Inverse methods for estimating primary input signals from time-averaged isotope profiles

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Abstract—Mammalian teeth are invaluable archives of ancient seasonality because they record along their growth axes an isotopic record of temporal change in environment, plant diet, and animal behavior. A major problem with the intra-tooth method is that intra-tooth isotope profiles can be extremely time-averaged compared to the actual pattern of isotopic variation experienced by the animal during tooth formation. This time-averaging is a result of the temporal and spatial characteristics of amelogenesis (tooth enamel formation), and also results from laboratory sampling. This paper develops and evaluates an inverse method for reconstructing original input signals from time-averaged intra-tooth isotope profiles. The method requires that the temporal and spatial patterns of amelogenesis are known for the specific tooth and uses a minimum length solution of the linear system $A\hat{m} = d$, where $d$ is the measured isotopic profile, $A$ is a matrix describing temporal and spatial averaging during amelogenesis and sampling, and $\hat{m}$ is the input vector that is sought. Accuracy is dependent on several factors, including the total measurement error and the isotopic structure of the measured profile. The method is shown to accurately reconstruct known input signals for synthetic tooth enamel profiles and the known input signal for a rabbit that underwent controlled dietary changes. Application to carbon isotope profiles of modern hippopotamus canines reveals detailed dietary histories that are not apparent from the measured data alone. Inverse methods show promise as an effective means of dealing with the time-averaging problem in studies of intra-tooth isotopic variation. Copyright © 2005 Elsevier Ltd

1. INTRODUCTION

Intra-tooth isotope variation tracks seasonal patterns of isotope variation in animal systems (Koch et al., 1989; Fricke and O’Neil, 1996), and the study of such variation is becoming a fundamental tool for studying ancient seasonality in climate, ecology, and behavior (Fricke et al., 1998; Kohn et al., 1998; Fox and Fisher, 2001; Balasse et al., 2002; Zazzo et al., 2002). The intra-tooth method involves sampling teeth along their growth axes; samples taken near the occlusal surface record an earlier portion of an animal’s life, those taken near the root record a later portion, and a series taken in between records isotopic variation in the animal for the duration of tooth formation. Already this method has led to a significant body of research in several fields: selected applications include the reconstruction of herd-management strategies of ancient pastoralists and seasonal environments in which ancient humans lived (Balasse et al., 2002), examination of cohort structure of fossil mammals (Zazzo et al., 2002), detection of seasonal dietary variation and migration in fossil mammals (Koch et al., 1998; Hoppe et al., 1999; Gadbury et al., 2000; Feranec and MacFadden, 2000), and estimation of oxygen isotope seasonality associated with climatic and tectonic change (Fricke et al., 1998; Kohn et al., 2002).

It has recently become apparent, however, that intra-tooth isotope profiles in tooth enamel are time-averaged compared to the actual pattern of isotopic variation—the input signal—experienced by animals during tooth formation (Fox and Fisher, 1998; Balasse, 2002; Passey and Cerling, 2002). Tooth enamel is the material of choice for isotopic studies of fossil mammals because of its resistance to isotopic alteration (Lee-Thorp and van der Merwe, 1987; Quade et al., 1992). It provides a time-averaged isotopic record because, during amelogenesis, each layer of enamel is deposited as a mineral poor matrix that gradually accumulates mineral over an extended period of time. Numerous studies of tooth enamel development in rats, pigs, steers, humans, and other animals show that the initial enamel matrix contains, by volume, a fraction (~20–30%) of the total hydroxyapatite content of mature enamel, and that there is a spatial maturation zone along the growth axis of the tooth where the enamel accumulates the remaining mineral (Hiller et al., 1975; Robinson et al., 1978; Suga et al., 1979; Deutsch and Pe’er, 1982; Sakae and Hirai, 1982; Suga, 1982; Robinson et al., 1987; Robinson et al., 1988; Passey and Cerling, 2002). This maturation zone often corresponds to a large portion of the overall crown height. For example, the lengths of the maturation zone (length of maturation) for cow and bison lower first molars studied by Passey and Cerling (2002) were at least 15 mm and 30 mm, respectively. The total crown height for these teeth is on the order of 35 mm to 45 mm, and taken with a tooth crown formation time of ~1 y (Brown et al., 1960), any volume of enamel will have isotopic composition that is the time average of several months (Balasse, 2002).

Passey and Cerling (2002) developed a series of equations that serve as a forward model allowing prediction of how primary input signals will appear as measured tooth enamel signals for different maturation parameters and sampling geometries. The model is specific to ever-growing teeth and is a type of running average that predicts that features of the input

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signal are increasingly time-averaged and attenuated in amplitude as the maturation length becomes longer (Fig. 1). The model predicts that isotope amplitudes of measured isotope profiles are as much a function of the environmental input signal amplitude as they are of maturation length, and shows that accounting for tooth enamel maturation and sampling geometry is critical for meaningful interpretation of intra-tooth isotope profiles.

In this paper, inverse methods are presented that allow for reconstruction of input signals based on measured isotope profiles. This inversion requires that the forward model describing sampling geometry and spatial-temporal averaging during amelogenesis be embodied in the form of a matrix called the averaging matrix. This matrix relates the input time series to the measured isotope profile and can be inverted to solve for the input time series. The forward model used throughout this paper is the constant growth rate, linear maturation model described in Passey and Cerling (2002). It should be noted here that by “input signal”, we refer to the isotopic composition of fluids in the animal’s body that are in isotopic equilibrium with the measured phase in tooth enamel. The term “input signal” does not refer to the instantaneous isotopic composition of, for instance, diet or drinking water. Other types of models (e.g., Kohn, 1996; Ayliffe et al., 2004) relate these inputs to the body fluid composition.

This paper describes a linear system that relates input and measured isotope signals, and then outlines the inverse methods used to estimate the input signal. These methods are tested using synthetic systems in which tooth enamel profiles are generated from hypothetical input signals, random error is added to the profiles to simulate measurement uncertainties, and profiles are inverted to give an estimate of the original hypothetical input signal. Comparison between the original and estimated input signals allows direct evaluation of the ability of the inverse methods to correctly recover input signals. As an important component of this paper, we evaluate the accuracy of the forward and inverse models by studying a tooth from a rabbit that underwent known dietary changes, and we estimate the diets of two modern Hippopotamus individuals based on carbon isotope profiles of lower canine teeth.

