Application

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Project info

Project title (Swedish)*

Modellering och identifiering av spektroskopiska signaler

Project title (English)*

Modelling and identification of spectroscopic signals

Abstract (English)*

The proposed research deals with the identification and modelling of spectroscopic signals, consisting of two main parts, namely the study of nuclear magnetic resonance (NMR) and of nuclear quadrupole resonance (NQR) signals. In both cases, the signals of interest result from the interaction between the quadrupole moment of the nucleus and the field gradient. For NMR, one applies both an electric and a magnetic field to the investigated substance, whereas, for NQR, one only applies the electric field. The latter case results in dramatically weaker signals as compared to the former, but also offers the possibility of obtaining unique signal signatures that allow for an unequivocal identification of many solid-state substances, such as most forms of high explosives, and many kinds of narcotics and medicines. In this work, we will examine both kinds of signals, addressing key areas of each method.

In the last decade, powerful methods in NMR spectroscopy have been developed to study protein dynamics involved in increasingly complex biological phenomena. These advancements have relied on lengthy experimental acquisition schemes, which are deemed necessary to obtain robust estimates of the relaxation rates of NMR coherences. In order to push the frontier towards increasingly complex systems, such as living cells or in-vitro reconstructed biochemical signalling pathways, it is required to drastically shorten the time frame of the data acquisition schemes. Traditional NMR spectroscopy samples the signals uniformly. However, recent results in compressive sensing have shown that one may achieve the same spectral resolution with a non-uniformly sampled signal, using only a fraction of the number of samples required in the uniform case. This amounts to very significant time savings, which make it possible to, for example, address challenging research questions in the context of living cells or other sensitive systems. We propose to develop a novel framework for acquiring and analysing multidimensional NMR spectra in order to achieve optimal sampling in terms of experiment time, signal-to-noise, resolution, and robustness of the determined parameter estimates and their associated uncertainties.

The signals resulting from NQR spectroscopy share many characteristics with NMR signals, and some solutions and methods for one of the techniques may also be used for the other. However, the practical usability of NQR spectroscopy is often seriously hampered by the corruption of strong interference signals, resulting from, for instance, radio transmissions or from piezoelectric or magneto-acoustic responses. As the NQR signal is so weak, these interference signals may be a thousand, or even a million, times stronger than the signal of interest, making it critical to find ways to alleviate this problem, especially when designing a non-shielded system. In the proposed work, we will further investigate this challenging problem, with the aim of developing a system that would allow for the detection of narcotics on or inside a body.

The proposed research is of a collaborative nature, and we will regularly during the work interact with leading NMR and NQR experts. These collaborations are already ongoing, and allow us access to both measurement data and expert knowledge in the fields.

Popular scientific description (Swedish)*

Den föreslagna forskningen berör spektroskopiska signaler. Dessa uppstår på grund av interaktioner mellan atomkärnor och applicerade elektriska och magnetiska fält, och möjliggör detaljerade studier av många former av substanser. Vår forskning har två huvudteman; dels hur man kan förbättra studier av levande protein och dels hur man kan detektera olika former av skadliga preparat, såsom narkotika eller sprängämnen.

Biologiska processer regleras av proteiner genom att dessa övergår från inaktiva till aktiva strukturer, som kan växelverka med andra molekyler, och på så sätt skicka signaler inom eller mellan celler. Möjligheten att påverka och styra dessa processer utgör grunden för utvecklingen av nya läkemedel och många biotekniska tillämpningar. Vår kunskap om de molekylära grunderna för ett proteins funktion ökar dramatiskt om vi vet hur proteinets struktur varierar dynamiskt över tiden. Kärnmagnetisk resonansspektroskopi (NMR, "nuclear magnetic resonance") är en unik metod för att studera proteiners dynamik. I NMR-experimenten mäter vi kärnspinnens resonansfrekvenser och relaxation. Nuvarande metoder inom NMR är dock relativt långsamma och okänsliga, vilket gör att dyrbar utrustning måste belastas med långa mätserier. Aktuella rön rörande grundläggande statistiska metoder för signalskattning har dock visat sig vara tillämpliga inom NMR och då potentiellt kunna ge högst betydande tidsvinster. Genom att vidareutveckla dessa metoder specifikt för mångdimensionell NMR kommer vi att uppnå mycket stora tidsvinster för tillämpningar mot proteindynamik. Vi kommer att kunna frångå den traditionella datainsamlingen, som i hög grad är repetitiv och 'överflödig' (och därmed långsam), och ersätta denna med en ny metod som är oregelbunden och sparsam (och därmed snabb). Våra nyutvecklade signalbehandlingsmetoder kommer att kunna lösa dagens problem med de allvarliga förvrängningar av NMR-signalerna som normalt uppstår då man frångår den traditionella datainsamlingen och istället ge en korrekt representation av NMR-signalerna. Utvecklingen av de statistiska signalbehandlingsmetoderna kommer att ske i nära samarbete med NMR-experter för att på bästa sätt bygga in den kunskap som finns a priori om de aktuella NMR-signalerna för varje givet protein. Vi kommer därmed att kunna skräddarsy datainsamlingen för varje protein och sedan analysera dessa data med våra nyutvecklade metoder, för att på så sätt kunna genomföra experimenten på dramatiskt mycket kortare tid än vad som varit möjligt tidigare och med bibehållen eller förbättrad noggrannhet och precision.

Ett matematiskt relaterat problem uppkommer vid studier av NQR ("nuclear quadrupole resonance"), som är en teknik som enbart använder ett elektriskt fält för att studera kärnspinnens resonanser. Fördelen med NQR är att man kan fokusera studier på enskilda substanser, utan att påverkas av andra ämnen som kan vara närvarande, även om dessa är snarlika det ämne man studerar. Till exempel innebär detta att man kan se skillnad på olika polymorfer av ett ämne. Denna selektivitet gör det möjligt att använda tekniken för att säkert identifiera många former av sprängämnen, narkotika och läkemedel. Man skulle därför kunna använda tekniken i en rad olika tillämpningar, såsom att detektera minor eller för att upptäcka förfalskade läkemedel. I det här projektet vill vi förbättra möjligheten att upptäcka och identifiera intressanta ämnen, speciellt genom att utveckla metoder för att reducera effekten av störningar. Tyvärr påverkas NQR-signaler avsevärt av störningar från t.ex. radiosändningar eller av närvaron av metall, och det är därför viktigt att ta fram tekniker för att försöka minska dessa störningars inverkan. Genom att hitta nya och bättre sätt att få fram den intressanta informationen, kommer vi att möjliggöra praktiskt användbara sensorer, t.ex. för att upptäcka svald narkotika. Under projektet kommer vi speciellt att studera just detta problem, som har flera betydande utmaningar, såsom att man inte kan bestråla personer med alltför kraftiga elektriska fält. Ett annat problem är att smugglad narkotika ofta är oren, vilket gör att man måste kunna detektera flera olika varianter av samma preparat. Denna del av arbetet kommer att utföras i nära samarbete med ledande NQR experter för att säkerställa tillgång till mätdata och expertkunskap.

Project period

Number of project years*

4

Calculated project time*

2016-01-01 - 2019-12-31

Classifications

Select a minimum of one and a maximum of three SCB-codes in order of priority.

Select the SCB-code in three levels and then click the lower plus-button to save your selection.

SCB-codes*

2. Teknik > 202. Elektroteknik och elektronik > 20205. Signalbehandling

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Enter a minimum of three, and up to five, short keywords that describe your project.

Keyword 1*

Spectroscopic signals

Keyword 2*

Statistical signal processing

Keyword 3*

Detection and estimation theory

Keyword 4

Keyword 5

Research plan

Ethical considerations

Specify any ethical issues that the project (or equivalent) raises, and describe how they will be addressed in your research. Also indicate the specific considerations that might be relevant to your application.

Reporting of ethical considerations*

Inga etiska överväganden är aktuella; arbetet är av en teoretisk natur.

The project includes handling of personal data

No

The project includes animal experiments

No

Account of experiments on humans

No

Research plan

Purpose and aims

The proposed research is concerned with the modeling and identification of nuclear quadrupole resonance (NQR) and nuclear magnetic resonance (NMR) spectroscopy signals. In both cases, the observed signal results from the interaction between the quadrupole moment of the nucleus and the field gradient. For NQR, one only utilizes an electric field, whereas, for NMR, one also makes use of a magnetic field. The latter makes a dramatic difference in the resulting signals, and whereas NQR will only yield very weak signals, and then only for solid state substances, NMR will generally result in signals with a high signal-to-noise ratio (SNR), even for liquid substances. However, even though the resulting signals are weak, NQR offers some benefits that NMR does not (and vice versa).

In this work, we strive to exploit the structure of the NQR and NMR signals to achieve an improved identification capability as compared to existing techniques. For NQR signals, the primary aim is to reduce the performance degradation resulting from interference and signal variabilities, whereas for NMR, we examine how efficient sampling schemes should be designed to improve the performance, as well as how the desired signal characteristics should be estimated. Our specific aims are to:

(i) Drastically reduce the required experimental time for NMR measurements without sacrificing accuracy in peak quantification, by both determining efficient non-uniform sampling (NUS) schemes and reliable identification techniques for NUS NMR signals;

(ii) Improve on the existing NQR signal models and determine ways of reducing the performance deterioration resulting from the presence of strong interference signals, with the aim of developing systems able to detect narcotics hidden on or inside the body.

The proposed research is of a collaborative nature, and the applicant has ongoing collaborations with four of the worlds foremost NQR groups, namely the groups of Prof. Althoefer, King's College London (KCL), Prof. Trontelj, the University of Ljubljana (UoL), Prof. Apih, the Institute Josef Stefan (IJS), and Prof. Itozaki, the University of Osaka (UoO). Similarly, the applicant collaborates on NMR research with Prof. Akke at Lund University (LU). These collaborations ensure that the applicant has access to both measurement data and expert knowledge in spectroscopy.

Survey of the field and preliminary results

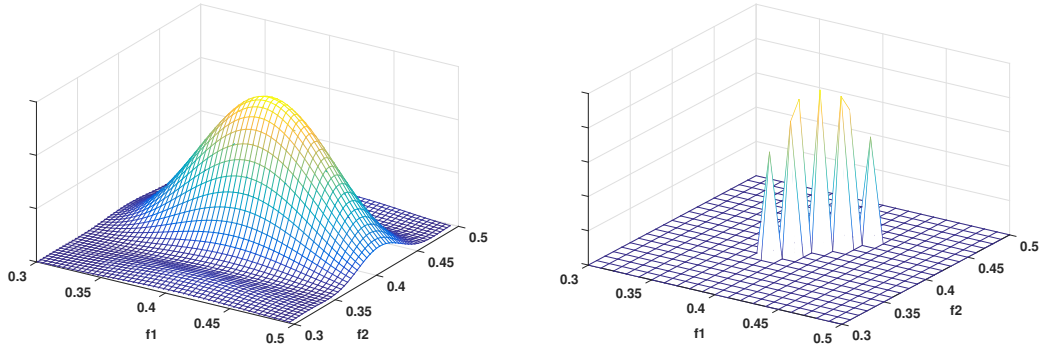
The proposed research in NMR spectroscopy is concerned with protein dynamics, which is essential for the majority of biological processes, including molecular recognition and enzyme catalysis [1]. It has recently been established that conformational fluctuations have a direct bearing on ligand binding affinities, which are of key importance for drug design [2]. Today, a large range of NMR methods is available for this purpose, with the majority of these involving NMR relaxation measurements. Traditional NMR relaxation methods all have the drawback of involving lengthy acquisition schemes, which impose heavy demands on instrument time and limits the usefulness for studies of samples with limited lifetimes, such as living cells. There are several reasons for the lengthy acquisitions: (i) every experiment typically comprises 10–30 two-dimensional (2D) NMR spectra with parametrically varied relaxation delays; (ii) each 2D spectrum needs to be sampled with very high resolution to resolve the large number of peaks

in a protein NMR spectrum, so as to achieve atomic-resolution information and accurate peak quantification; (iii) protein samples typically have low concentrations, which limits the inherent sensitivity; (iv) experiments often need to be repeated at different ligand concentrations, external magnetic field strengths, and sample temperatures. Notably, peak intensity versus relaxation time (delay) constitute the underlying data used to derive dynamic properties, which puts special demands on the accuracy of quantitative peak measurements.

Traditionally, NMR signals are sampled uniformly, such that the signal power is measured at regular intervals, and the majority of available techniques for analyzing NMR signals assume that the signals are measured in this way. Recently, NMR researchers have begun to examine the possibility of measuring the NMR signal using irregular sampling in some of the considered dimensions, such that the measured tensor contains fewer measurements in these dimensions as compared to the typical regular sampling. This development is due to recent research in sparse modeling and compressive sensing, showing that, theoretically, one may achieve the same spectral resolution with a NUS signal as one may with a uniformly sampled signal, although the former uses only a fraction of the number of samples required for the latter. This somewhat counter-intuitive result relies on that the measured signal is in some sense sparse, and that a sufficient number of the non-uniform samples are taken at the same rate as the regular sampling, in order to capture the high-frequency behavior of the signal, whereas only a few remaining samples are required to allow for a reconstruction of the signal [3, 4]. As a consequence, only a fraction of the samples normally required using a regular sampling are needed to achieve the same resolution.

This implies potentially dramatic time savings, possibly making it feasible to also perform in-cell dynamic studies. As an example, a recent study of a 4D NMR measurement that would have taken about 2.5 years to perform using a regular sampling, in order to achieve the desired resolution, was possible to construct in merely 90 hours using an irregular sampling [5]. In order to achieve this level of time savings, both the used sampling pattern and the method used for data reconstruction are crucial. As a result, many recent studies have examined the potential and the limitations of various sampling schemes and reconstruction methods of NUS signals (see, e.g., [6–9] and the references therein). Often, the used sampling schemes strive to use random and pseudo-random sampling patterns, as, in order to achieve an optimal reconstruction, the coherence between the sensing and the representation basis should be as low as possible.

For reconstruction, most examined techniques use a standard Fourier transformation matrix, such that the NMR spectral lines are modeled as non-decaying sinusoids, even though this will lead to spectral artifacts in the reconstruction. An example of this is shown in Figure 1, showing the spectral estimate of a single 2D NMR component using (a) the regular periodogram estimate and (b) a Lasso-based estimate, the latter being formed by imposing an ℓ_1 constraint on the resulting minimization (see, e.g., [7, 10–12] and the references therein). As seen from the figures, the decaying structure of the spectral line widens the spectral peak in the periodogram, further reducing its already inherently limited spectral resolution, while yielding a range of spurious spectral peaks in the Lasso estimate. To avoid such spectral leakage in a dictionary-based technique, such as the Lasso, one may extend the dictionary to contain candidate elements with different line-widths, allowing the minimization to select the dictionary atom with both the appropriate frequency and line-width, and some efforts on improving the sparse reconstruction



(a) **(b)**

Figure 1: Illustration of (a) the periodogram and (b) a Lasso-based spectral estimate.

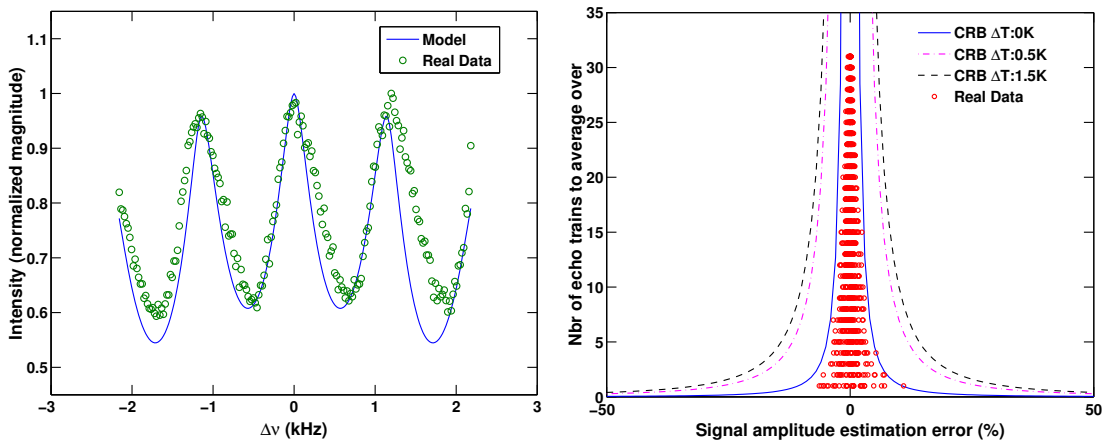
techniques in this way have been made (see, e.g., [11, 13] and[1] [C:13]). Simply extending the dictionary to contain a large range of line-widths for each frequency quickly becomes infeasible as the dimensionality of the problem grows, and therefore needs to be done with care, for instance using an iterative zooming approach, as suggested in [13], or using a dictionary learning approach reminiscent to the one we suggested in [C:13].

For NQR spectroscopy, the field is less developed, and there are still many open issues to be addressed. The use of only the electrical field in the measurement, as is done in NQR, implies that the resulting signals are much weaker than the corresponding NMR signals, but also that the signals are highly specific, and suffers from little or no interference from other materials that may be present [14]. This enables the technique to be used for unequivocal *close range* detection and identification of *solid-state* substances containing quadrupolar nuclei[2], allowing for a reliable identification of both the quantity of the substance of interest and of its purity. During the last decade, the applicant has worked closely with several of the world's most well-known NQR researchers, making notable progress in deriving reliable detection and identification algorithms for NQR signals (see [B:1] and the references therein). Much of this work has been aimed at formulating algorithms exploiting the signal structure of the observed signal optimally and at countering the typically very notable interference signals corrupting the measurements [J:13, J:24, J:27, J:30, J:31, J:36, B:1, C:11].

Together with the NQR groups at KCL and JSI, the applicant has also worked on refining the actual NQR signal model. It is well known that the frequencies of the spectral lines are temperature dependent and will deviate noticeably from their expected locations even for small temperature offsets [17]. Recently, we have also verified that the expected amplitudes of the spectral lines will change significantly as a result of this frequency deviation, resulting in varying signal intensities as the substance temperature varies [18]. This is illustrated for (the single

[1]Due to the page limitation, we have opted not to include the full citations to our own work here; instead, we refer to the applicant's list of publications. Thus, J:1, B:2, and C:3 refer to journal papers 1, book/book chapter 2, and conference paper 3 in the publication list, respectively.

[2]These account for over 50% of the elements in the periodic table, and, in particular, the most commonly occurring quadrupolar nucleus, ^{14}N, occurs in almost all high explosives, many forms of narcotics, and in nearly 80% of all medicines [15, 16].



(a) **(b)**

Figure 2: (a) Comparison of experimental and theoretical signal intensities as a function of the frequency offset (b) the 99% estimation accuracy as determined using the CRB of the NQR signal intensity at different offset frequencies.

line substance) sodium nitrate in Figure 2(a), where our new model is compared to measured signal intensities for varying frequency offsets. Such variations in the expected signal intensity will strongly affect the quality of the resulting parameter estimates. This is illustrated in Figure 2(b), which shows the 99% estimation accuracy, as determined by the Cramér-Rao lower bound (CRB) of the NQR signal intensity, at different offset frequencies, as compared to the estimated amplitude errors obtained from actual measurements. The figure thus shows the number of echo trains that needs to be averaged to achieve a desired estimation accuracy. As expected, the CRB is seen to accurately yield the expected variability for the on-resonance case, i.e., for the case without temperature uncertainties. However, if one examines the expected accuracy, even for a minor temperature deviation of half a degree, which corresponds to the first minimum of the amplitude modulation model in Figure 2(a), it is clear that one would need to average a lot more echo trains to achieve the same accuracy, thus much prolonging the required measurement time. This variability has long been overlooked; most likely as, for laboratory measurements, this form of deviations are of less concern, as one may then retune the system appropriately to maximize the signal intensities. However, for a practical system, this is likely not feasible, and it is thus of uttermost importance to consider such variabilities, especially if aiming to quantify the amount present of a given substance, such as in the detection of counterfeit medicines.

Another area of interest is the typical presence of notable radio-frequency interference and the effects of spurious signals due to, for instance, piezoelectric or magneto-acoustic responses. These interferences are often stationary narrowband signals, such as those resulting from radio transmissions, but may also be non-stationary [J:13, J:24, J:30, C:11]. Such signals may occur for different reasons. For example, when we investigated the NQR-based heroin detector at Heathrow[3], it was clear that the measurements were corrupted by signals resulting from the

[3]The applicant and researchers from KCL were asked by the British Home Office to assess and make recommendations for this system. Our conclusions were that the system's performance was inadequate primarily due to poor interference suppression, and that our techniques could likely improve it notably.

