Numerical examples, computational complexity and possible applications to other hyperbolic equations or systems, including time dependent problems, will be discussed.
All references are available at www.math.tamu.edu/∼popov/preprints.html

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Identification of Sparse Operators

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(joint work with Götz Pfander and Jared Tanner)

Motivated by the channel estimation problem in communication engineering (wireless communication and sonar) we consider the problem of identifying a matrix $\Gamma \in \mathbb{C}^{n\times m}$ from its action Γh on a single vector $h \in \mathbb{C}^m$. Clearly, without further knowledge Γ is completely determined only by its action on n basis vectors in $\mathbb{C}^m$, and our task seems impossible. However, physical considerations suggest that in certain practical situations (see also below) Γ can be well-represented by a short linear combination of a few basic matrices; in other words it has a sparse representation. In this situation one can exploit connections to sparse approximation and compressed sensing [5, 7] to efficiently reconstruct Γ.

Given a suitable set $\mathbf{\Psi}$ of N "elementary" matrices $\Psi_j \in \mathbb{C}^{n\times m}$, $j = 1,\dots,N$ (a matrix dictionary) we say that $\Gamma \in \mathbb{C}^{n\times m}$ has a k-sparse representation if

$$\Gamma = \sum_j x_j \Psi_j$$

for a vector $x \in \mathbb{C}^N$ whose support has at most cardinality k, formally $\|x\|_0 := |\{k, x_k \neq 0\}| \leq k$. The action of such a matrix Γ on a vector $h \in \mathbb{C}^m$ can be written as

$$\Gamma h = \sum_j x_j \Psi_j h \;=\; \Psi_h x$$

with the matrix $\mathbf{\Psi}_h = (\Psi_1 h|\dots|\Psi_N h) \in \mathbb{C}^{n\times N}$. Identification of Γ clearly amounts to reconstructing the sparse vector x from Γh. Unfortunately, the obvious approach of determining the vector x with shortest support (i.e. minimal $\|x\|_0$) that is consistent with the observation, $\Gamma h = \mathbf{\Psi}_h x$, yields an NP-hard combinatorial problem[2] and, thus, is not feasible in practice.

Several tractable alternative recovery algorithms have been proposed so far, most notably ℓ_1-minimization (Basis Pursuit), on which we will concentrate here.

Instead of solving a combinatorial optimization problem we consider the minimizer of the problem

$$\min_x \|x\|_1 = \sum_{j=1}^{N} |x_j| \quad \text{subject to} \quad \Gamma h = \mathbf{\Psi}_h x. \tag{1}$$

This minimization problem can be solved efficiently with convex optimization techniques [4].

Obvious questions concern the choice of h, and the maximal sparsity k that allows for recovery of x resp. identification of Γ by ℓ_1-minimization.

Our first result in this direction [11] deals with dictionaries of random matrices. Although in practice rather deterministic dictionaries will appear, it nevertheless provides some intuition of what can be expected, in particular, the maximal recoverable sparsity.

Theorem 1. Let h be a non-zero vector in $\mathbb{R}^m$.

(a) Let all entries of the N matrices $\Psi_j \in \mathbb{R}^{n\times m}$, $j = 1,\dots,N$, be chosen independently according to a standard normal distribution (Gaussian ensemble); or

(b) let all entries of the N matrices $\Psi_j \in \mathbb{R}^{n\times m}$, $j = 1,\dots,N$, be independent Bernoulli ± 1 variables (Bernoulli ensemble).

Then there exists a positive constant c such that

$$k \le c\,\frac{n}{\log\left(\frac{N}{n\varepsilon}\right)} \tag{2}$$

implies that with probability at least $1-\varepsilon$ all matrices Γ having a k-sparse representation with respect to $\mathbf{\Psi} = \{\Psi_j\}$ can be recovered from Γh by Basis Pursuit (1).

The proof of this theorem is based on estimating the so called restricted isometry constants [6] of the random matrix $\mathbf{\Psi}_h$.

