

Forward testing of differentiation matrices

Note: You will only be able to run this once you have written the functions `build_grid()` and `build_ops()`!

The discrete operators **D** and **G** are differentiation matrices. If **f** is a vector that is the discrete representation of a function $f(x)$, then **G*f** returns a discrete approximation of the derivative $\frac{\partial f}{\partial x}$.

For the one-dimensional examples below the discrete operators can be generated as follows:

```
clear, clc
set_demo_defaults
Grid.xmin = 0; Grid.xmax = 3; Grid.Nx = 10;
Grid = build_grid(Grid);
[D,G,C,I,M] = build_ops(Grid); L = D*G;
```

Here **Grid** is a structure that contains all information about the grid and `build_grid()` is a function that generates all the necessary information. The function `build_ops()` then generates the discrete operators for the grid. The matrix **L** corresponds to the Laplacian operator and hence to a second derivative matrix in 1D.

The other matrices returned by `build_ops()` are:

C = discrete curl (does not exist in 1D)

I = identity

M = mean matrix - computes arithmetic mean of cell centered values on the cell faces

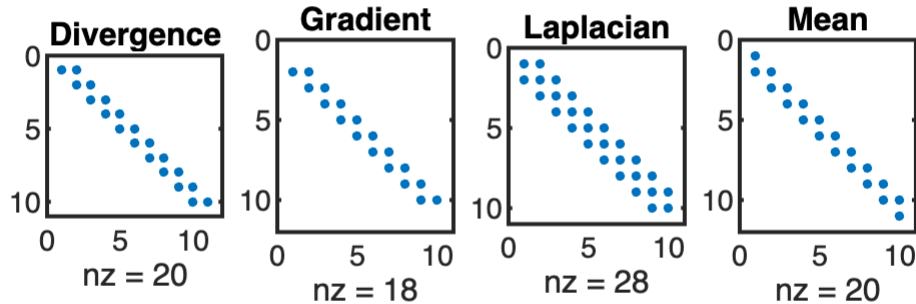
Visualizing the fill pattern of the operators

We can visualize the sparsity pattern of our matrices with the `spy()` function.

```
figure(1)
subplot 141
spy(D)
title 'Divergence'

subplot 142
spy(G)
title 'Gradient'

subplot 143
spy(L)
title 'Laplacian'
subplot 144
spy(M)
title 'Mean'
```



Not the Laplacian has the standard tri-diagonal structure expected for the 1D discretization of the second derivative.

Testing the discrete operators

We would like to establish that our discrete operators are correct, before moving on in our implementation. The obvious idea is to solve a particular boundary value problem (BVP) with a known analytic solution and to compare it with the numerical solution. However, this is not the optimal testing strategy, because the full numerical solution of a boundary value problem (BVP) requires both the discrete operators and the implementation of the boundary conditions. The BVP solution may be wrong, even if the discrete operators are correct, because the error might be in the implementation of boundary conditions.

To test only the correctness of the discrete operators, we can use the knowledge that they simply differentiate a function. The only caveat is that the derivative is **not** evaluated at the same location, due to the staggered grid!

To test the operators we need a finer grid.

```
Grid.xmin = 0; Grid.xmax = 3; Grid.Nx = 30;
Grid = build_grid(Grid);
[D,G,C,I,M] = build_ops(Grid); L = D*G;
```

