Temporal Learning, Modeling and Adaptation

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José Dorronsoro
Escuela Politécnica Superior
Universidad Autónoma de Madrid

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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 $X_1, \dots X_K$ are random variables, we can define $F(x_1, \dots x_K) = P(\{\omega : X_k(\omega) \leq x_k,\ k = 1, \dots, K\})$

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: $\{t\} = \{\dots, -1, 0, 1, \dots\}$
  - 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**: $\Omega = \{1, \dots, N\}$ is discrete and $P(X_{t+1} = j | X_t = i, X_{t-1} = i_{t-1}, \dots, X_{t-k} = i_{t-k}) = P(X_{t+1} = j | X_t = i)$
    - $p_{ij} = P(X_{t+1} = j | X_t = i)$ 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 $F_\tau(x_1, \dots, x_K)$ for $\tau = (t_1, \dots, t_K)$ of the SP X_t as $F_\tau(x_1, \dots, x_K) = P(\{\omega : X_{t_k}(\omega) \leq x_k,\ k = 1, \dots, K\})$
- The SP X_t is **strictly stationary** (SS) if for all K, τ and h we have for $\tau + h = (t_1 + h, \dots, t_K + h)$
$$F_\tau(x_1, \dots, x_K) = F_{\tau+h}(x_1, \dots, x_K)$$
- 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
$$\mu_t = \mu, \quad \gamma(t+h,t) = \gamma(h,0) \ \ \forall t,h$$
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

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

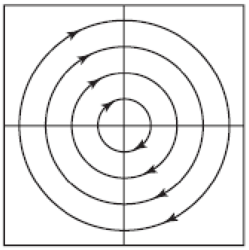
- Solution again given as $X(0) = x_0$ is $X(t) = e^{tA}x_0$
- If $A = \text{diag}\ (\lambda_1, \lambda_2)$ then
$$e^{tA} = \begin{pmatrix} e^{t\lambda_1} & 0 \\ 0 & e^{t\lambda_2} \end{pmatrix}$$
- Now A is a 2×2 matrix and its eigenanalysis is quite simple
- Thus, planar systems can be studied quite exhaustively

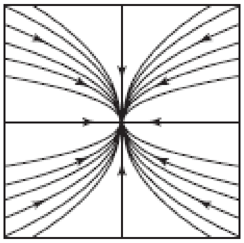
Phase Portraits

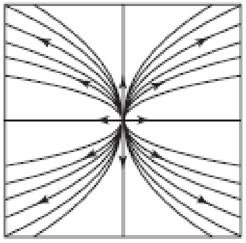
- The goal in the study of dynamical systems is often to understand their asymptotic behavior
- This is depicted using **phase portraits**
- The phase portrait of a planar system is a picture of a collection of representative solution curves in $\mathbf{R}^2$, which we call the **phase space**, for which 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:
$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}, \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}$$

- 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**

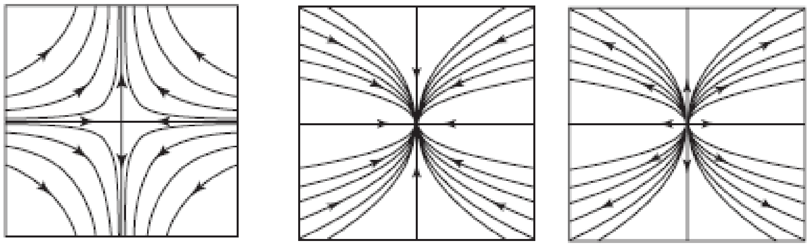
Real Distinct Eigenvalues III: Sources

- 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

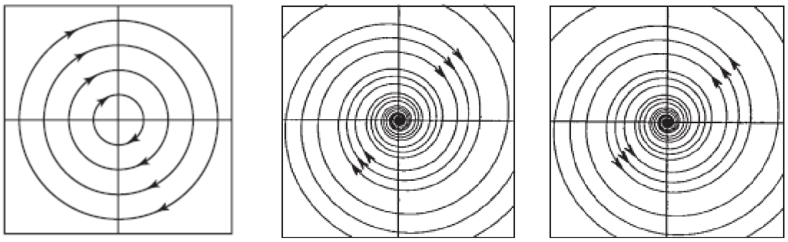
  $$X(t) = c_1 e^{\alpha t} \begin{pmatrix} \cos \beta t \\ -\sin \beta t \end{pmatrix} + c_2 e^{\alpha t} \begin{pmatrix} \sin \beta t \\ \cos \beta t \end{pmatrix}$$

- 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

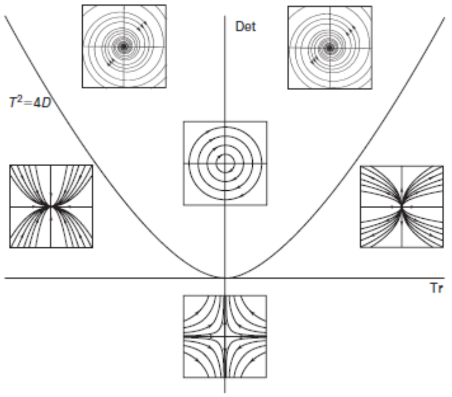
- It can be easily seen that the eigenvalue equation of a 2×2 matrix A is of the form
$$\lambda^2 - \text{ tr } A \; \lambda + \text{ det } A = \lambda^2 - \tau\lambda + \delta = 0$$
with solutions $\lambda_\pm = \frac{1}{2}\left(\tau \pm \sqrt{\tau^2 - 4\delta}\right)$
- As a consequence we have
  - 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

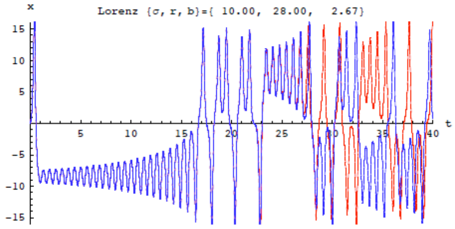
- First goal: a simple approximation to atmospheric flow that models as a two-dimensional fluid cell heated from below and cooled from above
- Further simplified to three independent variables: the rate of convectivity (x; **convection**: the process of heat transfer by a moving fluid), and the horizontal 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

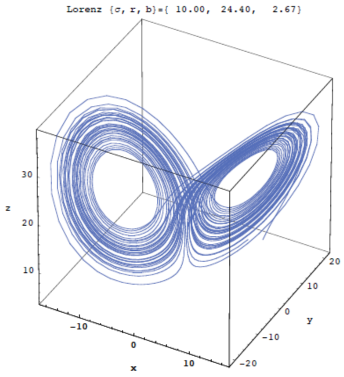
- Lorenz's significant parameters: $\sigma = 10$, $b = 8/3$, $r = 28$
- While being a deterministic system, it is very sensible to very small changes in initial conditions



- 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

$$\begin{tikzcd}
\text{Current state} \arrow[r, "Det.rule", "T"'] \arrow[d, shift right, "\mathrm{Rec}_k"'] & \text{Next state} \arrow[d, "\mathrm{Rec}_k"'] \\
(y_i, \dots, y_{i+k-1}) \arrow[u, shift right, "\mathrm{Rec}_k^{-1}"'] \arrow[r, "Prediction", "\mathrm{Rec}_k \circ T \circ \mathrm{Rec}_k^{-1}"'] & (y_{i+1}, \dots, y_{i+k})
\end{tikzcd}$$

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

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

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

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

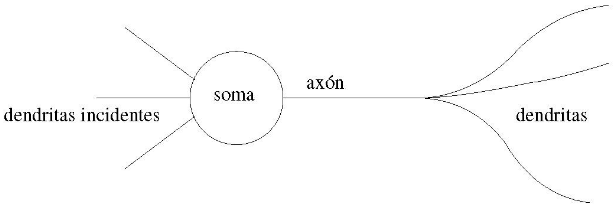
- Predicting temporal information coming from either a time series or a dynamical system ends up in building proper models over time delays
  - Quite often we can/have to add exogenous information that can improve our predictions
- We thus fall in a natural way into possibly non–linear regression models 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

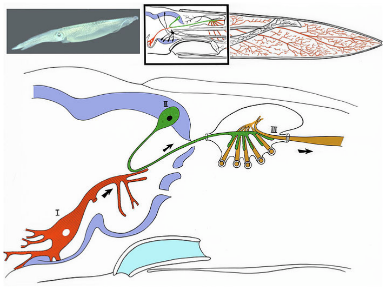
- Basic model: Ramón y Cajal's neuron (1900)



- 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

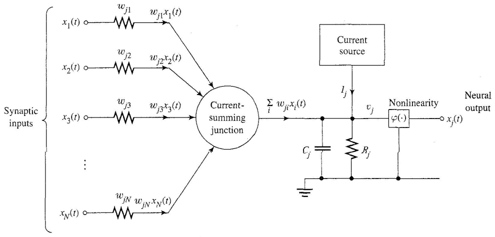
- They developed (circa 1935) the first model to describe the generation and propagation of electrical **action potentials** in neurons



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

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

- 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 $(x^p, y^p) = \left(x^{p(t)}, y^{p(t)}\right)$
  if $y^p w \cdot x^p \le 0$ 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

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

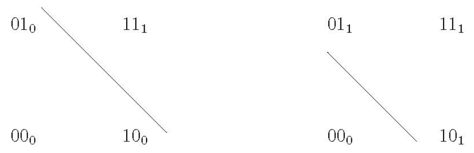
- Putting both together we have for all t for which x^t is erroneous

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

  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

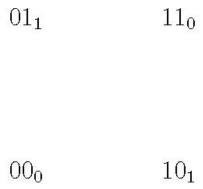
- Observation 1: A PCP can learn (obviously) only linearly separable problems; for instance, it can learn the AND and OR predicates



(a) AND

(b) OR

- But a PCP cannot learn the XOR predicate

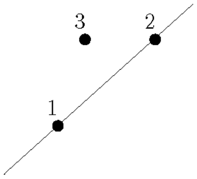


Dichotomies

- 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 $L\left(N, D\right)$ of linearly separable dichotomies is

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

Thus ...