2. METHODS

2.1. Description of the Linear System \( \text{Am} = \text{d} \)

Notation used throughout this paper is listed in Table 1. The maturation parameters \( l_m \) (length of maturation) and \( l_a \) (length of apposition) are introduced and described in Passey and Cerling (2002), and are illustrated in Figure A1.1. The primary input signal and the measured isotope data are related by a system of equations:

\[
\text{Am} = \text{d}. 
\]

The averaging matrix \( \text{A} \) is an \( M \times N \) matrix, the input isotopic time-series \( \text{m} \) is an \( M \times 1 \) vector, and the measured isotopic time-series \( \text{d} \) is an \( N \times 1 \) vector. The elements \( d_i \) that comprise \( \text{d} \) are the isotopic delta values of the measured isotope profile, and the elements \( m_i \) that make up \( \text{m} \) are the isotopic delta values of the input signal. The spatial and temporal characteristics of \( \text{A}, \text{m}, \) and \( \text{d} \), and special cases termed the open-ended and closed-ended cases, are described and illustrated in Appendix 1. Computation of the averaging matrix \( \text{A} \) is described and illustrated in the electronic annex (EA1).

2.2. Inversion of the Linear System \( \text{Am} = \text{d} \)

The conditions under which inversion is carried out in this paper are briefly outlined here and generally follow methods described by Menke (1989). For detailed background reading on discrete inverse theory, the reader is referred to Menke (1989). Linear systems for tooth enamel have more unknown parameters \( M \) than measured data \( N \). These systems are underdetermined, and there is an infinite number of solutions \( \text{m} \) that exactly predict \( \text{d} \). Most of these solutions are impractical because they have values that fall well outside of the expected isotope range for ecological systems. Accordingly, we use the a priori constraints that the best solutions have minimal model length, and that all parameters of a solution must fall within an isotope range acceptable for the system being studied. We also require that the measured data are not overpredicted or underpredicted by the estimated solution \( \text{m}_{\text{est}} \). A solution that allows these constraints to be satisfied is a least squares minimum model length solution, similar to Menke (1989), Eqn. 3.40:

\[
\text{m}_{\text{est}} = (\text{m}) + A^T [AA^T + e^2 I]^{-1} [\text{d}_{\text{meas}} - A(\text{m})]. \quad (2)
\]

where \( \text{m} \) is an a priori \( M \times 1 \) reference vector, \( e^2 \) is a damping factor, and \( I \) is an \( N \times N \) identity matrix. The square of solution length is defined by:

\[
L = [\text{m}_{\text{est}} - (\text{m})]^T [\text{m}_{\text{est}} - (\text{m})], \quad (3)
\]

and the prediction error by

\[
E_{\text{pred}} = [\text{d}_{\text{meas}} - \text{d}_{\text{pred}}]^T [\text{d}_{\text{meas}} - \text{d}_{\text{pred}}], \quad (4)
\]

where

\[
\text{Am}_{\text{est}} - \text{d}_{\text{pred}}. \quad (5)
\]
Inversion of intra-tooth isotope profiles

### 2.3. Laboratory Procedures

Computations were performed using MATLAB v. 5.2 on an 800 MHz Mac G4 PowerPC. A computer code, Emeas1_1, was developed that estimates measurement error using, as inputs, the sampling geometry parameters, measured isotope signal, and isotope ratio and sampling dimension uncertainties. Another code, mSolve1_1, was developed that calculates A, generates a reference vector, solves Eqn. 2 for the input signal, and calculates the prediction error of the generated input signal. These codes are given as MATLAB m-files in EA2 (Emeas1_1) and EA3 (mSolve1_1). EA4 describes how to use these codes.

All of the estimated input signals are presented in the figures as tooth-enamel equivalent isotope ratios. In reality, the input signals reflect body fluid composition and so will be depleted relative to tooth enamel. For carbon isotopes, tooth enamel hydroxyapatite is $-14\%$ enriched relative to diet (Cerling and Harris, 1999; Passey et al., in press) and 11 to $12\%$ enriched relative to breath CO$_2$.

Tooth enamel samples were hand-drilled from teeth using diamond impregnated drill bits. Samples were treated for 15 min in 3% H$_2$O$_2$ and 15 min in 0.1 M acetic acid (pH 2.9) or 0.1 M buffered acetic acid (pH 4.7). The rabbit samples were not treated because the enamel was thin ($\sim 100 \mu m$) and yielded only $\sim 500 \mu g$ of enamel powder per 2 mm sample. This is the amount necessary to make an isotopic analysis, and treatment would have resulted in excessive sample loss. Treatment tests presented in Passey et al. (2002) show little difference and a consistent isotopic offset between treated and untreated enamel using this procedure. Enamel was reacted at 90°C in a common acid bath (100% H$_3$PO$_4$) under positive helium pressure. The liberated CO$_2$ was analyzed using a Finnigan MAT 252 mass spectrometer at the University of Utah.

Growth rate of hippopotamus lower canines was measured on two female individuals (ages 48 and 8 yr) at the Toledo Zoo by filing a notch in the tooth at the gum line and monitoring subsequent growth. The canine of the older individual grew 14 to 15 mm in 394 days (13–14 mm/yr) and that of the younger individual grew 26 to 28 mm in 336 days (28–30 mm/yr).

As part of a larger study, several rabbits were raised on strictly controlled diets. Animal R2 was equilibrated to an isotopically homogeneous alfalfa diet ($^{13}$C = $-27.3\%$) at the Toledo Zoo by filing a notch in the tooth at the gum line and monitoring subsequent growth. The animal continued on the C$_4$-based diet until day 37, at which time it was switched back to the alfalfa. The animal was humanely sacrificed on day 72 by intravenous injection of sodium pentobarbitol. The animal was frozen following sacrifice, and later the lower incisors were removed, washed with distilled water, and dried. One incisor was sampled for isotopic analysis. Maturation parameters were determined on a lower incisor of a different animal using an X-ray microcomputed tomography method (Lin and Miller, 2001).

### 3. SENSITIVITY TESTING USING SYNTHEtic DATA

#### 3.1. Overview

In this section synthetic data are used to test the sensitivity of mtest to changes in modeling parameters. A hypothetical input signal m is made into synthetic measured data dmean, random error is added to the signal to simulate natural measurement uncertainties (Appendix 3), and then the signal is inverted to see if the resultant vector mtest is similar to m. This approach allows evaluation of how changes in (m), $e^2$, maturation parameters, error in sampling and isotope analysis, and closed- vs. open-ended profiles, influence the form of mtest.

Two different hypothetical input series are studied: the first is a $^{81}$Sr record for precipitation collected at Midway Airport (Chicago, Illinois) over the period 1967–1971 (ISOHIS, 2003), and the second is a sine wave with simple structure similar to that discussed by Kohn (2004).