Differentiating a function that satisfies the natural BC's

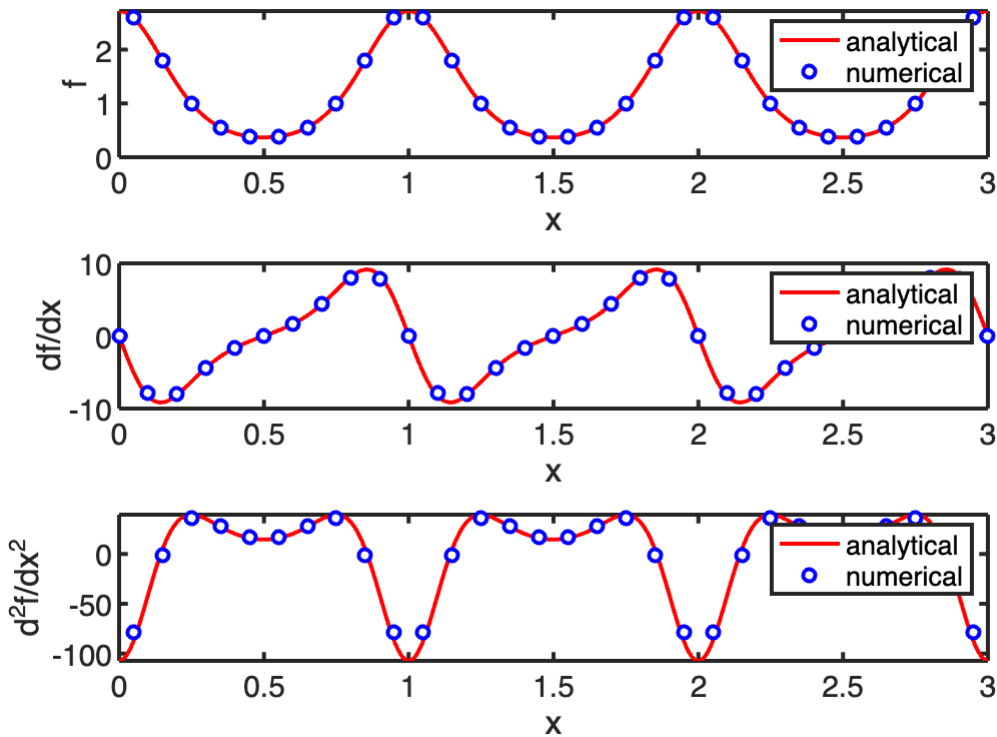
Consider the function $f(x) = e^{\cos(2\pi x)}$ on the domain $x \in [0, 3]$, which satisfies the natural boundary conditions, i.e., $df/dx = 0$ at the boundaries. These are the boundary conditions that are built into the discrete gradient G.

```
xa = linspace(Grid.xmin,Grid.xmax,3e2);
f = @(x) exp(cos(2*pi*x));
dfdx = @(x) -exp(cos(2*pi*x)).*sin(2*pi*x)*2*pi;
d2fdx2 = @(x) -2*pi^2*exp(cos(2*pi*x)).*(2*cos(2*pi*x)+cos(4*pi*x)-1);

figure(2)
subplot 311
plot(xa,f(xa),'r',Grid.xc,f(Grid.xc),'bo','markerfacecolor','w','markersize',6)
xlabel 'x'
ylabel 'f'
legend('analytical','numerical')

subplot 312
plot(xa,dfdx(xa),'r',Grid.xf,G*f(Grid.xc),'bo','markerfacecolor','w','marker size',6)
xlabel 'x'
ylabel 'df/dx'
legend('analytical','numerical')

subplot 313
plot(xa,d2fdx2(xa),'r',Grid.xc,L*f(Grid.xc),'bo','markerfacecolor','w','marker size',6)
xlabel 'x'
ylabel 'd^2f/dx^2'
legend('analytical','numerical')
```



The figure shows that discrete derivatives approximate the analytic derivatives well. Note that the two derivatives are evaluated at different locations:

1. First derivative is evaluated at cell faces.
2. Second derivative is evaluated at cell centers.

Differentiation a function that does NOT satisfy the natural BC's

Consider the function $g(x) = e^{\cos(2\pi x)}$, which does not satisfy the natural boundary conditions, i.e., the homogeneous Neumann boundary conditions of the discrete gradient operator G .

```

g = @(x) exp(sin(2*pi*x));
dgdxdx = @(x) exp(sin(2*pi*x)).*cos(2*pi*x)*2*pi;
d2gdxdx2 = @(x) 2*pi^2*exp(sin(2*pi*x)).*(-2*sin(2*pi*x)+cos(4*pi*x)+1);

figure(3)
subplot 311
plot(xa,g(xa),'r',Grid.xc,g(Grid.xc),'bo','markerfacecolor','w','markersize',6)
xlabel 'x'
ylabel 'g'
legend('analytical','numerical')

subplot 312

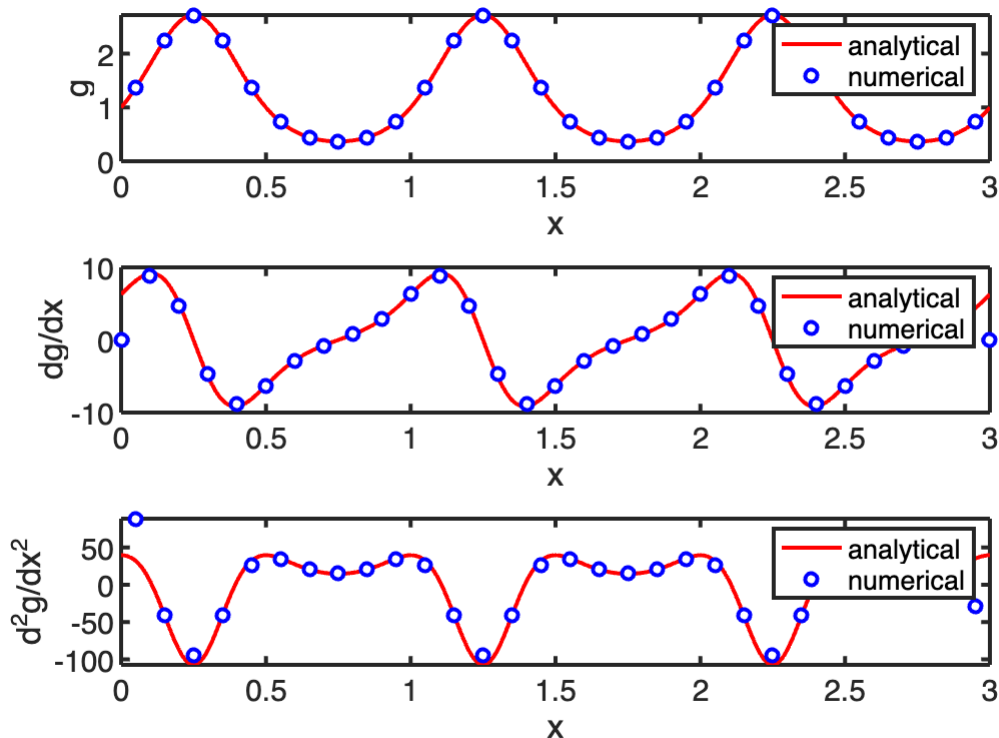
```

```

plot(xa,dgdx(xa),'r',Grid.xf,G*g(Grid.xc),'bo','markerfacecolor','w','marker
size',6)
xlabel 'x'
ylabel 'dg/dx'
legend('analytical','numerical')

subplot 313
plot(xa,d2gdx2(xa),'r',Grid.xc,L*g(Grid.xc),'bo','markerfacecolor','w','mark
ersize',6)
xlabel 'x'
ylabel 'd^2g/dx^2'
legend('analytical','numerical')

