

# Development of a test environment for constitutive models

## Introduction

In modern engineering applications polymeric materials play a significant role, as they for instance can be found in biomaterials and foams, just to mention a few. Their advanced mechanical properties call for elaborate constitutive models to describe the observed material behaviour. To achieve an accurate model representation the parameters in such a model need to be determined experimentally, see Figure 1.



Figure 1: Experimental setup of foam testing, typical application of foam, simulation results

## Project

The goal of the project is to develop a programme to fit a material model to experimental data. Thereby focus is placed on the Mooney–Rivlin model as it well describes the hyperelastic behaviour of many materials. In both a one-dimensional, incompressible and a three dimensional compressible format, the stress state for a given deformation shall be evaluated. A numerical derivative is found by systematically perturbing the deformation state, and with this a solution for the occurring multi-axial deformation is obtained iteratively. The algorithm for the numerical derivative shall also be used for the fitting of the material parameters to the experimental data.

A key ingredient in the programming is to define data structures, which allow to handle the matrix quantities, and to define the necessary corresponding operators. The code shall be designed in a modular fashion, such that the present Mooney–Rivlin model could easily be replaced by other constitutive models, if needed later on. For this project the programming language C is used.

## Project Assignment

### General procedure

The programming project in particular comprises five steps, which the group shall subsequently solve and briefly document.

- In weekly meetings the progress will be discussed. Bring your current results and be well prepared to explain occurring problems.
- The individual steps of the projects must be documented in a final report, which is due 6 March 2009.
- There will be a final discussion session of 30 min which each group in week 11 (9–13 March 2009). The exact time will be appointed during the course.
- The project tasks include simple plots to visualize the results. Because plotting curves in C may be very time-consuming, it is recommended to perform the visualization of the results using, for instance, Matlab.

### Work plan.

step	task	date
S1	One-dimensional model and simple fitting	4 February 2009
S2	Three-dimensional hyperelastic model	9 February 2009
S3	Numerical derivative	13 February 2009
S4	Uniaxial stress state	20 February 2009
S5	Curve fitting for uniaxial stress state	6 March 2009

**Final project report.** The final project report must be submitted by 6 March 2009. It only needs to be in note form, but make sure to include

- the group number and the names of all group members,
- the results of all problems asked for in the assignment,
- the source files containing the programming code written in C.

### Problems

The following problem steps are to be solved subsequentially.

#### S1 One-dimensional hyperelastic model and simple fitting

Consider an incompressible Mooney–Rivlin constitutive model, in which the stress function is defined as

$$\sigma = [G_1 + G_2\lambda^{-1}][\lambda^2 - \lambda^{-1}]. \quad (1)$$

when subjected to a uniaxial stretch ratio  $\lambda$ . Herein, the material parameters  $G_1$  and  $G_2$  represent the two elastic shear moduli.

- First assume  $G_1 = 100$  MPa and  $G_2 = 100$  MPa. For the stretch  $\lambda$  linearly varied over from 1 to 3 in steps of 0.1, determine the resulting stress.

b) Now the shear moduli  $G_1$  and  $G_2$  shall be fitted to the curve shown in Figure 2 using the algorithm of appendix C. The model response  $\sigma$  of Eq. (1) is thus stored in a column  $\underline{h}$  such that  $h_i = \sigma(\lambda_i)$  and the model input in a column  $\underline{\lambda}$ . Note that in the algorithm the column  $\underline{\theta} = [G_1 \ G_2]^T$  contains the shear moduli of the model to be identified using the fitting algorithm described.

- Summarize all the data quantities (arrays) you will need in your code.
- Read the experimentally measured data for the stretch  $\lambda_i$  and the corresponding stress  $\sigma_i$  from file `data_1b.txt` (columns:  $\lambda$ ,  $\sigma_{\text{exper}}$ ) and store them as  $\underline{\lambda}$  and  $\underline{m}$ , respectively.
- Analytically determine the derivatives of the model quantity with respect to the material parameters,  $\frac{\partial \sigma}{\partial G_i}$ . For the stretch  $\underline{\lambda}$  found in Figure 2, store these derivatives in the sensitivity matrix  $\underline{H} = \frac{\partial \underline{h}(\underline{\lambda}, \underline{\theta})}{\partial \underline{\theta}}$  using the notation of appendix A.
- Identify the two material parameters  $G_1$  and  $G_2$  with the Gauss–Newton algorithm of appendix C. The weighting matrices can be set to  $\underline{V} = \underline{I}$  and  $\underline{W} = \underline{\underline{Q}}$ .
- Plot and compare the model response for these parameters with the experimental behaviour.