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b = Passey and Cerling (2002).

a These parameters are also associated with spatial positions on the tooth, and have time significance.

We follow the “Morozov Discrepancy Principle” and choose a value of $e^2$, which gives a value for $E_{\text{pred}}$ that is the same as the estimated error level for sampling and isotope measurements (Groetsch, 1993). This allows solutions to be obtained that are neither overpredicted ($E_{\text{pred}} \ll$ measurement error, with too great a value for $L$) nor underpredicted ($E_{\text{pred}} \gg$ measurement error, with too small a value for $L$). Appendix 2 describes how measurement error is estimated, and Appendix 3 outlines the computational procedure used in this paper.

### Table 1. List of notations used in this paper.

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b = Passey and Cerling (2002).

a These parameters are also associated with spatial positions on the tooth, and have time significance.
3.2. Influence of Damping

In this section, the damping factor \( \varepsilon^2 \) is varied, the reference vector is held constant at the average value of the elements of \( \mathbf{d}_{\text{mean}} \) and the closed-ended case is assumed. Figure 2a shows the Midway isotope data and corresponding forward-modeled tooth enamel signal \( \mathbf{d}_{\text{mean}} \) for \( l_p = 240d \) and \( l_p = 90d \). The tooth enamel signal has maximum amplitude of 8.0‰, which is 47% of the amplitude of the Midway input signal. Inverse estimates of the input signal using Eqn. 2 with \( \varepsilon^2 = 0 \) are shown in Figure 2b; these estimates are very spiky because they must predict \( \mathbf{d}_{\text{mean}} + \sigma^2_{\text{ins}} \) with zero prediction error. Figure 2c and 2d shows inverse estimates with \( \varepsilon^2 = 0.005 \) and 0.01. These estimates are much smoother, and comparison with Figure 2a shows that they accurately capture the majority of the complexity in the true input signal. The total amplitude of the original input signal is 17.2‰; the average amplitude of the input signals in Figure 2c and 2d are 16.7‰ and 15.3‰, respectively, recovering 97 and 89% of the original amplitude.

The loss of recovered amplitude is proportional to the level of measurement error, with greater error requiring more damping, and hence lower amplitude. Figure 2e shows that the prediction error for \( \varepsilon^2 = 0 \) and \( \varepsilon^2 = 0.005 \) are less than the expected measurement error \( E_{\text{mean}} \), while that for \( \varepsilon^2 = 0.01 \) is similar. The solutions shown in Figure 2d are the most accurate solutions in this example.

Figure 3 shows the same progression with a sinusoidal input signal. Inverse estimates made with \( \varepsilon^2 = 0.0 \) blow up for such input signals because there is very little structure to constrain the wanderings of the input signal (Fig. 3b). This problem is analogous to a two-point running average of a signal that oscillates between two opposing values, for instance 100 and -100; the running average will be constant-valued at the average of those values. In the same way, the tooth enamel maturation process is a type of running average, so an input signal may oscillate between extreme values provided that they average out at the value of the measured signal. Figure 3c and 3d shows that introduction of the damping factor remedies this situation and gives estimates that are similar to the true input signal. The spikiness of these estimates compared to the input signal derives from the random sampling and isotope error added before solving for \( \mathbf{m}_{\text{est}} \). (Appendix 3) and demonstrates the less constrained nature of this simple profile compared to the more complex profile in Figure 2. This spikiness is an artifact that should generally be ignored, and an average of several propagations gives a smoother and more reasonable profile that is very similar to the input signal. Inversion of a measured signal with no error added beforehand yields an input signal that is indistinguishable from the original input signal shown in Figure 3a. Figure 3e indicates that a damping factor of \( -0.04 \) is appropriate for this system. The total amplitude of the original input signal is 4.0‰. The averaged inverse estimates in Figure 3c and 3d recover 3.9‰ (98%) and 3.5‰ (87%) of the original amplitude, again illustrating the relationship between increasing measurement error and decreasing recoverable amplitude.

Also note that the prediction error for the \( \varepsilon^2 = 0.0 \) solutions is greater than that for the \( \varepsilon^2 = 0.005 \) solutions; this stems from the fact that the prediction error results both from damping and random error propagation. In the undamped case (\( \varepsilon^2 = 0.0 \)), \( \mathbf{m}_{\text{est}} \) exactly predicts \( \mathbf{d}_{\text{mean}} + \sigma^2_{\text{ins}} \), so relative to \( \mathbf{d}_{\text{mean}} \) there is a finite amount of prediction error. This error decreases slightly when a very small damping factor is introduced, and again increases as the damping factor is increased.

3.3. Choice of Reference Vector

The inverse estimates discussed above are minimum-length solutions relative to a reference vector (\( \mathbf{m} \)) that is constant-valued at the average isotope value of the measured isotope profile. It is possible, however, that the “best” solution is one which has minimum length compared to a nonconstant reference vector. In some cases, solving relative to a variable reference vector brings about new solutions that are reasonable and which would not be observed using a constant reference vector. Such solutions cannot be ruled out if they have isotope values that fall within a realistic range. The ultimate reference vector is equivalent to the input signal, but unfortunately this is what is being solved for and is not known beforehand.

One way to generate a wider range of possible solutions is to solve relative to a randomly generated, nonconstant reference vector. The only constraints on such reference vectors are (1) they fall within the acceptable isotope range for the system being studied, and 2) they are not unrealistically spiky (i.e., rapid oscillations between, say, \( \delta^{13}C = -15\%e \) and 0‰ over a short period of time may be ecologically unlikely). An algorithm is included in the code mSolve1_1 (EA3) that generates random reference vectors within a specified isotope range, and with adjacent isotope parameters that differ by a randomly generated number that has normal distribution about a specified value. The computed solutions based on such reference vectors for the closed-ended case are shown in Figure 4a and 4b. For the highly structured Midway signal, there is little difference between these solutions and those generated using a constant reference vector (Fig. 2c). For the less structured sinusoidal signal, these inverse estimates are appreciably noisier and do not point to the existence of alternative solutions that are reasonable. A variable reference vector is important in some open-ended cases, however, as outlined in sections 3.4 and 4.2.

