notebooks (/github/waltherg/notebooks/tree/master)
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2013-12-03-Crank_Nicolson.ipynb (/github/waltherg/notebooks/tree/master/2013-12-03-Crank_Nicolson.ipynb)

This notebook demonstrates how IPython notebooks can be used to discuss the theory and implementation of numerical algorithms on one page.

With `ipython nbconvert --to markdown name.ipynb` a notebook like this one can be made into a blog post (http://georg.io/2013/12/Crank_Nicolson) in one easy step. To display the graphics in your resultant blog post use, for instance, your Dropbox Public folder (https://www.dropbox.com/help/16/en) that you can activate here (https://www.dropbox.com/enable_public_folder).

The Crank-Nicolson Method

The Crank-Nicolson method (http://en.wikipedia.org/wiki/Crank%E2%80%93Nicolson_method) is a well-known finite difference method for the numerical integration of the heat equation and closely related partial differential equations.

We often resort to a Crank-Nicolson (CN) scheme when we integrate numerically reaction-diffusion systems in one space dimension

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u),$$
$$\left.\frac{\partial u}{\partial x}\right|_{x=0,L} = 0,$$

where u is our concentration variable, x is the space variable, D is the diffusion coefficient of u, f is the reaction term, and L is the length of our one-dimensional space domain.

Note that we use Neumann boundary conditions (http://en.wikipedia.org/wiki/Neumann_boundary_condition) and specify that the solution u has zero space slope at the boundaries, effectively prohibiting entrance or exit of material at the boundaries (no-flux boundary conditions).

Finite Difference Methods

Many fantastic textbooks and tutorials have been written about finite difference methods, for instance a free textbook by Lloyd Trefethen (http://people.maths.ox.ac.uk/trefethen/pdetext.html).

Here we describe a few basic aspects of finite difference methods.

The above reaction-diffusion equation describes the time evolution of variable $u(x,t)$ in one space dimension (u is a line concentration). If we knew an analytic expression for $u(x,t)$ then we could plot u in a two-dimensional coordinate system with axes t and x.

To approximate $u(x,t)$ numerically we discretize this two-dimensional coordinate system resulting, in the simplest case, in a two-dimensional regular grid (http://en.wikipedia.org/wiki/Regular_grid). This picture is employed commonly when constructing finite differences methods, see for instance Figure 3.2.1 of Trefethen (http://people.maths.ox.ac.uk/trefethen/3all.pdf).

Let us discretize both time and space as follows:

$$t_n = n\Delta t,\ n = 0, \ldots, N-1,$$
$$x_j = j\Delta x,\ j = 0, \ldots, J-1,$$

where N and J are the number of discrete time and space points in our grid respectively. Δt and Δx are the time step and space step respectively and defined as follows:

$$\Delta t = T/N,$$
$$\Delta x = L/J,$$

where T is the point in time up to which we will integrate u numerically.

Our ultimate goal is to construct a numerical method that allows us to approximate the unknonwn analytic solution $u(x,t)$ reasonably well in these discrete grid points.

That is we want construct a method that computes values $U(j\Delta x, n\Delta t)$ (note: capital U) so that

$$U(j\Delta x, n\Delta t) \approx u(j\Delta x, n\Delta t)$$

As a shorthand we will write $U_j^n = U(j\Delta x, n\Delta t)$ and (j,n) to refer to grid point $(j\Delta x, n\Delta t)$.

The Crank-Nicolson Stencil

Based on the two-dimensional grid we construct we then approximate the operators of our reaction-diffusion system.

For instance, to approximate the time derivative on the left-hand side in grid point (j, n) we use the values of U in two specific grid points:

$$\left.\frac{\partial u}{\partial t}\right|_{x=j\Delta x, t=n\Delta t} \approx \frac{U_j^{n+1} - U_j^n}{\Delta t}.$$

We can think of this scheme as a stencil that we superimpose on our (x, t)-grid and this particular stencil is commonly referred to as forward difference (http://en.wikipedia.org/wiki/Finite_difference#Forward.2C_backward.2C_and_central_differences).

