Electromagnetic Relaxation Time Distribution Inverse Problems in the Time-domain

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Outline

1. **Maxwell's Equations**
   - Description
   - Simplifications

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   - Distributions

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4. **Forward Simulation**
   - Polynomial Chaos

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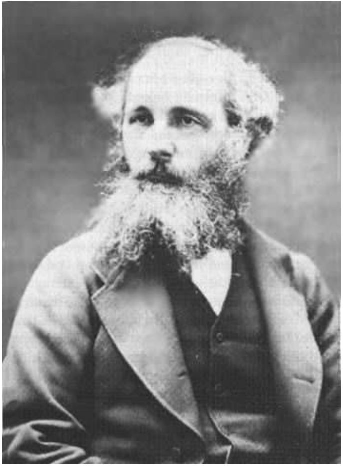
3. **Inverse Problem for Distributions**
4. **Forward Simulation**
   - Polynomial Chaos
5. **Inverse Problem Numerical Results**

Maxwell's Equations



- Maxwell's Equations were formulated circa 1870.
- They represent a fundamental unification of electric and magnetic fields predicting electromagnetic wave phenomenon.

Maxwell's Equations

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H} \qquad \text{(Ampere)}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \qquad \text{(Faraday)}$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Poisson)}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \text{(Gauss)}$$

$\mathbf{E} =$	Electric field vector	$\mathbf{D} =$	Electric displacement
$\mathbf{H} =$	Magnetic field vector	$\mathbf{B} =$	Magnetic flux density
$\rho =$	Electric charge density	$\mathbf{J} =$	Current density

Note: Need initial conditions and boundary conditions.

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$\boxed{\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} + \mathbf{P} \\ \mathbf{B} &= \mu \mathbf{H} + \mathbf{M} \\ \mathbf{J} &= \sigma \mathbf{E} + \mathbf{J}_s \end{aligned}}$$

$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Linear, Isotropic, Non-dispersive and Non-conductive media

Assume no material dispersion, i.e., speed of propagation is not frequency dependent.

$$\boxed{\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} \\ \mathbf{B} &= \mu \mathbf{H} \end{aligned}}$$

$$\epsilon = \epsilon_0 \epsilon_r \qquad \epsilon_r = \text{Relative Permittivity}$$

$$\mu = \mu_0 \mu_r \qquad \mu_r = \text{Relative Permeability}$$

$$c = 1/\sqrt{\epsilon\mu}$$

Maxwell's Equations in One Space Dimension

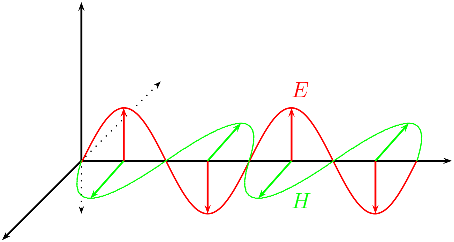
- The time evolution of the fields is thus completely specified by the curl equations

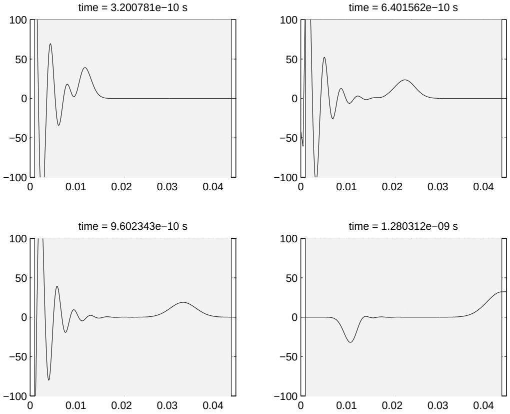
$$\begin{aligned} \epsilon \frac{\partial \mathbf{E}}{\partial t} &= \nabla \times \mathbf{H} \\ \mu \frac{\partial \mathbf{H}}{\partial t} &= -\nabla \times \mathbf{E} \end{aligned}$$

- Assuming that the electric field is polarized to oscillate only in the y direction, propagate in the x direction, and there is uniformity in the z direction:

Equations involving E_y and H_z.

$$\begin{aligned} \epsilon \frac{\partial E_y}{\partial t} &= -\frac{\partial H_z}{\partial x} \\ \mu \frac{\partial H_z}{\partial t} &= -\frac{\partial E_y}{\partial x} \end{aligned}$$





Snapshots of a windowed electromagnetic pulse with $f = 10GHz$ for the interrogation problem.