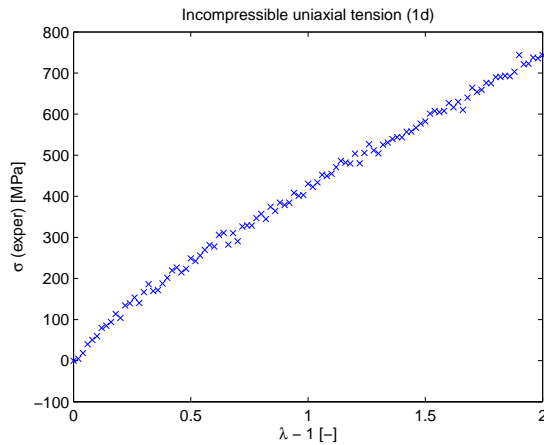


Figure 2: Measurements from a tensile test for the incompressible material, which is to be fitted in step 1b.

## S2 Three-dimensional hyperelastic model

For a three-dimensional hyperelastic Mooney–Rivlin model, the Cauchy stress  $\boldsymbol{\sigma}$  for an arbitrary deformation gradient tensor  $\mathbf{F}$  is given as:

$$\boldsymbol{\sigma} = \frac{1}{J} \left[ G_1 \tilde{\mathbf{B}}^d - G_2 (\tilde{\mathbf{B}}^{-1})^d \right] + K(J - 1)\mathbf{I}, \quad (2)$$

For this compressible model, the bulk modulus  $K$  represents a third material parameter. Furthermore,  $\tilde{\mathbf{B}} = J^{-2/3} \mathbf{F} \cdot \mathbf{F}^T$  is the isochoric left Cauchy–Green deformation tensor

and  $J = \det(\mathbf{F})$  is the volume ratio of the deformation. The required tensor operations can be found in appendix A.

- a) Identify the matrix operations that are needed to determine the Cauchy stress (2) for a known deformation gradient  $\mathbf{F}$ .
- b) Give all components of the Cauchy stress tensor for the following deformations for the scalar stretch  $\lambda = 1.1$ :

$$\underline{\mathbf{F}} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda^{-\frac{1}{2}} & 0 \\ 0 & 0 & \lambda^{-\frac{1}{2}} \end{bmatrix}; \quad \underline{\mathbf{F}} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix}. \quad (3)$$

Thereby use the following material parameters:  $G_1 = 100$  MPa,  $G_2 = 100$  MPa, and  $K = 200$  MPa.

- b) For these deformations also determine the equivalent deviatoric stress  $\sigma^{\text{eq}} = \sqrt{\frac{3}{2}\boldsymbol{\sigma}^{\text{d}} : \boldsymbol{\sigma}^{\text{d}}}$  and the hydrostatic stress  $\sigma^{\text{h}} = \frac{1}{3}\text{tr}(\boldsymbol{\sigma})$ .

### S3 Numerical derivative

For a constitutive model, a numerical derivative of the stress with respect to the deformation gradient,  $\frac{d\boldsymbol{\sigma}}{d\mathbf{F}}$ , can be obtained as follows:

$$\left. \frac{d\boldsymbol{\sigma}}{dF_{ij}} \right|_{\mathbf{F}} = \frac{\boldsymbol{\sigma}(\mathbf{F} + \delta F \vec{e}_i \vec{e}_j) - \boldsymbol{\sigma}(\mathbf{F})}{\delta F} \quad \text{for } i, j \in \{1, 2, 3\} \quad (4)$$

wherein  $\delta F$  is a perturbation applied to the deformation gradient componentwise.

- a) Write a programme that determines all the components of the numerical tangent for the three-dimensional Mooney–Rivlin model of the previous step. Store the stress and the deformation gradient tensors both in column format as

$$\underline{\boldsymbol{\sigma}} = [ \sigma_{11} \quad \sigma_{22} \quad \sigma_{33} \quad \sigma_{12} \quad \sigma_{23} \quad \sigma_{31} ]^{\text{T}}, \quad (5)$$

$$\underline{\mathbf{F}} = [ F_{11} \quad F_{22} \quad F_{33} \quad F_{12} \quad F_{23} \quad F_{31} \quad F_{21} \quad F_{32} \quad F_{13} ]^{\text{T}}, \quad (6)$$

respectively. Identify further arrays you need to initialize, while considering the notation of appendix A.

- b) Create a plot that displays the component  $\left. \frac{d\sigma_{11}}{dF_{11}} \right|_{\mathbf{F}}$  versus the perturbation  $\delta F$  for

$$\underline{\mathbf{F}} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda^{-\frac{1}{2}} & 0 \\ 0 & 0 & \lambda^{-\frac{1}{2}} \end{bmatrix} \quad \text{with } \lambda = 1.1. \quad (7)$$

Thereby vary  $\delta F$  from  $10^{-9}$  to  $10^0$  and use a logarithmic scale for the  $\delta F$ -axis.

#### S4 Uniaxial stress state

A material is subject to the prescribed stretch

$$U_{11} = \lambda(t) \quad (8)$$

under the condition of uniaxial tensile stress, with

$$\sigma_{22} = \sigma_{33} = \sigma_{12} = \sigma_{13} = \sigma_{23} = 0. \quad (9)$$

Since in this case no rotation occurs and no shearing modes are active, the deformation tensor boils down to

$$\mathbf{F} = \mathbf{U} \hat{=} \begin{bmatrix} U_{11} & 0 & 0 \\ 0 & U_{22} & 0 \\ 0 & 0 & U_{33} \end{bmatrix}, \quad (10)$$

which is a symmetric tensor with all diagonal components other than  $U_{11}$  unknown.

- a) To determine these unknown deformations in  $\mathbf{U}$ , write a programme that solves the following system of equations

$$\varrho(\underline{u}) = 0, \quad (11)$$

using an iterative Newton–Raphson scheme (see appendix B). Use the notation

$$\varrho = \begin{bmatrix} \sigma_{22} \\ \sigma_{33} \end{bmatrix}, \quad \underline{u} = \begin{bmatrix} U_{22} \\ U_{33} \end{bmatrix} \quad (12)$$

and numerically determine the tangent  $\frac{d\varrho}{d\underline{u}}$  for a perturbation of  $\delta u = 10^{-5}$ .

- b) Calculate the response for the stretch ratio  $\lambda \in [0; 2]$  in steps of  $\Delta\lambda = 0.02$ . Discretize the time into small increments and plot the following quantities versus  $\lambda - 1$ :

- the three stress components  $\sigma_{ii}$ ,
- the diagonal components of the stretch tensor  $\mathbf{U}$ ,
- the number of iterations needed for convergence and the residue  $\|\varrho\|_2$  after convergence.

#### S5 Fitting to experimental data

Apply the fitting algorithm of step 1, described in appendix C, now to the uniaxial model within the three-dimensional setting of the previous step, which provides the relation  $\sigma_{11}$ . While taking the bulk modulus  $K$  the same as before, the goal is to determine the shear moduli  $G_1$  and  $G_2$  in the model (2) based on the experimental response shown in Figure 3, as it was obtained under uniaxial loading conditions.

- a) • Read the experimental data from a file `data_5a.txt` (columns:  $\lambda$ ,  $\sigma$ ) and store the stretches in  $\underline{\lambda}$  and the corresponding stress measures in the column  $\underline{m}$ .

- Store the model response in  $\underline{h}$  such that  $h_i = \sigma_{11}(t_i)$  and the model input in  $\underline{\lambda}$  such that  $\lambda_i = \lambda(t_i)$ .
- Compute the sensitivity matrix  $\underline{H} = \frac{\partial \underline{h}(\underline{\lambda}, \underline{\theta})}{\partial \underline{\theta}}$  with respect to the sought-for set of parameters  $\underline{\theta} = [G_1 \ G_2]^T$  applying the same perturbation technique for a numerical derivative as in step 3.
- Determine the shear moduli of this material, plot the resulting model response and compare it to the experimental curve. Give the value of the (least squares) objective function (29) for this fit.