The spatial part of the Crank-Nicolson stencil (http://journals.cambridge.org/abstract_S0305004100023197) (or see Table 3.2.2 of Trefethen (http://people.maths.ox.ac.uk/trefethen/3all.pdf)) for the heat equation ($u_t = u_{xx}$) approximates the Laplace operator (http://en.wikipedia.org/wiki/Laplace_operator) of our equation and takes the following form

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x=j\Delta x, t=n\Delta t} \approx \frac{1}{2\Delta x^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n + U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}\right).$$

To approximate $f(u(j\Delta x, n\Delta t))$ we write simply $f(U_j^n)$.

These approximations define the stencil for our numerical method as pictured on Wikipedia (http://en.wikipedia.org/wiki/Crank%E2%80%93Nicolson_method).

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Applying this stencil to grid point (j, n) gives us the following approximation of our reaction-diffusion equation:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{D}{2\Delta x^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n + U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}\right) + f(U_j^n)$$

Reordering Stencil into Linear System

Let us define $\sigma = \frac{D\Delta t}{2\Delta x^2}$ and reorder the above approximation of our reaction-diffusion equation:

$$-\sigma U_{j-1}^{n+1} + (1+2\sigma)U_j^{n+1} - \sigma U_{j+1}^{n+1} = \sigma U_{j-1}^n + (1-2\sigma)U_j^n + \sigma U_{j+1}^n + \Delta t f(U_j^n$$

This equation makes sense for space indices $j = 1, \dots, J-2$ but it does not make sense for indices $j = 0$ and $j = J-1$ (on the boundaries):

$$j = 0: \quad -\sigma U_{-1}^{n+1} + (1+2\sigma)U_0^{n+1} - \sigma U_1^{n+1} = \sigma U_{-1}^n + (1-2\sigma)U_0^n + \sigma U_1^n + \Delta$$
$$j = J-1: \quad -\sigma U_{J-2}^{n+1} + (1+2\sigma)U_{J-1}^{n+1} - \sigma U_J^{n+1} = \sigma U_{J-2}^n + (1-2\sigma)U_{J-1}^n + \sigma$$

The problem here is that the values U_{-1}^n and U_J^n lie outside our grid.

However, we can work out what these values should equal by considering our Neumann boundary condition. Let us discretize our boundary condition at $j = 0$ with the backward difference (http://en.wikipedia.org/wiki/Finite_difference#Forward.2C_backward.2C_and_central_differences) and at $j = J-1$ with the forward difference (http://en.wikipedia.org/wiki/Finite_difference#Forward.2C_backward.2C_and_central_differences):

$$\frac{U_1^n - U_0^n}{\Delta x} = 0,$$
$$\frac{U_J^n - U_{J-1}^n}{\Delta x} = 0.$$

These two equations make it clear that we need to amend our above numerical approximation for $j = 0$ with the identities $U_0^n = U_1^n$ and $U_0^{n+1} = U_1^{n+1}$, and for $j = J-1$ with the identities $U_{J-1}^n = U_J^n$ and $U_{J-1}^{n+1} = U_J^{n+1}$.

Let us reinterpret our numerical approximation of the line concentration of u in a fixed point in time as a vector $\mathbf{U}^n$:

$$\mathbf{U}^n = \begin{bmatrix} U_0^n \\ \vdots \\ U_{J-1}^n \end{bmatrix}.$$

Using this notation we can now write our above approximation for a fixed point in time, $t = n\Delta t$, compactly as a linear system:

$$\begin{bmatrix} 1+\sigma & -\sigma & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -\sigma & 1+2\sigma & -\sigma & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -\sigma & 1+2\sigma & -\sigma & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\sigma & 1+2\sigma & -\sigma \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\sigma & 1+\sigma \end{bmatrix}$$
$$= \begin{bmatrix} 1-\sigma & \sigma & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ \sigma & 1-2\sigma & \sigma & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & \sigma & 1-2\sigma & \sigma & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma & 1-2\sigma & \sigma \end{bmatrix} \begin{bmatrix} U_0^n \\ U_1^n \\ U_2^n \\ \vdots \\ U_{J-2}^n \end{bmatrix}$$

