Error Estimate for Forward Differences

The expression for the FD approximation to the derivative of a function $f(x)$ at the point x_j is given by

$$\tilde{f}'_j = \frac{f_{j+1} - f_j}{x_{j+1} - x_j}\,, \tag{1}$$

where we use superposed tildes to denote approximations. Using Taylor's theorem with remainder we have the exact result

$$\tilde{f}'_j = f'_j + f''(\theta)h/2\,, \tag{2}$$

where θ is some (unknown) point between x_j and x_{j+1} and $h = x_{j+1} - x_j$. Thus the error in using the FD formula is $f''(\theta)h/2$. To be able to exploit this relation, we need to know $f''(\theta)$, which is not easy to know. Notwithstanding, we can estimate it.

Consider computing the derivative using a step size of h and then with a step size $h/2$. This will give two different approximations with exact error relations

$$\tilde{f}'_j(h) = f'_j + f''(\theta)h/2 \tag{3}$$

$$\tilde{f}'_j(h/2) = f'_j + f''(\bar{\theta})h/4\,, \tag{4}$$

where $\theta \in (x_j, x_j + h)$ and $\bar{\theta} \in (x_j, x_j + h/2)$ are both unknown. If we subtract these two results and ASSUME that $f''(x)$ is approximately constant between x_j and x_{j+1}, then

$$\tilde{f}'_j(h) - \tilde{f}'_j(h/2) \approx f''h/4\,. \tag{5}$$

Thus the error in $\tilde{f}'_j(h)$ is approximately $2(\tilde{f}'_j(h) - \tilde{f}'_j(h/2))$ or, equivalently, the error in $\tilde{f}'_j(h/2)$ is approximately $\tilde{f}'_j(h) - \tilde{f}'_j(h/2)$. This allows us to construct a simple function that computes the derivative to a "known" error tolerance. The algorithm is:

1. Compute an approximate derivative using h and $h/2$ for step sizes.
2. Estimate the absolute error as $|\tilde{f}'_j(h) - \tilde{f}'_j(h/2)|$
3. If the error satisfies a given tolerance, then return the approximation $\tilde{f}'_j(h/2)$
4. Else, decrease h and repeat.

A simple (divide-and-conquer) version would look like:

```
function df=myDer(f,x,h,tol)
% Usage: df=myDer(f,x,h,tol)
% Purpose: Estimate the f'(x) to a given tolerance
% Inputs: f -- function handle
%         x -- point
%         h -- starting step size (guess)
%       tol -- desired tolerance
% Output: df -- estimate of f'(x), such that |df - f'(x)| < tol


dfh  = (f(x+h)-f(x))/h;
dfh2 = (f(x+h/2)-f(x))/(h/2);

while abs(dfh-dfh2) >= tol  % Check error of dfh2
    h = h/2;
    dfh = (f(x+h)-f(x))/h;
    dfh2 = (f(x+h/2)-f(x))/(h/2);
end

df=dfh2;
end
```

One can derive an identical result for the backward difference formula. For the central difference formula one has a slightly different result that can be found by re-doing the above analysis using the Taylor series with remainder expression that is appropriate for central differences; viz.,

$$\tilde{f}_j' = f_j' + f'''(\hat{\theta})h^2/6\,, \tag{6}$$

for some $\hat{\theta} \in (x_{j-1}, x_{j+1})$. Note that to derive this relation one needs to use the Taylor series with remainder out to third order terms.