Identification of the Themophysical properties of Fish
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Introduction

The problem is to determine the thermal conductivity and heat capacity of a fish sample given its thermal history from freezing to thawing. This data is important both for food safety and for food quality during industrial processing. Fish is an example of a binary substance in that freezing takes place over a temperature range, not a single temperature. Steady state measurements are problematic so the problem is to recover the thermal properties from unsteady temperature profiles measured while the sample is either being progressively frozen or thawed [Nes]. This problem has a long history, having been presented at previous study groups, however a completely successful approach had not been found. This type of thermal inverse problem occurs elsewhere and there have been a number of recent papers of interest [Hua, Bud]. The main difficulty lies in the phase change and on its adverse effect on the regularisation of the inverse problem, which is necessarily ill-posed [Bec].

The experimental temperature measurements were taken in such a way that the fish sample can be treated as one-dimensional. (In fact the thermal properties will depend on the sample orientation, and heat flow in these experiments was typically transverse to muscle fibres.) The fish sample is assumed to be homogeneous in that direction so that the thermal properties are only temperature dependent. The unsteady heat equation for the temperature $T(x,t)$ is then

$$c(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(k(T)\frac{\partial T}{\partial x}) \;\; \forall (x,t) \in [0,L] \times [0,t_0]$$

$$\text{boundary conditions } T(0,t) = \tilde{T}^{obs}(0,t),\;\; T(L,t) = \tilde{T}^{obs}(L,t),$$

$$\text{initial conditions } T(x,0) = \tilde{T}^{obs}(x,0),$$

where $c(T)$ is the specific heat capacity *per unit volume*, $k(T)$ is the thermal conductivity, the domain is of length L, and the (suitably interpolated) observed temperatures $\tilde{T}^{obs}$ have been used to specify the boundary data and initial data.

Inverse Problem

Let the set of temperature observation time-space positions be $\Omega^{obs} = [x_\alpha, \alpha = 1, N] \times [t_\beta, \beta = 1, M]$. The problem is then to determine the coefficients $c(T), k(T)$, given the observed temperatures $T^{obs}(x,t)\ \forall (x,t) \in \Omega^{obs}$. Some form of regularisation of the inverse problem is required; the standard approach is a weighted least squares minimisation, i.e. choose $c(T), k(T)$ from some appropriate class of functions so as to minimise

$$F(c(T), k(T)) = \sum_{\beta=1}^{M} \sum_{\alpha=1}^{N} \left[(1/\sigma_{\alpha,\beta})^2 (T(x_\alpha, t_\beta) - T^{obs}(x_\alpha, t_\beta))^2 \right]$$

where the $\sigma_{\alpha,\beta}$ are estimates of the standard deviations of the errors for each of the temperature measurements.
To solve this problem we need to define

- a class of functions to be searched for $c(T), k(T)$, specified in terms of a finite parameter set $a_i, i = 1, p$;
- a numerical solution to the nonlinear heat equation;
- a nonlinear minimisation algorithm for F with respect to the $a_i, i = 1, p$.

These three elements of the determination of the inverse problem are described in the following sections.

Parameterisation

In the paper by Nesvadba [Nes] a function class consisting of cubic splines was used to allow for a completely general representation of $c(T), k(T)$; this was observed to be numerically unstable as the number of knots (i,e, the dimension of the space) was increased. Since the change of phase implies that both properties, but particularly $c(T)$ are rapidly varying in the "mushy" region this was a particular limitation. This rapid variation can easily destabilise the regularisation approach which relies on a degree of smoothness in the recovered coefficients. The second study group effort on this problem considered different minimisation techniques and an exponential parameterisation chosen to allow efficient representation of the mushy region; this was successful for synthetic data but not on the actual data, and the parameters appeared to contain unsuitable correlations making the minimisation impossible on real data [Wil]. The 1997 ESGI group produced a simpler and more robust parameterisation which avoided obvious interdependencies between parameters while capturing the physical features of the thermal properties. A seven-parameter representation was derived, with the following form;

