

Converting global derivatives to local derivatives

Juha Jeronen

March 25, 2012

TECHNICAL NOTE

1 Introduction

This document covers the global to local derivative conversions needed in finite element analysis of PDEs, when the basis functions are defined in terms of the local coordinates on the reference element.

First and second derivatives are discussed. First derivatives are sufficient for weak forms of second-order problems; second derivatives are required for fourth-order problems.

The idea is that the original PDE problem is written in terms of the global coordinates. In order to be able to apply the derivatives to the basis functions, which are defined in terms of the local coordinates on the reference element, the derivatives must be expressed in local coordinates.

2 First derivatives

See Haataja et al. [2002] and Hughes [2000] for more information.

2.1 Transformations

The coordinate transformation Jacobian in 2D of $(\xi, \eta) \mapsto (x(\xi, \eta), y(\xi, \eta))$ is

$$J = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix}. \quad (1)$$

Note the convention; this is the transpose of the standard Jacobian for reasons of convenience.

By the inverse function theorem, its inverse at the point $(x(\xi, \eta), y(\xi, \eta))$ is

$$J^{-1} = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\ \frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} \end{bmatrix}. \quad (2)$$

We use the chain rule. Let $f = f(\xi, \eta)$ once differentiable. Then

$$\frac{\partial f}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial f}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial f}{\partial \eta}. \quad (3)$$

$$\frac{\partial f}{\partial y} = \frac{\partial \xi}{\partial y} \frac{\partial f}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial f}{\partial \eta}. \quad (4)$$

Hence, we can use the inverse Jacobian (2) to convert. In vector notation, we have

$$\nabla_{(x,y)} f = J^{-1} \nabla_{(\xi,\eta)} f, \quad (5)$$

where the subscripted nablas refer to gradients taken in the coordinate system identified by the subscript.

2.2 Computing it in practice

The coordinate transform $(\xi, \eta) \mapsto (x, y)$ is known analytically (from the Galerkin interpolation of coordinates). We can thus compute the forward Jacobian (1) analytically at each desired point on each element. Taking its matrix inverse (separately at each desired point), we obtain values for (2), which can then be fed into (5). The obtained values are exact up to floating point rounding errors.

The local derivatives of each basis function $N_j(\xi, \eta)$ are also known analytically; these can be inserted to (5) directly.

3 Second derivatives

In the case where second derivatives are present, in addition to the inverse Jacobian, we will need the inverse Hessian of the coordinate mapping.

3.1 Transformations

Recall the chain rule, (3)–(4). To obtain $\partial^2 f / \partial x^2$, we apply (3) to itself:

$$\begin{aligned} \frac{\partial^2 f}{\partial x^2} &= \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial x} \right] = \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} \right] \\ &= \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} \right] + \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} \right] \\ &= \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial \xi} \right] \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \xi} \frac{\partial}{\partial x} \left[\frac{\partial \xi}{\partial x} \right] \\ &\quad + \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial \eta} \right] \frac{\partial \eta}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial}{\partial x} \left[\frac{\partial \eta}{\partial x} \right] \\ &= \left[\frac{\partial^2 f}{\partial \xi^2} \frac{\partial \xi}{\partial x} + \frac{\partial^2 f}{\partial \xi \partial \eta} \frac{\partial \eta}{\partial x} \right] \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \xi} \frac{\partial^2 \xi}{\partial x^2} \\ &\quad + \left[\frac{\partial^2 f}{\partial \xi \partial \eta} \frac{\partial \xi}{\partial x} + \frac{\partial^2 f}{\partial \eta^2} \frac{\partial \eta}{\partial x} \right] \frac{\partial \eta}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial^2 \eta}{\partial x^2} \end{aligned}$$

Cleaning up, we have

$$\frac{\partial^2 f}{\partial x^2} = \left[\frac{\partial \xi}{\partial x} \right]^2 \frac{\partial^2 f}{\partial \xi^2} + 2 \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial x} \frac{\partial^2 f}{\partial \xi \partial \eta} + \left[\frac{\partial \eta}{\partial x} \right]^2 \frac{\partial^2 f}{\partial \eta^2} + \frac{\partial^2 \xi}{\partial x^2} \frac{\partial f}{\partial \xi} + \frac{\partial^2 \eta}{\partial x^2} \frac{\partial f}{\partial \eta}. \quad (6)$$

