Scientific Computation

Spring, 2019

Lecture 10

Imperial College
London

Feedback

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https://goo.gl/forms/K5YEXbxZFTbUdfda2

Diffusion in networks

- With networks, we no longer have spatial derivatives

- Need to think about flux along a link between two nodes
- Then the rate of change at a node will be the sum of fluxes from its neighbors
- The diffusive flux from node j to node i is taken to be: $J_{ij} = -\mathcal{D}\left(f_i - f_j\right)$

  which leads to: $\frac{\partial f_i}{\partial t} = \sum_j J_{ij}$ and the sum is over all nodes with links to node i
- We can rewrite the sum using the network's adjacency matrix:

$$\frac{\partial f_i}{\partial t} = \sum_{j=1}^{N} A_{ij} J_{ij}$$

$$\frac{\partial f_i}{\partial t} = -\sum_{j=1}^{N} A_{ij} \mathcal{D}\left(f_i - f_j\right)$$

- And this is a representative model for diffusion/spreading in networks

Diffusion in networks

- **Can we further simplify the equation below?**

$$\frac{\partial f_i}{\partial t} = -\sum_{j=1}^{N} A_{ij}\mathcal{D}\left(f_i - f_j\right)$$

- **There are two "sum invariants" and we rewrite the equation as:**

$$\frac{\partial f_i}{\partial t} = \mathcal{D}\left(\sum_{j=1}^{N} A_{ij} f_j - f_i \sum_{j=1}^{N} A_{ij}\right)$$

- **For undirected graphs, the second sum is simply the degree of node i,** q_i
- **Define a diagonal matrix,** Q**, where the** (k,k) **element is the degree,** q_k
- **Then, our diffusion equation can be re-written as:**

$$\frac{\partial f_i}{\partial t} = -\mathcal{D}\left(\sum_{j=1}^{N} L_{ij} f_j\right),\ L = Q - A$$

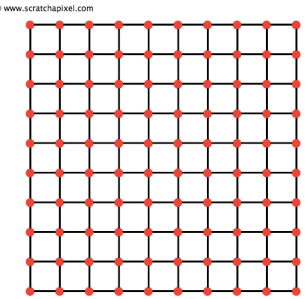
where L **is the *Laplacian* matrix**

- **Does the Laplacian matrix have any connection to the Laplacian operator?**

Laplacians

- Let's think about Laplacian operator on a 2D x-y grid
- Need to approximate $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}$ on discrete grid with spacing Δ:

$$x_i = i * \Delta,\ i = 0, 1, 2, ..., N + 1$$
$$y_j = j * \Delta,\ j = 0, 1, 2, ..., N + 1$$



- Use a 2nd-order finite-difference approximation:

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} \approx \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}$$
$$\left(\frac{\partial^2 T}{\partial y^2}\right)_{i,j} \approx \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2}$$
$$\Delta x = \Delta y = \Delta$$

The approximation error is $O(\Delta^2)$ – can use Taylor series expansions to show this

Rearranging, we have:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \approx \frac{T_{i+1,j} + T_{i,j+1} - 4T_{i,j} + T_{i-1,j} + T_{i,j-1}}{\Delta^2}$$

Laplacians

- Our 2-D grid can be re-interpreted as a graph
- Each node has four links (degree=4), so:

$$\sum_{j=1}^{N} L_{ij} T_{i,j} = 4T_{i,j} - T_{i-1,j} - T_{i+1,j} - T_{i,j+1} - T_{i,j-1}$$

- This is the negative of our approximate Laplacian operator with Δ=1
- So we can anticipate "diffusion-like" behavior with our model for spreading on graphs
- The Laplacian matrix also provides insight into the structure of graphs (e.g. connectivity)

Diffusion in networks

$$\frac{\partial f_i}{\partial t} = -\mathcal{D}\left(\sum_{j=1}^{N} L_{ij} f_j\right),\ L = Q - A$$