```



The figure shows that the derivatives are still well approximated in the interior of the domain. The error on the boundaries is large and does not reduce with increasing refinement of the grid. We will see later that the implementation of the boundary condition takes care of this problem.

Convergence with refinement

To check the convergence of the discrete operators compute the error between $\partial f/\partial x$ and $G*f$ and $\partial^2 f/\partial x^2$ and $D*G*f$ as the number grid points increases.

```

Nx = round(logspace(1,6,10));
error_grad = zeros(size(Nx)); error_lap = zeros(size(Nx));

for i = 1:length(Nx)

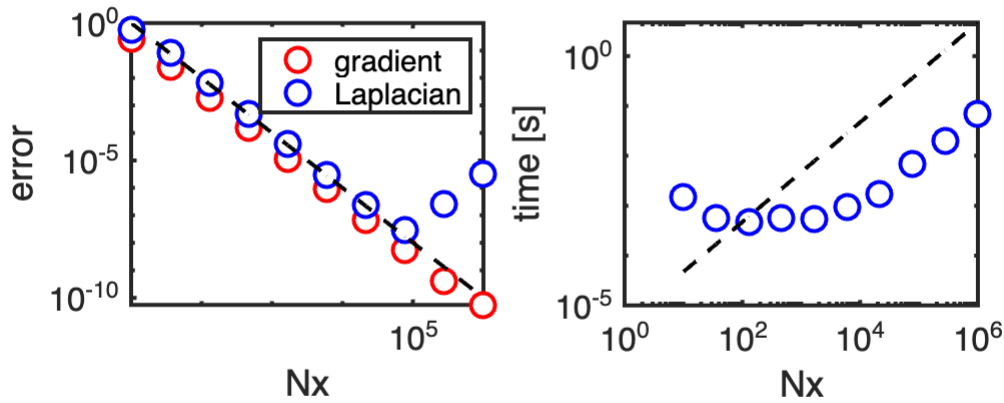
```

```

Grid.Nx = Nx(i); Grid = build_grid(Grid);
clear D G I
pause(1e-3)
tic;
[D,G,C,I,M] = build_ops(Grid);
time(i) = toc;
L = D*G;
error_grad(i) = norm(dfdx(Grid.xf)-G*f(Grid.xc))/norm(dfdx(Grid.xf));
error_lap(i) = norm(d2fdx2(Grid.xc)-D*G*f(Grid.xc))/
norm(d2fdx2(Grid.xc));
end

figure(4)
clf
subplot 121
loglog(Nx,error_grad,'ro','markerfacecolor','w'), hold on
loglog(Nx,error_lap,'bo','markerfacecolor','w')
semilogy(Nx,Nx.^(-2)*1e2,'k--')
xlabel 'Nx', ylabel 'error'
xlim([Nx(1)-1e-3 Nx(end)+1e-3])
legend('gradient','Laplacian')
pbaspect([1 .8 1])
subplot 122
loglog(Nx,time,'bo','markerfacecolor','w'), hold on
semilogy(Nx,min(time)*Nx/100,'k--')
xlabel 'Nx', ylabel 'time [s]'
set(gca,'xtick',[1e0 1e2 1e4 1e6])
pbaspect([1 .8 1])

```



The graph on the left shows the decline of the numerical error as a function of increasing grid refinement. The dashed line indicates the quadratic slope expected for that is expected for the central difference, which is second order accurate. Note, as the grid gets very fine ($N > 500,000$) the numerical rounding error takes over.

The graph on the right shows the time required to compute the discrete operators as the grid size increases with a dashed line indicating linear increase. The discrete operators can be assemble very efficiently using the [spdiags\(\)](#) function.

Auxillary functions

```
function [] = set_defaults()
    set(0, ...
        'defaultaxesfontsize', 18, ...
        'defaultaxeslinewidth', 2.0, ...
        'defaultlinelength', 2.0, ...
        'defaultpatchlinewidth', 2.0, ...
        'DefaultLineMarkerSize', 12.0);
end
```