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**Harold H. Szu
F. Jack Agee**
Editors

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Introduction

SPIE's conference on Independent Component Analyses, Wavelets, Neural Networks, Biosystems, and Nanoengineering (ICAN) was established as part of the Aerosense Symposium over a decade ago. Our conference, though relatively small, is well attended and covers basic math-bio-science-tech and societal needs. It takes a hard science approach to soft societal concerns, ranging from IT "digging knowledge" to biomedical wellness in senior home security, which will comprise about half a dozen papers in this volume and will likely become even more important in the following years! Onsite publication of the proceedings provides timely dissemination of the research to conference attendees, as well as to worldwide libraries; the publication of this volume coincides with the start of the conference: 13 April 2009.

Being co-chairs, we often face questions about our goals and focus for the future of the conference series. To state the question plainly, how has the conference endured, and how can it continue to endure and evolve in an uncertain future? The answer lies partly in the following secret: We have adapted a workable system tested by the Nobel Foundation for over half a century—passing the baton of honor.... "The past award recipients shall determine the new awardees." The role SPIE and the co-chairs serve is to act as facilitators for the decision process. A major difference between the systems is a lack of recourse in supporting the awardees. Thus we have improvised a temporary win-win-win solution: in order to prepare the interdisciplinary audience, state of the art knowledge is disseminated by both past and present award recipients, who are encouraged to teach short courses at the meetings.

The ICAN conference, now in its 16th year with SPIE, was established to address our desire to learn from Mother Nature. The question of where to begin is a difficult one and thus we began slowly, building year by year, learning from one another. This year the results have been impressive. From the 2009 Wavelet Pioneer Award Recipient Prof. Ronald Coifman (Yale University), we learn how to "steal a smart algorithm" from the ear-eye like Wavelet transform. In the same theme, we follow brain-like neural nets seeking to learn, from observable effects, the underlying hidden causes, explained by the 2009 ICAN Unsupervised Learning Award recipient Prof. Mark Girolami (University of Glasgow). After a decade, some are ready for the "implementation" and "test and evaluation" of these advances. With this in mind, we encourage you to consider the NIH-phobia problem explained by our 2009 Biomedical Wellness Award recipient Prof. Takeshi Yamakawa (Kuyshu Institute of Technology). We introduce so-called "Nano-Engineering," as elucidated by our 2009 Nano-Engineering Pioneer Award recipient Dr. Robert Shull (National Institute of Standards and Technology). Nano-engineers can take advantage of the transitional nanometer regime, which falls between classical

physics and quantum mechanics and is technically defined as 10^{-9} m = 10 angstrom = 20 hydrogen atoms. Finally, we are ready to emulate the most robust, and perhaps most efficient field in its own right, System Biology, as elucidated by our 2009 System Biology Award recipient Prof. Olaf Wolkenhauer (University of Rostock), during the last day of our end-to-end program.

We wish to thank all of last year's recipients who have graciously co-chaired an award selection process. The chairs include the former recipients in Wavlets: Prof. Mark Smith (Purdue) and Prof. Victor Wickerhauser (Washington University in St. Louis); ICA Unsupervised Learning Recipient Prof. Tzyy-Ping Jung (University of California, San Diego, in 2008); Nanoengineering Pioneers Prof. Toshio Fukuda (Nagoya University, Japan, in 2008) and BMW recipient Prof. Soo-Young Lee (Korea Advanced Institute of Science and Technology, Republic of Korea, in 2008).

The Conference could not be successful without your unselfish willingness to share and contribute to the conference series. We also thank SPIE's technical support and the thirty-member program committee, as well as the five conference co-chairs: Dr. F. Jack Agee (Rice University), Dr. Kitt C. Reinhardt (Air Force Office of Scientific Research), Prof. Fredric M. Ham (Florida Institute of Technology), Prof. Toshio Fukuda (Nagoya University, Japan), and Prof. Tzyy-Ping Jung (University of California, San Diego).

