Fully Bayesian analysis of multi-exponential decays in low resolution NMR

Proposal for ITT / SAMBa project on applications of "Massive Inference"

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Part 1: Nuclear Magnetic Resonance in Porous Media, and what we do with it



NMR can be done at many field strengths

9 T





bore imager

2 T



23 - 12 MHz – rock

0.3 T



permanent magnets

50 mT

2 MHz – "industry standard" for NMR in petrophysics

> \leq 2 MHz – Well logging





50 μT

no magnet

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400 MHz – a chemical spectroscopy system

MRI



core imager

petrophysics & well logging

Resonance Frequency ------



- Earth's Field NMR



Early wave MRI of rocks (1991-92)

Final oil saturation state (flowing) hydrocarbon image only



Saturation Gradients in Drainage of Porous Media: NMR Imaging Measurements

E. J. Fordham and L. D. Hall Herchel Smith Laboratory for Medicinal Chemistry, Cambridge University School of Clinical Medicine, Cambridge, CB2 2PZ, U.K.

> **T. S. Ramakrishnan** Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT 06877

M. R. Sharpe and C. Hall Schlumberger Cambridge Research, Cambridge, CB3 0HG, U.K.

AIChE Journal September 1993 Vol. 39, No. 9

2 Tesla / 85 MHz



(attempts at) Quantitative saturation profiles (1993)



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In combination with 1D MRI – profiles of T_1 -distributions

JOURNAL OF MAGNETIC RESONANCE, Series A 113, 139-150 (1995)

Imaging Multiexponential Relaxation in the $(y, \log_e T_1)$ Plane, with Application to Clay Filtration in Rock Cores

E. J. FORDHAM, * † A. SEZGINER, ‡ AND L. D. HALL†

Imaging: FT of echo data delivers profile

Relaxation: analysed for T_1 – distribution pixel-by-pixel





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Research

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2D relaxation time distributions - in the same EOR experiment





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T_1 - T_2 Interpretation in shales



... after Marc Fleury (IFP)

- Measure T_1 AND T_2 relaxation times
- Sensitive to molecular motion
- Frequency (magnet strength) dependent





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actual examples from organic shales





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2D Diffusion – T_2 distributions



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US Patent Application 12/731,005

Mitchell and Fordham, J. Magn. Reson (2011) doi: 10.1016/j.jmr.2011.07.020

That EOR experiment again: $D - T_2$ this time





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There's more ...





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More dimensions ...





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What's wrong with it all?

Poor resolution

- typically only integrals or moments are used
- Rock properties and fluid types the goal
- No error bars !!!! -
 - or any other uncertainty estimates
 - Point values on T₂ almost meaningless
- No easy way to include prior information
 - Bulk relaxation rates impose ceiling on T_{1,2}
 - $T_1 \ge T_2$ from physics
- Time/memory may become prohibitive in dimensions > 2



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Part 2: The mathematical problem



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Problem archetype and approaches

The archetype problem is the solution, for an unknown distribution $P(T_2, T_1) \ge 0$, of a

First Kind Fredholm integral equation with exponential kernel :

$$M\left(\tau_{1}^{(i)},\tau_{2}^{(j)}\right) = \int_{0}^{\infty} P(T_{2},T_{1})\exp\left(-\tau_{2}^{(j)}/T_{2}\right) \left[1 - \exp\left(-\tau_{1}^{(i)}/T_{1}\right)\right] dT_{2}dT_{1} + e\left(\tau_{1}^{(i)},\tau_{2}^{(j)}\right)$$

 $M(\tau_1^{(i)}, \tau_2^{(j)})$ experimental magnetization values at discrete sampling times $\tau_1^{(i)}, \tau_2^{(j)}$ for i = 1, ..., N; j = 1, ..., M $e(\tau_1^{(i)}, \tau_2^{(j)})$ experimental noise (Gaussian, white). Signal to Noise Ratio may be poor (0 dB in first experimental prototypes)

Different measurements involve different kernels – may or may not be separable $K(\tau_1, \tau_2; T_1, T_2) = k_1(\tau_1; T_1)k_2(\tau_2; T_2)$ Positivity condition $P(T_2, T_1) \ge 0$ may need to be relaxed (in some 2D contexts).

- Current routine practice: one of many (and evolving) *ad hoc* variants of Tikhonov regularisation [3,4,5,6,7]
- Attempts at uncertainty estimates:
- (i) confidence intervals on the overall data misfit (with explicit *rejection* of Bayesian priors) [8]
- (ii) direct estimation of petrophysically important moments, via the use of Mellin transforms [9, 10]
- (iii) Markov Chain Monte-Carlo (MC²) exploration of posterior probability spaces, but without close attention to the priors [11]
- Not attempted (so far !): Systematic treatment as a problem in Bayesian inference.



Apparatus for exploration of the problem:

• Potential apparatus:

Constraints on priors from independence of discretization [12]:

Random samples from a wide class of uncorrelated measures, appropriate as priors, are known to be "atomic" (i.e. encodable as a finite set of discrete masses) [12,13,14].

"Atomic" property is arguably reasonable in the context:

 T_2 is a routine proxy for pore "size" – but derives from "isolated" pore assumptions – clearly non-physical ! Dominant diffusion eigenmodes of fully inter-connected pore network a better model – and a finite discrete set may describe them

Practical implementations [15] use various "engines" for MC² exploration of posterior probability spaces. Concomitant estimates of the Bayesian "evidence" ("prior predictive") are also available.

LGPL codes "**BayeSys**" and "**MassInf**" available with documentation (John Skilling, 2004, Maximum Entropy Data Consultants Ltd)



Solution by Tikhonov Regularization

Measured magnetization data M_i & unknown distribution f(x) $M_i = \int_{x_a}^{x_b} f(x)k_i(x) dx + n_i$ i = 1, 2, ..., N

Kernel functions exponential decays (or similar variants)

$$k_i = \exp\left(-\tau_i/T_2\right)$$

 $k_i(x) \dots k_N(x)$ are "almost linearly dependent" such that matrix $G_{ij} = \int_{x_a}^{x_b} k_i(x)k_j(x) dx$ i, j = 1, 2, ..., N... is ill-conditioned.

Formal statement of (ill-conditioned) problem: $f = \frac{\operatorname{argmin}}{f \ge 0} ||Kf - \mathbf{d}||$

Regularized problem: $f^{(\alpha)} = \operatorname*{argmin}_{f \ge 0} \left(||Kf - \mathbf{d}||^2 + \alpha ||f||^2 \right)$

Seek f(x) minimising mean square misfit with regularising term, for some α selected by one of many *ad hoc* criteria

Key papers and reviews

IEEE TRANSACTIONS ON SIGNAL PROCESSING, VOL. 50, NO. 5, MAY 2002

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Contents lists available at SciVerse ScienceDirect

Progress in Nuclear Magnetic Resonance Spectroscopy

journal homepage: www.elsevier.com/locate/pnmrs

Solving Fredholm Integrals of the First Kind With Tensor Product Structure in 2 and 2.5 Dimensions

Lalitha Venkataramanan, Member, IEEE, Yi-Qiao Song, and Martin D. Hürlimann

The "Schlumberger algorithm" for separable kernels in 2D:

$$M(\tau,\tau_2) = \int \int k_1(x,\tau_1)k_2(y,\tau_2)\mathcal{F}(x,y)\,\mathrm{d}x\,\mathrm{d}y + e(\tau_1,\tau_2)$$

or in discretised matrix form:

 $M = K_1 F K_2' + E$

Separability applies to most 2D relaxation experiments but *not* all diffusion ones

Numerical estimation of relaxation and diffusion distributions in two dimensions J. Mitchell*, T.C. Chandrasekera, L.F. Gladden

Department of Chemical Engineering and Biotechnology, University of Cambridge, New Museums Site, Pembroke Street, Cambridge CB2 3RA, United Kingdom





Innocent questions that don't go away

The story:

- The problem is very ill-conditioned.
- We distort it to make it less so.
- The form of the regularising functional is a matter of taste.
- We fiddle the value of the regularising parameter α according to criteria which are also a matter of taste.
- The results "look" reasonable.
- They agree well enough with known distributions for synthetic data.

Innocent questions:

- We all know the inversion is highly ill-conditioned. What do these distributions really mean ?
- How reliable / accurate are they ?
- How do you choose the value of the "tuning knob" α ?
- How do you choose the regularising functional ? (square norm, curvature, entropy, UPEN ...)
- How much information do they contain ?
- How many measurements can you extract ?



Bayesian interpretation of Regularisation

Regularization problem:

$$f^{(\alpha)} = \operatorname*{argmin}_{f \ge 0} \left(||Kf - \mathbf{d}||^2 + \alpha ||f||^2 \right)$$

in which:
$$||Kf - \mathbf{d}||^2 = \sum_k (K_{kj}f_j - d_k)^2 = \sigma^2 \chi^2$$

Noise known to be white Gaussian, so *Likelihood* is:

$$\mathcal{P}(\mathbf{d}|\mathbf{f},I) = \exp\left(-\chi^2/2\right)/Z_L$$

Hence identify: $||Kf - \mathbf{d}||^2 = 2\sigma^2 L(\mathbf{f}; \mathbf{d}, \sigma)$ log-likelihood

log-prior

Similarly identify:

i.e. prior on distribution
$${f f}$$
 :

 $\alpha ||f||^2 = \alpha S(\mathbf{f}) \qquad \mathcal{P}(\mathbf{f}|I) \propto \exp(\alpha S(\mathbf{f}))$

likelihood prior inference $\mathcal{P}(H|DI) =$ $\mathcal{P}(D|HI)\mathcal{P}(H|I)$ evidence

Then by Bayes' Theorem: $\mathcal{P}(\mathbf{f}|\mathbf{d}, I) \propto \exp\left(-(L(\mathbf{f}; \mathbf{d}) - \alpha S(\mathbf{f}))\right)$ So minimising the argument $-Q = L - \alpha S$ or maximising $Q = \alpha S - L$ maximises posterior "inference" $\mathcal{P}(\mathbf{f}|\mathbf{d}, I) \propto \exp(Q)$ "Best" distribution maximises Q for $\mathbf{f} = \hat{\mathbf{f}} = f^{(\alpha)}$

Regularised distribution is "most probable" (maximum a posteriori probability or MAPP) – <u>assigning αS as log-prior</u>



So how *should* we assign the prior?

Entropic Prior

$$\mathcal{P}(\mathbf{f}|\alpha, \mathbf{m}) = \left(\frac{\alpha}{2\pi}\right)^{M/2} \exp\left(\alpha S(\mathbf{f}, \mathbf{m})\right)$$

where $S(\mathbf{f}, \mathbf{m}) = -\sum_{i=1}^{M} f_i \log\left(\frac{f_i}{m_i}\right)$

- Highly structured \mathbf{f} highly informative (low $\boldsymbol{\mathcal{P}}$ without data)
- Featureless f uninformative (high P without data)
- Shannon entropy should be a candidate
- Entropy the only form without spurious correlations
- Over-riding consideration should be *consistency*

Hence: "Quantified Maximum Entropy" or QME

Problems emerge:

- *Not* independent of pixelation / discretisation of domain
- Consistency requires independence of pixelation ...
 For any disjoint sub-domains $A \cap B = \emptyset$ Additivity: Positivity: $\Phi_{A \cup B} = \Phi_A + \Phi_B$ and $0 \le \Phi_C < \infty \quad \forall C$ Image: Construct on the second sec

Surprising consequences !



"Atomic" priors

J. R. Statist. Soc. B (1997) 59, No. 1, pp. 217–235

Prior Distributions on Measure Space

By SIBUSISO SIBISI† and JOHN SKILLING

University of Cambridge, UK

[Received March 1994. Final revision March 1996]



Fig. 1. Evolution of a sample from the Dirichlet prior

SUMMARY

A measure is the formal representation of the non-negative additive functions that abound in science. We review and develop the art of assigning Bayesian priors to measures. Where necessary, spatial correlation is delegated to correlating kernels imposed on otherwise uncorrelated priors. The latter must be infinitely divisible (ID) and hence described by the Lévy–Khinchin representation. Thus the fundamental object is the Lévy measure, the choice of which corresponds to different ID process priors. The general case of a Lévy measure comprising a mixture of assigned base measures leads to a prior process comprising a convolution of corresponding processes. Examples involving a single base measure are the gamma process, the Dirichlet process (for the normalized case) and the Poisson process. We also discuss processes that we call the supergamma and super-Dirichlet processes. Examples of multiple and continuum base measures are also discussed. We conclude with numerical examples of density estimation.



More on atomic priors

Proc. 15th Workshop on Maximum Entropy and Bayesian Methods (1996) pp 261-270 Kluwer

JOHN SKILLING AND SIBUSISO SIBISI University of Cambridge, Cavendish Laboratory Madingley Road, England CB3 0HE

Abstract. A "measure" is the mathematical concept underlying distributed quantities such as images, spectra, and probability distributions. Inference about a measure requires a suitable Bayesian prior. If the prior is to remain valid on indefinitely small cells, it must be "infinitely divisible", and in consequence samples from it will be "atomic" (being essentially a limited sum of delta functions). Infinitely divisible priors are described in terms of the distribution of delta function strengths via the Lévy-Khinchin representation. Such priors include the Poisson process, but not the Quantified Maximum Entropy prior that has been used as its continuous reformulation.

Figure 4. Subdivision of an *id*-process into atoms. A sample from a Gamma process with measure $\alpha = 5$ per cell is shown (top) with successive five-fold expansions of the central fraction.

Small probabilities of $\mathcal{O}(1)$ "flux" in a small cell *Not* $\mathcal{O}(1)$ probability of *small* flux





The "Massive Inference" method

The "Massive Inference" prior for measure *F*:

$$\mathcal{P}(F|\alpha,q) = e^{-\alpha} \left[\delta(F) + e^{-F/q} \sqrt{\frac{\alpha}{qF}} I_1\left(2\sqrt{\frac{\alpha F}{q}}\right) \right]$$

Properties:

- Satisfies requirement of "infinite divisibility"
- Delta-function at F = 0 forces posterior mode to be null ! Counter-example to MAPP: mode is not useful
- Mean values instead used for display / "best" distribution
- Two hyper-parameters:
 - α is Poisson Expectation number of "atoms" over domain range on which F is estimated
 - q is a dimensional flux unit (expected scale)



The "Massive Inference" method: sketch derivation



How is total flux ζ distributed ? (given *r* atoms)

$$\mathcal{P}(\zeta|r) = \begin{cases} \delta(\zeta) & r = 0\\ \mathrm{e}^{-\zeta} \zeta^{r-1} / (r-1)! & r > 0 \end{cases}$$

How many atoms *r* in cell δx ?