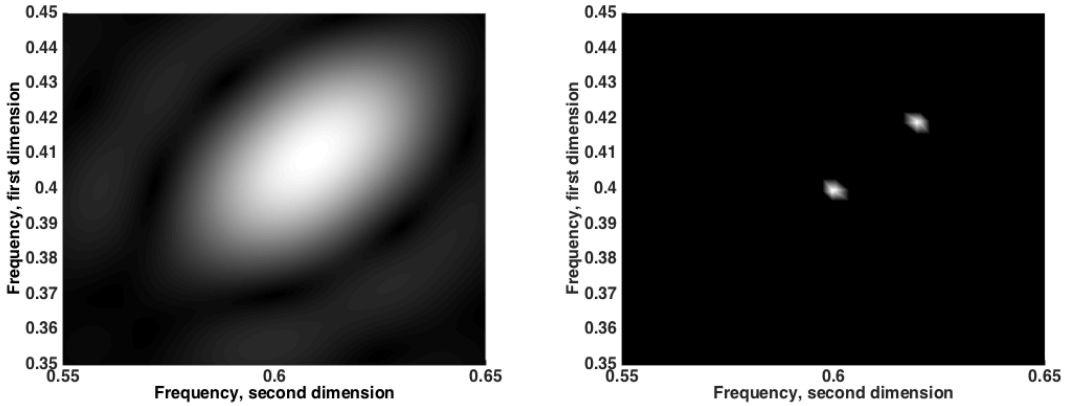


Figure 3: Estimates of two closely spaced modes using (a) the 2D periodogram and (b) the 2D SEMA.

conveyor belts and mechanical components within the sensor. Active electronics will also cause dramatic interference signals, which is important to consider for cases when electronic devices may be present within the scanned volume, such as when scanning a suitcase or a person.

Project description and some further preliminary results

(i) *Efficient identification of N-D NUS NMR signals*. As noted above, given the potential of NUS NMR spectroscopy, the problem of estimating the modes of N-D NUS NMR spectra is attracting significant interest. In [C:13], we introduced a sparse dictionary learning approach, termed SEMA, that allows for computationally efficient 2D spectral estimates yielding close to statistically efficient estimates. In forming these estimates, we split the required convex optimization into sub-problems using the ADMM technique (see, e.g., [19]). Figure 3 illustrates a typical estimate of a 2D NUS NMR signal of two closely spaced spectral lines, comparing the resulting 2D periodogram estimate with the SEMA estimate; as can be noted, the latter method does not suffer from the spectral leakage of the periodogram, nor from the spurious peaks commonly occurring in regular Lasso-based estimates, as illustrated (for a single spectral line) in Figure 1(b). As a part of the proposed research, we will extend on these results, aiming to formulate a computationally efficient N-D SEMA estimator. Using a similar dictionary learning approach as the one proposed in [C:13], we will extend the technique to allow for high-dimensional NUS tensor signals, as well as examine ways of computing the required steps in the algorithm efficiently, using the inherent structure of the resulting matrices, reminiscent of our earlier contributions in this area (see [J:12, J:15] and the references therein). We will also examine possibilities of using coordinate descent approaches for the ADMM subproblems [20], as well as using zooming techniques to compute local spectral estimates efficiently [21]. Another area of interest is the possible use of non-convex regression formulations; as was shown in [22], a major drawback of the Lasso algorithm is that it tends to produce biased estimates for larger coefficients. This can potentially be remedied by using a set of non-convex penalty

functions and the so-called DC (Difference of Convex functions) programming approach (see, e.g., [23]), or via smooth ℓ^0 approximations [24].

(ii) *Optimal sampling schemes for NMR*. As noted above, one may achieve notable performance gains by using a NUS scheme when measuring the NMR response in the indirect dimensions. Several studies to date have examined the performance of various (fixed) sampling schemes (see, e.g., [7–9, 25] and the references therein), most typically assuming that the signal contains pure spectral lines, neglecting the decaying structure of the signals. In the here proposed work, we aim instead to formulate an optimal sampling scheme for a given substance, taking the decaying signal structure into account. Using the multi-dimensional CRB for NUS NMR signals, as presented in [C:10], as a measure of performance for the parameters of interest, we will strive to form a sampling scheme in each indirect dimension that optimally captures these parameters, with the aim to allow for sampling schemes that are optimally formed to estimate the signal amplitudes, frequencies, or decays - or some combination of these characteristics. We have found that this may possibly be done by minimizing the loss resulting from the used sampling scheme over the set of all feasible sampling schemes. As a part of this study, we also aim at forming an adaptive sampling scheme, such that the next sampling point is selected optimally given the information retrieved from the earlier measurements, even if the exact characteristics of the substance at hand is unknown. The notion of forming a substance dependent adaptive sampling scheme has been examined in existing literature (see, e.g., [26,27] and the references therein), but then without any optimality criterion, and for given signal characteristics. Here, we propose instead to form such an adaptive scheme by extending upon the 1D results presented for adaptive compressed sensing in [28], such that one selects the following sample to minimize the CRB corresponding to the signal parameters, estimated using the observed measurements. For some experimental setups, one also wishes to vary the used flip-angle, such that the resulting sampling scheme depends on both the sampling times, in each dimension, and on the used flip-angles at each excitation pulse. Here, we will initially examine the problem of determining an adaptive multi-dimensional sampling scheme for fixed flip-angles, striving to extend upon the obtained results to also allow for a variable flip-angle scheme. The latter problem will first require that the signal model is extended to include the flip-angles, the derivation of the corresponding CRB, and to extend the adaptive sampling scheme accordingly.

(iii) *Improved estimation and identification of NQR signals*. In [J:2], we have presented results indicating that one may use the echo decay and the spectral line-width to determine the age, and possibly even the manufacturer, of pharmaceuticals. This is illustrated in Figure 4(a), which shows estimated parameters for two sets of paracetamol tablets, together with the corresponding CRB ellipses for two SNR values, clearly indicating that one may determine the age of the substance using the estimated line-width parameter, β. In Figure 4(b), we investigate this dependance further, showing how the line-width change with age[4]. In the proposed research, we wish to investigation this further, but also extend the

[4]Given the very limited data set, it is hard to draw any definite conclusions on how the line-width change with age; for illustration purposes, we show a possible exponential fit to the observed behavior, but clearly further work is needed to clarify how the line shape change with age.

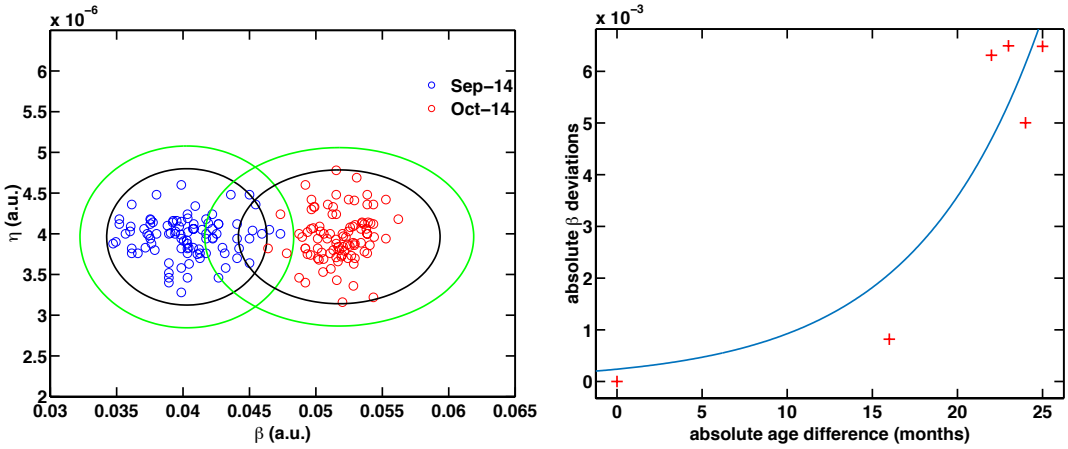


Figure 4: (a) Scatterplot of the line width (β) versus the echo train decay (η) for two batches of paracetamol of different age, along with their corresponding CRB ellipses for two SNR values, and (b) the absolute age difference versus the associated absolute β deviations from the reference/newest batch (red crosses). For illustration purposes, a possible exponential fit is shown (blue curve).

model to incorporate how the line shape depends on temperature (see, e.g., [29]). In connection with this, we will also examine the Voigt line shape model (see, e.g., [30, 31]); possibly, the Voigt line shape observed in some substances can partly be explained via variabilities in the line shape due to off-resonance effects, similar to those observed for the signal intensities [18], perhaps due to a temperature gradient over the observed sample (as the part of the substance that is close to the excitation coil will heat up during the experiment). In this work, we wish to examine these topics further[5]. As a part of this investigation, we will also extend upon the developed estimation algorithms to incorporate the refined signal model, including the one derived in [18] and for the possibility of Voigt line shapes.

(iv) *Detection of narcotics concealed on or in the body*. Another area of interest is the possibility to use atomic magnetometers for the detection of the NQR signal; recent work has indicated that one can expect an order of magnitude improvement of such a system (see, e.g., [32]), although the results are still quite preliminary. Together with UoL and UoO, we are examining this possibility, also to see if the signal or interference models need to be modified for such a system. In particular, we aim at examining the possibilities of using such a system to detect narcotics concealed in body cavities or swallowed in condoms, being common ways of smuggling such substances. This work has already been initiated together with researchers at the UoO, resulting in some preliminary findings on how to possibly deal with interference rejection for this setup [C:11].

(v) *Interference cancellation for unshielded NQR signals*. As discussed above, the NQR signals typically suffer from being corrupted by strong interference signals, in particular

[5]We note that much of the here proposed work may be done using the already measured data sets.

for non-shielded measurements. The applicant has in earlier work examined ways of reducing the influence of (primarily) stationary interference signals. In our efforts to examine narcotics hidden on or in the body, the screening will most likely need to be done without proper shielding, making the treatment of interference signals critical to the system. In particular, we strive to extend upon the work in [J:13], wherein we treat the subspaces spanned by both the signal of interest and the interference signals as only being partly known. In doing so, we will combine the notion of a persymmetric adaptive detector (see, e.g., [33, 34]), with sparse reconstruction techniques, exploiting that the interference signals are in general narrowband and may be well represented using a sparse framework. We also wish to examine how the ideas in [C:11] may be extended to allow for such partially known signals. In connection with this work, we will also examine the possibility of using a low-power non-resonance system to allow for a wider excitation, thereby allowing for the possible detection of multiple substances [35, 36]. This would imply that the observed signal should be modelled as a mixture from multiple substances, reminiscent of the ideas in [J:31], although we will strive to modify this model to instead use a sparse framework to model the signal mixture. As an alternative, we will examine how one may use multiple atomic magnetometers to excite a wider bandwidth, and we will examine possibilities to formulate a persymmetric adaptive multi-channel detector for this case.

Significance

The proposed work strives to make important contributions to the sampling and estimation of multidimensional NMR signals, being a current topic of great interest in the field. The possibility of developing optimal sampling schemes offers the potential of drastically reducing measurement times, as well as, hopefully, allow for studies of in-cell dynamics. Such possibilities would be of uttermost importance for the development of new medicines. The proposed studies in NQR focus on enabling devices to detect narcotics concealed on or in the body; currently, there are no non-invasive and non-ionizing techniques that allow for the latter problem. One of the main difficulties of such a system would be the development of reliable interference rejection techniques, and in particular for unshielded data. The proposed work strives to address this topic, as well as to improve the modeling of NQR signals in general.

References

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Interdisciplinarity

My application is interdisciplinary

☐

An interdisciplinary research project is defined in this call for proposals as a project that can not be completed without knowledge, methods, terminology, data and researchers from more than one of the Swedish Research Councils subject areas; Medicine and health, Natural and engineering sciences, Humanities and social sciences and Educational sciences. If your research project is interdisciplinary according to this definition, you indicate and explain this here.

Click here for more information

Scientific report

Scientific report/Account for scientific activities of previous project

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Budget and research resources

Project staff

Describe the staff that will be working in the project and the salary that is applied for in the project budget. Enter the full amount, not in thousands SEK.

Participating researchers that accept an invitation to participate in the application will be displayed automatically under Dedicated time for this project. Note that it will take a few minutes before the information is updated, and that it might be necessary for the project leader to close and reopen the form.

Dedicated time for this project

	Role in the project	Name	Percent of full time
1	Applicant	Andreas Jakobsson	30
2	Other personnel without doctoral degree	Doktorand	100

Salaries including social fees

	Role in the project	Name	Percent of salary	2016	2017	2018	2019	Total
1	Applicant	Andreas Jakobsson	30	342,991	353,281	363,880	374,796	1,434,948
2	Other personnel without doctoral degree	Doktorand	100	480,728	513,137	545,545	558,149	2,097,559
	Total			823,719	866,418	909,425	932,945	3,532,507

Other costs

Describe the other project costs for which you apply from the Swedish Research Council. Enter the full amount, not in thousands SEK.

Premises

	Type of premises	2016	2017	2018	2019	Total
1	Kontor	50,495	51,213	53,643	54,971	210,322
	Total	50,495	51,213	53,643	54,971	210,322

Running Costs

	Running Cost	Description	2016	2017	2018	2019	Total
1	Direkta kostnader	Dator	30,000				30,000
2	Direkta kostnader	Konferensresa	40,000	40,000	40,000	40,000	160,000
	Total		70,000	40,000	40,000	40,000	190,000

Depreciation costs

	Depreciation cost	Description	2016	2017	2018	2019

Total project cost

Below you can see a summary of the costs in your budget, which are the costs that you apply for from the Swedish Research Council. Indirect costs are entered separately into the table.

Under Other costs you can enter which costs, aside from the ones you apply for from the Swedish Research Council, that the project includes. Add the full amounts, not in thousands of SEK.

The subtotal plus indirect costs are the total per year that you apply for.