Similarly (by repeating the above for y , or simply by replacing each x by y in (6)), we have

$$\frac{\partial^2 f}{\partial y^2} = \left[\frac{\partial \xi}{\partial y} \right]^2 \frac{\partial^2 f}{\partial \xi^2} + 2 \frac{\partial \xi}{\partial y} \frac{\partial \eta}{\partial y} \frac{\partial^2 f}{\partial \xi \partial \eta} + \left[\frac{\partial \eta}{\partial y} \right]^2 \frac{\partial^2 f}{\partial \eta^2} + \frac{\partial^2 \xi}{\partial y^2} \frac{\partial f}{\partial \xi} + \frac{\partial^2 \eta}{\partial y^2} \frac{\partial f}{\partial \eta}. \quad (7)$$

Finally, for the mixed second derivative, we take (3) and differentiate it with respect to y . We assume C^2 continuity within each element so that the order of the differentiations does not matter. We have

$$\begin{aligned}
\frac{\partial^2 f}{\partial x \partial y} &= \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial x} \right] = \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} \right] \\
&= \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} \right] + \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} \right] \\
&= \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial \xi} \right] \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \xi} \frac{\partial}{\partial y} \left[\frac{\partial \xi}{\partial x} \right] \\
&\quad + \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial \eta} \right] \frac{\partial \eta}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial}{\partial y} \left[\frac{\partial \eta}{\partial x} \right] \\
&= \left[\frac{\partial^2 f}{\partial \xi^2} \frac{\partial \xi}{\partial y} + \frac{\partial^2 f}{\partial \xi \partial \eta} \frac{\partial \eta}{\partial y} \right] \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \xi} \frac{\partial^2 \xi}{\partial x \partial y} \\
&\quad + \left[\frac{\partial^2 f}{\partial \xi \partial \eta} \frac{\partial \xi}{\partial y} + \frac{\partial^2 f}{\partial \eta^2} \frac{\partial \eta}{\partial y} \right] \frac{\partial \eta}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial^2 \eta}{\partial x \partial y}
\end{aligned}$$

Again, cleaning up, we obtain

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial \xi}{\partial x} \frac{\partial \xi}{\partial y} \frac{\partial^2 f}{\partial \xi^2} + \left[\frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial y} + \frac{\partial \xi}{\partial y} \frac{\partial \eta}{\partial x} \right] \frac{\partial^2 f}{\partial \xi \partial \eta} + \frac{\partial \eta}{\partial x} \frac{\partial \eta}{\partial y} \frac{\partial^2 f}{\partial \eta^2} + \frac{\partial^2 \xi}{\partial x \partial y} \frac{\partial f}{\partial \xi} + \frac{\partial^2 \eta}{\partial x \partial y} \frac{\partial f}{\partial \eta}. \quad (8)$$

3.2 Computing it in practice

The inverse Hessian can be approximated by wlsqm (see separate document on the method). In a small neighbourhood of each point where we wish to obtain the inverse Hessian, we compute a few points $(x_j, y_j) = (x(\xi_j, \eta_j), y(\xi_j, \eta_j))$ in the forward direction, obtaining a point cloud of samples.

We then switch the roles of input and output in the point cloud: $(\xi_j, \eta_j) = (\xi(x_j, y_j), \eta(x_j, y_j))$. This is trivial because it is just a data set with a 1:1 correspondence between input and output. Splitting into two, this gives us the data sets $\xi_j = \xi(x_j, y_j)$ and $\eta_j = \eta(x_j, y_j)$. Note that the expressions for the functions ξ and η are not known, but are not needed.

We can then apply wlsqm to the data sets $(x_j, y_j, \xi(x_j, y_j))$ and $(x_j, y_j, \eta(x_j, y_j))$ to obtain approximations of the second derivatives of the unknown functions $\xi(x, y)$ and $\eta(x, y)$ at each desired point.

The values obtained for the inverse Hessian using this method contain some approximation error. This comes from the Taylor series fitting of wlsqm. Thus the “small neighbourhood” should be small enough to get reasonable derivative approximations, but not so small that rounding errors will dominate.

Also, more regular spacings of the points seem to give better derivatives. For this reason, the solver uses a 3×3 meshgrid in (ξ, η) coordinates. As for the size, in practice $\varepsilon = 10^{-4}$ for the radius of the neighbourhood along ξ (and same along η) seems a good value.

Finally, the local first and second derivatives of each basis function $N_j(\xi, \eta)$ are known analytically; these can be inserted to the formulas (6)–(8) directly.

References

- J. Haataja, J. Heikonen, Y. Leino, J. Rahola, J. Ruokolainen, and V. Savolainen. *Numeeriset menetelmät käytännössä (Numerical methods in practice)*. CSC, Espoo, 2nd edition, 2002. ISBN 952-9821-81-6. Available on the Internet. <http://www.csc.fi/oppaat/num.kayt/>.
- T. J. R. Hughes. *The Finite Element Method. Linear Static and Dynamic Finite Element Analysis*. Dover Publications, Inc., Mineola, N.Y., USA, 2000. ISBN 0-486-41181-8.