. This numerically supports the reliability of the adaptive scheme. To asses the efficiency, see Figure 1 (left). The computational cost is less than 2.5% of the CPU time of the reference solution. This is due to the reduction of degrees of freedom to less than 1% by grid coarsening. In Figure 1 (right) we see on top the solution computed with the adaptive scheme and in the middle the tree of detail coefficients after thresholding (where white means that the detail coefficient is zero). At the bottom the tree of detail coefficients that was used to calculate the current time step is shown. Each of these trees corresponds to an adaptive grid,

where a cell is refined, if detail coefficients are non-zero. The difference of the two grids is minimal, therefore we can conclude that the amount of over-prediction is small. We note that the resulting grid does not need to be graded, in contrast to MR-FV schemes. This allows for higher polynomial degrees and therefore higher compression ratios without having larger stencils, resulting in better computational performance.

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Tensor Product Approximation – For the Electronic Schrödinger Equation

Reinhold Schneider

Approximation by sums of tensor products of single variate functions, herein called tensor product approximation, offer a flexible tool for a data sparse approximation. The single variate component functions have to be optimized in a sense providing best, almost best or at least a reasonable accuracy. Recent developments in tensor product approximation [Ko] were motivated by problems in data compression and data analysis. But there are various partial differential equations in high dimensions, for example Fokker Planck equation, chemical master equation, boundary value problems with stochastic data and quantum dynamics. One of the most important highdimensional problems is the stationary electronic Schrödinger equation [He].

For convenience of exposition, we will regard a tensor U as a multivariate function of the form

$$U \;=\; U(\underline{x}) \;=\; U(x_1,\dots,x_d) \;:\; \mathcal{I}_1 \times \cdots \times \mathcal{I}_d \;\longrightarrow\; \mathbb{R}.$$

In the present talk we are dealing only with the representation or approximation of tensors $U \in \mathbb{R}^{n_1 \times \dots \times n_d}$ of order (or dimension) indexed by finite index sets $\mathcal{I}_i := \{1,\dots,n_i\}$ for all $i \in \{1,\dots,d\}$, where $d \in \mathbb{N}$ and $n_1,\dots,n_d$.

Unfortunately, besides in the elementary (matrix) case $d = 2$, classical concepts from tensor product approximation, such as the *canonical* or *Kronecker decomposition* also known as *CANDECOMP* or *PARAFAC*, see e.g. [Ko],

$$U(x_1, \ldots, x_d) = \sum_{i=1}^{r} U_i = \sum_{i=1}^{r} \bigotimes_{\nu=1}^{d} u_{i,\nu}(x_\nu) = \sum_{i=1}^{r} \bigotimes_{\nu=1}^{d} u_\nu(x_\nu, i) \ ,$$

suffer from various shortcomings from the theoretical as well as from the practical point of view, making the actual computation of a low-rank approximation a numerically hazardous task. This is in contrast the so-called *Tucker decomposition*, In essence the Tucker format is a subspace approximation. It has been shown, e.g. in [Lu], that the Tucker format provides an embedded manifold.

Since the representation of a tensor in the Tucker format requires $\mathcal{O}(r^d + dn)$, $n := \max\{n_\nu : 1 \le \nu \le d\}$, degrees of freedom (DOF), it does not overcome the curse of dimensionality, namely the scaling $\mathcal{O}(e^{\alpha d})$, $\alpha > 0$.

To overcome this dilemma, a new format built on a hierarchical structure for tensor decomposition has been introduced in [HT]. Independently Tyrtyshnikov and Oseledets [TT] developed the *TT format* (abbreviating "tree tensor" or "tensor train"). It is a special and simplest case of the more general hierachical Tucker format in [HT]. In the present talk we focuses on this representation exclusively. Independent from those recent developments, the TT format was considered in [Vi] in the form of matrix product states (MPS) in quantum information theory. A representation of a tensor $U \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ in the TT tensor format rewrites an order-d tensor in the form

$$U(x) = \sum_{k_1=1}^{r_1} \cdots \sum_{k_{d-1}=1}^{r_{d-1}} U_1(x_1, k_1) U_2(k_1, x_2, k_2) \ldots U_{d-1}(k_{d-2}, x_{d-1}, k_{d-1}) U_d(k_{d-1}, x_d),$$

where for $2 \le i \le d-1$, $U_i(k_{i-1}, x_i, k_i) \in \mathbb{R}^{r_{i-1} \times n_i \times r_i}$. For brevity of notation, it could rewritten by matrix products

$$U(\mathbf{x}) = \mathbf{U}_1(x_1) \cdots \mathbf{U}_\nu(x_\nu) \cdots \mathbf{U}_d(x_d) \ .$$

with matrices $\mathbf{U}_\nu(x_\nu) \in \mathbb{R}^{r_{\nu-1} \times r_\nu}$ [Vi]. In a recent paper [HRS-1], we have shown that the TT-format provides an embedded manifold, see. [HRS-1] for further details. In this paper, we have parametrized corresponding tangent spaces by introducing an appropriate gauge condition like in [Lu].

For solving elliptic linear equations or eigenvalue problems in the TT format, let us present a (block) relaxation scheme [HRS-2], similary as the *alternating least squares scheme* for the canonial format. Let us fix all tensors $U(x_\nu)$, $\nu \in \{1, \ldots, d\} \backslash \{j\}$, except the one for index j. We are going to optimize $U(k_{j-1}, x_j, k_j)$ in an micro-iteration step. We perform this procedure sequentially with $j = 1, \ldots, d$, then we repeat the relaxation procedure in the opposite direction. This scheme has the disadvantage that the ranks r_j. To adapt the individual ranks r_j, we modify the scheme, by concatenating two variables x_j, x_{j+1} into one (x_j, x_{j+1}), and searching for an optimized component $W(k_{j-1}, x_j, x_{j+1}, k_{j+1})$. In a decimation step we approximate $\mathbf{W}(x_j, x_{j+1}) = \mathbf{U}_j(x_j)\mathbf{V}_j(x_{j+1})$ by low rank, e.g. by

means of SVD, up to a tolerance ϵ_j. We keep $\mathbf{U}_j$ and proceed by computing $\mathbf{W}(x_{j+1}, x_{j+2})$ next.

The basic equation for a quantitative description of atomic and molecular physics is the *electronic Schrödinger equation* [He],

$$H\,\Psi \;=\; -\frac{1}{2}\sum_i \Delta_i \;-\; \sum_i^N \sum_{\nu=1}^K \frac{Z_\nu}{|x_i - a_\nu|} \;+\; \frac{1}{2}\sum_{i\neq j}^N \frac{1}{|x_i - x_j|}\;\Psi = E\Psi\ .$$

It describes the stationary and non-relativistic behavior of an ensemble of N electron exposed to an electric Coulomb field given by fixed nuclei. A quantity of major interest is the ground state energy of a given N-electron system, which is the eigenvalue E of the lowest eigenstate Ψ of the Schrödinger-Hamilton operator H. Since the corresponding wave function Ψ depends on at least $3N$ spatial variables, its numerical approximation is a rather difficult and challenging task. The electrons are Fermions, hence, their wavefunction Ψ obeys the *Pauli antisymmetry principle*, i.e. it must be antisymmetric with respect of permutation of particle variables $\mathbf{x}_i, s_i$, $\mathbf{x}_i \in \mathbb{R}^3, s_i = \pm\frac{1}{2}$, $i = 1, \ldots, N$. The hierarchical tensor formats introduced in [HT, TT] are sensitive w.r.t. permutation of variables. Therefore they are not appropriate for approximation of Ψ in their present form. We pursue an alternativ way [HRS-1], using the discrete Fock space $\mathcal{F}$ built by all Slater determinants

$$\Psi_{SL}[k_1, \ldots, k_N](\mathbf{x}_1, s_1; \ldots; \mathbf{x}_N, s_N) \quad := \quad \frac{1}{\sqrt{N!}}\det(\varphi_{k_i}(\mathbf{x}_j, s_j))_{i,j=1}^N$$

to a given orthonormal basis set $\{\varphi_i : i = 1, \ldots, d\}$ and $\mathcal{X}_h := \text{span}\,\{\varphi_i\}$,

$$\mathcal{F} := \bigoplus_{N=1}^d \mathcal{V}_{FCI}^N = \bigoplus_{N=1}^d \bigwedge_{i=1}^N \mathcal{X}_h == \{\Psi : \Psi = \sum_\mu c_\mu \Psi_\mu\}\ .$$

Labeling of indices $\mu \in \mathcal{I}$ by an binary string of length d [He]

$$\text{e.g.:}\;\; \mu \;\; = \;\; (0,0,1,1,0,\ldots) =: \sum_{i=0}^{d-1} \mu_i 2^i\ ,\ \mu_i = 0,1\ ,$$

- $\mu_i = 1$ means φ_i is (occupied) in $\Psi[\ldots]$.
- $\mu_i = 0$ means φ_i is absend (not occupied) in $\Psi[\ldots]$.

yields that the discrete Fock space could be parametrized by tensors

$$\mathcal{F} \simeq \{\mathbf{c} : \mu \mapsto \mathbf{c}(\mu_0, \ldots, \mu_{d-1}) = c_\mu\ ,\ \mu_i = 0,1\ \} = \bigotimes_{i=1}^d \mathbb{R}^2$$

With the aid of the 2×2 matrices

$$A := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\ ,\ A^T = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\ ,\ S := \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\ , I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\ ,$$

we can reformulate the calculus of second quantization introducing discrete creation (annihilation) operators

$$a_p^{(\dagger)} \simeq \mathbf{A}_p^{(T)} := I \otimes \ldots \otimes A_{(p)}^{(T)} \otimes S \otimes \ldots \otimes S$$

where $A_{(p)}$ means that A appears on the p-th position in the product.

