Principles of measurement and modeling in atmospheric chemistry

Earth and Planetary Sciences 236

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General properties of linear models:
Jacobian matrix and box models

Evidently the stepwise reduction of a problem with many compartments could be very difficult indeed. Fortunately, a straightforward procedure is available that allows us to solve any analogous problelm with arbitrary number of boxes, using simple matrix algebra.

The time-dependence of any model composed of n reservoirs (boxes) and fluxes between them given by linear functions of reservoir contents, can be written as

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dx₁/dt  =  Σk₁ᵢxᵢ
dx₂/dt  =  Σk₂ᵢxᵢ
...
dxⱼ/dt  =  Σkⱼᵢxᵢ
dxₙ/dt  =  Σkₙᵢxᵢ
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This is a familiar mathematical problem, a set of coupled, 1st-order, linear differential equations that can be written in matrix form,

$d\mathbf{X}/dt = \mathbf{K}*\mathbf{X}$,

where **bold** symbols denote matrices or vectors. For the initial value problem, where $\mathbf{X}(t=0) = \mathbf{X_0}$, it is easy to show that the solution is given compactly as

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X = exp(Kt) * X₀.                    (3.1)
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Here is the demonstration: the function **exp(Mt)** of a matrix is defined in terms of a power series analogous to exp(x), i.e.,

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exp(M) ≡ 1 + M + M²/2! + M³/3! + M⁴/4! + ....
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If we differentiate **exp(M)** with respect to a scalar (say, t), we see that

$d\,\mathbf{exp(M)}/dt = \mathbf{exp(M)} * d\mathbf{M}/dt$,

which proves the point for our case ($\mathbf{M} = \mathbf{K} * t$, $\mathbf{K}$ independent of t).

The infinite power series is evidently not a convenient form for computing **exp(K**t**)**. The task is simplified enormously if we take linear combinations of the x_i to define the eigenvectors of **exp(K**t**)**.

Quick Math "review"!

Recall that for each eigenvector X^e_i of an arbitrary matrix M,

`M * X`^e_i` =    `λ_i`X`^e_i

where the scalar λ_i is the ith *eigenvalue* corresponding to X^e_i. If we form the matrix of eigenvectors, X^e and its inverse, $(X^e)^{-1}$, then

`(X`^{e}`)`$^{-1}$`* M * X`^{e}` =`Λ`   ,`

where Λ is a diagonal matrix with elements λ_i (off-diagonal elements all 0).

An exercise: if **K** is a matrix with eigenvectors X^e_i and eigenvalues λ_i, what are the eigenvalues and eigenvectors of the matrix **exp(K**t**)**?

We obtain an elegant and useful result if we multiply equation (3.1) by $(X^e)^{-1}$ on the left,

$$X' (t) = exp(\Lambda * t) * X' (0). \qquad (3.2)$$

Here $exp(\Lambda * t)$ is the diagonal matrix of eigenvalues of the matrix **exp(K**t**)**, and
$X' \equiv (X^e)^{-1} * X$
represents the state variables (concentrations in the boxes) *expressed in terms of the eigenvectors*. (The demonstration that $exp(\Lambda * t)$ is obtained from $(X^e)^{-1} * exp(Kt) * X^e$ is left as an exercise.)

The CH$_4$ oxidation problem (from your homework...)
The Jacobian matrix, its role in linear models, and linearized approximations to nonlinear models

(Reference: Prather, M., *Geophys. Res. Letters 23,* 2597-2600, 1996)

In general a model describing the spatial distribution and temporal evolution any constituent in the earth-atmosphere system may be represented as a set of coupled differential equations, the mass continuity equations for each constituent at each point in the domain (Eq. 1).