**Harold Szu
F. Jack Agee**

Reversible Jump MCMC for Non-Negative Matrix Factorization with Application to Raman Spectral Decomposition

Mark Girolami *

girolami@dcs.gla.ac.uk

Department of Computing Science

University of Glasgow

Glasgow, G12 8QQ, Scotland UK

<http://www.dcs.gla.ac.uk/inference/>

March 4, 2009

Abstract

We present a fully Bayesian approach to Non-Negative Matrix Factorisation (NMF) by developing a Reversible Jump Markov Chain Monte Carlo (RJMCMC) method which provides full posteriors over the matrix components. In addition the NMF model selection issue is addressed, for the first time, as our RJMCMC procedure provides the posterior distribution over the matrix dimensions and therefore the number of components in the NMF model. A comparative analysis is provided with the Bayesian Information Criterion (BIC) and model selection employing estimates of the marginal likelihood. An illustrative synthetic example is provided using blind mixtures of images. This is then followed by a large scale study of the recovery of component spectra from multiplexed Raman readouts. The power and flexibility of the Bayesian methodology and the proposed RJMCMC procedure to objectively assess differing model structures and infer the corresponding plausible component spectra for this complex data is demonstrated convincingly.

1 INTRODUCTION

We consider the NMF problem (Paatero and Tapper, 1994; Lee and Seung, 2001) of representing a non-negative matrix \mathbf{X} as a product of two non-negative matrices, formulated as,

$$\mathbf{X} = \mathbf{AS} + \mathbf{E}, \quad (1)$$

*This is joint work with Mingjun Zhong

where $\mathbf{A} \in \mathcal{R}_+^{N \times M}$, $\mathbf{S} \in \mathcal{R}_+^{M \times T}$, and $\mathbf{E} \in \mathcal{R}^{N \times T}$ is the tolerance within each column and is assumed to follow a Normal distribution with zero mean and unknown diagonal covariance $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_N)$. Each row of \mathbf{S} designates one component and M is the number of components (NoC). Our aim is to obtain the joint posterior for M , \mathbf{A} , and \mathbf{S} . It is well known that this decomposition is non-unique and hence not likelihood identifiable, we therefore invoke weak identifiability by the use of proper priors within the Bayesian framework.

Some NMF algorithms based on gradient methods, e.g., (Lee and Seung, 2001), could be directly employed to obtain *Maximum a Posteriori* estimates of \mathbf{A} and \mathbf{S} given an assumed NoC M . Indeed a Bayesian approach to NMF, using Metropolis sampling, is proposed in (Moussaoui *et al.*, 2006) although no attempt at model-order inference was made in that work. All of these methods implicitly assume that the NoC are known *a priori*. Estimating NoC is essentially the model selection problem and in this paper we consider several possible approaches. It is required to compute the posterior distribution of M given observed data \mathbf{X} , which is proportional to the marginal likelihood $p(\mathbf{X}|M)$. However, the integral $p(\mathbf{X}|M) = \int p(\mathbf{X}, \mathbf{\Theta}|M) d\mathbf{\Theta}$ is analytically intractable for the current problem, where we denote $\mathbf{\Theta} = \{\mathbf{A}, \mathbf{S}, \mathbf{\Lambda}\}$. The BIC of (Schwarz, 1978) is a method of obtaining an asymptotic approximation of the marginal likelihood and could be simply employed with any number of standard NMF algorithms although as will be demonstrated in subsequent sections this approximation is not without its shortcomings. The use of the Thermodynamic Integral identity forms the basis for estimates of the log-marginal likelihood which have been shown to improve upon estimators using samples from the posterior density, see (Friel and Pettitt, 2008) and references therein. For example estimating the marginal likelihood using the harmonic mean identity can yield highly unstable estimators and ways to circumvent this problem have been proposed in (Raftery *et al.*, 2007). (Green, 1995) proposed the general RJMCMC methodology which is a generalized Metropolis-Hastings algorithm allowing trans-dimensional exploration of model and parameter space. Green's method considers M as a random variable, and the posterior of all the model parameters, i.e., $P(M, \mathbf{\Theta}|\mathbf{X})$, is the invariant distribution. The outputs of the RJMCMC algorithm are then both the samples of $\mathbf{\Theta}$ and M .

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Nanomagnetism: What Is It? And Why Should You Care?