The discrete (full CI) Schrödinger equation is casted into the variational form [HRS-1].

$$\boxed{\mathbf{c} = (c(\mu)) = \operatorname{argmin}\{\langle \mathbf{Hc}, \mathbf{c}\rangle : \langle \mathbf{c}, \mathbf{c}\rangle = 1 \ , \ \mathbf{Pc} = N\mathbf{c}\} \ .}$$

With the discrete Hamiltonian $\mathbf{H}$ and particle number operator $\mathbf{P} = \sum_{p,q=1}^{d} \mathbf{A}_p^T \mathbf{A}_q$,

$$\mathbf{H} = \sum_{p,q=1}^{d} h_p^q \mathbf{A}_p^T \mathbf{A}_q + \sum_{p,q,r,s=1}^{d} g_{r,s}^{p,q} \mathbf{A}_r^T \mathbf{A}_s^T \mathbf{A}_p \mathbf{A}_q \ .$$

where h_p^q and $g_{r,s}^{p,q}$ denote the well known one and two electron integrals,

$$h_q^p := \langle \varphi_q, (\frac{-1}{2}\Delta - V_{core})\varphi_p \rangle \ , \ g_{r,s}^{p,q} := \frac{1}{2}\langle \varphi_r(\mathbf{x}, s_1)\varphi_s(\mathbf{y}, s_2), \frac{\varphi_p(\mathbf{x}, s_1)\varphi_q(\mathbf{y}, s_2)}{|\mathbf{x} - \mathbf{y}|} \rangle \ ,$$

the tensorized problem can be tackled by recent tensor product approximation techniques, e.g. the TT-format and the introduced relaxation method. The modified relaxation method applied to this problem resembles exactly the DMRG (density matrix renormalization group) method introduced in [SW] for spin chains.

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Sparse Tensor Discretizations of PDEs with Stochastic Data

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(joint work with Albert Cohen, Ronald DeVore, Viet Ha Hoang)

We present recent results on the regularity, on the best N-term approximation and on numerical solution algorithms for PDEs which depend on a vector y of possibly countably many parameters $(y_j)_{j\geq 1}$. In a bounded Lipschitz domain $D \subset \mathbb{R}^d$, we study the parametric, elliptic problem

$$-\mathrm{div}_x(a(x,y)\nabla_x u) = f(x) \quad \text{for} \quad x \in D, \tag{1}$$

and, for $0 \leq t \leq T$ and for $x \in D$, its parabolic analog

$$u_t - \mathrm{div}_x(a(x,y)\nabla_x u) = f(x) \quad u|_{t=0} = u_0, \tag{2}$$

and the corresponding parametric wave equation

$$u_{tt} - \mathrm{div}_x(a(x,y)\nabla_x u) = f(x)\ , \quad u|_{t=0} = u_0, \quad u_t|_{t=0} = u_1\ . \tag{3}$$

For simplicity, we consider homogeneous Dirichlet boundary conditions $u|_{\partial D} = 0$. Here, $D \subset \mathbb{R}^d$ is a bounded Lipschitz domain and the diffusion coefficient $a(x,y)$ depends on the parameter vector $y \in U := [-1,1]^{\mathbb{N}}$ in an affine manner

$$a(x,y) = \bar{a}(x) + \sum_{j=1}^{\infty} y_j \psi_j(x), \tag{4}$$

where $\psi_j \in L^\infty(D)$. Such coefficients arise, for example, in the parametric expansion of random diffusion coefficients by Karhúnen-Loève expansions. We impose the uniform ellipticity assumption UEA(r,R)

$$0 < r \leq a(x,y) \leq R < \infty, \quad x \in D, \quad y \in U \tag{5}$$

which implies, in particular, that $(\|\psi_j\|_{L^\infty(D)})_{j\geq 1} \in \ell^1(\mathbb{N})$. Under UEA$(r,R)$, for every $y \in U$ there exist unique solutions $u(\cdot,y) \in V$ where $V := H^1_0(D)$ for (1), and, for (2), (3), V is a suitable Bochner space, such as $L^2(0,T;H^1_0(D)) \cap H^1(0,T;H^{-1}(D))$ for (2).

We are interested in the numerical approximation of (1), (2) and (3) on the infinite-dimensional parameter space U. To this end, we show that the solution map $U \ni y \to u(\cdot;y) \in V$ is measurable, as a map from the measurable space $(U,\mu(dy))$ (with $\mu(dy) = \otimes_{j\geq 1}\frac{dy_j}{2}$ denoting the uniform probability measure on U) into V and, moreover, that is it *analytic* as a V-valued function of y, with precise estimates on the size of the analyticity domains in terms of the $\|\psi_j\|_{L^\infty(D)}$.

Under UEA(r,R), the parametric solution $u(\cdot,y)$ admits, as V-valued function, unconditionally convergent series expansions into several function systems in the infinite-dimensional parameter domain U. For example, we show in [CDS1, CDS2, HS1, HS2] that $u(\cdot,y)$ admits a Legendre expansion

$$u(\cdot,y) = \sum_{\nu\in\mathcal{F}} u_\nu(\cdot) L_\nu(u), \quad u_\nu(\cdot) := \int_U u(\cdot,y) L_\nu(y) d\mu(y) \in V \tag{6}$$

where the set $\mathcal{F} = \{\nu \in \mathbb{N}_0^{\mathbb{N}} : |\nu|_1 < \infty\}$ of "finitely supported" multiindices denotes all sequences of nonnegative integers with finitely many nonzero entries. In (6), the tensorized Legendre polynomials $L_\nu(y)$ are defined as

$$\forall \nu \in \mathcal{F}: \qquad L_\nu(y) := \prod_{j\geq 1} L_{\nu_j}(y_j) \tag{7}$$

with $L_n(t)$ denoting the Legendre polynomial of degree $n \in \mathbb{N}_0$ on $(-1,1)$ with normalization $\int_{-1}^{1} L_n(t)\frac{dt}{2} = 1$. The series (6) converges unconditionally in the Bochner space $L^2(U,\mu(dy);V)$. Our main results in [CDS2, HS1, HS2] quantify sparsity of the coefficient sequence $(u_\nu)_{\nu\in\mathcal{F}}$ in the Legendre expansion (6) in terms of the p-summability of the sequence $\|\psi_j\|_{L^\infty(D)}$:

Theorem 1. *Assume $(UEA)(r,R)$ and that for some $0 < p \leq 1$,*

$$\sum_{j\geq 1} \|\psi_j\|_{L^\infty(D)}^p < \infty \tag{8}$$

Then $(\|u_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F})$ for the same value of p as in (8).

Thus, the sequence of Legendre coefficients of the polynomial chaos type expansion (6) of the parametric solution $u(\cdot,y)$ on the infinite dimensional parameter space U inherits exactly the sparsity of the input's coefficient function sequence ψ_j. There are two proofs of Theorem 1: in [CDS1], analyticity was quantified by estimates on the growth of derivatives of the solution w.r. to y_j, whereas in [CDS2, HS1, HS2], analyticity was quantified by a continuation argument and p-summability was shown to follow from derivative-free estimates on the Legendre coefficients $u_\nu(\cdot)$ by Cauchy's integral formula.

The p-summability of $(\|u_\nu\|_V)_{\nu\in\mathcal{F}}$ in Theorem 1 immediately implies, via a classical argument due to Stechkin (see, e.g., [DeV] and the references there) that the map $U \ni y \to u(\cdot,y) \in V$ can be approximated as follows.

Theorem 2. *If $(\|\psi_j\|_{L^\infty(D)})_{j\geq 1} \in \ell^p(\mathbb{N})$, then for every $N \in \mathbb{N}$ there exists an index set $\Lambda_N^* \subset \mathcal{F}$ of cardinality not exceeding N such that the N-term approximation converges with rate $r := 1/p - 1/2 \geq 1/2$, i.e. for all N it holds*

$$\|u - \sum_{\nu\in\Lambda_N^*} u_\nu L_\nu\|_{L^2(U,\mu(dy);V)} \leq \|(\|u_\nu\|_V)\|_{\ell^p(\mathcal{F})}\, N^{-(1/p-1/2)} \tag{9}$$

This result is to be contrasted with the rate $N^{-1/2}$ obtained, for example, by Monte-Carlo (MC) sampling the parametric problems at N points in U with respect to the probability measure $\mu(dy)$: if the coeffiecient sequence is p-summable with exponent $p = 1$ (which is a minimal necessary condition for UEA(r,R) to hold and, hence, for well-posedness of the parametric problems), N term truncated polynomial chaos type expansions yield the same convergence rate as MC sampling, at the expense of N coefficient functions in V to be determined. Theorem 2 indicates, however, that as soon as the sequence $(\|\psi_j\|_{L^\infty(D)})_{j\geq 1} \in \ell^p(\mathbb{N})$ with $p < 1$, the polynomial chaos type N-term approximations offer the rate $r = 1/p - 1/2 > 1/2$.

In the recent papers [CDS1, CDS2, HS1, HS2], we also obtained apriori estimates for $\|(\|u_\nu\|_V)\|_{\ell^p(\mathcal{F})}$ in terms of $\big\|(\|\psi_j\|_{L^\infty(D)})_{j\geq 1}\big\|_{\ell^p(\mathbb{N})}$. We remark that earlier results [TS] showed even superalgebraic N-term convergence rates of Taylor expansions of $u(\cdot,y)$ about $y=0\in U$, albeit under the substantially stronger assumption of *exponential decay* of $(\|\psi_j\|_{L^\infty(D)})_{j\geq 1}$. These results open the perspective of efficient numerical approximations of solutions to the parametric problems (1), (2), (3) on the infinte dimensional parameter space U. In [CDS1, CDS2], results analogous to (9) were also obtained for *best N-term Taylor expansions* of $U\ni y\to u(\cdot,y)\in V$ about $y=0\in U$ (see the abstract of A. Cohen in this volume for a statement of these results).

To develop viable numerical algorithms, two additional questions must be addressed: first, the localization of (sequences of) (near) optimal index sets $\Lambda_N\subset\mathcal{F}$ of cardinality not exceeding N and, second, the numerical approximation of the "active" coefficients u_ν, $\nu\in\Lambda_N$. The first question allows several answers: based on the sharp apriori estimates of the Legendre coefficients u_ν in (6), in [ABS], under the assumption of monotonic decay of the fluctuation sequence $\|\psi_j\|_{L^\infty(D)}$ an algorithm was proposed for the *apriori localization of index sets Λ_N of cardinality not exceeding N* with log-linear complexity in $\#(\Lambda_N)$ such that Galerkin projections of the parametric solutions in $L^2(U,\mu(dy);V)$ onto truncated Legendre expansions achieve the optimal rate r (see also [Acta]). A second approach which yields quasi optimal index sequences $(\Lambda_N)_{N\geq 1}\subset\mathcal{F}$ is based on variants of the bulk-chasing algorithms which were developed in the context of adaptive Finite Element Methods (FEM). This is subject of current research.

Finally, the *discretization of the "active" coefficients u_ν, $\nu\in\Lambda_N$*, from a dense, one-parameter family $(V_h)_{h>0}\subset V$ with $\dim V_h<\infty$ is considered. If $(V_h)_{h>0}$ is *hierarchic* (as is the case with e.g. FEM on nested families of triangulations, wavelets, spectral methods or *hp*-FEM) with approximation rate $t>0$ for solutions u belonging to a smoothness space $W\subset V$ (as, e.g., $W=(H^2\cap H^1_0)(D)$), i.e. $\inf_{v\in V_h}\|u-v\|_V\leq CM^{-t}$ for $M=\dim(V_h)\to\infty$, we show in [CDS2] that for the sequence $(\Lambda_N^*)_{N\geq 1}$ of optimal active coefficients u_ν, there exists a sequence $(h_\nu)_{\nu\in\Lambda_N^*}$ of discretization parameters such that the corresponding sparse tensor approximations satisfy

$$\|u-\sum_{\nu\in\Lambda_N^*}u_{\nu,h_\nu}\|_{L^2(U,\mu(dy);V)}\leq CN_{tot}^{-\min\{r,t\}} \tag{10}$$

where $N_{tot}=\sum_{\nu\in\Lambda_N^*}\dim(V_{h_\nu})$ denotes the total number of degrees of freedom. The estimate (10) requires the regularity $(\|u_\nu\|_W)_{\nu\in\mathcal{F}}\in\ell^p(\mathcal{F})$ for the same value of p as in Theorem 2 for (1), (2), (3) (see [CDS2, HS1, HS2]).

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Adaptive Wavelet Schemes for Evolution Problems

Rob Stevenson
(joint work with Christoph Schwab, Nabi Chegini)

This talk will be concerned with the numerical solution of linear evolution equations, in particular parabolic equations. In general, even for a smooth source term and initial condition, the solution of such a problem has a reduced smoothness near the bottom and walls of the space-time cylinder. As a consequence, standard discretization methods based on uniform meshes will converge at reduced rates.

A general approach to retrieve the best possible rate allowed by the order of the discretization is to apply *adaptive* methods. Standard methods for solving time evolution problems first discretize in space and then in time (method of lines), or first in time and then in space (Rothe's method). As a consequence, with these time marching methods it seems hard to be able to arrive at an optimal distribution of the "mesh-points" or degrees of freedom simultaneously over space *and* time.

Therefore, we consider a simultaneous space-time variational formulation of the parabolic problem. This formulation is well-posed in the sense that it defines a boundedly invertible operator between a Hilbert space and the dual of another Hilbert space. We equip both Hilbert spaces – being Bochner spaces or intersections of those – by Riesz bases that are tensor products of temporal and spatial wavelet bases. In this way, we arrive at an equivalent, well-posed bi-infinite matrix vector problem. We solve this problem with an *adaptive wavelet method* applied to the *normal equations*.

The advantages of our approach are two-fold: Firstly, thanks to the tensor-product construction of the basis, there is a nearly neglectable penalty in asymptotic computational complexity due to the additional time dimension, an effect that is well-known for so-called *sparse-grid* or *hyperbolic cross* approximation methods. Secondly, the adaptive wavelet method is proven to converge at the best possible rate, in linear complexity.

Our approach was investigated earlier in [SS09], and on a more heuristical level, in [GO07]. Compared to the first work, here we introduce an alternative variational formulation in which the initial condition is incorporated more naturally. Furthermore, we design a new wavelet basis with respect to which any parabolic differential operator of second order with constant coefficient gives rise to a bi-infinite system matrix that is *truly sparse*. Having such a matrix largely simplifies the implementation and improves the quantitative properties of the adaptive wavelet method. We present numerical results for an ordinary differential equation and for the heat equation.

Finally, we will show that the instationary Stokes equations can also be given a well-posed space-time variational formulation, so that our approach applies to these equations as well.

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Existence and Equilibration of Global Weak Solutions to Kinetic Models of Dilute Polymers

Endre Süli

(joint work with John W. Barrett)

We show the existence of global-in-time weak solutions to a general class of coupled FENE-type bead-spring chain models that arise from the kinetic theory of dilute solutions of polymeric liquids with noninteracting polymer chains. The class of models involves the unsteady incompressible Navier–Stokes equations in a bounded open Lipschitz domain Ω in $\mathbb{R}^d$, $d = 2$ or 3, for the velocity $\underset{\sim}{u}$ and the pressure p of the fluid, with the divergence of the elastic extra-stress tensor $\underset{\approx}{\tau}$ appearing on the right-hand side of the Navier–Stokes momentum equation. Let k denote the product of the Boltzmann constant and the absolute temperature. The extra-stress tensor $\underset{\approx}{\tau}$ stems from the random movement of the polymer chains and is defined by the Kramers expression

$$\underset{\approx}{\tau}(\underset{\sim}{x},t) = k\left(\sum_{i=1}^{K}\int_D \psi(\underset{\sim}{x},\underset{\sim}{q},t)\,\underset{\sim}{q}_i\,\underset{\sim}{q}_i^{\mathrm{T}}\,U_i'\left(\tfrac{1}{2}|\underset{\sim}{q}_i|^2\right)\,\mathrm{d}\underset{\sim}{q} - \int_D \psi(\underset{\sim}{x},\underset{\sim}{q},t)\,\underset{\approx}{I}\,\mathrm{d}\underset{\sim}{q}\right),$$

through the associated probability density function $(\underset{\sim}{x},\underset{\sim}{q},t) \in \Omega\times D\times[0,T] \mapsto \psi(\underset{\sim}{x},\underset{\sim}{q},t) \mapsto \mathbb{R}_{\geq 0}$ that satisfies a Fokker–Planck-type parabolic equation on $\Omega \times D \times [0,T]$, a crucial feature of which is the presence of a center-of-mass diffusion term, with diffusion coefficient $\varepsilon > 0$. Here $D := D_1 \times \cdots \times D_K$ is the configuration

space, defined as the Cartesian product of D_i, $i = 1, \ldots, K$, where each D_i is a bounded open ball of radius $\sqrt{b_i}$, with $b_i > 2$, centred at the origin $\underset{\sim}{0} \in \mathbb{R}^d$.

We require no structural assumptions on the drag term in the Fokker–Planck equation; in particular, the drag term need not be corotational. With a square-integrable and divergence-free initial velocity datum $\underset{\sim}{u}_0$ for the Navier–Stokes equation and a nonnegative initial probability density function ψ_0 for the Fokker–Planck equation, which has finite relative entropy with respect to the Maxwellian M, we prove the existence of a global-in-time weak solution $t \mapsto (\underset{\sim}{u}(t), \psi(t))$ to the coupled Navier–Stokes–Fokker–Planck system, satisfying the initial condition $(\underset{\sim}{u}(0), \psi(0)) = (\underset{\sim}{u}_0, \psi_0)$, such that $t \mapsto \underset{\sim}{u}(t)$ belongs to the classical Leray space and $t \mapsto \psi(t)$ has bounded relative entropy with respect to M and $t \mapsto \psi(t)/M$ has integrable Fisher information (w.r.t. the measure $\mathrm{d}\nu := M(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}$) over any time interval $[0, T]$, $T > 0$. If the density of body forces $\underset{\sim}{f}$ on the right-hand side of the Navier–Stokes momentum equation vanishes, then $t \mapsto (\underset{\sim}{u}(t), \psi(t))$ decays exponentially in time to $(\underset{\sim}{0}, M)$ in the $\underset{\sim}{L}^2 \times L^1$ norm, at a rate that is independent of $(\underset{\sim}{u}_0, \psi_0)$ and of ε. The precise statements of these results are given below.

Let $\mathcal{O}_i \subset [0, \infty)$ denote the image of D_i under the mapping $\underset{\sim}{q}_i \in D_i \mapsto \frac{1}{2}|\underset{\sim}{q}_i|^2$, and consider the *spring-potential* $U_i \in C^2(\mathcal{O}_i; \mathbb{R}_{\geq 0})$, $i = 1, \ldots, K$. Clearly, $\mathcal{O}_i = \left[0, \frac{b_i}{2}\right)$. We shall suppose that $U_i(0) = 0$ and that U_i is monotonic increasing and unbounded on $\mathcal{O}_i$ for each $i = 1, \ldots, K$. The elastic spring-force $\underset{\sim}{F}_i : D_i \subseteq \mathbb{R}^d \to \mathbb{R}^d$ of the ith spring in the chain is defined by $\underset{\sim}{F}_i(\underset{\sim}{q}_i) = U_i'(\frac{1}{2}|\underset{\sim}{q}_i|^2)\,\underset{\sim}{q}_i$, $i = 1, \ldots, K$.

