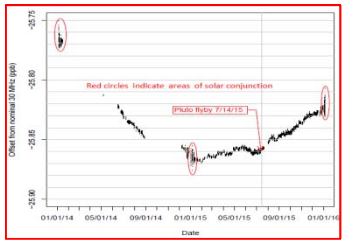
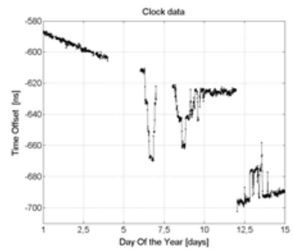
Metrology: from physics fundamentals to quality of life

July 2016

International School of Physics

Statistical tools for time varying quantities





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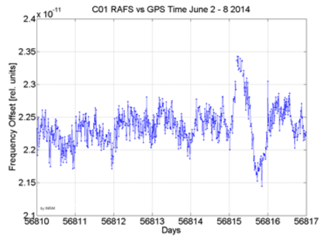
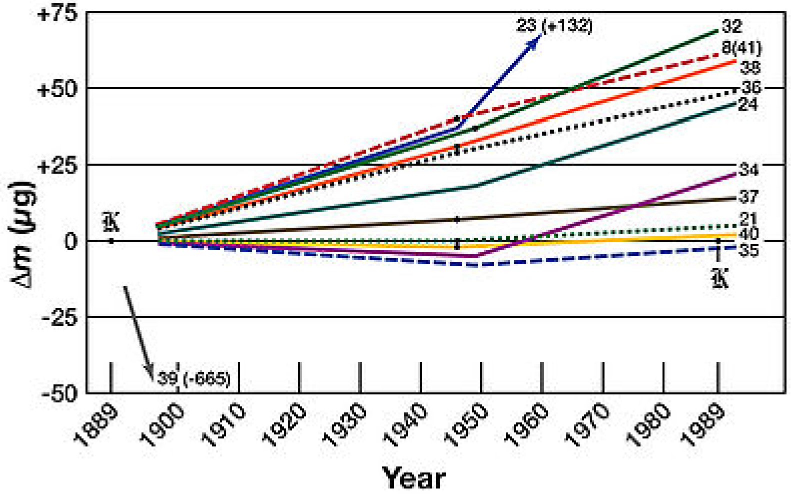
Torino Italy

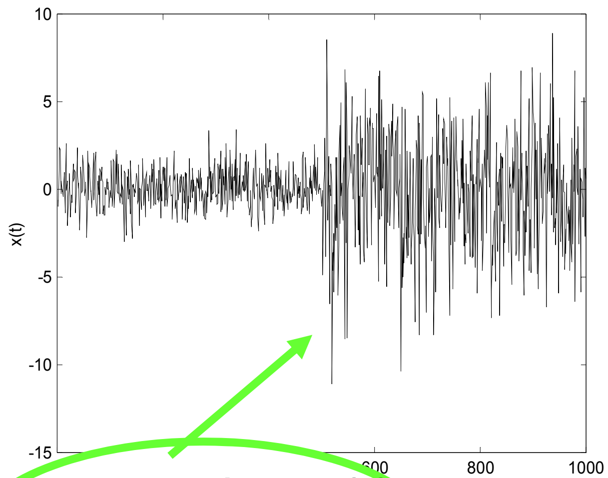


Varenna 2016

Repeated measurements reveal always something

- *stationarity*
- *aging*
- *slow drift*
- *abrupt change*
- *failure*





around t = 500
the noise
increases

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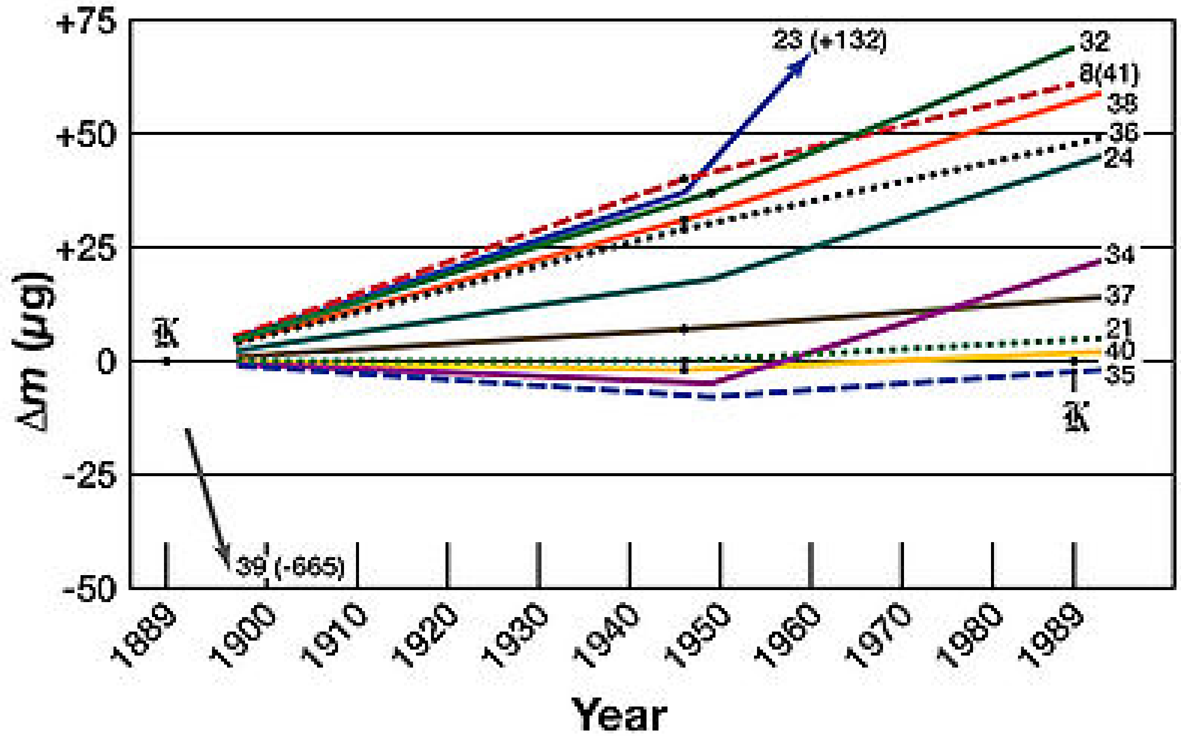
Changes may cause disturbance: the mass of the International Prototype Kilogram



Masses of the entire worldwide ensemble of prototypes have been slowly diverging from each other.

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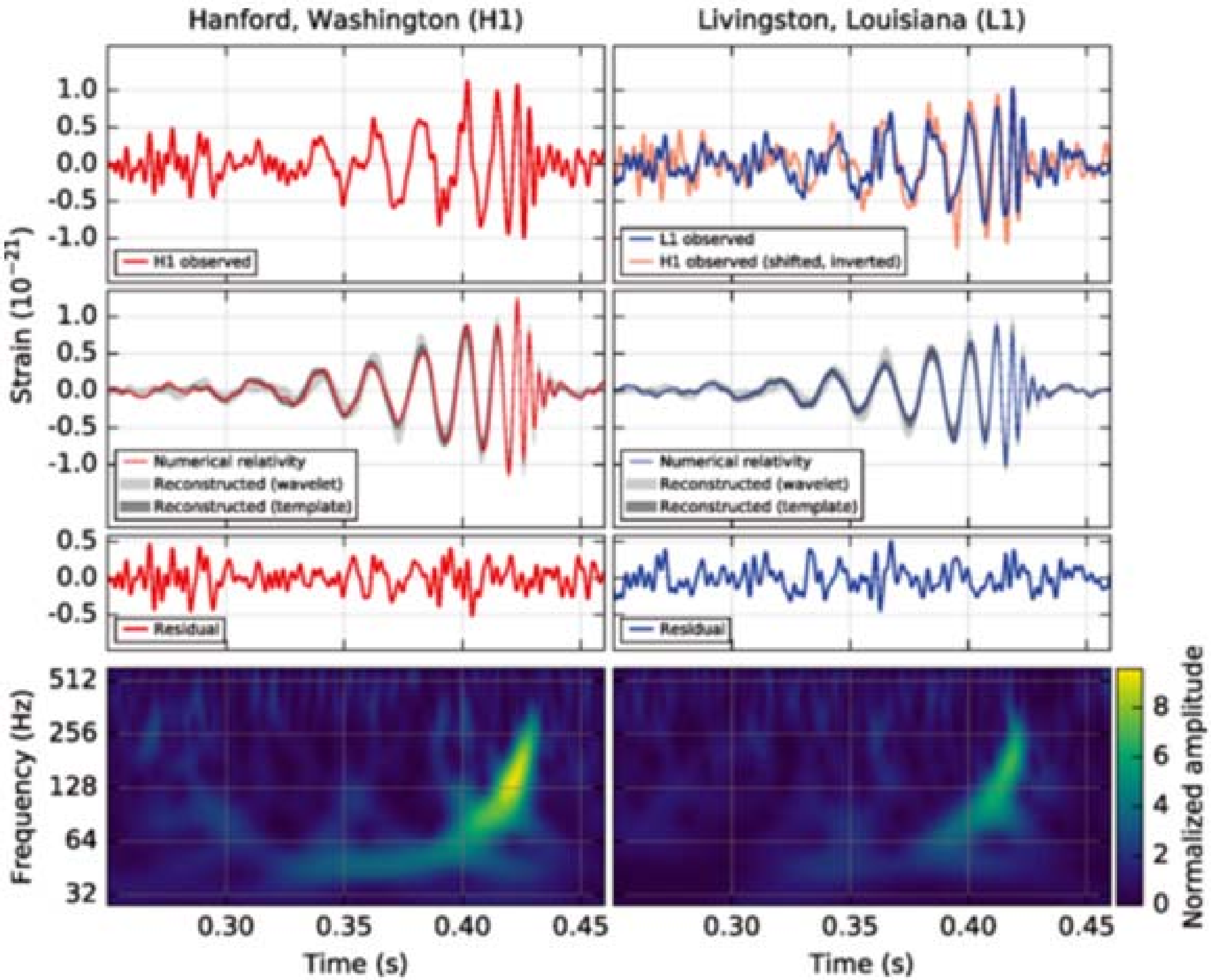
Or may reveal new physics



LIGO Sees First Gravitational Waves

Or just give the complete picture

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Statistical and Mathematical Tools

noise filtering

simulation

long term analysis

- to **estimate** the behaviour of a physical quantity and its possible impact on complex systems
- to **predict** the behaviour
- to **control** the behaviour

→

uncertainty propagation

identifying drift

data validation

assessing noise

calibration intervals

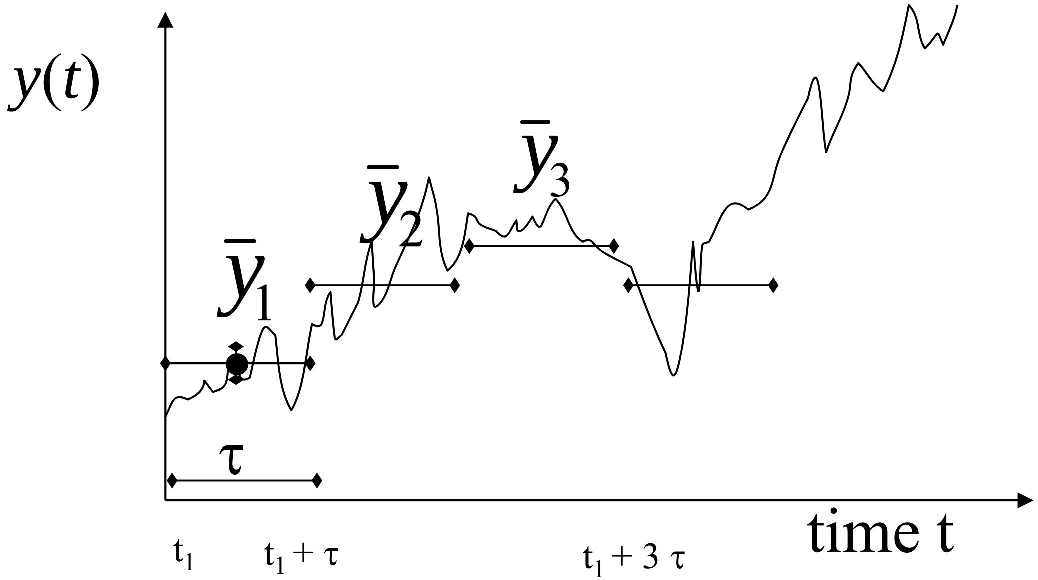
outliers

missing data reconstruction

P. Tavella, "Statistical and mathematical tools for atomic clocks", Metrologia 45, 6, (2008) S183-S192

Repeating measurements

The uncertainty on the single measure can be evaluated according to the GUM: Guide for Uncertainty in Measurement



instability is more impacting than single measure uncertainty

Instability is more impacting than single measure uncertainty

Instability can be due to the measurement process,
to the reference standard, to device under test, ot to the measurand

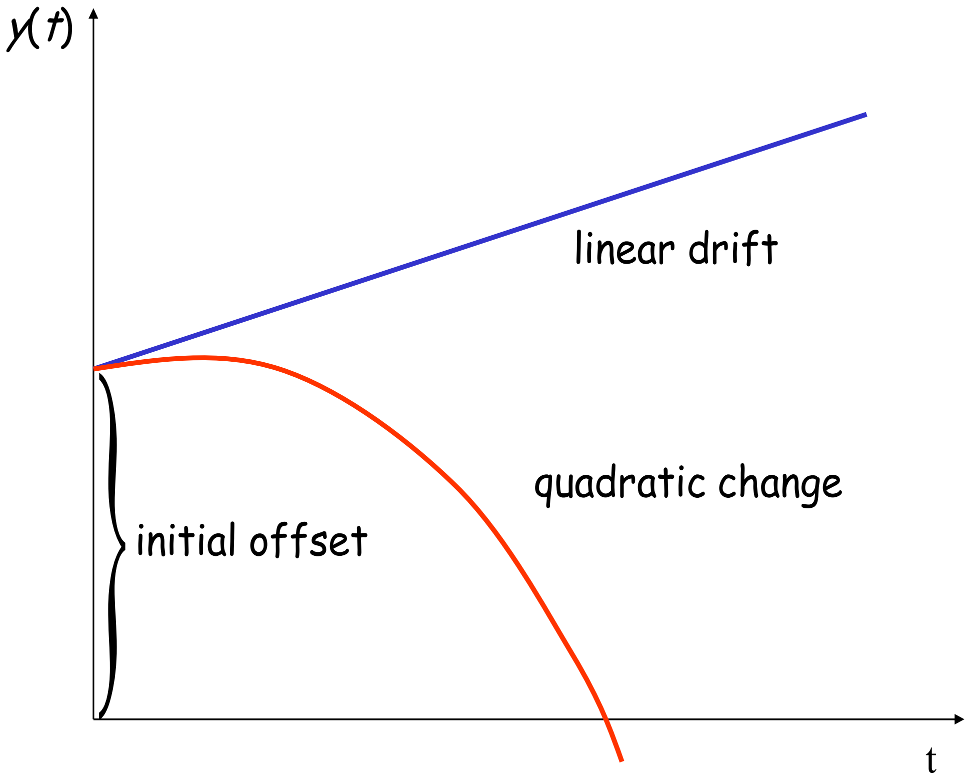
- If we want to produce and sell a reference measurement standard or measuring device

- If we want to use the standard as primary reference for calibrating other devices

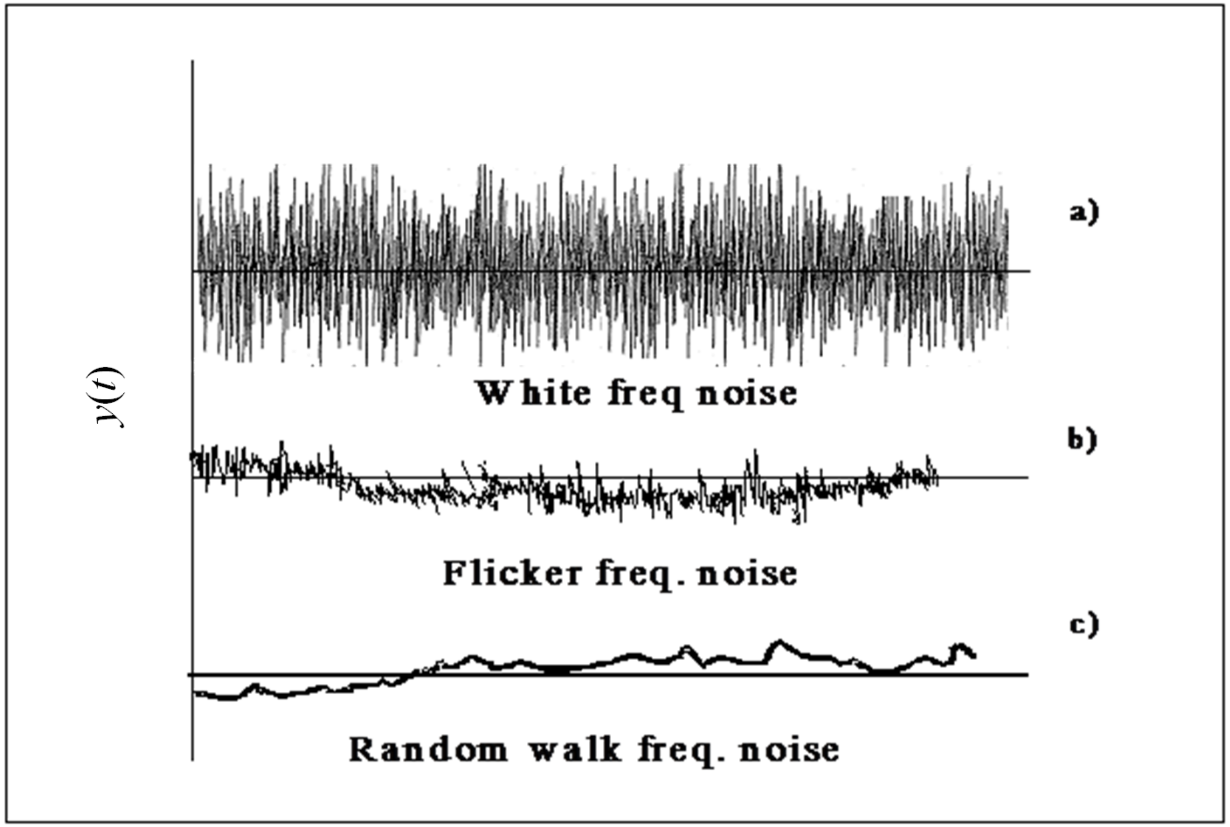
- If we want to carry out precise measure to test fundamental physics

- If we use the standard or the measurement device in a complex system, as space, health, environment applications

Time series of measures may contain polynomial component to be treated by least square estimation techniques (batch, recursive…)



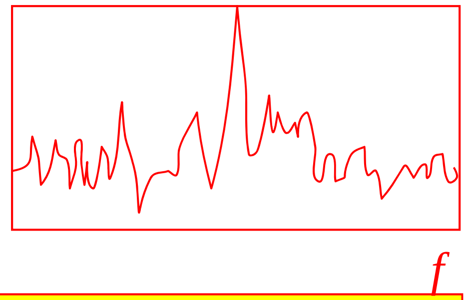
but stochastic components are also present and sometime dominant



At each instant the measure y(t) is a random variable

Appropriate mathematical tools for describing the stochastic noises:

- Spectral analysis of noise

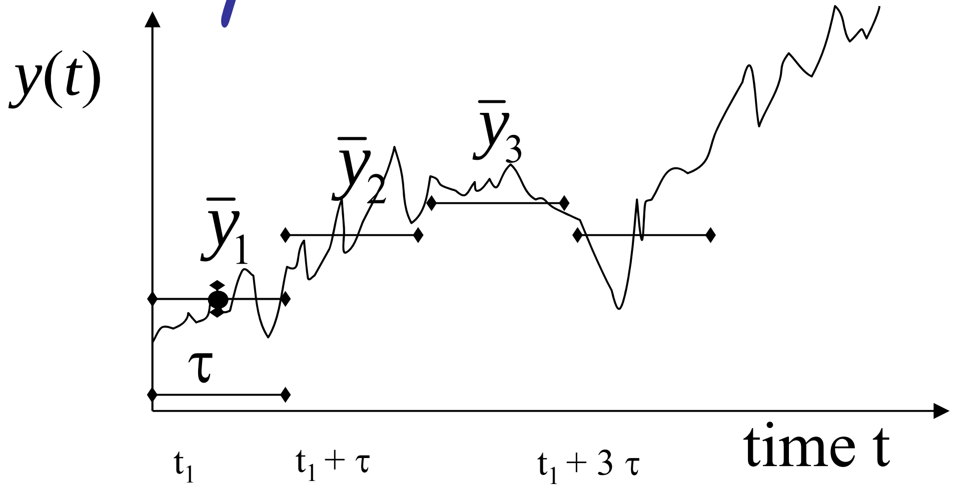


decomposition in elementary frequencies

- Filtered variances such as the Allan variance

dispersion of the average frequency values

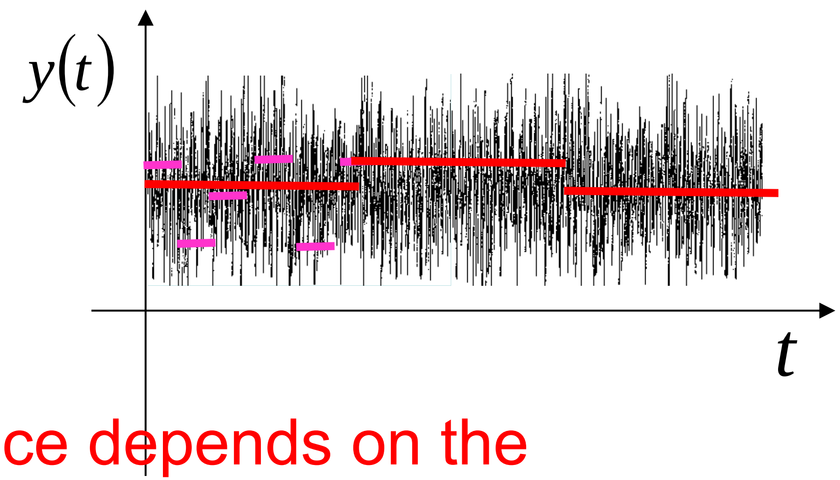
Instability - dispersion - variability



The variance is the measure of dispersion

$$\sigma^2(\tau) = \frac{\sum_{i=1}^{N} (\bar{y}_i - \mu)^2}{N}$$

First case of typical noisy behaviour (short term noise):



If the “noise” is stationary, the estimation of the variance converges as N grows

For longer observation interval τ, the variability diminishes
The “noise” is white and

$$\sigma^2(\tau) \propto \frac{1}{\tau}$$

The variance depends on the observation interval τ

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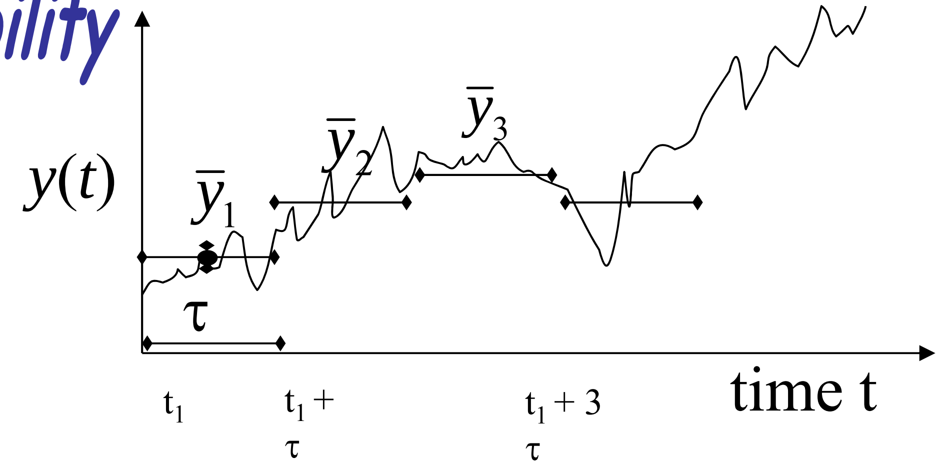
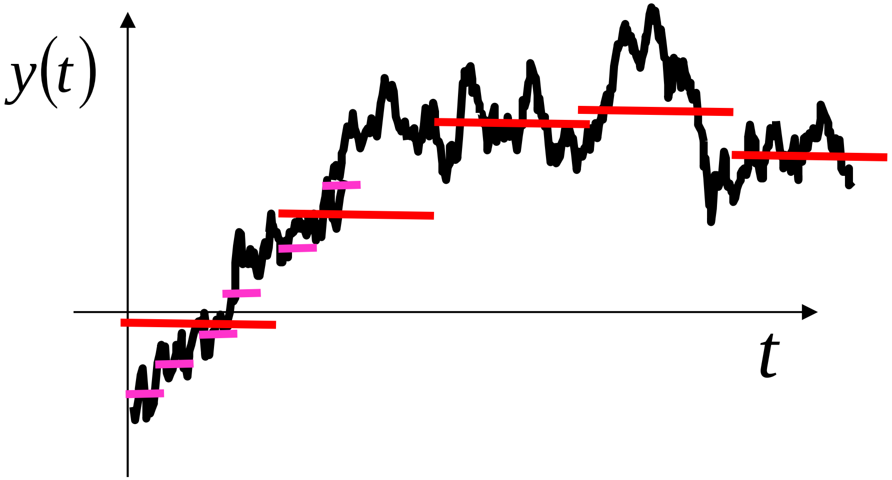
Instability - dispersion - variability

The variance is the measure of dispersion

$$\sigma^2(\tau) = \frac{\sum_{i=1}^{N} (\bar{y}_i - \mu)^2}{N}$$



Other typical noisy behaviour (long term noise)



If the "noise" is not strictly stationary, e.g. a random walk, the estimation of the variance do not converge and depends on N the number of samples (for any τ)

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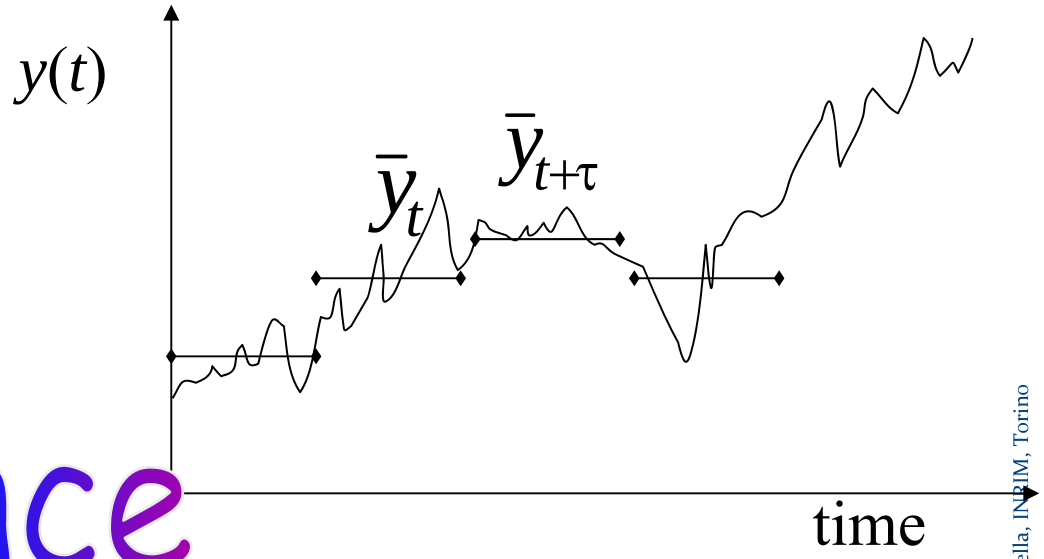
If the “noise” is not strictly stationary, e.g. a random walk, the estimation of the variance do not converge and depends on N the number of samples (for any τ)

IDEA of Allan and Barnes (1966) let’s agree on the number of samples N=2

$$\sigma^2(N=2,\tau)=\frac{\sum_{i=1}^{2}(\bar{y}_i-\mu)^2}{2}=\frac{1}{2}(\bar{y}_1-\bar{y}_2)^2$$

and let’s average many 2-sample variances

$$\sigma_y^2(\tau)=\frac{1}{2}\left\langle\left(\bar{y}_{t+\tau}-\bar{y}_t\right)^2\right\rangle$$

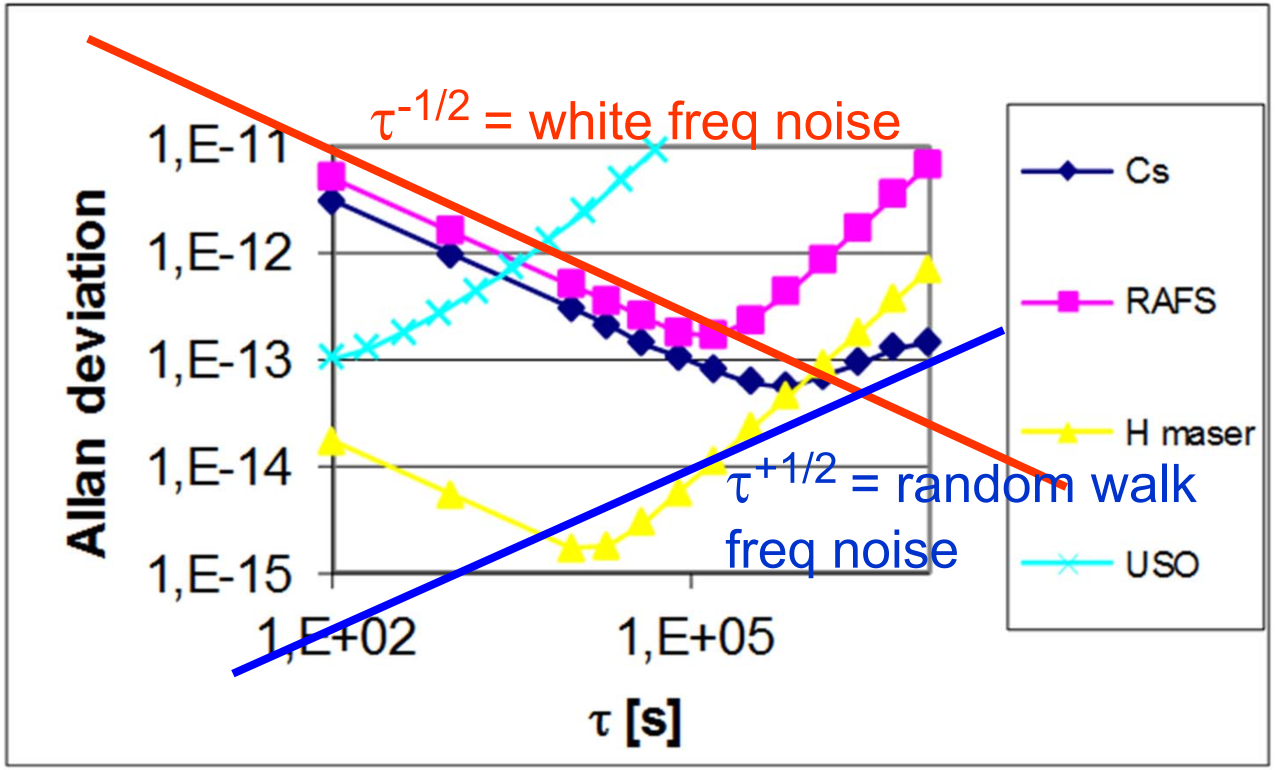


Allan variance

stability of the mean values (on τ intervals), actually variance of increments

J. Levine, P. Tavella, G. Santarelli, “Introduction to the Special Issue on Celebrating the 50th Anniversary of the Allan Variance”, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. 63, No. 4, Pag 511 – 512, April 2016

With the Allan deviation we understand which type of noise is (mostly) affecting the measures, usually applied to the frequency of the atomic clocks



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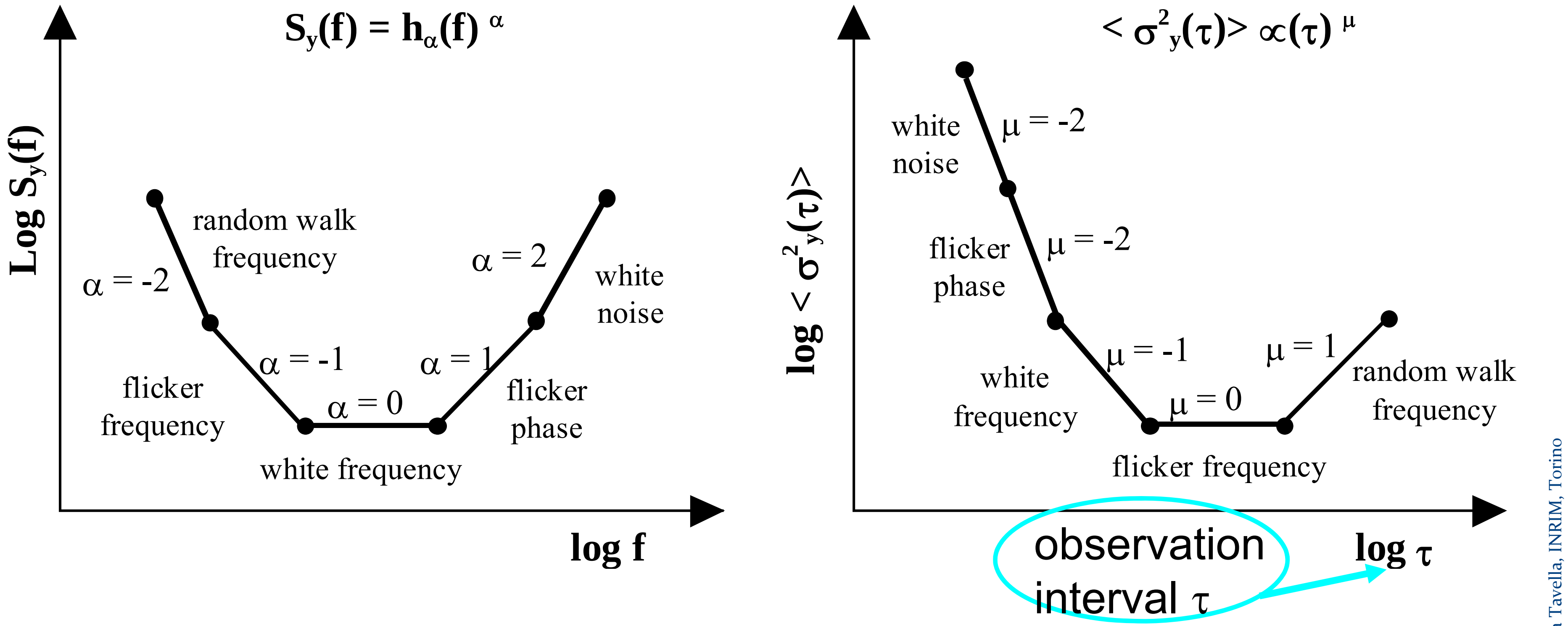
Allan variance <-> spectral density



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What we learnt

1- In some cases, the frequency instability is more impacting than single measure uncertainty

2. The instability variance depends on the observation interval τ

3. In some cases, the noise is non strictly stationary and the classical variance is not an appropriate tool. The Allan variance was proposed and important properties were found

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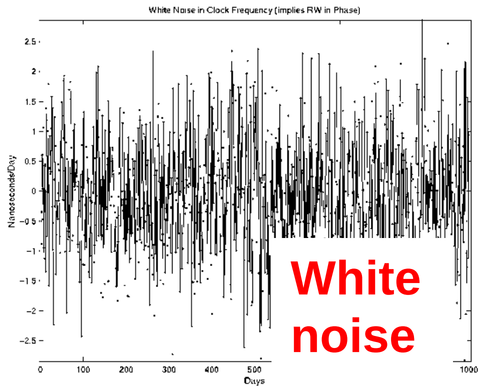
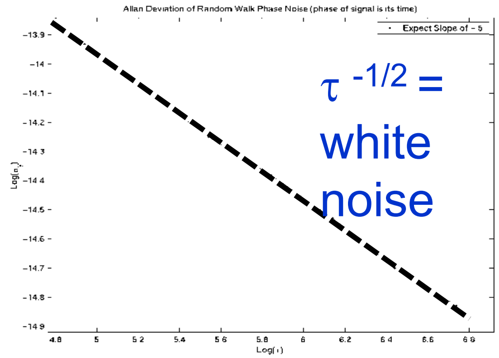
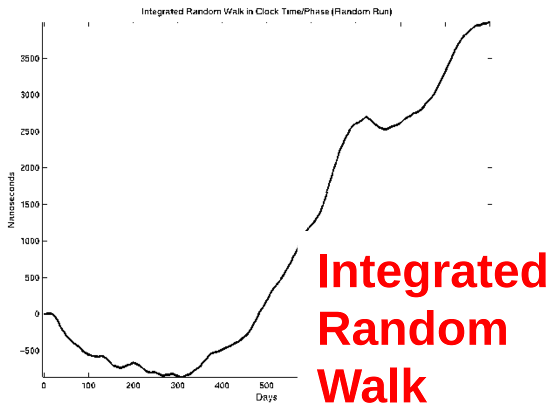
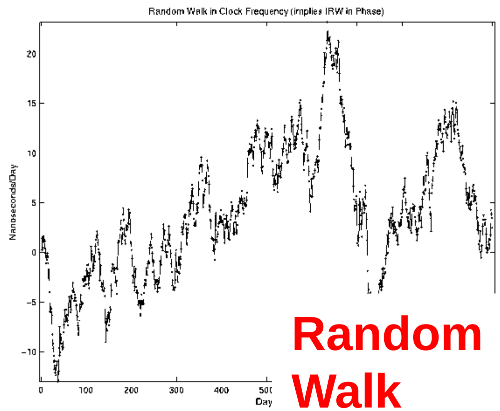
Most common noise are white, random walk, and integrated random walk

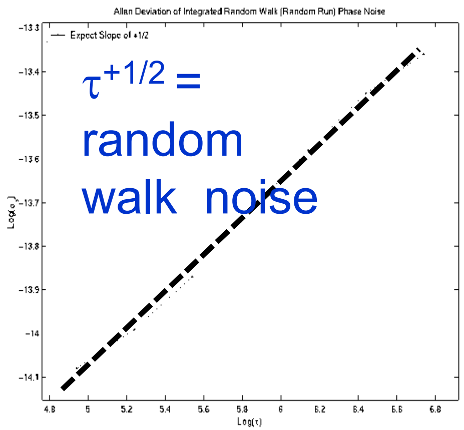
Time offset = Integral of Frequency offset Allan Deviation









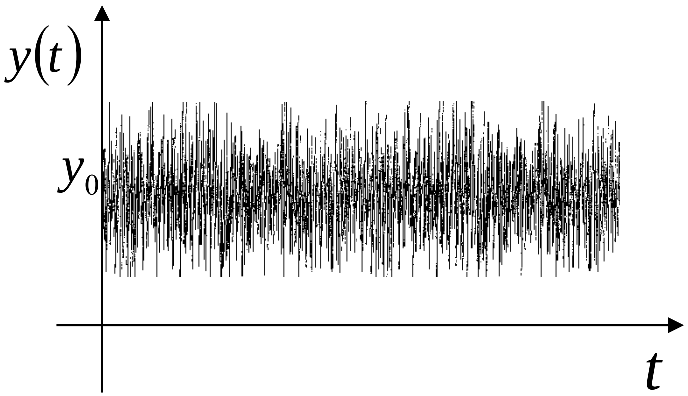


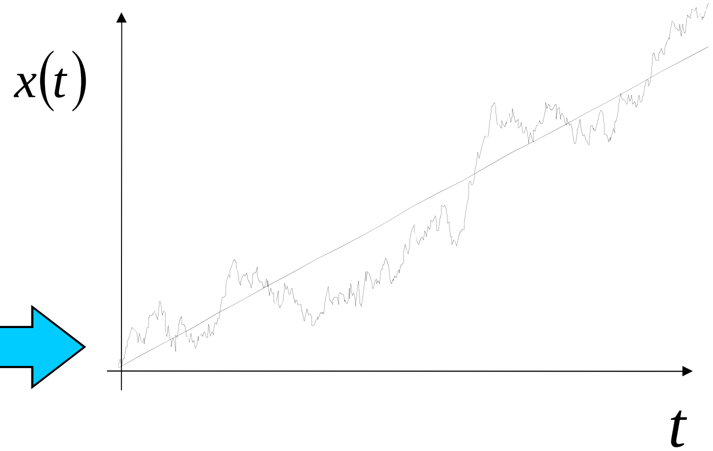
The mathematical model for deterministic and stochastic behaviour

A mathematical model for determinist and stochastic behaviour

White noise plus constant offset and its integrated effect

Velocity	Position
$y(t) = y_0 + \xi(t)$	$x(t) = x_0 + y_0(t - t_0) + \int_{t_0}^{t} \xi(s)ds$





White Frequency Noise
+ constant initial offset

$$\xi(t) : N(0, \sigma^2)$$

Strainght Line +
Random Walk on Time Offset

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Mathematical context: notations

Random Walk

Wiener Process $W(t)$

(Brownian Motion)

White Noise $\xi(t)$

"derivative" of a Wiener process

$$\xi(t)dt = dW(t)$$

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$$\xi(t)dt = dW(t)$$

$$x(t) = x_0 + y_0(t - t_0) + \int_{t_0}^{t} \xi(s)ds$$

$$y(t) = \frac{dx(t)}{dt} = y_0 + \xi(t)$$

Stochastic calculus

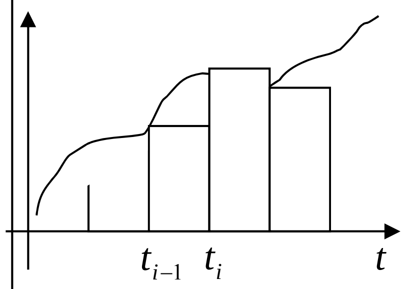
$$dx(t) = y_0 dt + \sigma\, dW(t)$$

Riemann integral

Stochastic integral

$$x(t) = \int_{t_0}^{t} y_0 dt + \sigma \int_{t_0}^{t} dW(t)$$

Stochastic integral



$$\approx \lim_{\delta \to 0} \sum_{i=1}^{n} \left(W(t_i) - W(t_{i-1})\right)$$

$$\delta = t_i - t_{i-1}$$

It depends on the choice of t_i

Itô stochastic integration

White is the derivative of Wiener or Random Walk

Integrated (White noise plus Random Walk noise)

$$dx(t) = y_0 dt + \sigma \; dW(t)$$

$$\begin{cases} dx_1(t) = x_2(t)dt + \sigma_1 \; dW_1(t) \\ dx_2(t) = a \; dt + \sigma_2 \; dW_2(t) \end{cases}$$

Wiener noise on the phase ← White noise on the frequency

Integrated Wiener on the phase ← Wiener on the frequency

Quadratic ageing

with initial conditions $\begin{cases} x_1(0) = x_0 \\ x_2(0) = y_0 \end{cases}$

$$x_1(t) = \text{time offset} = \text{integrated effect as position}$$

$$x_2(t) = \text{a component of frequency offset or of velocity}$$

In case of integrated white and random walk the exact solution exists:

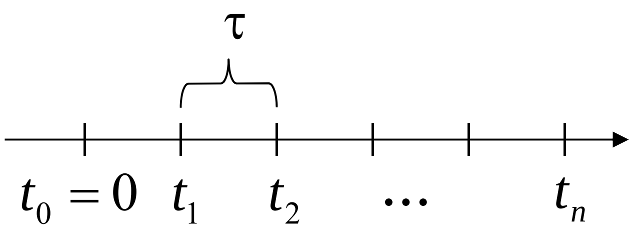
$$\begin{cases} x_1(t) = x_0 + y_0 t + a\frac{t^2}{2} + \sigma_1 W_1(t) + \sigma_2 \int_0^t W_2(s)\,ds \\ x_2(t) = y_0 + a\,t + \sigma_2 W_2(t) \end{cases}$$

White Freq. noise ($\sigma_1 W_1(t)$)

RW Freq. noise ($\sigma_2 \int_0^t W_2(s)\,ds$)

Iterative solution useful

for **simulations**, filter, …



$$\begin{cases} X_1(t_{k+1}) = X_1(t_k) + X_2(t_k)\tau + a\frac{\tau^2}{2} + \sigma_1 \mathrm{W}_{1,k}(\tau) + \sigma_2 \int_{t_k}^{t_{k+1}} W_2(s)\,ds \\ X_2(t_{k+1}) = X_2(t_k) + a\,\tau + \sigma_2 \mathrm{W}_{2,k}(\tau) \end{cases}$$

correlated processes ($\mathrm{W}_{2,k}(\tau)$ and $\int_{t_k}^{t_{k+1}} W_2(s)\,ds$)

with initial conditions

$$\begin{cases} X_1(0) = x_0 \\ X_2(0) = y_0 \end{cases}$$

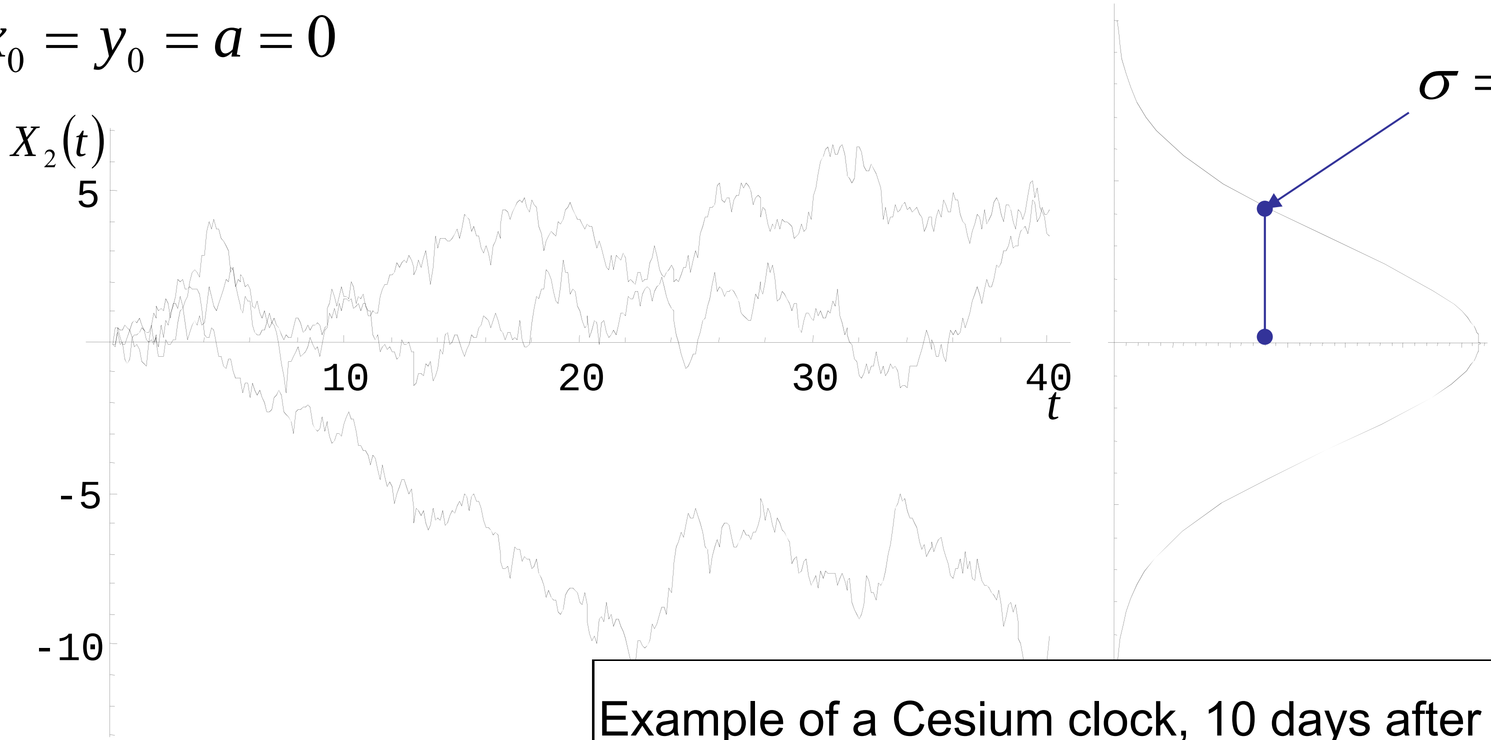
L. Galleani, L. Sacerdote, P. Tavella, C. Zucca, “A mathematical model for the atomic clock error”, Metrologia Volume 40 (3), 2003, S257-S264

Random Walk prediction

Diffusion coefficient linked to Allan Deviation

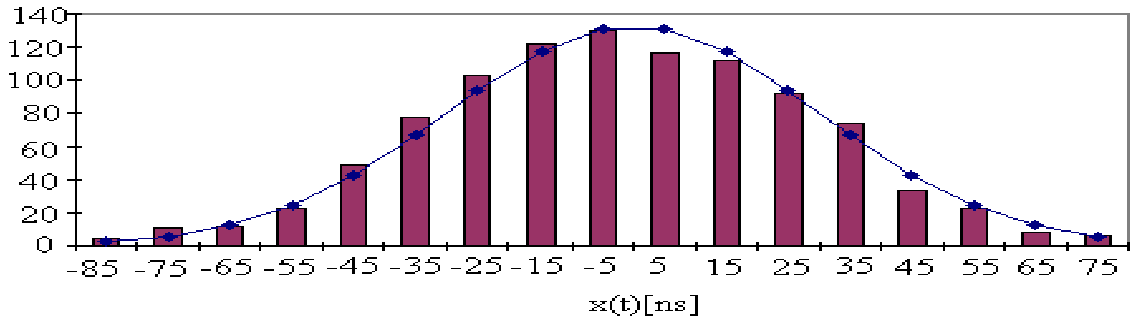
$$x_0 = y_0 = a = 0$$

$$\sigma = \sqrt{\sigma_2^2 t}$$



The prediction error at epoch *t* can be evaluated

Example of a Cesium clock, 10 days after synchronisation



G. Panfilo, P. Tavella, "Atomic Clock Prediction based on stochastic differential equations", Metrologia 45, 6, (2008) S108-S116

P. Tavella, C. Zucca "The Clock Model and its Relationship with the Allan and related Variances", IEEE Trans. UFFC Ultras. Ferroel. Freq. Control, vol. 52, no. 2, Feb. 2005, pp. 288-295

Other stochastic process may be useful as the Ornstein–Uhlenbeck process

The O-U process is the solution of the following sde

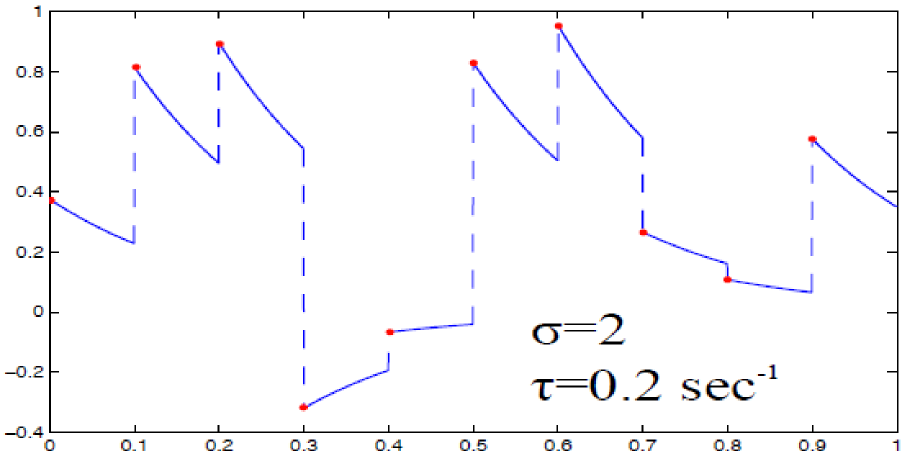
$$dU_t = -\frac{1}{\tau} U_t dt + \sigma dW_t.$$

the parameter σ measures how much *noisy* is the process. For τ:

Exact iterative formula (U at discrete times $t_{n+1} = t_n + h$)

$$U_n = U_{n-1} \cdot e^{-\frac{h}{\tau}} + \sqrt{\frac{\sigma^2 \tau}{2} \left(1 - e^{-\frac{2h}{\tau}}\right)}\, \xi_k$$

where $\{\xi_k\}$ are i.i.d. standard normal r.v.



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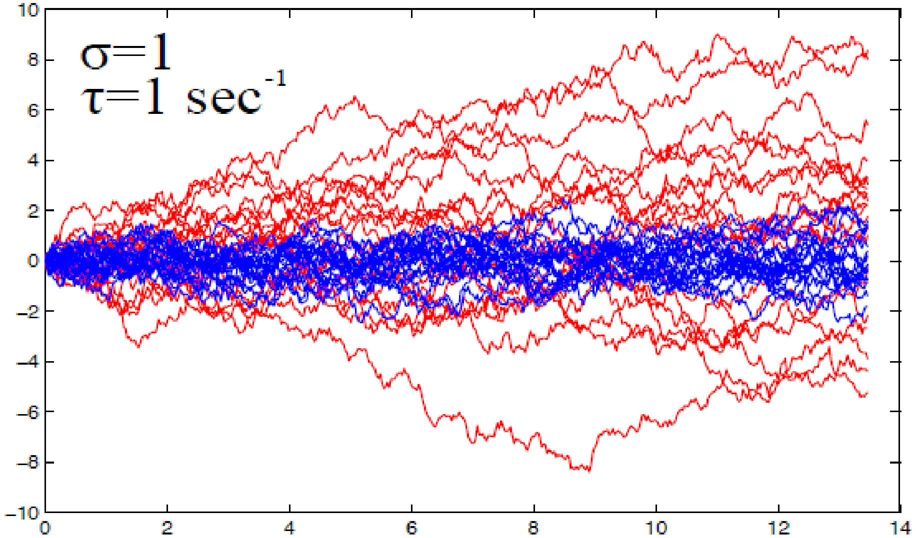
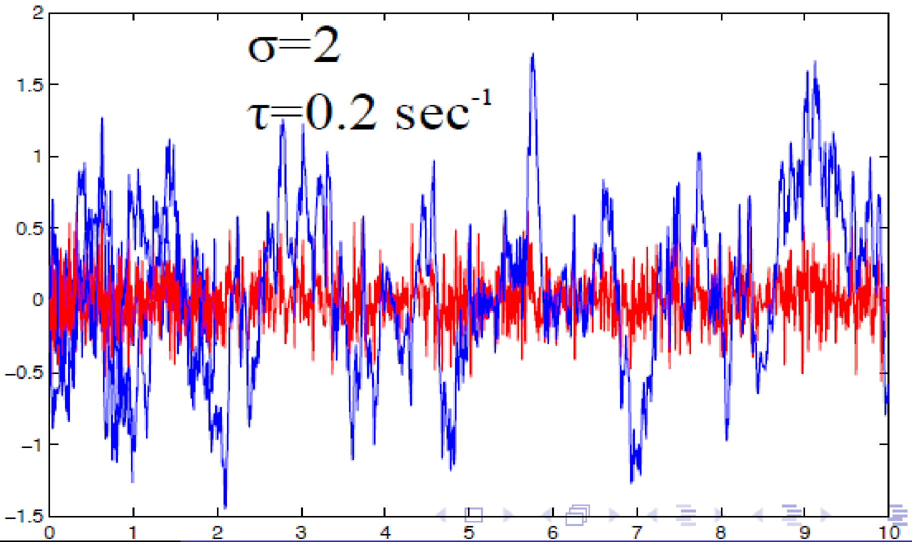
Other stochastic process may be useful as the Ornstein–Uhlenbeck process

limit behaviors:

- O-U w.r.t. Brownian Motion $(\tau \rightarrow \infty)$ e.g. phase data of a white of frequency



- O-U w.r.t. White Noise $(\tau \rightarrow 0)$



E. Bibbona, G. Panfilo, P. Tavella, "The Ornstein-Uhlenbeck Process as a Model of the Filtered White Noise", Metrologia 45, 6, (2008) S117-S126

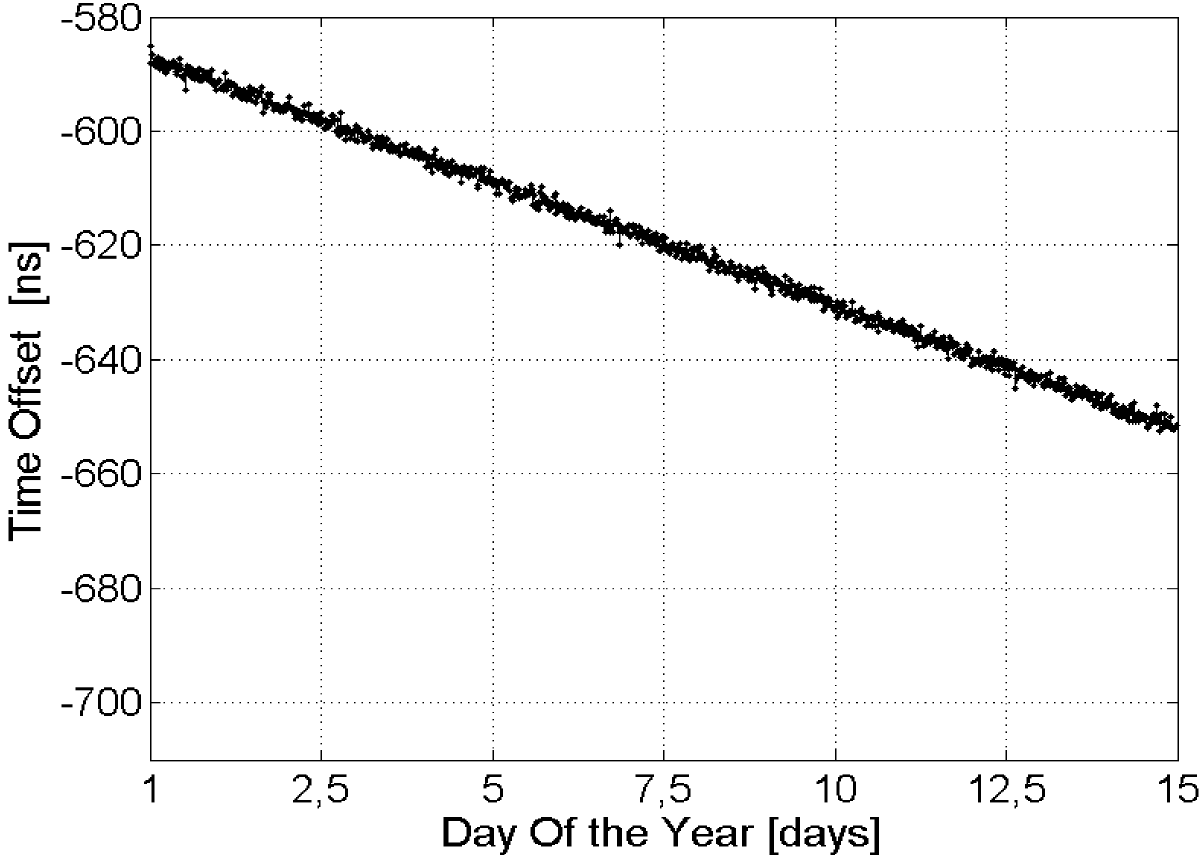
What we learnt

1- Deterministic and stochastic behaviour can be modeled by stochastic differential equations(SDE)

2. The exact (or approximat) solution of the SDE allows the dynamic behaviour estimation, simulation, and prediction

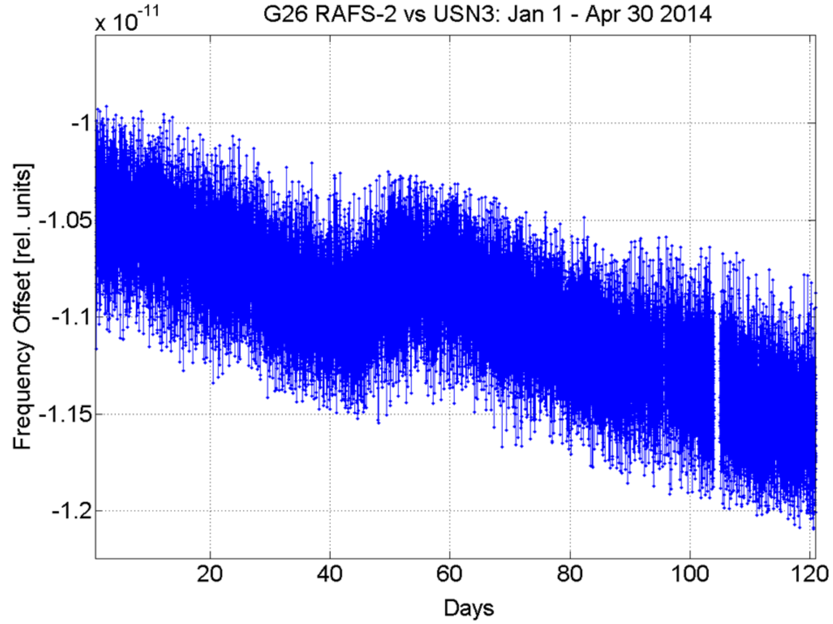
3. The noises imbedded in the model has usually zero mean value, they do not impact on the prediction but on the uncertainty of the predicted values
(therefore allowing to evaluate confidence intervals)

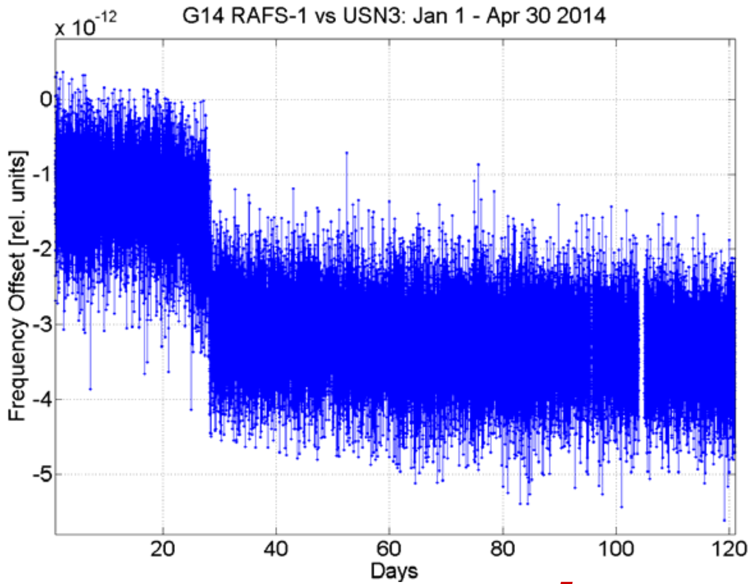
Will the well understood and modeled behaviour last forever?

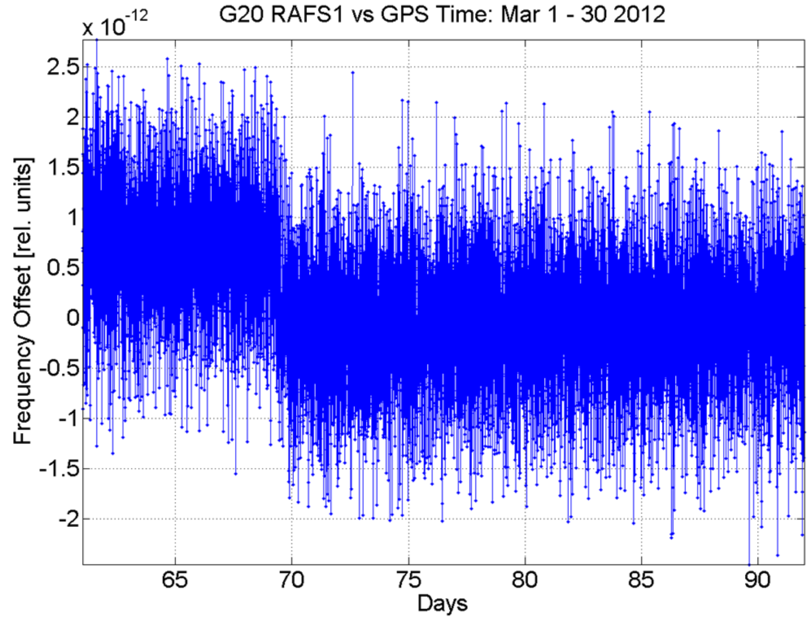


Example of GPS space clocks

Possible causes of nonstationarities on space clocks are manoeuvres and tests on board, environmental variations, eclipses, etc. In other cases, the nonstationarities may be due to the clock itself.







Frequency jumps are observed

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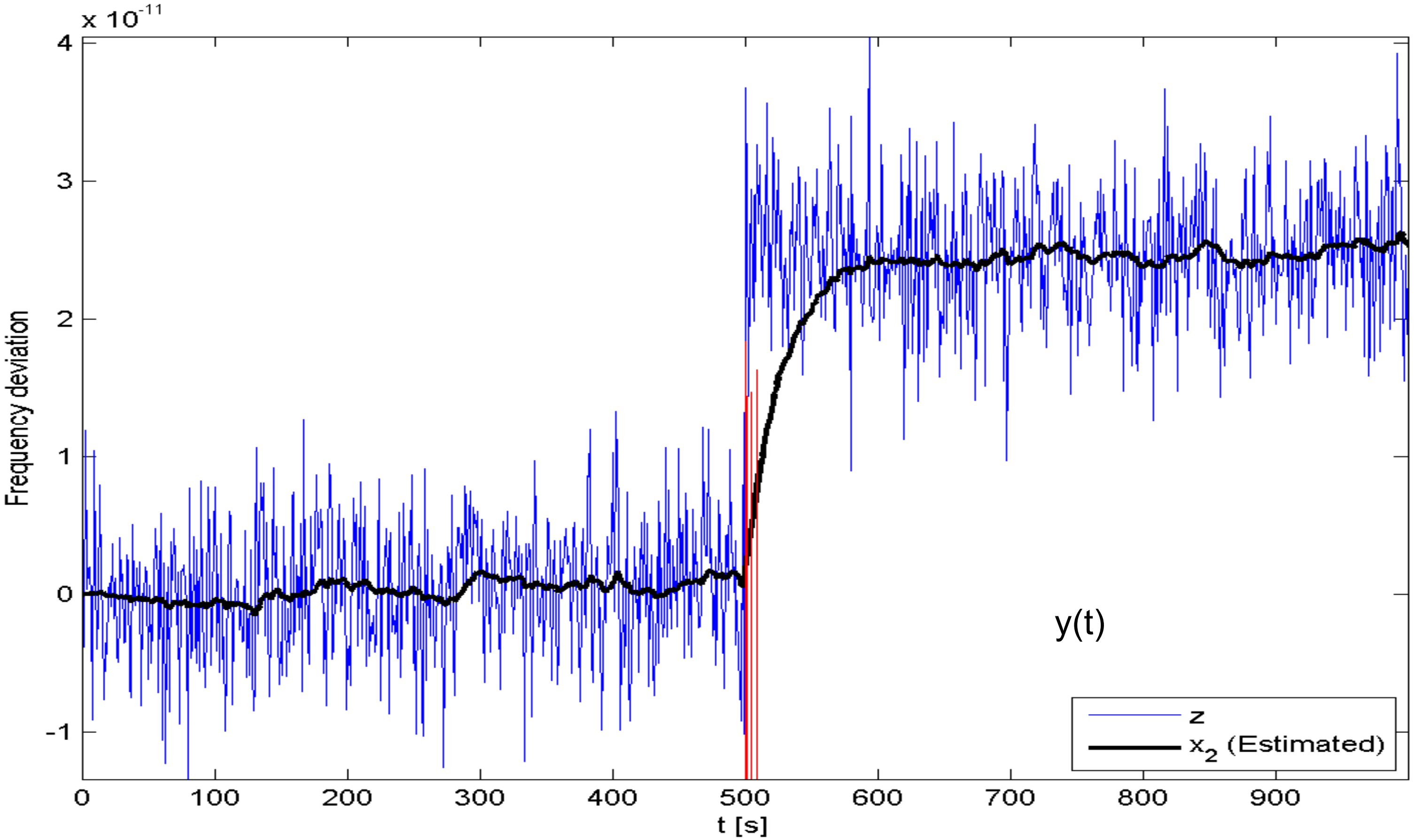
WE NEED A FREQUENCY JUMP DETECTOR



Q. Wang, F.Droz, P. Rochat, "Robust Clock Ensemble for Time and Frequency Reference System", presented at the EFTF/IFCS Denver 2015

L.Galleani,P.Tavella."Detection of Atomic Clock Frequency Jumps with the Kalman Filter," IEEE Transactions on Ultrasonics, Ferroelectr, Freq Control March 2012. vol. 59, no. 3, p. 504-509, March 2012

Huang X, Gong H, Ou G, Detection of weak frequency jumps for GNSS onboard clocks, IEEE Trans Ultrasonics, Ferroelectr Freq Control. 2014 May;61(5):747-55

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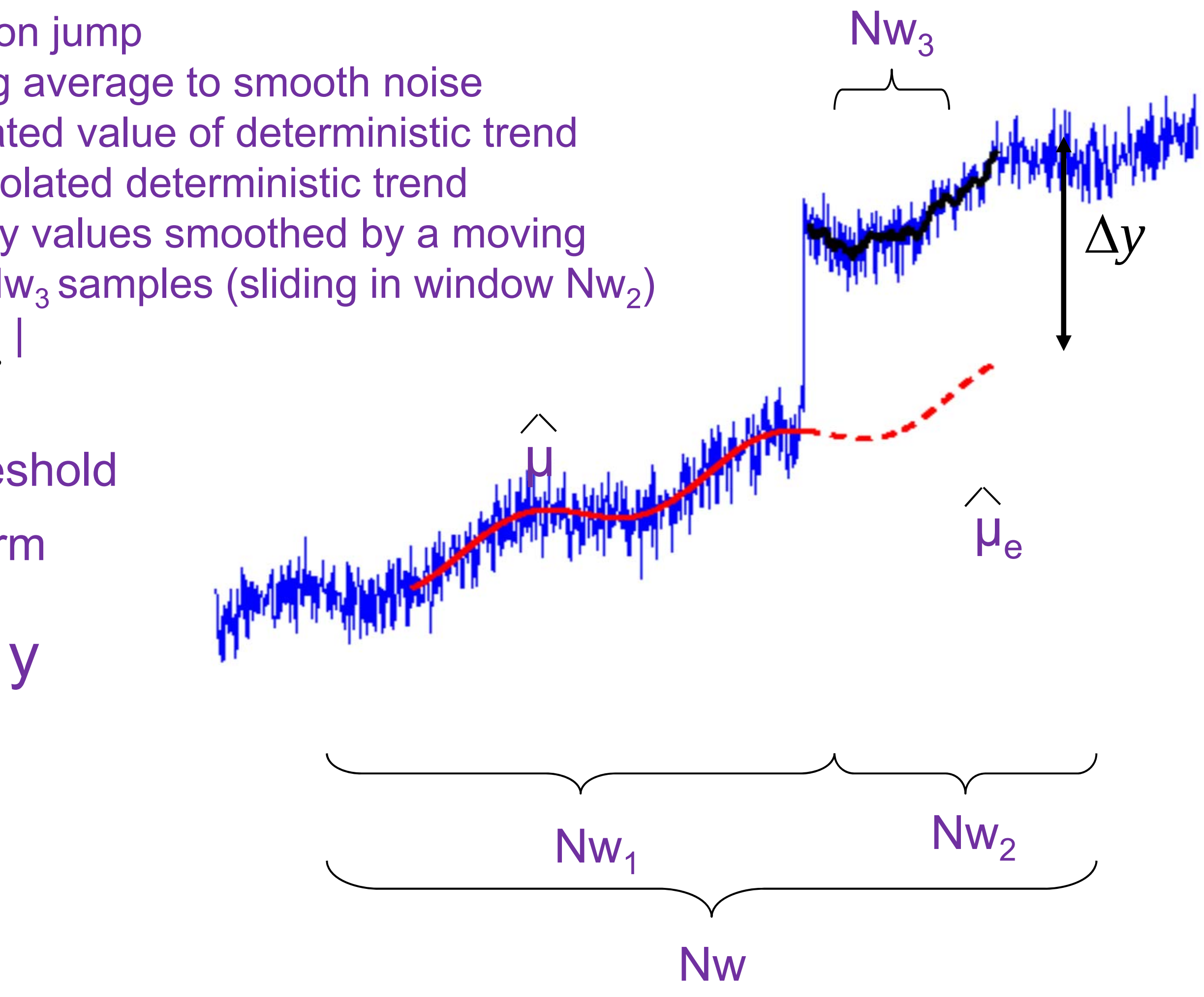
From the past we best predict the future and then we compare prediction with measures (or mean of measures)

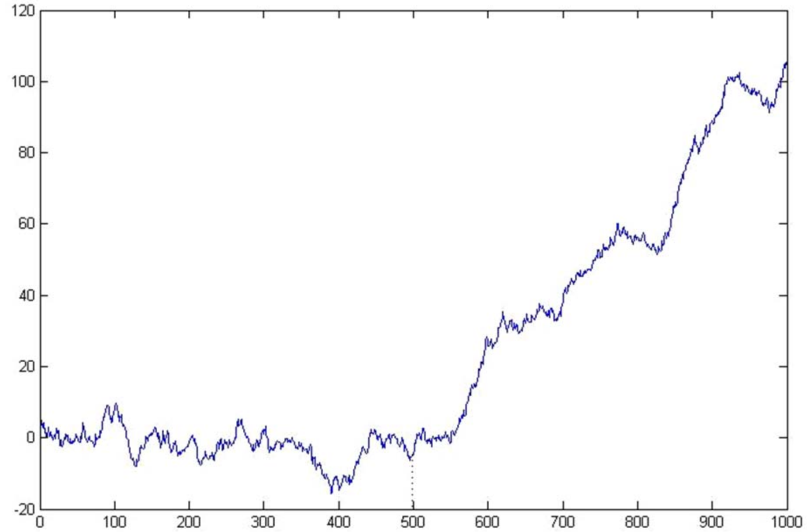
Nw = full data set
Nw_1 = estimation of deterministic behaviour
Nw_2 = check on jump
Nw_3 = moving average to smooth noise
$\hat{\mu}$ = estimated value of deterministic trend
$\hat{\mu}_e$ = extrapolated deterministic trend
y_s = frequency values smoothed by a moving average on Nw_3 samples (sliding in window Nw_2)
$\Delta y = | y_s - \hat{\mu}_e |$

If Δy > threshold

➡ Alarm



QUICKEST DETECTION METHOD (optimal stopping)
FOR A WIENER PROCESS



θ

Assume that the quantity evolution can be modeled by a Wiener process X and observe a trajectory with a drift changing from 0 to $\mu \neq 0$ at some random time θ.

Task: find a stopping time τ of X that is as close as possible to the unknown time θ.

Peskir, G. and Shiryaev, A. *Optimal Stopping and Free-Boundary Problems* Lectures in Mathematics. ETH Zürich Birkhäuser (2006); Shiryaev, A. *Optimal Stopping Rules* Springer (1978)

QUICKEST DETECTION METHOD (optimal stopping) FOR A WIENER PROCESS

We write a risk function

$$V(\pi) = \inf_{\tau} \left(P(\tau < \theta) + cE[\tau - \theta]^+ \right)$$

$P(\tau < \theta)$ probability of false alarm

$E[\tau - \theta]^+$ average delay in detecting the anomaly

c a suitable constant

We want $P(\tau < \theta)$ and also $E[\tau - \theta]^+$ to be small

- To avoid false alarms
- To minimize the detection delay

The minimization problem

$$V(\pi) = \inf_{\tau} \left(P(\tau < \theta) + cE[\tau - \theta]^{+} \right)$$

can be written as an optimal stopping problem

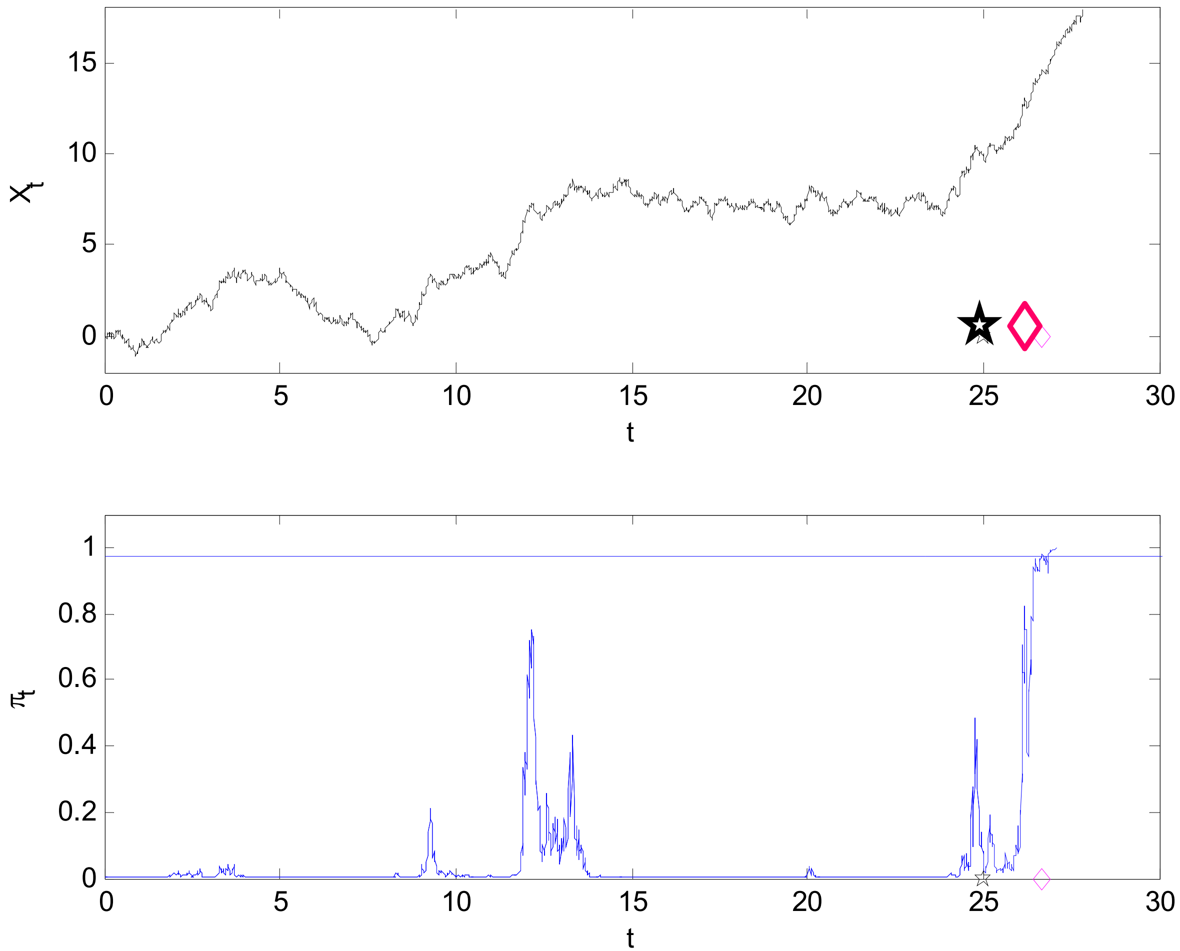
$$V(\pi) = \inf_{\tau} E\left[1 - \pi_{\tau} + c\int_0^{\tau} \pi_t dt \right]$$

where $\pi_t = P_\pi(\theta \leq t | \mathcal{F}_t^X)$ with $P_\pi(\pi_0 = \pi) = 1$

is the a posteriori probability process, probability that by epoch *t* the process *X* has changed drift.

The original process *X* has changed drift when the process π is crossing the boundary A.
The optimization problem has been transformed into a first passage time, becoming an analytical problem.

A theorem demonstrates that the exact solution exists and studying the additional process π we can optimally estimate the epoch of the insurgence of the new drift μ

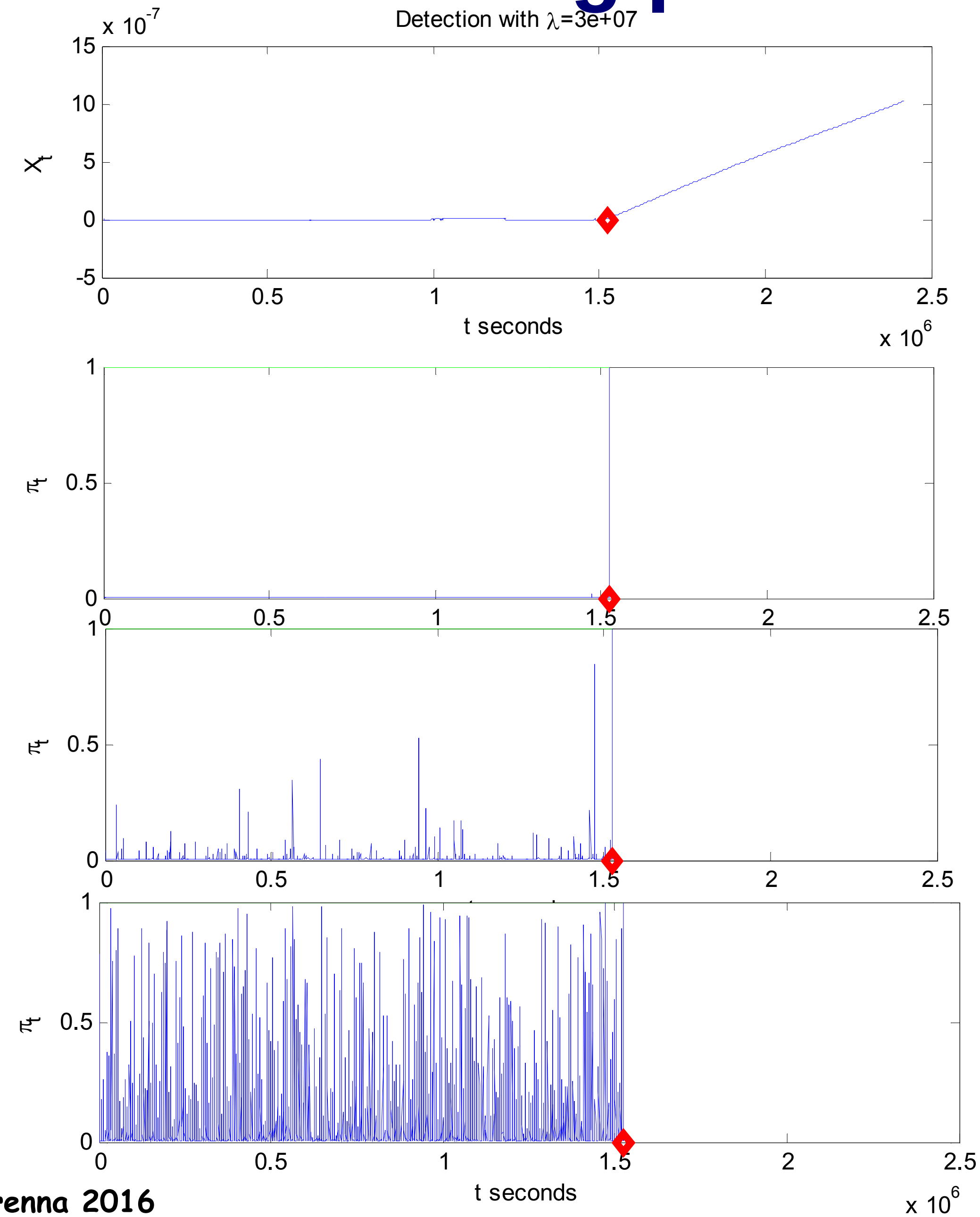


★ $=\theta= 25$

◊ $=\tau=26.63$

$\mu=3,\ \sigma^2=1.$

Tuning parameter values



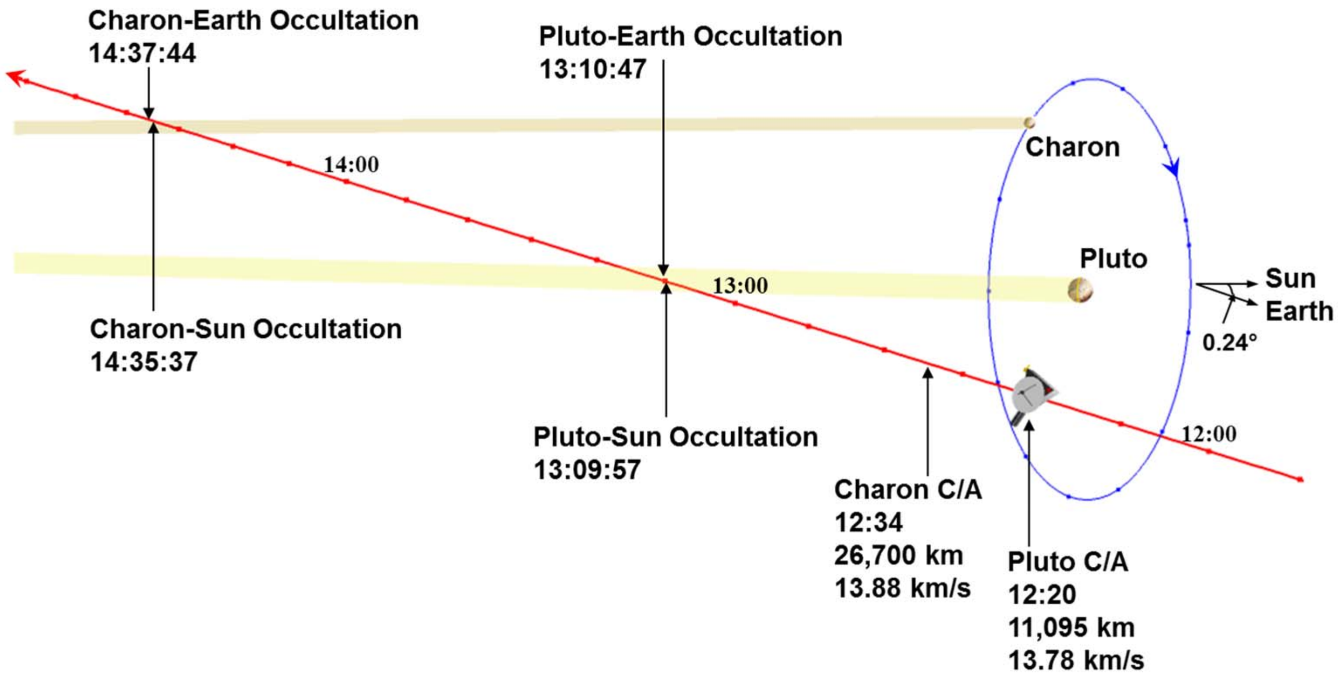
We apply the optimal stopping with different values of $E(\theta)=1/\lambda$.

$E(\theta)$=3*10^7(one event a year)
$\tau=5087.5$

$E(\theta)$=10^6 (one event every 28 days)
$\tau=5087.5$

$E(\theta)$=1500 (one event every 25 min)
$\tau=5086.5$

Example of optimal stopping



The NASA New Horizon spacecraft was launched on Jan 19th, 2006 to meet Pluto on July 14, 2015 The measurement system required an ultra-stable oscillator (Quartz Crystal) with very high frequency stability

G.L.Weaver, J. R. Jensen, C. Zucca, P. Tavella, V. Formichella, G. Peskir, “Estimation of the dynamics of frequency drift in mature ultra-stable oscillators: a study based on the in-flight performance from New Horizons, in proc ION PTTI Precise Time and Time Interval meeting, Monterey CA, Jan 2016

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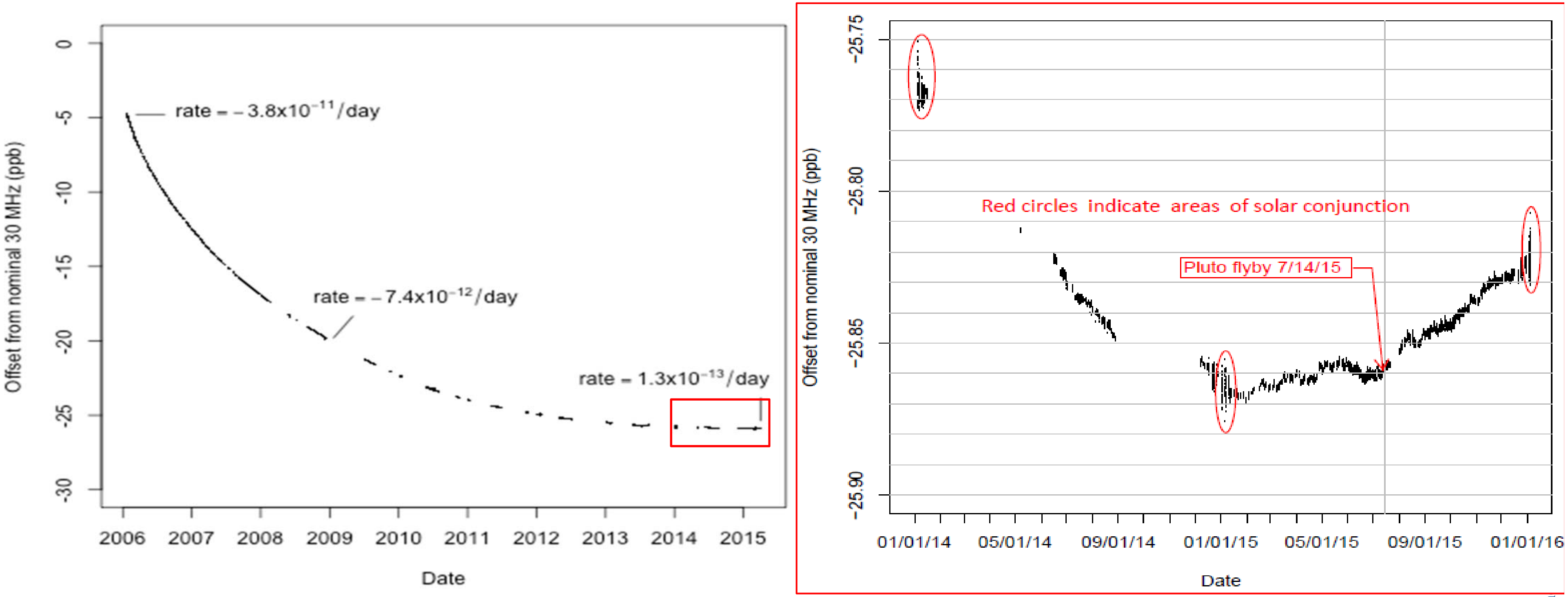
Quartz frequency was changing rate?



- The gaps in the data are those periods when the spacecraft was in hibernation and no tracking was performed.
- During 2015, the frequency of the Quartz was measured almost continuously in preparation for the Pluto-Charon encounter.
- A reversal in the frequency rate asks for recovery actions

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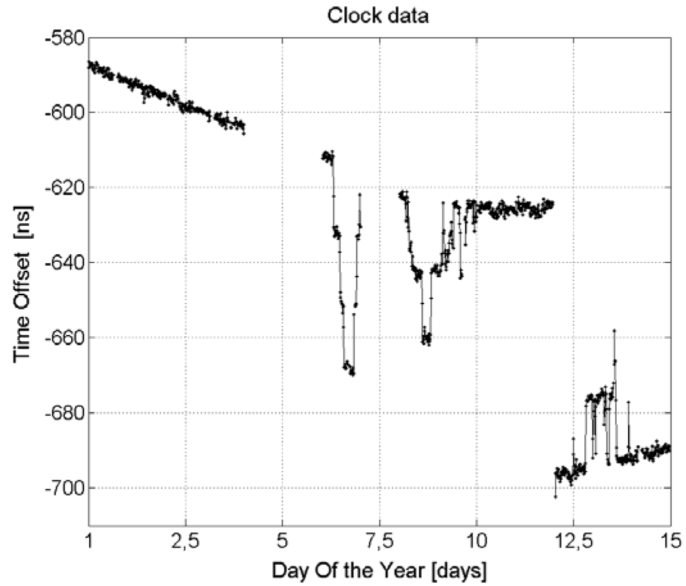
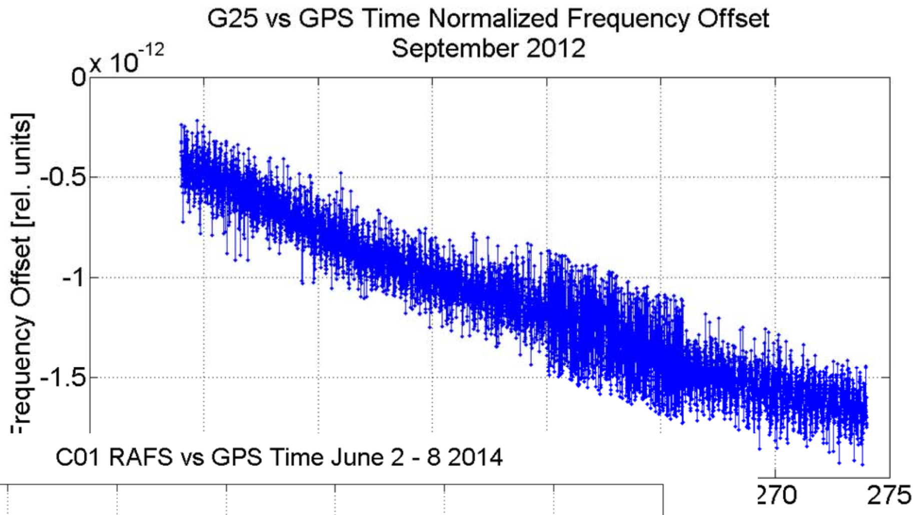
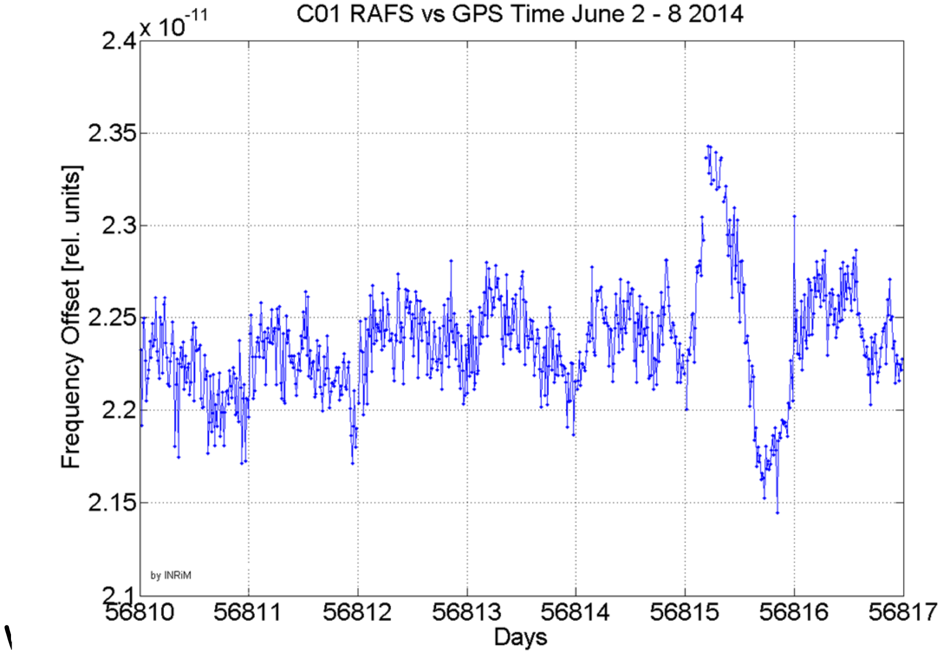
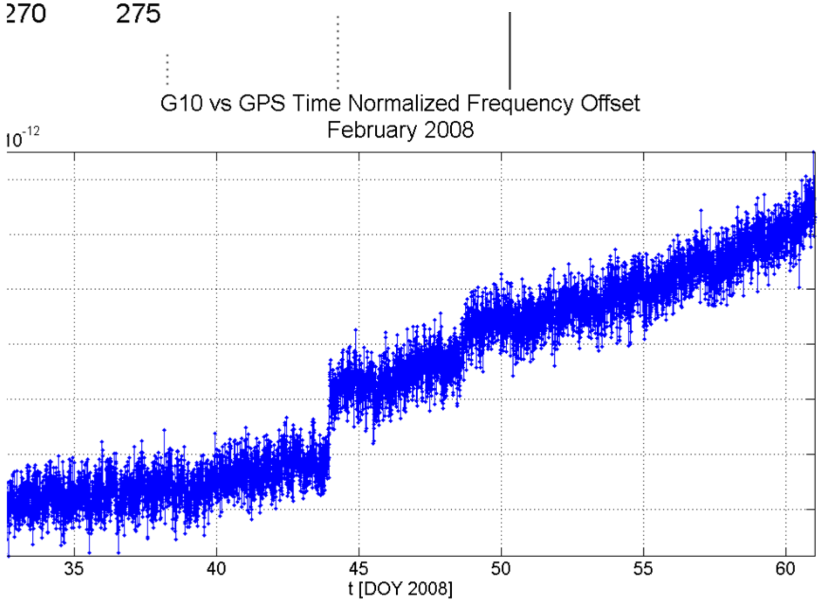
Will the well understood and modeled behaviour last forever?









We need a
dynamical characterization of the noise

Time and Frequency spectral analysis
for example

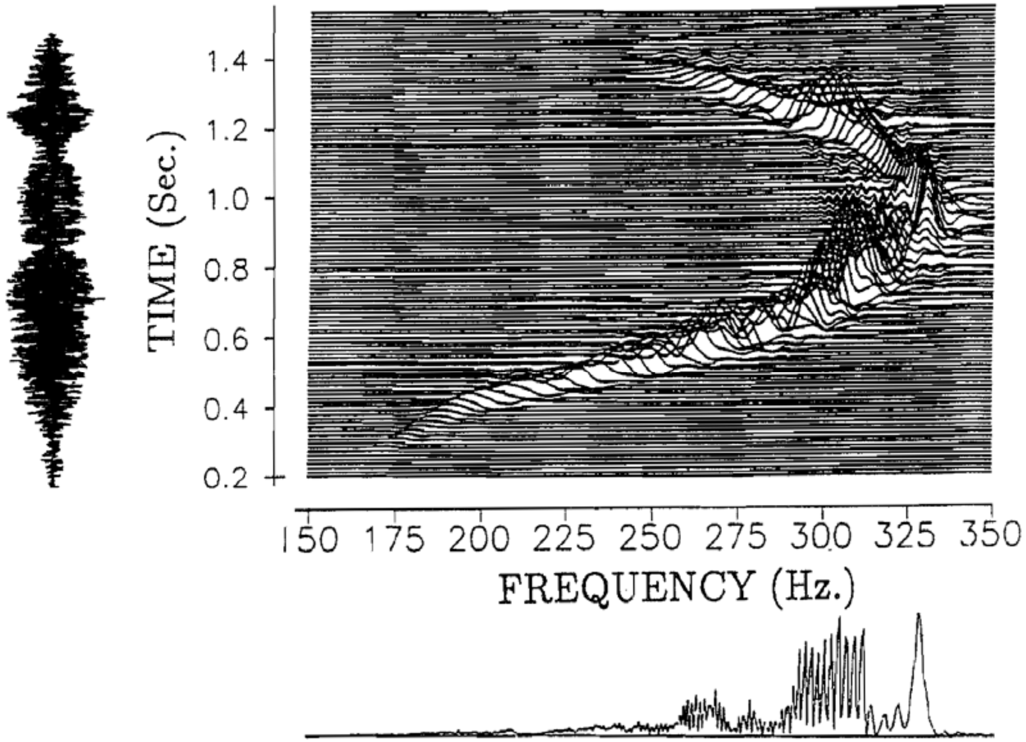
Not only estimating which frequencies existed

But also estimating when they existed

Time-frequency analysis

It describes how the frequencies of a signal change with time

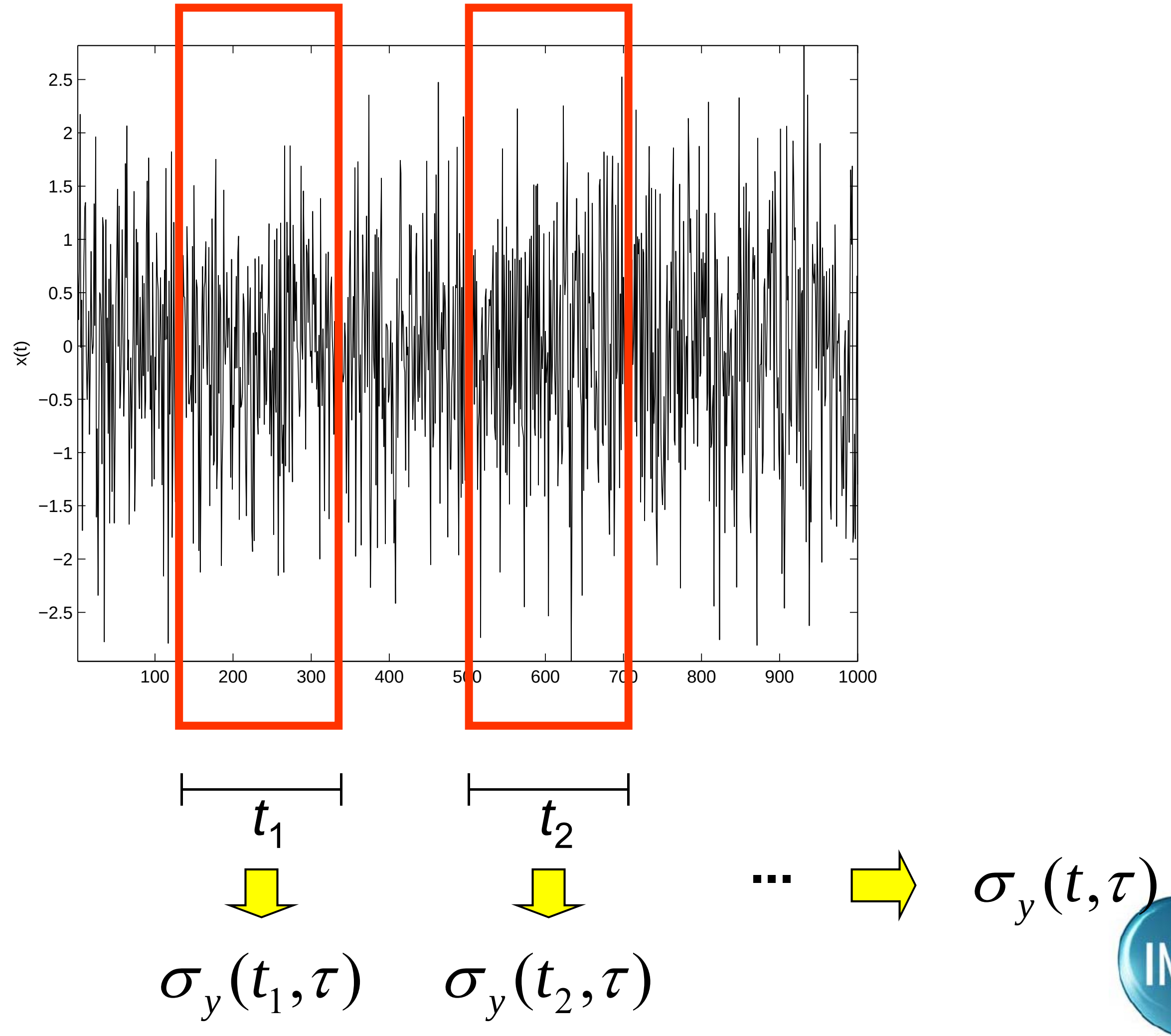
Bowhead whale



L. Cohen, *Time-frequency analysis*, Prentice-Hall, 1995

A Dynamic Allan variance

sliding the Allan variance estimator on the data



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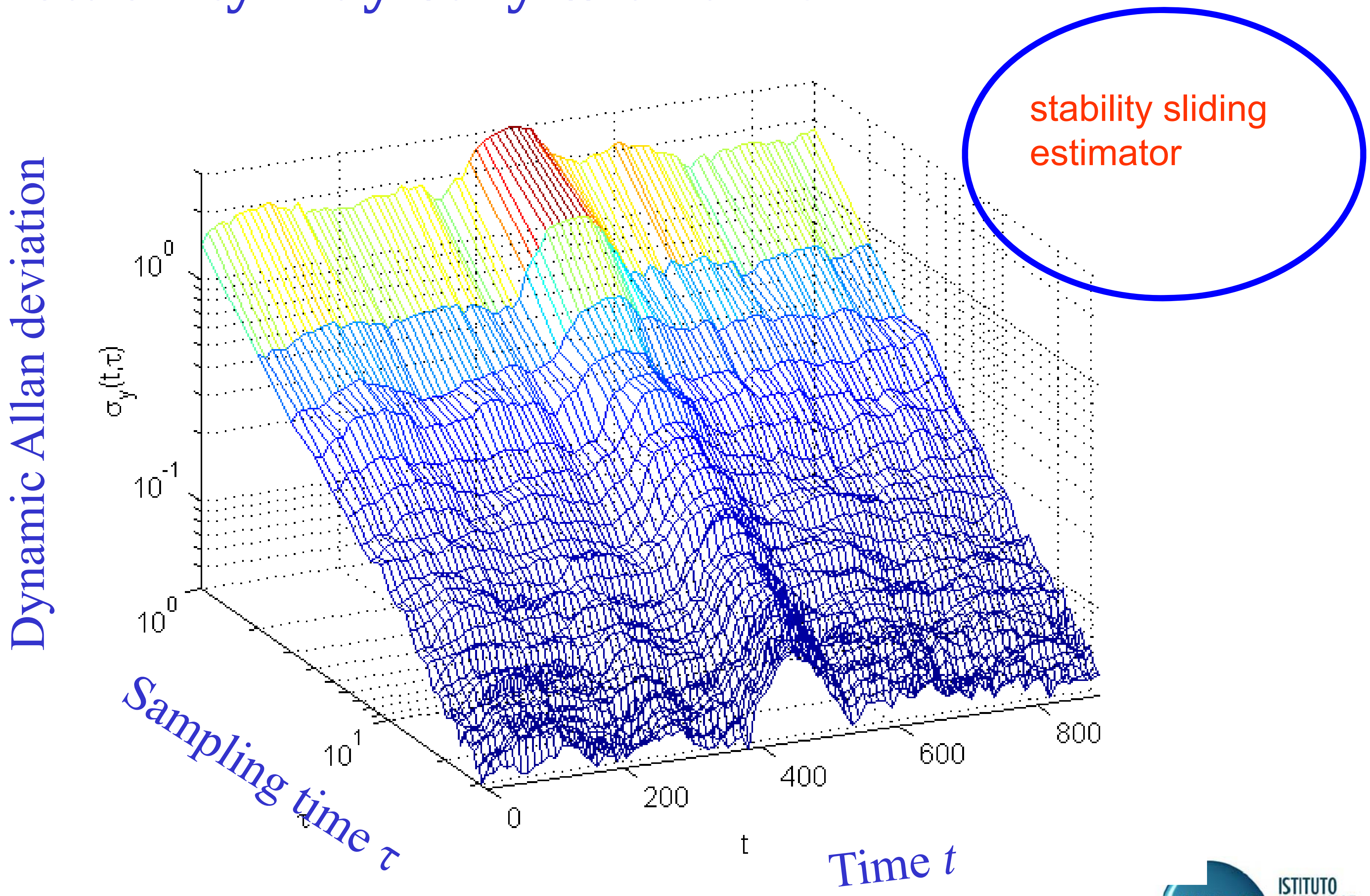
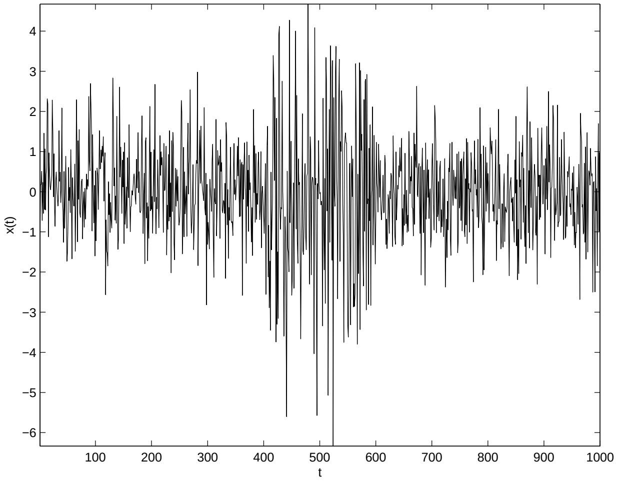
stability may vary with time

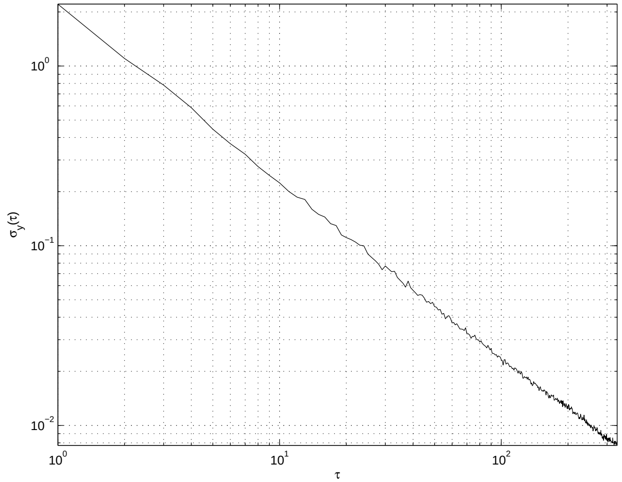


L. