6 An analysis of data driven damage mechanics

In a general case, where the 1D object is assumed to be made of several linear elastic materials (heterogeneous material for instance), the distance function becomes

$$\Pi = \frac{1}{2}(\mathbb{1}\sigma - \sigma^*)^T D^{-1}(\mathbb{1}\sigma - \sigma^*) + \frac{1}{2}(\epsilon - \epsilon^*)^T D(\epsilon - \epsilon^*) + \lambda(\mathbb{1}^T\epsilon - \frac{u_D}{le}), \tag{156}$$

where $\sigma \in \mathbb{R}$ is the mechanical stress, $\epsilon, \sigma, \sigma^* \in \mathbb{R}^N$ (N is the number of elements) are the vectors of mechanical strains, material strains, and material stresses, respectively. The last term indicates the compatibility condition, where u_D is the applied displacement and le is the element length. $\mathbb{1} = (\underbrace{1, 1, \ldots, 1}_{\text{N times}})^T$. $D \in \mathbb{R}^{N\times N}$ denotes the metric.

Mechanical given material

Variation of Π wrt σ gives

$$\mathbb{1}^T D^{-1}(\mathbb{1}\sigma - \sigma^*) = 0 \implies \sigma = \frac{\mathbb{1}^T D^{-1}\sigma^*}{\mathbb{1}^T D^{-1}\mathbb{1}}. \tag{157}$$

Variation wrt ϵ and λ gives

$$D(\epsilon - \epsilon^*) + \mathbb{1}\lambda = 0, \quad \mathbb{1}^T\epsilon = u_D/le, \tag{158}$$

which means

$$\lambda = \frac{\mathbb{1}^T\epsilon^* - \frac{u_D}{le}}{\mathbb{1}^T D^{-1}\mathbb{1}}. \tag{159}$$

Using the above, ϵ can be seen to be

$$\epsilon = \epsilon^* - \frac{D^{-1}\mathbb{1}\mathbb{1}^T}{\mathbb{1}^T D^{-1}\mathbb{1}}\epsilon^* + \frac{D^{-1}\mathbb{1}}{\mathbb{1}^T D^{-1}\mathbb{1}}\frac{u_D}{le}. \tag{160}$$

Material given mechanical

If the bar is made of piece wise linear materials, the material state can be expressed in terms of the mechanical state by taking the partial derivative of Π wrt the material states as (see later examples for explicit forms)

$$\epsilon^* = A\mathbb{1}\sigma + B\epsilon + C, \tag{161}$$

$$\sigma^* = K\mathbb{1}\sigma + L\epsilon + M, \tag{162}$$

where $A, B, K, L \in \mathbb{R}^{N\times N}$, and $C, M \in \mathbb{R}^N$. It has been assumed that the material behavior can be expressed as $\sigma^* = m\epsilon^* + c$.

Combining the above

Using all the above, the data driven algorithm can be written as

$$\sigma^{k+1} = S\left(K\mathbb{1}\sigma^k + L\epsilon^k + M\right), \tag{163}$$

$$\epsilon^{k+1} = R(A\mathbb{1}\sigma^k + B\epsilon^k + C) + c\frac{u_D}{le}, \tag{164}$$

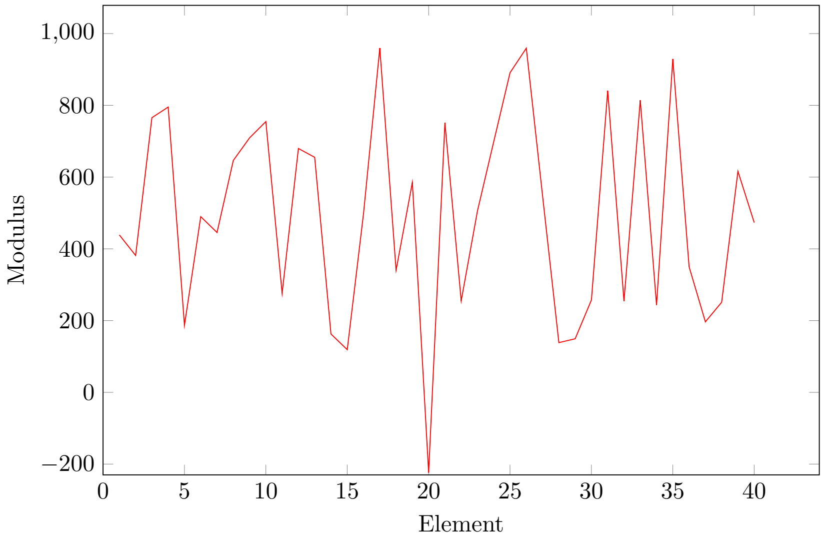

Figure 5: Modulus as a function of element number.

where

$$S = \frac{\mathbb{1}^T D^{-1}}{\mathbb{1}^T D^{-1}\mathbb{1}}, \quad R = I - \frac{D^{-1}\mathbb{1}\mathbb{1}^T}{\mathbb{1}^T D^{-1}\mathbb{1}}, \quad c = \frac{D^{-1}\mathbb{1}}{\mathbb{1}^T D^{-1}\mathbb{1}}.$$

Defining $s = [\sigma\ \epsilon^T]^T$, the above can be written as

$$s^{k+1} = \begin{bmatrix} SK\mathbb{1} & SL \\ RA\mathbb{1} & RB \end{bmatrix} s^k + r. \tag{165}$$

The speed of convergence hence depends on the spectral radius of the coefficient matrix.

A heterogeneous bar

Consider a case where a 1D bar is meshed with N elements and each element is assigned a different material "database" that is linear. In the current case, the number of elements has been chosen to be 40. The modulus of the material database of each of the elements of the bar plotted as a function of the element number can be seen in figure 5. It shall be noted that the modulus of one of the elements has been taken to be negative to simulate softening.

The eigen values of the coefficient matrix has been obtained for different choices of the metric D. In one case, it is taken as $D = EI$, where I is the identity matrix and $E = 1000$, a higher value than all the modulii. In the other case, $D = \mu I$, where $\mu = \frac{\sum_{i=1}^{N} E_i}{N}$, where E_i is the modulus of the i^{th} element. In the third case, $D = diag(E_1, E_2, E_3, \ldots, E_N)$, where $diag$ denotes a diagonal matrix with the entries specified.

The eigen values obtained has been plotted in figure 6. It can be seen that for the third case, the spectral radius is 0.5, while in the other cases, it is close to 1, with the second case better than the first.

6.1 Damage

Consider the case of a bar meshed with N+1 elements. Assume now that the current state of bar is such that out of these N+1 elements, one of them has undergone damage while the others are

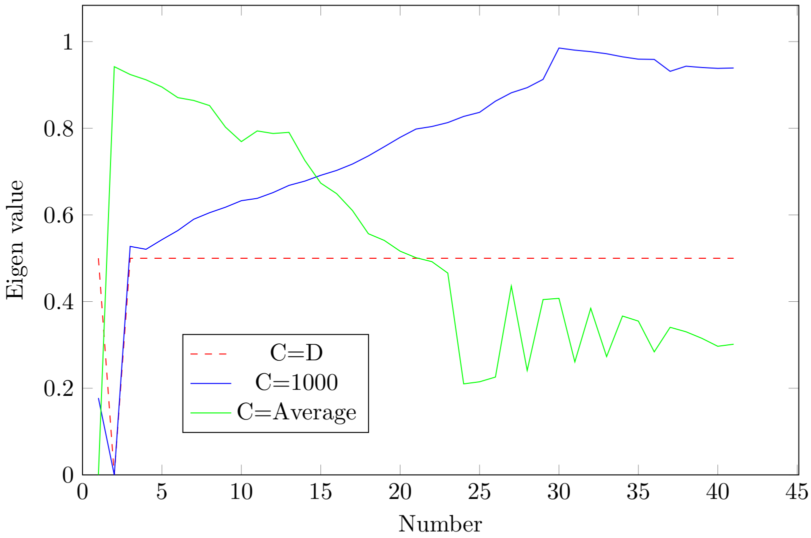

Figure 6: Eigen values for different cases.

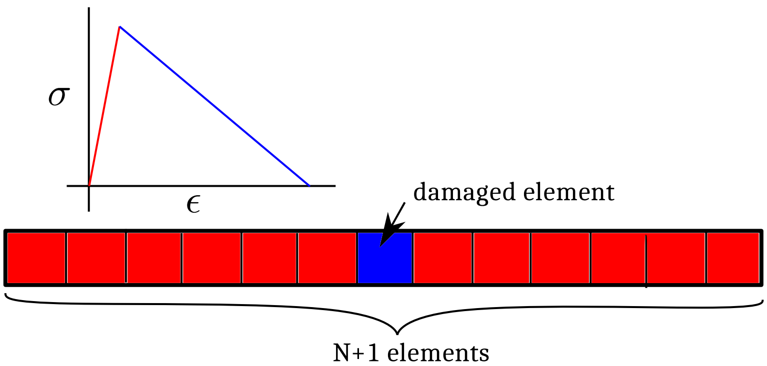

Figure 7: Softening 1D example (local).

intact. Also, the current displacement is such that the damaged element is on the yield surface and the other N elements are on the initial elastic branch.

At this instance, when the loading (applied displacement in this case) is increased, the damaged element is expected to damage further with increasing strains in this element while the other N elements are expected to travel further downward on the initial elastic branch. See figure 7.

In this case, the data driven problem can be written as

$$\min \left\{ N \left[\frac{1}{2C_1}(\sigma - \sigma_1^*)^2 + \frac{C_1}{2}(\epsilon_1 - \epsilon_1^*)^2 \right] + n \left[\frac{1}{2C_2}(\sigma - \sigma_2^*)^2 + \frac{C_2}{2}(\epsilon_2 - \epsilon_2^*)^2 \right] \right\}, \tag{166}$$

where equilibrium has been imposed implicitly by taking the mechanical stresses to be the same in all the elements. C_1 and C_2 are the parameters of the metric whose effect is to be studied. σ_1^*, ϵ_1^*, and σ, ϵ_1 correspond to the material and mechanical states for the elements on the elastic branch while σ_2^*, ϵ_2^*, and σ, ϵ_2 correspond to the material and mechanical states for the element on the damage branch.

The compatibility equation becomes

$$N\epsilon_1 + n\epsilon_2 = \frac{u_D}{le}, \tag{167}$$

where u_D is the applied displacement and le is the element length (uniform mesh considered).

It will be assumed that the material states are related as

$$\sigma_1^* = E\epsilon_1^* \tag{168}$$

on the initial elastic branch (for the red elements) and

$$\sigma_2^* = m\epsilon_2^* + c, \tag{169}$$

for the blue elements on the softening branch. $m < 0$ and c are appropriately chosen.

Material states given mechanical states

On elastic branch

The values of σ^* and ϵ^* given σ and ϵ, where $\sigma^* = E\epsilon^*$, can be found by using

$$\frac{\partial}{\partial \epsilon^*}\left[\frac{1}{2C_1}(\sigma - E\epsilon_1^*)^2 + \frac{C_1}{2}(\epsilon_1 - \epsilon_1^*)^2\right] = 0. \tag{170}$$

Using this, it can be seen that

$$\epsilon_1^* = \frac{E\sigma + C_1^2\epsilon_1}{E^2 + C_1^2} \text{ and } \sigma_1^* = E\epsilon_1^*. \tag{171}$$

On softening branch

Here, $\sigma^* = m\epsilon^* + c$ and $m < 0$. Similar to above, the values of material states can be found as

$$\epsilon_2^* = \frac{m\sigma - mc + C_2^2\epsilon_2}{m^2 + C_2^2} \text{ and } \sigma_2^* = m\epsilon_2^* + c. \tag{172}$$

It can be seen that when $m = E$ and $c = 0$, the above equation boils down to equation 171.

The above equations can be written together in matrix form as

$$s^* = Cs + d, \tag{173}$$

where $s^* = \begin{bmatrix}\epsilon_1^* & \epsilon_2^* & \sigma_1^* & \sigma_2^*\end{bmatrix}^T$, $s = \begin{bmatrix}\epsilon_1 & \epsilon_2 & \sigma\end{bmatrix}^T$.

$$C = \begin{bmatrix} C_1^2/(E^2+C_1^2) & 0 & E/(E^2+C_1^2) \\ 0 & C_2^2/(m^2+C_2^2) & m/(m^2+C_2^2) \\ EC_1^2/(E^2+C_1^2) & 0 & E^2/(E^2+C_1^2) \\ 0 & mC_2^2/(m^2+C_2^2) & m^2/(m^2+C_2^2) \end{bmatrix},\ d = \begin{bmatrix} 0 \\ -mc/(m^2+C_2^2) \\ 0 \\ cC_2^2/(m^2+C_2^2) \end{bmatrix}.$$

Mechanical states given material states

In this case, the minimization is carried out with respect to σ, ϵ_1 and ϵ_2 in the presence of the constraint equation 167. The mechanical states in terms of material states can be expressed as

$$s = As^* + b, \tag{174}$$

where

$$A = \begin{bmatrix} C_1/(C_1+NC_2) & -C_2/(C_1+NC_2) & 0 & 0 \\ -NC_1/(C_1+NC_2) & NC_2/(C_1+NC_2) & 0 & 0 \\ 0 & 0 & NC_2/(C_1+NC_2) & C_1/(C_1+NC_2) \end{bmatrix},$$

$$b = \begin{bmatrix} C_2u_D/(C_1+NC_2)/le & C_1u_D/(C_1+NC_2)/le & 0 \end{bmatrix}^T.$$