Dispersive Dielectrics

- Recall
$$\mathbf{D} = \epsilon\mathbf{E} + \mathbf{P}$$
where **P** is the dielectric polarization.
- We can generally define **P** in terms of a convolution
$$\mathbf{P}(t, \mathbf{x}) = g \star \mathbf{E}(t, \mathbf{x}) = \int_0^t g(t - s, \mathbf{x}; q)\mathbf{E}(s, \mathbf{x})ds,$$
where g is a general dielectric response function (DRF), and **q** is some parameter set.
- Debye model
$$g(t, \mathbf{x}) = \epsilon_0(\epsilon_s - \epsilon_\infty)/\tau \;\; e^{-t/\tau}$$
or equivalently,
$$\tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)\mathbf{E}$$
where $q = \{\epsilon_\infty, \epsilon_s, \tau\}$ and, in particular, τ is called the relaxation time.

Frequency Domain

- Converting to frequency domain via Fourier transforms

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

becomes

$$\hat{\mathbf{D}} = \epsilon(\omega)\hat{\mathbf{E}}$$

where $\epsilon(\omega)$ is called the complex permittivity.

- Debye model gives

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + i\omega\tau}$$

- Cole-Cole model (heuristic generalization)

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + (i\omega\tau)^{1-\alpha}}$$

Unfortunately, the Cole-Cole model corresponds to a fractional order differential equation in the time domain, and simulation is not straight-forward.

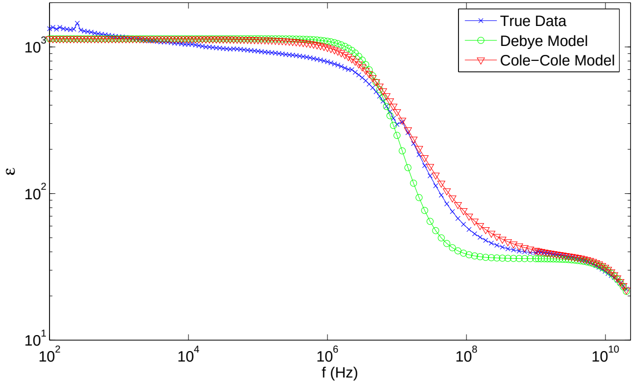


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity.

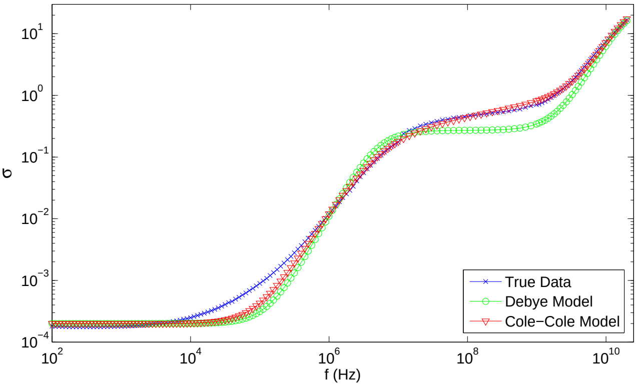


Figure: Imaginary part of $\epsilon(\omega)$, σ, or the conductivity.

Motivation

- Broadband wave propogation suggests time-domain simulation.
- The Cole-Cole model corresponds to a fractional order ODE in the time-domain and is difficult to simulate.
- Debye is efficient to simulate, but does not represent permittivity well.
- Better fits to data are obtained by taking linear combinations of Debye models (multi-pole Debye), idea comes from the known existence of multiple physical mechanisms.
- An alternative approach is to consider the Debye model but with a (continuous) distribution of relaxation times.
- Empirical measurements suggest a log-normal distribution.

Distributions of Parameters

To account for the effect of possible multiple parameter sets q, consider

$$h(t, \mathbf{x}; F) = \int_{\mathcal{Q}} g(t, \mathbf{x}; q) dF(q),$$

where $\mathcal{Q}$ is some admissible set and $F \in \mathfrak{P}(\mathcal{Q})$.
Then the polarization becomes:

$$\mathbf{P}(t, \mathbf{x}) = \int_0^t h(t-s, \mathbf{x}; F) \mathbf{E}(s, \mathbf{x}) ds.$$

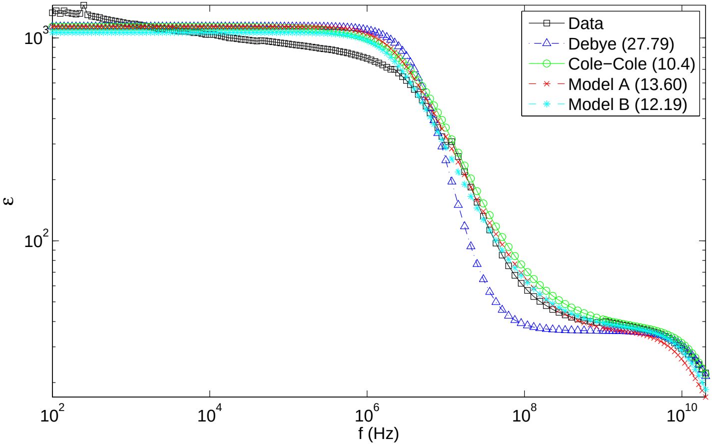


Figure: Real part of $\epsilon(\omega)$, called simply ϵ, or the permittivity. Model A refers to the Debye model with a uniform distribution on τ.

Random Polarization

We define the random polarization $\mathcal{P}(x, t; \tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E$$

where τ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.

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for a uniform distribution.
The electric field depends on the macroscopic polarization, which we take to be the expected value of the random polarization at each point (x, t)

$$P(x, t; F) = \int_{\tau_a}^{\tau_b} \mathcal{P}(x, t; \tau) f(\tau) d\tau.$$

Well-Posedness of Forward Problem

- Existence and uniqueness of solutions to weak formulation of the forward problem follows as a special case of work in [BBL00]
- Continuous dependence of $(E, \dot{E})$ on F in the Prohorov metric shown in [BG05]

Time-domain Inverse Problem

- Given data $\{\hat{E}\}_j$ we seek to determine a probability measure F^*, such that

$$F^* = \min_{F \in \mathfrak{P}(\mathcal{Q})} \mathcal{J}(F),$$

where, for example,

$$\mathcal{J}(F) = \sum_j \left(E(t_j; F) - \hat{E}_j \right)^2.$$

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- Continuity of $F \to (E, \dot{E}) \implies$ continuity of $F \to \mathcal{J}(F)$
- Compactness of $\mathcal{Q} \implies$ compactness of $\mathfrak{P}(\mathcal{Q})$ with respect to the Prohorov metric
- Therefore, a minimum of $\mathcal{J}(F)$ over $\mathfrak{P}(\mathcal{Q})$ exists [BG05]

Numerical Approximation of Random Polarization

To solve the inverse problem for the distribution of relaxation times, we need a method of accurately and efficiently simulating $P(x, t; F)$.

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- Could apply a quadrature rule to the integral in the expected value. Results in a linear combination of individual Debye solves.

Numerical Approximation of Random Polarization

To solve the inverse problem for the distribution of relaxation times, we need a method of accurately and efficiently simulating $P(x, t; F)$.

- Could apply a quadrature rule to the integral in the expected value. Results in a linear combination of individual Debye solves.
- Alternatively, we can use a method which separates the time derivative from the randomness and applies a truncated expansion in random space, called Polynomial Chaos. Results in a linear system.