- Notice that for D fixed,
$$\frac{L\left(N,D\right)}{2^N} \to 0$$
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

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

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

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

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

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

  - 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**

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

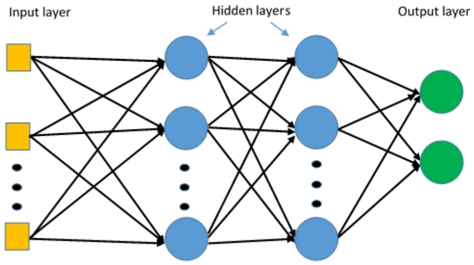
  with ρ_k a **learning rate** and G some vectorial function
  - When $G(W) = \nabla L(W)$ we have **gradient descent**
  - When $G(W) = \mathcal{H}(W)^{-1}\nabla L(W)$ we obtain **Newton's method**
  - When the entire sample S is used at each iteration, we speak of **batch learning**
  - When only single 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

3.3 Classical MLPs

MLP Architecture

- General layout:
  - An input layer (input)
  - One or several hidden layers
  - One output layer
- Feedforward connections only
- Example: TensorFlow Playground

MLP Connections



- No feedback or lateral conections
- Fully connected layers
- Linear unit connections and (usually) non linear activations inside each unit
- General processing: layered and feedforward
- In practice (1990s), one hidden layer and only sometimes two
- Later (around 2010): Deep Networks with “many” (from 3 to 10) layers
- Combined effect of sucesive layers: potentially highly non–linear transformation

Unit Activation and Output

- The **activations** of a unit in layer h receives the **outputs** from processing in the previous layer

$$a_i^h = \sum_{j=1}^{n_{h-1}} w_{ij}^h o_j^{h-1} + b_i^h,$$

- In matrix/vector form:

$$a^h = w^h o^{h-1} + b^h$$

- **Output** of a unit: non linear processing of its activation $o_i^h = \varphi(a_i^h)$
- In matrix form:

$$o^h = \varphi(a^h),$$

where f is applied over each unit

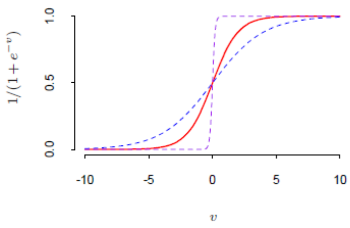
Activation Functions

- Choices for f:
  - Heaviside (in Rosenblatt’s Perceptrons): $\varphi(a) = 0$ if $a \leq 0$, $\varphi(a) = 1$ if $a > 0$

- Identity/linear: $\varphi(a) = a$
- Sigmoid:
$$\varphi(a) = \sigma(a) = \frac{1}{1 + e^{-a}}$$
- Hyperbolic tangent:
$$\varphi(a) = \tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$
- Rectified Linear Units (ReLUs): $\varphi(a) = r(a) = \max(0, a)$

Sigmoid and Hyperbolic Tangent

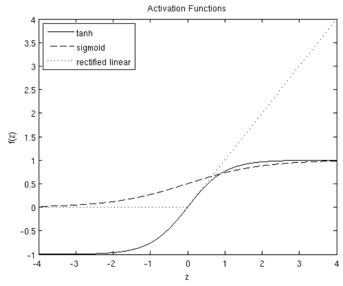
- Sigmoid and tanh: smooth version of Heaviside step function



- Classical choices:
  - Hyperbolic tangent for hidden units
  - Linear outputs for modelling (and sometimes) classification problems
  - Sigmoid outputs for classification problems

ReLUs

- ReLU transfer function: $r(x) = \max(0, x)$



From Stanford's UFLDL Tutorial

- We have $r'(x)$ either 0 or 1 (hoping $x = 0$ never happens!!)

  - Many gradient elements will go to 0

The Simplest MLP I

- The Single Hidden Layer(SHL) MLP
  - D inputs (determined by the problem at hand)
  - One hidden layer with H units (number to be chosen) and tanh activation
  - One or several linear or sigmoid outputs (according to the problem at hand)
- Input–hidden processing: denoting inputs by x and the hidden unit ouput as o,

$$o^h = \tanh \left(b_h^H + \sum_{j=1}^{D} w_{hj}^H x_j \right)$$

  - In matrix/vector form: $o = \tanh\ \left(w^H x + b^H \right)$

The Simplest MLP II

- Hidden–output processing: assuming 1–dimensional targets, we have for the outputs $\widehat{y}$

$$\widehat{y} = \sum_{h=0}^{H} w_h^O o_h + b^O,$$

  - In vector form: $\widehat{y} = w^O \cdot o + b^O$
- Global process:

$$\widehat{y} = f(x; w^O, w^H, b^O, b^H) = b^O + \sum_h w_h^O \tanh \left(b_h^H + \sum_j w_{hj}^H x_j \right)$$

  - Or in matrix/vector form

$$\widehat{y} = f(x; w^O, w^H, b^O, b^H) = b^O + w^O \cdot \tanh\ \left(b^H + w^H x \right)$$

MLPs and Universal Approximation

- We say that $\mathcal{F} = \{f(x; W)\}$ is a **Universal Approximation Family** over a domain $\mathcal{R}$ if

  For any $\epsilon > 0$ and any reasonable ϕ, we can find an $f(x; W_{\phi,\epsilon})$ s.t.

$$\int (\phi(x) - f(x; W_{\phi,\epsilon}))^2 p(x) dx \leq \epsilon$$

- Notice that Universal Approximation is just what we need in regression

- In fact a **Single Hidden Layer (SHL) MLP with enough hidden units is an effective universal approximator**
- But we have to be able to build them

MLP Error Function

- MSE is the standard error function for regression MLPs

$$\begin{aligned} e(W) &= \frac{1}{2} E_{x,y}\left[(y - f(x;W))^2\right] = E_{x,y}\left[e^{\ell}(x,y;W)\right] \\ &= \int e^{\ell}(x,y;W) p(x,y) dx dy \end{aligned}$$

  with $e^{\ell}(x,y;W)$ denotes the **local error**

$$e^{\ell}(x,y;W) = \frac{1}{2}(y - \widehat{y})^2 = \frac{1}{2}(y - f(x;W))^2$$

MSE Gradient

- The general idea would be to obtain W^* as a solution of $\nabla e(W) = 0$, where we have

$$\begin{aligned} \nabla e(W) &= E_{x,y}\left[\nabla_W e^{\ell}(x,y;W)\right] \\ &= E_{x,y}\left[\nabla_W f(x;W)(f(x;W) - y)\right] \end{aligned}$$

  for we have

$$\begin{aligned} \nabla_W e^{\ell}(x,y;W) &= -(y - f(x;W)\ \nabla_W f(x;W) \\ &= \nabla_W f(x;W)(f(x;W) - y) \end{aligned}$$

- We have therefore two tasks:
  - Compute ∇e
  - Exploit it to build MLPs
- We will exploit $\nabla e(W)$ through **optimization methods** after we compute it

SHL Forward Pass I

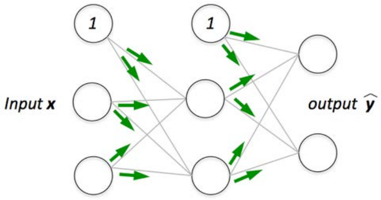
- We apply the preceding to a single hidden layer MLP with
  - A single output unit and input–to–hidden weight matrix $w^H = (w^H_{hj})$ and bias b^H vector and
  - A hidden–to–output weight vector $w^O = (w^O_1, \dots, w^O_H)$ and scalar bias b^O
- Recall that the forward pass can be computed as follows
  - $a = w^H x + b^H$, $o = \varphi(a)$,

    - ∗ Or unit–wise: $a_h = \sum w^H_{hi} x_i + b^H_i$, $o_h = \varphi(a_h)$
  - $\hat{y} = w^O \cdot o + b^O = \sum_h w^O_h o_h + b^O$

- Straightforward to program

SHL Forward Pass II

- Graphically we have the following scheme:



From Sebastian Raschka's A Visual Explanation of the Back Propagation Algorithm for Neural Networks, KDnuggets

SHL Generalized Errors

- In general we have
$$\frac{\partial e^\ell}{\partial w_{ij}} = \frac{\partial e}{\partial a_i}\frac{\partial a_i}{\partial w_{ij}} = \frac{\partial e}{\partial a_i} o_j = \delta_i o_h$$
- Thus, the key is to compute the δ_i, which we do for MSE
- In the output layer $e^\ell = \frac{1}{2}(y - \widehat{y})^2$ and $a^O = \widehat{y}$, and thus,
$$\delta^O = \frac{\partial e^\ell}{\partial a^O} = \frac{\partial e^\ell}{\partial \widehat{y}} = \widehat{y} - y$$
- Therefore, in the output layer we have
$$\frac{\partial e^\ell}{\partial w^O_h} = (\widehat{y} - y)\frac{\partial a^O}{\partial w^O_h} = (\widehat{y} - y) o^H_h$$

SHL Gradient Backprop I

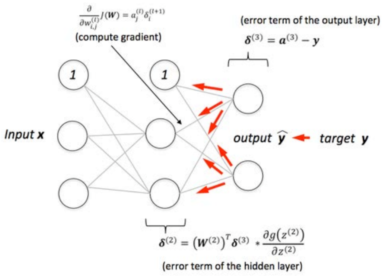
- In the hidden layer we **backpropagate** $\delta^O = \widehat{y} - y$ to get
$$\delta^H_h = \frac{\partial e^\ell}{\partial a^H_h} = \frac{\partial e^\ell}{\partial a^O}\frac{\partial a^O}{\partial a^H_h} = (\widehat{y} - y)\frac{\partial a^O}{\partial a^H_h} = \delta^O \frac{\partial a^O}{\partial a^H_h}$$
- And. moreover,
$$\frac{\partial a^O}{\partial a^H_h} = \frac{\partial a^O}{\partial o^H_h}\frac{\partial o^H_h}{\partial a^H_h} = \frac{\partial a^O}{\partial o^H_h}\varphi'(a^H_h) = w^O_h \varphi'(a^H_h)$$

- Moreover, $o_j^D = x_j$ and, therefore,

$$\frac{\partial e^\ell}{\partial w_{hj}^H} = \frac{\partial e^\ell}{\partial a_h^H}\frac{\partial a_h^H}{\partial w_{hj}^H} = \delta_h^H x_j = (\widehat{y} - y) w_h^O \varphi'(a_h^H) x_j$$

SHL Gradient Backprop II

- Graphically we have the following scheme:


$\frac{\partial}{\partial w_{i,j}^{(l)}} J(\boldsymbol{W}) = a_j^{(l)} \delta_i^{(l+1)}$
(compute gradient)
(error term of the output layer)
$\boldsymbol{\delta}^{(3)} = \boldsymbol{a}^{(3)} - \boldsymbol{y}$
1
1
Input x
output $\widehat{\boldsymbol{y}}$
target y
$\boldsymbol{\delta}^{(2)} = (\boldsymbol{W}^{(2)})^T \boldsymbol{\delta}^{(3)} * \frac{\partial g(z^{(2)})}{\partial z^{(2)}}$
(error term of the hidden layer)

From Sebastian Raschka's A Visual Explanation of the Back Propagation Algorithm for Neural Networks, KDnuggets

Takeaways on Clasical MLPs

1. They have a layered structure with outputs computed in a **forward pass** using differentiable activations
2. Usual activations: sigmoid, tanh, linear
3. MLPs are **universal approximators**: this is indispensable for regression but has to be handled with care
4. MSE is the usual regression cost; cross entropy is used in classification
5. The error function gradients are computed by **backpropagation** of generalized errors
6. Backprop is basically a very simple procedure than can be **largely automated**
7. Once an MLP is defined (feedforward and backward passes), MLP training reduces to a (usually difficult and costly) **optimization problem**

3.4 From MLPs to DNNs

NN's Second Spring

- There was a very intense academic interest in the (by now) standard MLPs in the 1990's
  - Several NN conferences and journals appear
- MLP working and training became well understood

  - Although losing much of neuronal plausibility

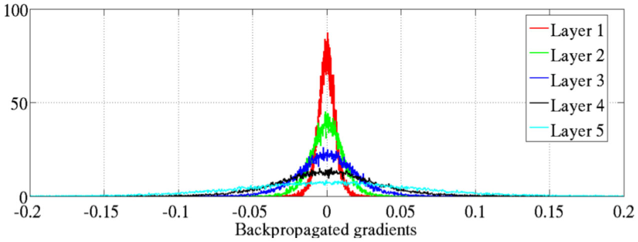
- MLPs found relevant applications in many fields
  - They were incorporated into data science tools and products
  - Although hyperparameter selection was (is) costly and had (has) to be done very carefully

NN's Golden Autumn?