- How do we find solutions?
- Need initial values to be specified for each node
- Then, this is a system of linear constant-coefficient ODEs
  - i.e. it's an eigenvalue problem
- For undirected networks, the Laplacian is real-valued and symmetric
  - So its eigenvalues are real (they are also non-negative)

Diffusion in networks

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- **Need initial values to be specified for each node**
- **Then, this is a system of linear constant-coefficient ODEs**
  - **i.e. it's an eigenvalue problem**
- **For undirected networks, the Laplacian is real-valued and symmetric**
  - **So its eigenvalues are real (they are also non-negative)**
- **How do we compute eigenvalues in Python?**
  - np.linalg.eig
  - scipy.sparse.linalg.eig
- **What are the advantages/disadvantages of the two functions?**

Diffusion in networks

$$\frac{\partial f_i}{\partial t} = -\mathcal{D}\left(\sum_{j=1}^{N} L_{ij} f_j\right), \; L = Q - A$$

- **An example:**

```
In [3]: G  = nx.erdos_renyi_graph(15,0.2)


In [6]: A = nx.adjacency_matrix(G)

In [7]: A.todense()
Out[7]:
matrix([[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
        [0, 0, 0, 0, 1, 0, 0, 0, 1, 1, 0, 1, 0, 1, 0],
        [0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 1, 1, 0, 1, 1],
        [0, 0, 0, 0, 1, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0],
        [0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
        [0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0],
        [0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
        [0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1],
        [0, 1, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0],
        [0, 1, 1, 1, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0],
        [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
        [0, 1, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0],
        [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
        [0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
        [0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0]],
```

Diffusion in networks

$$\frac{\partial f_i}{\partial t} = -\mathcal{D}\left(\sum_{j=1}^{N} L_{ij} f_j\right), \; L = Q - A$$

- **An example:**

```
In [22]: Q = A.toarray().sum(axis=1)

In [23]: L = np.diag(Q)-A.toarray()

In [27]: e,v = np.linalg.eig(L)

In [28]: e
Out[28]:
array([8.46780548e+00, 6.22084072e+00, 5.59130087e+00, 4.25530240e+00,
       3.73535212e+00, 1.66002435e-15, 2.55436419e+00, 2.37762994e+00,
       1.87790207e+00, 1.69700500e+00, 1.46423645e+00, 8.66087659e-01,
       8.92173104e-01, 0.00000000e+00, 0.00000000e+00])
```

- **Unaddressed questions:**
  - **There are three eigenvalues with value zero – are these important? What is their physical interpretation?**
  - **What should be done with the eigenvectors?**

Dynamical process on networks

- **Previously, we considered *linear* diffusion:** $\frac{\partial f_i}{\partial t} = -\mathcal{D}\left(\sum_{j=1}^{N} L_{ij} f_j\right),\ L = Q - A$
- **Often, the most interesting/important problems involve *nonlinear* dynamics:**

$$\frac{\partial f_i}{\partial t} = \mathcal{F}(t, f_j, A_{ij}),\ \ i, j \in 0, 1, ..., N-1$$

- **How can we solve problems of this form?**
  - **Generally, no analytical solution, need to find approximated numerical solution**

Dynamical process on networks

- **Previously, we considered *linear* diffusion:** $\frac{\partial f_i}{\partial t} = -\mathcal{D}\left(\sum_{j=1}^{N} L_{ij} f_j\right),\ L = Q - A$
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- **How can we solve problems of this form?**
  - **Generally, no analytical solution, need to find approximated numerical solution**

- **Basic idea: discretize time,** t = 0, dt, …, N*Δt, **and starting from** f(0) **march forward in time and compute** f(Δt), … f(N*Δt)

- **Explicit Euler method:** $f_i(t_0 + \Delta t) = f_i(t_0) + \Delta t \frac{df_i}{dt}|_{t_0} + O(\Delta t^2)$

$$f_i(t_0 + \Delta t) \approx f_i(t_0) + \Delta t \mathcal{F}(t_0, f_j(t_0), A_{ij})$$