A Crank-Nicolson Example in Python

Let us apply the CN method to a two-variable reaction-diffusion system that was introduced by Mori *et al.* (http://www.sciencedirect.com/science/article/pii/S0006349508704442):

$$\frac{\partial u}{\partial t} = D_u \frac{\partial^2 u}{\partial x^2} + f(u,v),$$
$$\frac{\partial v}{\partial t} = D_v \frac{\partial^2 v}{\partial x^2} - f(u,v),$$

with Neumann boundary conditions

$$\left.\frac{\partial u}{\partial x}\right|_{x=0,L} = 0,$$
$$\left.\frac{\partial v}{\partial x}\right|_{x=0,L} = 0.$$

The variables of this system, u and v, represent the concetrations of the active form and its inactive form respectively. The reaction term $f(u,v)$ describes the interchange (activation and inactivation) between these two states of the protein. A particular property of this system is that the inactive has much greater diffusivity that the active form, $D_v \gg D_u$.

Using the CN method to integrate this system numerically, we need to set up two separate approximations

$$A_u \mathbf{U}^{n+1} = B_u \mathbf{U}^n + \mathbf{f}^n,$$
$$A_v \mathbf{V}^{n+1} = B_v \mathbf{V}^n - \mathbf{f}^n,$$

with two different σ terms, $\sigma_u = \frac{D_u \Delta t}{2\Delta x^2}$ and $\sigma_v = \frac{D_v \Delta t}{2\Delta x^2}$.

Import Packages

For the matrix-vector multiplication, vector-vector addition, and matrix inversion that we will need to carry out we will use the Python library NumPy (http://www.numpy.org/). To visualize our numerical solutions, we will use pyplot (http://matplotlib.org/api/pyplot_api.html).

In [1]:
```
import numpy
from matplotlib import pyplot
```

Numpy allows us to truncate the numerical values of matrices and vectors to improve their display with `set_printoptions` (http://docs.scipy.org/doc/numpy/reference/generated/numpy.set_printoptions.html).

In [2]:
```
numpy.set_printoptions(precision=3)
```

Specify Grid

Our one-dimensional domain has unit length and we define `J = 100` equally spaced grid points in this domain. This divides our domain into `J-1` subintervals, each of length `dx`.

In [153]:
```
L = 1.
J = 100
dx = float(L)/float(J-1)
x_grid = numpy.array([j*dx for j in range(J)])
```

Equally, we define `N = 1000` equally spaced grid points on our time domain of length `T = 200` thus dividing our time domain into `N-1` intervals of length `dt`.

In [154]:
```
T = 200
N = 1000
dt = float(T)/float(N-1)
t_grid = numpy.array([n*dt for n in range(N)])
```

Specify System Parameters and the Reaction Term

We choose our parameter values based on the work by Mori *et al.* (http://www.sciencedirect.com/science/article/pii/S0006349508704442).

In [155]:
```
D_v = float(10.)/float(100.)
D_u = 0.01 * D_v

k0 = 0.067
f = lambda u, v: dt*(v*(k0 + float(u*u)/float(1. + u*u)) - u)
g = lambda u, v: -f(u,v)

sigma_u = float(D_u*dt)/float((2.*dx*dx))
sigma_v = float(D_v*dt)/float((2.*dx*dx))

total_protein = 2.26
```

Specify the Initial Condition

As discussed by Mori *et al.* (http://www.sciencedirect.com/science/article/pii/S0006349508704442), we can expect to observe interesting behaviour in the steady state of this system if we choose a heterogeneous initial condition for u.

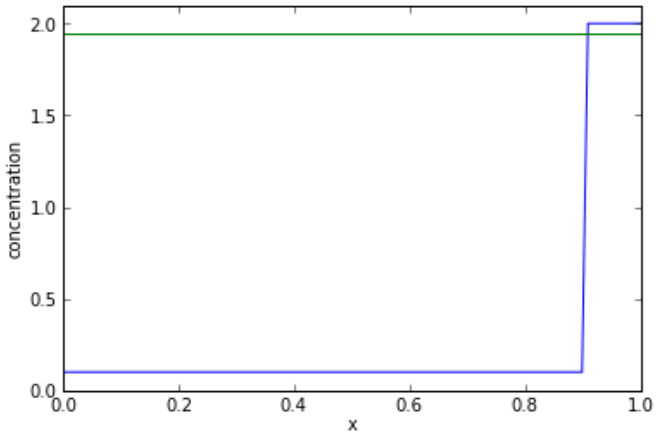
Here, we initialize u with a step-like heterogeneity:

In [156]:
```
no_high = 10
U =  numpy.array([0.1 for i in range(no_high,J)] + [2. for i in ra
V = numpy.array([float(total_protein-dx*sum(u))/float(J*dx) for i
```

Note that we make certain that total protein amounts equal a certain value, `total_protein`. The importance of this was discussed by Walther *et al.* (http://link.springer.com/article/10.1007%2Fs11538-012-9766-5).

Let us plot our initial condition for confirmation:

In [157]:
```
ylim((0., 2.1))
xlabel('x'); ylabel('concentration')
pyplot.plot(x_grid, U)
pyplot.plot(x_grid, V)
pyplot.show()
```



The blue curve is the initial condition for U, stored in Python variable `U`, and the green curve is the initial condition for V stored in `V`.

Create Matrices

The matrices that we need to construct are all tridiagonal so they are easy to construct with `numpy.diagflat` (http://docs.scipy.org/doc/numpy/reference/generated/numpy.diagflat.html).

In [158]:
```
A_u = numpy.diagflat([-sigma_u for i in range(J-1)], -1) +\
      numpy.diagflat([1.+sigma_u]+[1.+2.*sigma_u for i in range(J-
      numpy.diagflat([-sigma_u for i in range(J-1)], 1)

B_u = numpy.diagflat([sigma_u for i in range(J-1)], -1) +\
      numpy.diagflat([1.-sigma_u]+[1.-2.*sigma_u for i in range(J-
      numpy.diagflat([sigma_u for i in range(J-1)], 1)

A_v = numpy.diagflat([-sigma_v for i in range(J-1)], -1) +\
      numpy.diagflat([1.+sigma_v]+[1.+2.*sigma_v for i in range(J-
      numpy.diagflat([-sigma_v for i in range(J-1)], 1)

B_v = numpy.diagflat([sigma_v for i in range(J-1)], -1) +\
      numpy.diagflat([1.-sigma_v]+[1.-2.*sigma_v for i in range(J-
      numpy.diagflat([sigma_v for i in range(J-1)], 1)
```

To confirm, this is what `A_u` looks like:

In [159]:
```
print A_u
```

```
[[ 1.981 -0.981  0.    ...,  0.     0.     0.   ]
 [-0.981  2.962 -0.981 ...,  0.     0.     0.   ]
 [ 0.    -0.981  2.962 ...,  0.     0.     0.   ]
 ...,
 [ 0.     0.     0.    ...,  2.962 -0.981  0.   ]
 [ 0.     0.     0.    ..., -0.981  2.962 -0.981]
 [ 0.     0.     0.    ...,  0.    -0.981  1.981]]
```

Solve the System Iteratively

To advance our system by one time step, we need to do one matrix-vector multiplication followed by one vector-vector addition on the right hand side.