We shall further suppose that for $i = 1, \ldots, K$ there exist constants $c_{ij} > 0$, $j = 1, 2, 3, 4$, and $\gamma_i > 1$ such that the (normalized) Maxwellian M_i, defined by

$$M_i(\underset{\sim}{q}_i) = \frac{1}{\mathcal{Z}_i} \mathrm{e}^{-U_i(\frac{1}{2}|\underset{\sim}{q}_i|^2)}, \qquad \mathcal{Z}_i := \int_{D_i} \mathrm{e}^{-U_i(\frac{1}{2}|\underset{\sim}{q}_i|^2)}\,\mathrm{d}\underset{\sim}{q}_i\,,$$

and the associated spring potential U_i satisfy

$$\text{(1a)} \qquad c_{i1}\,[\mathrm{dist}(\underset{\sim}{q}_i, \partial D_i)]^{\gamma_i} \leq M_i(\underset{\sim}{q}_i) \leq c_{i2}\,[\mathrm{dist}(\underset{\sim}{q}_i, \partial D_i)]^{\gamma_i} \quad \forall \underset{\sim}{q}_i \in D_i,$$

$$\text{(1b)} \qquad c_{i3} \leq [\mathrm{dist}(\underset{\sim}{q}_i, \partial D_i)]\,U_i'(\tfrac{1}{2}|\underset{\sim}{q}_i|^2) \leq c_{i4} \quad \forall \underset{\sim}{q}_i \in D_i.$$

The Maxwellian in the model is then defined by $M(\underset{\sim}{q}) := \prod_{i=1}^K M_i(\underset{\sim}{q}_i)$ where $\underset{\sim}{q} := (\underset{\sim}{q}_1, \ldots, \underset{\sim}{q}_K) \in D$. Let $\underset{\sim}{H}$ and $\underset{\sim}{V}_\sigma$ denote, respectively, the closure of divergence-free d-component $\underset{\sim}{C}_0^\infty(\Omega)$ functions in the norm of $\underset{\sim}{L}^2(\Omega)$ and $\underset{\sim}{H}^\sigma(\Omega) \cap \underset{\sim}{H}_0^1(\Omega)$, $\sigma \geq 1$. When $\sigma = 1$, we write $\underset{\sim}{V}$ instead of $\underset{\sim}{V}_1$. For a function space X, X' will denote the dual space of X and $\langle \cdot, \cdot \rangle_X$ the duality pairing between X' and X.

Let $\mathcal{F}(s) := s(\log s - 1) + 1$, $s > 0$; and $\mathcal{F}(0) := 1$. We adopt the notation $\widehat{\psi} := \psi/M$, and introduce the following assumptions on the data:

$$\begin{aligned} &\partial\Omega \in C^{0,1}; \quad \underset{\sim}{u}_0 \in \underset{\sim}{H}; \quad \widehat{\psi}_0 := \frac{\psi_0}{M} \geq 0 \ \text{ a.e. on } \Omega \times D \quad \text{with} \\ &\mathcal{F}(\widehat{\psi}_0) \in L^1_M(\Omega \times D) \quad \text{and} \quad \int_D M(\underset{\sim}{q})\,\widehat{\psi}_0(\underset{\sim}{x}, \underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q} = 1 \quad \text{for a.e. } \underset{\sim}{x} \in \Omega; \\ &\gamma_i > 1, \quad i = 1, \ldots, K \quad \text{in (1a,b)}; \quad \text{and} \quad \underset{\sim}{f} \in L^2(0, T; \underset{\sim}{V}'). \end{aligned} \tag{2}$$

Here, $L^p_M(\Omega \times D)$, for $p \in [1, \infty)$, denotes the Maxwellian-weighted L^p space over $\Omega \times D$ with norm

$$\|\widehat{\varphi}\|_{L^p_M(\Omega\times D)} := \left\{ \int_{\Omega\times D} M\, |\widehat{\varphi}(\underset{\sim}{x}, \underset{\sim}{q})|^p \, \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x} \right\}^{\frac{1}{p}}.$$

Theorem 1. *Let the assumptions* (2) *hold. Then, there exists a pair of functions* $(\underset{\sim}{u}, \widehat{\psi})$ *such that*

$$\underset{\sim}{u} \in L^\infty(0,T;\underset{\sim}{L}^2(\Omega)) \cap L^2(0,T;\underset{\sim}{V}) \cap H^1(0,T;\underset{\sim}{V}'_\sigma), \quad \sigma \geq \tfrac{1}{2}d,\ \sigma > 1,$$

and

$$\widehat{\psi} \in L^1(0,T;L^1_M(\Omega\times D)) \cap H^1(0,T;M^{-1}H^s(\Omega\times D)'), \quad s > 1 + \tfrac{1}{2}(K+1)d,$$

with $\widehat{\psi} \geq 0$ *a.e. on* $\Omega \times D \times [0,T]$,

$$\int_D M(\underset{\sim}{q})\, \widehat{\psi}(\underset{\sim}{x}, \underset{\sim}{q}, t)\, \mathrm{d}\underset{\sim}{q} = 1 \quad \textit{for a.e. } (x,t) \in \Omega \times [0,T],$$

whereby $\widehat{\psi} \in L^\infty(0,T;L^1_M(\Omega\times D))$*; and finite relative entropy and Fisher information, i.e.,*

$$\mathcal{F}(\widehat{\psi}) \in L^\infty(0,T;L^1_M(\Omega\times D)) \quad \textit{and} \quad \sqrt{\widehat{\psi}} \in L^2(0,T;H^1_M(\Omega\times D));$$

such that the pair of functions $(\underset{\sim}{u}, \widehat{\psi})$ *is a global weak solution to the Navier–Stokes–Fokker–Planck system in the sense that, for all* $\underset{\sim}{w} \in L^2(0,T;\underset{\sim}{V}_\sigma)$,

$$\int_0^T \left\langle \frac{\partial \underset{\sim}{u}}{\partial t}, \underset{\sim}{w} \right\rangle_{V_\sigma} \mathrm{d}t + \int_0^T \int_\Omega \left[\left[(\underset{\sim}{u} \cdot \underset{\sim}{\nabla}_x) \underset{\sim}{u} \right] \cdot \underset{\sim}{w} + \nu \underset{\approx}{\nabla}_x \underset{\sim}{u} : \underset{\approx}{\nabla}_x \underset{\sim}{w} \right] \mathrm{d}\underset{\sim}{x}\, \mathrm{d}t$$
$$= \int_0^T \left[\langle \underset{\sim}{f}, \underset{\sim}{w} \rangle_V - k \sum_{i=1}^K \int_\Omega \underset{\approx}{C}_i (M\, \widehat{\psi}) : \underset{\approx}{\nabla}_x \underset{\sim}{w}\, \mathrm{d}\underset{\sim}{x} \right] \mathrm{d}t,$$

where $\nu > 0$ *is the kinematic viscosity and* $\underset{\sim}{f}$ *the density of body forces; and, for all* $\widehat{\varphi} \in L^2(0,T;H^s(\Omega\times D))$,

$$\int_0^T \left\langle M \frac{\partial \widehat{\psi}}{\partial t}, \widehat{\varphi} \right\rangle_{H^s(\Omega\times D)} \mathrm{d}t + \int_0^T \int_{\Omega\times D} M \left[\varepsilon \underset{\sim}{\nabla}_x \widehat{\psi} - \underset{\sim}{u}\, \widehat{\psi} \right] \cdot \underset{\sim}{\nabla}_x \widehat{\varphi}\, \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x}\, \mathrm{d}t$$
$$+ \frac{1}{2\lambda} \int_0^T \int_{\Omega\times D} M \sum_{i=1}^K \sum_{j=1}^K A_{ij}\, \underset{\sim}{\nabla}_{q_j} \widehat{\psi} \cdot \underset{\sim}{\nabla}_{q_i} \widehat{\varphi}\, \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x}\, \mathrm{d}t$$
$$- \int_0^T \int_{\Omega\times D} M \sum_{i=1}^K [(\underset{\approx}{\nabla}_x \underset{\sim}{u})\, \underset{\sim}{q}_i]\, \widehat{\psi} \cdot \underset{\sim}{\nabla}_{q_i} \widehat{\varphi}\, \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x}\, \mathrm{d}t = 0.$$

Here, $\lambda > 0$ *is the Weissenberg number and* $(A_{ij})_{i,j=1}^K$ *the symmetric positive definite Rouse matrix. The initial conditions* $\underset{\sim}{u}(\cdot,0) = \underset{\sim}{u}_0(\cdot)$ *and* $\widehat{\psi}(\cdot,\cdot,0) = \widehat{\psi}_0(\cdot,\cdot)$ *are satisfied in the sense of weakly continuous functions, in the function spaces* $C_w([0,T];\underset{\sim}{H})$ *and* $C_w([0,T];L^1_M(\Omega\times D))$*, respectively.*

The weak solution $(\underset{\sim}{u}, \widehat{\psi})$ *satisfies the following energy inequality for* $t \in [0,T]$*:*

$$\|\underset{\sim}{u}(t)\|^2_{L^2(\Omega)} + \nu \int_0^t \|\underset{\approx}{\nabla}_x \underset{\sim}{u}(s)\|^2_{L^2(\Omega)}\,\mathrm{d}s + 2k \int_{\Omega\times D} M\mathcal{F}(\widehat{\psi}(t))\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}$$
$$+ 8k\,\varepsilon \int_0^t \int_{\Omega\times D} M|\underset{\sim}{\nabla}_x \sqrt{\widehat{\psi}}|^2\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\,\mathrm{d}s + \frac{2a_0 k}{\lambda}\int_0^t \int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_q \sqrt{\widehat{\psi}}|^2\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\,\mathrm{d}s$$
$$\leq \|\underset{\sim}{u}_0\|^2_{L^2(\Omega)} + \frac{1}{\nu}\int_0^t \|\underset{\sim}{f}(s)\|^2_{V'}\,\mathrm{d}s + 2k\int_{\Omega\times D} M\mathcal{F}(\widehat{\psi}_0)\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}.$$