- This went on strongly until the late 90's when
  - New relevant contributions decreased
  - New competitors appeared: Boosting, SVMs, Random Forests, Gradient Boosting Regression, ...
- A nagging issue were deeper MLPs
  - One hidden layer MLPs were enough for most applications
  - But nobody knew how to train MLPs with three or more hidden layer

Vanishing Gradients

- One main obstacle was **vanishing gradients**:
  - Consider the distribution of gradient values in a 5 layer MLP



From Glorot & Bengio, AISTATS 2010

  - Gradients in the last (5–th) layer are nonzero but vanish as we go back towards the first layer
  - Training ceases to have any effect and learning stalls at an early, bad minimum

Towards Deep Networks

- Deep Nets: (initially) standard MLPs with 3 or more layers, either fully connected or **convolutional**
- Training impossible even in early 2000:

  - Poor results over limited HW
  - Addressable problems better solved by single layer nets

- First breakthrough around 2007: deep MLP **unsupervised pretraining** using stacked RBMs (Hinton) or autoencoders (Bengio)
- Easier fine-tunning afterwards by standard backprop

The Boom

- Interest in NNs was rekindled and around 2010 the floodgates opened:
  - Large nets with huge number of weights
  - New convolutional layers, regularizations, initializations or activations
  - New techniques appear ... that are not that different from the old ones
- **New mood**: what was impossible before is now much easier and leads to better results
- Major breakthroughs were achieved in significant problems in computer vision and speech recognition

What Is New In DNNs?

- New and fancy network structures:
  - **Convolutional layers** (with non–differentiable components)
  - More flexible feedforward connections
- **Automated symbolic backprop derivation**
- Network size: huge number of weights
- Very large sample size (sometimes)
- New cost functions
- New (non differentiable) activations: ReLUs
- New regularization: **dropout**, dropconnect
- Recognition that a **good weight initialization is critical**

Changes In DNN Training

- Some things have to change:
  - Batch training becomes unfeasible for huge samples/networks
  - Strict online learning may become impractical as single patterns may get lost in a huge network
- Minibatch training balances these extremes:

  - Choose a minibatch size M (a new DNN parameter?) and at each iteration randomly select M sample patterns
  - Perform SGD or some variant over the minibatch
  - Or even a second order method such as CG

- But other things much remain the same

Changes In DNN Training II

- Backprop is still the backbone of gradient computation
  - But it is no longer programmed but derived automatically by **symbolic differentiation**
  - Easily extended to convolutional layer weights
  - Imaginatively extended to non–differentiable elements: just pretend that they are so!
- Minibatch–based Stochastic Gradient Descent (SGD) still is the primary optimization approach
- And several hyper–parameters may still have to be chosen, with no clear cut procedures
- In any case, we review next some of the most important new things

3.5 Advanced DNN Techniques

Initialization

- If layers with M_i units used, the standard procedure Glorot–Bengio (`xavier`) is

$$W_i \sim U\left[-\frac{\sqrt{6}}{\sqrt{M_i + M_{i+1}}}, \frac{\sqrt{6}}{\sqrt{M_i + M_{i+1}}}\right]$$

- It ensures $Var\left(\frac{\partial e}{\partial w_i}\right) \simeq Var\left(\frac{\partial e}{\partial w_i'}\right)$ across successive layers when tanh activations are used
- Gradient vanishing is thus avoided
- Pretraining no longer indispensable (at least for large training data sets)

Dropout Regularization

- The extremely large weight numbers of Deep Neural Networks (DNNs) make regularization mandatory
- First choice: standard Tikhonov regularization (i.e., **weight decay**) for regression DNNs with linear output units

- **Dropout** in other fully connected layers, replacing standard output processing $o_i^\ell = f(a_i^\ell) = f(w_i^\ell o^{\ell-1} + b_i^\ell)$ by

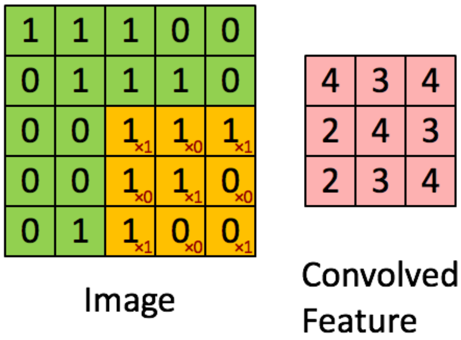
$$o_i^\ell = f(a_i^\ell) = f\left(w_i^\ell(o^{\ell-1} \odot r^\ell) + b_i^\ell\right),$$

  with each r_j^ℓ being 1 with probability p

  - It somehows sub-samples a larger network at each layer
  - Output errors are backpropagated but the final optimal weights w^* are downscaled as $w_f^* = pw^*$
  - It adds **randomness** to the final DNN model (and some **independence** for two different models)

Convolutional Layers

- Starting assumption: patterns organized in features having a one–, two– or multi–dimensional structure
- Basic processing: to apply a $K \times K$ convolutional filter w over an image patch x_j as $y_j = f(w * x_j + b)$



From Stanford's UFLDL Tutorial

Convolutional Layers II

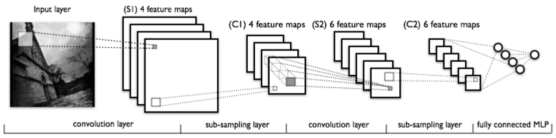
- An $M \times N$ input "image" x is transformed into an $(M - K + 1) \times (N - K + 1)$ output $x' = C(x)$
- This is done over Q input **feature maps** $x_1, \ldots, x_Q$ and creates R output feature maps $x'_1, \ldots, x'_R$
- Then a **pooling** transformation $P(x')$ is applied over $K' \times K'$ patches of each x'_j
  - Possible pooling transforms: averages, max
- We have to learn $Q \times R$ pairs of $K \times K$ filters (w_ℓ, b_ℓ)

  - And decide on K, K' and the pooling transformation

- The forward pass has a cost of $O(Q \times M \times N \times K^2 \times R)$ per pattern, which can be quite costly

Deep Convolutional NNs

- Important goals may be achieved: invariance preservation, structural feature extraction, balancing layer sizes
- Deep Convolutional NNs combine the previous steps
  - An initial number of convolutional layers, followed by
  - A number of fully connected inner product layers and, finally
  - A readout layer that yields the NN's response



A typical architecture for image processing. From Convolutional Neural Networks (LeNet) tutorial

- Possibly with connections and weights in the millions

Training Time and Technology

- Training time is a key issue as it usually shoots up:
  - Samples may be very large
  - Networks may be huge even for moderate samples
  - More hyperparameters may have to be optimized
- Heavy duty computing needed:
  - Multicore machines: very handy for hyperparameter selection; less so for single network tranining
  - Same true for cloud computing environments
  - GPUs: crucial for single network training
- Best: machines/computing centers with many GPUs

Ad Hoc Programming Tools

- Do–it–yourself programming no longer possible
- Increasingly better tools are being available with very fast evolution

- Initially PyLearn+Theano
- Next Caffe: C++ base with Python interface
- Now Keras: Python platform capable of running on top of Theano and Google's TensorFlow
- Plus open releases by large companies
  - Google‘s TensorFlow (plus TensorBoard)
  - Facebook's Torch, on top of the Lua language
  - Microsoft's cntk environment

Deep Nets as DAGs

- The layers of a feedforward net are nodes in a linear graph
  - Backprop is straightforward on such a graph
- But it is also very easy in nets with layers in a DAG
  - They connect different input nodes to different outputs at varying depths and with different layer processing
  - The backprop path is also straightforward
  - And the backprop components at each layer node can be "collated" to the full network gradient
- We just "program" the DAG net defining layer nodes and connecting them in a DAG
  - Then a compiling step yields the forward pass and the backward gradient
- End result: fairly fancy networks
  - Perhaps useful; certainly very costly to train

And Much Better Technologies

- Advanced hardware is a must:
  - GPUs, multicore machines, cloud
- High–level programming:
  - Python as data preprocessing/pipelining + DNN model definition + experimental setup setting + results visualization
  - Python based high–level layers to symbolic GPU backends: Keras (coding in Python), TensorBoard (point and click?)
  - Git as the code and ideas exchange tool
- New skills in high demand, perhaps having more to do with advanced systems handling than with ML
- To read on: M. Nielsen's Neural Networks and Deep Learning online book

3.6 The Golden Era?

Renewed, Huge Interest

- Things go from a mild NN stagnation around 2000 to big explosion in the 2010s
- Relatively large number of contributions and widely attented workshops in mayor conferences (ICML, NIPS)
- Strong groups in leading companies (Google, Baidu, Facebook, Microsoft)
- Great scientific (and mediatic) success: Deep learning. LeCun, Bengio & Hinton (Nature, May 2015)
- New field arising: **Representation Learning**
- New (possible and perhaps more plausible) connections with computational neuroscience (at least for image and audio recognition?)

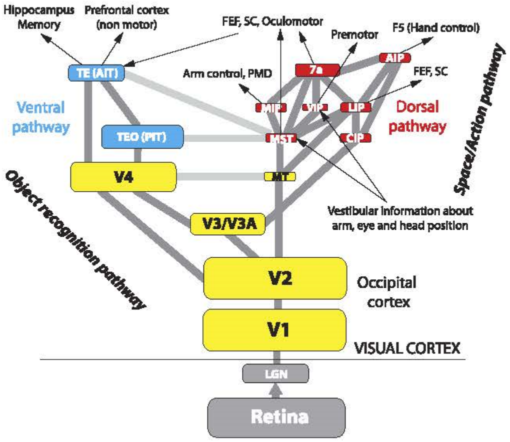
Great Successes

- DNNs define a rich and suggestive paradigm with impressive results in several fields
  - They vastly improve the previous state of the art (Viterbi models) in speech recognition,
  - They consistently give the best results in the latest Image Net Large Scale Visual Recognition Challenges
- Google is particularly active:
  - Caption generation from images
  - Smart Reply: automatically recommendation of responses to messages in Gmail
  - Learning to play video console games: Nature, February 2015
  - Public release of TensorFlow (plus MOOC in Udacity)
  - Beating humans at go ten years in advance: Nature, January 20156

Right Now

- Great hype and substantial entry barriers
  - Of course knowledge has to be acquired (perhaps not too different from before)
  - But large computational (and technical) resources are indispensable
  - And perhaps their natural habitat are problems with extremely large training databases
- Cutting edge Deep Nets are big, complicated and nervous animals, but also full of promise
- Plausible goal: train (teach?) networks to process information in a hierarchical way

What Are DNNs Aiming At?