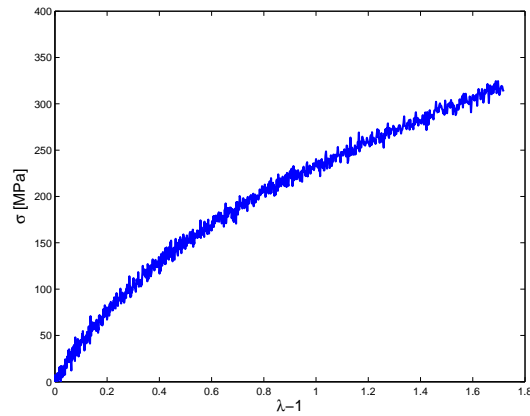


Figure 3: Experimental measurements from tensile test for the compressible material under uniaxial stress, which is to be fitted in step 5a.

- b) Describe the structure of the programme and how the constitutive model can be replaced by an arbitrary other model.

## Appendix A: Notation and tensor/matrix operations

### Tensor operations

We consider the stress/strain state of a material point in a global Cartesian coordinate system with unit vector basis  $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ .

**Products between tensors.** For two second-order tensors  $\mathbf{A} = A_{ij} \vec{e}_i \vec{e}_j$  and  $\mathbf{B} = B_{jk} \vec{e}_j \vec{e}_k$  the following products are defined. Thereby Einstein's summation convention holds, which prescribes a summation over equal indices.

- tensor product

$$\mathbf{C} = \mathbf{A} \cdot \mathbf{B} = A_{ij} B_{jk} \vec{e}_i \vec{e}_k = C_{ik} \vec{e}_i \vec{e}_k \quad (13)$$

- scalar product

$$c = \mathbf{A} : \mathbf{B} = A_{ik} B_{ki} \vec{e}_i \vec{e}_k \quad (14)$$

**Operations on tensors.** The operations on second order tensors are evaluated for the matrix representation with respect to the Cartesian basis defined above.

- transpose

$$\mathbf{A}^T \rightarrow \underline{\mathbf{A}}^T := \begin{bmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{bmatrix} \quad (15)$$

- determinant

$$\begin{aligned} \det \mathbf{A} \rightarrow \det \underline{\mathbf{A}} &:= \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} \\ &= A_{11}A_{22}A_{33} - A_{11}A_{23}A_{32} - A_{12}A_{21}A_{33} \\ &\quad + A_{12}A_{23}A_{31} + A_{13}A_{21}A_{32} - A_{13}A_{22}A_{31} \end{aligned} \quad (16)$$

- inverse

$$\begin{aligned} \mathbf{A}^{-1} \rightarrow \underline{\mathbf{A}}^{-1} &:= \frac{1}{\det \underline{\mathbf{A}}} \begin{bmatrix} \begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix} & \begin{vmatrix} A_{13} & A_{12} \\ A_{33} & A_{32} \end{vmatrix} & \begin{vmatrix} A_{12} & A_{13} \\ A_{22} & A_{23} \end{vmatrix} \\ \begin{vmatrix} A_{23} & A_{21} \\ A_{33} & A_{31} \end{vmatrix} & \begin{vmatrix} A_{11} & A_{13} \\ A_{31} & A_{33} \end{vmatrix} & \begin{vmatrix} A_{13} & A_{11} \\ A_{23} & A_{21} \end{vmatrix} \\ \begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix} & \begin{vmatrix} A_{12} & A_{11} \\ A_{32} & A_{31} \end{vmatrix} & \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} \end{bmatrix} \\ &= \frac{1}{\det \underline{\mathbf{A}}} \begin{bmatrix} A_{22}A_{33} - A_{23}A_{32} & A_{13}A_{32} - A_{33}A_{12} & A_{12}A_{23} - A_{22}A_{13} \\ A_{23}A_{31} - A_{21}A_{33} & A_{11}A_{33} - A_{13}A_{31} & A_{13}A_{21} - A_{11}A_{23} \\ A_{21}A_{32} - A_{22}A_{31} & A_{12}A_{31} - A_{11}A_{32} & A_{11}A_{22} - A_{12}A_{21} \end{bmatrix} \end{aligned} \quad (17)$$