Theorem 2. *Let the assumptions of Theorem 1 hold and let* M *satisfy the Bakry–Émery condition; i.e. there exists* $\kappa > 0$ *such that* $\mathsf{Hessian}(-\log M(\underset{\sim}{q})) \geq \kappa\,\mathsf{Id}$*, in the sense of symmetric* $Kd \times Kd$ *matrices, on* D*. Then, for any* $T > 0$*,*

$$\|\underset{\sim}{u}(T)\|^2_{L^2(\Omega)} + \frac{k}{|\Omega|}\|\widehat{\psi}(T) - 1\|^2_{L^1_M(\Omega\times D)}$$
$$\leq \mathrm{e}^{-\gamma_0 T}\left[\|\underset{\sim}{u}_0\|^2_{L^2(\Omega)} + 2k\int_{\Omega\times D} M\mathcal{F}(\widehat{\psi}_0)\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right] + \frac{1}{\nu}\int_0^T \|\underset{\sim}{f}\|^2_{V'}\,\mathrm{d}s,$$

where $\gamma_0 := \min\left(\frac{\nu}{C_{\mathsf{P}}^2}, \frac{\kappa\,a_0}{2\lambda}\right)$ *and* C_{P} *is the constant in the Poincaré inequality* $\|\underset{\sim}{w}\|_{L^2(\Omega)} \leq C_{\mathsf{P}}\|\underset{\approx}{\nabla}_x \underset{\sim}{w}\|_{L^2(\Omega)}$*,* $\underset{\sim}{w} \in \underset{\sim}{V}$*. In particular if* $\underset{\sim}{f} \equiv \underset{\sim}{0}$ *then*

$$\|\underset{\sim}{u}(T)\|^2_{L^2(\Omega)} + \frac{k}{|\Omega|}\|\widehat{\psi}(T) - 1\|^2_{L^1_M(\Omega\times D)} \leq \mathrm{e}^{-\gamma_0 T}\left[\|\underset{\sim}{u}_0\|^2_{L^2(\Omega)} + 2k\int_{\Omega\times D} M\mathcal{F}(\widehat{\psi}_0)\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right].$$

The FENE potential $U_i(s) = -\frac{b_i}{2}\log\left(1 - \frac{2s}{b_i}\right)$, $s \in \mathcal{O}_i := \left[0, \frac{b_i}{2}\right)$, $b_i > 2$, $i = 1, \ldots, K$, satisfies the hypotheses of the two theorems above. For further details, we refer to [BS2010]. In the case of Hookean-type springs existence and decay results analogous to Theorems 1 and 2 above hold. The numerical approximation of these high-dimensional problems is the subject of ongoing research.

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Multiscale Solutions in Critical Spaces: A Constructive Proof of the Closed Range Theorem

Eitan Tadmor

We begin with a prototype example. Let $L^d_{\#}(\mathbb{T}^d)$ denote the Lebesgue space of periodic functions with zero mean over the d-dimensional torus $\mathbb{T}^d$. Given $f \in L^d_{\#}(\mathbb{T}^d)$, we seek a uniformly bounded solution, $U \in L^\infty(\mathbb{T}^d, \mathbb{R}^d)$, of the problem

$$div\, U = f, \qquad U \in L^\infty(\mathbb{T}^d, \mathbb{R}^d). \tag{1a}$$

A classical solution is given by $U = \nabla\Delta^{-1}f$, which in addition to (1a), satisfies the irotationality constraint,

$$curl\, U = 0. \tag{1b}$$

Clearly, this solution lies in $W^1(L^d_\#)$. But since $W^1(L^d_\#)$ is *not contained* in L^∞, the solution may — and in fact does fail to satisfy the uniform bound sought for the solution of (1a). Thus, the question is whether (1a) admits a uniformly bounded solution by giving up on the additional constraint of irotationality (1b). The existence of such solutions was proved by Bourgain and Brezis, [BB03, Proposition 1] using a straightforward but non-constructive duality argument based on the closed range theorem. We present here another duality-based approach for the existence of such solutions. Our approach is *constructive*: the solution U is constructed as the sum, $U = \sum \mathbf{u}_j$, where the $\{\mathbf{u}_j\}$'s are computed *recursively* as appropriate minimizers,

$$\mathbf{u}_{j+1} = \underset{\mathbf{u}}{arg\,min} \left\{ \|\mathbf{u}\|_{L^\infty} + \lambda_1 2^j \big\| f - div\,\big(\sum_{k=1}^{j} \mathbf{u}_k\big) - div\,\mathbf{u} \big\|^d_{L^d} \right\}, \quad j = 0, 1, \ldots,$$

and λ_1 is a sufficiently large parameter specified below.

This construction is in fact a special case of our main result which applies to general linear problems of the form

$$\mathcal{L}U = f, \quad f \in L^p_\#(\Omega), \quad \Omega \subset \mathbb{R}^d,\ 1 < p < \infty. \tag{2}$$

Here, $\mathcal{L} : \mathbb{B} \mapsto L^p_\#(\Omega)$ is a linear operator densely defined on a Banach space $\mathbb{B}$ with a closed range in $L^p_\#(\Omega)$. The subscript $\{\cdot\}_\#$ indicates an appropriate subspace, $L^p_\#(\Omega) = L^p(\Omega) \cap \mathrm{Ker}(\mathcal{P})$. Here, $\mathcal{P} : L^p \mapsto L^p$ is a linear operator whose null is "compatible" with the range of $\mathcal{L}$ so that the dual of $\mathcal{L}$ is injective, namely, there exists $\beta > 0$ such that

$$\|g - \mathcal{P}^* g\|_{L^{p'}} \le \beta \|\mathcal{L}^* g\|_{\mathbb{B}^*}, \qquad \forall g \in L^{p'}(\Omega). \tag{3}$$

The closed range theorem combined with the open mapping principle tell us that equation (2) has a bounded solution, $U \in \mathbb{B}$. Our main result [Ta10] is a constructive proof for the existence of such solutions in this setup.

Theorem 1. *Assume that the apriori estimate* (3) *holds. Then, for any given* $f \in L^p_\#(\Omega), 1 < p < \infty$, *equation* (2) *admits a solution of the form* $U = \sum_{j=1}^{\infty} \mathbf{u}_j \in \mathbb{B}$,

$$\|U\|_{\mathbb{B}} \lesssim \beta \|f\|_{L^p}, \tag{4}$$

where the $\{\mathbf{u}_j\}$*'s are constructed recursively as minimizers of*

(5)

$$\mathbf{u}_{j+1} = \underset{\mathbf{u}}{arg\,min} \left\{ \|\mathbf{u}\|_{\mathbb{B}} + \lambda_{j+1} \big\| r_j - \mathcal{L}\mathbf{u} \big\|^p_{L^p} \right\}, \quad r_j := f - \mathcal{L}\big(\sum_{k=1}^{j} \mathbf{u}_k\big), \ \ j = 0, 1, \ldots.$$

Here, $\{\lambda_j\}_{j\geq 1}$ *can be taken as any exponentially increasing sequence,* $\lambda_{j+1} := \lambda_1\zeta^j,\ j=0,1,\ldots$ *with a sufficiency large* $\lambda_1 \gtrsim \dfrac{\beta}{\|f\|_{L^p}^{p-1}}$.

Remark 1. *The description of* U *as the sum* $U=\sum \mathbf{u}_j$ *provides a multiscale* hierarchical decomposition *of a solution for* (2). *The role* $\{\lambda_j\}$*'s as the different scales associated with the* $\mathbf{u}_j$*'s, is realized in terms of the "energy bound"*

$$\sum_{j=1}^{\infty}\frac{1}{\zeta^j}\|\mathbf{u}_j\|_{\mathbb{B}} \lesssim \beta\|f\|_{L^p},\quad f\in L^p_{\#}(\Omega),\qquad \lambda_{j+1}=\lambda_1\zeta^j. \tag{6}$$

Remark 2. *We emphasize that the hierarchical construction* $U=\sum \mathbf{u}_j$ *does* not *require apriori knowledge of the constant* β *appearing in the duality estimate* (3). *If the initial scale* λ_1 *is underestimated then the hierarchical expansion will yield zero hierarchical terms,* $\mathbf{u}_j\equiv 0, j=1,2,\ldots$, *until reaching the critical scale* $\lambda_1 2^{j_0} \gtrsim \beta\|f\|_{L^p}^{1-p}$ *which will dictate the initial non-zero step of the hierarchical decomposition,* $U=\sum_{j=j_0}\mathbf{u}_j$. *The value of a finite* β *is only needed to guarantee that the hierarchical construction will indeed pick up at some finite scale* λ_{j_0}.

Bounded solutions of $div\, U=f\in L^p_{\#}$

Let $\mathcal{P}$ denote the averaging projection, $\mathcal{P}g:=\overline{g}$ where $\overline{g}$ is the average value of g. Given $f\in L^p_{\#}(\mathbb{T}^d):=\big\{g\in L^p(\mathbb{T}^d)\ |\ \overline{g}=0\big\}$, then according to theorem 1, we can construct hierarchical solutions of

$$div\, U=f,\qquad f\in L^p_{\#}(\mathbb{T}^d),\quad 1<p<\infty, \tag{7}$$

in an appropriate Banach space, $U\in\mathbb{B}$, provided the corresponding apriori estimate (3) holds, namely, there exists a constant $\beta>0$ (which may vary of course, depending on p,d and $\mathbb{B}$), such that

$$\|g-\overline{g}\|_{L^{p'}}\leq \beta\|\nabla g\|_{\mathbb{B}^*},\qquad \forall g\in L^{p'}(\mathbb{T}^d). \tag{8}$$

We specify two cases of such relevant $\mathbb{B}$'s.

#1. **Solutions of (7) in** L^{p^*}. By Sobolev inequality

$$\|g-\overline{g}\|_{L^{p'}(\mathbb{T}^d)}\leq\beta\|\nabla g\|_{L^{(p^*)'}(\mathbb{T}^d,\mathbb{R}^d)},\quad \frac{1}{p^*}=\frac{1}{p}-\frac{1}{d},\quad d\leq p<\infty,\quad \forall g\in L^{p'}(\mathbb{T}^d),$$

where the case $p=d$ corresponds to the Sobolev-Gagliardo-Nirenberg inequality, $\|g-\overline{g}\|_{L^{d'}(\mathbb{T}^d)}\leq\beta\|g\|_{BV(\mathbb{T}^d)}$. We distinguish between two cases.