From Kruger et al., PAMI 35, 2013

- Model: information processing in the visual cortex

The Ideal Deep Net

- Desired working:
  - The first and intermediate layers extract information substructures
  - The final layers recompose into cognitive content
- Ultimate goal: to replicate the cortex's workings to
  - Decompose a complex tasks in elementary subtasks
  - Solve each one separately and
  - Merge these subsolutions on a complex and rich representation
- That is, to achieve a kind of cognitive "Map Reduce"
- And Deep Learning is clearly behind the **renewed conversation on AI** and its implications

Renewing The AI Conversation

- Decomposing and merging is similar to what it is being done in other AI fields (such as self driving cars)
- But also in the automatization of industrial and (increasingly) service processes
- Very likely with important economic and social disruptions
- Two very recent examples: OpenAI, NIPS 2015 Symposium

What May Come Next?

- OpenAI: *... to advance digital intelligence ... to benefit humanity ... unconstrained by ... financial return ...*
  - Research Director: I. Sutskever (U. Toronto–Hinton, U. Stanford–Ng, Google)
  - Sponsors: Elon Musk (Tesla), Reid Hoffman (LinkedIn), Peter Thiel (PayPal)
  - Up to 1 billion dollars pledged
- NIPS 2015 symposium Algorithms Among Us: The Societal Impacts of Machine Learning, with among others
  - Nick Bostrom, Future of Humanity Institute–Oxford U.
  - Andrew Ng, Stanford–Coursera–Baidu, The Economic Impact of Machine Learning (podcast)
  - Erik Brynjolfsson, MIT, The Second Machine Age
- But after much hype, some clearer thinking is arising: Michael Jordan on AI, IA and II

4 Unconstrained Smooth Optimization

4.1 Classical Methods

Back to Optimization

- General optimization theory is a key tool in Machine Learning (ML)
- There are two optimization set ups in ML
  - **Unconstrained** optimization, slightly simpler and that of MLPs
  - **Constrained** optimization, wider and more complex
- In ML we have also to consider the optimization of differentiable and also non differentiable error functions
- MLP optimization: unconstrained and differentiable
- And also **batch**, i.e., over the entire sample, **mini–batch** over subsamples or **on line**, pattern by pattern

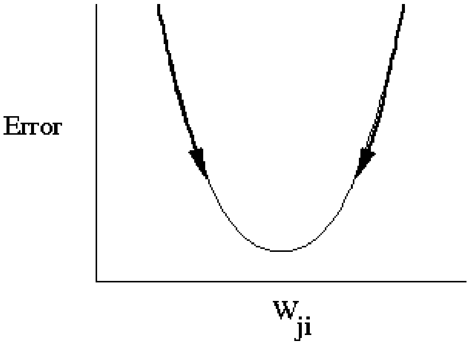
Gradient Descent

- We recall that $-\nabla e$ is the maximum descent direction
- First idea: to build a (hopefully convergent) sequence W^k iterating (small) steps along $-\nabla e(W^k)$

Gradient Descent II

- In more detail, we start from a random W^0 and compute

$$W^{k+1} = W^k - \rho_k \nabla_W e(W^k)$$



- ρ_k is the **learning rate** (LR)
- With a small ρ_k we ensure $e(W^{k+1}) < e(W^k)$ (although with possibly a very small descent)
- We can get a better iteration $W^{k+1} = W^k - \rho_k^* \nabla_W e(W^k)$ using a ρ_k^* given by

  $$\rho_k^* = \arg\min_\rho e(W^k - \rho \nabla_W e(W^k));$$

  this is known as **line minimization**
- These GD methods are called **first order methods** in part because they only use ∇e

Newton's Method

- Assume a quadratic function $q(w) = aw^2 + bw + c$ with $a > 0$ and a minimum at some w^*
- We can reach w^* from some w with a step Δw such that

  $$0 = q'(w + \Delta w) = 2a(w + \Delta w) + b$$
- We have thus $\Delta w = \frac{-b-2aw}{2a}$, that is

  $$w^* = w - \frac{2aw + b}{2a} = w - \frac{1}{q''(w)} q'(w)$$
- This leads to **Newton's method**: minimize a general f iteratively using steps

  $$w^{k+1} = w^k - \rho_k \frac{1}{f''(w^k)} f'(w^k)$$

  with ρ_k a suitable learning rate

Multidimensional Newton's Method

- For a d dimensional W, the Taylor expansion of e at an optimum W^* is

$$e(W) \approx e(W^*) + \frac{1}{2}(W - W^*)^t \cdot \mathcal{H}(W^*) \cdot (W - W^*)$$

  - $\mathcal{H}(W^*)$ is the **Hessian** of e at W^* and $\nabla e(W^*) = 0$

- It follows that $\nabla e(W) \approx \mathcal{H}(W^*) \cdot (W - W^*)$ and, therefore,

$$W^* \approx W - \mathcal{H}(W^*)^{-1} \nabla_W e(W)$$

- This suggest to derive the W^k by

$$W^{k+1} = W^k - \rho_k \mathcal{H}(W^k)^{-1} \nabla_W e(W^k)$$

  which is known as **Newton's Method** (NM)

Variants of Newton's Method

- Theoretically NM converges very fast near W^*, but
  - Far from W^* convergence is not guaranteed
  - Moreover $\mathcal{H}(W^k)$ may not be invertible
  - Besides, computing $\mathcal{H}(W^k)$ is cumbersome and costly
- The **Gauss–Newton (GN)** approximation

$$\mathcal{H}(W) \simeq E[\nabla e(W) \nabla e(W)^\tau],$$

  holds for any quadratic cost and simplifies the third problem
- The **Levenberg–Marquardt (LM)** method deals with the other two problems combining
  - Gradient descent "away" from W^*
  - Gauss–Newton "near" W^*

  although "away" and "near" have to be properly addressed

One–dimensional GN Approximation

- Assume $e(w) = \frac{1}{2} \int (f(x; w) - y)^2 p(x, y) dxdy$; then

$$e'(w) = \int (f(x; w) - y) \frac{\partial f}{\partial w}(x, y) p(x, y) dxdy$$

- Near a minimum w^* we may expect $f(x; w) \simeq y$ and, therefore,

$$\begin{aligned} e''(w) &= \int \left(\frac{\partial f}{\partial w}\right)^2 p(x,y)dxdy \\ &\quad + \int (f(x;w) - t)\frac{\partial^2 f}{\partial w^2}(x,y)p(x,y)dxdy \\ &\simeq \int \left(\frac{\partial f}{\partial w}\right)^2 p(x,y)dxdy > 0 \end{aligned}$$

- Thus, for square errors, we can use first derivates to approximate $e''(w)$

General GN Approximation I

- In the general case we have

$$\nabla e(W) = E\left[\nabla f(x;W)\left(f(x;W) - y\right)\right]$$

- And, therefore,

$$\begin{aligned} \nabla^2 e(W) &= E\left[\nabla^2 f(x;W)\left(f(x;W) - y\right)\right] + \\ &\quad E\left[\nabla f(x;W)\nabla f(x;W)^\tau\right] \end{aligned}$$

- The second term is easy to compute once we have ∇f
- If $W \approx W^*$, $f(x;W) \approx y$; therefore $f(x;W) - y \approx 0$,
  - We can ignore the first, more complex, term

General GN Approximation II

- We arrive at $\nabla^2 e(W) \simeq E\left[\nabla f(x;W)\nabla f(x;W)^\tau\right]$ or, equivalently,

$$\mathcal{H}_{(i,j)(p,q)}(W) = \left(\frac{\partial^2 e}{\partial w_{ij}\partial w_{pq}}(W)\right) \simeq \left(E\left[\frac{\partial f}{\partial w_{pq}}\frac{\partial f}{\partial w_{ij}}\right]\right)_{(i,j)(p,q)}$$

- $\mathcal{J} = E\left[\nabla f(x;W)\nabla f(x;W)^\tau\right]$ is **Fisher's information matrix**
- Often only its diagonal is considered and we have

$$\mathcal{H}_{(i,j)(i,j)}(W) = \left(\frac{\partial f}{\partial w_{ij}}\right)^2$$

- Pending: how do we know we are either near or far from the optimum?
- The **Levenberg–Marquardt** method tries to address this

Some Linear Algebra

- A square matrix Q is **semidefinite positive** if $u^t Q u \geq 0$ for all vectors u
- If $u^t Q u = 0$ iff $u = 0$, Q is **definite positive**
  - $Q = gg^t$ is semidefinite but not definite positive
  - If Q is semidefinite positive, $Q + \lambda I$ is definite positive for $\lambda > 0$
- If Q is definite positive, it can be diagonalized as $Q = U^t \Lambda U$ with U orthonormal and Λ diagonal with all its elements positive
- If Q is definite positive, Q is invertible
- A smooth f has a minimum at x^* iff $\nabla f(x^*) = 0$ and $H_f(x^*)$ is definite positive
- Thus, after a rotation, f can by locally approximated by a parabolic hypersurface

Levenberg–Marquardt Optimization I

- By construction, Fisher's matrix is semidefinite positive:

$$\begin{aligned} u^t \mathcal{J} u &= E\left[u^t \nabla f(x;W) \ \nabla f(x;W)^\tau u\right] \\ &= E\left[\left(u^t \nabla F(x;W)\right)^2\right] \geq 0 \end{aligned}$$

- Thus for any $\lambda > 0$, $\mathcal{J} + \lambda I$ is definite positive and, hence, invertible
- We can approximate Newton's iterations by

$$W^{k+1} = W^k - \rho_k \left(\mathcal{J}(W^k) + \lambda_k I\right)^{-1} \nabla_W e(W^k)$$

Levenberg–Marquardt Optimization II

- When $W^k \simeq W^*$, $\mathcal{I}(W^k) \simeq \mathcal{H}(W^k)$
  - If we take $\lambda_k \simeq 0$, we essentially perform a Newton step
- When W^k is far from W^*, we take $\lambda_k \gg 1$
  - We then essentially have $\mathcal{J} + \lambda_k I \approx \lambda_k I$ and thus

$$(\mathcal{J} + \lambda_k I)^{-1} \approx \frac{1}{\lambda_k} I$$

  - Therefore we essentially perform gradient descent
- The **Levenberg–Marquardt** method combines those options "detecting" when to apply each of them