Total budget

Specified costs	2016	2017	2018	2019	Total, applied	Other costs	Total cost
Salaries including social fees	823,719	866,418	909,425	932,945	3,532,507		3,532,507
Running costs	70,000	40,000	40,000	40,000	190,000		190,000
Depreciation costs					0		0
Premises	50,495	51,213	53,643	54,971	210,322		210,322
Subtotal	944,214	957,631	1,003,068	1,027,916	3,932,829	0	3,932,829
Indirect costs	407,894	413,689	433,318	444,052	1,698,953		1,698,953
Total project cost	1,352,108	1,371,320	1,436,386	1,471,968	5,631,782	0	5,631,782

Explanation of the proposed budget

Briefly justify each proposed cost in the stated budget.

Explanation of the proposed budget*

In the proposed project, funding is sought for one Ph.D. student as well as funds for the applicant's participation in the project. The costs include 50.04% employment costs (where appropriate). The indirect costs are computed at 45.64% of the budget. Rooms are included at 5.65%. The costs include a projected salary increase of 3% for Jakobsson, as well as the expected salary increase according to the Ph.D. salary scheme.

Other funding

Describe your other project funding for the project period (applied for or granted) aside from that which you apply for from the Swedish Research Council. Write the whole sum, not thousands of SEK.

Other funding for this project

Funder	Applicant/project leader	Type of grant	Reg no or equiv.	2016	2017	2018	2019

CV

Professor Andreas Jakobsson

Curriculum Vitae, March 10, 2015

1. Higher education degrees:
   - Ph.D., Signal processing, Uppsala University, 2000.
   - Tekn. Licentiate, Signal processing, Uppsala University, 1997.
   - M.Sc., Computer Science and Engineering, Lund Institute of Technology, 1993.
2. Doctoral degree
   - "Model-Based and Matched-Filterbank Signal Analysis", Ph.D. thesis, Uppsala University, February 2000. Advisor: Prof. Petre Stoica.
3. Postdoctoral work
   - Post-doc (20%), Royal Institute of Technology, Sweden, 2001-2002.
4. Appointments as docent/professor
   - Professor in Mathematical Statistics, Lund University, Sweden, 2008.
   - Professor in Signal Processing, Karlstad University, Sweden, 2006
   - Docent, Signal Processing, Karlstad University, 2005.
5. Current position
   - Professor in Mathematical Statistics, Lund University, Sweden, permanent position. Position includes 20% research during 2015. Head of division since 2013.
6. Previous positions
   - [2006-2008] Professor in Signal Processing, Karlstad University, Sweden.
   - [2004-2006] Associate Professor, Karlstad University, Sweden.
   - [2002-2003] Lecturer, King's College London, UK.
   - [2001-2002] Post-doc (20%), Royal Institute of Technology, Sweden.
   - [1999-2002] Senior R&D Engineer, Global IP Sound AB, Sweden.
7. Interruptions in research
   - [2007] Parental leave for 3 months.
   - [2001-2002] Parental leave for 10 months.
8. Supervision - Ph.D. students

   Current students, with expected year of graduation
   - Rachele Anderson, Lund University, 2019. Co-supervisor.
   - Unn Dahlén, Lund University, 2019. Co-supervisor.

- Johan Brynolfsson, Lund University, 2017. Co-supervisor.
- Johan Swärd, Lund University, 2017. Main supervisor.
- Ted Kronvall, Lund University, 2017. Main supervisor.
- Georgia Kyriakidou, King's College London, 2015. External supervisor.

Finished students, with graduation year

- Stefan Ingi Adalbjörnsson, Lund University, 2014. Main supervisor.
- Naveed Butt, Lund University, 2011. Main supervisor.
- Erik Gudmundson, Uppsala University, 2010. Co-supervisor.
- Samuel Somasundaram, King's College London, 2007. External supervisor.
- Thomas Bowles, Cardiff University, 2006. Co-supervisor.
- Zhuo Zhang, Cardiff University, 2005. Main supervisor.

9. Supervision - Post-docs
   - Dr Naveed Butt, 2011-2014.
   - Dr Erik Gudmundson, 2010-2014
   - Dr Samuel Somasundaram, 2007-2008.
10. Other points of merit
    - During 2007-2008, Dr Jakobsson was a member of the University Board at Karlstad University. During 2004-2008, he was responsible for the graduate program in Electrical Engineering at Karlstad University, Sweden. During 2009-2013, he was the deputy program manager for the M.Sc. program in Engineering Mathematics at Lund University, Sweden.
    - During spring 2008, Dr Jakobsson held a visiting professorship at King's College London, UK. During 2004-2009, he held an Honorary Research Fellowship at Cardiff University, UK. Dr Jakobsson has acted as an expert for the IAEA in China, as well as for the British HMRC's evaluation of NQR equipment at Heathrow airport, UK.
    - Dr Jakobsson is a member of The Royal Swedish Physiographic Society, a Senior Member of IEEE, and an Associate Editor for Elsevier Signal Processing (2011-). He has previously also been an Associate Editor for the IEEE Transactions on Signal Processing (2006-2010), the IEEE Signal Processing Letters (2007-2011), the Research Letters in Signal Processing (2007-2009), and the Journal of Electrical and Computer Engineering (2009-2014). He has also been a member of the IEEE Sensor Array and Multichannel (SAM) Signal Processing Technical Committee (2008-2013).

Publication list

Professor Andreas Jakobsson

List of Publications, March 11, 2015

The following list contains the applicant's work published since 2007. Conference papers on work also published in journal papers have been excluded from the list. The five publications that are most important to the proposed project are marked with ($\star$). Citations have been computed using the Google Scholar, and thus include self-citations.

1. Peer-reviewed articles

1. S. D. Somasundaram, N. R. Butt, A. Jakobsson, and L. Hart, "Evaluation of Computationally Efficient Robust Adaptive Beamforming for Passive Sonar", to appear in *IEEE Journal of Oceanic Engineering. Number of citations: 0*
2. G. Kyriakidou, A. Jakobsson, K. Althoefer, and J. Barras, "Batch-Specific Discrimination using Nuclear Quadrupole Resonance Spectroscopy", to appear in *Analytical Chemistry. Number of citations: 0* ($\star$)
3. S I. Adalbjörnsson, J. Swärd, J. Wallin, and A. Jakobsson, "Estimating Periodicities in Symbolic Sequences Using Sparse Modeling", to appear in *IEEE Transactions on Signal Processing. Number of citations: 0*
4. S. I. Adalbjörnsson, A. Jakobsson, and M. G. Christensen, "Multi-Pitch Estimation Exploiting Block Sparsity", *Elsevier Signal Processing*, Vol. 109, pp. 236-247, April 2015. *Number of citations: 0* ($\star$)
5. G. O. Glentis, K. Zhao, A. Jakobsson, H. Abeida, and J. Li, "SAR Imaging via Efficient Implementations of Sparse ML Approaches", *Elsevier Signal Processing*, Vol. 95, pp.15-26, Feb. 2014. *Number of citations: 3*
6. J. R. Jensen, G. O. Glentis, M. G. Christensen, A. Jakobsson, and S. H. Jensen, "Fast LCMV-based Methods for Fundamental Frequency Estimation', *IEEE Transactions on Signal Processing*, Vol. 61, No. 12, pp. 3159-3172, Dec. 2013. *Number of citations: 1*
7. K. Angelopoulos, G. O. Glentis, and A. Jakobsson, "Computationally Efficient Sparsity-Inducing Coherence Spectrum Estimation of Complete and Non-Complete Data Sets", *Elsevier Signal Processing*, Vol. 93, No. 5, pp. 1221-1234, May 2013. *Number of citations: 4*
8. G. O. Glentis, K. Zhao, A. Jakobsson, and J. Li, "Non-Parametric High-Resolution SAR Imaging", *IEEE Transactions on Signal Processing*, Vol. 71, No. 7, pp. 1614-1624, April 2013. *Number of citations: 9*