Polynomial Chaos: Simple example

Consider the first order, constant coefficient, linear ODE

$$\dot{y} = -ky, \quad k = k(\xi) = \xi, \quad \xi \sim \mathcal{N}(0,1).$$

We apply a Polynomial Chaos expansion in terms of orthogonal Hermite polynomials H_j to the solution y:

$$y(t,\xi) = \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi), \quad \phi_j(\xi) = H_j(\xi)$$

then the ODE becomes

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) = -\sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi),$$

Triple recursion formula

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) = -\sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi),$$

We can eliminate the explicit dependence on ξ by using the triple recursion formula for Hermite polynomials

$$\xi H_j = jH_{j-1} + H_{j+1}.$$

Thus

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j + \alpha_j(t)(j\phi_{j-1} + \phi_{j+1}) = 0.$$

Galerkin Projection onto span($\{\phi_i\}_{i=0}^{p}$)

Taking the weighted inner product with each basis gives

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\langle\phi_j,\phi_i\rangle_W + \alpha_j(t)\big(j\langle\phi_{j-1},\phi_i\rangle_W + \langle\phi_{j+1},\phi_i\rangle_W\big) = 0,$$

$$i = 0,\ldots,p.$$

Where

$$\langle f(\xi), g(\xi)\rangle_W = \int f(\xi)g(\xi)W(\xi)d\xi.$$

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Where

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Using orthogonality, $\langle\phi_j,\phi_i\rangle_W = \langle\phi_i,\phi_i\rangle_W\delta_{ij}$, we have

$$\dot{\alpha}_i\langle\phi_i,\phi_i\rangle_W + (i+1)\alpha_{i+1}\langle\phi_i,\phi_i\rangle_W + \alpha_{i-1}\langle\phi_i,\phi_i\rangle_W = 0, \quad i = 0,\ldots,p,$$

Deterministic ODE system

Letting $\vec{\alpha}$ represent the vector containing $\alpha_0(t), \ldots, \alpha_p(t)$ (and assuming $\alpha_{p+1}(t)$, etc. are identically zero) the system of ODEs can be written

$$\dot{\vec{\alpha}} + M\vec{\alpha} = \vec{0},$$

with

$$M = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & p \\ & & & 1 & 0 \end{bmatrix}$$

The mean value of $y(t, \xi)$ is $\alpha_0(t)$.

Generalizations

For any choice of family of orthogonal polynomials, there exists a triple recursion formula. Given the arbitrary relation

$$\xi \phi_j = a_j \phi_{j-1} + b_j \phi_j + c_j \phi_{j+1}$$

(with $\phi_{-1} = 0$) then the matrix above becomes

$$M = \begin{bmatrix} b_0 & a_1 & & & \\ c_0 & b_1 & a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & a_p \\ & & & c_{p-1} & b_p \end{bmatrix}$$

Generalizations

Consider the non-homogeneous ODE

$$\dot{y} + ky = g(t), \quad k = k(\xi) = \sigma\xi + \mu, \quad \xi \sim \mathcal{N}(0,1).$$

then

$$\dot{\alpha}_i + \sigma\left[(i+1)\alpha_{i+1} + \alpha_{i-1}\right] + \mu\alpha_i = g(t)\delta_{0i}, \quad i = 0, \dots, p,$$

or the deterministic ODE system

$$\dot{\vec{\alpha}} + (\sigma M + \mu I)\vec{\alpha} = g(t)\vec{e_1}.$$

Exponential convergence

- Any set of orthogonal polynomials can be used in the truncated expansion, but there may be an optimal choice.
- If the polynomials are orthogonal with respect to weighting function $f(\xi)$, and k has PDF $f(k)$, then it is known that the PC solution converges exponentially in terms of p.
- In practice, approximately 4 are generally sufficient.

Generalized Polynomial Chaos

Table: Popular distributions and corresponding orthogonal polynomials.

Distribution	Polynomial	Support
Gaussian	Hermite	$(-\infty, \infty)$
gamma	Laguerre	$[0, \infty)$
beta	Jacobi	$[a, b]$
uniform	Legendre	$[a, b]$