Equations for spatially distributed models of trace species (Example: GEOS-CHEM):

$$dx_k/dt = p_k - \nabla \bullet \Phi_K \qquad (1)$$

$$dX/dt = \mathbf{P} - \nabla \bullet \Phi \tag{2}$$

$$\mathbf{J}_{ik} = \partial(dX/dt)_i/\partial x_k = \partial(\mathbf{P})_i/\partial x_k - \partial(\nabla \Phi)_i/\partial x_k \tag{3}$$

$$d(X^o(t) + D(t))_i/dt = d(X^o(t))_i/dt + \Sigma_{k=1:nm}J_{ik}D_k + \text{2nd order terms} \tag{4}$$
$$(\textit{Note}\ d(X^o(t))_i/dt \equiv 0)$$

$$d\mathbf{D}/dt = \mathbf{J}\ \mathbf{D} \tag{5}$$

$$dA^k/dt = -c_k\ A^k$$
$$(=> A^k(t) = A^k(0)\ \exp(-c_kt)\ ) \tag{6}$$

$$D(0) = \Sigma_{k=1:nm}d_kA^k$$
$$(=> D(t) = \Sigma_{k=1:nm}d_kA^k\ \exp(-c_kt)\ ) \tag{7}$$

The continuity equation (1) for the concentration of each species at a given spatial location (or box). X_k, can be expressed in terms of its local net chemical production $P_{k'}$ and its transport tendency, $\nabla \Phi_k$ the flux divergence. The chemical or biological rates (P_k), and the velocity field defining the transport rates $(\nabla \Phi_k)$, constitute the conceptual (bigeochemical) model and the inputs.

If we have m species and n spatial gridpoints (boxes), the individual equations (1) can be written as a single vector equation (Eq. 2), $\mathbf{X}$ being a vector of species concentrations x_k where $k=i+m(j-1)$, $i = 1{:}m$ is the species index and $j = 1{:}n$ is the spatial (box) index. The vector $\mathbf{P}$ represents the individual P_k. (function of different species at the same location); and the vector $\nabla \Phi$, the individual $\nabla \Phi_k$.

The nm x nm Jacobian matrix $\mathbf{J}$ is defined in (Eq. 3) as the partial derivative of each of the equations (Eq. 1) with respect to each independent variable' x_k . Let the vector of chemical species $X°(t)$ be a timedependent solution to Eq. 2, and solve for a perturbation $X^o + D$ by expanding equation (2) in a Taylor series (Eq. 4). Only the chemical terms (viz. for CO_2, the solubility, equilibrium coefficients, etc) are nonlinear and appear in (Eq. 4) with secondorder terms.

To firstorder the perturbation vector D satisfies the matrix equation (Eq. 5). If a perturbation A^k is an eigenvector of J with eigenvalue c_k, then the vector solution to (Eq. 5) decays, maintaining its spatial pattern, as a simple exponential (Eq. 6).

The natural modes in the model are the eigenvectors A^k (k=l:nm), a linearly independent set that spans the nmdimensional space of chemical species. Any perturbation D has a unique expansion with coefficients d^k in terms of these eignevectors, and decays with an ensemble of decay frequencies corresponding to the eigenvalues (Eq. 7). These modes are basic properties of the model, unlike the behavior of a particular perturbation. The vectors A^k are independent of the perturbation D provided that the Jacobian varies slowly: $J[X\ D] \sim J[Xo]$, i.e. the second-order terms in (4) are negligible.

- *In a fully linear system (like the CO_2 box models) J is constant and the time evolution of ANY state, not just a small perturbation around the stationary state, may be described by the decay of a single set of natural modes (Eq. 7).*

[Note that a real asymmetric matrix like J can have positive, negative, or complex eigenvalues. Provided that all eigenvalues are negative ($c < 0$) any perturbation decays. If there is a single positive eigenvalue of J[X] then the system would be (at least) locally unstable since any realistic perturbation would excite the unstable mode. Although complex eignevalues may appear in natural systems, giving oscillating "clocks" (Nitzan and Ross 1973), this case will not be considered in EPS236.]