Takeaways on Basic Methods

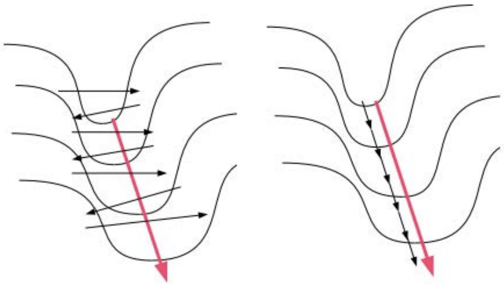
1. Gradient descent is the simplest method but possibly also the slowest

2. Newton's method is fastest but may be very costly in full form (and Hessian computation is messy)
3. Gauss–Newton approximates Hessian computation for square error
4. Levenberg–Marquardt switches between gradient descent and Gauss–Newton
5. Most of the previous methods require the (usually tricky) selection of a learning rate

4.2 Advanced Optimization

Accelerating Gradient Descent

- A possibility on the error surface of a NN is to have many long, narrow ravines
- Gradients will then bounce in the narrow section, but may be very small along the wider one



Momentum

- **Momentum** (or the **Heavy Ball** method) pushes them forward in the wider section
- Momentum tries to maintain descent's inertia with a term $\Delta^k = W^k - W^{k-1}$, i.e.,

$$W^{k+1} = W^k - \rho_k \nabla_W e(W^k) + \mu_k \Delta^k$$

  - We have to deal with the new parameter μ
- The goal is to keep W^k advancing in "plateaux", i.e., small gradient zones
- Momentum can be seen as a crude approximation of a CG step
- Nice explanation at Why Momentum Really Works

Nesterov's Accelerated Gradient

- Let's rewrite momentum in two steps
  1. Define $\tilde{\Delta}^{k+1} = -\rho_k \nabla_W e(W^k) + \mu_k \tilde{\Delta}^k$ and

2. Apply
$$W^{k+1} = W^k + \tilde{\Delta}^{k+1} = W^k - \rho_k \nabla_W e(W^k) + \mu_k \tilde{\Delta}^k$$

- **Nesterov's Accelerated Gradient** is a variant of this
$$\tilde{\Delta}^{k+1} = -\rho_k \nabla_W e(W^k + \mu_k \tilde{\Delta}^k) + \mu_k \tilde{\Delta}^k;\ W^{k+1} = W^k + \tilde{\Delta}^{k+1}$$
- In convex optimization it improves GD and is highly recommended in Deep Network training
- Deep Learning has also produced new methods such as Adagrad, Adadelta or **Adam**

Adam

- At each step t Adam uses a new random mini–batch to
  - Update exponentially smoothed averages m_t of the gradient g_t and v_t of the the squared gradient $g_t^2 = g_t \odot g_t$ as
$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t,\ v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2;$$
  - Compute bias corrections $\widehat{m}_t$, $\widehat{v}_t$ as
$$\widehat{m}_t = \frac{1}{1-\beta_1^t} m_t,\ \widehat{v}_t = \frac{1}{1-\beta_2^t} v_t;$$
  - Update weights as $W_t = W_{t-1} - \alpha \frac{\widehat{m}_t}{\sqrt{\widehat{v}_t} + \epsilon}$
- One can show $E[m_t] \simeq (1-\beta_1^t) E[g_t]$ and $E[v_t] \simeq (1-\beta_2^t) E[g_t^2]$
- Default values $\alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999$, and $\epsilon = 10^{-8}$ usually work fine

Understanding Adam

- What is going on in Adam?
- At each step we work with estimates of the average local gradient:
$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t \simeq E[\nabla_W f];$$
- Then $v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2 \simeq E[(\nabla_W f)^2] \simeq \sigma^2(g_t)$
- Thus, we can see Adam as a kind of "normalized" gradient descent
- Or since we can expect $E[\nabla^2_{W^2} f] \simeq E[(\nabla_W f)^2]$, we can see Adam as a more conservative "cousin" of Gauss–Newton's steps
  - Recall that the denominator in GN would be $\sigma^2(g_t) \simeq v_t$ instead of $\sqrt{v_t}$

Convergence of Adam

- When applying Adam we have at step t an error function e_t (the current minibatch loss) and a weight estimate w_t

- Define $w_T^* = \arg\min_{w\in\{w_1,\ldots,w_T\}} \sum_1^T e_t(w)$
- The **regret** until time T is then $R(T) = \sum_1^T \left(e_t(w_t) - e_t(w_T^*)\right)$
- Then it can be shown that $\frac{R(T)}{T} = O\left(\frac{1}{T}\right)$
- Notice that for a large T and full batches $\frac{1}{T}\sum_1^T e_t(w) \simeq e(w)$
- And since $w_T^* \simeq \arg\min \frac{1}{T}\sum_1^T e_t(w)$, we can expect $w_T^* \simeq w^*$

When to Stop Training

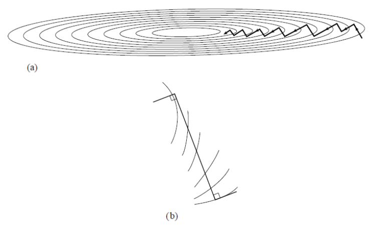
- Typically the $e(W_k)$ error diminishes towards an asymptotic minimum
  - If many units are used, we arrive to 0 which usually implies overfitting
- First solution: to use a separate **validation subset** V and stop training when the error in V, i.e., the **validation error** starts growing
  - But: How to choose V? What do we do for small samples?
- Second solution (better): get a good regularization and forget about overfitting
  - A low CV error is also a low validation error
  - Now training stops because of reasons such as computational cost, but not because of overfitting risk

Advanced Methods

- There are many more proposals in unconstrained optimization
- The **Conjugate Gradient** (CG) and **Quasi–Newton** (QN) methods are important in MLP training
- The basic idea in CG is to replace gradient descent directions $g_k = -\nabla e(W_k)$ with new conjugate directions that try to keep somehow the previous “good directions”
- The basic idea in QN is to iterate as in NM but with simple approximations $\mathcal{A}_k$ to $\mathcal{H}^{-1}(W^k)$ that converge to $\mathcal{H}^{-1}(W^*)$
- When training “small” NNs the Limited-memory Broyden–Fletcher–Goldfarb–Shanno (L-BFGS) QN variant is often used

Conjugate Gradient I

- In a narrow valley, GD plus line minimization may be inefficient, as the next gradient is perpendicular to the previous one
- Thus a bad initial gradient choice slows down gradient descent
- **Conjugate Gradient** (CG) tries to avoid this by using better descent directions



From Press et al., *Numerical Recipes in C*, chap. 10.

Conjugate Gradient II

- In GC we start at a random W^0 and $h_0 = g_0 = -\nabla e(W^0)$ and at each step we compute

$$W^{k+1} = \arg\min_{\rho} e(W^k - \rho h_k), \quad g_{k+1} = -\nabla e(W^{k+1})$$

- The new descent direction h_k is $h_{k+1} = g_{k+1} + \gamma_k h_k$ with

$$\gamma_k = \frac{(g_{k+1} - g_k) \cdot g_{k+1}}{g_k \cdot g_k}$$

- For a **quadratic** $e(W) = c + b \cdot W + \frac{1}{2} W^t A W$,
  - The h_k verify $g_i \cdot g_j = h_i \cdot h_j = h_i^t A h_j = 0$ for all i and $j < i$,
  - This ensures that a minimum is reached in $D = \dim(W)$ steps
- For a general e we have to reset h periodically

Quasi–Newton Methods I

- In QN one builds iteratively approximations $\mathcal{A}_k$ to the inverse Hessians $\mathcal{H}(W^k)^{-1}$ to which Newton's steps are applied
- The general form for $\mathcal{A}_k$ is

$$\mathcal{A}_{k+1} = \mathcal{A}_k + \mathcal{L}(W^{k+1}, W^k, g^{k+1}, g^k)$$

  with $\mathcal{L}$ having a ± simple algebraic form
- There are several formulae to update the $\mathcal{A}_k$: Broyden–Fletcher–Goldfarb–Shannon (BFGS), Davidon–Fletcher–Powell (DFP), ...
- In all of them we want that $\mathcal{A}^* = \lim \mathcal{A}_k$ to verify $\mathcal{A}^* \simeq \mathcal{H}(W^*)^{-1}$

Quasi–Newton Methods II

- For a quadratic f QN arrives at the optimum W^* in a finite number of steps but has a memory cost which is quadratic on D

- **Limited BFGS** (LBFGS) doesn't store the approximations $\mathcal{A}_k$ but a number of vectors instead that are recursively updated and used to compute the $\mathcal{A}_k$
- Therefore, its memory cost is linear and LBFGS can thus be used in problems with large $\dim(W)$
- For a general f the theoretical convergence rates of CG and QN are equivalent to those of GD
- In practice, both QN and CG are faster, with QN requiring less iterations but at a larger $O(d^2)$ cost per iteration

Takeaways on Advanced Optimization

1. Momentum tries to improves the gradient descent direction when learning moves on a ravine of the error surface
2. Conjugate Gradient is a stronger, more sound version of momentum
3. The Quasi–Newton matrices converge to the inverse of the Hessian
4. CG adds a moderate cost to standard GD; QN is costlier
5. Momentum requires hyper–parameter tuning; GD and QN do not (good!!)
6. Second order methods such as Conjugate Gradient and **Quasi–Newton** avoid learning rates and are more efficient but costlier
7. Limited Broyden–Fletcher–Goldfarb–Shanno (L-BFGS) is currently the option of choice for "small" MLPs
8. Minibatch accelerated gradient descent or Adam dominate on "large", big data MLPs

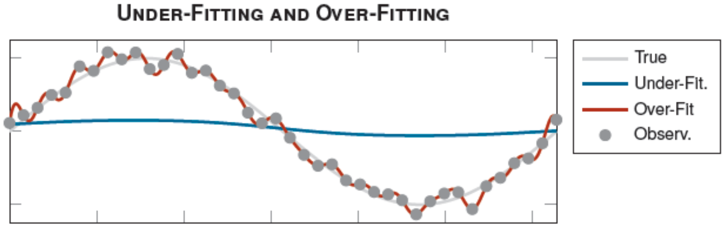
4.3 Overfitting and Regularization

Overfitting in MLPs

- Since MLPs are a UAF, they can also approximate the noise in the sample
  - Given $S = \{(x^p, y^p)\}$ if we allow enough hidden units in a SHL MLP we can arrive to a W^* s.t. $y^p = f(x^p; W^*)$
  - We get thus a sample error $\hat{e}(W^*) = 0$ but possibly with a very high generalization error
- I.e., MLPs may have very small bias but possibly large variance

Regularization vs Overfitting

- Why is there overfitting?
  - Because we may end up having too many weights with respect to sample size
  - Because we allow these weights to explore the entire weight space