(i) The case $d<p<\infty$: the equation $div\, U=f\in L^p_{\#}(\mathbb{T}^d)$ has a hierarchical solution $U\in L^{p^*}(\mathbb{T}^d,\mathbb{R}^d)$, with the same integrability as the irrotational Helmholtz solution, $\nabla\Delta^{-1}f\in W^{1,p}(\mathbb{T}^d,\mathbb{R}^d)\subset L^{p^*}(\mathbb{T}^d,\mathbb{R}^d)$.

(ii) The case $d=p$: the equation $div\, U=f\in L^d_{\#}(\mathbb{T}^d)$ has a solution $U\in L^{\infty}(\mathbb{T}^d,\mathbb{R}^d)$. This is the the prototype example discussed in the beginning of the introduction. According to the intriguing observation of Bourgain & Brezis, [BB03, Proposition 2], there exists no bounded right inverse $K: L^d_{\#}\mapsto L^{\infty}$ for the operator div, and therefore, there exists no *linear* construction of solutions

$f \mapsto U$ (in particular, $\nabla\Delta^{-1} f$ cannot be uniformly bounded). Theorem 1 provides a *nonlinear* hierarchical construction of such solutions.

#2. **Solutions of (7) in $L^\infty \cap \dot{W}^{1,d}$.** A central question raised and answered in [BB03] is whether (7) has a solution which captures the *joint* regularity, $U \in \mathbb{B} = L^\infty \cap \dot{W}^{1,d}(\mathbb{T}^d, \mathbb{R}^d)$. To this end, one needs to verify the duality estimate (8), which now reads

$$\|g - \overline{g}\|_{L^{d'}(\mathbb{T}^d)} \leq \beta \|\nabla g\|_{L^1 + \dot{W}^{-1,d'}(\mathbb{T}^d, \mathbb{R}^d)}, \qquad \forall g \in L^{d'}(\mathbb{T}^d). \tag{9}$$

This key estimate was proved in [BB03] and theorem 1 converts (9) into a *constructive* proof of:

Corollary 1. *The equation $div\, U = f \in L^d_\#(\mathbb{T}^d)$ admits a solution $U \in L^\infty \cap \dot{W}^{1,d}(\mathbb{T}^d, \mathbb{R}^d)$, given by the hierarchical decomposition $U = \sum_{j=1} \mathbf{u}_j$, which is constructed by the refinement step,*

$$\mathbf{u}_{j+1} = arg\min_{\mathbf{u}} \left\{ \|\mathbf{u}\|_{L^\infty \cap \dot{W}^{1,d}} + \lambda_1 \zeta^j \big\| f - div\big(\sum_{k=1}^{j} \mathbf{u}_k\big) - div\, \mathbf{u} \big\|^d_{L^d} \right\},$$

for $j = 0, 1, 2 \ldots$, with $\zeta > 1$ and $\lambda_1 \gtrsim \beta \|f\|^{1-d}_{L^d}$.

Remark 3. *We note that the duality estimate* (9) *is in fact a byproduct of Bourgain & Brezis* **construction** *of $L^\infty \cap \dot{W}^{1,d}$ solutions for $div\, U = f$,* [BB03, theorem 1]*: their construction, which is based on Littlewood-Paley decomposition, is rather involved. Corollary 1 offers a simpler construction of such solutions which could be implemented in actual computations based on the construction of minimizers for, $\vee_{div}(r, \lambda; L^\infty, L^d_\#) := inf_{\mathbf{u}} \big\{ \|\mathbf{u}\|_{L^\infty} + \lambda \|r - div\, \mathbf{u}\|^d_{L^d} \big\}$.*

Since the proof of the dual estimate (9) *in $d > 2$ dimensions is indirect, a specific value of β is not known. As noted earlier, however, the hierarchical construction can proceed without a precise knowledge of β: if one sets $\lambda_1 = \|f\|^{1-d}_{L^d}$ and this initial scale underestimates a correct value of $\beta > 1$, then it will take at most $j_0 \sim \log(\beta)$ steps before picking-up non-trivial terms in the hierarchical decomposition, $U = \sum_{j=j_0} \mathbf{u}_j$.*

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Complexity of Recovering Functions of Few Variables in High Dimension

Przemek Wojtaszczyk

We have a function f defined on $[0,1]^N$ where N is big. We assume that there exists a g on $[0,1]^\ell$ with ℓ small and integers $j_1 < j_2 < \cdots < j_\ell \le N$ such that

$$f(x_1,\dots,x_N) = g(x_{j_1},\dots,x_{j_\ell}) \qquad \text{exact case}$$

or

$$\|f(x_1,\dots,x_N) - g(x_{j_1},\dots,x_{j_\ell})\|_\infty \le \epsilon \qquad \text{approximate case}$$

We know ℓ (or an estimate for ℓ). We do not know g, $j_1, j_2, \dots, j_\ell$ nor ϵ. We assume g is smooth.

We want to find a subset $\mathfrak{B} \subset [0,1]^N$ of small cardinality such that values $f(P)$ with $P \in \mathfrak{B}$ will allow us to find $\hat{f} := \tilde{g}(x_{j'_1},\dots,x_{j'_\ell})$ which is a good approximation to f in *sup norm.*

- Even in the exact case we cannot expect to find $j_1,\dots,j_\ell$. There may be coordinates of g that do not show when we take our point values.
- Obviously there is no hope to recover g exactly.
- Our algorithms are rather theoretical

This was discussed in a recent paper [DPW] with R.DeVore and G.Petrova.

Here we are interested in the number of points needed.

Let $h = 1/L$ with L an integer. Lattice of equally spaced points $\mathcal{L} := \{i/L \ : \ 0 \le i \le L\} \subset [0,1]$ and $\mathcal{L}^\ell \subset [0,1]^\ell$ and $/\mathcal{L}N \subset [0,1]^N$. For each h, we have a nice linear operator $A_h : C(\mathcal{L}^\ell) \to C([0,1]^\ell)$ such that:

(1) $\|A_h\| \le C_0$, for all $L = 1, 2, \dots$.
(2) If g depends on $k \le \ell$ variables then $A_h(g)$ depends only on these variables. So, $A_h(g) = g$, for any $g \equiv const$.

We consider the following approximation class:

$$\mathcal{A}^s := \mathcal{A}^s((A_h)) = \{g \in C([0,1]^\ell) : \ \|g - A_h(g|\mathcal{L}^\ell)\|_\infty \le Ch^s\},$$

with semi-norm $|g|_{\mathcal{A}^s} := \sup_h \left\{h^{-s}\|g - A_h(g|\mathcal{L}^\ell)\|_\infty\right\}$.

For natural A_h's those are real smoothness spaces.

Now let us describe main results from [DPW]. For $g \in \mathcal{A}_s$ we get $\hat{f}$ so that *in the exact case* we get the estimate

$$\|f - \hat{f}\|_\infty \le |g|_{\mathcal{A}_s} h^s$$

and *in the approximate case* we get

$$\|f - \hat{f}\|_\infty \le |g|_{\mathcal{A}_s} h^s + K(C_0,\ell)\epsilon$$

	Exact	*Approximate*
Adaptive pts	$C(\ell)(L+1)^\ell \log N$	$C(\ell)(L+1)^\ell \log N + C'(\ell)\log^2 N$
$Non-adaptive$	$C(\ell)(L+1)^{\ell+1}\log^2 N$	$C(\ell)(L+1)^{\ell+1}\log^2 N$

So the question: *Do we really need more points in the nonadaptive case then in adaptive?*

To get $\hat{f}$ we need two things

(1) Active variables $j_1, j_2, \dots, j_\ell$.
(2) Values of g in points from $\mathcal{L}$.

This will give us approximation up to Ch^s. Even when we know $j_1, \dots, j_\ell$ for (2) we need at least $(L+1)^\ell$ points.

How much do we have to pay to find appropriate coordinates?

I will discuss only the non-adaptive case.

Theorem (Approximate case) *Suppose that $f \in C([0,1]^N)$ and there exists a function $g \in \mathcal{A}^s$ and a coordinates $j_1, \dots, j_\ell$ such that $\|f - \tilde{g}\|_{C([0,1]^N)} \le \epsilon$ where $\tilde{g}(x_1, \dots, x_N) = g(x_{j_1}, \dots, x_{j_\ell})$. There exists a set $\mathfrak{B} \subset \mathcal{L}^N$ such that*

(1) $\#\mathfrak{B} \le C(\ell)(L+1)^\ell \log N$
(2) *Using values $f(P)$ for $P \in \mathfrak{B}$ we can get function $\hat{f} \in C([0,1]^N$ which depends only on ℓ variables and such that*

$$\|f - \hat{f}\|_{C([0,1]^N)} \le |g|_{\mathcal{A}^s} h^s + C\epsilon,$$

where C is the constant dependent on the approximation process A_h and ℓ.

In the exact case we can have constants $C(\ell)$ and C smaller and the procedure to find $\hat{f}$ is more userfriendly.

Description of $\mathfrak{B}$

Let $\mathcal{A}$ be a collection of partitions $\mathbf{A}$ of $\{1, 2, \dots, N\}$. $\mathcal{A}$ is *ν–separating* if

(1) each $\mathbf{A}$ consists of ν disjoint sets $A_1, \dots, A_\nu$
(2) given any ν distinct integers $i_1, \dots, i_\nu \in \{1, \dots, N\}$, there is a partition $\mathbf{A}$ in $\mathcal{A}$ such that each set in $\mathbf{A}$ contains precisely one of the integers $i_1, \dots, i_\nu$.

There exist such collections $\mathcal{A}$ of cardinality $\le 2\nu e^\nu \ln N$

We fix a 2ℓ–separating collection $\mathcal{A}$.

