Temporal Learning, Modeling and Adaptation

April 2018

José Dorronsoro
Escuela Politécnica Superior
Universidad Autónoma de Madrid

Contents

1 Time Series Review

1.1 Stochastic Processes

Temporal Information Processing?

- First interpretation: the **processing of information that has a time structure**, i.e., time series
- Time series (TS): a time–ordered sequence of scalar or vector values X_t
- The temporal structure determines the behavior of X_t and must be taken into account to model it
- Second interpretation: the **temporal processing of information**
- Even if they do not have a temporal structure, data are (almost always) generated sequentially
- Examples: streaming data, on–line learning
- In both cases we get back to Machine Learning (although with different objectives)
  - Clearly so in on–line learning
  - After some roundabouts in practical TS modelling
- We deal first with time structured data

Time Series Contexts

- Two different TS origins:
  - **Stochastic generation**: the observed TS is a realization of a **stochastic process**
  - **Dynamical system evolution**: the observed TS is the trajectory of the solution of a continuous or discrete dynamical system (DS) from given initial conditions
- Different worlds (stochastic vs deterministic) but sometimes are hard to tell them apart
- Very different tools and perspectives
  - For stochastic TS we worry about **stationarity, ergodicity, spectral densities**; linear models and short term prediction are the main goals
  - For DS we worry about **sinks, sources, stability, attractors, chaos**; the main goal is non–linear long term behavior, often very sensible to initial conditions
- We begin with (general) stochastic processes and then briefly review the (much simpler) ARMA models

Basic Tools

- Probability Space: triplet made up of a set Ω, a subset $\mathcal{A}$ of 2^{Ω} and a probability P defined in $\mathcal{A}$

  - We associate $\mathcal{A}$ with the events to which we can assign a probability
  - If Ω is discrete, usually $\mathcal{A} = 2^{\Omega}$ (i.e., all possible subsets of Ω)
- Two subsets $A, B \in \mathcal{A}$ are **independent** if $P(A \cap B) = P(A)P(B)$
- Random variable: a function $X : \Omega \to \mathbf{R}$
  - As such X is deterministic; it is its arguments that are random
- Mean of X: $\overline{X} = \mu_x = E_P[X]$
- If $\mu_X < \infty$, its variance is $var(X) = E_P[(X - \mu_X)^2] = E_P[X^2] - \mu_X^2$
- The order k moment of X is $E_P[X^k]$

Computing Expectations

- What do we mean by $E_P[X]$?
- In simple cases it is clear:
  - If Ω discrete, $E_P[X] = \sum X(\omega)P(\{\omega\})$
  - If X takes discrete values $\{x_n\}$, $E_P[X] = \sum x_n P(\{\omega : X(\omega) = x_n\})$
- In general, one defines the expectation of X in terms of the **distribution function** of X

$$F(x) = F_X(x) = P(\{\omega : X(\omega) \leq x\})$$

  - Clearly $F(x)$ is increasing
  - If x is one–dimensional and F is derivable, $F'(x) = f(x)$ is its **density**
- Then for a general one–dimensional continuous X, $E[X]$ is defined as a **Stieltjes integral** of x with respect to F: $E[X] = \int x dF_X(x) = \int x dF(x)$
  - If F is differentiable, $E[X] = \int x f(x) dx$
  - We can also define $E_X[g(X)] = E[g(X)] = \int g(x) dF(x)$

Joint Distribution Function

- Given two r.v. X, Y their **joint distribution** $F(x, y)$ is defined as

$$\begin{aligned} F(x,y) &= F_{X,Y}(x,y) = P(\{\omega : X(\omega) \leq x, Y(\omega) \leq y\}) \\ &= P(\{X(\omega) \leq x\} \cap \{Y(\omega) \leq y\}) \end{aligned}$$

  - Then $\int_{y=-\infty}^{\infty} dF(x,y) = F(x,\infty) = P(\{\omega : X(\omega) \leq x\}) = F_X(x)$
  - If $F(x, y)$ is differentiable, $\frac{\partial^2 F}{\partial x \partial y} = f(x, y)$ is the joint density
- We can define $E_{X,Y}[g(X, Y)] = \int g(x, y) dF(x, y)$ also as a Stieltjes integral
  - If $F(x, y)$ differentiable, $\int g(x, y) dF(x, y) = \int g(x, y) f(x, y) dx dy$

- X, Y are said to be **independent** if the subsets $\{x_1 \leq x \leq x_2\}$ and $\{y_1 \leq y \leq y_2\}$ are independent
  - Then $F(x, y) = F_X(x)F_Y(y)$
- Similarly, if $X_1, \ldots X_K$ are random variables, we can define $F(x_1, \ldots x_K) = P(\{\omega : X_k(\omega) \leq x_k,\ k = 1, \ldots, K\})$

Stochastic Processes

- A **stochastic/random process** (SP) is a family $\{X_t\}$ of random variables on a common probability space $(\Omega, \mathcal{A}, P)$
  - We will consider discrete time: $\{t\} = \{\ldots, -1, 0, 1, \ldots\}$
  - If we fix a $\omega_0 \in \Omega$, a **sample path** or **realization** of a SP is the sequence $\{x_t = X_t(\omega_0)\}$
- Examples of SPs
  - **White noise**: X_t are independent variables with 0 mean and finite variance
  - **Brownian Motion**: $X_0 \equiv 0$, the increments $X_t - X_s$ are independent, $X_t - X_s = N(0, \sqrt{t-s}\ I)$
  - **Markov models**: $\Omega = \{1, \ldots, N\}$ is discrete and $P(X_{t+1} = j | X_t = i, X_{t-1} = i_{t-1}, \ldots, X_{t-k} = i_{t-k}) = P(X_{t+1} = j | X_t = i)$
    - $p_{ij} = P(X_{t+1} = j | X_t = i)$ is the **transition** matrix
- Kolmogorov's Theorem ensures the existence of underlying SPs
- But if the different X_t behave differently, it will be difficult to say much about them

Stationarity

- We can define the joint distributions $F_\tau(x_1, \ldots, x_K)$ for $\tau = (t_1, \ldots, t_K)$ of the SP X_t as $F_\tau(x_1, \ldots, x_K) = P(\{\omega : X_{t_k}(\omega) \leq x_k,\ k = 1, \ldots, K\})$
- The SP X_t is **strictly stationary** (SS) if for all K, τ and h we have for $\tau + h = (t_1 + h, \ldots, t_K + h)$
$$F_\tau(x_1, \ldots, x_K) = F_{\tau+h}(x_1, \ldots, x_K)$$
- If X_t is SS, $\mu_t = \int x dF_t(x) = \int x dF_{t+h}(x) = \mu_{t+h}\ \forall h$
- The **autocovariances** of X_t are
$$\begin{aligned} \gamma(r, s) &= cov(X_r, X_s) = E[(X_r - \mu_r)(X_s - \mu_s)] \\ &= \int (x - \mu_r)(x' - \mu_s) dF_{r,s}(x, x'), \end{aligned}$$
- If X_t is SS, $\gamma(r, s) = \gamma(r + h, s + h) = \gamma(r - s, 0)\ \forall r, s, h,$

Stationarity II

- Also $\gamma(r,s) = \gamma(s,r)$
- SS is very desirable, but perhaps too restrictive
- We relax it to just **stationarity** (S) (or weakly/second order stationarity) if we simply impose

$$\mu_t = \mu, \;\; \gamma(t+h,t) = \gamma(h,0) \;\; \forall t,h$$

  We just write $\gamma(h)$ instead of $\gamma(h,0)$
- In particular $\gamma(0) = var[X_t]$ for all t
- Moreover, if $\mu_t = 0$, $\gamma(h) \leq \gamma(0)$
- If we define the **autocorrelations** $\rho(h) = \gamma(h)/\gamma(0)$, we have $\rho(h) \leq 1$

Ergodicity

- The time series $\{x_t\}$ given as a realization of a S SP X_t is the only information that we have if we want to compute the statistics of all X_t
- Ergodicity makes possible to estimate moments of X_t from the time series values
- An intuitive idea is to estimate μ by the mean $\hat{\mu}_k = \frac{1}{2k+1}\sum_{-k}^{k} x_t$, for considering the RV $M_K = \frac{1}{2k+1}\sum_{-k}^{k} X_t$, we have

$$E[M_K] = \frac{1}{2k+1}\sum_{-k}^{k} E[X_t] = \frac{1}{2k+1}\sum_{-k}^{k} \mu = \mu$$