$$c(T) = \begin{cases} c_1 & T < T_1 \\ c_1 + 2La(T - T_1)/(T_2 - T_1)^2 & T_1 \leq T \leq T_2 \\ c_2 & T_2 < T \end{cases}$$

$$k(T) = \begin{cases} k_1 & T < T_1 \\ k_1 + (k_2 - k_1)(T - T_1)^2/(T_2 - T_1)^2 & T_1 \leq T \leq T_2 \\ k_2 & T_2 < T \end{cases}$$

where T_1 and T_2 bracket the mushy region. It is easily seen that La is the effective latent heat of the sample since

$$\int_{T_1}^{T_2} c(T)dT = c_1(T_2 - T_1) + La.$$

Clearly $c(T)$ is discontinuous at $T = T_2$, the temperature corresponding to the depressed freezing point of the water component of the fish sample. The thermal conductivity is continuous, with continuous first derivative at $T = T_1$ and discontinuous first derivative at $T = T_2$. A similar parameterisation of $c(T)$ had been produced by Bonacina [Bon] for a binary fluid however he used a piecewise constant function for $k(T)$.

The above parameterisation was considered simple but representative and could be extended (e.g. by allowing linear variation outside the mushy region) if found to effective when combined with the least-squares regularisation of the inverse problem. Since the heat equation in the temperature regions outside the mushy region depends only on the thermal diffusivity $\kappa(T) = k(T)/c(T)$ it follows that only the ratios k_1/c_1 and k_2/c_2 can be determined from temperature measurements, so that in practice the parameterisation is reduced to 5 independent parameters $\{\kappa_1 = k_1/c_1, \kappa_2 = k_2/c_2, T_1, T_2, La\}$.

Note that the enthalpy $H(T) = \int_0^T c(T)dT$ takes a particularly simple form

$$H(T) = \begin{cases} c_1 T & T < T_1 \\ c_1 T + La(T - T_1)^2/(T_2 - T_1)^2 & T_1 \le T \le T_2 \\ c_1 T_2 + La + c_2(T - T_2) & T_2 < T \end{cases}$$

The Kirchoff transformation variable $V(T) = \int_0^T k(T)dT$ is also easily evaluated,

$$V(T) = \begin{cases} k_1 T & T < T_1 \\ k_1 T_1 + \frac{1}{3}(k_2 - k_1)(T - T_1)^3/(T_2 - T_1)^2 & T_1 \le T \le T_2 \\ k_1 T_1 + \frac{1}{3}(k_2 - k_1)(T_2 - T_1) + k_2(T - T_2) & T_2 < T \end{cases}$$

The enthalpy transformation can be explicity inverted, $H \longmapsto T$, as follows

$$T = \begin{cases} H/c_1 & H < H_1 \\ T_1 + \frac{\sqrt{\{c_1^2 + \frac{4La(H-H_1)}{(T_2-T_1)^2}\}} - c_1}{2La/(T_2-T_1)^2} & H_1 \le H \le H_2 \\ T_2 + (H - c_1 T_2 + La)/c_2 & H_2 < H \end{cases}$$

where $H_1 = c_1 T_1$ and $H_2 = c_1 T_2 + La$. This saves some work in the numerical solution procedure described next.

Numerical solution of the Nonlinear Heat Equation

The enthalpy method combined with the Kirchoff transformation reformulates the heat equation in a way suitable for numerical approximation and avoids the need to use front tracking methods to follow the phase boundary. Using the definitions above, the heat equation becomes

$$\frac{\partial H(T)}{\partial t} = \frac{\partial^2 V(T)}{\partial x^2} \quad \forall (x,t) \in [0, L] \times [0, T_0]$$

$$\text{boundary conditions } H(0,t) = \int_0^{T^{obs}(0,t)} c(T)dT, \;\; H(L,t) = \int_0^{T^{obs}(L,t)} c(T)dT$$

$$\text{initial conditions } H(x,0) = \int_0^{\tilde{T}^{obs}(x,0)} c(T)dT.$$

These equations can be readily approximated on a uniform mesh of N_x points $\Omega = [x_1, x_2, ...x_{N_x}]$ by a mesh function $T_j^n \approx T(x_i, n\Delta t)$, where Δt is the timestep, using backward-Euler time stepping and central finite differences. The solution procedure is then

- Calculate initial enthalpies $H_j^0, j = 1, N_x$ and $V_j^0, j = 1, N_x$.
- Update the enthalpies for $n = 0, 1, ...$ using

$$H_j^{n+1} = H_j^n + (\Delta t/\Delta x^2)(V_{j+1}^n + V_{j-1}^n - 2V_j^n)$$

- Calculate corresponding temperature updates T_j^{n+1}, and hence V_j^{n+1} by inverting the enthalpy transformation.

Numerical results

The least squares minimisation was solved using the NAG Library routines E04FCF (a robust Newton-type nonlinear solver); function evaluations only were provided i.e. gradients were calcualated using finite differences. The numerical investigation was limited in that two of the 5 independent parameters were specified in advance (from known experimental values), namely the thermal diffusivities κ_1 and κ_2 in the frozen/thawed regions respectively. A summary of the results obtained are given below for a set of measured temperature profiles provided by P. Nesvadba:

- Thermal diffusivities were set to $\kappa_1 = k_1/c_1 = 2.38/(2.4 \times 10^6))m^2/sec$ and $\kappa_2 = k_2/c_2 = 0.55/(4.1 \times 10^6))m^2/sec$.
- Starting values for the mushy region $[T_1, T_2]$ and for the effective latent heat La were $T_1 = -46°C, T_2 = -2°C, La = 331 \times 10^6 joules$
- The minimisation terminated with values $T_1 = -8.4°C, T_2 = -1.2°C, La = 351 \times 10^6 joules/m^3$. A different set of starting values converged to similar parameter values.
- The observed and fitted temperature profiles are shown in Figures 1 & 2, and the residuals at each (x_α, t_β) measurement point are shown in Figure 3.

The fit to the measured data is remarkably good, with the movement of the phase change "kink" in the temperature profiles well captured. The residuals appear to show some systematic features implying that there may be a small systematic modelling error; one possible cause would be a degree of spatial inhomogeneity in the fish sample.

Further Work

- A full 5 - parameter minimisation should be carried and the results checked for correlations in the parameters; this can be conveniently carried out by using the NAG Library routine EO4YCF to return estimates of the variance-covariance matrix.
- The numerical approximation of the heat equation could easily be improved through adaptive and more accurate (e.g. Crank-Nicolson) timestepping.
- A Levenberg-Markardt approach to the least squares minimisation could give better results than the Newton-style algorithm used in EO4FCF.
- The gradients of the F with respect to the parameters $\{k_1/c_1, k_2/c_2, T_1, T_2, La\}$ should be evaluated analytically, either by solving pde's for the sensitivities $\partial T/\partial a_i$, $i = 1, 5$, obtained by appropriate differentiation of the heat equation, or by using the adjoint approach [Hua] which would only require one additional pde to be solved, at the cost of storing the numerical solution for each timestep.
- It would be good practice to use this approach to optimise the design of the actual experiments themselves, for example in the timing and the location of the temperature measurement points. This would be abasis for systematically improving the accuracy of the themophysical properties deduced from the parameter estimation process itself.

