

# Tensor Flattening

Julian Panetta

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We discuss how symmetric rank 2 and rank 4 tensors are flattened into vectors and matrices so that contractions can be implemented efficiently as dot products and matrix multiplies. We use summation notation for our tensors, where summation over repeated indices is implied. The range of indices is 0..2 in 3D and 0..1 in 2D.

## 1 Voigt Notation

Our approach is to use Voigt notation with zero indexing.

### 1.1 Symmetric Rank 2 Tensors

In this notation, symmetric rank 2 tensors are flattened into vectors in the order:

$$\text{3D: } \begin{pmatrix} 0 & 5 & 4 \\ 5 & 1 & 3 \\ 4 & 3 & 2 \end{pmatrix} \quad \text{2D: } \begin{pmatrix} 0 & 3 \\ 3 & 1 \end{pmatrix}.$$

For example, strain tensors are flattened as:

$$\text{3D: } \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{pmatrix} \mapsto \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix}, \quad \text{2D: } \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} \\ \epsilon_{xy} & \epsilon_{yy} \end{pmatrix} \mapsto \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{xy} \end{pmatrix}$$

This flattening is implemented by the following formula for flattened index  $\bar{ij}$  in  $N$  dimensions:

$$\bar{ij}(i, j) = \begin{cases} i & \text{if } i = j \\ \frac{N(N+1)}{2} - \left(i + \frac{j(j-1)}{2} + 1\right) & i < j \\ \bar{ij}(j, i) & i > j \end{cases}.$$

We can also go the other direction by solving for the upper triangle  $(i, j)$  associated with  $\bar{ij}$ . This is done by picking the largest  $j$  possible (to ensure we're in the upper triangle), and then solving for the  $i$  index:

$$j(\bar{ij}) = \begin{cases} \bar{ij} & \text{if } \bar{ij} < N \\ \left\lfloor \frac{1 + \sqrt{1 + 8\left(\frac{N(N+1)}{2} - 1 - \bar{ij}\right)}}{2} \right\rfloor & \text{otherwise} \end{cases} \quad i(\bar{ij}) = \begin{cases} \bar{ij} & \text{if } \bar{ij} < N \\ \frac{N(N+1)}{2} - 1 - \bar{ij} - \frac{j(\bar{ij})(j(\bar{ij})-1)}{2} & \text{otherwise} \end{cases}.$$

## 1.2 Symmetric Rank 4 Tensors

The symmetric rank 2 tensor flattening induces a flattening of symmetric rank 4 tensors that act on symmetric rank 2 tensors by double contraction. We consider tensors with the symmetries of an elasticity tensor:

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}. \quad (1)$$

The idea is to flatten this tensor into a matrix so that matrix multiplication can implement double contraction on both the left and the right:  $E : \epsilon = E_{ijkl}\epsilon_{kl}$  and  $\epsilon : E = \epsilon_{ij}E_{ijkl}$ . Since  $\epsilon_{kl}$  is flattened into vector entry  $\overline{kl}$ , we want entries  $E_{**kl}$  to end up in matrix column  $\overline{kl}$  so that entries are paired properly for the left double contraction. Likewise, the right double contraction requires  $E_{ij**}$  to end up in matrix row  $\overline{ij}$ . Accordingly, we flatten rank 4 tensors  $E_{ijkl}$  into the matrix:

$$D_{\overline{ij}\overline{kl}} = E_{ijkl} \quad \text{where } i = i(\overline{ij}), j = j(\overline{ij}), k = i(\overline{kl}), l = j(\overline{kl})$$

The minor symmetries ( $i \leftrightarrow j$  and  $k \leftrightarrow l$ ) of tensor  $E_{ijkl}$  mean no information is lost in this conversion, and the major symmetry  $ij \leftrightarrow kl$  means  $D$  is a symmetric matrix.

## 1.3 Examples

A general rank 4 tensor looks like:

$$\begin{aligned} \text{3D: } E_{ijkl} &= \begin{pmatrix} \begin{pmatrix} E_{0000} & E_{0001} & E_{0002} \\ E_{0010} & E_{0011} & E_{0012} \\ E_{0020} & E_{0021} & E_{0022} \end{pmatrix} & \begin{pmatrix} E_{0100} & E_{0101} & E_{0102} \\ E_{0110} & E_{0111} & E_{0112} \\ E_{0120} & E_{0121} & E_{0122} \end{pmatrix} & \begin{pmatrix} E_{0200} & E_{0201} & E_{0202} \\ E_{0210} & E_{0211} & E_{0212} \\ E_{0220} & E_{0221} & E_{0222} \end{pmatrix} \\ \begin{pmatrix} E_{1000} & E_{1001} & E_{1002} \\ E_{1010} & E_{1011} & E_{1012} \\ E_{1020} & E_{1021} & E_{1022} \end{pmatrix} & \begin{pmatrix} E_{1100} & E_{1101} & E_{1102} \\ E_{1110} & E_{1111} & E_{1112} \\ E_{1120} & E_{1121} & E_{1122} \end{pmatrix} & \begin{pmatrix} E_{1200} & E_{1201} & E_{1202} \\ E_{1210} & E_{1211} & E_{1212} \\ E_{1220} & E_{1221} & E_{1222} \end{pmatrix} \\ \begin{pmatrix} E_{2000} & E_{2001} & E_{2002} \\ E_{2010} & E_{2011} & E_{2012} \\ E_{2020} & E_{2021} & E_{2022} \end{pmatrix} & \begin{pmatrix} E_{2100} & E_{2101} & E_{2102} \\ E_{2110} & E_{2111} & E_{2112} \\ E_{2120} & E_{2121} & E_{2122} \end{pmatrix} & \begin{pmatrix} E_{2200} & E_{2201} & E_{2202} \\ E_{2210} & E_{2211} & E_{2212} \\ E_{2220} & E_{2221} & E_{2222} \end{pmatrix} \end{pmatrix} \\ \text{2D: } E_{ijkl} &= \begin{pmatrix} \begin{pmatrix} E_{0000} & E_{0001} \\ E_{0010} & E_{0011} \end{pmatrix} & \begin{pmatrix} E_{0100} & E_{0101} \\ E_{0110} & E_{0111} \end{pmatrix} \\ \begin{pmatrix} E_{1000} & E_{1001} \\ E_{1010} & E_{1011} \end{pmatrix} & \begin{pmatrix} E_{1100} & E_{1101} \\ E_{1110} & E_{1111} \end{pmatrix} \end{pmatrix} \end{aligned}$$

After accounting for the symmetries of an elasticity tensor (1), these tensors really only have 21 and 6 unique entries in 3D and 2D respectively:

$$\begin{aligned} \text{3D: } E_{ijkl} &= \begin{pmatrix} \begin{pmatrix} E_{0000} & E_{0001} & E_{0002} \\ E_{0001} & E_{0011} & E_{0012} \\ E_{0002} & E_{0012} & E_{0022} \end{pmatrix} & \begin{pmatrix} E_{0001} & E_{0101} & E_{0201} \\ E_{0101} & E_{1101} & E_{1201} \\ E_{0201} & E_{1201} & E_{2201} \end{pmatrix} & \begin{pmatrix} E_{0002} & E_{0201} & E_{0202} \\ E_{0201} & E_{1102} & E_{1202} \\ E_{0202} & E_{1202} & E_{2202} \end{pmatrix} \\ \begin{pmatrix} E_{0001} & E_{0101} & E_{0201} \\ E_{0101} & E_{1101} & E_{1201} \\ E_{0201} & E_{1201} & E_{2201} \end{pmatrix} & \begin{pmatrix} E_{0011} & E_{1101} & E_{1102} \\ E_{1101} & E_{1111} & E_{1112} \\ E_{1102} & E_{1112} & E_{1122} \end{pmatrix} & \begin{pmatrix} E_{0012} & E_{1201} & E_{1202} \\ E_{1201} & E_{1112} & E_{1212} \\ E_{1202} & E_{1212} & E_{2212} \end{pmatrix} \\ \begin{pmatrix} E_{0002} & E_{0201} & E_{0202} \\ E_{0201} & E_{1102} & E_{1202} \\ E_{0202} & E_{1202} & E_{2202} \end{pmatrix} & \begin{pmatrix} E_{0012} & E_{1201} & E_{1202} \\ E_{1201} & E_{1112} & E_{1212} \\ E_{1202} & E_{1212} & E_{2212} \end{pmatrix} & \begin{pmatrix} E_{0022} & E_{2201} & E_{2202} \\ E_{2201} & E_{1122} & E_{2212} \\ E_{2202} & E_{2212} & E_{2222} \end{pmatrix} \end{pmatrix} \\ \text{2D: } E_{ijkl} &= \begin{pmatrix} \begin{pmatrix} E_{0000} & E_{0001} \\ E_{0001} & E_{0011} \end{pmatrix} & \begin{pmatrix} E_{0001} & E_{0101} \\ E_{0101} & E_{1101} \end{pmatrix} \\ \begin{pmatrix} E_{0001} & E_{0101} \\ E_{0101} & E_{1101} \end{pmatrix} & \begin{pmatrix} E_{0011} & E_{1101} \\ E_{1101} & E_{1111} \end{pmatrix} \end{pmatrix} \end{aligned}$$

And flattening to a symmetric matrix as described gets a single copy of each of these entries in the upper triangle:

$$\begin{aligned} \text{3D: } D_{\overline{ij} \overline{kl}} &= \begin{pmatrix} E_{0000} & E_{0011} & E_{0022} & E_{0012} & E_{0002} & E_{0001} \\ E_{0011} & E_{1111} & E_{1122} & E_{1112} & E_{1102} & E_{1101} \\ E_{0022} & E_{1122} & E_{2222} & E_{2212} & E_{2202} & E_{2201} \\ E_{0012} & E_{1112} & E_{2212} & E_{1212} & E_{1202} & E_{1201} \\ E_{0002} & E_{1102} & E_{2202} & E_{1202} & E_{0202} & E_{0201} \\ E_{0001} & E_{1101} & E_{2201} & E_{1201} & E_{0201} & E_{0101} \end{pmatrix} \\ \text{2D: } D_{\overline{ij} \overline{kl}} &= \begin{pmatrix} E_{0000} & E_{0011} & E_{0001} \\ E_{0011} & E_{1111} & E_{1101} \\ E_{0001} & E_{1101} & E_{0101} \end{pmatrix}. \end{aligned}$$

Here  $D$  is used to denote the matrix holding the flattened elasticity tensor, as is standard in engineering literature.

## 2 Implementing Double Contraction

### 2.1 The Missing Factor of 2

We have flattened with the goal of using dot products to implement double contraction of two rank 2 tensors and matrix-vector multiplication to implement double contraction of a rank 4 tensor and a rank 2 tensor. However we're not done yet: the off diagonal entries aren't handled properly! Consider a double contraction of a stress tensor with a strain tensor in 3D:

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} : \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{pmatrix} = \sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + \sigma_{zz}\epsilon_{zz} + 2(\sigma_{yz}\epsilon_{yz} + \sigma_{xz}\epsilon_{xz} + \sigma_{xy}\epsilon_{xy})$$

Notice the factor of 2 on the off-diagonals, which isn't present in the dot product of the two tensors in flattened form:

$$\begin{pmatrix} \sigma_{xx} & \sigma_{yy} & \sigma_{zz} & \sigma_{yz} & \sigma_{xz} & \sigma_{xy} \end{pmatrix} \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix} = \sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + \sigma_{zz}\epsilon_{zz} + \sigma_{yz}\epsilon_{yz} + \sigma_{xz}\epsilon_{xz} + \sigma_{xy}\epsilon_{xy}$$

A similar problem happens with a double contraction of a rank 4 tensor with a rank 2 tensor. Consider entries of the symmetric stress tensor  $\sigma = E : \epsilon$ :