- If the variance σ_k^2 of $\hat{\mu}_k$ tends to 0, $\hat{\mu}_k$ **tends to μ in MSE** and we say that X_t is **mean–ergodic**
- **Slutsky's theorem**: A S SP X_t with covariance $\gamma(k)$ it is mean–ergodic iff $\lim \frac{1}{k+1}\sum_{0}^{k} \gamma(j) = 0$

Covariance Ergodicity

- Assuming $\mu = 0$, the intuitive variance estimation is now

$$\hat{v}_k = \frac{1}{2k+1}\sum_{-k}^{k} x_t^2,$$

  which is the mean of the SP X_t^2
- Now if X_t is a S SP, so is X_t^2 and we can apply again Slutsky's theorem
- The covariance $\gamma^2(k)$ of X_t^2 is $\gamma^2(k) = E[X_k^2 X_0^2] - E[X_0^2]^2$
- The Slutsky's condition for **covariance ergodicity** is now $\lim \frac{1}{k+1}\sum_{0}^{k} \gamma^2(j) = 0$ or, equivalently,

$$\lim \frac{1}{k+1}\sum_{0}^{k} E[X_j^2 X_0^2] = E[X_0^2]^2$$

1.2 Basic TS Models

AR and MA Models

- An **autoregressive** (AR) model of order p is a SP X_t with 0 mean where $X_t = \sum_1^p \phi_j X_{t-j} + \epsilon_t$, with ϵ_t white noise with variance σ^2
- If B denotes the **time delay** operator $BX_t = X_{t-1}$, we can write the above as

$$\epsilon_t = X_t - \sum_1^p \phi_j X_{t-j} = (I - \sum_1^p \phi_j B^j)\ X_t = \Phi(B)\ X_t$$

- A **moving average** (MA) model of order q is a SP X_t where $X_t = \epsilon_t + \sum_1^q \theta_j \epsilon_{t-j}$, with ϵ_t again white noise
- Just as before, we can write a MA (q) SP X_t as

$$X_t = \epsilon_t + \sum_1^q \theta_j \epsilon_{t-j} = (I + \sum_1^q \theta_j B^j)\ \epsilon_t = \Theta(B)\ \epsilon_t$$

Stationarity of AR and MA Models

- It is easy to see that if X_t is a S SP, $Y_t = \sum_0^q \theta_j X_{t-j}$ is also a S SP
- Thus any MA (q) SP is S
- If the series $\sum_0^\infty |\theta_j|$ converges and X_t is a S SP, the SP $Y_t = \sum_0^\infty \theta_j X_{t-j} = \sum_0^\infty \theta_j B^j X_t$ is also S
- What about AR (p) processes?
- If X_t is $AR(1)$ we have $\epsilon_t = X_t - \phi X_{t-1} = (1-\phi B)X_t$ or, formally, $X_t = (1-\phi B)^{-1}\ \epsilon_t = \sum_0^\infty \phi^j B^j\ \epsilon_t$
- If $|\phi| < 1$ the series converges; thus an $AR(1)$ process is S if $|\phi| < 1$ (in fact iff)
- Notice that the root $1/\phi$ of $\Phi(z) = 1 - \phi z$ lies outside the unit circle
- For a general AR (p) SP X_t we have formally $X_t = (\Phi(B))^{-1}\epsilon_t$, and **we can invert $\Phi(B)$ into a convergent series if the polynomial $\Phi(z)$ has all its roots outside the unit circle**
- Thus an AR (p) process X_t is S if(f) $\Phi(z)$ has all its roots outside the unit circle

ARMA Models

- An **ARMA** (p, q) model is a SP X_t s.t.

$$X_t = \sum_1^p \phi_i X_{t-i} + \sum_1^q \theta_j \epsilon_{t-j} + \epsilon_t,$$

  with ϵ_t white noise

- We can rewrite the above as $\epsilon_t + \sum_1^q \theta_j \epsilon_{t-j} = X_t - \sum_1^p \phi_i X_{t-i}$, i.e.

$$\Theta(B)\epsilon_t = \Phi(B)X_t$$

  for some polynomials Φ, Θ

- Formally we have $X_t = \Phi(B)^{-1}\Theta(B)\epsilon_t$, which we can express as

$$X_t = \sum_0^\infty \gamma_j B^j \Theta(B)\epsilon_t = \sum_0^\infty \delta_i B^i \epsilon_t$$

  if $\Phi(z)$ has all its roots outside the unit circle

- Thus an ARMA (p, q) process X_t is S if(f) $\Phi(z)$ has all its roots outside the unit circle

Covariance Functions

- Q1: How easy is to identify an ARMA process?
  - Right now this a too general question
- Q2: are there simple ways to characterize ARMA processes?
  - Yes: through their covariances
- In fact, covariances are sort of a **signature** of S SPs
- **Theorem**: a function $K : Z \to C$ is the autocovariance function of a (possibly complex) S TS iff it is **Hermitian and semi–definite positive**, i.e.,
  - $K(h) = \overline{K(-h)}$ and
  - For any $n \geq 0$ and $a \in C^n$, $a^t K(n) a \geq 0$, where $K(n)$ is the $n \times n$ matrix $K(n)_{ij} = K(i-j)$
- We can thus focus our attention on Hermitian and semi–definite positive functions

Spectral Covariance Representation

- **Riesz–Herglotz Theorem**: a function $\gamma : Z \to C$ is hermitian and semi–definite positive (i.e., an autocovariance function) iff

$$\gamma(h) = \int_{-\pi}^{\pi} e^{ih\omega} dF(\omega)$$

  with F a right–continuous, non decreasing function on $[-\pi, \pi]$ with $F(-\pi) = 0$

- Such an F is called the **spectral distribution** of γ
- If we can write $F(\omega) = \int_{-\pi}^{\omega} f(u)du$, we say that f is the **spectral density** of γ and then $\gamma(h) = \int_{-\pi}^{\pi} e^{ih\omega} f(\omega)d\omega$
- Notice that then $f(\omega) = F'(\omega) \geq 0$

- With (considerable) more work we can arrive at a spectral representation of a S SP X_t

Spectral Densities

- Spectral densities are much easier to handle
- If $\gamma(h)$ is summable (i.e., $\sum_h |\gamma(h)| < \infty$), Fourier series theory implies that

$$f(\omega) = \frac{1}{2\pi} \sum_{-\infty}^{\infty} \gamma(h) e^{ih\omega}$$

- An immediate consequence is that an absolutely summable $\gamma(h)$ is the autocovariance function of a S TS X_t iff $f(\omega) = \sum_{-\infty}^{\infty} \gamma(h) e^{ih\omega} > 0$
- Moreover, if X_t is real, f is symmetric
- Thus, S TSs with "simple" γ should have spectral densities easy to compute
- For instance, if ϵ_t is white noise with variance σ^2, its spectral density is $\sigma^2/2\pi$
- This is also the case for MA and (with more work) AR processes

Autocovariances of MA Processes

- MA processes have the simplest autocovariances:

  If X_t is a zero–mean S SP whose autocovariances verify $\gamma(h) = 0$ if $|h| > q$, then it is a MA(q) process

- More generally, if $\sum_0^{\infty} |\theta_k| < \infty$,

$$X_t = \sum_0^{\infty} \theta_k \epsilon_{t-k}$$

  is called a MA(∞) process

- It is relatively easy to check that its autocovariances verify

$$\gamma(h) = \sigma^2 \sum_0^{\infty} \theta_j \theta_{j+|h|}$$

Autocovariances of AR Processes

- The situation is more complicated for AR(p) processes
- Their covariances cannot be written in closed form unless p is small
- Usually they are all non zero
- To get them, recall that if X_t is AR(p) and $\Phi(z)$ has all its roots outside the unit circle, then we can write $\Phi(B)X_t = \epsilon_t$