3.4. Open-Ended Cases

Inverse estimates for the proximal values of a profile may be poorly constrained for open-ended cases (Appendix 1), especially when the reference vector is allowed to vary. Figure 4c shows the open-ended sinusoidal signal solved relative to three different reference vectors. The dashed, gray, and solid black lines are inverse estimates solved relative to a constant-valued reference vectors with values of \( -13.5\%e \), \( -5.5\%e \), and 1‰, respectively. This figure shows that the proximal values are more sensitive to changes in the reference vector than are the distal values. The three solutions predict the measured data equally well, and are equally valid solutions under the minimum-length constraint. Figure 4c illustrates that, for open-ended cases, solving relative to a variable reference vector may illuminate possible solutions that are both reasonable and very different from those estimated using a constant reference vector. These solutions are important to generate because the form or the primary input signal following the proximal most samples is very poorly constrained, and may make excursions that
Inversion of healthy isotope profiles

Fig. 2. Inversion of synthetic tooth enamel data generated with rainfall data from Midway Airport, Chicago (ISOHIS, 2003). (a) Input signal (rainfall data, black circles) modeled as tooth enamel (white circles) with $L_x = 240$ days, $L_y = 90$ days, $\Delta x = 30$ days, and $\Delta z = 1/3 L_z$ (that is, depth of each sample is 1/3 thickness of enamel). Closed-ended case is assumed. (b) Four different inverse estimates (solid lines) of the input signal using $\varepsilon^2 = 0$, with reference vector constant valued at $-8.3\%$ (average value of measured signal), and with random errors $\sigma_{\text{meas}}$, $\sigma_x$, $\sigma_z$, of 0.1%, 3 days, and 1/5 $L_z$, respectively. (c) and (d) Same inversion conditions as (b), but with $\varepsilon^2 = 0.005$ and 0.01, respectively. (e) Comparison between the estimated measurement error $E_{\text{meas}}$ and the prediction error $E_{\text{pred}}$ for each damping level. These are percentile box plots, showing the minimum, mean, and maximum (solid lines) and 25th and 75th percentiles (dashed lines) for 100 random error propagations ($E_{\text{meas}}$) or 25 error propagations followed by inversion ($E_{\text{pred}}$).
Fig. 3. Inversion of synthetic tooth enamel data generated using a sine wave. (a) Input signal (black circles) modeled as tooth enamel (white circles) with $l_x = 14$ mm, $l_y = 6$ mm, $\Delta x = 1$ mm, and $\Delta y = 1/2$ $l_x$. Closed-ended case is assumed. (b) Four inversion estimates (solid lines) of the input signal using $\varepsilon^2 = 0$, with reference vector constant valued at $-6.2\%$, and with random errors $\sigma_m, \sigma_x,$ of $0.05\%$, $0.2$ mm, and $1/5$ $l_x$, respectively. (c) and (d) Same inversion conditions as (b), but with $\varepsilon^2 = 0.005$ and $0.042$, respectively. Gray lines are the average of 25 estimated input signals. (e) Percentile box plot representation of the measurement error and the prediction error for each example.
depart from the pattern of variation observed in the better constrained part of the profile.

Another important case where a variable reference vector is critical is the “short” profile, or a profile where the length of maturation is similar to the length of the entire profile. The open-ended solution may be very poorly constrained in this case, as can be visualized from Figure 4c if it is imagined that the distal half of the measured profile is missing.

4. INVERSE MODELING OF RABBIT AND HIPPO PROFILES

4.1. Overview

The following section explores the inversion of three different carbon isotope profiles measured on teeth from modern mammals. Inversion of these “real” signals is potentially more troublesome than inversion of hypothetical signals because of uncertainties in growth rates, maturation parameters, sampling geometry, and mass spectrometry. Each of the profiles is unique and illustrates different problems associated with inverse methods. The first profile is from a rabbit that underwent a controlled feeding experiment and has a known input signal. This profile illustrates the case where more than one type or class of solutions can equally well predict the same profile. The second profile is a modern hippo canine (K00-AS-167) that shows the potential for a single data point to cause a major excursion in the modeled input signal. The third profile is a modern hippo canine that gives rise to a quasi-repeating input signal that may be an artifact of inverse methods and that is subjected to extensive testing before accepting the solution. The approach suggested in the following section is to be skeptical of the initial inversion estimate, and to accept the solution only after it proves to be robust to deliberate minor changes in model parameters that reflect uncertainty in those parameters.

4.2. R2 Rabbit Profile

Rabbit R2 was given a controlled dietary change as outlined in section 2.3. The breath data from this experiment serves as a known input signal, and allows the forward model of Passey and Cerling (2002) to be evaluated. The breath data were measured as a function of time, whereas the tooth enamel data are measured as a function of distance from the proximal margin of the tooth. This discrepancy was reconciled by determining the growth rate of the tooth using day 72 and day 14 to find the relation that best fits the data. The latter relation was determined by matching the position of the initial increase in δ13C indicated by modeling (Fig. 5b and 5c) with the timing of the dietary changes.

Fig. 4. Inversion of synthetic tooth enamel data using variable reference vectors. (a) Same model conditions as in Figure 2c, but with randomly generated reference vectors that are allowed to vary between 0 and −20‰, with adjacent parameters differing by a random number drawn from a Gaussian distribution with a standard deviation of 3‰. (b) Same model conditions as in Figure 3d, but with $\epsilon = 0.01$ and a random reference vector between 2 and −15‰ with adjacent parameters linked by a 1‰ standard deviation. (c) Estimated input signals for an open-ended tooth enamel profile. Each estimated input vector is the average of 25 estimated input signals. Dashed line: reverence vector constant valued at −13.5‰; solid line: reverence vector constant valued at −5.5‰; thick grey line: reference vector constant valued at 1‰.
switch to C₄ feed. Figure 5a shows the breath data, the measured tooth enamel data, and the predicted tooth enamel signal based on lₙ₀ = 5 mm and lₙ₁ = 1.8 mm. The predicted and measured tooth enamel signals are very similar, suggesting that the forward model of Passey and Cerling (2002) is reasonably accurate for this rabbit incisor. The fact that the model was developed using maturation patterns from a hippo canine (K00-AS-167) suggests the potential applicability of the model to ever-growing teeth from a wide range of mammals.

A significant deviation between the measured and forward modeled tooth enamel is for the two samples between 20 mm and 15 mm (Fig. 5a). Here the measured data are depleted (or proximally shifted) compared to the model prediction. This could result from a number of factors, including too small a value for finit, or a temporary decrease in the growth rate of the tooth following the switch to C₄ feed. The latter would not be surprising given that two other rabbits involved in the study refused the new feed for 2 to 3 days following the switch, and that the breath data from R2 show a brief return to depleted values following the initial isotope increase, possibly indicating partial food refusal and reliance on C₃ energy reserves in the body. We also note that the sample depth uncertainty for all samples in the profile is very large because the enamel itself is only ~100 μm thick.