Choose Poisson prior of expectation / mean $\mu = \alpha \, \delta x$

$$\mathcal{P}(r) = e^{-\mu} \mu^r / r!$$
 $r = 0, 1, 2, ...$

How large ($\zeta_i = F_i/q$) are each of the *r* atoms ?

$$\mathcal{P}(\zeta_i) = \exp(-\zeta_i)$$
 $i = 1, 2, ..., r$
Fotal flux in cell width δx is $\zeta = \sum_{i=1}^r \zeta_i$

How is total flux ζ distributed ? (any *r* atoms in cell δx)

$$\mathcal{P}(\zeta) = \sum_{r=0}^{\infty} \mathcal{P}(\zeta|r) \mathcal{P}(r)$$
Number of atoms r
in cell summed
away analytically
$$= e^{-\mu} \left[\delta(\zeta) + e^{-\zeta} \sqrt{\mu/\zeta} I_1 \left(2\sqrt{\mu\zeta} \right) \right]$$

Hence previous page ($F = \text{dimensionless flux} \times \text{flux quantum}$)

$$\mathcal{P}(F|\alpha,q) = e^{-\alpha} \left[\delta(F) + e^{-F/q} \sqrt{\frac{\alpha}{qF}} I_1 \left(2\sqrt{\frac{\alpha F}{q}} \right) \right]$$



Computational engines



- Markov Chain Monte Carlo algorithms
- exploring Hilbert (space-filling) curves
- Implemented in Public Domain (LGPL) codes BayeSys and MassInf
- © John Skilling 2004
- Further development since 2004 bibliography incomplete !
- May be more advanced codes available commercially

(Maximum Entropy Data Consultants Ltd)

How Far Can We Go?

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Bibliography

- [1] W E Kenyon (1997). Petrophysical principles of applications of NMR Logging. *The Log Analyst*, March-April 1997, 21-43
- [2] J Mitchell, L F Gladden, T C Chandrasekera & E J Fordham (2014). Low-field permanent magnets for industrial process and quality control. *Prog Nucl Mag Res Spectros*, **76**, 1-60
- [3] A N Tikhonov & V Y Arsenin (1977). *Solutions of ill-posed problems.* London, Wiley.
- [4] E J Fordham, A Sezginer & L D Hall (1995). Imaging multiexponential relaxation in the $(y, \log T_1)$ plane, with application to clay filtration in rock cores. J Mag Res Ser A 113 139-150
- [5] L Venkataramanan, Y-Q Song & M D Hürlimann (2002). Solving Fredholm integrals of the first kind with tensor product structure in 2 and 2.5 dimensions. *IEEE Trans Signal Process* **50** 1017–1026
- [6] J Mitchell, T Chandrasekera & L F Gladden (2012).
 Numerical estimation of relaxation and diffusion distributions in two dimensions.
 Prog Nucl Mag Res Spectros 62 34–50
- [7] V Bortolotti, R J S Brown, P Fantazzini, G Landi & F. Zama (2016).
 Improved inversion of two-dimensional NMR relaxation data with the UPEN principle.
 Proc. 13th Int. Conf. on Magnetic Resonance in Porous Media

- [8] R L Parker & Y-Q Song (2005). Assigning uncertainties in the inversion of NMR relaxation data. *J Mag Res* **174** 314-324
- [9] L Venkataramanan T M Habashy D E Freed & F K Gruber (2012). Continuous moment estimation of CPMG data using Mellin transform. *J Mag Res* **216** 43-52
- [10] F K Gruber, L Venkataramanan, T M Habashy & D E Freed (2013). Estimation of petrophysical and fluid properties using integral transforms in NMR. J Mag Res 228 104–115
- [11] M Prange & Y-Q Song (2010). Understanding NMR *T*₂ spectral uncertainty. *J Mag Res* **204** 118–123
- [12] S Sibisi & J Skilling (1997). Prior distributions on measure space. *J Roy Stat Soc B* **59**(1) 217-235
- [13] T S Ferguson (1973). A Bayesian analysis of some nonparametric problems. Ann. Statistics 1(2) 209-230
- [14] J F C Kingman (1993). Poisson Processes, OUP.
- [15] Skilling, J. (2004) **BayeSys** and **MassInf** (2004).

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