9. K. Angelopoulos, G. O. Glentis, and A. Jakobsson, "Computationally Efficient Capon- and APES-based Coherence Spectrum Estimation", *IEEE Transactions on Signal Processing*, Vol. 60, No. 12, pp. 6674-6681, Dec. 2012. *Number of citations: 3*

10. S. D. Somasundaram, A. Jakobsson, and N. H. Parsons, "Robust and Automatic Data-Adaptive Beamforming for Multi-Dimensional Arrays", *IEEE Transactions on Geoscience and Remote Sensing*, Vol. 50, No. 11, pp. 4642-4656, Nov. 2012. *Number of citations: 10*

11. A. Jakobsson, G. O. Glentis, and E. Gudmundson, "Computationally Efficient Time-Recursive IAA-Based Blood Velocity Estimation", *IEEE Transactions on Signal Processing*, Vol. 60, No. 7, pp. 3853-3858, July 2012. *Number of citations: 7*

12. G. O. Glentis and A. Jakobsson, "Superfast Approximative Implementation of the IAA Spectral Estimate", *IEEE Transactions on Signal Processing*, Vol. 60, No. 1, pp. 472-478, Jan. 2012. *Number of citations: 21*

13. A. Svensson and A. Jakobsson, "Adaptive Detection of a Partly Known Signal Corrupted by Strong Interference", *IEEE Signal Processing Letters*, Vol. 18, No. 12, pp. 729-732, Dec. 2011. *Number of citations: 8* ($\star$)

14. M. G. Christensen, J. L. Højvang, A. Jakobsson, and S. H. Jensen, "Joint Fundamental Frequency and Order Estimation using Optimal Filtering", *EURASIP Journal on Advances in Signal Processing*, Vol. 13, 2011. *Number of citations: 20*

15. G. O. Glentis and A. Jakobsson, "Efficient Implementation of Iterative Adaptive Approach Spectral Estimation Techniques", *IEEE Transactions on Signal Processing*, Vol. 59, No. 9, pp. 4154-4167, Sept. 2011. *Number of citations: 36*

16. N. R. Butt, M. Nilsson, A. Jakobsson, M. Nordberg, A. Pettersson, S. Wallin, and H. Östmark, "Classification of Raman Spectra to Detect Hidden Explosives", *IEEE Geoscience and Remote Sensing Letters*, Vol. 8, No. 3, pp. 516-520, 2011. *Number of citations: 15*

17. E. Gudmundson, A. Jakobsson, J. A.. Jensen, and P. Stoica, "Blood Velocity Estimation Using Ultrasound and Spectral Iterative Adaptive Approaches", *Elsevier Signal Processing*, Vol. 91, No. 5, pp. 1275-1283, May 2011. *Number of citations: 19*

18. G. O. Glentis and A. Jakobsson, "Time-Recursive IAA Spectral Estimation", *IEEE Signal Processing Letters*, Vol. 18, No. 2, pp. 111-114, February 2011. *Number of citations: 28*

19. M. G. Christensen and A. Jakobsson, "Optimal Filter Designs for Separating and Enhancing Periodic Signals", *IEEE Transactions on Signal Processing*, Vol. 58, No. 12, pp. 5969-5983, December 2010. *Number of citations: 27*

20. N. R. Butt and A. Jakobsson, "Coherence Spectrum Estimation from Non-Uniformly Sampled Sequences", *IEEE Signal Processing Letters*, Vol. 17, No. 4, pp. 339-342, April 2010. *Number of citations: 25*

21. E. Gudmundson, P. Stoica, J. Li, A. Jakobsson, M. D. Rowe, J. A. S. Smith, and J. Ling, "Spectral Estimation of Irregularly Sampled Exponentially Damped Sinusoids with Applications to RF Spectroscopy", *Journal of Magnetic Resonance*, Vol. 203, pp. 167-176, 2010. *Number of citations: 17*

22. M. G. Christensen, A. Jakobsson and S. H. Jensen, "Sinusoidal Order Estimation using Angles between Subspaces", *EURASIP Journal on Advances in Signal Processing*, vol. 2009, Article ID 948756, 11 pages, 2009. *Number of citations: 30*

23. F. Gran, A. Jakobsson and J. A.. Jensen, "Adaptive spectral Doppler estimation", *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, Vol. 56, No. 4, pp. 700-714, April 2009. *Number of citations: 21*

24. S. D. Somasundaram, A. Jakobsson and N. R. Butt, "Countering Radio Frequency Interference in Single Sensor Quadrupole Resonance", *IEEE Geoscience and Remote Sensing Letters*. Vol. 6, No. 1, pp. 62-66, January 2009. *Number of citations: 20*

25. M. G. Christensen, J. H. Jensen, A. Jakobsson and S. H. Jensen, "On Optimal Filter Designs for Fundamental Frequency Estimation", *IEEE Signal Processing Letters*, Vol. 15, pp. 745-748, 2008. *Number of citations: 17*

26. N. R. Butt, A. Jakobsson, S. D. Somasundaram and J. A. S. Smith, "Robust Multichannel Detection of Mixtures Using Nuclear Quadrupole Resonance", *IEEE Transactions on Signal Processing*, Vol. 56, No. 10, pp. 5042-5050, October 2008. *Number of citations: 4*

27. S. D. Somasundaram, A. Jakobsson, M. D. Rowe, J. A. S. Smith, N. R. Butt and K. Althoefer, "Robust Detection of Stochastic Nuclear Quadrupole Resonance Signals", *IEEE Transactions on Signal Processing*, Vol. 56, No. 9, pp. 4221-4229, September 2008. *Number of citations: 21*

28. M. G. Christensen, P. Stoica, A. Jakobsson and S. H. Jensen, "Multi-Pitch Estimation", *Signal Processing*, Vol. 88, No. 4, pp. 972-983, April 2008. *Number of citations: 50*

29. N. R. Butt, S. D. Somasundaram, A. Jakobsson and J. A. S. Smith, "Frequency-Selective Robust Detection and Estimation of Polymorphic QR Signals", *Signal Processing*, Vol. 88, No. 4, pp. 834-843, April 2008. *Number of citations: 8*

30. S. D. Somasundaram, A. Jakobsson and E. Gudmundson, "Robust NQR Signal Detection Allowing for Amplitude Uncertainties", *IEEE Transactions on Signal Processing*, Vol. 56, No. 3, pp. 887-894, March 2008. *Number of citations: 13*