References

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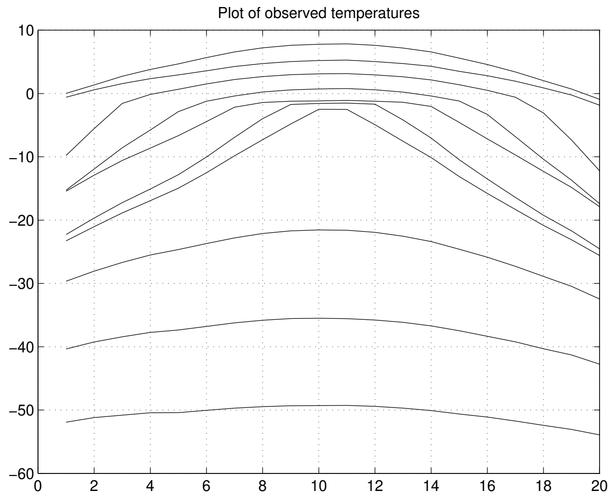
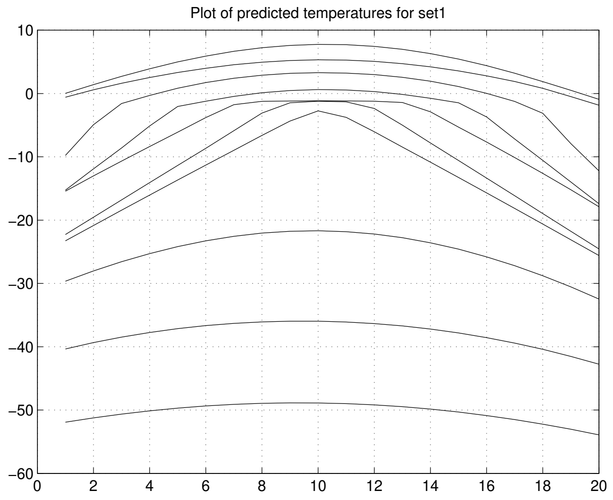


(a) Measured temperatures



(b) Predicted temperatures

Figure 1: Comparison between the experimentally measured temperatures (a) and the final set of predicted temperatures (b) after least-squares minimisation with $T_1 = -8.4°C, T_2 = -1.2°C, La = 351 \times 10^6 joules/m^3$

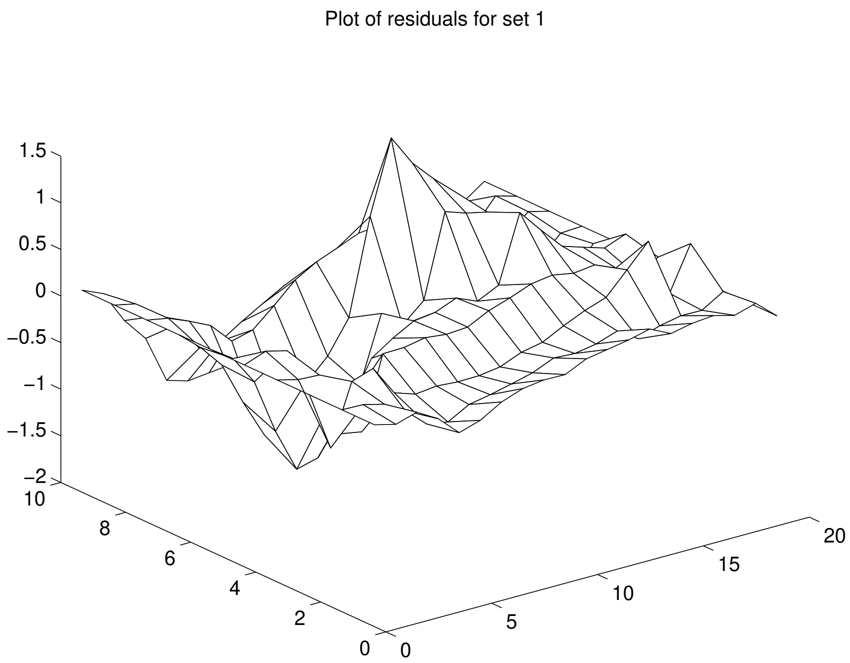


Figure 2: Temperature residuals after least-squares minimisation plotted at each measurement point (x_α, t_β); ideally, they would appear completely uncorrelated. The systematic left-right feature indicates (not unexpectedly) that the mathematical model does not quite fit the experiment