For any $\mathbf{A} = (A_1, A_2, \dots, A_{2\ell}) \in \mathcal{A}$ and $V \subset \{1, \dots, 2\ell\}$ with $\#V = \ell$ we construct points

$$\mathcal{P}_{\mathbf{A},V} = \{P = \sum_{i \in V}^{\ell} \alpha_i \chi_{A_i}, \ : \ \ \alpha_i \in \mathcal{L}\}$$

i.e. P has coordinate value α_i at each coordinate index in A_i for $i \in V$ and other coordinates are equal to 0. We put $\mathcal{P}_{\mathbf{A}} = \bigcup_V \mathcal{P}_{\mathbf{A},V}$ and $\mathfrak{B} = \bigcup_{\mathbf{A} \in \mathcal{A}} \mathcal{P}_{\mathbf{A}}$.

Finding $\hat{f}$ We put $\|\phi\|_{\mathfrak{B}} = \max\{|\phi(P)| \ : \ P \in \mathfrak{B}\}$.

For a set $A \subset \{1,\dots,N\}$, $\#A = \ell$ and $x \in \mathcal{L}^N$ we put

$$\begin{aligned}\alpha(f,A,x) &= \max\{f(P) \ : \ P \in \mathfrak{B} \ \text{ and } \ P|A = x|A\}\\ \beta(f,A,x) &= \min\{f(P) \ : \ P \in \mathfrak{B} \ \text{ and } \ P|A = x|A\}\end{aligned}$$

and we define

$$h_A(x) = \frac{\alpha(f,A,x) + \beta(f,A,x)}{2}. \tag{1}$$

Clearly each h_A depends only on variables from A.

We define set A_0 as $\operatorname{argmin}_A \|f - h_A\|_{\mathfrak{B}}$. From the very definition $\|f - h_{A_0}\|_{\mathfrak{B}} \le \|f - h_B\|_{\mathfrak{B}}$ where $B =: \{j_1,\dots,j_\ell\}$. We check that $\|f - h_B\|_{\mathfrak{B}} \le 2\epsilon$. We put $\hat{f} = h_{A_0}$ so

$$\|f - \hat{f}\|_{\mathfrak{B}} \le 2\epsilon.$$

Why this works? We define

$$\operatorname{osc}(B \setminus A_0) =: \max\{|f(P) - f(P')| \ : \ P, P' \in \mathcal{L}^N, \ P|(B \setminus A_0)^c = P'|(B \setminus A_0)^c.$$

Proposition: *We have* $\operatorname{osc}(B \setminus A_0) \le 8\epsilon$.

Proof: If $\operatorname{osc}(B \setminus A_0) > 8\epsilon$ we can fix $P, P' \in \mathcal{L}^N$ such that P and P' differ only on $B \setminus A_0$ and $8\epsilon < |f(P) - f(P')|$. Since $\#B, \#A_0 \le \ell$ we fix $Q, Q' \in \mathfrak{B}$ such that $Q|B = P|B$ and $Q'|B = P'|B$ and $Q|A_0 \setminus B = 0 = Q'|A_0 \setminus B$. Note that $Q|A_0 = Q'|A_0$. Now we have

$$\begin{aligned}8\epsilon &< |f(P) - f(P')| \le |g(P) - g(P')| + 2\epsilon\\ &= |g(Q) - g(Q')| + 2\epsilon \le |f(Q) - f(Q')| + 4\epsilon\\ &\le |h_{A_0}(Q) - h_{A_0}(Q')| + 8\epsilon = 8\epsilon\end{aligned}$$

This contradiction completes the proof.

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On the Regularity and Approximability of Electronic Wave Functions

Harry Yserentant

Approximating the solutions of the electronic Schrödinger equation is one of the basic tasks of quantum chemistry. The electronic Schrödinger equation describes the motion of a finite set of electrons in the field of a given number of clamped nuclei. Its solutions are the eigenfunctions of the Hamilton operator

$$H \ = \ -\ \frac{1}{2}\sum_{i=1}^{N} \Delta_i \ + \ V_{ne} \ + \ \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N} \frac{1}{|x_i - x_j|} \tag{1}$$

that is written down here in atomic units. It acts on functions with arguments $x_1, \ldots, x_N$ in the three-dimensional space, which are associated with the positions of the considered electrons. The external potential

$$V_{ne} = -\sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|x_i - a_\nu|} \tag{2}$$

covers the interaction of the electrons with the nuclei that are kept fixed at the positions $a_1, \ldots, a_K$. The Z_ν are the charges of the nuclei in multiples of the electron charge. The problem with this equation is its high dimensionality which immediately rules out classical discretization methods for partial differential equations as they are used in engineering applications. To overcome this curse of dimensionality, procedures like the Hartree-Fock method or density functional theory based methods have been developed over the decades. While these methods are applied with much success, they suffer, however, either from modeling errors or from the fact that it is not clear how the accuracy can be systematically improved without the effort truly exploding for larger numbers of electrons. It is therefore rather surprising that simple expansions of the electronic wave functions can be constructed whose convergence rate, measured in terms of the number of determinants involved, is independent of the number of electrons and does not fall below that for a two-electron system [4]. It is even possible to reach a convergence rate as for the case of a single electron adding a simple regularizing factor that depends explicitly on the interelectronic distances [5].

The wave functions depend on the three-dimensional position vectors $x_1, \ldots, x_N$ of the electrons that split into the coordinates $x_{i,1}$, $x_{i,2}$, and $x_{i,3}$. Accordingly, we label partial derivatives doubly, that is, by multi-indices

$$\alpha = (\alpha_1, \ldots, \alpha_N), \quad \alpha_i = (\alpha_{i,1}, \alpha_{i,2}, \alpha_{i,3}). \tag{3}$$

The differentiation operator D^α of order $|\alpha| = \sum_{i,\nu} \alpha_{i,\nu}$ reads in this notation

$$\mathrm{D}^\alpha = \prod_{i=1}^{N}\prod_{\nu=1}^{3}\Big(\frac{\partial}{\partial x_{i,\nu}}\Big)^{\alpha_{i,\nu}}. \tag{4}$$

The key to the mentioned results is the existence of high-order weak derivatives of the solutions representing bound states and, as the domain of definition is unbounded, the rapid decay of these derivatives. To describe the differentiability properties, let $\mathcal{A}$ be the set of the multi-indices $\alpha = (\alpha_1, \ldots, \alpha_N)$ for which

$$\alpha_{i,1} + \alpha_{i,2} + \alpha_{i,3} \le 1. \tag{5}$$

The maximum order that the assigned differentiation operators D^α can reach is N and grows therefore with the number of electrons; their order is, however, at most one in the components of the position vectors of the single electrons i. Subsets of this set of multi-indices are the set $\mathcal{A}_-$ consisting of the α in $\mathcal{A}$ with components $\alpha_i = 0$ for all electrons i with spin $+1/2$ and the correspondingly defined set $\mathcal{A}_+$ consisting of the α in $\mathcal{A}$ with components $\alpha_i = 0$ for the electrons i with spin $-1/2$. The corresponding operators D^α intermix only partial derivatives with respect to

coordinates of electrons of the same spin. One of our main results [2, 3] is that the weak derivatives

$$\mathrm{D}^\alpha u, \quad \frac{\partial}{\partial x_{i,\nu}} \mathrm{D}^\alpha u \tag{6}$$

of the bound state solutions u of the electronic Schrödinger equation exist for all α in $\mathcal{A}_-$ and in $\mathcal{A}_+$ and are square integrable. Moreover, they decay exponentially in the L_2-sense [4], that is, the functions

$$\exp\left(\gamma \sum_{i=1}^{N} |x_i|\right) \mathrm{D}^\alpha u, \quad \exp\left(\gamma \sum_{i=1}^{N} |x_i|\right) \frac{\partial}{\partial x_{i,\nu}} \mathrm{D}^\alpha u, \tag{7}$$

with a coefficient $\gamma > 0$ depending on the distance of the eigenvalue under consideration to the bottom of the essential spectrum, are square integrable. A more precise formulation and a proof can be found in [4].

This proof utilizes that the admissible wave functions are by the Pauli principle antisymmetric under the exchange of electrons of same spin. Thus they vanish where such electrons meet, which counterbalances the singularities of the electron-electron interaction potential there. The singularities at the places where electrons of distinct spin meet are considerably stronger. This is the reason why it is not possible to show that the derivatives (6) and their exponentially weighted counterparts (7) are square integrable for all multi-indices α in the set $\mathcal{A}$. To overcome this problem, the electron correlation has to be taken into account explicitly. We partition the solutions u of the electronic Schrödinger equation into a regular part

$$u_0(x) \;=\; \exp\left(-\sum_{i<j} \phi(x_i - x_j)\right) u(x) \tag{8}$$

and a universal factor that covers the electron cusps already to a large extent. The function ϕ has to satisfy some technical conditions [5] that mainly concern the decay behavior of its first and second-order derivatives and its behavior at the origin. A possible example is

$$\phi(x_i - x_j) \;=\; \ln\Big(1 + \frac{1}{2}\,|x_i - x_j|\Big), \tag{9}$$

or even simpler than this,

$$\phi(x_i - x_j) \;=\; \frac{1}{2}\,|x_i - x_j|. \tag{10}$$

The crucial point is that the weak derivatives

$$\mathrm{D}^\alpha u_0, \quad \frac{\partial}{\partial x_{i,\nu}} \mathrm{D}^\alpha u_0 \tag{11}$$

and even their exponentially weighted counterparts (7) are square integrable for all multi-indices α in the set $\mathcal{A}$ introduced above, not only for the multi-indices α in $\mathcal{A}_-$ and $\mathcal{A}_+$. This reflects the fact that the regularizing factor largely compensates the singular behavior of the wave functions at the points where two or more electrons meet [5]. Approximations of the wave functions u can thus be found first

approximating their regular parts (8) and then dividing the result by the given universal factor. With the sparse grid techniques described in [4] it is possible to approximate the regular parts of the wave functions, and with that indirectly also the wave functions themselves, with an order of convergence that comes arbitrarily close to that for the one-electron case.