(*Ph.D. Thesis of Carlos Alaíz*)

- We can avoid this wandering if we limit W's growth, for which we add a **regularization** term $g(W)$ to $e(W)$ that depends on and grows with $\|W\|$
- Working with $e_R(W) = e(W) + g(W)$ we have to **balance** the minimization of $e(W)$ and that of $g(W)$
- This balanced learning results in better generalization

L_2 Regularization

- Here too the simplest regularization procedure adds a quadratic penalty to the square error e

$$e_R(W) = e(W) + \frac{\lambda}{2}\|W\|^2,$$

  with λ the **weight decay** factor

  - Also known as Tikhonov's regularization or Ridge Regression for linear models

- The desired effect is to constrain the evolution of W:
  - We expect $e(W^*) \simeq \frac{\lambda}{2}\|W^*\|^2$ and, hence, $\|W^*\|^2 \lesssim \frac{2e(W^*)}{\lambda}$
  - In fact, the regularized loss can be seen as the Lagrangian of the constrained problem $\min_W e(W)$ subject to $\|W\|^2 \leq \rho$ for some $\rho > 0$
- The gradient becomes $\nabla e_R(W) = \nabla e(W) + \lambda W$
- And the Hessian is $\mathcal{H}_R(W) = \mathcal{H}(W) + \lambda I$

Regularized Algorithms

- The preceding methods apply straightforwardly to e_R
- Gradient descent becomes

$$W^{k+1} = W^k - \rho_k(\nabla_W e(W^k) + \lambda W^k)$$

- Newton steps are now

$$W^{k+1} = W^k - \rho_k \left(\mathcal{H}(W^k) + \lambda I\right)^{-1} \left(\nabla_W e(W^k) + \lambda W^k\right)$$

- And the Gauss–Newton approximation to $\mathcal{H}_R(W)$ is

$$\mathcal{H}_R(W) = \mathcal{H}(W) + \lambda I \sim E[\nabla f(W) \nabla f(W)^\tau] + \lambda I$$

  that is definite positive and, hence, invertible

How to choose λ

- Again, the correct choice of λ is crucial
- A small $\lambda \ll 1$ results in a small regularization effect and overfitting risk appears
- A large $\lambda \gg 1$ causes learning to forget about $e(W)$ and the model will be essentially constant and will underfit
- Usually λ is chosen by:
  - Exploring a discrete set of values λ_j,
  - That fall in a preselected range $[\Lambda_0, \Lambda_1]$,
  - Using **cross validation** (CV)
- The same is essentially done for any other hyper–parameter

MLP Ensembles

- Recall that $e(W)$ does not have a single minimum
- Moreover, the final MLP depends on the random initial W^0
- And mini–batch training adds extra randomness to the final model
- This suggests
  - To start from K independent initial weights and get K optimal weight sets W_k^*
  - To output the average $f_e(x) = \frac{1}{K} \sum_1^K f(x; W_k^*)$
- We expect outputs of the form $\widehat{y}_k^p = y^p + \epsilon_k^p$ with the ϵ_k^p independent
- Hence $\frac{1}{K} \sum_k \epsilon_k^p \simeq 0$ and $\frac{1}{K} \sum_k \widehat{y}_k^p \simeq y^p$

Takeaways on MLP Regularization

- MLPs have a high risk of overfitting
- Thus, they must be **regularized** to avoid overfitting
- The regularization hyperparameter is chosen through **cross validation**
- MLP training has two random components: the initial point and minibacth selection
- They do not thus converge to a single optimum
- MLP ensembles can take advantage of this
- They imply extra costs but ensembles are embarrassingly parallelizable

4.4 Bias & Variance in Regression

Sample Dependence

- Important: **everything is sample dependent** for if we change S we get a different model
- We get sample–dependent weights $\widehat{w} = \widehat{w}_S$ and model $\widehat{f}_S(x) = \widehat{f}_S(x; \widehat{w}_S)$
- We must to control their dependence on the concrete S sample used to build it
- Moreover, we must apply our model on new, **unseen** samples
- We must have a sample generating procedure that ideally gives homogeneous samples S, S', and a robust model building methodology
- They should (reasonably) guarantee that
$$\widehat{f}_S(x) \simeq \widehat{f}_{S'}(x)$$

Sample Bias and Variance

- If we had several samples $S_1, \ldots, S_M$ we could work with the averages of the $\widehat{f}_{S_m}(x)$ models, i.e.,
$$\frac{1}{M}\sum_1^M \widehat{f}_{S_m}(x) \simeq E_S[\widehat{f}_S(x)] = \widehat{f}_N(x)$$
which approximate the **samples' average** $\widehat{f}_N(x)$ of f_s at x
- The variance of the $\widehat{f}_S(x)$ estimates is then
$$V_N(x) = E_S\left[(\widehat{f}_S(x) - \widehat{f}_N(x))^2\right]$$
- Ideally we would like to have a small model **bias** $\widehat{f}_N(x) - \phi(x)$ and a small model **variance** $V_N(x)$
- Then we would have $\widehat{f}_s(x) \simeq \phi(x)$ and $\widehat{f}_s(x)$ would change little with S

Expected Prediction Error

- Q: at a fixed x, **what error we may expect for models built over size N samples?**
- The **expected prediction error** (EPE) at a fixed x over all such samples is
$$\begin{aligned} EPE(x) = E_{Y|x,S}[(y - \widehat{f}_S(x))^2] &= E_{n,S}[(n + \phi(x) - \widehat{f}_S(x))^2] \\ &= E_n[n^2] + E_S[(\phi(x) - \widehat{f}_S(x))^2] \\ &= \sigma^2 + E_S[(\phi(x) - \widehat{f}_N(x) + \widehat{f}_N(x) - \widehat{f}_S(x))^2] \\ &= \sigma^2 + \\ &\quad (\phi(x) - \widehat{f}_N(x))^2 + \\ &\quad E_S[(\widehat{f}_S(x) - \widehat{f}_N(x))^2] \end{aligned}$$

Bias vs Variance

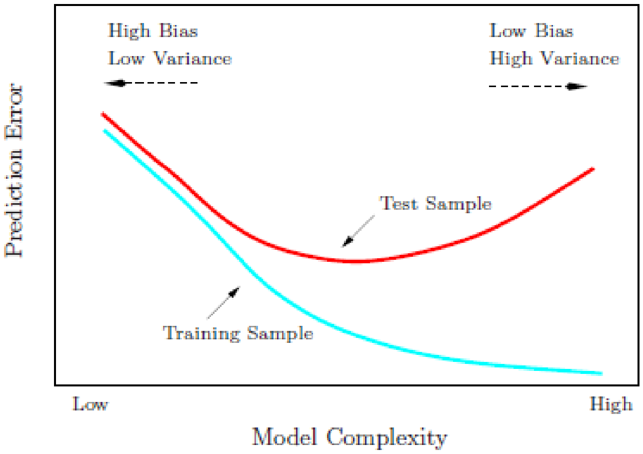
- We do not have control on σ^2 but

  The **bias** term $(\phi(x) - \widehat{f}_N(x))^2$ should be small if the family $\mathcal{F}$ is flexible enough

  The **variance** term $E_S[(\widehat{f}_S(x) - \widehat{f}_N(x))^2]$ should be small for simple models
- Thus ideally we want **highly flexible, low bias models** that also have **small across sample variance**
- But usually flexibility comes from having many model parameters (i.e., highly complex models)
- That, in turn, may change substantially when computed across different samples

The Bias–Variance Tradeoff

- There is thus a **tradeoff** between bias (low for complex models) and variance (low for simple models)



Taken from *Hastie et al., p. 38*

Evaluating Expected Model Performance

- The previous theoretical considerations give **very important practical insights**
- Measuring a model's **generalization** performance **only** over the training sample S results in misleading error values
- Ideal goal: to have M subsamples S_m and
  - Compute $\widehat{f}_M(x) = \frac{1}{M}\sum_m \widehat{f}_{S_m}(x) \simeq \widehat{f}_N(x)$

  - Get the error estimate $\widehat{e} = \frac{1}{N}\sum_p (y^p - \widehat{f}_M(x^p))^2$ over a new sample $\{(x^p, y^p)\}$

- Since usually we only have a single S, we apply **Cross Validation** (CV) to get more realistic generalization error estimates

Cross Validation

- In Cross Validation (CV) we
  - Randomly split the sample S in M subsets $S_1, \dots, S_M$
  - Work with M **folds**: pairs (S_m, S_m^c), with
    $$S_m^c = S - S_m = \cup_{i \neq m} S_i$$
  - Build M different models using the S_m^c as training subsets
  - Compute their errors e_m on the folds' validation subsets S_m
  - Use these errors' average as a first estimate of the true model performance

- CV can and must be used in any model building procedure

- Most data science packages have tools to simplify this

- We will also use CV to find **optimal model hyperparameters**

Takeaways on Bias, Variance and CV

1. We have stressed that **any model estimation is sample–dependent** and that this has to be controlled

2. We have introduced the **bias** and **variance** as the two key components of any model error

3. We have discussed **bias–variance trade–off**

4. We have introduced **Cross Validation** here as a tool to estimate a **model's generalization performance**

5. We have also introduced **Cross Validation** as a tool to estimate a **model's hyperparameters**

5 Convergence of MLP Training

5.1 Computational Costs of MLPs

MLPs and Big Data?

- Many Vs in Big Data: **Volume, Velocity**, Variety, Veracity, Value, ...