- Multiplying both sides by X_{t-k} and taking expectations, we can get recurrence relations for $\gamma(k)$
- Easy exercise: compute them for $X_t = \phi X_{t-1} + \epsilon_t$, $\phi < 1$
- Nevertheless, AR and MA spectral densities are simpler to find

Spect. Densities of AR and MA Processes

- If we have $Y_t = \sum_{-\infty}^{\infty} \psi_j Z_{t-j} = \sum_{-\infty}^{\infty} \psi_j B^j Z_t$, with ψ_j real and Z_t is S with zero mean and spectral density (spd) f_Z, then Y_t is S with spectral distribution

$$F_Y(\omega) = \int_{-\pi}^{\omega} \left| \sum_{-\infty}^{\infty} \psi_j e^{-iju} \right|^2 f_Z(u)du = \int_{-\pi}^{\omega} \left| \sum_{-\infty}^{\infty} \psi_j \left(e^{-iu}\right)^j \right|^2 f_Z(u)du$$

  and $f_Y(\omega) = F'_Y(\omega) = \left| \sum_{-\infty}^{\infty} \psi_j \left(e^{-i\omega}\right)^j \right|^2 f_Z(\omega)$

- Since for an AR(p) X_t we have $\epsilon_t = \Phi(B)X_t$, it follows that

$$\frac{\sigma^2}{2\pi} = |\Phi(e^{-i\omega})|^2 f_X(\omega) \Rightarrow f_X(\omega) = \frac{\sigma^2}{2\pi} \frac{1}{|\Phi(e^{-i\omega})|^2}$$

- And since for a MA(q) X_t we have $X_t = \Theta(B)\epsilon_t$, its spd is $f_X(\omega) = \frac{\sigma^2}{2\pi}|\Theta(e^{-i\omega})|^2$

Spectral Densities of ARMA Processes

- For an ARMA(p, q) X_t we have $Y_t = \Phi(B)X_t = \Theta(B)\epsilon_t$, and putting together the previous equalities, we get

$$f_Y(\omega) = |\Phi(e^{-i\omega})|^2 f_X(\omega) = \frac{\sigma^2}{2\pi}|\Theta(e^{-i\omega})|^2$$

- Working things out we arrive at a rational spectral density

$$f_X(\omega) = \frac{\sigma^2}{2\pi} \frac{|\Theta(e^{-i\omega})|^2}{|\Phi(e^{-i\omega})|^2} = \frac{\sigma^2}{2\pi} \left| \frac{\Theta(e^{-i\omega})}{\Phi(e^{-i\omega})} \right|^2$$

- Since rational functions (and polynomials) are dense in $C([-\pi, \pi])$, a process with a symmetric continuous spd can be approximated in an appropriate sense by ARMA(p, q) or MA(q) processes
- But this has more theoretical than practical interest

ARIMA Models

- In general, time series are not stationary, with a typical instance being SP of the form $X_t = m_t + s_t + Y_t$, with m_t the **trend**, s_t a (periodic) **seasonal** component and Y_t a S SP

- The removal of m_t is problem dependent, with a frequent choice being the application of some power Δ^d of the difference operator $\Delta X_t = \Delta_1 X_t = X_t - X_{t-1}$
- A seasonal component with period S (i.e., $s_t = s_{t+S}$) can be removed applying the operator Δ_S, i.e. $\Delta_S X_t = X_t - X_{t-S}$
- An ARIMA (p, d, q) model is a SP X_t such that $\Delta^d X_t$ is an ARMA (p, q) model
- A seasonal ARIMA $(p, d, q) \times (P, D, Q)_S$ SP X_t can be formally expressed as

$$\Phi(B^S)\Phi(B)\Delta_S^D\Delta^d(X_t) = \Theta(B^S)\Theta(B)\epsilon_t$$

ARX and NARX Models

- Thus things get progressively more complicated and drift towards **system identification**, i.e., to use statistical methods to build mathematical models of dynamical systems from measured data
- Moreover, there may be some other inputs U_t that we may want to incorporate to our model
- In an autoregressive with exogenous inputs (ARX) model we assume that our target X_t has the form

$$X_t = \sum_1^D \phi_j X_{t-j} + \sum_0^{D'} \theta_{j'} U_{t-j'} + \epsilon_t$$

- Issues such as stationarity or ergodicity start to fade ...
- In a non linear ARX (NARX) the target X_t is a non linear function of the $X_{t-j}, U_{t-j'}$:

$$X_t = \Phi(X_{t-1}, \ldots, X_{t-D}, U_t, U_{t-1}, \ldots, U_{t-D'}) + \epsilon_t$$

- Besides being reasonable by themselves, they also appear when studying dynamical systems

2 Dynamical Systems

2.1 Linear Differential Equations

From AR to Dynamical Systems

- If in an AR process we impose $\epsilon_t = 0$ we are left with the difference equation $x_t = \sum_1^p \alpha_j x_{t-j}$
- In general, we say that a system $X_t \in \mathbf{R}^d$ follows a discrete differential equation if $X(t+1) = x_{t+1} = F(x_t) = F(X(t))$
- In turn writing $X'(t) \simeq X(t+1) - X(t) = F(X(t)) - X(t) = G(X(t))$, we arrive to a system of differential equations $X' = G(X)$

- Differential equation systems have behind a rich (and sometimes difficult) theory
- Basic examples: linear systems

Linear Systems

- An **autonomous linear system** is given by

$$X' = AX, \quad X(0) = x_0 \tag{1}$$

  for a $d \times d$ matrix A
- Basic example: (homogeneous) harmonic oscillator $x'' + ax' + bx = 0$
- Setting $y = x'$ we have $x' = y$, $y' = -bx - ay$; that is, for $X = (x, y)^t$, we have

$$X' = \begin{pmatrix} 0 & 1 \\ -b & -a \end{pmatrix} X = AX$$

- The **exponential** of a matrix B is $e^B = \sum_0^\infty \frac{B^n}{n!}$
- The general solution of (1) when $X(0) = x_0$ is $X(t) = e^{tA}x_0$

The Linearity Principle

- The eigenanalysis of A is the basic tool to study linear systems:
  if $Av_0 = \lambda v_0$, then $V(t) = e^{\lambda t}v_0$ is a solution with $V(0) = v_0$
- Now assume that λ_1, λ_2 are distinct eigenvalues of A with eigenvectors v_1, v_2, and let $x_0 = \alpha_1 v_1 + \alpha_2 v_2$
- Then we can find the solution of $X' = AX$ with $X(0) = x_0$ by writing

$$X(t) = \alpha_1 e^{\lambda_1 t} v_1 + \alpha_2 e^{\lambda_2 t} v_2$$

- This is a particular case of the **Linearity Principle**:

  If $Y_1(t), Y_2(t)$ are solutions of $X' = AX$ and $Y_1(0), Y_2(0)$ are linearly independent, then $X(t) = \alpha Y_1(t) + \beta Y_2(t)$ is the unique solution that satisfies $X(0) = \alpha Y_1(0) + \beta Y_2(0)$
- Simplest linear systems: **planar** systems in $\mathbf{R}^2$

Higher Dimensional Systems

- In principle for any $d \times d$ matrix A, $e^{tA}x_0$ yields the (unique) solution of $X' = AX$ with $X(0) = x_0$
- However the eigenstructure of a general A is more complicated than in the planar case
- Simplest situation: A has d **distinct eigenvalues**
- Then A can be transformed as $M = TAT^{-1}$ into a matrix M made up of a diagonal block and a series of 2–dimensional diagonal blocks $\begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}$

- The structure of M when there are repeated eigenvalues is given by the (more complicated) **Jordan form** of A
- However, matrices with distinct eigenvalues are what is to be expected:

  The subset of matrices with d distinct eigenvalues is an **open and dense** *subset of the set of $d \times d$ matrices*

Non Autonomous Linear Systems

- The general form of a non autonomous linear system is $X' = A(t)X$, with $A(t)$ a time varying $d \times d$ matrix
- A general discussion of such systems is not possible; a simpler situation is that of **forced linear system** (FS)

$$X' = AX + G(t),\ X(0) = x_0$$

- The time independent system $X' = AX$ is the **homogeneous equation** (HE)
- If we know a particular solution Z of the FS and X is a solution of the HE, $Y = Z + X$ is another solution of the FS with initial condition $X(0) + Z(0)$
- Conversely, if Y, Z are solutions of the FS, $X = Y - Z$ is a solution of the HE with $X(0) = Y(0) - Z(0)$
- Since $e^{tA}x_0$ gives the general solution of the HE, **it is enough to find a particular solution to the FS**

Variation of Parameters

- Given the FS $X' = AX + G(t),\ X(0) = x_0$, a first try to solve it is to guess a particular solution; this is the method of **undetermined coefficients**
- However such a guess is not usually easy; the method of **variation of parameters** yields a (theoretical) general solution
- The solution of the above FS for $X(0) = x_0$ is given by

$$X(t) = e^{tA}\left(x_0 + \int_0^t e^{-sA}G(s)ds\right)$$

- The difficulty is, of course, to compute the integral!!