Robert D. Shull

Metallurgy Division, Materials Science and Engineering Laboratory
National Institute of Standards and Technology
Gaithersburg, MD 20899-8552

ABSTRACT

The advent of the age of nanotechnology has caused a great deal of excitement in the scientific community, especially since the National Nanotechnology Initiative in the USA was unveiled by President Clinton in 2001, as it was generally regarded as the next frontier in materials science. The argument for its support was overwhelming, and in hindsight all the unique new material properties and phenomena that have been discovered since that time make all this activity worth while. Magnetic research and discoveries have been no exception, and such developments are reported in this publication. Interestingly, much more money has been spent in supporting this activity outside of the United States than inside the United States.

Keywords: ferromagnetism, superparamagnetism, magnetic refrigeration, transformers, generators, spintronics

1. INTRODUCTION

The magnetic character of a material can change significantly when some material dimension is reduced to the nanoscale. These changes include new phenomena, different size dependencies, and unusual property combinations. Usually, these properties are not logical extensions of large scale behavior extrapolated to small sizes. The reasons for these differences fall into three main categories. (1) Quantum confinement, where a particle restricted to being confined in a small region in space will quantize its allowed energy levels to values that are discretely different from those the particle possesses at freedom. (2) The increased importance of the interface atoms in dictating what the bulk properties will be. (3) The presence of a nanometer-sized critical length in the property being evaluated. Critical magnetic length scales include the magnetic exchange length, domain wall width, and single domain size. Due to the fact that magnets are endemic to our society and are largely responsible for enabling our present way of life, the above changes can affect our daily lives. Therefore, it is imperative one understands why and how magnetic properties might change as the structural length scale reduces to the nanometer level, so that one can take advantage of them for improving our health and standard of living.

2. DISCOVERIES

One major impact on our lives is the potential availability of multi-terrabit/in² computer hard disc storage. As the size of the magnetic regions is made smaller down to <12 nm, terrabit storage becomes feasible. Unfortunately, in order to keep each of those bits independent of the other neighboring ones, a new magnetic phenomena is created called superparamagnetism.¹ This state only exists if ferromagnetic regions become nanometer in size and are independent of other ferromagnetic regions, just like the new recording media would become as it is nanostructured to a sufficiently small size. In this new magnetic state, high magnetization is achieved as an external magnetic field is applied to the material, just like in a normal ferromagnet (but smaller in magnitude), but once the external magnetic field is removed the magnetization is also lost. Consequently, the material ceases being able to retain any magnetic information. Until one reaches this superparamagnetic limit, however, large improvements in storage density can be obtained.

Another exciting application of nanostructured materials is the use of nanometer-diameter ferromagnetic particles for magnetically directed drug delivery, hyperthermia treatment and magnetic resonance imaging (MRI) contrast enhancement.² These are possible, because nanometer-sized particles are small enough to move freely through the intervascular system in order to find and attach to targeted diseased cells. Attachment is accomplished by functionalizing the outer surface of the nanoparticles with a molecule, like a protein that recognizes these cells. If a drug is also attached to the magnetic particle, then drugs are delivered directly to where they are needed without flooding the whole body with them and limiting the dosage possible. If an alternating magnetic field is applied to the body after attachment of the magnetic particles to the targeted cells, the resulting localized heating can be used to kill the diseased cells. Also, the magnetic fields emanating from the nanoparticles can interfere with the external magnetic field applied in a MRI machine and thereby provide a mechanism for obtaining greater contrast in the MRI images. The improved resolution would then enable earlier detection of anomalies, which usually translates to earlier treatment and greater likelihood of survival by the patient. Again, all these new possibilities are possible due to the small size of the magnetic species.

A great deal of energy is lost as heat whenever the voltage of the power source (like the home wall outlet) is reduced to that needed to operate the electrical device, like a hair dryer, connected to it. That is because the transformer used to step down the voltage is inefficient, due to a non-zero magnetic coercivity of the ferromagnet in it. It has been found that one can obtain much lower coercivities in that ferromagnetic transformer core if the grain size of the material is reduced to nanometer sizes.³ This new phenomenon is caused by the fact that as the material's magnetization is reversed when the field is reversed in an alternating current device, the magnetic domain walls during reversal can move through the ferromagnet easier when the grain size is very small. This change from conventional behavior is due to the loss of magnetocrystalline anisotropy as the material is nanostructured, and the elimination of the grain boundaries as effective pinning sites for the moving domain walls. As there are transformers in every electrical device, like refrigerators, computers, televisions, cell phones, electric lights, etc., small improvements in the efficiency of the transformer can result in huge energy savings.

At the present time, electricity is created primarily through the use of generators. This device consists of a permanent magnet, e.g., a "hard" ferromagnet, which is moved in relation to a stationary coil of wire. The greater the magnetic strength of that ferromagnet, the greater the voltage generated. With the advent of nanometer control in the preparation of materials, a new paradigm has been found for developing much more powerful permanent magnets. This new material is a composite of nanometer-sized pieces of a hard ferromagnet and nanometer-sized pieces of a "soft" ferromagnet (like the material in a transformer core).⁴ The new innovation is that by having nanometer-sized components in this composite there will be vastly increased interface area, resulting in the magnetic exchange interaction between the two species across these interfaces becoming the predominant factor determining how that composite material will reverse its magnetization in response to an external field. This strong exchange interaction forces the magnetization to reverse by rotating the magnetization vector as compared to the easier mechanism of a domain with reversed magnetization forming and the wall surrounding it moving through the material. Therefore, the much higher saturation magnetization of the "soft" ferromagnet results in the composite possessing a much larger saturation value than does the original pure hard ferromagnet, while the coercivity doesn't change much. The area enclosed in the hysteresis loop for this composite (essentially the saturation value multiplied by the coercivity) is therefore much enhanced. Consequently, the generator using this nanocomposite will be much more efficient.

Conventional refrigeration systems are based on the expansion and compression of a gas. Unfortunately this type of process is an irreversible process, and cannot possibly achieve Carnot efficiency, which is the best one can obtain. An alternative method, based on a reversible cycle, is that of using a magnetic field to order and disorder the magnetic spins in a magnetizable material, thereby changing the entropy of those two states and enabling the transfer of heat from one heat reservoir to another. As a consequence of its reversibility, Carnot efficiencies are possible. However, for this to be a viable alternative to vapor compression systems, good magnetic refrigerants need to be found which have large entropies at low magnetic fields and high temperatures. Magnetic nanocomposites, especially those which possess a superparamagnetic state, have been found to have advantages in both of those directions.⁵ Because the magnetic susceptibility of these materials is much larger than that for a system with isolated spins, e.g. paramagnets, for a given

external magnetic field application, they can achieve much larger spin alignments and bigger entropy changes during the application of the field. The figure of merit for magnetic refrigerants is the magnetocaloric effect, and these superparamagnetic nanocomposites possess enhanced magnetocaloric effects at low fields and higher temperatures than conventional low temperature refrigerants. Since refrigeration and air conditioning are the major sources of energy use in the home, modest improvements in refrigeration efficiency can translate into huge energy savings throughout the world and less reliance on carbon-based energy sources.

With the advent of methods to controllably prepare thin films and devices with atomic-scale resolution, it has become possible to prepare thin film composites with vastly dissimilar magnetic and electronic characters placed adjacent to each other. These can result in quite different bulk electronic and magnetic character, as described above. One particularly exciting possibility is using the electron spin rather than its charge for controlling electrical operation of devices has become a viable idea. This is called the area of spin electronics, or “spintronics.” Such novel systems could revolutionize the electronics industry because they are scalable to very small size, have infinite cycling ability, and do not lose their spin orientations when the power is turned off. Already, spin-dependent scattering in the form of the “giant magnetoresistance effect”⁶ has been observed and taken advantage of in the form of very high sensitivity magnetic recording read heads, which has enabled the availability of multi-gigabit computer hard drives. Now, work is progressing quickly to use the spin in an electron to exert a torque on the magnetic spin in the material being traversed, thereby enabling fast reliable switching and novel magnetic random access memory (MRAM).⁷

3. SUMMARY

The new possibilities enabled by nanostructuring electronic and magnetic materials have only just begun, and will certainly expand many-fold in the future. This also carries the danger of being a disruptive technology since new nanomagnetic devices may well obsolete present devices. Such was the case of the advent of the GMR read head. Of the approximately 30 companies making hard discs at the time of the GMR discovery, only about three remain at the time of this publication. Consequently, it is important to pay close attention to developments in the area of nanomagnetism for both its potential of opening up new areas of application and its potential for making present technology obsolescent.

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