Complex Systems

Lecture 1

Two types of complex systems

1. A homogeneous system with many degrees of freedom
2. A complex adaptive system
   John Holland invented this field

Complex Systems are nonlinear systems with many degrees of freedom that exhibit interesting behaviors

Incapability of self-organization is a key feature of a complex system

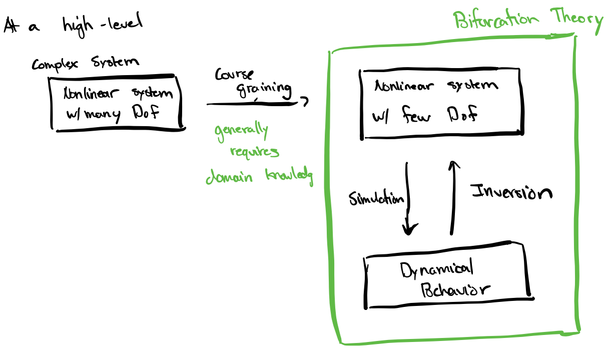
Emergence occurs due to stable states

- Find fixed points
- Analyze their stability

3 cores of the course

- Bifurcation Theory
- Inverse Theory
- Coding/Modeling

At a high-level



Lecture 2

Population growth

① Exponential Model

$$\frac{dx}{dt} = r x$$

← growth rate

$$X(t) = X(0)\exp(rt)$$

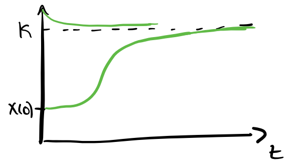
② Logistic Model

$$r \to r(1 - X/K)$$

↖ carrying capacity

When $x > K$, $r < 0$ and population decreases

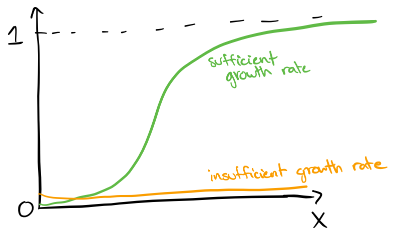
$$\dot{X} = rX\left(1 - X/K\right)$$



③ Insect Outbreak Model

$$\dot{X} = pX\left(1 - \frac{X}{K}\right) - \frac{X^2}{1+X^2}$$

↖ death rate

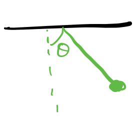


General Framework

$$\dot{X}_1 = f_1(X_1 \dots X_n)$$
$$\dot{X}_2 = f_1(X_1 \dots X_n)$$
$$\vdots$$
$$\dot{X}_n = f_n(X_1 \dots X_n)$$

Examples:

Swinging Pendulum



$$\ddot{\theta} + \frac{g}{L}\sin\theta = 0$$

$$\Rightarrow \quad \dot{x}_1 = x_2$$
$$\dot{x}_2 = \theta \frac{g}{L} \sin x_1$$

Forced Harmonic Oscillator

$$m\ddot{x} + b\dot{x} + kx = F\cos(t)$$

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = 1/m\left(-kx_1 - bx_2 + F\cos(x_3)\right)$$
$$\dot{x}_3 = 1$$

Consider $\dot{x} = \sin(x)$ w/ $x = x_0 a$ $t = 0$

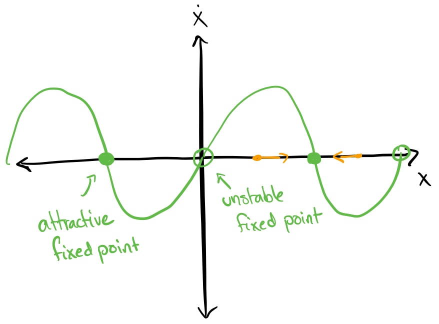
$$\frac{dx}{dt} = \sin(x)$$

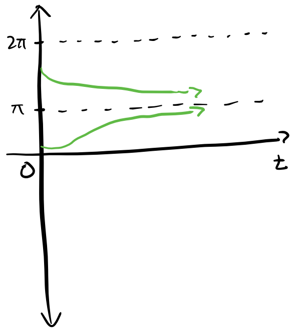
$$dt = \frac{dx}{\sin x}$$

$$t = \ln\left|\tan\left(\frac{x}{2}\right)\right| + C$$

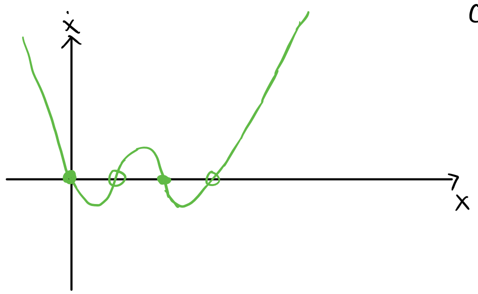
$$= \ln\left|\frac{\tan(x/2)}{\tan(x_0/2)}\right|$$

Alternatively →





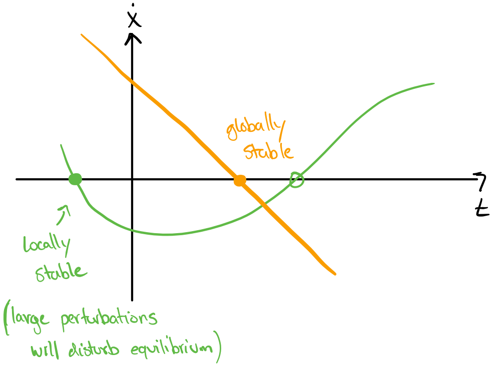
Consider $\dot{x} = x(x-1)(x-2)(x-3)$



Phase Portrait

Crossing from pos − neg implies stable fixed point

Locally vs. globally stable fixed points



Initial Value ODE

$$\frac{du}{dt} = au \qquad u = u_0 \text{ @ } t = 0$$

$$u(t) = u_0 e^{at}$$

Three schema to solve initial value ODE's

- finite difference → approximate soln using a finite set of points
- finite element
- spectral

} approximate solution using a finite set of solutions

↖ trig functions

Finite Difference

Estimate $\frac{du}{dt} \approx \frac{u(t+\Delta t) - u(t)}{\Delta t}$

$$u(t+\Delta t) = \frac{du}{dt} \cdot \Delta t + u(t)$$

Lecture 3

Important considerations in numerical methods

- Stability
- Accuracy
- Efficiency

Suppose we have the ODE $\frac{du}{dt} = au$ with initial value $u(0) = u_0$

Analytically $\rightarrow$ $u(t) = u_0 e^{at}$

Finite Difference (Forward Euler's Method)

$$\frac{U(t+\Delta t) - U(t)}{\Delta t} = aU$$

$$\frac{U_{n+1} - U_n}{\Delta t} = a U_n$$

n is the number of time steps

$$U_{n+1} = U_n + a\Delta t U_n$$

$$= (1 + a\Delta t) U_n \longrightarrow U_n = (1 + a\Delta t)^n U_0$$

growth factor

$$= \left(1 + \frac{at}{n}\right)^n U_0 \xrightarrow[n \to \infty]{} e^{at} U_0$$

We require $|G| < 1$ for a stable integration

$$\longrightarrow \Delta t < \frac{2}{|a|}$$

Finite Difference via Euler's Method

forward : $\frac{U_{n+1} - U_n}{\Delta t} = aU_n$

backward : $\frac{U_n - U_{n-1}}{\Delta t} = a U_n$

$$\longrightarrow U_n = \frac{1}{1 - a\Delta t} U_{n-1}$$

$|G| < 1$ for $Re(a) < 0$

absolute stability

Consider a general ODE : $\frac{du}{dt} = f(t, u)$

contains information we know

Forward Euler : $U_n = U_{n-1} + \Delta t\, f(t_{n-1}, U_{n-1})$

explicit time-stepping

Backward Euler : $U_n - \Delta t\, f(t_n, U_n) = U_{n-1}$

implicit time-stepping

Explicit time-stepping methods often have time-step conditions for stability

Implicit time-stepping methods are often A-stable but at the cost of computability

Accuracy of Euler's Method

$$U(t) = U(0) + U'(t) + \frac{1}{2} U''(t)^2 + \cdots$$

$$U(\Delta t) = U(0) + U'(\Delta t) + \frac{1}{2} U''(\Delta t)^2 + \cdots$$

$$\longrightarrow \frac{U(\Delta t) - U(0)}{\Delta t} = U' + \underbrace{\frac{1}{2} U'' \Delta t + \cdots}_{\text{Approximation error}} \propto O(\Delta t)$$

order 1 method

Methods to Improve Error

1. Multistep Method

$$\frac{U_{n+1} - U_n}{\Delta t} = \alpha f(t_n, U_n) + \beta f(t_{n-1}, U_{n-1})$$

$$\frac{U_{n+1} - U_n}{\Delta t} = U' + \frac{1}{2} \Delta t\, U'' + O(\Delta t^2)$$

We know $f_n = f(t_n, u_n) = u'(n\Delta t)$

$$f_{n-1} = u'((n-1)\Delta t)$$

$$= u'(n\Delta t) - \Delta t\, u'' + \frac{1}{2}(\Delta t)^2 u''' + \dots$$

$$\alpha f_n + B f_{n-1} = (\alpha + B)\, u'(n\Delta t) - B\,\Delta t\, u'' + O(\Delta t^2)$$

$$\alpha + B = 1$$

$$B = -1/2 \;\longrightarrow\; \alpha = 3/2$$

$$u_{n+1} = u_n + \Delta t\left(\frac{3}{2} f_n - \frac{1}{2} f_{n-1}\right)$$

↳ predictor-corrector method for PDE

2. Runge-Kutta

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{1}{2}\left[f(t_n, u_n) + f(t_{n+1}, u_n + \Delta t\, f(t_n, u_n))\right]$$

Average of current value and estimated next value

Runge-Kutta can be extrapolated to a 4th order R-K method

Tests when using numerical solvers

1. Benchmark test
   - Test a problem with a known solution
   - Use this test to understand the limitations/parameters of the code
2. Convergence test

Lecture 4

Multistep

$$\frac{u_{n+1} - u_n}{\Delta t} = u' + \frac{1}{2}\Delta t\, u'' + O(\Delta t^2) \quad \leftarrow \text{taylor expansion}$$

$$u_{n+1} = u_n + \Delta t\; u'$$

$\nwarrow$ $\frac{3}{2} f_n - \frac{1}{2} f_{n-1}$

$$u' = f(t, u)$$

$\nearrow$ $\frac{du}{dt}$

$$f_n = u'(n\Delta t)$$

$\swarrow$ $-dt$

$$f_{n-1} = u'((n-1)\Delta t) \underset{\text{taylor expansion}}{=} u'(n\Delta t) - \Delta t\, u'' + \frac{1}{2}(\Delta t)^2 u''' + \dots$$

1-D dynamical systems

Three step analysis

1. Identify steady state solutions $\left(\frac{d}{dt} = 0 \text{ or } \frac{\partial}{\partial t} = 0\right)$
2. Determine stability of solutions
   Linear stability analysis
3. Move on to finite amplitude analysis
   Numerical Integration

Suppose x^* is a fixed point

$$\eta(t) = x(t) - x^* \quad \leftarrow \text{small perturbation from } x^*$$

$$\dot{\eta}(t) = \frac{d}{dt} x(t)$$

$$= \dot{x} = f(x)$$

$$= f(x^* + \eta) \quad \swarrow \text{apply } x(t) = \eta(t) + x^*$$

taylor expansion

$$= \underbrace{f(x^*)}_{=0} + \eta f'(x^*) + O(\eta^2)$$

$$\dot{\eta} = \eta f'(x^*) + O(\eta^2)$$

if $f'(x^*) \neq 0$

$$\dot{\eta} = \eta f(x^*)$$

growth exponent

$$\dot{u} = au \longrightarrow \eta(t) \propto \exp\left(f'(x^*)t\right)$$

$f'(x^*) < 0 \longrightarrow x^*$ is stable fixed point

$= 0 \longrightarrow x^*$ is a neutral fixed point

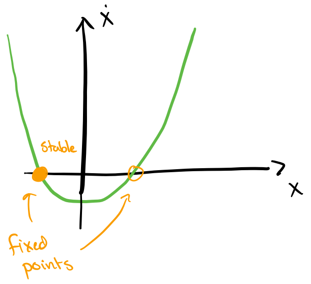
$> 0 \longrightarrow x^*$ is an unstable fixed point

$|f'(x^*)|$ tells us the degree of stability

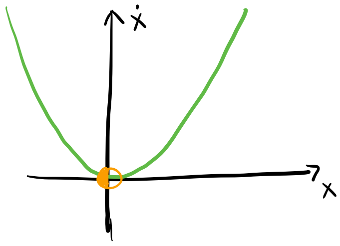
$\frac{1}{|f'(x^*)|}$ is the characteristic time scale (time required to vary significantly in the neighboor hood of x^*)

Consider $\dot{x} = r + x^2$

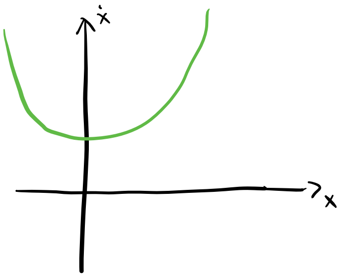
$r < 0$



$r = 0$

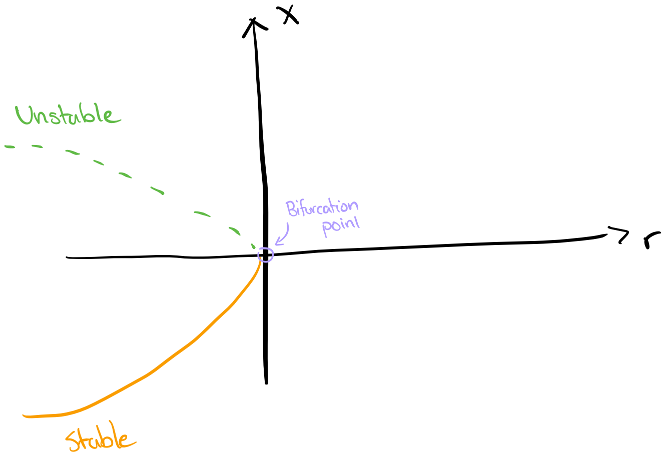


$r > 0$

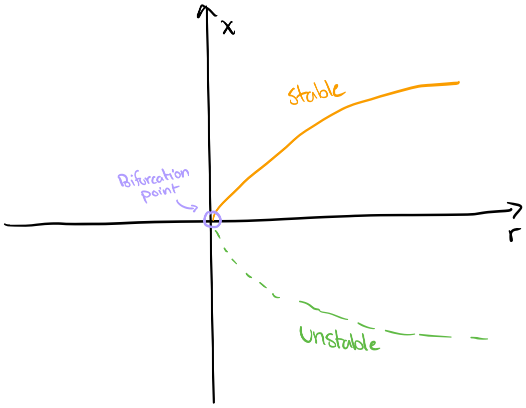


Saddle-Node Bifurcation

$\dot{x} = r + x^2$



$\dot{x} = r - x^2$



$$\dot{x} = f(x, r)$$

$$= \underbrace{f(x^*, r_c)}_{=0} + (x - x^*) \underbrace{\frac{\partial f}{\partial x}\bigg|_{x^*, r_c}}_{\substack{0 \\ \text{must be } 0 \\ \text{when bifurcation} \\ \text{takes place}}} + (r - r_c) \frac{\partial f}{\partial r}\bigg|_{x^*, r_c} + \frac{1}{2}(x - x^*)^2 \frac{\partial^2 f}{\partial x^2}\bigg|_{x^*, r_c} + \underbrace{\frac{1}{2}(r - r_c)^2 \frac{\partial^2 f}{\partial r^2}\bigg|_{x^*, r_c} + \frac{1}{2}(r - r_c)(x - x^*) \frac{\partial^2 f}{\partial r \partial x}}_{\text{ignore since they are } 2^{nd} \text{ order terms}}$$

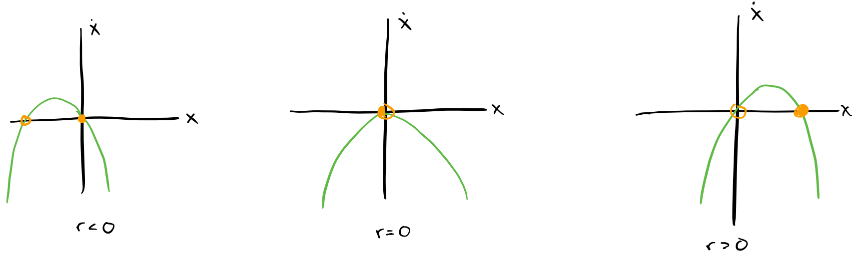
taylor expansion

$$= a(r - r_c) + b(x - x^*)^2$$

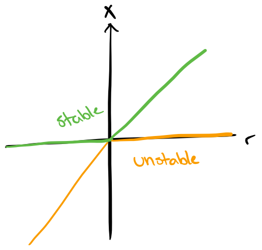
Lecture 5

Transcritical Bifurcation

normal form : $\dot{x} = rx - x^2$



Position of fixed point by r



$$\dot{x} = rx\left(1 - \frac{x}{K}\right)$$
$$= rx - \frac{r}{K}x^2$$
$$= \frac{r}{K}(Kx - x^2)$$

$r > 0,\ K > 0$

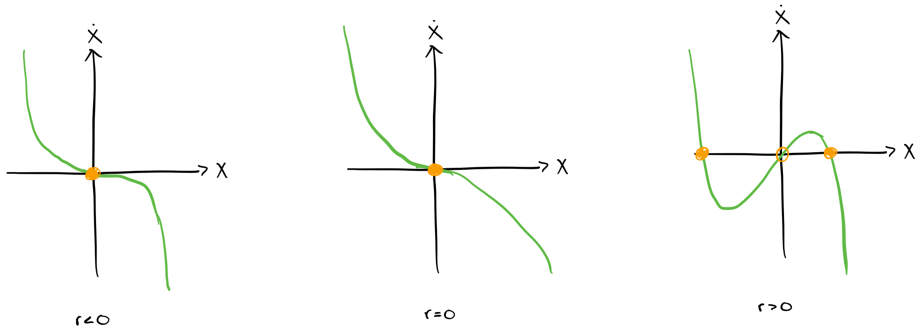
$$\dot{x} = \underbrace{rx(1-x)}_{\text{resource growth}} - \underbrace{px}_{\text{consumption}}$$
$$= r\left(\frac{r-p}{r}x - x^2\right)$$

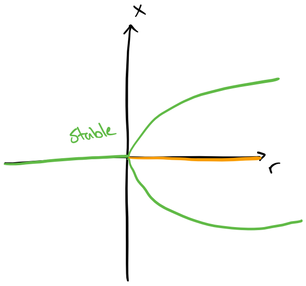
SIS model

Supercritical pitchfork bifurcation

normal form : $\dot{x} = rx - x^3$

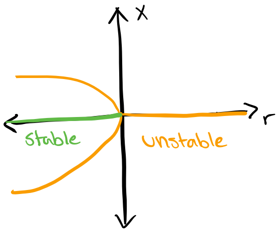
invariant over reflective symmetry $(x = -x)$





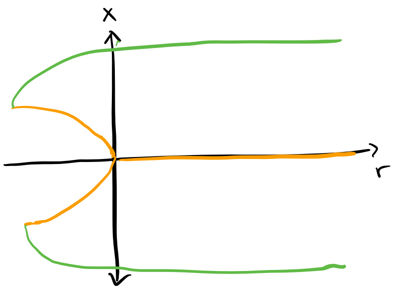
Subcritical Pitchfork bifurcation

normal form : $\dot{x} = rx + x^3$ (reflectionally invariant)



Usually implies higher order structure

For example : $\dot{x} = rx + x^3 \longrightarrow \dot{x} = rx + x^3 - x^5$



System exhibits hysteresis

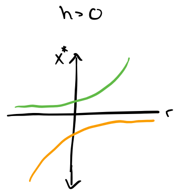
Imperfect Bifurcation

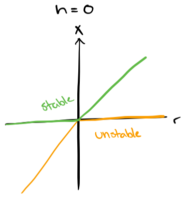
$\underbrace{\dot{x} = rx - x^2}_{\text{transcritical}} + h$ ← perturbation

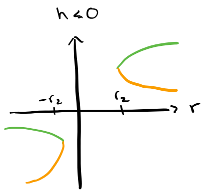
$\dot{x} = 0 \longrightarrow x^* = \frac{1}{2}\left(r \pm \sqrt{r^2 + 4h}\right)$

$r^2 + 4h \geq 0$

$\longrightarrow r^2 \geq -4h$







$$\dot{x} = f(x,r) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{m!n!} \frac{\partial^{m+n}}{\partial x^m \partial r^n} \frac{\partial^{m+n}}{\partial x^m \partial r^n} \Bigg|_{x^*, r_c} (x - x^*)^m (r - r_c)^n$$

taylor expansion

$$= \underbrace{f(x^*, r_c)}_{\substack{0 \\ \text{fixed point}}} + \underbrace{f_x(x^*, r_c)}_{\substack{0 \\ \text{tangential condition}}}(x - x^*) + f_r(x^*, r_c)(r - r_c) + \frac{1}{2} f_{xx}(x^*, r_c)(x - x^*)^2 + \dots$$

ignore higher order terms

transition from stable to unstable requires passage through 0

Additional Conditions yield other bifurcation types

① $f_r \neq 0, f_{xx} \neq 0 \longrightarrow \dot{x} = rx + x^2$ (Saddle node)

② Add $f(0,r) = 0 \longrightarrow \dot{x} = rx + x^2$ (transcritical)

③ Add $f(0,r) = 0$ and $f(-x,r) = f(x,r) \longrightarrow \dot{x} = r \pm x^3$ (pitchfork)

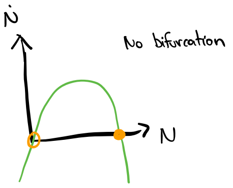
Lecture 6

Population Dynamics

① $\dot{N} = RN \quad R > 0$

② $\dot{N} = RN\left(1 - \frac{N}{K}\right)$ ← logistic model

carrying capacity



growth rate

harvesting rate

③ $\dot{N} = RN\left(1 - \frac{N}{K}\right) - H(N) - (H_0)$

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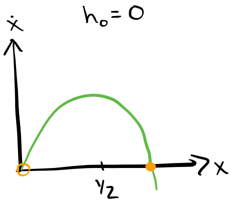
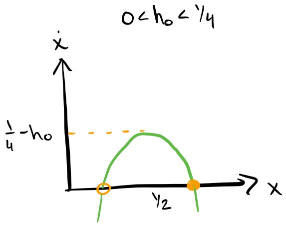
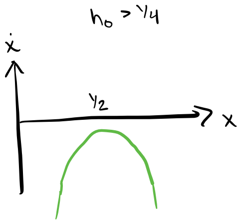
Nondimensionalization (reduce dimensionality)

$x = \frac{N}{K}, \quad t' = Rt, \quad h = \frac{H}{RK}$

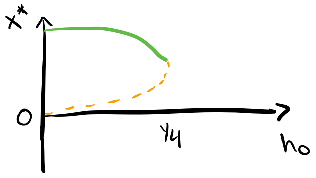
$\dot{x} = x(1-x) - h_0$ ← rewriting with one variable





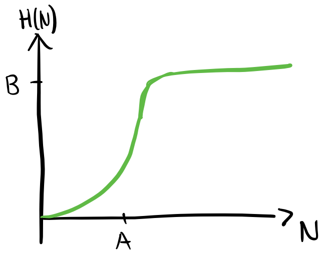


Saddle-Node



Insect Outbreak Model

$$H(N) = \frac{BN^2}{A^2+N^2} \quad (A, B > 0)$$



$$\dot{N} = RN\left(1-\frac{N}{K}\right) - \frac{BN^2}{A^2+N^2}$$

$$\dot{x} = x(1-x) - \frac{1}{RK}\,\frac{BK^2x^2}{A^2+K^2x^2}$$

$$t' = \frac{Bt}{A}, \quad x = \frac{N}{A}, \quad r = \frac{RA}{B}, \quad k = \frac{K}{A} \longleftarrow$$ Buckingham π algorithm

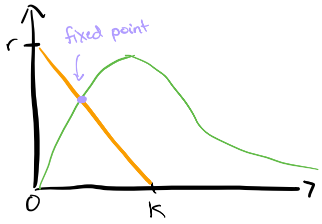
$$\dot{x} = rx\left(1-\frac{x}{k}\right) - \frac{x^2}{1+x^2}$$

Solving for fixed points

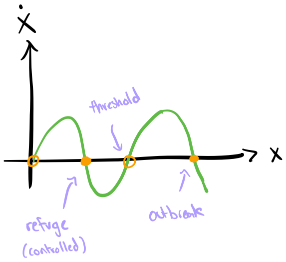
$$\dot{x} = 0 \Rightarrow$$

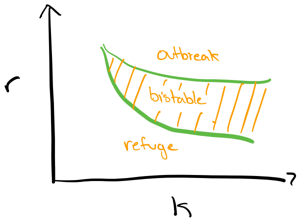
$$x\left[r\left(1-\frac{x}{k}\right) - \frac{x}{1+x^2}\right] = 0$$

$$x = 0 \quad \text{or} \quad r(1-x/k) = \frac{x}{1+x^2}$$



Depending on slope of the line we transition from 1→2→3→2→1





Lecture 7

Code Structure for Agent modeling

① Initial set up

② Iteration

③ Ending

Setup Variables

- Domain size
- Population size
- Initial infections
- Time for recovery
- time steps

Define at beginning

Infection occurs when susceptible and infected agents occupy the same location

Review of Linear Algebra

$$\frac{d\vec{x}}{dt} = f(\vec{x})$$

$$\approx Ax + b \leftarrow \text{first order taylor expansion}$$

$$A = [a_{ij}] \text{ where } a_{ij} = \left.\frac{\partial f_i}{\partial x_i}\right|_{x=x_0}$$

$$b = f(x_0)$$

Consider the initial value problem

$$\frac{dv}{dt} = 4v - 5w$$

$$\text{w/ } V(0) = V_0 \text{ and } W(0) = W_0$$

$$\frac{dw}{dt} = 2v - 3w$$

$$\text{Let } \vec{u} = \begin{bmatrix} v \\ w \end{bmatrix}, \quad \frac{du}{dt} = A\vec{u} \quad \text{where } A = \begin{bmatrix} 4 & -5 \\ 2 & -3 \end{bmatrix}$$

Can we find a,b and λ s.t.

$$\frac{d}{dt}(av + bw) = \lambda(av + bw)$$

$$U = av + bw \implies \frac{dU}{dt} = \lambda U \longrightarrow U = U(0)\exp(\lambda t)$$

$$a\frac{dv}{dt} + b\frac{dw}{dt} = a(4v - 5w) + b(2v - 3w)$$

$$= (4a + 2b)v + (-5a - 3b)w$$

$$= \lambda a v + \lambda b w$$

Requires

$$\begin{aligned} \lambda a &= 4a + 2b \\ \lambda b &= -5a - 3b \end{aligned} \longrightarrow \begin{bmatrix} 4 & 2 \\ -5 & 3 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \lambda \begin{bmatrix} a \\ b \end{bmatrix}$$

eigenvalue problem!

Lecture 8

For the system studied previously,

$$a_1\frac{dv}{dt} + b_1\frac{dw}{dt} = \lambda_1(a_1 v + b_1 w)$$

$$a_2\frac{dv}{dt} + b_2\frac{dw}{dt} = \lambda_2(a_2 v + b_2 w)$$

$$\underbrace{\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix}}_{T} \underbrace{\begin{bmatrix} \frac{dv}{dt} \\ \frac{dw}{dt} \end{bmatrix}}_{\dot{\vec{u}}} = \underbrace{\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}}_{\Lambda} \underbrace{\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix}}_{T} \underbrace{\begin{bmatrix} V \\ W \end{bmatrix}}_{\vec{u}}$$

$$\text{Suppose } \vec{U} = T\vec{u}$$

$$\dot{\vec{U}} = \Lambda \vec{U}$$

Function of a matrix

Always defined via taylor series expansion

E.g. $\exp(tA)$

$$e^{tA} = I + tA + \frac{1}{2!}(tA)^2 + \dots$$

Properties of exponential Matricies

① $e^{sA} e^{tA} = e^{(s+t)A}$

② $e^{tA} e^{-tA} = I$

③ $\frac{d}{dt} e^{tA} = Ae^{tA}$

Consider the eigenvalue decomposition of A

$A = S \Lambda S^{-1}$

$A^k = S \Lambda^k S^{-1}$

Suppose $\frac{du}{dt} = A\vec{u}$ w/ $u(0)$

$\vec{u} = e^{tA} \vec{u}(0)$

$= Se^{t\Lambda} S^{-1} \vec{u}(0)$

Nonnormal Matricies

$\dot{\vec{u}} = A\vec{u}$

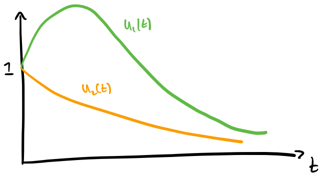
$A = \begin{bmatrix} -1 & 5 \\ 0 & -2 \end{bmatrix}$ $\vec{u}(0) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$= S \Lambda S^{-1}$

$$S = \begin{bmatrix} 1 & -0.9806 \\ 0 & 0.1961 \end{bmatrix} \quad \Lambda = \begin{bmatrix} -1 & 0 \\ 0 & -2 \end{bmatrix}$$

x_1 x_2

$$u(t) = S \begin{bmatrix} e^{-t} & 0 \\ 0 & e^{-2t} \end{bmatrix} S^{-1} \vec{u}(0)$$



← behavior is due to unequal decay rates of u_1 and u_2 and the coordinate transformation to u_1, u_2

Lecture 9

Linear Systems in 2-D

Rotation is now possible

Consider

$\dot{\vec{x}} = A\vec{x}$

$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ $\vec{x} = \begin{pmatrix} x \\ y \end{pmatrix}$

Linear Spring

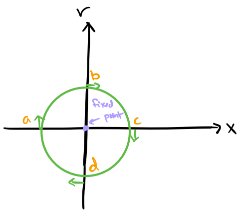
$m\ddot{x} + kx = 0$

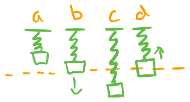
$\dot{x} = v$

$\dot{v} = -\frac{k}{m}x = -w^2 x$

$w = \sqrt{k/m}$

We can look at $(\dot{x}, \dot{v})$





$X_0 = V_0 = 0$ ← system is stationary

$X_0 \neq 0$ or $V_0 \neq 0$ ← system rotates in phase plane

We refer to fixed points of this type as closed orbit

implies periodic motion

In terms of linear algebra

$$\begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -w^2 & 0 \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix}$$

$$\det(A-\lambda I) = \begin{vmatrix} a-\lambda & b \\ c & d-\lambda \end{vmatrix} = 0$$

$$\lambda^2 - \tau\lambda + \Delta = 0$$

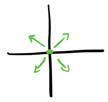
$$\tau = tr(A)$$

$$\Delta = \det(A)$$

$$\lambda_{1,2} = \frac{\tau \pm \sqrt{\tau^2 - 4\Delta}}{2}$$

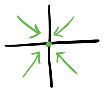
$\tau^2 - 4\Delta > 0$ ⟶ real eigen values

Case 1: Both positive



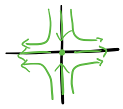
two dimensional
analog of unstable fixed point

Case 2: Both negative



two dimensional
analog of stable fixed point

Case 3: 1 positive, 1 negative



Saddle fixed point

$\tau^2 - 4\Delta < 0$ ⟶ complex eigenvalues

$$\lambda_{12} = \frac{\tau \pm i\omega}{2} \qquad \omega = \sqrt{4\Delta - \tau^2}$$

For our original example

$$\tau = 0$$

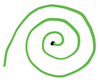
$$\Delta = \omega^2$$

$$\lambda_{1,2} = \pm i\omega$$

$\tau = 0$

center

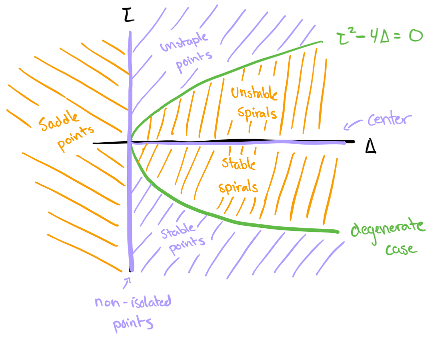
$\tau < 0$



Stable spiral

$\tau > 0$

Unstable spiral



Lecture 10

General 2-D Systems

$$\begin{cases} \dot{x}_1 = f_1(x_1, x_2) \\ \dot{x}_2 = f_2(x_1, x_2) \end{cases}$$

Existence and Uniqueness Theorem

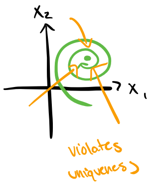
For an initial value problem $\dot{\vec{x}} = \vec{f}(\vec{x})$ w/ $\vec{X}(0) = X_0$,

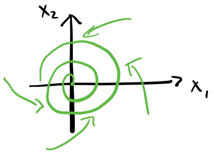
if $\vec{f}$ and all of its partial derivatives are continuous in an open + connected set

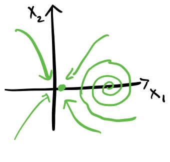
then, the IVP has a solution X(t) on some time interval $(-\tau, \tau)$ about 0.

Furthermore, X(t) is unique.

Consider the following 2-D phase portraits







Limit cycles are defined by isolated closed trajectory

Consider a perturbation of a general 2-D system

$$\dot{x} = f(x,y)$$
$$y = g(x,y)$$

$$u = x - x^*, \quad v = y - y^*$$

$$\dot{u} = \dot{x} = f(x^*+u, y^*+v)$$

Taylor Expansion

$$= \underbrace{f(x^*,y^*)}_{\text{0 bc fixed point}} + u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} + O(u^2, v^2, uv)$$

$$\dot{v} = \frac{u\partial g}{\partial x} + v\frac{\partial g}{\partial y}$$

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} \frac{\partial f}{dx} & \frac{\partial f}{\partial y} \\ \frac{\partial g}{dx} & \frac{\partial g}{\partial y} \end{pmatrix}\Bigg|_{(x^*,y^*)} \begin{pmatrix} u \\ v \end{pmatrix} + (\text{higher order terms})$$

Jacobian

① Competitive Lotka - Volterra Model (rabbit and sheep)

$$\dot{x} = x(3-x-2y) = 3x\left(1 - x/3\right) - 2xy \quad \leftarrow \text{Rabbit}$$
$$\dot{y} = y(2-x-y) = 2y\left(1 - y/2\right) - xy \quad \leftarrow \text{Sheep}$$

growth rate ↗ ↑ carrying capacity ↖ competition

1. Fixed Points

$\dot{x} = \dot{y} = 0$

$\rightarrow (0,0), (0,2), (3,0), (1,1)$

2. Jacobian

$$J = \begin{pmatrix} 3-2x-2y & -2x \\ -y & 2-x-2y \end{pmatrix}$$

@ (0,0)

$$J = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$$

$\tau = 5$

$\Delta = 6$

Unstable fixed point

@ (0,2)

$$J = \begin{pmatrix} -1 & 0 \\ -2 & -2 \end{pmatrix}$$

$\tau = -3$

$\Delta = 2$

Stable fixed point

@ (3,0)

$$J = \begin{pmatrix} -3 & -6 \\ 0 & -1 \end{pmatrix}$$

$\tau = -4$

$\Delta = 3$

Stable fixed point

@ (1,1)

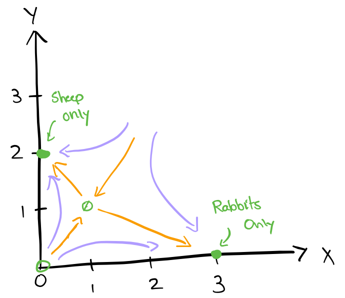
$$J = \begin{pmatrix} -1 & -2 \\ -1 & -1 \end{pmatrix}$$

$\tau = -2$

$\Delta = -1$

Saddle point

(need to find eigenvectors to fully characterize point)



Lecture 11

Non-linear 2-D Systems

$$\begin{cases} \dot{x} = f(x,y) \\ \dot{y} = g(x,y) \end{cases}$$

① Find fixed points

② Linear Stability Analysis

$$J = \begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix}\Bigg|_{x^*,y^*}$$

Lotka-Volterra predator-prey model

$$\dot{x} = ax - bxy \qquad a,b,c,d > 0$$
$$\dot{y} = cxy - dy$$

$x \leftarrow$ prey

$y \leftarrow$ predator

We can rewrite our equations

$$\dot{x} = ax\left(1 - \frac{b}{a}y\right)$$
$$y = cy\left(x - \frac{d}{c}\right)$$

① Find Fixed points

$x = y = 0$

$x = d/c \,,\; y = a/b$

② Jacobian

$$J = \begin{pmatrix} a-by & -bx \\ cy & cx-d \end{pmatrix}$$

$x = y = 0$

$$J_1 = \begin{pmatrix} a & 0 \\ 0 & -d \end{pmatrix}$$

↖ Saddle-point

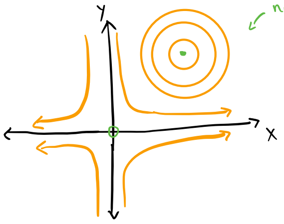
$x = d/c \,,\; y = a/b$

$$J_2 = \begin{pmatrix} 0 & -\frac{bd}{c} \\ \frac{ac}{b} & 0 \end{pmatrix}$$

$T = 0 \qquad \Delta = ad > 0$

Center

③ Phase Portrait



↙ not necessarily circular

Lyapunov Stability

① Local Stability ← Similar to linear stability analysis

② Global Stability

$$\frac{dx}{dt} = x(a-by) \qquad \frac{dy}{dt} = y(cx-d)$$

$$\frac{x(a-by)}{dx} = \frac{1}{dt} = \frac{y(cx-d)}{dy}$$

$$\frac{a-by}{y}\,dy = \frac{(cx-d)}{x}\,dx$$

Integrating each side

$$a\ln y - by = cx - d\ln x + C$$

$$C = a\ln y - by - cx + d\ln x$$

↖ Conservative System

SIR - model

susceptible, infected, recovered

$$\dot{S} = -\underset{\substack{\uparrow \\ \text{infection} \\ \text{rate}}}{\mu} IS$$

$$\dot{I} = \mu IS - \overset{\substack{\text{recovery} \\ \text{rate} \\ \swarrow}}{\alpha} I$$

$$\dot{R} = \alpha I$$

$$M = S + I + R$$

① Fixed points

$\dot{S} = \dot{I} = 0$

$$\begin{cases} IS = 0 \\ \mu IS = \alpha I \end{cases}$$

$I^{*} = 0$

$S^{*} =$ anything > 0

② Jacobian

$$J = \begin{pmatrix} -\mu I & -\mu S \\ \mu I & \mu S - \alpha \end{pmatrix} \Bigg|_{I^*, S^*} = \begin{pmatrix} 0 & -\mu S^* \\ 0 & \mu S^* - \alpha \end{pmatrix}$$

$\tau = \mu S^* - \alpha$

$\Delta = 0$

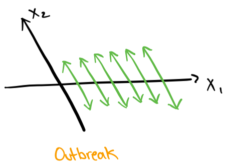
$\lambda = 0, \tau$

$\lambda_1 = 0, \quad x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

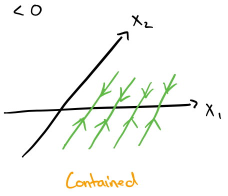
$\lambda_2 = \tau, \quad \vec{x}_2 = \begin{bmatrix} 1 \\ \frac{\alpha}{\mu S^*} - 1 \end{bmatrix}$

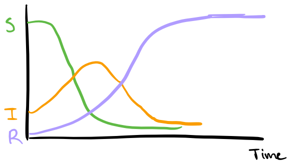
$\frac{-\tau}{\mu S^*}$

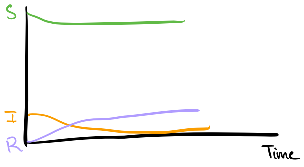
$\tau > 0$



$\tau < 0$







No steady state in the model

Lecture 12

Bifurcations in 2-D systems

- Saddle Node (zero eigenvalue Bifurcation)

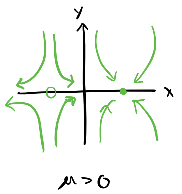
$\dot{x} = \mu - x^2$

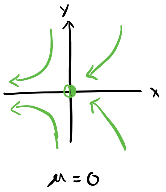
$\dot{y} = -y$

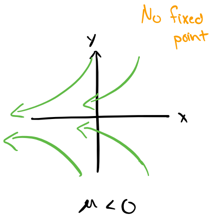
$\xrightarrow{\text{fixed points}} (x^*, y^*) = (\pm\sqrt{\mu}, 0)$

w/ $\mu > 0$

$J = \begin{pmatrix} -2x & 0 \\ 0 & -1 \end{pmatrix}$





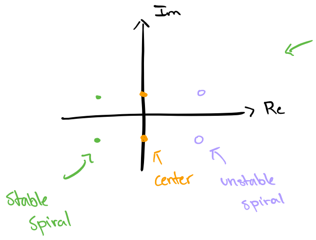


- Pitchfork

$\lambda_{1,2} = \frac{1}{2}\left(\tau \pm \sqrt{\tau^2 - 4\Delta}\right)$

$\tau = tr(A)$

$\Delta = det(A)$



← Hopf Bifurcation

Supercritical Hopf Bifurcation

Bifurcation parameter

normal form : $\dot{r} = \mu r - r^3$

$\dot{\theta} = w + br^2$

fixed points : $r = 0, \pm\sqrt{\mu}$ $(\mu > 0)$

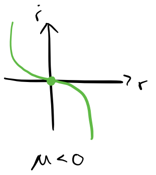
$\downarrow$ $w = 0$ $\quad$ $\downarrow$ $w = -b\mu$ ← satisfy $\dot{\theta} = w + br^2$

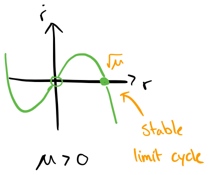
Converting to Cartesian

$\dot{x} = \mu x - wy$

$\dot{y} = wx + \mu y$

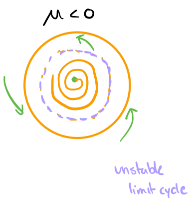
$\longrightarrow A = \begin{pmatrix} \mu & -w \\ w & \mu \end{pmatrix} \quad \lambda = \mu \pm iw$

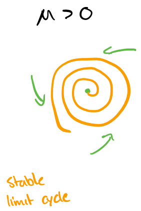




Subcritical Hopf Bifurcation

$$\dot{r} = \mu r + r^3 - r^5$$
$$\dot{\theta} = \omega + br$$





Lecture 13

Liénard Theorem

$$\frac{d^2x}{dt^2} + f(x)\frac{dx}{dt} + g(x) = 0$$

if

① $g(x) > 0$ for all $x > 0$

② $\lim_{x \to \infty} F(x) = \lim_{x \to \infty} \int_0^x f(s)\,ds = \infty$

③ $F(x)$ has exactly one positive root at some value p and $F(x) < 0$ for $0 < x < p$ and $F(x) >$ and monotonic for $x \geq p$

Then the system exhibits a limit cycle

Van der Pol Oscillator ← Obeys Lienard's Theorem

$$\frac{d^2x}{dt^2} - \epsilon(1-x^2)\frac{dx}{dt} + x = 0 \qquad \epsilon > 0$$

$$\begin{cases} \dot{x} = \epsilon(x - \tfrac{1}{3}x^3) - y \\ \dot{y} = x \end{cases}$$

reduces to harmonic oscillator when $\epsilon = 0$

$$\ddot{x} = \epsilon(\dot{x} - x^2 \dot{x}) - \dot{y}$$
$$= \epsilon(1-x^2)\dot{x} - x$$

Fixed Points

$$J = \left.\begin{pmatrix} \epsilon(1-x^2) & -1 \\ 1 & 0 \end{pmatrix}\right|_{(0,0)} = \begin{pmatrix} \epsilon & -1 \\ 1 & 0 \end{pmatrix}$$

$\tau = \epsilon \quad \Delta = 1$

Applying Lienard Transformation

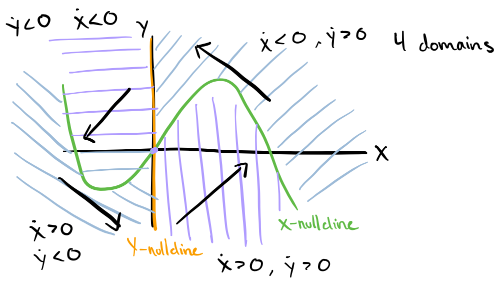
$$y = x - \frac{x^3}{3} - \dot{x}/\epsilon$$

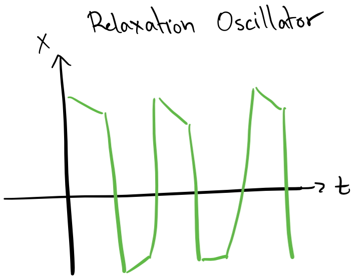
$$\begin{cases} \dot{x} = \epsilon(x - \tfrac{1}{3}x^3 - y) \\ \dot{y} = x/\epsilon \end{cases}$$

Null clines

$\dot{x} = 0 \longrightarrow y = x(1 - x^3/3)$ ← x-nullcline

$\dot{y} = 0 \qquad x = 0$ ← y-null cline





Lecture 14

Brusselator

A,B present in abundance

X,Y catalysts

① $A \rightarrow X$

② $B + X \rightarrow Y + D$

③ $2X + Y \rightarrow 3X$ ← auto catalytic reaction

④ $X \rightarrow C$

Rate Equations

$$[\dot{X}] = \underset{\textcircled{1}}{[A]} + \underset{\textcircled{2}}{[X]^2[Y]} - \underset{\textcircled{3}}{[B][X]} - \underset{\textcircled{4}}{[X]}$$

$$[\dot{Y}] = [B][X] - [X]^2[Y]$$

2-D Dynamical System

$$\dot{x} = a + \dot{x}^2 y - bx - x$$

$$\dot{y} = bx - x^2 y$$

① Fixed Points

$$(x^*, y^*) = (a, b/a)$$

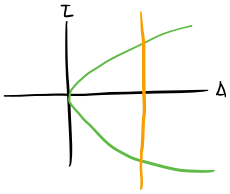
② Linear Stability Analysis

$$J = \begin{pmatrix} 2xy - b - 1 & x^2 \\ b - 2xy & -x^2 \end{pmatrix} \Bigg|_{(a,b/a)} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix}$$

$$\tau = b - 1 - a^2$$

$$\Delta = -a^2 b + a^2 + ba^2 = a^2$$

$$\lambda_{12} = \frac{\tau \pm \sqrt{\tau^2 - 4\Delta}}{2}$$



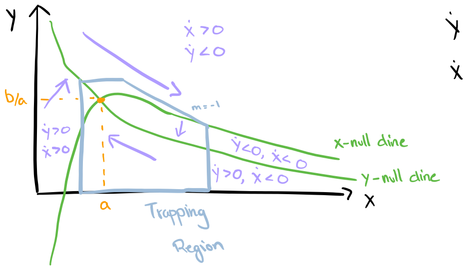
Poincare – Bendixson Theorem

Given a 2-D dynamical system $\dot{x} = f(x)$. If $x(t)$ is a solution that stays in a bounded region, $x(t)$ converges to an equilibrium point ($f(x) = 0$) or to a single periodic cycle as $t \rightarrow \infty$

Null Clines of Brusselator

$$\dot{x} = 0 \Rightarrow y = \frac{x + bx - a}{x^2}$$

$$\dot{y} = 0 \Rightarrow y = b/x$$



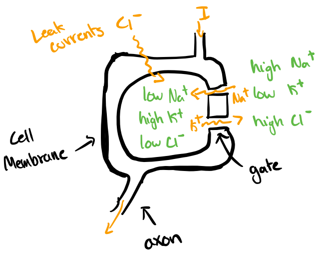
$\dot{y} < 0$ when we are above y-null cline

$\dot{x} > 0$ when we are above x-null cline

Lecture 15

Biological Neuron Model

Hodgkin-Huxley Model (1952)



Original model is 4-D

Simplified Persistent Sodium and Potassium Model

$$C\dot{V} = I - \underbrace{g_L(V-E_L)}_{\text{leaky current}} - \underbrace{g_{Na}\, m_\infty(V)\,(V-E_{Na})}_{\text{Na - diffusion}} - \underbrace{g_K n (V-E_K)}_{\text{K - diffusion}}$$

$$\dot{n} = \frac{n_\infty(V) - n}{I(V)}$$

g_L, g_{Na}, g_K are constants of the cell

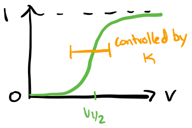
I is a bifurcation parameter

V is membrane voltage

E_L, E_{Na}, E_K are constants of the cell (Nernst Equilibrium Potential)

C is conductance of the cell

$$m_\infty(V) = \frac{1}{1+\exp\left(\frac{V_{1/2}-V}{K}\right)}$$ "activation function"



$$n_\infty(V) = \frac{1}{1+\exp\left(\frac{V_{1/2}-V}{K}\right)}$$ "activation function"

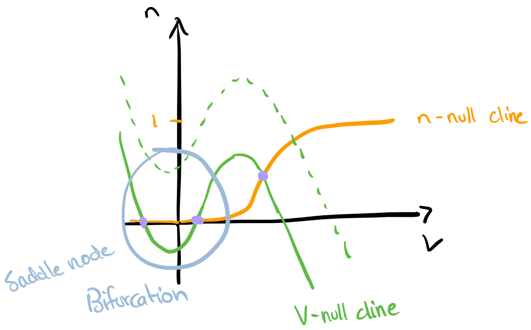
$$I(V) = C_{base} + C_{amp}\exp\left(\frac{-(V_{max}-V)^2}{\sigma^2}\right)$$ ← response to time scale

No analytic solutions for fixed point, instead we solve for null clines and find their intersections

Null Clines

$\dot{n} = 0 \longrightarrow n = n_\infty(V)$

$\dot{V} = 0 \longrightarrow n = \dfrac{I - g_L(V-E_L) - g_{Na}\, m_\infty(V)(V-E_{Na})}{g_K(V-E_K)}$



Finite Difference Method of Linear Stability Analysis

$$J = \left.\begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix}\right|_{(x^*,y^*)}$$

$\uparrow$

$$\left.\frac{\partial g}{\partial x}\right|_{x^*,y^*} \approx \frac{f(x^*+\Delta x, y^*) - f(x^*,y^*)}{\Delta x}$$

Finite difference

Don't need to calculate Jacobian anymore

Lecture 16

2-D Fixed points

$\lambda_1, \lambda_2 \neq 0$ ← ignoring degeneracies

1. $\lambda_1 < 0,\ \lambda_2 < 0$ Stable
2. $\lambda_1 > 0,\ \lambda_2 < 0$ Saddle point
3. $\lambda_1 > 0,\ \lambda_2 > 0$ Unstable point
4. $Re(\lambda_1) < 0,\ \lambda_2 = \lambda_1^*$ Stable spiral
5. $Re(\lambda_1) > 0,\ \lambda_2 = \lambda_1^*$ Unstable spiral

3-D fixed points ← Ignoring 0 and degenerate cases

1. $0 > \lambda_1 > \lambda_2 > \lambda_3$ stable fixed point
2. $\lambda_1 > 0 > \lambda_2 > \lambda_3$ Saddle point (+ − −) line divergence
3. $\lambda_1 > \lambda_2 > 0 > \lambda_3$ Saddle point (++−) plane divergence
4. $\lambda_1 > \lambda_2 > \lambda_3 > 0$ unstable fixed point
5. $0 > \lambda_1 > Re(\lambda_2, \lambda_3)$ or $0 > Re(\lambda_1, \lambda_2) > \lambda_3$ Stable Spiral spiral plane + convergent to plane
6. $\lambda_1 > 0 > Re(\lambda_2, \lambda_3)$ Spiral - Saddle (+ − −) spiral plane + divergent to plane
7. $Re(\lambda_1, \lambda_2) > 0 > \lambda_3$ Spiral - Saddle (++−) Unstable spiral plane + convergent to plane
8. $\lambda_1 > Re(\lambda_2, \lambda_3) > 0$ or $Re(\lambda_1, \lambda_2) > \lambda_3 > 0$ Unstable Plane

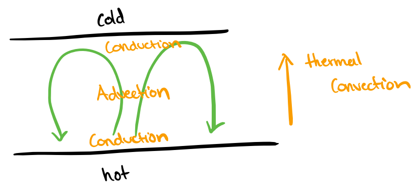
Lorenz System

known for exhibiting deterministic chaos

$$\frac{dX}{dt} = f(X)$$

$$\begin{cases} \dot{x} = \sigma(y - x) \\ \dot{y} = rx - y - xz \\ \dot{z} = xy - bz \end{cases}$$

Model is based on Convection currents



System is defined by

① Prandtl number

$$P_r = \frac{\nu}{\kappa} = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}}$$

← kinematic viscosity

↖ thermal diffusivity

↙ dependent on material

② Rayleigh Number

$$= \frac{\alpha \rho g \Delta T D^3}{\kappa \mu}$$

thermal expansivity ↓ density ↓ temperature contrast ↙ ← system height

↖ dynamic viscosity

$$= \frac{D^2/\kappa}{\mu/(\alpha \rho g \Delta T D)} = \frac{\text{diffusion time scale}}{\text{advection time scale}}$$

↑ Rayleigh Number : Advection time scale preferred

↓ Rayleigh Number : Diffusion preferred

Returning back to the Lorenz model

$$\begin{cases} \dot{x} = \overset{P_r}{\sigma}(y - x) \\ \dot{y} = rx - y - xz \\ \dot{z} = xy - bz \end{cases}$$

↖ normalized Ra

↖ related to aspect ratio

$$r = \frac{R_a}{R_{a_{crit}}} \leftarrow \sim 10^3$$

x ~ velocity of fluid particle

y ~ temp variation of particle

z ~ thermal boundary area

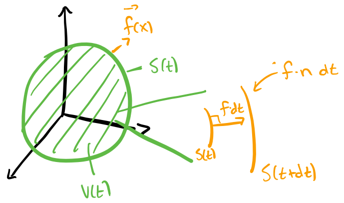
Lecture 17

Fate of volume in the phase space

for any 3D system $\frac{d\vec{x}}{dt} = \vec{f}(\vec{x})$

Pick an arbitrary closed surface $S(t)$ of volume $V(t)$ in the phase space

$$\dot{x} = \sigma(y-x)$$
$$\dot{y} = rx - y - xz$$
$$\dot{z} = xy - bz$$



① Find Fixed Points

$$\dot{x} = \dot{y} = \dot{z} = 0$$

Conduction

Convection

$$\begin{cases} ① & x^* = y^* = z^* = 0 \\ ② & x^* = y^* = \pm\sqrt{b(r-1)}, \quad z^* = r-1 \end{cases}$$

(C^+, C^-)

$r > 1$

$$V(t+dt) = V(t) + \int_S (f\cdot n\,dt)\,dA$$

$$\rightarrow \dot{V} = \lim \frac{V(t+dt) - V(t)}{dt} = \int_S f\cdot n\,dA \xrightarrow{} \int_V \nabla\cdot f\,dV$$

gauss theorem

$$\nabla\cdot f = \frac{\partial}{\partial x}\left(\sigma(y-x)\right) + \frac{\partial}{\partial y}(rx - y - xz) + \frac{\partial}{\partial z}(xy - bz) = -\sigma - 1 - b \underline{< 0}$$

$$\dot{V} = -(\sigma + b + 1)V$$

$$V(t) = V_0 \exp\left(-(\sigma+b+1)t\right)$$ ← phase volume decreases quickly

Stability of the Origin

$$J = \begin{pmatrix} -\sigma & \sigma & 0 \\ r & -1 & 0 \\ 0 & 0 & -b \end{pmatrix}$$

$$\tau = -\sigma - 1 \quad < 0$$
$$\Delta = \sigma(1-r)$$

$\underline{r < 1}$

$\Delta > 0$

$\tau^2 - 4\Delta = (\sigma-1)^2 + 4\sigma r > 0$

Stable Fixed Point

$\underline{r = 1}$

$\Delta = 0$

Non-isolated point

③ $\underline{r > 1}$

$\Delta > 0$

(+--) Saddle point

Stability of C^+ and C^-

$$J = \begin{pmatrix} -\sigma & \sigma & 0 \\ 1 & -1 & \mp\sqrt{b(r-1)} \\ \pm\sqrt{b(r-1)} & \pm\sqrt{b(r-1)} & -b \end{pmatrix}$$

$$\det(J - \lambda I) = f(\lambda) = \lambda^3 + (\sigma+b+1)\lambda^2 + (r+\sigma)b\lambda + 2b\sigma(r-1) = 0$$

$r > 1$ $(r \approx 1)$ ⟶ Stable fixed point $\lambda_1, \lambda_2, \lambda_3 < 0$

Hopf Bifurcation

$r \nearrow$ ⟶ Stable spiral $\lambda_1 < Re(\lambda_2, \lambda_3) < 0$

$r \nearrow\nearrow$ ⟶ (++- spiral saddle) $\lambda_1 < 0, \quad Re(\lambda_2, \lambda_3) > 0$

Consider the case where $\mathrm{Re}(\lambda_2, \lambda_3) = 0$

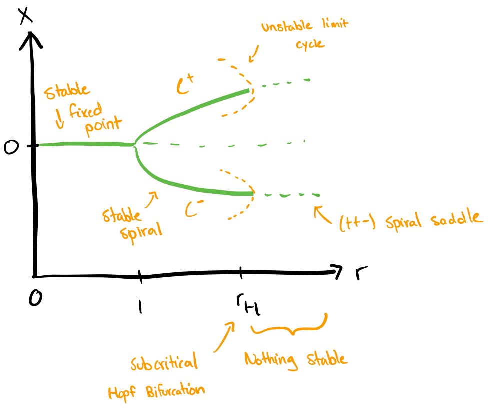
$$\lambda = \pm i w \qquad w \in \mathbb{R}$$

$$f(iw) = 0$$

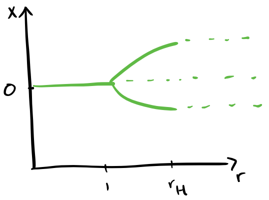
$$\mathrm{Re}(f(iw)) = 0 \longrightarrow w^2 = \frac{2b\sigma(r-1)}{\sigma+b+1}$$

$$\mathrm{Im}(f(iw)) = 0 \longrightarrow w^2 = b(r+\sigma)$$

$$r_H = \frac{\sigma(\sigma+b+3)}{\sigma-b-1} \quad (>1)$$



Lecture 18



$$L(x) = x^2 + y^2 + (z - r - \sigma)^2$$

Lyapunov function

$$\frac{1}{2}\frac{dL}{dt} = x\dot{x} + y\dot{y} + (z - r - \sigma)\dot{z}$$
$$= -\sigma x^2 - y^2 - bz^2 + b(r+\sigma)z$$

Negative outside of ellipsoid E

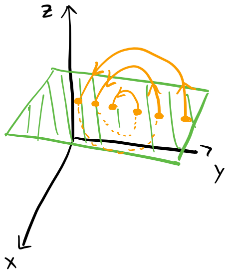
$$\sigma x^2 + y^2 + b(z-(r+\sigma))^2 = b^2(r+\sigma)^2$$

convention
$\sigma = 10$
$b = 8/3$

→ All trajectories eventually enter and remain inside S

→ $r > r_H$ all solutions are bounded

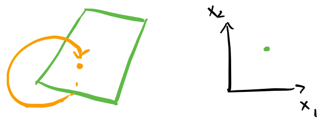
Poincaré Section



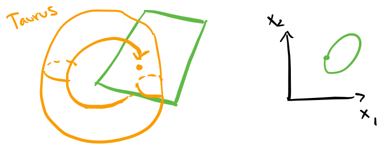
Set of intersection points define a poincaré section

3 types

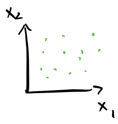
1) Periodic
Limit cycle



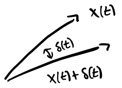
2) Quasiperiodic Flows (w/ Two Fundamental frequencies)



3) Aperiodic



Deterministic chaos is characterized by extreme sensitivity to initial conditions



$$|\delta(t)| \sim |\delta(0)| e^{\lambda t}$$ ← lyapunov exponent

positive lyapunov exponent indicates chaos

$|\delta_0|$ ← Uncertainity in the initial state

a ← measure of our tolerance

$$t_{\text{Horizon}} \sim O\left(\frac{1}{\lambda} \ln \frac{a}{|\delta_0|}\right)$$

time until solutions diverge

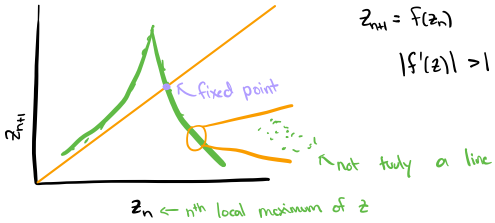
Lecture 19

Deterministic Chaos

Deterministic system with aperiodic long-term behavior that exhibits sensitive dependence on initial conditions

Lorenz system can be studied by looking at local maximum of each coordinate

Lorenz Map



$$z_{n+1} = f(z_n)$$

$$|f'(z)| > 1$$ everywhere

if $f(z_n) = z^*$, then the system exhibits periodic behavior

Lorenz map has finite thickness which allows for deterministic chaos

Perturbation around fixed point

$$z_n = z^* + \eta_n$$

$$\eta_{n+1} = f'(z^*)\eta_n$$

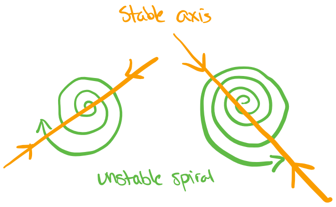
since this is greater than 1

$$|\eta_{n+1}| > |\eta_n|$$

Saddle spirals allow for deterministic chaos

require stretching: unstable spiral

falling: stable axis



Lecture 20

Controlling Chaos

Lorenz Equations

$$\begin{rcases} \dot{x} = \sigma(y-x) \\ \dot{y} = rx - y - xz + p(t) \\ \dot{z} = xy - bz \end{rcases}$$ 3 fixed points $(0,0,0)$, C^+, C^-

$$\dot{\vec{x}} = f(\vec{x}, p(t)) \simeq \underset{\substack{\parallel \\ 0 \\ \text{fixed point}}}{f(\vec{x}_F)} + A(\vec{x} - \vec{x}_F) + \vec{b}\, p(t)$$

$$A = \left.\frac{\partial f}{\partial x}\right|_{x=x_F} = \begin{pmatrix} -\sigma & \sigma & 0 \\ r & -1 & 0 \\ 0 & 0 & b \end{pmatrix} \qquad \vec{b} = \left.\frac{\partial f}{\partial p}\right|_{x=x_F} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Finite-Difference Approximation

$$\frac{\vec{x}_{k+1} - \vec{x}_k}{\Delta t} = A(\vec{x}_k - \vec{x}_F) + \vec{b}\, \underbrace{P_k}_{\vec{q}^T(\vec{x}_k - \vec{x}_F)}$$

$$\underbrace{\vec{x}_{k+1} - \vec{x}_F}_{d\vec{x}_{k+1}} = \underbrace{\vec{x}_k - \vec{x}_F}_{d\vec{x}_k} + \Delta t (\Delta + \vec{b}\vec{q}^T)(x_k - x_F)$$

$$|d\vec{x}_{k+1}| < |d\vec{x}_k|$$

Let's consider eigenvectors of A

$\lambda_a > 0, \lambda_s < 0 \quad (r > 1)$

$$A'\vec{e}_i = \lambda_i \vec{e}_i$$

$$A'[\vec{e}_v, \vec{e}_s] = [\vec{e}_v, \vec{e}_s] \begin{bmatrix} \lambda_v & 0 \\ 0 & \lambda_s \end{bmatrix}$$

$$A' = [\vec{e}_v, \vec{e}_s] \begin{bmatrix} \lambda_v & 0 \\ 0 & \lambda_s \end{bmatrix} [e_v, e_s]^{-1} \leftarrow \begin{bmatrix} g_v^T \\ g_s^T \end{bmatrix}$$

Constrained vectors

$$A' = \lambda_v e_v g_v^T + \lambda_s e_s g_s^T$$

← eigenvalue expansion

$$d\vec{x}'_{k+1} = d\vec{x}'_k + \underbrace{\Delta t(A' + \vec{b}'\vec{q}'^T) d\vec{x}'_k}_{\vec{e}_v}$$

$$g_v^T (A' + \vec{b}'\vec{q}'^T) dx'_F = 0$$

$$\vec{q}' = \frac{-\lambda_v \vec{g}_v}{\vec{g}_v^T \vec{b}'}$$

← Constrained vector

$$p(t) = \begin{cases} 0 & \text{if } |\vec{q}', dx_F| > p^* \\ q' \, d\vec{x}_k & \text{otherwise} \end{cases}$$

Lecture 21

Review of Statistics

$$p(a,b) = \frac{\text{cov}(a,b)}{\sigma(a)\,\sigma(b)}$$

↑ correlation coefficient

I am

Single Variable Statistics

$$\mathbb{E}(x) = \frac{1}{m} \sum_{i=1}^{m} x_i = \bar{x}$$

$$\sigma^2(x) = \mathbb{E}((x - \bar{x})^2)$$

Multivariate Case

Variance is replaced by a covariance matrix

$$\Sigma = \begin{bmatrix} \sigma^2(x_1) & \text{cov}(x_1,x_2) & & \\ \text{cov}(x_1,x_2) & \ddots & & \\ & & \ddots & \\ & & & \ddots \end{bmatrix} = S^{-1} \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{bmatrix} S$$

↖ eigenvalue decomposition

$$\lambda_1 \geq \lambda_2 \geq \dots \lambda_n \geq 0$$

Consider $y = A\vec{x} + b$

$$\mathbb{E}(y) = A\,\mathbb{E}(x) + b$$

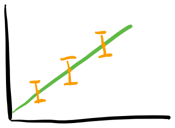
$$\sigma^2(y) = A\,\sigma^2(x)\,A^T$$

→ skipping algebra

Lecture 22

Linear Inverse Theory

Least Squares Regression



$y = a + bx$

$\sigma(a), \sigma(b), \text{cov}(a,b)$

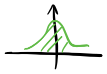
Suppose we have n samples

$(x_1, y_1), \dots (x_n, y_n)$

model via $f(x)$

Linear Regression Assumptions

① Data Errors have gaussian distributions



$$P(y) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(\frac{-(y-\mu)^2}{2\sigma^2}\right)$$

② All data errors are independent

Allows us to calalate likelihood functions

$$P(y_1, y_2, \ldots y_n) = P(y_1)P(y_2)\ldots P(y_n)$$

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{[y_i - y(x_i, \{a_j\})]^2}{2\sigma_i^2}\right)$$

$$-\log P = \sum_{i=1}^{N}\left(\underbrace{\frac{[y_i - y(x_i, \{a_j\})]^2}{2\sigma_i^2}}_{\substack{\text{minimize this term} \\ \text{to find MLE}}} + \frac{1}{2}\log(2\pi\sigma_i^2)\right)$$

③ No error in $\{x_i\}$

Linear Model

$$y(x, \{a_j\}) = \sum_{j=1}^{N} a_j \mathbb{X}_j(x)$$

$$\chi^2 = \sum_{i=1}^{N}\left[\frac{x_i - \sum_j a_j \mathbb{X}_j(x_1)}{\sigma_i}\right]^2$$

Goal is to find $\frac{\partial \chi^2}{\partial a_j} = 0$

Simplify this calculation using matricies

$$\vec{y} = \begin{bmatrix} y_1/\sigma_1 \\ \vdots \\ y_n/\sigma_n \end{bmatrix} \quad \vec{\sigma} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} \quad K = \begin{bmatrix} \frac{\mathbb{X}_i(x_i)}{\sigma_1} & \cdots & \frac{\mathbb{X}_m(x_i)}{\sigma_1} \\ \vdots & & \\ \vdots & \cdots & \frac{\mathbb{X}_m(x_N)}{\sigma_N} \end{bmatrix}$$

$$\chi^2 = |y - K\vec{a}|^2$$

$$= y^T y - y^T K a - a^T K^T y + \vec{a}^T K^T a$$

Review of Matrix Calculus

$$\frac{\partial(x^T y)}{\partial x} = \vec{y}^T$$

$$\frac{\partial(x^T y)}{\partial y} = \vec{x}^T$$

$$\frac{\partial(x^T A x)}{\partial x} = x^T A^T + x^T A$$

if $A = A^T$

$$= 2x^T A$$

$$\frac{\partial \chi^2}{\partial \vec{a}} = -y^T K - (K^T y)^T + 2a^T K^T K = 0$$

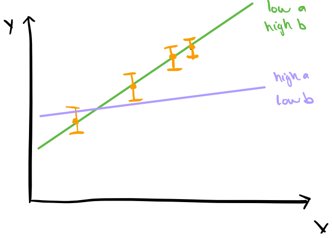
$$K^T K a = K^T y$$

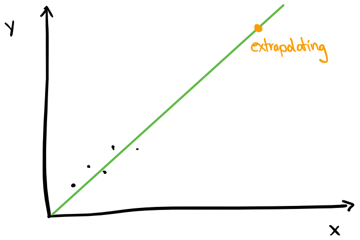
$$\boxed{a = (K^T K)^{-1} K^T y}$$

Closed Form of OLS

Lecture 23

$$\vec{a} = \underbrace{(K^T K)^{-1}}_{\text{cov}(A)} K^T \vec{y}$$

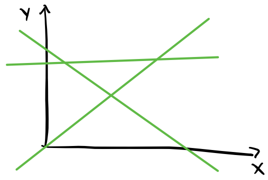




$y = a_1 + a_2 x$

$\sigma^2(y) = \sigma^2(a_1) + \sigma^2(a_2) + 2x\,\mathrm{cov}(a_1, a_2)$

Overdetermined System



$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0.9 \end{pmatrix}$$

Our closed form OLS solution only works for purely overdetermined systems

Singular matricies don't have unique solutions

Constructing a Hermetian matrix S

$$S = \left[\begin{array}{c|c} 0 & A \\ \hline A^+ & 0 \end{array}\right]$$

guaranteed to have an orthogonal set of eigenvectors with real eigenvalues

Lecture 24

Linear Model

$A\vec{x} = \vec{b}$ data

$$\left[\begin{array}{c|c} 0 & A \\ \hline A^+ & 0 \end{array}\right] \begin{bmatrix} u_i \\ v_i \end{bmatrix} = \lambda_i \begin{bmatrix} \vec{u}_i \\ \vec{v}_i \end{bmatrix} \begin{matrix} \} \text{ N - data space} \\ \} \text{ M - model space} \end{matrix}$$

If $\lambda_i \neq 0$ | $\lambda_i = 0$

$A\vec{v}_i = \lambda_i \vec{u}_i$ | $Au_i = 0$

$A^+\vec{u}_i = \lambda_i \vec{v}_i$ | $A^+\vec{u}_i = 0$

Consider

$$\left.\begin{aligned} A^+A\, v_i &= \lambda_i^2 v_i \\ AA^+ u_i &= \lambda_i^2 u_i \end{aligned}\right\} \text{True for all } \lambda_i$$

both Hermetian

Consider

$V = [v_1, v_2, \dots v_m]$ and $U = [u_1, u_2, \dots u_N]$

$V^+V = VV^+ = I_m$ | $U^+U = UU^+ = I_N$

v_i's are orthogonal | u_i's are orthogonal

Reconstruct Sections

$\underbrace{V}_{m\times m} = [\underbrace{V_p}_{m\times p}, \underbrace{V_0}_{m\times(m-p)}]$ | $\underbrace{U}_{N\times N} = [\underbrace{U_p}_{N\times p}, \underbrace{U_0}_{N\times(N-p)}]$

$V_p^+ V_p = I_p$ | $U_p^+ U_p = I_p$

$V_p V_p^+ \neq I_N$ | $U_p U_p^+ \neq I_N$

We can define

$$\Lambda_p = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_p \end{bmatrix}$$

So that

$$AV_p = U_p \Lambda_p \qquad AV_0 = 0$$

$$A^+ U_p = V_p \Lambda_p \qquad A^+ U_0 = 0$$

$$AV = A[V_p, V_0] = [U_p, U_0] \begin{bmatrix} \Lambda_p & 0 \\ 0 & 0 \end{bmatrix}$$

$$A = [U_p, U_0] \begin{bmatrix} \Lambda_p & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_p^+ \\ V_0^+ \end{bmatrix}$$

$$= U_p \Lambda_p V_p^+ \leftarrow \text{Single Value decomposition}$$

$$U_0^+ A = 0$$

$$U_0^+ A x = 0$$

$$U_0^+ (\underset{\text{model prediction}}{Ax}) = 0$$

$\vec{b}$ is the data vector

$$b = \sum_{i=1}^{N} \alpha_i \vec{v}_i$$

U_0 is the source of discrepancy between model prediction and data

V_0 is source of non-uniqueness

$$AV_0 = 0 \quad \text{so} \quad A\vec{v}_i = 0 \quad i = p+1, \dots M$$

$$A\left(\vec{x} + \sum_{i=1}^{M} \alpha_i v_i\right) = A\vec{x}$$

Generalized Inverse

Exact Inverse of A

$$A^{-1} = V \Lambda^{-1} U$$

General Inverse

$$A_g^{-1} = V_p \Lambda_p^{-1} U_p^+ \leftarrow \text{Moore - Penrose Psuedo Inverse}$$

Properties of Psuedo-Inverse

① No V_0, No U_0

$$A_g^{-1} = V_p \Lambda^{-1} U_p^+ = V \Lambda U^+ = A^{-1}$$

② No V_0, but $U_0 \neq 0$ (Overdetermined)

$$A^+ A = V_p \Lambda_p^2 V_p^+$$

$$(A^+ A)^{-1} = V_p \Lambda_p^{-2} V_p^+$$

$$A^+ A \, x = A^+ b$$

$$x = (A^+ A)^{-1} A^+ b = (V_p \Lambda_p^{-2} \underbrace{V_p^+)(V_p}_{I_M} \Lambda_p U_p^+) b = V_p \Lambda_p^{-1} U_p^+ b = A_g^{-1} b$$

③ No U_0, $V_0 \neq 0$ Underdetermined

$$\downarrow$$

$$U_p U_p^+ = UU^+ = I_N$$

$$V_p^+ V_p = I_p, \quad V_p V_p^+ = I_M$$

$$A\vec{x} = A(A_g^{-1} b) = (U_p \Lambda_p \underbrace{V_p^+)(V_p}_{I_p} \Lambda_p^{-1} U_p^+) b$$

$$= b$$

$X_g = A_g^{-1} b$ is restricted to V_p-space

$$X_g = V_p \Lambda_p^{-1} U_p \vec{b}$$

$$= c_1 v_1 + c_2 v_2 + \dots + c_p v_p$$

$$x = x_g + \sum_{i=p+1}^{M} \alpha_i \vec{v}_i$$

$$|x|^2 = |x_g|^2 + \sum \alpha_i^2 \geq |x_g|^2$$

$X_g \rightarrow$ minimum norm solution

④ $V_0 \neq 0$, $U_0 = 0$

$$X_g = A_g^{-1} \vec{b}$$

$$= V_p \Lambda^{-1} U_p b$$

simultaneously minimizes $\|b-Ax\|$ in data space and $\|x\|$ in model space

Lecture 25

Generalized Inverse

$$\vec{x}_g = V_p \Lambda_p U_p^{+} \vec{b}$$

Resolution is the relationship between inverse and true solution

model resolution

$$A\vec{x} = b$$

$$A_g^{-1} A x = A_g^{-1} b$$

recall: $\vec{x}_g = A_g^{-1} b$

$$\vec{x}_g = \underbrace{A_g^{-1} A}_{\text{ideally } I} x$$

model resolution matrix

$$\vec{x}_g = V_p \Lambda_p^{-1} \overbrace{\underbrace{U_p^{+}}_{I} U_p}^{I} \Lambda_p V_p^{+} = V_p V_p^{+} \underset{\text{generally}}{\neq I_p}$$

Data Resolution

$$A\vec{x}_g = \vec{b}_g$$

$$A(A_g^{-1}\vec{b}) = \vec{b}_g$$

$$\vec{b}_g = \underbrace{U_p U_p^{+}}_{\text{data resolution matrix}} \vec{b}$$

Model Uncertainity

$$\vec{y} = A\vec{x} + b$$

$$\sigma^2(y) = A\sigma^2(x)A^T$$

$$\vec{x}_g = A_g^{-1}\vec{b}$$

$$\sigma^2(x_g) = (V_p \Lambda_p^{-1} U_p^{+})\, \sigma^2(b)\, (U_p \Lambda_p^{-1} V_p^{+})$$

If data errors are independent and identical

$$\sigma^2(b) = \sigma_b^2 I_N$$

$$\sigma^2(x_g) = \sigma_b^2 V_p \Lambda_p^{-2} V_p^{+}$$

Send small $|\lambda_i|$ to 0

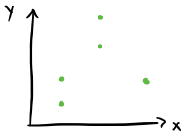
trade-off between model stability and resolution

Example: 5 data points

Fit a 4-parameter model

$$y = a + bx + cx^2 + dx^3$$

x	y
1	1.1
1	2.0
2	3.9
2	5.0
3	2



mixed-determined case

$A\vec{m} = \vec{d}$ ← ignore data error

$$\begin{array}{c} \\ 1 \\ 1 \\ 2 \\ 2 \\ 3 \end{array}
\begin{array}{c} \begin{array}{cccc} 1 & x & x^2 & x^3 \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \\ 1 & 2 & 4 & 8 \\ 1 & 3 & 9 & 27 \end{bmatrix} \end{array}
\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 1.1 \\ 2 \\ 3.9 \\ 5 \\ 2 \end{bmatrix}$$

Least-squares

$$m = (A^TA)^{-1} A^T \vec{d} = \begin{bmatrix} 4.1 \\ -2.2 \\ 21.1 \\ -2.0 \end{bmatrix}$$

$\det(A^TA) = 2\times10^{-12}$

Generalized Inverse

$$m = A_g^{-1} d = V_p \Lambda_p^{-1} U_p^{+} d = \begin{bmatrix} -1.2 \\ 0.92 \\ 2.8 \\ -0.91 \end{bmatrix}$$

Lecture 26

We can linearize the general relationship

$$\vec{G}(\vec{x}) = b \longrightarrow \vec{G}(\vec{x}) = \underset{\text{initial guess}}{\vec{G}(\vec{x}_0)} + \underset{A}{\left.\frac{\partial G}{\partial x}\right|_{\vec{x}_0}} \underbrace{(x - x_0)}_{\delta x}$$

$$A\,\delta x = b - G(x_0) = \delta \vec{b}$$

Probability Review

joint prob: $p(x,y)$

Conditional prob: $p(x|y)$

$$p(x,y) = p(x|y) \cdot p(y)$$

① Frequentist Approach

total # Events = N

total # of event x is n

$$P(x) = \lim_{N \to \infty} \frac{n}{N} \quad \leftarrow \text{Only applicable to repeatable schema}$$

Championed by R.A. Fisher (1920's - 1930's)

Uses bootstrap approach for computation

② Bayesian Approach

$$p(x|y) = \frac{p(y|x)\,p(x)}{p(y)} \quad \leftarrow \text{Bayes' Rule}$$

$$\left.\begin{aligned} p(\text{model}\,|\,\text{data}) &= \frac{p(\text{data}\,|\,\text{model})\;p(\text{model})}{p(\text{data})} \\ &= \frac{(\text{likelihood})(\text{prior})}{(\text{evidence})} \end{aligned}\right\} \text{Bayesian model}$$

Formalized by H. Jeffreys in his 1939 "Theory of Probability"

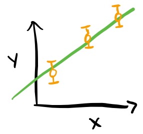
Uses Markov chain Monte Carlo for computation

If there is no prior

$p(\vec{m}|\vec{d})$ is maximized by

$$\max_{m}\, p(\vec{m}|\vec{d}) = \max_{m}\, (\vec{d}|\vec{m}) \quad \nwarrow \text{maximum likelihood estimate}$$

Consider the model $y = ax + b$



$$p(a,b) = p(\vec{d}\,|\,(a,b)) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_i}} \exp\left(- \frac{(y_i - (a+bx_i))^2}{2\sigma_i^2} \right)$$

$$\mathbb{E}(a) = \iint a\; p(a,b)\; da\, db$$

$$\mathbb{E}(b) = \iint b\; p(a,b)\; da\,db$$

$$\sigma^2(a) = \iint a^2\, p(a,b)\, da\,db - \mathbb{E}(a)^2$$

$$\sigma^2(b) = \iint b^2\, p(a,b)\, da\, db - \mathbb{E}(b)^2$$

$$\text{cov}(a,b) = \iint (a - \mathbb{E}(a))(b - \mathbb{E}(b))\, p(a,b)\, da\,db$$

Bayesian approach can solve systems with error in x and y coordinates

$$\sigma_i^2 = \text{Var}(y - (a+bx_i)) = \text{var}(y_i)$$

$$\downarrow$$

$$= \text{Var}(y_i) + b^2\,\text{var}(x_i)$$

$$\mathbb{E}(m) = \int_M m \ \text{prob}(\vec{m})\, dM = \int_M m\, p(\vec{m}|\vec{d})\, dM = \int_M m \ \frac{\overset{\text{likelihood}}{p(\vec{d}\,|\vec{m})}\ \overset{\text{prior}}{p(m)}}{p(d)}\, dM = \exp\left(-\frac{1}{2}\ \underset{\text{cost/misfit function}}{\chi^2(\vec{d},\vec{m})}\right)$$

Lecture 27

It is computationally inefficient to solve the model given many parameters

Instead, we can use statistical methods to estimate the solution

Conjugate Gradient Descent

taylor expansion

$$f(\vec{x}) = f(\vec{x}_0) + \sum_i \frac{\partial f}{\partial x_i} x_i + \frac{1}{2}\sum_{i,j} \frac{\partial^3 f}{\partial x_i \partial x_j} x_i x_j + \dots$$

$$\doteq \underset{f(x_0)}{c} - \underset{\begin{bmatrix} -\frac{\partial f}{\partial x_1} \\ \vdots \\ -\frac{\partial f}{\partial x_n} \end{bmatrix}_{x_0}}{\vec{b}}{}^T x + \frac{1}{2} x^T \underset{\text{Hessian Matrix}}{A} x$$

$$A_{ij} = \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right|_{x=x_0}$$

First Order Minimization

$$\nabla f = -b + Ax = 0$$

$$Ax = b \quad \longleftarrow \text{simplifies to Linear algebra}$$

Rewrite

$$x = \sum_i \alpha_i p_i$$

@ some intermediate step

$$x_k = x_{k-1} + \alpha_k P_k$$

$$= \underset{[P_1, P_2, \dots P_{k-1}]}{P_{k-1}}\ \underset{\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{k-1} \end{bmatrix}}{y} + \alpha_k P_k$$

Assume x_k minimizes $f(x_{k-1})$ and we want to minimize $f(x_k) = f(x_{k-1} + \alpha_k P_k)$

$$f(x_k) = f(x_{k-1} + \alpha_k P_k)$$

$$= f(x_{k-1}) + \underbrace{\alpha_k y^{+} P_{k-1}^T A p_k}_{\text{rather complicated}} + \frac{1}{2}\alpha_k^2 p_k^T A p_k - \alpha_k p_k b$$

Select vectors p s.t. the complicated term vanishes

$$p_j A p_i = 0$$

p_j is A conjugate to p_i

Algorithm

① Pick an initial direction $\vec{p}_1$ @ $x = x_0$

② $\alpha_1 = \dfrac{p_1^T b}{p_1 A p_1}$ $\quad x_1 = \alpha_1 p_1$

Pick a direction

Minimize along that directio

Rinse and repeat ?

③ Pick new direction p_2

repeat

- Calculate steepest descent @ x_1

$$r_1 = b - Ax_1$$

- Construct

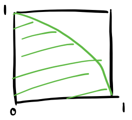
$$p_2 = r_1 + B_2 p_1$$

$$\longrightarrow B_2 = -\frac{p_1^T A p r_1}{p_1^T A p_1}$$

④ $\alpha_2 = \frac{P_2^T b}{P_2^T A P_2}$, $X_2 = X_1 + \alpha_2 P_2$

Lecture 28

Monte - Carlo Integration



N random points

n points w/ $x^2 + y^2 \leq 1$

$\lim_{N \to \infty} \frac{n}{N} = \frac{\pi}{4}$

$$\int_V f(x)\, dV = V \underbrace{\int f(x) \cdot \overset{\text{prob}}{\frac{1}{V}}\, dV}_{\langle f(x) \rangle}$$

$$\approx V \langle f \rangle \pm V \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}} \quad \text{error} \sim O(N^{-1/2})$$

monte carlo integration

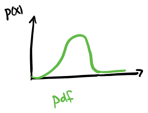
If there is a function $p(x)$ s.t. $f \approx \propto p(x)$ and $\int_0^1 p(x)\, dx = 1$

then $\int f\, dV = \int \left(\frac{f}{p}\right) p\, dV$

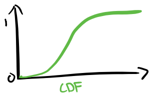
$$\approx \frac{V}{N} \sum_{i=1}^{N} \frac{f(x_i)}{p(x_i)} \pm V \sqrt{\frac{\langle (\frac{f}{p})^2 \rangle - \langle \frac{f}{p} \rangle^2}{N}}$$

importance Sampling : producing random points based on provided probability

① Transformation Method



pdf



CDF

Select random uniform number for y-axis and then back calalate associated x value

Only works for 1-D case

② Rejection Method

for p(x), find f(x) s.t. $f(x) \geq p(x)\ \forall x$

comparison function

Step 1: Draw a sample X from f(x)

select f(x) s.t. this is easy

compute $R = \frac{p(x)}{f(x)}$

Step 2: Draw a random # from [0,1] w/ uniform distribution and label it r

if $r \leq R$, accept new X, otherwise go back to 1

More general than transformation method but still limited to low dimensionality cases

③ Markov Chain Monte Carlo

Metropolis Algorithm

1. pick an initial point $\vec{X}_0$ and calalate $p(X_0)$
2. perturb it to get a new point $\vec{X}'$ and calculate $p(\vec{X}')$
   proposal
3. Select a random number r from uniform (0,1)

$$\begin{cases} \text{if } r \leq \frac{p(X')}{p(X_0)}, \text{ accept } \vec{X}' \text{ and set } X_1 = X' \\ \text{otherwise}, \quad \vec{X}_1 = X_0 \end{cases}$$

4. Repeat steps 1-3

Markov Chain

Stochastic process that satisfies the markov property

$$P(X_{t+1} = S_j \mid X_t = S_{i_t}, X_{t-1} = S_{i_{t-1}}, \ldots X_0 = S_{i_0}) = P(X_{t+1} = S_j \mid X_t = S_{i_t})$$

Markov Property

finite sample space : $\{S_1, S_2, \ldots S_n\}$

transition probability

$P_{ij}(t) = P(X_t = S_j \mid X_{t-1} = S_i)$

If $P_{ij}(t) = P_{ij}$ for all t, we have a stationary chain

Transition Matrix : $P = [P_{ij}]$

non-negative, $\sum_j P_{ij} = 1$ (row sum)

Stochastic Matrix

k-th step probability distribution vector

$$p(k) = \begin{bmatrix} P_1(k) \\ \vdots \\ P_n(k) \end{bmatrix} \quad P_j(k) = P(X_n = S_j)$$

$$p^T(k) = p^T(k-1)\, P = \underset{\overset{\nearrow}{\text{initial}}}{p^T(0)}\, P^k$$

Lecture 29

$$p^T(k) = p^T(0)\, P^k$$

P is the transition matrix

Stochastic matrix (row-sum = 1)

ρ is the spectral radius

$\nwarrow$ largest eigenvalue

$$|\lambda| \le \|P\|$$

$$|\lambda| \le 1$$

Right Eigenvector

$$P\vec{e} = \vec{e}$$

$(1, \vec{e})$ or $(1, \vec{e}/n)$

Left Eigenvector (Stationary distribution vector)

$$\pi^T P = \pi^T$$

If $1 > |\lambda_2| \ge |\lambda_3| \ge \dots$ P (primitive)

$$P = S \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} S^{-1} \quad , \lim_{k\to\infty} P^k = S \begin{bmatrix} 1 & & & 0 \\ 0 & 0 & & \\ & & 0 & \\ 0 & & & 0 \end{bmatrix} S^{-1}$$

$$PS = S \begin{bmatrix} 1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & \ddots \end{bmatrix} \qquad S^{-1}P = \begin{bmatrix} 1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \end{bmatrix} S^{-1}$$

$$\lim_{k\to\infty} P^k = S \begin{bmatrix} 1 & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} S^{-1}$$

$$\vec{e}\vec{\pi}^T = \begin{bmatrix} \pi_1 & \pi_2 & \cdots & \pi_n \\ \pi_1 & \pi_2 & & \pi_n \\ \vdots & \vdots & & \vdots \\ \pi_1 & \pi_2 & & \pi_n \end{bmatrix}$$

$$\lim_{k\to\infty} p^T(k) = \lim_{k\to\infty} p^T(0) P^k = p^T(0)\, \vec{e}\pi^T = \pi^T$$

If P is not primitive

$(|\lambda_2| = \dots = |\lambda_p| = 1$ for some $p)$

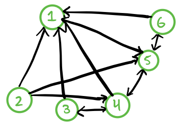
$\lim_{k\to\infty} P^k$ doesn't converge

P is cesàro - summable

$$\lim_{k\to\infty} \frac{I + P + \dots P^k}{k} = \vec{e}\vec{\pi}^T$$

$\nwarrow$ fraction of time spent at each position

Page Rank



If there are n external links in their current visiting state the next action is randomly taken from n+1 choices

$$P = \begin{bmatrix} 1/2 & 0 & 0 & 0 & 1/2 & 0 \\ 1/4 & 1/4 & 0 & 1/4 & 1/4 & 0 \\ 1/3 & 0 & 1/3 & 1/3 & 0 & 0 \\ 1/4 & 0 & 1/4 & 1/4 & 1/4 & 0 \\ 1/4 & 0 & 0 & 1/4 & 1/4 & 1/4 \\ 1/3 & 0 & 0 & 0 & 1/3 & 1/3 \end{bmatrix} \longrightarrow \vec{\pi} = \begin{bmatrix} 0.3529 \\ 0 \\ 0.0504 \\ 0.1345 \\ 0.3361 \\ 0.1261 \end{bmatrix}$$

Lecture 30

Markov Chain Monte Carlo Continued

$$P = [P_{ij}]$$

$$\pi^T \underset{\substack{\uparrow \\ \text{nxn} \\ \text{matrix}}}{P} = \underset{\substack{\nwarrow \\ \text{nx1 vector} \\ \text{(some pdf)}}}{\pi^T}$$

Detailed Balance

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \forall ij$$

Suppose that $X_k = S_i$ and we need to construct X_{k+1}

① Let $H = [h_{ij}]$ be an arbitrary stochastic matrix

$\leftarrow$ proposal matrix

pick Y according to $P(Y = S_j \mid X_k = S_i) = h_{ij}$

② Let $A = [a_{ij}]$ be a matrix w/ entries satisfying $0 \le a_{ij} \le 1$

$\uparrow$ acceptance probabilities

given $Y = S_j$, we set

$$X_{k+1} = \begin{cases} S_j & \text{w/ prob } a_{ij} \\ X_k & \text{w/ } 1 - a_{ij} \end{cases}$$

$$P_{ij} = \begin{cases} h_{ij} a_{ij} & \text{if } i \neq j \\ 1 - \sum_{k \neq i} h_{ik} a_{ik} & \text{if } i = k \end{cases}$$

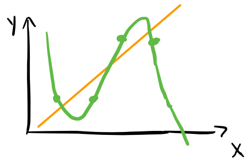
$$a_{ij} = \min\left(1, \frac{\pi_j h_{ji}}{\pi_i h_{ij}}\right)$$

$\nwarrow$ metropolis hastings

If H is symmetric

$$a_{ij} = \min\left(1, \frac{\pi_j}{\pi_i}\right)$$

Lecture 31



Bias - Variance Estimation Methods

- Splitting data into training and test data

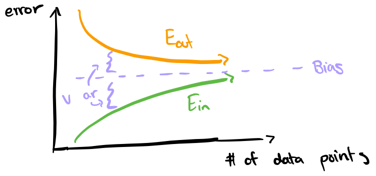
Error in training data is called fitting error

in - sample Error, E_{in}

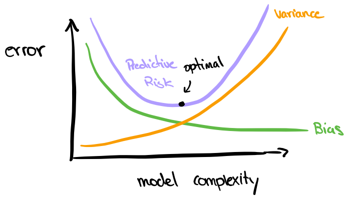
Error in test set is called prediction error

out - of - sample Error, E_{out}

For a given model complexity



For a given # of data



Shannon's Information Entropy

Information

$I(p_i)$ <— function of probability

Properties

① $I(p)\downarrow$ as $p\uparrow$

rare events have more meaning

② $I(1) = 0$

③ $I(p) \geq 0$

④ $I(p_1, p_2) = I(p_1) + I(p_2)$

$p_1 \perp p_2$ <— independence

$I(p) = \log(1/p) = -\log p$ <— simplest form

$\mathbb{E}[I(p)] = \int p - \log p \; dp$

information entropy

takes the same form as thermodynamic entropy

Kullback-Leibler Divergence

used to find difference between two pdfs

$g(x) \longrightarrow$ true pdf for x

entropy $\longrightarrow$ $-\int g(x) \log g(x) \, dx$

$f(x) \longrightarrow$ estimator

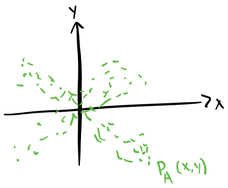
$$I(g,f) = -\int g(x) \log f(x) \, dx - \left(-\int g(x) \log g(x) \, dx\right)$$

$$= \int g(x) \log \frac{g(x)}{f(x)} \, dx$$

$= 0$ iff $g = f$

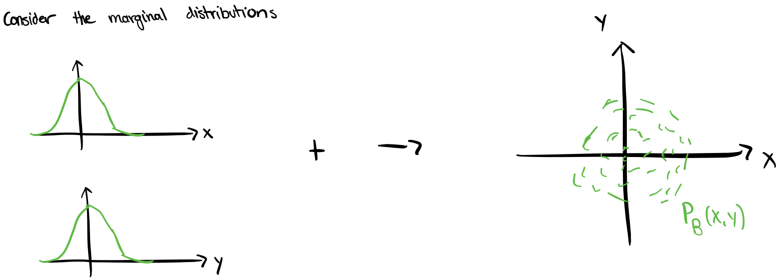
"distance" between pdfs

Non-linear Measure of Correlation



Linear correlation is 0

Consider the marginal distributions



"Mutual Information" $MI \equiv I(P_B; P_A)$

Normalize Mutual Information to find non-linear correlation

$$\frac{MI}{\sqrt{H(x)H(y)}}$$ $0 \leq \_ \leq 1$

Information entropy

To minimize $I(g;f)$

$$I(g;f) = \underbrace{\int g(x) \log g(x) \, dx}_{\text{constant}} - \underbrace{\int g(x) \log f(x) \, dx}_{\text{focus on this term}}$$

Estimate $\int g(x) \log f(x) \, dx \approx \frac{1}{n} \sum_{i=1}^{n} \log f(x_i)$

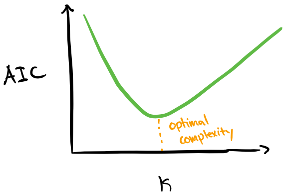
$$I(g;f) \approx \text{constant} - \frac{1}{n} \sum_{i=1}^{n} \log f(x_i) + \text{bias}$$

Aikake IC

$\approx \frac{k}{n}$ <— model parameters

Aikake Information Criteria

$$AIC \equiv -2 \sum_{i=1}^{n} \log f(x_i) + 2K$$



Lecture 32

Schmidt & Lipton (Science, 2009)

- Experimental data from physical systems

Consider a system with variables $X(t), Y(t)$, and $Z(t)$

Observed partial derivatives

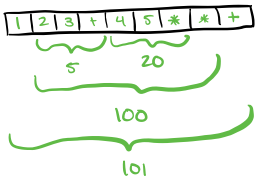
$$\frac{\Delta X}{\Delta Y} \approx \frac{dx/dt}{dy/dt} \quad , \quad \cdots$$

Theoretical partial derivatives

$f = f(x,y,z)$ ← estimated function

$$\frac{dx}{dy} = \frac{df/dy}{df/dx}$$

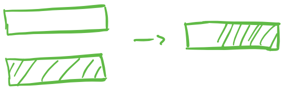
Stack-based calculator



Genetic Algorithm is parameter exploration based on darwinian evolution

- point mutation: randomly change instruction
- cross-over : mix two different code samples

} select prob of occurence



Brunton et. al (PNAS, 2016)

- Timeseries data → governing equation

$X(t), Y(t), Z(t)$ $$\frac{d\vec{x}}{dt} = f(\vec{x})$$

① Prepare data set

$X(t)$ → training set → $\frac{dX_T}{dt}$

$X(t)$ → validation set

② Build a library Θ

$$\vec{X}_T = \begin{bmatrix} \vdots & \vdots & \vdots \\ X(t) & Y(t) & Z(t) \\ \vdots & \vdots & \vdots \end{bmatrix}$$

$$\Theta = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ & X(t) & Y(t) & Z(t) & X^2 & Y^2 & Z^2 & XY & XZ & YZ & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

↗ constant term

③ Conduct Sparse Regression

$$\begin{bmatrix} \vdots \\ \frac{dx}{dt} \\ \vdots \end{bmatrix} = \begin{bmatrix} \Theta \end{bmatrix} \begin{bmatrix} \vec{x} \end{bmatrix}$$

$$\begin{bmatrix} \vdots \\ dy/dt \\ \vdots \end{bmatrix} = \begin{bmatrix} \Theta \end{bmatrix} \begin{bmatrix} \vec{y} \end{bmatrix}$$

$$\begin{bmatrix} \vdots \\ dz/dt \\ \vdots \end{bmatrix} = \begin{bmatrix} \Theta \end{bmatrix} \begin{bmatrix} \vec{z} \end{bmatrix}$$

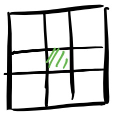
remove
extraneous
indicies

repeat sparse regression

Lecture 33

Cellular Automata (Von Neumann)

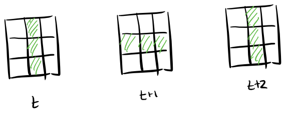
Game of Life (John Conway)

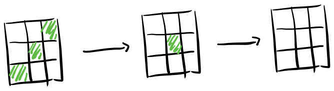


Each cell can be alive or dead

1. Any live cell with fewer than 2 neighbors dies
2. Any live cell with more than 3 neighbors dies
3. Any cell with 2 or 3 neighbors remains unchanged
4. Any dead cell with exactly 3 neighbors comes to life

Blinker





Ferreria & Fotanani (Phys Review E, 2002)

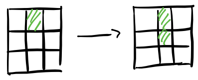
A prebiotic model for a surf-bonded autocatalytic chemical network

3 Rules

① Decay

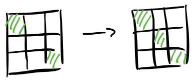
$A \xrightarrow{1} 0$

② Autocatalysis



$A+E \xrightarrow{s} 2A$

③ Cooperative Replication



$2A \xrightarrow{\mu} 3A$

$x = [A]$

$$\frac{dx}{dt} = -x + sx(1-x) + \mu x^2(1-x)$$

fixed point

$$-x(1-s(1-x) - \mu x(1-x)) = 0$$

$$x=0,\ \frac{1}{2\mu}\left(\mu - s \pm \sqrt{(\mu+s)^2 - 4\mu}\right)$$

$$\left.\frac{dx}{dt}\right|_{x=0} = s-1$$

$s<1$ --> $x=0$ is stable

$s>1$ --> $x=0$ is unstable