2.2 Planar Systems

Planar Systems

- A planar system is an autonomous linear system in $\mathbf{R}^2$, that is a function $X(t) \in \mathbf{R}^2$ such that

$$X' = AX,\quad X(0) = x_0$$

- Solution again given as $X(0) = x_0$ is $X(t) = e^{tA}x_0$
- If $A = \text{diag}\,(\lambda_1, \lambda_2)$ then

$$e^{tA} = \begin{pmatrix} e^{t\lambda_1} & 0 \\ 0 & e^{t\lambda_2} \end{pmatrix}$$

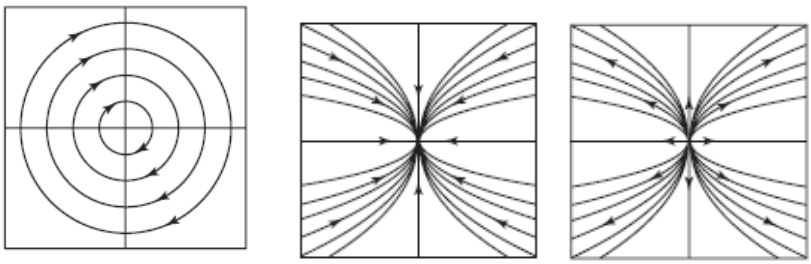
- Now A is a 2×2 matrix and its eigenanalysis is quite simple
- Thus, planar systems can be studied quite exhaustively

Phase Portraits

- The goal in the study of dynamical systems is often to understand their asymptotic behavior
- This is depicted using **phase portraits**
- The phase portrait of a planar system is a picture of a collection of representative solution curves in $\mathbf{R}^2$, which we call the **phase space**, for which a general idea of their evolution can be derived
- **Critical points** (and **equilibrium solutions**) arise when $0 = X' = AX$, with 0 the only critical point if $\det A \neq 0$

Examples of Phase Portraits

- Here are some examples associated at particular planar systems



- We can arrive to a complete understanding of the behavior of planar systems mapping the eigenanalysis of A into phase portraits

Planar Systems in Canonical Form

- Eigen values of a 2×2 matrix A: either two distinct real eigenvalues, or two repeated real eigenvalues, or two complex conjugate eigenvalues
- A 2×2 matrix A is in **canonical form** if it has one of the following forms:

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \quad \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}, \quad \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}$$

- We will split the analysis of these cases according to the eigenvalues of A:
  - A has two distinct real eigenvalues, i.e., the first matrix with $\lambda_1 \neq \lambda_2$
  - A has two complex conjugate eigenvalues, i.e., the second matrix
  - A has a single repeated real eigenvalue, i.e., the first matrix with $\lambda_1 = \lambda_2$ or the third matrix
- These cases will determine the limit behavior of the solutions of a general $X' = AX$

Real Distinct Eigenvalues I: Saddle Points

- If there are two non zero, distinct real eigenvalues λ_1, λ_2, we have

$$X(t) = \exp\left(t \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}\right) x_0 = \begin{pmatrix} e^{\lambda_1 t} & 0 \\ 0 & e^{\lambda_2 t} \end{pmatrix} x_0 = \begin{pmatrix} \alpha e^{\lambda_1 t} \\ \beta e^{\lambda_2 t} \end{pmatrix}$$

- There are three important cases: i) $\lambda_1 < 0 < \lambda_2$, ii) $\lambda_1 < \lambda_2 < 0$, iii) $0 < \lambda_1 < \lambda_2$
- In the case $\lambda_1 < 0 < \lambda_2$,
  - The solutions $\alpha e^{\lambda_1 t}$ tend to 0 as $t \to \infty$: they lie in the **stable** line
  - The solutions $\beta e^{\lambda_2 t}$ tend away from 0 as $t \to \infty$: they lie in the **unstable** line
  - The solutions for $\alpha, \beta \neq 0$ tend to $\pm\infty$ getting closer to the unstable line
- The origin is the only equilibrium point, which we call a **saddle point**

Real Distinct Eigenvalues II: Sinks

- When $\lambda_1 < \lambda_2 < 0$, both solutions $\alpha e^{\lambda_1 t}, \beta e^{\lambda_2 t} \to 0$ when $t \to \infty$
- For a general solution $X(t) = \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \alpha e^{\lambda_1 t} \\ \beta e^{\lambda_2 t} \end{pmatrix}$, writing $x(t) = \alpha_1 e^{\lambda_1 t}$, $y(t) = \alpha_2 e^{\lambda_2 t}$, we have

$$\frac{dy}{dx} = \frac{y'}{x'} = \frac{\lambda_2 \alpha_2 e^{\lambda_2 t}}{\lambda_1 \alpha_1 e^{\lambda_1 t}} = \frac{\lambda_2 \alpha_2}{\lambda_1 \alpha_1} e^{(\lambda_2 - \lambda_1) t}$$

  which tends to $\pm\infty$ when $\alpha_2 \neq 0$
- Thus the trajectories **tend to 0 tangentially to the Y axis**
- The origin, again the only equilibrium point, is now called a **sink**

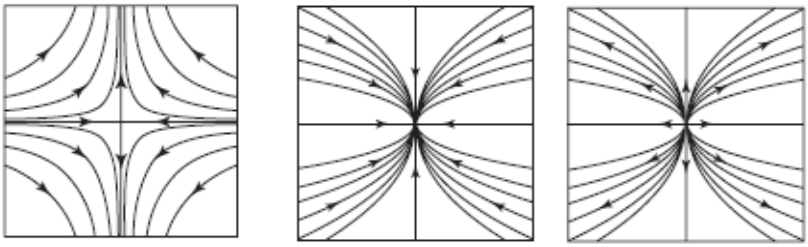
Real Distinct Eigenvalues III: Sources

- When $0 < \lambda_2 < \lambda_1$, a similar analysis yields
  - Both solutions $\alpha e^{\lambda_1 t}, \alpha e^{\lambda_2 t} \to \infty$ when $t \to \infty$
  - Writing as before $x(t) = \alpha_1 e^{\lambda_1 t}$, $y(t) = \alpha_2 e^{\lambda_2 t}$, we have that $\frac{y'}{x'}$ tends to 0 when $\alpha_2 \neq 0$

- Thus the trajectories **tend to ∞ away from 0 tangentially to the Y axis initially and becoming "horizontal"** as $t \to \infty$
- The origin, again the only equilibrium point, is now called a **source**
- When one of the eigenvalues, say $\lambda_1 = 0$, the X–axis defines an equilibrium line
- The other solutions tend to ∞ away from the axis if $\lambda_2 > 0$ or to 0 otherwise

Saddles, Sinks and Sources

- We depict saddles (left), sinks and sources (right) for planar systems in canonical form



From Hirsch et al., *Differential equations dynamical systems and an introduction to chaos.*

Complex Eigenvalues

- When $A = \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}$ the eigenvalues are $\alpha \pm i\beta$
- This yields two real solutions

$$e^{\alpha t} \begin{pmatrix} \cos \beta t \\ -\sin \beta t \end{pmatrix}, \quad e^{\alpha t} \begin{pmatrix} \sin \beta t \\ \cos \beta t \end{pmatrix}$$

  and the general solution

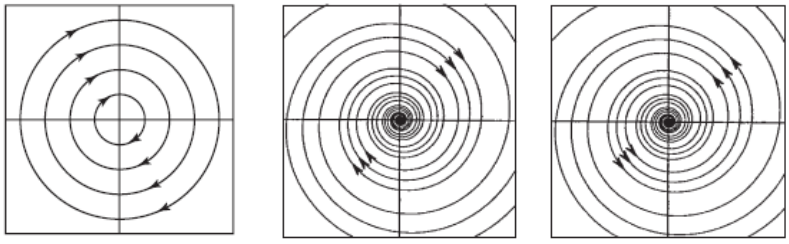
$$X(t) = c_1 e^{\alpha t} \begin{pmatrix} \cos \beta t \\ -\sin \beta t \end{pmatrix} + c_2 e^{\alpha t} \begin{pmatrix} \sin \beta t \\ \cos \beta t \end{pmatrix}$$

- If $\alpha = 0$, we have $\|X(t)\|^2 = c_1^2 + c_2^2$, i.e., the solutions **cycle** around 0
- If $\alpha \neq 0$, we get spirals that turn towards the origin when $\alpha < 0$ or away from it when $\alpha > 0$

  That is, we get **spiral sinks or sources**

Circles and Spiral Sinks and Sources

- We depict circles (left) and spiral sinks and sources (right) for planar systems in canonical form



From Hirsch et al., *Differential equations dynamical systems and an introduction to chaos.*

Repeated Real Eigenvalue

- We get a single repeated eigenvalue λ when we have

$$A = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \text{ or } A = \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}$$

- In the first case the solutions are $X(t) = e^{\lambda t}V$ for any $V = X(0)$;
  thus the trajectories are straight lines through $(0, 0)$ that either tend to 0 when $\lambda < 0$ or to ∞
- The solutions in the second case are obtained by the method of **undetermined coefficients**: they are assumed of the form $x(t) = \alpha e^{\lambda t} + \mu t e^{\lambda t}$ for some α, μ
- Plugging this into the equation results in

$$X(t) = \alpha e^{\lambda t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \mu e^{\lambda t} \begin{pmatrix} t \\ 1 \end{pmatrix}$$

- If $\lambda < 0$ the solutions $\to 0$ as $t \to \infty$; if $\lambda > 0$ they $\to \infty$
- In either case the solutions tend toward or away from $(0, 0)$ in a direction tangent to $(1, 0)$

Changing Coordinates

- Assume we want to solve $X' = AX, X(0) = x_0$ for a general matrix A
- We can find an invertible matrix T such that $M = TAT^{-1}$ is in canonical form
- Let Y be a solution of $Y' = MY$ with $Y(0) = y_0 = Tx_0$; setting $X = T^{-1}Y$ we obtain a solution of $X' = AX$ with $X(0) = T^{-1}y_0$
- Conversely, $Y = TX$ converts solutions of $X' = AX$, $X(0) = x_0$ into solutions of $Y' = TAT^{-1}Y$ with $Y(0) = y_0$
- The transformation T changes the initial coordinates X into the canonical form coordinates $Y = TX$

- Therefore the phase portraits for general planar systems $X' = AX$ can be derived from the phase portraits of canonical form system $Y' = MY$ by applying the T^{-1} coordinate change
- We thus obtain equilibrium points, sinks, sources, cycles or spirals that correspond to appropriate coordinate changes of the ones in canonical form

The Trace–Determinant Plane I

- It can be easily seen that the eigenvalue equation of a 2×2 matrix A is of the form

$$\lambda^2 - \text{ tr } A\ \lambda + \text{ det } A = \lambda^2 - \tau\lambda + \delta = 0$$

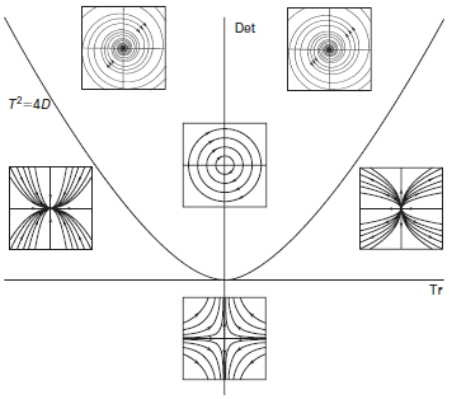
  with solutions $\lambda_\pm = \frac{1}{2}\left(\tau \pm \sqrt{\tau^2 - 4\delta}\right)$
- As a consequence we have
  - Complex conjugate eigenvalues when $\tau^2 < 4\delta$
  - Real different eigenvalues when $\tau^2 > 4\delta$
  - Real repeated eigenvalues when $\tau^2 = 4\delta$
- The parabola $\delta = \tau^2/4$ separates complex (above) from real (on or below) eigenvalues

The Trace–Determinant Plane II

- The real part of the complex eigenvalues above is $\tau/2$ and, therefore
  - We have a spiral sink if $\tau < 0$ and a spiral source when $\tau > 0$
  - We get a circle when $\tau = 0$
- Below the parabola we have a saddle when $\delta = \lambda_-\lambda_+ < 0$
- When $\delta > 0$, since $|\tau| > \sqrt{\tau^2 - 4\delta}$, we have sign $\lambda_\pm =$ sign τ; thus
  - We get a (real) source point when $\tau > 0$
  - We get a (real) sink point when $\tau < 0$
- One eigenvalue is 0 when $\delta = 0$ but $\tau \neq 0$ while both are 0 if $\delta = \tau = 0$

The Trace–Determinant Plane III

- The following plane diagram summarizes the preceding discussion



From Hirsch et al., *Differential equations dynamical systems and an introduction to chaos.*

2.3 Nonlinear Dynamical Systems

Nonlinear Dynamical Systems

- A dynamical system (DS) is a procedure that describes the behavior in time of all points of a given space (Euclidean space, manifolds, ...)
  - They are characterized by the **flow**, a function $\Phi_t : \mathbf{R}^d \to \mathbf{R}^d$ that takes x into $x_t = X(t) = \Phi_t(x)$
  - We call them **discrete or continuous** depending on how we consider time change
- Basic example: $\Phi_t(x)$ being the solution of a system of ordinary differential equations (ODE) $X' = F(X)$
- The behavior of general non linear DSs (NDS) may be quite complicated:
  - Most NDS are impossible to solve analytically
  - Some do not have solutions with a given initial value, some may have infinitely many ones
  - Solutions need not be defined for all time values t as they may tend to ∞ in finite time

Basic Results on ODEs

- **Existence and Uniqueness**: If F is C^1, given t_0 and x_0, there exists an $\epsilon > 0$ and a unique solution $X : (t_0 - \epsilon, t_0 + \epsilon) \to \mathbf{R}^d$ such that $X(t_0) = x_0$
  - Proved by the Picard iteration technique
  - We can show that we have a unique solution defined on a maximal time domain
  - However, the solution may not be defined for all t even for nice F

- **Continuous Dependence of Solutions**: If F is C^1 and $X(t)$ is a solution defined on $[t_0, t_1]$ with $X(t_0) = x_0$, then there is a neighborhood U of x_0 and a constant K such that if $y_0 \in U$, then there is a unique solution $Y(t)$ defined on $[t_0, t_1]$ with $Y(t_0) = y_0$ and for all $t \in [t_0, t_1]$

$$|Y(t) - X(t)| \leq K|y_0 - x_0|e^{K(t-t_0)}$$

  - In particular the flow $\Phi_t(x)$ is continuous in X

- **Continuous Dependence on Parameters**: If $X' = F(X, a)$ and F is C^1 on a and x, the flow $\Phi_t(X, a)$ depends continuously on a

Phenomena on Nonlinear DS

- This is almost as far as the general theory goes: many more tools have been developed but are often applicable only on concrete systems ...
- Moreover new issues and non standard behavior appear: **bifurcations, strange attractor, chaotic systems**, ...
- Chaos (Lorenz): *When the present determines the future, but the approximate present does not approximately determine the future*
- The Lorenz's system opened the way to the consideration of these phenomena

Lorenz's System I

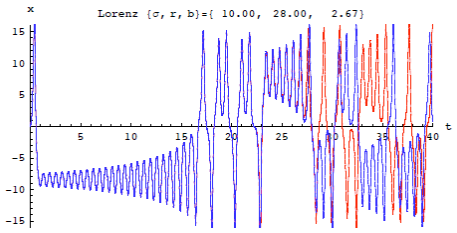
- First goal: a simple approximation to atmospheric flow that models as a two-dimensional fluid cell heated from below and cooled from above
- Further simplified to three independent variables: the rate of convectivity (x; **convection**: the process of heat transfer by a moving fluid), and the horizontal and vertical temperature variation (y and z, respectively)
- Equations: for parameters σ, b, r

$$\dot{x} = \sigma(y - x);\ \dot{y} = r\ x - y - x\ z;\ \dot{z} = x\ y - b\ z$$

- The asymptotic behavior is relatively simple in some cases
  - $r < 1$: all solutions of the Lorenz system tend to the equilibrium point at the origin or
  - $1 < r < r^* = \sigma\left(\frac{\sigma+b+3}{\sigma-b-1}\right)$: the two non–zero equilibrium points $Q_\pm$, i.e., the solutions of $F(Q) = 0$, are sinks

Lorenz's System II

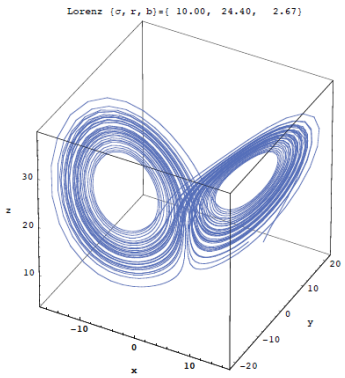
- Lorenz's significant parameters: $\sigma = 10$, $b = 8/3$, $r = 28$
- While being a deterministic system, it is very sensible to very small changes in initial conditions



- Butterfly effect: the flap of a butterfly's wing in Brazil can result in a tornado in Texas

Lorenz's Attractor

- All non–equilibrium solutions tend eventually to the so-called **Lorenz attractor**, roughly speaking an invariant set that "attracts" all nearby solutions



Discrete Dynamical Systems

- The theory of continuous DS focuses on the asymptotic behavior of solutions, assuming of course the system to be known
- If we are interested in (practical) prediction purposes we turn our attention to **discrete** DS (DDS)
- A Discrete Dynamical System is a pair $(\mathcal{X}, T)$ made up of the **state space** $\mathcal{X}$ (i.e., the set of all possible system states, that we assume bounded) and the map $T : \mathcal{X} \to \mathcal{X}$
- Starting at an $x_0 \in \mathcal{X}$ we get a **trajectory** or **orbit** $\{x_0, T(x_0), T^2(x_0), \ldots\}$ of the system
- A way to catch the behaviour of a DDS is to study the asymptotic behavior of orbits
- Long-term system properties are described in terms of **attractors**

Attractors of DDSs

- As for planar systems, the simplest cases are those of attracting points or cycles, but much more complicated attractors are possible
- In broad terms, we say that a compact set A is an **attractor** of a DDS with fundamental neighborhood U if
  - **Invariance**: for all $x \in A$ and all n, $T^n(x) \in A$
  - **Attractivity**: there is an open subset V s.t. $A \subset V$ and if $x \in V$, $T^n(x) \in V$ for all n and $\cap_n T^n(V) = A$
  - **Transitivity**: given any points $y_1, y_2 \in A$ and open neighborhoods U_j of y_j in U, there is a solution curve starting at U_1 and passing through U_2
- When we talk about evolution on the attractor, we actually mean in a neighborhood of the attractor

DS Reconstruction I

- In practice the dynamical system itself is rarely known and its study has to be done from a single orbit
- Moreover, instead of an orbit usually the most we can get is a time series of **measurements**

$$Y = \{y_0, y_1, y_2, \ldots\} = \{f(x_0), f(T(x_0)), f(T^2(x_0)), \ldots\}$$

  derived from a **read out map** $f : \mathcal{X} \to \mathbf{R}$
- In fact we often want a model $g : \mathbf{R}^k \to \mathbf{R}$ that helps us to predict the behavior of Y
- Q: Can we get it?

DS Reconstruction II

- At first sight we would need to know X to do any reconstruction
- So the first question could be:

  Can we reconstruct the internal state of the system from such a TS?
- But getting X is hopeless; we may at most answer another question:

  Can we get a somewhat equivalent representation of the internal state X from the TS?
- Tool: **reconstruction maps over time delays**
- For a fixed k define

$$R_k(x) = (f(x), f(T(x)), \ldots, f(T^{k-1}(x))$$

- Then $R_k(x_i) = (y_i, \ldots, y_{i+k-1})$

Takens Theorem

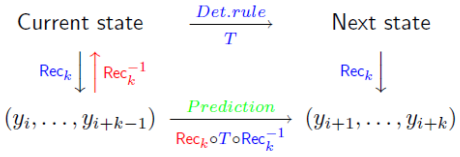
- Assume $\mathcal{X}$ is bounded and set $\mathcal{T} \times \mathcal{F}$ be the Cartesian product of the spaces of C^1 mappings T and C^1 readouts f; then

  There is an open dense subset $U \subset \mathcal{T} \times \mathcal{F}$ such that if $(T, f) \in U$ and $k > 2$ dim$(\mathcal{X})$, the reconstruction map R_k is a C^1 embedding of $\mathcal{T}$ in $\mathbf{R}^k$ with a C^1 inverse

- The density of U implies that such an embedding exists "very near" any (T, f)
- Moreover, **the embedding preserves the structural properties of** T: the image $R_k(A)$ of an attractor A is an attractor (embedded) in $\mathbf{R}^k$ and the observed orbit has the "same properties" of the underlying one
- More importantly, we have a path to predict the next state of the time series

From Takens Theorem to Predictions

- We have the following diagram



S. Laur, Time Series of Deterministic Dynamic Systems, 2004

- Setting $G = R_k^{-1} \circ F \circ R_k$, we have

$$(y_{i+1}, \ldots, y_{i+k-1}, y_{i+k}) = G(y_i, \ldots, y_{i+k-1}),$$

  i.e., there is a function $g = G_1$ s.t. $y_{t+1} = g(y_t, \ldots, y_{t-k+1})$ for all t

Time Series Prediction

- To exploit the preceding we need
  - A way to estimate an appropriate k
  - A way to estimate the function g
- The **correlation dimension** $cdim(A)$ of the attractor can be used to estimate an adequate k_0: since $cdim(A) = cdim(R_k(A))$, we may look for a k_0 after which $cdim(R_k(A))$ stabilizes
  - Often this is easier said than done!!
- In any case, we get back to non–linear regression problems and ...

- We may look to say, MLPs (o SVR) models to approximate the non–linear AR model $y_{i+k} = g(y_i, \ldots, y_{i+k-1})$

Back to TS Prediction by ML

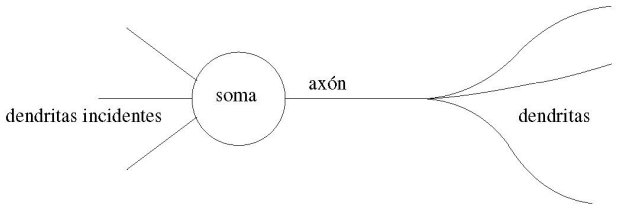
- Predicting temporal information coming from either a time series or a dynamical system ends up in building proper models over time delays
  - Quite often we can/have to add exogenous information that can improve our predictions
- We thus fall in a natural way into possibly non–linear regression models that we may try to build using ML models
  - The temporal structure should be preserved for instance when choosing train/test splits
  - But this structure is often no longer taken into account after that
- ML models are usually built parameterizing the desired model as $f(x, w)$, defining a loss $L(w|S)$ over a sample S and minimizing L iteratively
- Handling temporal information comes thus back when actually training models
  - Because of sample patterns appearing sequentially
  - Or just in the iterative way model building proceeds
- We turn now to these issues

3 From Perceptrons to Deep Networks

3.1 Rosenblatt's Perceptrons

Basic Neural Models

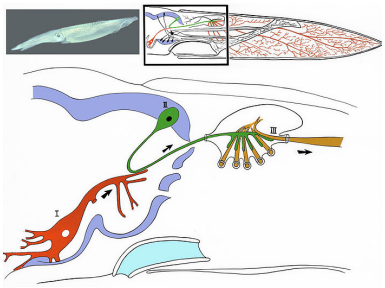
- Basic model: Ramón y Cajal's neuron (1900)



- Basic behavior: the neuron either fires or stays at rest depending basically on its inputs
- The brain has about 10^{11} neurons with each one having about 7,000 connections, often recurrent

Hodgkin–Huxley

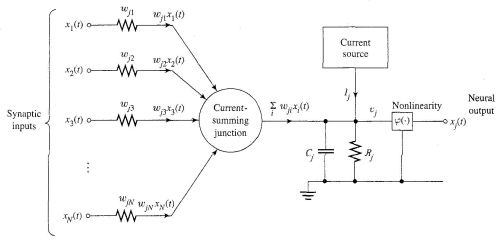
- They developed (circa 1935) the first model to describe the generation and propagation of electrical **action potentials** in neurons



From Wikipedia's Squid Giant Synapse

Electronic Neuron

- Electronic version: McCulloch–Pitts (1940)



  - Since $I = \frac{V}{R} = wV$, with w the conductance, the McC–P neuron output is

$$H\left(\sum_{j=1}^{N} w_j V_j + I\right) = V$$

    with the Heaviside function H ensuring a 0–1 output

- The **perceptron** is a mathematical formulation of the McC–P neuron where **the conductances are to be learned**

Rosenblatt's Perceptron

- Given a sample $S = \{(x^p, y^p)\}$ with $y^p = \pm 1$, Rosenblatt's Perceptrons (PCPs) are linear machines $w \cdot x$ such that

$$w \cdot x^p > 0 \quad \text{if} \quad y^p = 1$$
$$w \cdot x^p < 0 \quad \text{if} \quad y^p = -1$$

- This can be seen as a **homogeneous** classification problem
- In more compact form we want for all p

$$y^p \;\; w \cdot x^p > 0$$

- If such a **separating** w exists, it can be computed in many ways
- Rosenblatt's goal was to **learn** w, i.e., to arrive at a separating w by repeatedly examining the (x^p, y^p) and adjusting w if necessary

Rosenblatt's Delta Rule

- The **Delta Rule** algorithm

```
Start with w = 0
While stopping condition not met:
   Get a new pattern (x^p, y^p) = (x^{p(t)}, y^{p(t)})
   if y^p w · x^p ≤ 0 then:
      w = w + y^p x^p
```

- Writing w for the new vector and w' for the previous one, notice that

$$y^p \;\; w \cdot x^p = y^p \;\; w' \cdot x^p + \|x^p\|^2 > y^p \;\; w' \cdot x^p$$

Novikov's Theorem

- It states that if the sample S is linearly separable, the Delta rule yields a separating w in a finite number of steps
- More precisely, if for some separating hyperplane w with $\|w\| = 1$ we have $\min_p y^p w \cdot x^p = \gamma > 0$, then

  a separating w' can be found after at most $T = R^2/\gamma^2$ wrong classifications, where $R = \max_p \|x^p\|$

- Notice that γ is the margin of the w hyperplane. Thus, if

$$\gamma^* = \min_{\|w\|=1} m(w, S) = \min_{\|w\|=1} \min_p y^p w \cdot x^p$$

  is the **maximum margin**, we will need at most $R^2/(\gamma^*)^2$ iterations to train a Perceptron

- The maximum margin hyperplane gives the best (smallest) Novikov bound
- And problems with smaller margins require more iterations

Proof Sketch

- We consider only time–labelled wrong patterns, i.e., x^t is the t–th pattern such that $y^t w^{t-1} \cdot x^t \leq 0$
- We then have $\|w^t\|^2 \leq \|x^t\|^2 + \|w^{t-1}\|^2$, which leads to

$$\|w^t\|^2 \leq \|x^t\|^2 + \ldots + \|x^1\|^2 + \|w^0\|^2 \leq tR^2$$

  if $w^0 = 0$ and $\|x^p\| \leq R$ for all p
- Similarly, if w' is a 1–norm separating hyperplane i.e., $\min_p y^p w' \cdot x^p = \gamma > 0$ for all p, we have

$$w^t \cdot w' \geq \gamma + w^{t-1} \cdot w' \geq \ldots \geq t\gamma + w^0 \cdot w'$$

- Putting both together we have for all t for which x^t is erroneous

$$t\gamma \leq w^t \cdot w' \leq \|w^t\| \leq \sqrt{t}R$$

  which implies $t \leq R^2/\gamma^2$
- Thus, the Delta Rule can stop after at most R^2/γ^2 iterations

Problems with Perceptrons

- Observation 1: A PCP can learn (obviously) only linearly separable problems; for instance, it can learn the AND and OR predicates

(a) AND *(b)* OR

- But a PCP cannot learn the XOR predicate

01_1 11_0

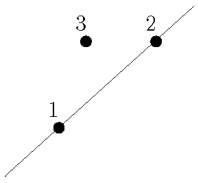
00_0 10_1

Dichotomies

- Observation 2: for PCPs to be useful, linearly separable problems must be frequent
- Q: how frequent are they?
- A dichotomy for $S = \left\{x^1, x^2, \ldots, x^N\right\}$ is any separation of S in two classes
- It corresponds to any asignment of the ± 1 values to the x^p
- The total number of dichotomies is 2^N
- Thus, the total number of 2-class problems over S is 2^N

Cover's Theorem

- The points in S are in general position if there are not $D+1$ patterns in a $D-1$–dimensional hyperplane



- **Theorem** If S is in general position, the number $L(N, D)$ of linearly separable dichotomies is

$$L(N, D) = \left\{ \begin{array}{ll} 2^N & \text{si } N \leq D+1 \\ 2\sum_{i=0}^{D} \binom{N-1}{i} & \text{si } N \geq D+1 \end{array} \right\}$$

Thus ...

- Notice that for D fixed,

$$\frac{L(N, D)}{2^N} \to 0$$

  as $N \to \infty$
- In practice we can expect $N \gg D$ and the fraction of separable dichotomies will be very small
- Thus, linear PCPs will not be useful
- But a one hidden layer PCP can solve XOR and, in fact, separate any convex region

- And a two hidden layers PCP can separate any polyhedral region and hence solve any classification problem
- The same is essentially true for regression problems
- **But:** no algorithm is known to learn these 2–hidden layer PCPs

Why Not Try to Minimize Some Loss?

- Rosenblatt's Perceptrons are natural **online** machines:
  - Patterns appear sequentially and each may change the current weights
- We can also define a perceptron loss over a given sample as

$$L(w|S) = -\sum_{\{p:y^p w\cdot x^p<0\}} y^p w\cdot x^p$$

- The local error would thus be $-y^p w\cdot x^p$ when $y^p w\cdot x^p<0$ and 0 otherwise
- Since $\nabla_w - y^p\ w\cdot x^p = -y^p\ x^p$, the Delta Rule can be seen as a kind of local gradient descent on the loss $L(w|S)$
- However $L(w|S)$ is not differentiable and it is not clear what to make of $\nabla_w L(w|S)$ ...

What Can We Do?

- First option: build trainable PCPs replacing the Heaviside function
  - Work with differentiable PCP transfer function
  - Transform PCP training into a differentiable optimization problem
  - This is what we will do next
- Second option: work with linear models but somehow ensure that $d \gg N$
  - Have to overcome that in practice we usually have $N \gg d$
  - Transform the original d–dimensional features x in new D–dimensional ones such that $D \gg d$
  - This is the goal of kernel–based Support Vector Machines

3.2 Linear and Logistic Regression

Improving on the PCP: Linear Regression

- The simplest way to avoid the non–differentiability of Heaviside function is simply to drop it and work with a straight linear model $f(x,w) = w_0 + w\cdot x$
- Rosenblatt's loss doesn't make sense anymore but we could try seeing the y^p as targets and then minimize the **mean squared error** loss

$$\widehat{e}(w_0,w) = \frac{1}{2N}\sum_p (y^p - w_0 - w\cdot x^p)^2$$

  which ends up being a simple quadratic form

- The **linear regression** problem reduces to **minimize** $\widehat{e}_S(W)$, i.e.,
- Building linear classifiers with targets $y = \pm 1$ is not a good idea
- But for general regression targets linear regression is the natural starting point

Improving on the PCP: Logistic Regression

- A second alternative could be to replace Heaviside's function by the sigmoid or **logistic function**
$$\sigma(z) = \frac{1}{1+e^{-z}}$$
with values between 0 and 1
- Then, the perceptron's output could be seen as a posterior probability
$$P(1|x) = \frac{1}{1+e^{-(w_0+w\cdot x}}$$
which leads to **Logistic Regression**
- We briefly review next how to solve them

Linear Regression

- To simplify notation we drop the w_0 term centering the x and y
- If Y is the $N \times 1$ **target** vector and we organize the sample S in a $N \times d$ **data matrix** X, the sample mse is given by
$$\begin{aligned}\widehat{e}(w) &= \frac{1}{2N}\sum_p (w\cdot x^p - y^p)^2 = \frac{1}{2N}(Xw-Y)^t(Xw-Y)\\ &= \frac{1}{2N}(w^tX^tXw - 2w^tX^tY + Y^tY)\end{aligned}$$
- Since $\widehat{e}(w)$ is convex, we get the optimum w^* by solving $\nabla\widehat{e}(w) = 0$
- It is easy to see that
$$\nabla\widehat{e}(w) = \frac{1}{N}X^tXw - \frac{1}{N}X^tY = \widehat{R}w - \widehat{b}$$

Solving the Normal Equations

- The optimal $\widehat{w}^*$ must verify the **normal equations**
$$\nabla\widehat{e}(\widehat{w}) = \widehat{R}\,\widehat{w} - \widehat{b} = 0,$$
where $\widehat{R} = \frac{1}{N}X^tX$, $\widehat{b} = \frac{1}{N}X^tY$
- Over the original, non–centered data matrix we have
$$\widehat{R} = \frac{1}{N}(X-\overline{X})^t(X-\overline{X});$$
i.e., $\widehat{R}$ is the **sample covariance matrix**

- If $\widehat{R}$ is invertible, we just solve the linear system $\widehat{R}\,\widehat{w} - \widehat{b} = 0$
- And obtain the sample–dependent optimal $\widehat{w}^*$ as

$$\widehat{w}^* = \widehat{R}^{-1}\widehat{b} = \left(X^t X\right)^{-1} X^t Y$$

Linear Models and Big Data

- In Big Data it may not possible to solve analytically the normal equations
  - Covariance matrices over large datasets or dimensions may not be easily computed
  - Iterative (temporal? dynamical?) numerical methods are needed
- The simplest numerical alternative is **gradient descent**:
  - Starting from some random W^0 we iteratively compute

$$W^{k+1} = W^k - \rho_k \nabla\widehat{e}(W^k) = W^k - \frac{\rho}{N}\left(X^t X W^k - X^t Y\right)$$

  - Component wise: $w_i^{k+1} = w_i^k - \rho_k \frac{\partial \widehat{e}}{\partial w_i}(W^k)$
  - ρ_k is the **learning rate**
- If $W^k \to W^*$, then $\nabla\widehat{e}(W^*) = 0$
  - Since our problems have obviously minima, this should be enough

Logistic Regression (LR)

- We assume

$$P(1|x) = \frac{1}{1 + e^{-(w_0 + w\cdot x)}}$$

  - Then $0 \leq P(1|x) \leq 1$ for any x
- We then have

$$P(0|x) = 1 - P(1|x) = \frac{e^{-(w_0+w\cdot x)}}{1 + e^{-(w_0+w\cdot x)}} = \frac{1}{1 + e^{w_0+w\cdot x}}$$

  - Notice that if $w_0 + w \cdot x = 0$, $P(1|x) = P(0|x) = 0.5$
- The ratio $\frac{P(1|x)}{P(0|x)} = e^{w_0+w\cdot x}$ is called the **odds** of x and its log the **log odds** or **logit**
- Thus, the basic assumption in LR is that the **logit is a linear function** $w_0 + w \cdot x$ of x
- We have the model $f(x; w)$; we need a loss function $L(w)$ to minimize for which we use the sample's **likelihood**

Sample's Likelihood

- Assume a sample $S = \{(x^p, y^p)\}$, with y^p either 1 or 0

- If the $Y = \{y^p\}$ labels are derived **independently** from a LR model with weights w_0, w applied to the $X = \{x^p\}$, we have

$$\begin{aligned} P(Y|X; w_0, w) &= \prod_{p=1}^{N} P(y^p|x^p; w_0, w) \\ &= \left\{ \prod_{y^p=1} P(1|x^p) \right\} \left\{ \prod_{y^p=0} P(0|x^p) \right\} \\ &= \prod_{p=1}^{N} P(1|x^p)^{y^p} \;\; P(0|x^p)^{1-y^p} \end{aligned}$$

  because

  - If $y^p = 1$, $P(1|x) = P(1|x^p)^{y^p} \;\; P(0|x^p)^{1-y^p}$ and
  - If $y^p = 0$, $P(0|x) = P(1|x^p)^{y^p} \;\; P(0|x^p)^{1-y^p}$

Max Log–Likelihood Estimation

- The log–likelihood of w_0, w given S is then

$$\begin{aligned} \ell(w_0, w; S) &= \log P(Y|X; w_0, w) \\ &= \sum_p \{ y^p \;\; \log p(1|x^p) + (1 - y^p) \;\; \log p(0|x^p) \} \\ &= \sum_p y^p \;\; \log \frac{p(1|x^p)}{p(0|x^p)} + \sum_p \log p(0|x^p) \\ &= \sum_p y^p \;\; (w_0 + w \cdot x^p) - \sum_p \log(1 + e^{w_0 + w \cdot x^p}) \end{aligned}$$

- The optimal $\widehat{w}_0^*, \widehat{w}^*$ should have given us the likeliest sample which makes it sensible to estimate them as

$$\widehat{w}_0^*, \widehat{w}^* = \arg\min_{w_0, w} \;\; -\ell(w_0, w; S)$$

- Extra bonus: $-\ell$ is a convex differentiable function of (w_0, w) and, thus, it is enough to solve $\nabla \ell(w_0, w) = 0$

Newton–Raphson Solution

- However, $\nabla \ell(W) = \nabla \ell(w_0, w) = 0$ doesn't admit a closed form solution but only an iterative, numerical one
- We apply the **Newton–Raphson** iterative method, here equivalent to the general **Newton method** for function minimization
- Starting with an initial random W^0, Newton's iterations are

$$W^{k+1} = W^k + (\mathcal{H}_\ell(W^k))^{-1} \nabla \ell(W^k)$$

- $\mathcal{H}_\ell(W^k)$ denotes the Hessian of ℓ at W^k, which may or may not be invertible
  - Everything is fine if the W^k are close enough to the optimum W^* but far away things may get tricky
- Just as before, we can add a regularization term $\frac{\alpha}{2}\|W\|^2$ to avoid invertibility problems
- The iterations in Logistic Regression are again typical of many of the model building methods used in Machine Learning

Learning in ML

- The general approach to **learning** is the following:
  - A **model** $f(x;W)$ is chosen
  - Given a sample $S = \{(x^1, y^1), \ldots, (x^N, y^N)\}$, we define a **sample dependent loss function**

$$L(W) = L(W|S) = L\left(y^1, \ldots, y^N, f(x^1; W), \ldots, f(x^N; W)\right)$$

- $L(W)$ is often minimized from some W^0 by **iterations**

$$W^{k+1} = W^k - \rho_k G(W^k, S)$$

  with ρ_k a **learning rate** and G some vectorial function
  - When $G(W) = \nabla L(W)$ we have **gradient descent**
  - When $G(W) = \mathcal{H}(W)^{-1}\nabla L(W)$ we obtain **Newton's method**
  - When the entire sample S is used at each iteration, we speak of **batch learning**
  - When only single patterns (x^p, y^p) or small subsamples are used, we speak of **on–line** or **minibatch learning**
- In all cases, learning could be seen as the evolution of a DS in weight space