31. S. D. Somasundaram, A. Jakobsson and J. A. S. Smith, "Analysis of NQR Signals from Mixtures", *Signal Processing*, Vol. 88, No. 1, pp. 146-157, January 2008. *Number of citations: 10*

32. A. Jakobsson, M. G. Christensen and S. H. Jensen,"Frequency Selective Sinusoidal Order Estimation", *IET Electronic Letters*, Vol. 43, No. 21, pp. 1164-1165, October 2007. *Number of citations: 4*

33. A. Jakobsson and M. Mossberg, "Using Spatial Diversity to Detect Narcotics and Explosives Using NQR Signals", *IEEE Transactions on Signal Processing*, Vol. 55, No. 9, pp. 4721-4726, September 2007. *Number of citations: 7*

34. M. G. Christensen, A. Jakobsson and S. H. Jensen, "Joint High-Resolution Fundamental Frequency and Order Estimation", *IEEE Transactions on Audio, Speech and Language Processing*, Vol. 15, No. 5, pp. 1635-1644, May 2007. *Number of citations: 59*

35. A. Jakobsson, S. R. Alty, and J. Benesty, "Estimating and Time-Updating the 2-D Coherence Spectrum", *IEEE Transactions on Signal Processing*, Vol. 55, No. 5, pp. 2350-2354, May 2007. *Number of citations: 17*

36. S. D. Somasundaram, A. Jakobsson, J. A. S. Smith and K. Althoefer, "Exploiting Spin Echo Decay in the Detection of Nuclear Quadrupole Resonance Signals", *IEEE Transactions on Geoscience and Remote Sensing*, Vol. 45, No. 4, pp. 925-933, April 2007. *Number of citations: 32* ($\star$)

2. Peer-reviewed conference contributions

1. T. Kronvall, M. Juhlin, S. I. Adalbjörnsson, and A. Jakobsson, "Sparse Chroma estimation for Harmonic Audio", *40th International Conference on Acoustics, Speech, and Signal Processing*, Brisbane, April 19-24, 2015. *Number of citations: 0*

2. J. Swärd, J. Brynolfsson, A. Jakobsson, and M. Hansson-Sandsten, "A Sparse Semi-Parametric Chirp Estimator", *48th Asilomar Conference on Signals, Systems and Computers*, Pacific Grove, Nov. 2-5, 2014. *Number of citations: 0*

3. S. I. Adalbjörnsson, J. Swärd, A. Jakobsson, and T. Kronvall, "A Sparse Approach for Estimation of Amplitude Modulated Sinusoids", *48th Asilomar Conference on Signals, Systems and Computers*, Pacific Grove, Nov. 2-5, 2014. *Number of citations: 0*

4. S. D. Somasundaram and A. Jakobsson, "Degradation of Covariance Reconstruction-Based Adaptive Beamformers in the Presence of Interferer Steering Vector Errors", *Sensor Signal Processing for Defense*, Edinburgh, Sept. 8-9, 2014. *Number of citations: 0*

5. J. Brynolfsson, J. Swärd, A. Jakobsson, and M. Sandsten, "Smooth 2-D Frequency Estimation using Covariance Fitting", *22nd European Signal Processing Conference* , Lisbon, Portugal, September 1-5, 2014. *Number of citations: 0*

6. G. Kyriakidou, A. Jakobsson, E. Gudmundson, A. Gregorovič, J. Barras, and K. Althoefer, "Improved modeling and bounds for NQR spectroscopy signals", *22nd European Signal Processing Conference* , Lisbon, Portugal, September 1-5, 2014. *Number of citations: 0*

7. T. Kronvall, S. I. Adalbjörnsson, and A. Jakobsson, "Joint DOA and Multi-pitch estimation via Block Sparse Dictionary Learning", *22nd European Signal Processing Conference* , Lisbon, Portugal, September 1-5, 2014. *Number of citations: 0*

8. G. O. Glentis, J. Karlsson, A. Jakobsson, and J. Li, "Efficient Spectral Analysis in the Missing Data Case using Sparse ML Methods", *22nd European Signal Processing Conference* , Lisbon, Portugal, September 1-5, 2014. *Number of citations: 0*

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3. J. Barras, A. Jakobsson, E. Gudmundson, M. D. Rowe, I. J. F. Poplett, J. Luznik, V. Jazbinsek, J. Pirnat, J. Seliger, Z. Trontelj, J. A. S. Smith, and K. Althoefer, "The Emerging Field of Medicines Authentication by Nuclear Quadrupole Resonance Spectroscopy", *Counterfeit Medicines Volume II: Detection, Identification and Analysis*, Eds. P. Wang and A. I. Wertheimer, ILM Publications, 2013. *Number of citations: 0*

4. M. G. Christensen and A. Jakobsson,"Multi-pitch estimation", *Morgan & Claypool*, 2009. *Number of citations: 112* ($\star$)

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2. A. Jakobsson, S. D. Somasundaram and J. A. S. Smith, "Analysing NQR Signals in the Presence of Multiple Polymorphic Forms", Publication No. WO 2008 029119.

3. A. Jakobsson and M. Mossberg, “Method and System for Detection of Possibly Harmful Items”, Publication No. WO 2008 008035.

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CV

Name: Andreas Jakobsson	**Doctorial degree:** 2000-02-11
Birthdate: 19701116	**Academic title:** Professor
Gender: Male	**Employer:** No current employer

Research education

Dissertation title (swe)

Dissertation title (en)

Model-based and matched-filterbank signal analysis

Organisation	Unit	Supervisor
Uppsala universitet, Sweden Sweden - Higher education Institutes	Inst för teknikvetenskaper	Petre Stoica
Subject doctors degree	**ISSN/ISBN-number**	**Date doctoral exam**
20205. Signalbehandling	91-554-4571-3	2000-02-11

Publications

Name: Andreas Jakobsson	**Doctorial degree:** 2000-02-11
Birthdate: 19701116	**Academic title:** Professor
Gender: Male	**Employer:** No current employer

Jakobsson, Andreas has not added any publications to the application.

Register

Terms and conditions

The application must be signed by the applicant as well as the authorised representative of the administrating organisation. The representative is normally the department head of the institution where the research is to be conducted, but may in some instances be e.g. the vice-chancellor. This is specified in the call for proposals.

The signature*from the applicant*confirms that:

- the information in the application is correct and according to the instructions form the Swedish Research Council
- any additional professional activities or commercial ties have been reported to the administrating organisation, and that no conflicts have arisen that would conflict with good research practice
- that the necessary permits and approvals are in place at the start of the project e.g. regarding ethical review.

The signature *from the administrating organisation* confirms that:

- the research, employment and equipment indicated will be accommodated in the institution during the time, and to the extent, described in the application
- the institution approves the cost-estimate in the application
- the research is conducted according to Swedish legislation.

The above-mentioned points must have been discussed between the parties before the representative of the administrating organisation approves and signs the application.

Project out lines are not signed by the administrating organisation. The administrating organisation only sign the application if the project outline is accepted for step two.

Applications with an organisation as applicant is automatically signed when the application is registered.