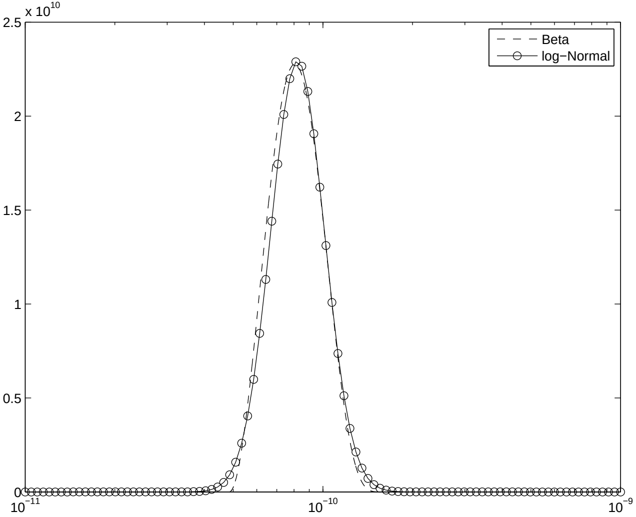

Figure: Shape of Beta distribution can mimic log-normal, but with finite support.

Random Polarization

We can apply Polynomial Chaos method to our random polarization

$$\tau \dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E, \quad \tau = \tau(\xi) = r\xi + m$$

with, e.g., $\xi \sim \text{Beta}(a, b)$, resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0(\epsilon_s - \epsilon_\infty)E\vec{e_1} =: \vec{g}$$

or

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

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or

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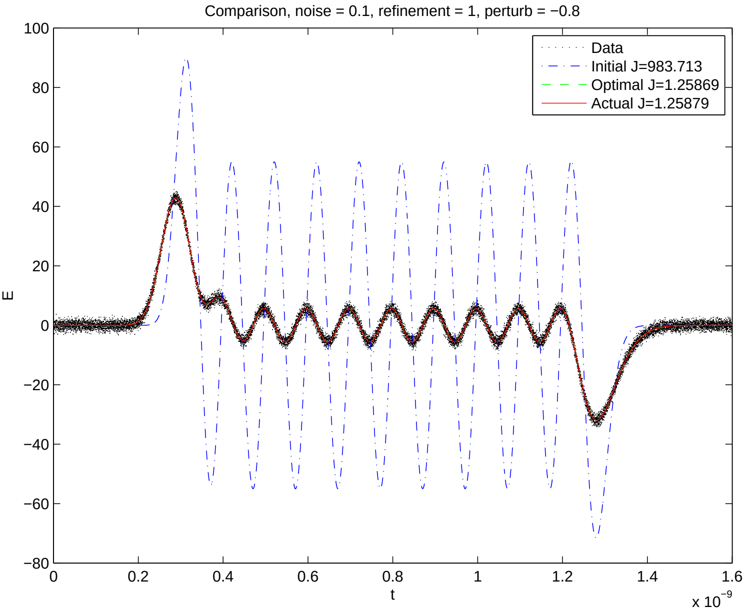
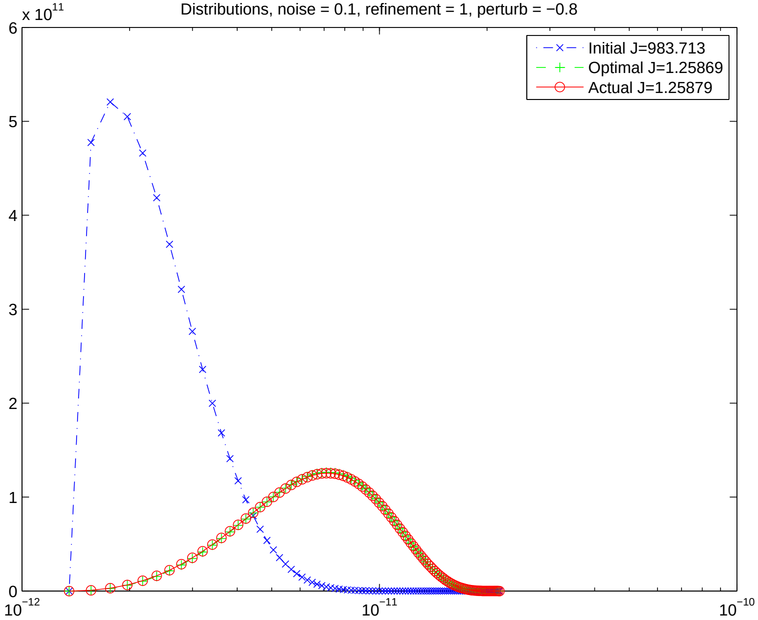
The macroscopic polarization, the expected value of the random polarization at each point (t, x), is simply