Inversion of the measured signal gives a range of input signals that fall between two end members, both accurately reconstructing the stepped nature of the diet change but differing in the shape of the signal preceding this change. One end member (Fig. 5b) has a depletion between 20 and 17 mm that is not indicated by the breath data (although it is possible that the once per day afternoon breath sampling for R2 undersampled this feature). The other end member (Fig. 5c) does not show the strong depletion between 20 mm and 17 mm. This type of solution is clearly better in light of the breath data. One basis for selecting the second type of solution in the absence of a priori knowledge of the input signal is the shorter solution length compared to the first type of solution. Another basis for selecting the second type is that increasing the damping factor and sampling error quickly removes the depletion seen in the first type, and the majority of the estimated input signals become more like the second type of signals.

4.3. K00-AS-167 Hippo Profile

The K00-AS-167 sample was collected in August 2000 at Arabuko-Sokoke National Park, Kenya and is discussed in Passey and Cerling (2002). The profile is closed-ended because the ever-growing tooth was still forming at the time the animal died (Appendix 1). A liberal sample length uncertainty σₓ of 1 mm, and a depth uncertainty σᵧ of 20% enamel thickness (1/5 lᵧ) are assumed. These uncertainties help to compensate for the mismatch between the idealized rectangular sample volume adjacent parameters linked by a random number from a normal distribution with 1‰ standard deviation. (c) Four inversion estimates generated under the same conditions and representing a class of solutions that do not show the depletion at 20 to 18 mm.
assumed by the model, and the actual sample morphology attained by hand drilling.

For hippo profiles, we discuss only the carbon isotope data, which has a reproducibility of \( \sim 0.05\% \) for duplicate analyses of the same sample powder and \( \sim 0.07\% \) for analyses of adjacent milled samples with the same x coordinate and \( \Delta x \) and \( \Delta z \) values. Oxygen isotope data are reported in Passey and Cerling (2002) and for unknown reasons have very poor reproducibility \( \sim 0.3\% \) for both profiles, despite tooth enamel standards having good reproducibility \( < 0.1\% \) within the same sample runs. The noisy nature of the oxygen isotope data precludes meaningful inversion for these profiles.

The initial inversions of the carbon isotope data (Fig. 6a) indicate two intervals of increased \( C_4 \) feeding at 440 to 400 mm and 220 to 200 mm. However, scrutiny of the data shows that both of these excursions are caused when pairs of measured isotope parameters with similar values precede a rapid change in the isotope value of the profile. Figure 6b shows that a change in the measured isotope parameter at \( \sim 210 \) mm before inversion greatly reduces the \( C_4 \) excursion. Because the presence of these excursions depends heavily on few data, they should be regarded as suspect. We resampled and reanalyzed the tooth between \( \sim 230 \) and 160 mm, and also reanalyzed the original samples from the entire profile. We discovered that in the original data, one sample at 240 mm had been analyzed twice but counted as two consecutive samples and that the value at 210 mm was slightly more negative \( (\sim 0.2\%) \) than the new value. Figure 6c shows the average and \( 1\sigma \) range of 75 inverse estimates on the correct data with the sampling and maturation uncertainties listed in the caption. These results show that a small amount of error in the measured isotope profile can sometimes have a large effect on the estimated input signals.

4.4. K00-AS-168 Hippo Profile

The K00-AS-168 profile is a hippo canine that was also collected at Arabuko in August 2000. The tusk is slightly smaller, and the profile is closed-ended. We assume the same sampling and isotope error as for the K00-AS-167 profile.

The initial inversions of this profile (Fig. 7a) show an interesting and unexpected signal that is quasi-repeating. In our experience, we have found that such repeating signals can be model artifacts that have a wavelength similar to the length of maturation, and that are triggered by small peaks in the measured data and misfit between the assumed and real maturation parameters. These problems are often associated with relatively flat profiles such as the middle portion of K00-AS-168. We therefore provisionally view the inversions in Figure 7a as suspect, and accordingly subject the system to a series of sensitivity tests to see if the repeating signal holds.

Figure 7b shows the same data inverted assuming three different lengths of maturation. We perform this sensitivity testing because we estimated and did not measure the actual lengths of maturation for this tooth. The figure shows that the positions of peaks 1, 2, and 4b are essentially unchanged by the different maturation parameters (although the valley between 1 and 2 is significantly wider for \( l_{\text{m}} = 45 \)). Peaks 3 and 4a change position as a function of maturation length, and the amplitude of peak 2 decreases with increasing maturation length. Overall, the results shown in Figure 7b suggest that peaks 1, 2, and 4b are robust features despite uncertainty in length of maturation, that the amplitude of peak 2 is uncertain, and that the remainder of the peaks are of questionable significance given the uncertainty in maturation parameters.

Another approach is to test whether certain features in the data trigger the oscillations in the inverse estimates. A very suspect feature in the measured data is the two-point peak at 120 to 100 mm. It is possible that the existence of this peak not only gives rise to peak 2 but causes a rebound on either side, which in turn gives rise to peaks 1 and 3, and possibly propagates to peak 4. In Figure 7c, the upper inverse estimate was modeled with this peak and treated as an open-ended profile, with all subsequent samples removed (proximal 12 samples). Peaks 3, 4a, and 4b remain and are slightly altered by this treatment. The middle-inverse estimate in Figure 7c was carried out with the 120 to 100 mm samples included, but with no subsequent samples (final 9 samples removed), and under open-ended conditions. The resulting profile is very similar to that shown in Figure 7a, indicating that the final several samples do not lead to artifacts in the inversion estimate. The lower inversion in Figure 7c was carried out with the entire measured profile, but with the 120 to 100 mm peak subdued to form a smoother profile. The result is also very similar to Figure 7a, with the exception that peak 2 is decreased in amplitude. The results of these experiments suggest that the peaks in the estimated input signals are robust features and are not triggered by isolated features in the measured data. Figure 7d shows the best estimate input signal for the K00-AS-168 profile that includes sampling and isotopic uncertainties, and also those associated with uncertainty in maturation parameters.

5. DISCUSSION

Inversion of the hypothetical profiles (Figs. 2, 3, and 4) and the rabbit profile (Fig. 5) led to estimates of the input signals that were, in all cases, much more similar to the original input signals than were the raw isotope data alone. However, the modeling results clearly illustrate that different isotope profiles respond differently to inversion, with some giving more accurate results than others. For some such as the Midway profile (Figs. 2 and 4), the form of \( m_{\text{est}} \) is insensitive to \( (m) \) and \( \sigma \), such that variations in these parameters have little influence on \( m_{\text{est}} \), and the solutions are essentially unique. Generally speaking, these profiles have a high degree of structure in the sense that they have many excursions and inflections. For other profiles, the form of \( m_{\text{est}} \) is more sensitive to \( (m) \) and \( \sigma \). These include smooth or “flat” profiles such as the sine wave in Figure 2, or square profiles such as the rabbit data (Fig. 4).