The slowest-decaying modes are often of the greatest interest in biogeochemical models. The analysis using the Jacobian matrix **J** and its eigenvalues allows immediate recognition of the extent to which a particular perturbation excites slowly-decaying modes and defines the rate of relaxation, which will typically provide the time response for significant environmental changes.

The analysis also helps us to see how changes in model structure may affect the behavior of the model. For example, if spatial resolution is increased, new modes appear for each new degree of freedom. However, these represent nearest-neighbor interactions that usually decay quickly. The longlived perturbations should change little unless the basic manner of interaction among the compartments is altered.

Summary

- Many models of the ocean-atmosphere system conceptually divide the domain into reservoirs, e.g. CO_2 in the atmosphere, the surface ocean, the deep ocean, etc., assume that these compartments are each well-mixed and represent fluxes between reservoirs as linear functions of the reservoir contents.
- The result is a *linear model* that can be repesented mathematically as a set of coupled first-order linear differential equations with constant coefficients.
- The time-dependent solution of this system for an initial-value boundary condition is given by a set of eigenvectors ("modes") of the coefficient matrix.

- If mass is distributed in the system in proportion to the weights in an eigenvector, the perturbation will decay over time as a simple exponential with time constant equal to the reciprocal of the corresponding eigenvalue.
- Any perturbation to the system may be represented as a sum of perturbations of the normal modes, each of which evolves independently as a simple exponential in time with time constant equal to the inverse of the associated eigenvalue.

Piecewise linear approximation in the Jacobian formulation

We are interested in solving the equation

$$\frac{d\underline{x}}{dt} = \underline{F}\left(\{x_k\}\right)$$

where $F_i = \sum_k K_{ik} x_k$ for the linear model case. At some chosen point $\underline{x}^o$,

$$\frac{d\underline{x}^o}{dt} = \underline{F}\left(\{x_k{}^o\}\right) \equiv \underline{F}^o$$

Expand F in a Taylor series about $\underline{x}^o$: $\underline{F} \approx \underline{F}^o + \Sigma_k \left[\frac{\partial F}{\partial x_k} \right]_{x_k = x^o{}_k} (x_k - x^o{}_k)$, and

$$\frac{d(\underline{x} - \underline{x}^o)}{dt} = \underline{F} - \underline{F}^o \approx \Sigma_k \left[\frac{\partial F}{\partial x_k} \right]_{x_k = x^o{}_k} (x_k - x^o{}_k) .$$

Since we wish to know $\frac{d\underline{x}}{dt}$, we have:

$$\frac{d\underline{x}}{dt} = \underline{F}^o + \Sigma_k \left[\frac{\partial F}{\partial x_k} \right]_{x_k = x^o{}_k} (x_k - x^o{}_k) .$$

For example, if $F_i = a\, x_j{}^2$, then the Jacobian term becomes $2\,a\,x^o{}_j$.

Box model solution with forcing term:

$$\frac{d\underline{c}}{dt} = \underline{\underline{K}}\,\underline{c} + \underline{P}$$

P held
constant

$$\underline{c}_p(t) = -\underline{\underline{K}}^{-1}\underline{P}$$

$$\underline{c}(t) = \left(\exp(\underline{\underline{K}}t) - 1\right)\underline{\underline{K}}^{-1}\underline{P}$$

If P is a function of time: ....

$$\underline{c}(t) = \exp(\underline{\underline{K}}t)\left(\underline{c}(0) + \underline{\underline{K}}^{-1}\underline{P}\right) - \underline{\underline{K}}^{-1}\underline{P}$$

each time step

1. Any external forcing of a system can be represented as the sum of pulse input, i.e. a sum of initial-value perturbations, and therefore the general solution for such a model subjected to arbitrary forcing is given by a superposition of decaying normal modes initiated at different times.
2. The behavior of more complex systems in which fluxes between reservoirs are not simple linear functions can usually be approximated by a linear system, particularly for small perturbations around some stationary state. The coefficient matrix described above becomes, in this more general case, the first term in a Taylor series i.e. the Jacobian matrix.