- trace

$$\text{tr}\mathbf{A} \rightarrow \text{tr}\underline{\mathbf{A}} = A_{ii} = A_{11} + A_{22} + A_{33} \quad (18)$$

- deviator

$$\mathbf{A}^d = \mathbf{A} - \frac{1}{3}\text{tr}\mathbf{A} : \mathbf{I} \quad (19)$$

### General matrix/column operations

- inverse of a  $2 \times 2$  matrix  $\underline{\mathbf{A}} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$

$$\underline{\mathbf{A}} = \frac{1}{\det \underline{\mathbf{A}}} \begin{bmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{bmatrix} \quad (20)$$

- 2-norm of a column

$$\|u\|_2 = \sqrt{\underline{u}^T u} = \sqrt{\sum_i u_i^2} \quad (21)$$

### How to store derivatives

Store the numerical derivatives in a matrix  $\underline{\mathbf{K}}$  where the rows refer to the component of the quantity itself and the columns refer to the quantity with respect to which the derivative is taken.

- numerical derivative of step 3,  $K_{ij} = \frac{d\sigma_i}{dF_j}$ :

$$\underline{\mathbf{K}} = \frac{d\sigma}{d\tilde{\mathbf{F}}} = \begin{bmatrix} \frac{d\sigma_{11}}{dF_{11}} & \frac{d\sigma_{11}}{dF_{22}} & \frac{d\sigma_{11}}{dF_{33}} & \frac{d\sigma_{11}}{dF_{12}} & \frac{d\sigma_{11}}{dF_{23}} & \frac{d\sigma_{11}}{dF_{31}} & \frac{d\sigma_{11}}{dF_{21}} & \frac{d\sigma_{11}}{dF_{32}} & \frac{d\sigma_{11}}{dF_{13}} \\ \frac{d\sigma_{22}}{dF_{11}} & \frac{d\sigma_{22}}{dF_{22}} & \frac{d\sigma_{22}}{dF_{33}} & \frac{d\sigma_{22}}{dF_{12}} & \frac{d\sigma_{22}}{dF_{23}} & \frac{d\sigma_{22}}{dF_{31}} & \frac{d\sigma_{22}}{dF_{21}} & \frac{d\sigma_{22}}{dF_{32}} & \frac{d\sigma_{22}}{dF_{13}} \\ \frac{d\sigma_{33}}{dF_{11}} & \frac{d\sigma_{33}}{dF_{22}} & \frac{d\sigma_{33}}{dF_{33}} & \frac{d\sigma_{33}}{dF_{12}} & \frac{d\sigma_{33}}{dF_{23}} & \frac{d\sigma_{33}}{dF_{31}} & \frac{d\sigma_{33}}{dF_{21}} & \frac{d\sigma_{33}}{dF_{32}} & \frac{d\sigma_{33}}{dF_{13}} \\ \frac{d\sigma_{12}}{dF_{11}} & \frac{d\sigma_{12}}{dF_{22}} & \frac{d\sigma_{12}}{dF_{33}} & \frac{d\sigma_{12}}{dF_{12}} & \frac{d\sigma_{12}}{dF_{23}} & \frac{d\sigma_{12}}{dF_{31}} & \frac{d\sigma_{12}}{dF_{21}} & \frac{d\sigma_{12}}{dF_{32}} & \frac{d\sigma_{12}}{dF_{13}} \\ \frac{d\sigma_{23}}{dF_{11}} & \frac{d\sigma_{23}}{dF_{22}} & \frac{d\sigma_{23}}{dF_{33}} & \frac{d\sigma_{23}}{dF_{12}} & \frac{d\sigma_{23}}{dF_{23}} & \frac{d\sigma_{23}}{dF_{31}} & \frac{d\sigma_{23}}{dF_{21}} & \frac{d\sigma_{23}}{dF_{32}} & \frac{d\sigma_{23}}{dF_{13}} \\ \frac{d\sigma_{31}}{dF_{11}} & \frac{d\sigma_{31}}{dF_{22}} & \frac{d\sigma_{31}}{dF_{33}} & \frac{d\sigma_{31}}{dF_{12}} & \frac{d\sigma_{31}}{dF_{23}} & \frac{d\sigma_{31}}{dF_{31}} & \frac{d\sigma_{31}}{dF_{21}} & \frac{d\sigma_{31}}{dF_{32}} & \frac{d\sigma_{31}}{dF_{13}} \end{bmatrix} \quad (22)$$