To facilitate this, we rewrite our reaction term so that it accepts concentration vectors $\mathbf{U}^n$ and $\mathbf{V}^n$ as arguments and returns vector $\mathbf{f}^n$.

As a reminder, this is our non-vectorial definition of f

```
f = lambda u, v: v*(k0 + float(u*u)/float(1. + u*u)) - u
```

In [160]:
```
f_vec = lambda U, V: numpy.multiply(dt, numpy.subtract(numpy.multi
                     numpy.add(k0, numpy.divide(numpy.multiply(U,U
```

Let us make certain that this produces the same values as our non-vectorial `f`:

In [161]:
```
print f(U[0], V[0])
```

```
0.00996135898275
```

In [162]:
```
print f(U[-1], V[-1])
```

```
-0.0623832232232
```

In [163]:
```
print f_vec(U, V)
```

```
[ 0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0.01   0
  0.01   0.01  -0.062 -0.062 -0.062 -0.062 -0.062 -0.062 -0.062 -0
 -0.062 -0.062]
```

Accounting for rounding of the displayed values due to the `set_printoptions` we set above, we can see that `f` and `f_vec` generate the same values for our initial condition at both ends of our domain.

We will use `numpy.linalg.solve` (http://docs.scipy.org/doc/numpy/reference/generated/numpy.linalg.solve.html) to solve our linear system each time step.

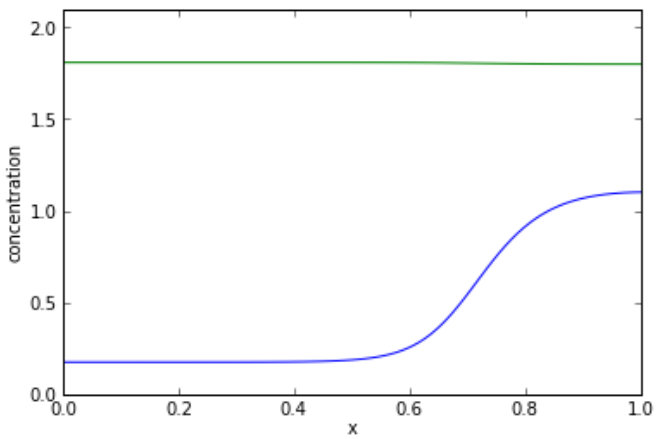
While we integrate our system over time we will record both U and V at each time step in `U_record` and `V_record` respectively so that we can plot our numerical solutions over time.

In [164]:
```
U_record = []
V_record = []

U_record.append(U)
V_record.append(V)

for ti in range(1,N):
    U_new = numpy.linalg.solve(A_u, B_u.dot(U) + f_vec(U,V))
    V_new = numpy.linalg.solve(A_v, B_v.dot(V) - f_vec(U,V))

    U = U_new
    V = V_new

    U_record.append(U)
    V_record.append(V)
```

Plot the Numerical Solution

Let us take a look at the numerical solution we attain after N time steps.

In [165]:
```
ylim((0., 2.1))
xlabel('x'); ylabel('concentration')
pyplot.plot(x_grid, U)
pyplot.plot(x_grid, V)
pyplot.show()
```



And here is a kymograph (http://en.wikipedia.org/wiki/Kymograph) of the values of U. This plot shows concisely the behaviour of U over time and we can clear observe the wave-pinning behaviour described by Mori *et al.* (http://www.sciencedirect.com/science/article/pii/S0006349508704442). Furthermore, we observe that this wave pattern is stable for about 50 units of time and we therefore conclude that this wave pattern is a stable steady state of our system.

In [169]:
```
U_record = numpy.array(U_record)
V_record = numpy.array(V_record)

fig, ax = subplots()
xlabel('x'); ylabel('t')
heatmap = ax.pcolor(x_grid, t_grid, U_record, vmin=0., vmax=1.2)
```