We will now concentrate on the matrix dictionary of time–frequency shifts, which appears naturally in the channel identification problem in wireless communications [3] or sonar [13]. Due to physical considerations wireless channels may indeed be modeled by sparse linear combinations of time–frequency shifts $M_\ell T_p$, where the translation operators T_p and modulation operator M_ℓ on $\mathbb{C}^n$ are given by

$$(T_p h)_q = h_{p+q \mod n} \quad \text{and} \quad (M_\ell h)_q = e^{2\pi i \ell q/n} h_q.$$

The system of time–frequency shifts $\mathbf{G} = \{M_\ell T_p : \ell, p = 0,\dots,n-1\}$ forms a basis of $\mathbb{C}^{n\times n}$ and for any non-zero h, the vector dictionary $\mathbf{G}_h = (M_\ell T_p h)_{\ell,p=0,\dots,n-1}$ is a Gabor system [9]. Below, we focus on the so-called Alltop window h^A [1, 10] with entries

$$h^A_q := \frac{1}{\sqrt{n}} e^{2\pi i q^3/n}, \quad q = 0,\dots,n-1, \tag{3}$$

and the randomly generated window h^R with entries

$$h_q^R := \frac{1}{\sqrt{n}}\epsilon_q, \quad q = 0, \dots, n-1, \tag{4}$$

where the ϵ_q are independent and uniformly distributed on the torus $\{z \in \mathbb{C}, |z| = 1\}$.

Invoking existing recovery results [8, 14] and results on the coherence of the Gabor systems $\mathbf{G}_{h^A}$ [10] and $\mathbf{G}_{h^R}$ [11], we obtain

Theorem 2. (a) Let $n \geq 5$ be prime and h^A be the Alltop window defined in (3). If $k < \frac{\sqrt{n}+1}{2}$ then BP recovers from Γh^A all matrices Γ having a k-sparse representation with respect to the time–frequency shift dictionary.

(b) Let n be even and choose h^R to be the random unimodular window in (4). Let $t > 0$ and suppose

$$k \leq \frac{1}{4}\sqrt{\frac{n}{C\log(n) + t}} + \frac{1}{2}$$

with $C = 2\log(4) \approx 2.77$. Then with probability of at least $1 - e^{-t}$ BP recovers from Γh^R all matrices $\Gamma \in \mathbb{C}^{n\times n}$ having a k-sparse representation.

Although this theorem provides a first recovery result, it is not yet satisfactory as the maximal sparsity which guarantees recovery is quite small – on the order of $\sqrt{n}$ – compared to (2), where it is of the order $n/\log(N/n)$ which in our case, $N = n^2$, is $n/\log(n)$. By passing from worst case analysis to a probability model on the sparse coefficient vector x one can apply recent work by Tropp based on the coherence [15] in order to achieve an improvement. Indeed, if the support set Λ is chosen at random as well as the signs of the non-zero coefficients x_j, $j \in \Lambda$, then for both h^A and h^R one has recovery with high probability of the true coefficient vector x provided

$$k \leq c\frac{n}{\log(n)^{1+u}}$$

for some $c, u > 0$ (governing the probability of recovery). We refer to [11] for a precise formulation.

In case of the randomly generated vector h^R we were able to improve further on the above recovery results by removing the randomness in the coefficient vector x [12].

Theorem 3. Let $\Gamma \in \mathbb{C}^{n\times n}$ be k-sparse with respect to the time-frequency shift dictionary $\mathbf{G}$. Choose h^R at random. There exists a constant $C > 0$ such that

$$k \leq C\frac{n}{\log(n/\epsilon)} \tag{5}$$

implies that with probability at least $1-\epsilon$ Basis Pursuit (1) recovers Γ from Γh^R.

The above theorem is based on a careful analysis of the singular values of a submatrix consisting of k columns of $\mathbf{G}_{h^R}$ [12]. It would be interesting to investigate an analog for the deterministic Alltop window h^A.

Numerical experiments for both h^A and h^R in [11] suggest that recovery is possible with high probability for most signals provided $k \leq \frac{n}{2\log(n)}$.

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Adaptive Coupled Cluster Method and CI Method for the Solution of the Electronic Schroedinger Equation

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The electronic Schrödinger equation plays a fundamental role in molecular physics. It describes the stationary non-relativistic quantum mechanical behavior of an N electron system in the electric field generated by the nuclei. The *Coupled Cluster Method* has been developed for the numerical computation of the ground state energy and wave function. It provides a powerful tool for high accuracy electronic structure calculations. The present paper aims to provide a convergence analysis of this method. Under additional assumptions quasi-optimal convergence of the projected coupled cluster solution to the full CI solution and also to the exact wave function can be shown in the Sobolev H^1 norm. The error of the ground state energy computation is obtained by an Aubin Nitsche type approach.