- Velocity: information flows in data streams that require fast processing and feed back
  - MLPs are rather fast
  - Less than linear models but much more so than SVMs

- Volume is probably the greatest attractive of Big Data
  - Huge samples and/or very large pattern dimension
  - Large impact in model training

Volume in MLPs

- Parallelism is the first answer to Big Volume
- On a standalone machine it may be
  - Passive: let the SO distribute work among several cores, or use low level parallelized libraries such as Linpack or BLAS for linear algebra
  - Active: explicitly exploit a problem's parallelism programming an algorithm in, say, OpenMP
- It is easy to passively parallelize the training of several MLPs
  - But memory costs multiply
- Training an isolated MLP is not parallelizable:
  - There is a sequential layer dependence in Backprop
  - It is the same for training iterations

MLP Complexity

- MLPs are fast to apply but costly to train
- How can we train MLPs over large sample sizes/dimensions?
- MLP traning cost is determined by
  - Its **architecture**, that determines the number of weights to fit and that is usually dependent on the input dimension D
  - The full or mini–batch **sample size** N, that determines the cost of the averages to be computed
  - The **training method**, with more or less iterations that, in turn, are more or less costly

Forward Pass Complexity

- The number of weights in a single hidden layer (SHL) MLP with D inputs, L outputs and one hidden layer with H units is

$$(D+1) \times H + (H+1) \times L \simeq H(D+L)$$

  - In regression, $L = 1$, so the weight number is $O(DH)$ for a regression SHL MLP
- Each extra $H_1 \times H_2$ hidden layer adds $(H_1 + 1) \times H_2 \simeq H_1 H_2$ weights

- For a general MLP the cost in FP operations of a forward pass is $\simeq N \times (\sum_h H_h \times H_{h-1})$
  - Very fast on GPUs

The Cost of Computing ∇e^ℓ

- Computing a local gradient ∇e^ℓ in a SHL MLP with square error and L outputs requires to compute
  - LH components for the hidden to output connections, with a $O(1)$ cost each, for $\frac{\partial e^\ell}{\partial w^O_{ih}} = (\widehat{y}_i - y_i)o_h$
  - DH components for the input to hidden connections with essentially an $O(1)$ cost each, for $\frac{\partial e^\ell}{\partial w^H_{h,j}} = \left(\sum_{i=1}^L \delta_i w^O_{ih}\right) \sigma^{'}(a_h)x_j$
- The overall cost of computing ∇e^ℓ is thus

$$O(LH + DH) \simeq O(DH)$$

  for usually $L = O(D)$
- More layers with H_h units add a cost $O(H_{h-1} \times H_h)$

The Cost of Computing ∇e

- For a sample S of size N, the cost of computing ∇e over S of a SHL MLP is $O(N(DH + HL))$
  - This is the same if the entire batch or several minibatches are used
- And each extra layer adds a cost $O(N \times H_{h-1} \times H_h)$
- This is of the same order of magnitude than the cost of the forward pass
- This also dominates the $O(H_{h-1} \times H_h)$ cost of updating the (H_{h-1}, H_h) weights in gradient descent
  - The updating costs for other methods (GN, CG, QN) are higher
- And all these costs have to be multiplied by the number of training **epochs**

Training Complexity

- The important term in the overall training cost is nEps × cost of ∇e, with nEps the number of epochs
  - One epoch = one pass on the entire sample
- Thus, the **globally dominant term** in a SHL MLP is

$$\text{nEps} \times \text{costof } (\nabla e) = O(\text{nEps } N(DH + HL))$$

  with N here the entire sample size

- And an extra cost

$$O(\text{nEps} \times N \times H_{h-1} \times H_h)$$

  for each extra hidden layer

- Thus, training many layered, large MLPs can be **very costly**
  - But it is linear on sample size

Takeaways on MLP's Cost

- MLP complexity is determined by its architecture $\{H_h\}$, training procedure and sample size N
- The forward and backward MLP passes have basically the same complexity
- Their cost per pattern and layer is $H_{h-1} \times H_h$
- For gradient descent these costs are multiplied by the number nEps of epochs
- First order methods essentially do not add extra complexity
- Second order methods add extra per iteration costs but will require less iterations
- Single MLP training is not easily parallelizable
- GPUs can greatly improve MLP processing costs

5.2 On Line Learning of MLPs

Handling Huge Sample Training

- Two consequences of a large N are
  - Sample doesn't fit in memory and we have to split it somehow
  - Global gradient is no longer feasible and we have to exploit its average $\nabla e = E[\nabla e^\ell]$ over local gradients
- The fist problem has been always present in fields such as analog signal filtering
- Solution: adaptive or **on line**, i.e., pattern by pattern, weight updates
  - Not used today: Currently medium–to–large NNs are trained using **mini–batches**
  - But allows a relatively simple setting for a theoretical analysis

Adaptive Filtering

- The signal processing solution to not having storage: **adaptive lineal filters** (ADALINE)

$$W^{k+1} = W^k - \rho_k(\hat{y}_k - y_k)X^k = W^k - \rho_k \nabla e^\ell(X^k, y_k; W^k)$$

- This is just local gradient descent in linear regression

- This makes sense also for MLPs
- On Line Learning $\equiv$ local gradient descent

On Line Learning of MLPs

- Starting from W^0, at time $\tau = 1, 2, \ldots$
  - We get a random pattern $X^p = x^{p(\tau)}$ and its target target y^p
  - We compute $\hat{y}^\tau = F(x^p, W^\tau)$ and $\nabla e^\ell(x^p, y^p; W^\tau)$
  - We update $W^{\tau+1} = W^\tau - \rho_\tau \nabla e^\ell(x^p, y^p; W^\tau)$
- SHL MLP complexity is now $O(\text{nIters} \times DHL)$ and nIters $> N$ is to be expected:
  - A batch epoch has the same cost of N on line iterations
- But now we do not have to store or even to know the entire sample
- And N on line iterations usually are more effective than a batch epoch

Variants in On Line Learning

- It is straightforward to include quadratic regularization

$$W^{\tau+1} = W^\tau - \rho_\tau \left(\nabla e^\ell(x^p, y^p; W^\tau) + \lambda W^\tau\right)$$

- As well as momentum

$$W^{\tau+1} = W^\tau - \rho_\tau \nabla e^\ell(x^p, y^p; W^\tau) + \mu_\tau \Delta^\tau$$

- Moreover the MLP is constantly updated
- We can work with **minibatches** with a fixed number of patterns instead of isolated ones
  - The same tricks and stopping criteria of batch learning apply and also CG is often possible over minibatches
- But: is there convergence?

Learning as a Random Variable Evolution

- In on line learning
  - The initial weight W^0 is random
  - The pattern $x^{p(t)}$ received at time t is also random
- Thus, the sequence W^t is a **realization of a random variable** $\mathcal{W}^t$
- We have deal with random variable convergence theory ...
- Rather heavy going, with many, more or less related, definitions

Convergence of Random Variables

- The basic limit concepts have to be adapted when dealing with random variables
- Set up: probability space $(\Omega, \mathcal{A}, P)$
- Pointwise limits are trickier so one starts with mean convergence
- $X_n \to X$ **in the r–th mean**, $r \geq 1$, (usually $r = 2$ or $r = 1$) if

$$E_P[|X_n - X|^r] = \int |X_n(\omega) - X(\omega)|^r dP(\omega) \to 0$$

- For a general probability space $(\Omega, \mathcal{A}, P)$ and suitable f, $E_P[f] = \int f(\omega) dP(\omega)$ can be properly defined
- Situation here: ω is given as a feature vector x and dP has a density $p(x)$; the previous definition becomes

$$E_P[|X_n - X|^r] = \int |X_n(x) - X(x)|^r p(x) dx \to 0$$

Pointwise Convergence of Random Variables

- We say $X_n \to X$ **almost surely** (AS) if

$$P(\{\omega : \lim X_n(\omega) = X(\omega)\}) = 1$$

  - It is the closest to the standard pointwise convergence
  - Has many synonimes: convergence **almost everywhere, strongly** or (slightly confusing) **with probability 1**

- An equivalent definition is that for all $\epsilon > 0$

$$\lim_n P(\{\omega : \sup_{m \geq n} |X_m(\omega) - X(\omega)| \geq \epsilon\}) = 0$$

- We say $X_n \to X$ **in probability** if for all $\epsilon > 0$

$$\lim P(\{\omega : |X_n(\omega) - X(\omega)| \geq \epsilon\}) = 0$$

- Convergence AS is thus stronger than convergence in probability
- In fact, convergence AS surely implies convergence in probability

Convergence in Distribution

- We say $X_n \to X$ **in distribution** if $\lim F_{X_n}(x) = F_X(x)$ at every x where F is continuous
- Synonimes: convergence **in law** or **weakly**

- The continuity requirement aims to avoid degenerate cases
  - If $X_n = \chi_{[0,1/n]}$, they converge in distribution (and pointwise) to $X \equiv 0$, for which $F_X(0) = 1$ while $F_{X_n}(0) = 0$
  - But 0 is not a point of continuity of F_X
- Convergence in distribution does not imply convergence of the density functions
- But convergence of the density functions implies convergence in distribution
- **Lévy's Theorem**: the sequence X_n converges in distribution to X iff the sequence of corresponding characteristic functions ϕ_n converges pointwise to the characteristic function ϕ of X

Relationships

- Recall that convergence almost surely implies convergence in probability
- Convergence in probability implies convergence in distribution
- Convergence in the mean for $r \geq 1$ implies convergence in probability (by Markov's inequality)
- If $r > s \geq 1$, convergence in the r–th mean implies convergence in the s–th mean
- Convergence in probability (and, hence, in the mean) implies convergence a.s. for some subsequence X_{n_k}
- If the X_n are bounded by an integrable Z and converge a.s. to X, they also converge in the r–th mean
- But the other implications are false

Limit Theorems

- **Weak Law of Large Numbers:** if the X_n are i.i.d., then the sample mean $\overline{X}_N = \frac{1}{N}\sum_1^N X_n$ converges in probability (weakly) to $\mu = E[X_n]$
- **Strong Law of Large Numbers:** if the X_n are i.i.d., then the sample mean $\overline{X}_N = \frac{1}{N}\sum_1^N X_n$ converges a.s. (strongly) to $\mu = E[X_n]$
- Besides weaker, the weak LLN is easier to prove
- **Central Limit Theorem:** if the X_n are i.i.d. with mean μ and variance σ^2, then the random variable $\sqrt{N}(\overline{X}_N - \mu)$ converges in distribution to a Normal $N(0, \sigma^2)$
- The LLN tells us that the sample mean converges; the CLT tells us how the sample mean error (approximately) behaves

Convergence of On Line Learning

- The end result is that the random variable sequence $\mathcal{W}^t$ converges in mean square to an W^* s.t. $0 = \nabla e(W^*)$

- That is, W^* is (very likely) a local minimum of e
- Theoretical foundation in the **Strong Law of Large Numbers:**

  If the X^n are i.i.d., then the sample mean $\overline{X}_N = \frac{1}{N}\sum_1^N X^n$ converges a.s. (strongly) to $\mu = E[X^n]$

Stochastic Optimization (SO)

- In a deeper look, assume the following:
  - We want to solve the equation $g(w) = 0$ that has a single root w^*
  - Where we don't know $g(w)$ ...
  - But can get an **oracle**, i.e., a random estimate $\hat{g}(X^n, w)$ with X^n i.i.d. such that $E[\hat{g}(X, w)] = g(w)$.
- Then, starting at a random W^0 and for some sequence ρ_k, we define

$$W^{k+1} = W^k - \rho_k \hat{g}(X^k, W^k)$$

  and hope for the best

Robbins–Monro SO

- Robbins and Monro showed that $W^k \to w^*$ in square mean (and, hence, in probability) if (among others)
  1. g is non decreasing and $g'(w^*) > 0$,
  2. $\sum \rho_k = \infty, \sum \rho_k^2 < \infty$
- For a D dimensional extension we assume the Jacobian $J_g(w^*)$ to be positive definite
- We need a dictionary to translate this to on line MLP training
- But first let's try to understand it on a simple situation

Why it Works?