- **Accuracy: global error ~** dt **→ smaller time step, more accurate solution**
- **Stability: for** s**: unconditionally unstable → for large enough N, solution becomes unbounded (blows up)**

Time-marching methods

- **Basic idea: discretize time,** t = 0, dt, …, N*Δt**, and starting from** f(0) **march forward in time and compute** f(Δt), … f(N*Δt)

- **Explicit Euler method:** $f_i(t_0 + \Delta t) = f_i(t_0) + \Delta t \frac{df_i}{dt}|_{t_0} + O(\Delta t^2)$

$$f_i(t_0 + \Delta t) \approx f_i(t_0) + \Delta t \mathcal{F}(t_0, f_j(t_0), A_{ij})$$

- **Accuracy: global error ~** Δt **→ smaller time step, more accurate solution**
- **Stability: for dy/dt = y: unconditionally unstable → for large enough N, solution becomes unbounded (blows up)**

- **Runge-Kutta methods provide better accuracy and stability**
  - **Evaluate function at sub-steps and construct approximation using this "extra information"**

Time-marching methods

Runge-Kutta methods provide better accuracy and stability

- **Evaluate function at sub-steps and construct approximation using this "extra information"**
- **4th-order RK for** dy/dt = f(t,y):

$$y(t_0 + \Delta t) = y(t_0) + \tfrac{1}{6}k_1 + \tfrac{1}{3}(k_2 + k_3) + \tfrac{1}{6}k_4$$

$$k_1 = \Delta t f(t_0, y(t_0))$$

$$k_2 = \Delta t f(t_0 + \Delta t/2, y(t_0) + k_1/2)$$

$$k_3 = \Delta t f(t_0 + \Delta t/2, y(t_0) + k_2/2)$$

$$k_4 = \Delta t f(t_0 + \Delta t, y(t_0) + k_3)$$

- **Error ~** Δt^4
- ***Conditionally* stable for dy/dt=y (bounded solutions for sufficiently small** Δt**)**
- **Requires 4 function evaluations per time step**
- **Was once *very* widely used**

Time-marching methods

Variable time-step Runge-Kutta methods are very popular

- **Similar to RK4, however time-step is automatically adjusted to ensure a specified accuracy**
- **In Matlab: ODE23 and ODE45 (also available in scipy.integrate)**

Time-marching methods

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- **Similar to RK4, however time-step is automatically adjusted to ensure a specified accuracy**
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- **Explicit time-marching methods (like R-K methods) can struggle with systems of nonlinear ODEs**
- **These systems often contain rapidly varying components which affect stability much more than accuracy**
- **Then, should look to *implicit* methods:**

- **Implicit Euler method:** $f_i(t_0 + \Delta t) \approx f_i(t_0) + \Delta t \mathcal{F}(t_0 + \Delta t, f_j(t_0 + \Delta t), A_{ij})$

- **Accuracy: global error ~ Δt → smaller time step, more accurate solution**
- **Stability: for dy/dt = ay: *unconditionally stable* → bounded solution for any time-step**
- **Requires solution of system of equations each time step**

Time-marching methods

Variable time-step implicit methods are also widely available

- **Again, time-step is automatically adjusted to ensure a specified accuracy**
- **In Matlab: ODE23s and ODE15s (also available in scipy.integrate)**

Time-marching methods

Variable time-step implicit methods are also widely available

- **Again, time-step is automatically adjusted to ensure a specified accuracy**
- **In Matlab: ODE23s and ODE15s (also available in scipy.integrate)**

- **We will use scipy.integrate.odeint (in this week's lab)**
  - **Have to specify: 1) initial conditions**
    2) time span
    3) function which evaluates RHS of ODEs
  - **Can specify: 1) error tolerance**
    2) times at which to return solution
    3) many other parameters

Look at online documentation!