The accuracy of estimated input signals is a function of many factors, including measurement error, sampling resolution, uncertainty in maturation parameters, and the structure of the input signal itself. Importantly, accuracy may also vary with respect to the type of information sought: is total isotope amplitude the most important parameter, or are rates of change and patterns of variation more significant for the application at hand? The Midway precipitation and sinusoidal test cases (section 3.2; Figs. 2 and 3) show that accuracy in terms of recovered amplitude is largely a function of the degree of damping necessitated by measurement error. Greater than 95% of the
primary input signal amplitude was recovered for both cases when the damping factor was small, which mimics a case with low measurement error, and ~90% amplitude was recovered when the damping factor was increased to a level consistent with the measurement error for each system. The R1 rabbit profile (Fig. 5) is very accurate in terms of reconstructing the stepped changes in diet, but is less accurate in terms of total amplitude because of uncertainty in a model parameter that precedes the dietary change. However, if single-point excursions in modeled input signals are ignored (which may be a good rule given results from the R1 and K00-AS-167 modeling), the estimated input signal for R1 is, for the intents and purposes of ecological reconstruction, indistinguishable from the primary input signal.

The accuracy of the hippopotamus profiles (Figs. 6 and 7) is obviously more difficult to evaluate because there is no a priori knowledge of the input signal. Uncertainty in maturation parameters reduces accuracy, as may the assumption of a constant growth rate. The hippopotamus canine teeth have large zones of maturation (~65 mm) compared to their growth rates (~30 mm/yr; section 2.3). This means that each portion of enamel is the time average of ~2 yr, and the consequence is that very short-lived isotope excursions, even if they are very pronounced, will be overprinted by subsequent mineralization to the point that they are below the background level for isotopic analysis. Therefore, with respect to fine details, the accuracy of these profiles is limited, but this is due to measurement limitations rather than error in inverse methods. With respect to long-term patterns, the accuracy is likely to be much better.

Because of the complexity of intra-tooth isotope systems, simple equations cannot be used to determine the accuracy of inverse results, and there is no universal cutoff level in terms of profile length, sampling interval, or measurement uncertainty that can be used to determine whether a profile is suitable for inversion. The complexity of these systems necessitates a model-based approach for gauging the accuracy or sensitivity of each unique profile with respect to inversion.

The approach suggested here for determining the accuracy of inverse results is similar to that outlined in sections 3 and 4.2: begin with an input signal (which may be synthetic or the estimated input signal from the profile in question), forward-model the signal with appropriate uncertainties in maturation parameters into hypothetical tooth enamel signals, add random error that is reflective of the measurement error for the system, and then use inverse methods to estimate "new" input signals. The similarity between the new signals and original signal will illustrate the accuracy of the inverse results. Accuracy can be gauged in several ways depending on the specific application, for example, as the percent recovered of the original amplitude or the sum of the squared differences between each original and each estimated data point ($\Delta$ prediction error). Features in the original input signal that cannot be reproduced in the new input signals must be regarded as unrecoverable, given the uncertainty in the system, or as meaningless artifacts of the original inversion.

6. CONCLUSIONS

A method has been presented that enables tooth enamel maturation and sampling parameters to be embodied into the...
form of a linear system that allows both forward and inverse modeling of measured and input isotope signals. The inverse modeling is based on the fundamental assumption that the best model solutions are those with minimized length. Application of these inverse methods to hypothetical data shows that meaningful results can be recovered on this basis of this assumption. Application of the methods to measured tooth enamel profiles shows that features can be recovered that are not apparent in the raw data alone, that a controlled feeding experiment supports the forward model described in Passey and Cerling (2002), and that inversion can accurately recover the input signal in living systems.

Inverse methods open the door to more meaningful interpretation of intra-tooth isotope profiles, but are capable of producing both accurate and inaccurate solutions. This is not surprising in the light that tooth enamel systems are underdetermined and that there are an infinite number of possible solutions for each one. The fact that numerous solutions can be produced means that it is important for workers to clearly describe the conditions under which solutions are generated. The method presented here is to use a minimum-length solution and to damp the solution so that the prediction error is comparable to the measurement error. This leads to, in many cases, a stable solution that is accurate and relatively insensitive to further increases in damping.

The forward model used in this paper is simplistic, assuming constant growth rate and constant dimensions of maturation parameters. Obtaining more detailed information about the temporal and spatial patterns of mineral uptake during amelogenesis is an important goal that will enhance the utility of intra-tooth isotope methods. The inverse methods utilized here are independent of the forward model and should be applicable to a variety of teeth when forward models for those teeth become available.

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APPENDIX 1

Representing Isotope Profiles as Am = d

Intra-tooth isotope profiles can be approximated as simple linear systems as described in this section. The averaging matrix A is an M x N matrix that describes the sampling and maturation parameters that relate the input signal to the measured signal. The input isotope signal m is described by an M x 1 vector, and the measured isotope signal d by an N x 1 vector (Figure A1.1).

The elements d, that comprise d are the isotope delta values of the
measured isotope profile, and the elements $m_i$ that make up $m$ are the isotope delta values of the input signal that will be solved for. Each $d_i$ has a length dimension along the growth axis $\Delta x_i$, a width dimension perpendicular to the growth axis $\Delta y_i$ (that is also parallel to features such as linear hypoplasia), and a depth dimension perpendicular to the enamel surface $\Delta z_i$ (Figure A1.1). The $\Delta x_i$ value, as used in this paper and in the computer codes developed for this research, is the interval along the $x$-axis that each sample represents; if samples are milled contiguously as in Figure A1.1, $\Delta x_i$ is equivalent to the length in the $x$-direction of each sample volume. If samples are not milled contiguously, i.e., if there is a space of unmilled enamel between each sample pit, the value $\Delta x_i$ must be defined as the interval starting at the midpoint between sample $d_{i-1}$ and $d_i$, and ending at the midpoint between $d_{i+1}$ and $d_i$. Each $d_i$ is additionally defined by a mean position on the tooth $x_i$, $y_i$, and $z_i$, each measured relative to an arbitrary line or surface, for example, the cervical margin for $x_i$, a line parallel to the growth axis for $y_i$, and the outside enamel surface for $z_i$. In this paper, we assume that lines parallel to the $y$-axis are isochronous with respect to mineral deposition such that there is no systematic isotopic variation in the $y$-direction, and we do not make use of the $\Delta y_i$ and $y_i$ parameters. This assumption is yet to be tested rigorously, although data in Balasse (2003) show that isotopic differences caused by different sampling strategies with respect to the $y$-axis are minor compared to total isotopic variation along the growth ($x$) axis. It is also assumed that all samples are milled from the outside enamel surface, which allows the $z_i$ term to be dropped because the parameter $\Delta z_i$ completely describes the $z$ position of the sample relative to the enamel surface. The convention used throughout this paper is that sample depth $\Delta z_i$ is expressed in units of $l_a$, where $0.25l_a$ is a sample milled to half the thickness of the enamel, $0.5l_a$ is a sample milled to half the thickness of the enamel, $0.25l_a$ is quarter-thickness depth, and so on.