- Assume we want to solve the equation $g(w) = w - \mu$ where we do not know μ, but can get random estimates $\hat{g}(X_n, w) = w - X_n$ with X_n i.i.d. s.t. $E[X_n] = \mu$
- It is obvious that $E[\hat{g}(X, w)] = g(w)$
- Then, starting at $W_0 = 0$ and for $\rho_k = \frac{1}{k+1}$, let's define

$$W_{k+1} = W_k - \frac{1}{k+1}(W_k - X_{k+1});$$

- Then, unwinding the recurrence we arrive at

  $$W_{k+1} = \frac{1}{k+1}\sum_{1}^{k+1} X_j,$$

  which, by the LLN converges to the root $\mu = E[X]$ of $w - \mu = 0$

- Thus Robbins–Monro essentially reduces here to the LLN

Stochastic Optimization and MLPs

- We begin with $e(w) = E[e^{\ell}(\cdot, w)]$, which is smooth with (we hope) a minimum w^*
- As g we take $g(w) = \nabla e(w) = E_X[\nabla e^{\ell}(x, w)]$ (unknown) and $\hat{g}(x, w) = \nabla e^{\ell}(x, w)$ (known)
- Then we have $E_X[\hat{g}(x, w)] = g(w)$
- Its Jacobian $J_g(w) = \mathcal{H}_e(w)$ is definite positive at and near w^*
- Starting at a random W^0 we take the X^k as i.i.d. and build the r.v. sequence for appropriate ρ_k

  $$W^{k+1} = W^k - \rho_k \nabla e^{\ell}(X^k, W^k)$$

- Robbins–Monro then ensures that the W^k converge in mean square to an w^* s.t. $0 = g(w^*) = \nabla e(w^*)$, which by local convexity must then be a minimum of e

Takeaways on Online Learning

1. Training standalone MLPs is difficult to parallelize (or to be done under a MapReduce scheme)
2. On the other hand, simple parallel training of several MLPs is very easy
3. Very large samples require on line or (usually) mini–batch training
4. Theoretical results on Stochastic Gradient Descent imply convergence (in a random variable sense)
5. But training may be slow and unstable
6. And choosing the right learning rate may be tricky

5.3 Convergence Rates

Convex Functions

- f is **convex** if $f(\lambda w + (1-\lambda)w') \leq \lambda f(w) + (1-\lambda) f(w')$
- Arquetypical example: positive quadratic form $q(w) = \frac{1}{2} w^t Q w + b \cdot w + c$, with Q positive (semi–) definite
  - We expect that $f(w) \simeq q(w)$ near a minimum w^* of a C^2 f

- Convex functions are the natural ground to study minimization problems
- Convex functions have global minima: if w^* is a local minimum of a convex f, it is also a global minimum since if w^* is a local minimum, λ small and for any other w

  $$f(w^*) \leq f((1-\lambda)w^* + \lambda w) \leq (1-\lambda)f(w^*) + \lambda f(w),$$

  and this implies implies $f(w^*) \leq f(w)$
- Consequence: the minimum f^* of a convex f is unique (although the arg min may be not)
- And also, if f is C^1, w^* is a minimum of f iff $\nabla f(w^*) = 0$

Strong / Strongly Smooth Functions

- Hyperplane bound: if f is convex and C^1, for any pair x, y

  $$f(y) \geq f(x) + \nabla f(x)(y-x) \tag{2}$$
- We say that f is μ–**strongly convex** (μ–SC) if there is a $\mu > 0$ such that for any pair x, y

  $$f(y) \geq f(x) + \nabla f(x)(y-x) + \frac{\mu}{2}\|y-x\|^2$$
- We say that f is L–**strongly smooth** (L–SS) if there is an $L > 0$ such that for any pair x, y

  $$f(y) \leq f(x) + \nabla f(x)(y-x) + \frac{L}{2}\|y-x\|^2$$

  - If ∇f is Lipschitz with constant L, f is then L–strongly smooth

Gradient Descent for SSC Functions

- If f is L-SSC and $x_{k+1} = x_k - \alpha \nabla f_k$

  $$f_{k+1} \leq f_k - \nabla f_k \cdot (\alpha \nabla f_k) + \frac{L}{2}\|\alpha \nabla f_k\|^2 = f_k + \left(\frac{\alpha^2 L}{2} - \alpha\right)\|\nabla f_k\|^2$$
- The optimal step is thus $\alpha = \frac{1}{L}$ and then

  $$f_{k+1} \leq f_k - \frac{1}{2L}\|\nabla f_k\|^2 \tag{3}$$

  and the f_k decrease (unless $\nabla f_k = 0$)
- Writing $x_k = x$, $p = x_{k+1}$, from this we can deduce that for any z

  $$f(p) - f(z) \leq \frac{L}{2}\|x-z\|^2 - \frac{L}{2}\|p-z\|^2$$

  which we prove next

Bounds for SSC Gradient Descent

- Notice that $\nabla f(x) = L(p-x)$ and using (2) and (3)

$$\begin{aligned} f(p) - f(z) &\leq -\nabla f(x)\cdot(z-x) - \frac{1}{2L}\|\nabla f(x)\|^2 \\ &= -L(p-x)\cdot(z-x) - \frac{L}{2}\|p-x\|^2 - \\ &\quad \frac{L}{2}\|z-x\|^2 + \frac{L}{2}\|z-x\|^2 \\ &= \frac{L}{2}\|z-x\|^2 - \frac{L}{2}\|z-p\|^2 \end{aligned}$$

- Taking $z = x^*$, it follows that

$$f_{k+1} - f^* \leq \frac{L}{2}\|x_k - x^*\|^2 - \frac{L}{2}\|x_{k+1} - x^*\|^2$$

GD Convergence Rate for SSCFs

- Summing things up for $k = 0, \ldots, K-1$, we have

$$\begin{aligned} \sum_0^{K-1}(f_{k+1} - f^*) &\leq \frac{L}{2}\left(\sum_0^{K-1}\left\{\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2\right\}\right) \\ &= \frac{L}{2}\left(\|x_0 - x^*\|^2 - \|x_K - x^*\|^2\right) \end{aligned}$$

  and since the f_k decrease we arrive at

$$f_K - f^* \leq \frac{1}{K}\sum_0^{K-1}(f_{k+1} - f^*) \leq \frac{L\|x_0 - x^*\|^2}{2K}$$

- I.e., for a L SSC convex f, the gradient descent sequence f_K converges to f^* with a $O\left(\frac{1}{K}\right)$ rate

Contractive Gradient Descent

- We say that a transformation T is η–**contractive** if $\|T(x) - T(y)\| \leq \eta\|x-y\|$, with $\eta < 1$
- **Fixed point convergence:** If T is η–contractive, then the sequence $x_k = T^k(x_0)$ converges to x^* and $\|x_k - x^*\| \leq \eta^k\|x_0 - x^*\|$
- If a C^2 f is μ–SC and L–SSC, then $\mu I \preceq \nabla^2 f(z) \preceq LI$ for any z
- Writing gradient steps in terms of the operator $G_\alpha(x) = x - \alpha\nabla f(x)$, we have

$$\begin{aligned} G_\alpha(y) - G_\alpha(x) &= y - x - \alpha(\nabla f(y) - \nabla f(x)) \\ &= (I - \alpha\nabla^2 f(z))(y-x) \\ &\leq \|I - \alpha\nabla^2 f(z)\|\|y-x\| \\ &\leq \max\{|1-\alpha\mu|, |1-\alpha L|\}\ \ \|y-x\| \end{aligned}$$

  where z is some point intermediate between x and y

GD for α–SC and L–SSC Functions

- In other words, G_α is η_α–contractive with $\eta_\alpha = \max\{|1-\alpha\mu|, |1-\alpha L|\}$
- It is easy to see that the optimal α^* that minimizes η_α is $\alpha^* = \frac{2}{\mu+L}$, for which we have

$$\eta_{\alpha^*} = \frac{L-\mu}{L+\mu} = \frac{\kappa-1}{\kappa+1}$$

  with $\kappa = \frac{L}{\mu}$ the **condition number** of $\nabla^2 f$ at any z

- Thus, if f is α–SC and L–SSC we achieve a **linear** convergence rate

$$\|x_K - x^*\| \leq \left(\frac{\kappa-1}{\kappa+1}\right)^K \|x_0 - x^*\|$$

Optimal Convergence Rates for GD

- We can construct L–SSC functions f in $\mathbf{R}^{2k+1}$ such that GD verifies

$$f_k - f^* \geq \frac{C(x_o, x^*, f^*)}{k^2}$$

- We can also construct μ–SC, L–SSC functions f such that GD verifies

$$\|x_k - x^*\| \geq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k \|x_0 - x^*\|$$

- Q: can we improve GD as to attain these bounds?

The Heavy Ball Method

- The iterations of the Heavy Ball (or Momentum) method are

$$x_{k+1} = x_k - \alpha \nabla f(x_k) + \beta(x_k - x_{k-1})$$

- If f is μ–SC and L–SSC and we take

$$\alpha = \arg\max_{\alpha'} \{|1-\sqrt{\alpha'\mu}|, |1-\sqrt{\alpha' L}|\} = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2}$$

  and also

$$\beta = \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^2$$

  then the contraction factor becomes $\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$, i.e.

$$\|x_k - x^*\| \leq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k \|x_0 - x^*\|$$

Nesterov's Method

- The iterations in Nesterov's method are

$$y_{k+1} = x_k + \beta_{k+1}(x_k - x_{k-1}), \;\; x_{k+1} = y_{k+1} - \frac{1}{L}\nabla f(y_{k+1})$$

  where the β_k are defined as

$$\beta_{k+1} = \frac{t_k - 1}{t_{k+1}}, \;\; t_{k+1} = \frac{1}{2}\left(1 + \sqrt{1 + 4t_k^2}\right)$$

  starting with $y_1 = x_0$, $t_1 = 1$

- Then, if f is L–SSC, Nesterov's iterations verify

$$f_k - f^* \leq \frac{2L\|x_0 - x^*\|^2}{(k+1)^2}$$

- Moreover, the x_k converge weakly to x^*

Nesterov's Method for SSCFs

- There is also a version of Nesterov for μ–SC, L–SSC functions f in which we take

$$\begin{aligned} y_{k+1} &= x_k + \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}(x_k - x_{k-1}), \\ x_{k+1} &= y_{k+1} - \frac{1}{L}\nabla f(y_{k+1}) \end{aligned}$$

- For these we have

$$f_k - f^* \leq L\left(1 - \frac{1}{\sqrt{\kappa}}\right)^k \|x_0 - x^*\|^2$$

Optimal Convergence for Stochastic GD

- If f is C^1 and convex, and we set $\tilde{x}_k = \frac{1}{k}\sum_1^k x_j$, then

$$f(\tilde{x}_k) - f^* \leq \frac{C}{\sqrt{k}}$$

- If, moreover, f is SSC, then

$$E[\|x_k - x^*\|^2] \leq \frac{C}{k}$$