Solver

The alternate minimization process involves solving the equations 174 and 173 alternately. Hence, using 173 in 174

$$s^k = ACs^{k-1} + Ad + b. \tag{175}$$

At convergence, $s^k = s^{k-1} = s$. Hence, the exact solution satisfies

$$s = (I - AC)^{-1}(Ad + b). \tag{176}$$

Using the equation 175 starting from the first iteration, the solution at the kth iteration can be expressed as

$$s^k = (AC)^k s^0 + \left\{[-(AC)^k + I](I - AC)^{-1}\right\}(Ad + b). \tag{177}$$

Using equation 176 in the above,

$$s^k = s + (AC)^k[s^0 - s], \tag{178}$$

where s is the exact solution and s^0 is the initial iterate. Hence, the error at the kth iteration can be expressed as

$$e^k = (AC)^k[s^0 - s], \tag{179}$$

Analysis

From equation 179, it can be seen that the rate of convergence of the algorithm depends on the spectral radius of the matrix AC. For instance, since the initial iterate s^0 can be arbitrary, if it is aligned along the Eigen vector of the matrix AC corresponding to the largest Eigen value, the algorithm will converge as long as the spectral radius of the matrix AC, ρ, is smaller than 1. How fast the algorithm converges depends on how small the spectral radius is. If ρ is closer to 1, the algorithm converges slowly. ρ, in turn, depends on C_1 and C_2. Hence, the choice of metric affects the rate of convergence of the algorithm. Whether the algorithm converges is also determined by the choice of C_1 and C_2.

Linear elasticity

In this case, $m = E$, $c = 0$ and $C_1 = C_2 = E$. The spectral radius of the matrix AC is 0.5. Hence, the algorithm converges (as expected) and the rate convergence is also fast(er).

With damage

Since a value of $C_1 = E$ gives a smaller spectral radius for the elastic branch, the same value has been used in the case where there is damage. For the initial simulations, C_2 has been chosen to be E as well. For this choice, the spectral radius is 0.9999. The algorithm hence converges, but the rate of convergence is expected to be (very) small. For instance, the figure 8 illustrates the paths taken by the mechanical and material states for two different values of C_2 within a load increment. For $C_2 = E$, as mentioned earlier, the spectral radius of the matrix AC is 0.999. Hence, the successive iterates (mechanical states in red circles) are very close to each other.

Since the stopping criterion is based on whether the successive material states change, the solution with $C_2 = E$ will have been judged to be converged even before the actual solution is reached. From figure 8, it can actually be seen that if the mechanical states are extrapolated further, the point of intersection with the material states will correspond to the analytical

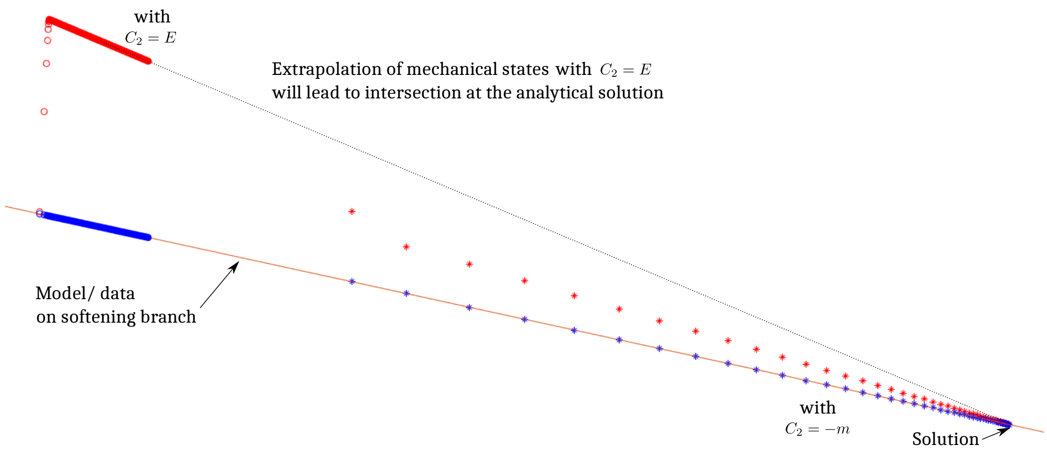

Figure 8: Mechanical and material states of the element on the damage branch. Circles indicate the results with $C_2 = E$ and the asterisks indicate the results with $C_2 = -m$. Red indicates the mechanical states and blue, the material states.

solution. The number of iterations required to reach this point will be very large, of the order of 200000. Similar conclusion can be drawn if the material data are discrete.