Each $d_i$ has a time dimension $\Delta t_i$ that is determined by the length $\Delta x_i$ of $d_i$ (Figure A1.1) and the growth rate of the tooth. This paper uses a constant growth rate, which may be valid for some ever-growing teeth but is certainly not valid for all teeth. Each $m_i$ has a length dimension $\Delta x_i$, mean position at the outer enamel surface $x_i$, and mean position at

\[
\begin{align*}
\text{fractional contribution to } d_i \text{ from:} \\
&\begin{bmatrix}
 0.25 & 0.30 & 0.20 & 0.20 & 0.05 \\
 0 & 0.26 & 0.32 & 0.21 & 0.21 \\
 0 & 0 & 0.33 & 0.40 & 0.27 \\
 0 & 0 & 0 & 0.45 & 0.55 \\
\end{bmatrix}
\end{align*}
\]

\[
\begin{align*}
&\begin{bmatrix}
m_0 \\
m_1 \\
m_2 \\
m_3 \\
m_4 
\end{bmatrix} = \\
&\begin{bmatrix}
d_1 \\
d_2 \\
d_3 \\
d_4 
\end{bmatrix}
\end{align*}
\]

\[
A = (N = 4) \\
M = 5
\]

Fig. A1.1. Illustration of the spatial relationship between $A$, $m$, and $d$. Each $m$ represents the average isotopic composition of the body during the time that the volume was initially deposited as tooth enamel matrix. Each $d$ is the final isotopic composition of mature tooth enamel. The position and length of each $m$ is determined by the position and length of each $d$. The parameters $l_m$ and $l_a$ are the length of maturation and length of apposition (Passey and Cerling, 2002). The $y$-direction is perpendicular to the plane of the page. As discussed in the Appendix 1, this scenario represents the closed-ended case, where the youngest enamel is completely immature because the animal died while the tooth enamel was forming. Note that the parameter $m_0$ is a preceding input parameter and does not have a corresponding $d_0$. Inversion of intra-tooth isotope profiles
the enamel dentine junction (EDJ) x i - l a. The isotope ratio m i is the average isotopic composition of the animal during the time that the enamel matrix in volume m i was initially deposited. Although not used in this paper, it is possible for m i to have width y i and position y i, whereas the z dimension has no meaning.

The first and last elements in m represent the earliest and latest input isotope parameters influencing d, respectively. Likewise, the first and last elements in d are the distal and proximal samples from the tooth, respectively. The distal end of the tooth is the occlusal or wear surface, and the proximal end is the cervical margin.

There are always more m’s than d’s (i.e., M > N). The parameter m N in Figure A1.1 influences the isotopic composition of d N by virtue of the z dimension of sampling. Such parameters are referred to as “preceding” input parameters, and the number of these depends on the relationship between sampling depth and length of apposition, with greater depths and longer lengths of apposition resulting in more preceding m’s.

The averaging matrix A is a function of maturation parameters such as l a and l m, and sampling parameters defined by the vectors x, y, and z (vectors specifying the x-, y-, and z-positions of each sample) and Δx, Δy, and Δz (vectors specifying the length Δx, width Δy, and depth Δz of each sample). Each d i is a function of several m i’s, and A determines the relative contribution of each m i to each d i.

Calculation of the elements in A is performed by the code mSolv1_1, using as inputs l a, l m, and a parameter that specifies the degree to which the profile is open-ended, and the vectors Δx and Δz. The basic theory is behind the calculation of A is outlined in EA1.

Open-Ended and Closed-Ended Cases

The proximal volume in a milled profile (d N) may be fully mineralized or only partially mineralized. If it is fully mineralized (Figure A1.2), its isotopic composition is determined by the isotopic composition of the animal during a subsequent time interval represented by the length of maturation l m. Figure A1.2 shows that m N - 1, m N, and m N + 1 contribute to the isotopic compositions of d N, d N - 1, and d N - 2. The model elements m i near this boundary are less constrained than elements in the tooth interior. This is referred to as the open-ended case. The elements distal to and including m N + 1 are referred to as "open-ended" input parameters.

The closed-ended case arises when the proximal volume d N is immature enamel matrix. This sample volume is deposited just before death and sees no subsequent mineral overprinting, so the isotopic composition of d N is a function of m N and perhaps preceding m’s, as shown in Figure A1.1, but is not a function of subsequent m’s. The model elements m i near this boundary are more constrained than elements in the tooth interior. A continuum exists between the open- and closed-ended cases corresponding to d N’s with varying degrees of mineral content.

APPENDIX 2

Estimating Measurement Error

Measurement error is an estimated quantity that is dependent on the reproducibility of isotope analysis and on the precision of sampling positions and dimensions. The measurement error r i for any sample in a measured profile is the sum of the uncertainty in the mass spectrometer analysis and the isotope uncertainty induced by sampling error. This latter quantity is largely a slope-dependent error: for absolutely flat isotope profiles (isotope slope = 0), errors in the x- and z-position of samples will have no effect on the isotope ratio of the sample, whereas for rapidly changing isotope profiles, such errors will significantly influence the measured isotope ratio of the sample (Figure A2.1).
Fig. A2.1. Slope-dependent isotope error. For portions of a profile where the isotope value quickly changes, a lateral error in sampling will translate into a finite isotope error. No isotope error will result from sampling error when the isotope slope is zero. (a) Isotope error associated with errors in the x-position (along the growth axis) of samples. Samples indicated by gray boxes are shifted by 0.5 cm from samples indicated by white boxes. In one case this leads to a 0.5‰ isotope error (left side), and in another leads to no isotope error (right side). (b) Isotope error associated with errors in the z-position (sample depth) of samples. Solid line is the isotope value at the outside enamel surface, and dashed line is the isotope value at the enamel-dentine junction (EDJ). The later is equivalent to the value of the outside enamel surface at a position $x - l_a$. The samples indicated by white boxes are milled from the outside half of the enamel thickness, while those indicated by gray boxes are milled from the inside half of the enamel thickness. In one case, this leads to a 1‰ isotope difference (left side), and in another leads to a 0.2 to 0.3‰ difference (right side).
To calculate the x-position slope-dependent error, the slope of the isotope profile along the x-axis must be estimated. For the first and last data points in an isotope profile, this slope is estimated by the first and second, and penultimate and ultimate samples, respectively:

\[ s_i^1 = \frac{d_i - d_i}{\frac{1}{2} \Delta x_i + \Delta x_i} \quad \text{(A2.1a)} \]

\[ s_i^0 = \frac{d_n - d_{n-1}}{\frac{1}{2} \Delta x_{n-1} + \Delta x_{n-1}} \quad \text{(A2.1b)} \]