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} E_{0000}\epsilon_{xx} + E_{0011}\epsilon_{yy} + E_{0022}\epsilon_{zz} + 2(E_{0012}\epsilon_{yz} + E_{0002}\epsilon_{xz} + E_{0001}\epsilon_{xy}) \\ E_{0011}\epsilon_{xx} + E_{1111}\epsilon_{yy} + E_{1122}\epsilon_{zz} + 2(E_{1112}\epsilon_{yz} + E_{1102}\epsilon_{xz} + E_{1101}\epsilon_{xy}) \\ E_{0022}\epsilon_{xx} + E_{1122}\epsilon_{yy} + E_{2222}\epsilon_{zz} + 2(E_{2212}\epsilon_{yz} + E_{2202}\epsilon_{xz} + E_{2201}\epsilon_{xy}) \\ E_{0012}\epsilon_{xx} + E_{1112}\epsilon_{yy} + E_{2212}\epsilon_{zz} + 2(E_{1212}\epsilon_{yz} + E_{1202}\epsilon_{xz} + E_{1201}\epsilon_{xy}) \\ E_{0002}\epsilon_{xx} + E_{1102}\epsilon_{yy} + E_{2202}\epsilon_{zz} + 2(E_{1202}\epsilon_{yz} + E_{0202}\epsilon_{xz} + E_{0201}\epsilon_{xy}) \\ E_{0001}\epsilon_{xx} + E_{1101}\epsilon_{yy} + E_{2201}\epsilon_{zz} + 2(E_{1201}\epsilon_{yz} + E_{0201}\epsilon_{xz} + E_{0101}\epsilon_{xy}) \end{pmatrix}.$$

Again, our flattened version of this operation (applying matrix  $D$  to the flattened strain vector) gets almost the correct answer, but it misses the factor of 2 on the off-diagonal strain contributions:

$$D\mathbf{e} := D \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix} = \begin{pmatrix} E_{0000}\epsilon_{xx} + E_{0011}\epsilon_{yy} + E_{0022}\epsilon_{zz} + E_{0012}\epsilon_{yz} + E_{0002}\epsilon_{xz} + E_{0001}\epsilon_{xy} \\ E_{0011}\epsilon_{xx} + E_{1111}\epsilon_{yy} + E_{1122}\epsilon_{zz} + E_{1112}\epsilon_{yz} + E_{1102}\epsilon_{xz} + E_{1101}\epsilon_{xy} \\ E_{0022}\epsilon_{xx} + E_{1122}\epsilon_{yy} + E_{2222}\epsilon_{zz} + E_{2212}\epsilon_{yz} + E_{2202}\epsilon_{xz} + E_{2201}\epsilon_{xy} \\ E_{0012}\epsilon_{xx} + E_{1112}\epsilon_{yy} + E_{2212}\epsilon_{zz} + E_{1212}\epsilon_{yz} + E_{1202}\epsilon_{xz} + E_{1201}\epsilon_{xy} \\ E_{0002}\epsilon_{xx} + E_{1102}\epsilon_{yy} + E_{2202}\epsilon_{zz} + E_{1202}\epsilon_{yz} + E_{0202}\epsilon_{xz} + E_{0201}\epsilon_{xy} \\ E_{0001}\epsilon_{xx} + E_{1101}\epsilon_{yy} + E_{2201}\epsilon_{zz} + E_{1201}\epsilon_{yz} + E_{0201}\epsilon_{xz} + E_{0101}\epsilon_{xy} \end{pmatrix}$$

Finally, by symmetry, an identical problem happens when implementing the double contraction  $\epsilon_{ij}E_{ijkl}$  as  $\mathbf{e}^T D$ .

## 2.2 Solving the Problem

There are several ways to introduce the factors of two. We can double the right half of the  $D$  matrix, but this breaks its symmetry. We can leave  $D$  unchanged, but work with “engineering strain”  $(\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, 2\epsilon_{yz}, 2\epsilon_{xz}, 2\epsilon_{xy})^T$ , but this means strain and stress are flattened differently, which could lead to mistakes. We could weight the off diagonal terms of all symmetric rank 2 tensors by  $\sqrt{2}$  (this is called Kelvin or Mandel notation) but this also requires modifying the  $D$  matrix—though this time in a symmetric way.

Instead of any of these, we choose to work with true, unmodified strain/stress quantities and the original, symmetric  $D$ , but to include a “shear doubling” matrix that doubles the off-diagonal entries each time a double contraction is taken. This means off diagonals of strain and stress are flattened the same way,  $D$  remains symmetric, and entries in  $D$  give the corresponding elasticity coefficients directly instead of some scaling of them. This shear doubling matrix is given by

$$\text{3D: } S = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \quad \text{2D: } S = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

## 2.3 Examples

Finally, we show examples of double contraction implemented by matrix vector multiplies and inner products. We use  $F$  to denote the flattening operation mapping symmetric rank 2 tensors to vectors and symmetric rank 4 tensors to symmetric matrices. Letting  $\mathbf{e} = F(\epsilon)$  and  $\mathbf{s} = F(\sigma)$  (flattened stress and strain tensors), we show various identities of our notation:

$$\begin{aligned} \mathbf{s} &= F(\sigma) = F(E : \epsilon) = F(E_{ijkl}\epsilon_{kl}) = D\mathbf{S}\mathbf{e}, \\ \sigma : \epsilon &= \sigma_{ij}\epsilon_{kl} = \mathbf{s}^T \mathbf{S}\mathbf{e}, \\ \epsilon : E : \epsilon &= \epsilon_{ij}E_{ijkl}\epsilon_{kl} = \mathbf{e}^T S D \mathbf{S}\mathbf{e}, \\ F(A : B) &= F(A_{ijpq}B_{pqkl}) = F(A)SF(B) \end{aligned}$$

Note, however, that the last operation does not result in a tensor with major symmetries unless  $A_{ijpq} = B_{pqij}$ . This means that the matrix representing the flattened result is not necessarily symmetric.

## 3 Quadruple Contraction

We can also implement quadruple contraction in flattened form:

$$A_{ijkl}B_{ijkl}$$

This is useful in several settings, including computing the Frobenius norm of a tensor. Each term of the contraction will be an entry of  $F(A)$  multiplied by the corresponding entry of  $F(B)$ —we just need to determine how many times each flattened entry appears. That is, we can compute the contraction by instead sum over entries of the flattened tensor, weighting each term by how many components are flattened down to that particular entry. This can be determined from the minor symmetries alone; major symmetry just causes a symmetric flattened tensor as opposed to flattening more components of the tensor to a single flattened entry.

Below are the counts of how many tensor components are represented by each flattened entry:

$$\text{3D: } \begin{pmatrix} 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 2 & 2 & 2 \\ 2 & 2 & 2 & 4 & 4 & 4 \\ 2 & 2 & 2 & 4 & 4 & 4 \\ 2 & 2 & 2 & 4 & 4 & 4 \end{pmatrix}, \quad \text{2D: } \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix}$$

This per-entry weighting can be applied to a flattened tensor by “shear doubling” both the rows and columns,

$$SF(A)S,$$

allowing us to implement the quadruple contraction as a double contraction of the scaled flattened tensors:

$$A_{ijkl}B_{ijkl} = [SF(A)S] : F(B) = [F(A)S] : [SF(B)] = [SF(A)] : [F(B)S]$$

In linear algebra terms, this is:

$$A_{ijkl}B_{ijkl} = \text{tr}(SF(A)^T SF(B)) = \text{tr}(F(A)^T SF(B)S)$$

### 3.1 Examples

As an example, we compute the squared Frobenius norm of an orthotropic elasticity tensor:

$$\text{3D: } F(E) = \begin{pmatrix} E_{0000} & E_{0011} & E_{0022} & 0 & 0 & 0 \\ E_{0011} & E_{1111} & E_{1122} & 0 & 0 & 0 \\ E_{0022} & E_{1122} & E_{2222} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{0202} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{0101} \end{pmatrix}, \quad \text{2D: } F(E) = \begin{pmatrix} E_{0000} & E_{0011} & 0 \\ E_{0011} & E_{1111} & 0 \\ 0 & 0 & E_{0101} \end{pmatrix}$$

In 3D the Frobenius norm is

$$\|E\|_F^2 = E_{ijkl} : E_{ijkl} = \|S^{1/2}F(E)S^{1/2}\|_F^2 = E_{0000}^2 + E_{1111}^2 + E_{2222}^2 + 2E_{0011}^2 + 2E_{0022}^2 + 2E_{1122}^2 + 4E_{1212}^2 + 4E_{0202}^2 + 4E_{0101}^2,$$

and in 2D:

$$\|E\|_F^2 = E_{ijkl} : E_{ijkl} = \|S^{1/2}F(E)S^{1/2}\|_F^2 = E_{0000}^2 + E_{1111}^2 + 2E_{0011}^2 + 4E_{0101}^2.$$

Notice that the only difference between  $\|E\|_F^2$  and  $\|F(E)\|_F^2$  for orthotropic tensors is the weight of 4 on the “shear” terms.