Changing $C_2 = -m$ (arbitrarily, after evaluating the spectral radius of AC with different combinations) results in a spectral radius of 0.9722. In this case, it can be seen that the solution tends to the analytical solution rapidly. The gap between the successive iterations is finite as well. Hence, convergence can be expected with discrete finite material data. $C_2 = m$ gives a spectral radius of 0.5 regardless of the mesh size. (see figures 8, 9).

From the above, it can be seen that the choice of metric plays a crucial role in the rate of convergence of the data driven solution.

Plasticity

A similar exercise can be done in the case of plasticity. In this case, the material states on the plastic branch satisfy $\sigma^* = m\epsilon^* + c$, $m > 0, c > 0$. Simulations have been carried out using $C_2 = E$ and $C_2 = m$. The results can be seen in the figure below.

The spectral radius in both the cases are 0.995 and 0.5 respectively. ρ in the first case increases further and approaches 1 as the mesh is refined. In the second case, it remains at 0.5 regardless of mesh size.

7 Modified method (?)

The DD equations in this case are

$$B^T DMBu - B^T DM\epsilon^* + B^T C^T \lambda_d = 0, \tag{180}$$

$$\sigma - \sigma^* + DB\eta = 0, \tag{181}$$

$$B^T M\sigma - B^T C^T \lambda_d = 0, \tag{182}$$

$$-CB\eta = 0. \tag{183}$$

Combining the second and third of the above,

$$B^T M\sigma^* - B^T MDB\eta - B^T C^T \lambda_d = 0. \tag{184}$$

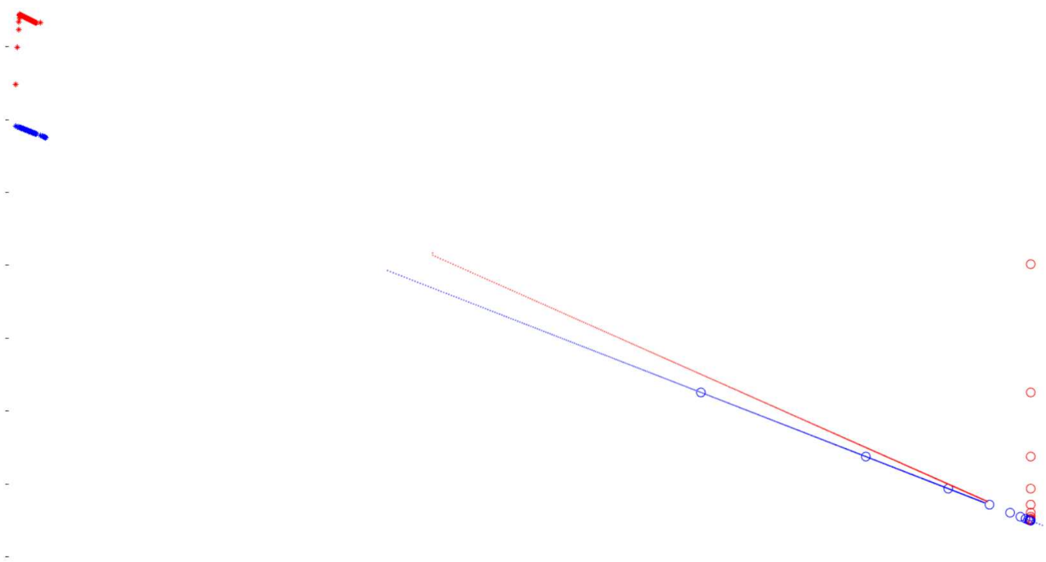

Figure 9: Mechanical and material states of the element on the damage branch. Circles indicate the results with $C_2 = m$ and the asterisks indicate the results with $C_2 = E$, dots when $C_2 = -m$. Red indicates the mechanical states and blue, the material states.

The Hessian is defined as

$$H = \begin{bmatrix} K & 0 & 0 \\ 0 & -K & -B^T C^T \\ 0 & -CB & 0 \end{bmatrix}, r = \begin{bmatrix} B^T DMBu - B^T DM\epsilon^* + B^T C^T \lambda_d \\ B^T M\sigma^* - B^T MDB\eta - CB\lambda_d \\ -CB\eta \end{bmatrix}, \tag{185}$$

where $K = B^T MDB$.

(Approximate) Variational form

The functional to be minimized is (?)

$$\Pi = d + \int \eta^T B^T \sigma - \int \eta^T B^T C^T \lambda_d + \int u^T B^T C^T \lambda_d^* + \int \lambda \left(CBu - 1/\ell_c \right) \tag{186}$$