For other samples, the slope is estimated on the basis of three points:

\[ s_i^t = \frac{1}{\frac{1}{2} \Delta x_{i-1} + \Delta x_i + \frac{1}{2} \Delta x_{i+1}} \left( d_i - d_{i-1} + d_{i+1} \right) \quad 1 < i < N \quad \text{(A2.1c)} \]

The units of slope are ‰/U length, so multiplication of the slope’s absolute value by length (x-position) error gives an isotope error.

Calculation of sampling depth (z-position) error is based on the assumption that the isotopic composition of enamel is constant along appositional surfaces (i.e., Fig. 3; Passey and Cerling, 2002). This assumption has not been rigorously tested, but may be supported by data in Hoppe (2004), and may possibly be valid for some species and not for others. The assumption allows for the observation that an isotope profile sampled at the enamel-dentine junction (EDJ) is shifted in the proximal direction of distance l, compared to the same profile sampled at the outside enamel surface (Figure A2.1b), and is equivalent to the concept of “proximal shift” discussed in Passey and Cerling (2002). Therefore, the isotopic difference between the outside enamel surface and the EDJ can be approximated as the isotopic difference between the outside enamel and the EDJ.

The units of slope are ‰/U length, so multiplication of the slope’s absolute value by length (x-position) error gives an isotope error. The units of slope are ‰/U length, so multiplication of the slope’s absolute value by length (x-position) error gives an isotope error. The units of slope are ‰/U length, so multiplication of the slope’s absolute value by length (x-position) error gives an isotope error.

The slope-dependent sample length and sample depth errors are combined with the analytical isotope error to give the overall error \( r_i \):

\[ r_i = \sqrt{\left( \frac{s_i^1}{\sigma_{\Delta x}} \right)^2 + \left( \frac{s_i^0}{\sigma_{\Delta x}} \right)^2 + \sigma_{ms}^2} \quad \text{(A2.2)} \]

where \( \sigma_{\Delta x} \) and \( \sigma_{ms} \) are the 1σ precisions of the length, depth, and mass spectrometer measurements, respectively. The total measurement error is analogous to the prediction error and is given by:

\[ E_{\text{meas}} = r_{\text{meas}} \cdot r_i \quad \text{(A2.3)} \]

where \( r_{\text{meas}} \) is the measurement error vector composed of the elements \( r_i \).

### APPENDIX 3

#### Outline of Modeling Procedure

The sequence of events for inverse modeling used in this paper is as follows. First, isotope profile data are organized into the vectors \( \mathbf{d} \), \( \Delta z \), and \( \Delta x \), maturation parameters \( l_m \) and \( l_a \) are determined or estimated, the degree to which which the profile is open-ended is determined, and estimates are made of the 1σ isotope measurement and sampling dimension precisions. These data are then placed into the MATLAB codes Emea1_1 and mSolv1_1 (EA2 and EA3, respectively).

Next, the code Emeas1_1 is used to estimate the measurement error \( E_{\text{meas}} \). The code performs Monte-Carlo error propagation with the following equation:

\[ r_i = \sqrt{\left( \frac{s_i^1}{\sigma_{\Delta x}} \right)^2 + \left( \frac{s_i^0}{\sigma_{\Delta x}} \right)^2 + \sigma_{ms}^2} \quad \text{(A3.1)} \]

This equation differs from Eqn. A2.2 in that \( \sigma_{\Delta x}, \sigma_{\Delta z}, \) and \( \sigma_{ms} \) are random numbers drawn from normal distributions with standard deviations \( \sigma_{\Delta x}, \sigma_{\Delta z}, \) and \( \sigma_{ms} \) respectively. A random vector \( \mathbf{r}_{\text{meas}} \) is generated using Eqn. A3.1, and this is used in Eqn. A2.3 to calculate the measurement error. This is done many times (−100) to create a probability distribution of \( E_{\text{meas}} \). Because \( E_{\text{meas}} \) is equivalent to the square of a Gaussian variable, the distribution of \( E_{\text{meas}} \) is approximately chi-squared.

Next, the code mSolv1_1 is used to generate numerous solutions \( \mathbf{m}_{\text{meas}} \). The code adds random error \( \sigma_{ms} \) to each \( d_i \) using a normally distributed random number generator with standard deviation \( \sigma_{ms} \). Sampling geometry error is similarly incorporated by adding normally distributed random sample length and sample depth errors \( \sigma_{s}^z \) and \( \sigma_{s}^d \) to each sample length and depth before calculation of \( \mathbf{A} \). A random reference vector \( \mathbf{m} \) is generated based on user-specified parameters, and the system is then solved for \( \mathbf{m}_{\text{meas}} \) using Eqn. 2 with a user-specified value for \( \epsilon \). This process is repeated several times, producing a range of solutions \( \mathbf{m}_{\text{meas}} \) each associated with a unique \( \mathbf{d}_{\text{meas}} = \mathbf{m} \), and a combination. This range of solutions is important for estimating the degree of variability among the solutions, and may reveal the existence of separate classes or types of solutions that have different form but predict the measured data equally well.

Finally, mSolv1_1 calculates \( E_{\text{pred}} \) for each inverse estimate, and the user compares the resulting probability distribution of \( E_{\text{pred}} \) with that of \( E_{\text{meas}} \). If the distributions of \( E_{\text{pred}} \) and \( E_{\text{meas}} \) are similar, the associated solutions are accepted and possibly subjected to additional tests such as those described in sections 3 and 4. If the distributions are different, the value for \( \epsilon \) is adjusted until the resulting solutions yield a distribution of \( E_{\text{pred}} \) that is consistent with \( E_{\text{meas}} \), in accordance with the Morozov Discrepancy Principle (section 2.2).

Electronic annex EA4 explains in detail how the inverse modeling is accomplished using the MATLAB codes Emea1_1 (EA2) and mSolv1_1 (EA3).

#### ELECTRONIC ANNEX