We remark that the same kind of results as for the regular parts (8) of the eigenfunctions u also hold for their modifications

$$u_1(x) \;=\; \exp\left(2\sum_{i,\nu} Z_\nu\,\phi(x_i - a_\nu) \;-\sum_{i<j}\phi(x_i - x_j)\right) u(x) \tag{12}$$

that contain an additional term smoothing the singularities at the positions of the nuclei. This observation might be helpful in the approximation of the wave functions in view of their analytic structure [1] outside the points where more than two particles meet.

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Approximating Electronic Wave Functions by Wavelets

Andreas Zeiser

The non-relativistic electronic Schrödinger equation describes the chemical behavior of molecules very accurately. However depending on the number of electrons N a function in $3N$ variables has to be discretized in order to solve the governing eigenvalue equation. Therefore classical discretization schemes fail due to the curse of dimensionality. Recently it has been shown that the eigenfunctions posses a certain high derivatives which in addition also decay exponentially [Ys1, Ys2]. Now approximating the wave function with anisotropic wavelets one can exploit this regularity and obtain approximation rates which are independent of the number of electrons [Ze].

Let $u(\vec{\boldsymbol{x}})$, $\vec{\boldsymbol{x}} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$, $\boldsymbol{x}_i \in \mathbb{R}^3$, be a bounded state of the electronic Schrödinger equation with N electrons. Now decomposing u according to

$$u(\vec{\boldsymbol{x}}) = \exp\big(-\sum_{i,\nu} Z_\nu|\boldsymbol{x}_i - \boldsymbol{a}_\nu|_2 + 1/2\sum_{i,j}|\boldsymbol{x}_i - \boldsymbol{x}_j|_2\big)\, u_0(\vec{\boldsymbol{x}}),$$

Yserentant showed [Ys1, Ys2] that both u and u_0 are in weighted Sobolev spaces of mixed order, that is $u \in H^{1/2,1}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w_\gamma\big)$ and $u_0 \in H^{1,1}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w_\gamma\big)$ for some γ. Here $w_\gamma = \prod \exp(\gamma|\boldsymbol{x}_i|_2)$ denotes an exponential weight function.

Given a positive weight function w and integers m, k the weighted Sobolev spaces $H^{k,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ of mixed order are defined as the set of all measurable functions such that

$$\|u\|^2_{\mathrm{mix},w,k,m} := \sum_{\boldsymbol{\alpha}\in\vec{A}^{k,m}} \int_\Omega \big|\partial^{\vec{\boldsymbol{\alpha}}} u(\vec{\boldsymbol{x}})\big|^2 \cdot w(\vec{\boldsymbol{x}})\,\mathrm{d}\vec{\boldsymbol{x}}$$

is finite. Here the index set $A^{k,m}$ is given by

$$A^{k,m} = \big\{\vec{\boldsymbol{\alpha}} + \vec{\boldsymbol{\beta}} \;\big|\; \max_{i=1,\dots,N} |\boldsymbol{\beta}_i|_1 \le k, \sum_{i=1}^N |\boldsymbol{\alpha}_i|_1 \le m\big\} \subset \big(\mathbb{N}^d\big)^N.$$

That is in addition to m order of isotropic smoothness we are allowed to differentiate the function in each variable $\boldsymbol{x}_i$ another k times. Weighted Sobolev spaces of mixed order with fractional order of smoothness are defined through interpolation theory.

Our goal now is to characterize these spaces in terms of wavelet coefficients and use these discrete norm for constructing efficient approximations. For that purpose we assume that we are given a biorthogonal and compactly supported multiresolution analysis $\{\psi_\lambda \mid \lambda \in \nabla\}$, $\{\tilde\psi_\lambda \mid \lambda \in \nabla\}$. Here the multi-index $\lambda = (\varepsilon, j, \boldsymbol{k})$ consists of the type ε, the level j and the translation $\boldsymbol{k}$. We furthermore assume that for $0 \le s < \tau$ the norm equivalence

$$\|u\|^2_{H^s(\mathbb{R}^d)} \sim \sum_{\lambda\in\nabla} 2^{2j(\lambda)s}\,|u_\lambda|^2, \quad u_\lambda = \langle\tilde\psi_\lambda, u\rangle$$

holds for Sobolev spaces $H^s(\mathbb{R}^d)$. Here $j(\lambda)$ denotes the level of the wavelet ψ_λ. Wavelets which satisfy these assumptions are well known, see for example [Co]. One may take for example Daubechies wavelets, biorthogonal spline wavelets or orthogonal spline multiwavelets. By taking the anisotropic tensor product

$$\psi_{\vec\lambda} = \bigotimes_{i=1}^N \psi_{\lambda_i}, \quad \tilde\psi_{\vec\lambda} \;\text{ analogously}$$

with multi-index $\vec\lambda = (\lambda_1, \dots, \lambda_N)$ we construct a biorthogonal multiresolution analysis $\{\psi_{\vec\lambda} \mid \vec\lambda \in \nabla^N\}$, $\{\tilde\psi_{\vec\lambda} \mid \vec\lambda \in \nabla^N\}$ in dN variables.

As a first central result we characterize the spaces $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ in terms of wavelet coefficients. Defining

$$\kappa_{\mathrm{iso}}(\vec\lambda) = 2^{|\vec j(\vec\lambda)|_\infty}, \quad \kappa_{\mathrm{mix}}(\vec\lambda) = 2^{|\vec j(\vec\lambda)|_1}, \quad \kappa_{s,m}(\vec\lambda) = \kappa^s_{\mathrm{mix}}(\vec\lambda)\cdot\kappa^m_{\mathrm{iso}}(\vec\lambda).$$

the discrete norm

$$|||u|||^2_{\mathrm{mix},w,m,s} = \sum_{\vec\lambda\in\nabla^N} w(\vec{\boldsymbol{x}}_{\vec\lambda})\,\kappa^2_{s,m}(\vec\lambda)\,|u_{\vec\lambda}|^2, \quad u_{\vec\lambda} = \langle\tilde\psi_{\vec\lambda}, u\rangle_{L^2(\mathbb{R}^{dN})}.$$

is an equivalent norm on $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$. Here we have to assume that the weight functions is regular enough, i.e. there exists a constant C_w such that for all $\vec{\boldsymbol{x}}, \vec{\boldsymbol{y}} \in \mathbb{R}^{dN}$ with $|\vec{\boldsymbol{x}} - \vec{\boldsymbol{y}}|_\infty \leq 1$

$$w(\vec{\boldsymbol{y}}) \leq C_w \; w(\vec{\boldsymbol{x}}).$$

In order to proof the assertion we first introduce a localized norm (see for example [Tr]) on overlapping cubes of equal size covering the whole space. This equivalent norm is a weighted sum of unweighted mixed norms on these cubes. Now we can use the results on unweighted Sobolev spaces of mixed order [GK] and the fact that both the primal as well as the dual wavelets are compactly supported to show the norm equivalence.

Using this norm equivalence we can construct approximations to functions $u \in H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$. For that purpose set

$$u_L = \sum_{\vec{\lambda} \in \Phi_L} u_{\vec{\lambda}} \psi_{\vec{\lambda}}, \quad u_{\vec{\lambda}} = \langle \tilde{\psi}_{\vec{\lambda}}, u \rangle,$$

where the index set Φ_L is defined by $\Phi_L = \big\{ \vec{\lambda} \in \nabla^N \;\big|\; w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa^{2s}_{\mathrm{mix}}(\vec{\lambda}) \leq 2^{2L} \big\}$. Then using the norm equivalence twice

$$\|u - u_L\|_m \lesssim 2^{-L} \|u\|_{\mathrm{mix},w,s,m}$$

That is we can achieve arbitrary accuracy.

In order to estimate the convergence rate we have to fix the weight function w. In view of the regularity result on the bounded states of the electronic Schrödinger equation we analyze the case for the family w_γ of exponential weight functions. In this case the set of indices Φ_L form a sparse grid in both the position as well as the level of the wavelet. In particular the number of elements can be estimated by

$$\sharp \Phi_L \lesssim \gamma^{-dN} \cdot L^{N-1} \, 2^{dL/s}.$$

Relating the error of approximation to the number of elements in the index set we finally can show the second central result: for each $\varepsilon > 0$ we can construct an approximation u_ε such that $\|u - u_\varepsilon\|_m \leq \varepsilon \, \|u\|_{\mathrm{mix},w_\gamma,s,m}$. Moreover the number of terms can be bounded by

$$\sharp u_\varepsilon \lesssim \gamma^{-dN} \cdot C_\gamma^{dn_\xi/(2s)} \cdot |\log \varepsilon|^{N-1} \cdot \varepsilon^{-d/s}.$$

Or stated the other way round for an approximation u_n of u containing n terms we can achieve an error of

$$\|u - u_n\|_m \lesssim (\log n)^{s(N-1)} \cdot n^{-s/d}.$$

The rate of convergence is up to logarithmic factors independent of the number of dimensions N.

In the case of bounded states of electronic wave functions these approximation results can readily be applied. However the convergence rate can be improved if

one takes the antisymmetry of the wave function into account. Due to the Pauli principle

$$u(P\vec{\boldsymbol{x}}) = \operatorname{sign}(P)\, u(\vec{\boldsymbol{x}}),$$

where P is any permutation in the symmetric group S_N satisfying $P(\vec{\sigma}) = \vec{\sigma}$ for a fixed spin configuration $\vec{\sigma} \in \{\pm 1/2\}^N$. This finally leads to an approximation rate of

$$\|u - u_n\|_1 \lesssim e^{2\sqrt{2/3\ \log_2 n}} \cdot n^{-1/6}.$$

for the full wave function and

$$\|u_0 - u_{0,n}\|_1 \lesssim e^{4/3\,\sqrt{2/3\ \log_2 n}} \cdot n^{-1/3}.$$

for the more regular part u_0. The rate of convergence is therefore independent on the number of electrons, the curse of dimensionality is therefore broken.

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