- numerical derivative of step 4,  $K_{ij} = \frac{d\sigma_i}{du_j}$ :

$$\underline{\mathbf{K}} = \frac{d\sigma}{d\tilde{\mathbf{u}}} = \begin{bmatrix} \frac{d\sigma_{22}}{dU_{22}} & \frac{d\sigma_{22}}{dU_{33}} \\ \frac{d\sigma_{33}}{dU_{22}} & \frac{d\sigma_{33}}{dU_{33}} \end{bmatrix} \quad (23)$$



## Appendix B: Newton–Raphson scheme

The iterative Newton–Raphson scheme is used to find a solution  $\underline{u}$  for the following non-linear set of equations:

$$\underline{\sigma}(\underline{u}) = \underline{\rho}. \quad (24)$$

Because the real solution  $\underline{u}$  of this equation is yet unknown, consider an estimate  $\underline{u}^*$ . A Taylor expansion around this estimate reads

$$\underline{\sigma}(\underline{u}^* + \delta\underline{u}) = \underline{\sigma}(\underline{u}^*) + \left. \frac{d\underline{\sigma}}{d\underline{u}} \right|_{\underline{u}^*} \delta\underline{u} + \dots \quad (25)$$

If the higher order terms are ignored, the update on the estimate,  $\delta\underline{u}$ , can be obtained as:

$$\delta\underline{u} = - \left[ \left. \frac{d\underline{\sigma}}{d\underline{u}} \right|_{\underline{u}^*} \right]^{-1} \underline{\sigma}(\underline{u}^*). \quad (26)$$

With this a new, better estimate is obtained from:

$$\underline{u}^* := \underline{u}^* + \delta\underline{u}. \quad (27)$$

Starting with an initial estimate, the solution (26) and the update (27) are repeated until the estimated solution is sufficiently close to the real solution and convergence has been obtained. Use as a criterion for convergence:

$$\frac{\|\delta\underline{u}\|_2}{\|\underline{u}^*\|_2} \leq 10^{-6}, \quad (28)$$

## Appendix C: Fitting algorithm

The Gauss–Newton fitting algorithm that is also given in section 3.3.2 of the lecture notes “Continuum Mechanics for Advanced Manufacturing Technologies” is used to determine the parameters of the model that best fit the experimentally obtained response of the material.

Let the difference between the measured data points for the stress  $\underline{m}$  and the model prediction for this response  $\underline{h}$  be given by  $\underline{\xi} = \underline{m} - \underline{h}$ . Furthermore, the difference between the estimated parameters  $\underline{\theta}$  and an initial estimate  $\underline{\theta}_0$  is given by  $\underline{\zeta} = \underline{\theta}^0 - \underline{\theta}$ . With the fitting algorithm, the following quadratic objective function will be minimized:

$$G(\underline{\theta}) = \underline{\xi}^T \underline{V} \underline{\xi} + \underline{\zeta}^T \underline{W} \underline{\zeta}, \quad (29)$$

where  $\underline{V}$  and  $\underline{W}$  are weighting matrices (which are positive definite and symmetric).

The model sensitivity to variations in the parameters is given by:

$$\underline{H} = \frac{\partial \underline{h}(\underline{\lambda}, \underline{\theta})}{\partial \underline{\theta}} \quad (30)$$

Then, a new estimate for the model parameters can be obtained from

$$\underline{\theta} := \underline{\theta} + \delta\underline{\theta} \tag{31}$$

with

$$\delta\underline{\theta} = \underline{K}^{-1} (\underline{H}^T \underline{V}\xi + \underline{W}\zeta) \tag{32}$$

and

$$\underline{K} = \underline{H}^T \underline{V}\underline{H} + \underline{W}. \tag{33}$$

The parameter estimate  $\underline{\theta}$  is being updated until the updates are sufficiently small. Use as a criterion for convergence:

$$\frac{\|\delta\underline{\theta}\|_2}{\|\underline{\theta}\|_2} \leq 10^{-4}. \tag{34}$$