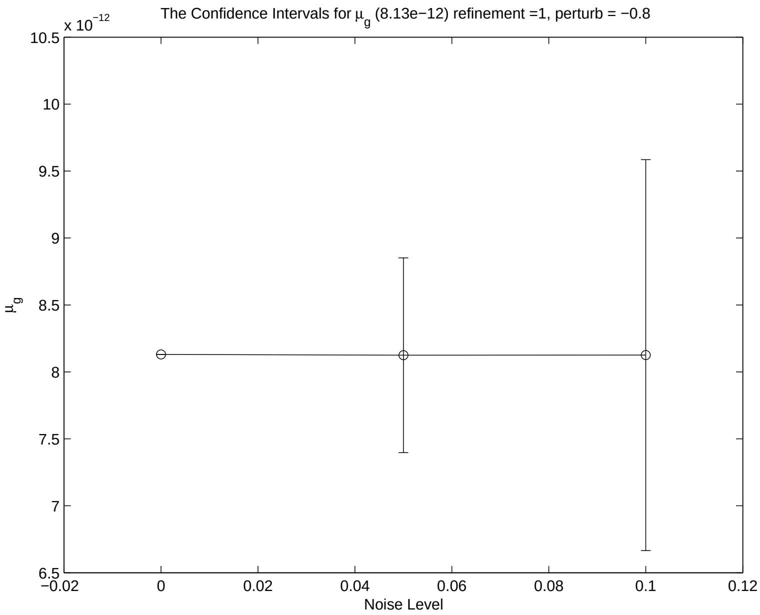
$$P(t, x; F) = \alpha_0(t, x).$$



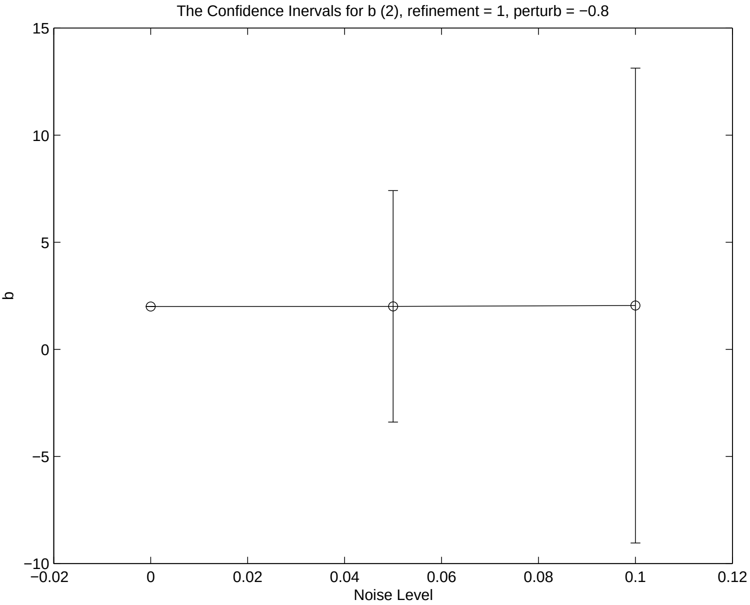
Comparison of simulations to data.



Comparison of initial to final distribution.



Estimates for the mean of the relaxation time distribution (RTD).



Estimates for (a function of) the variance of the RTD.

Comments on Time-domain Inverse Problems for Distributions

- Previous work showed that estimation methods worked well for discrete distributions and continuous uniform distribution and Gaussian distributions (using quadrature)
- We are able to accurately determine the mean in the Beta distributions with confidence in spite of noise
- Variance information is highly sensitive to noise and may be unreliable in practice with current data
- Need to test with very broad bandwith signal
- Next step is to combine multiple polarization poles (mixtures of distributions)
- Goal is to distinguish dry skin from wet skin and possibly determine moisture content from reflection data using broad band (THz-range) pulse modelled as a log-normal distribution of frequencies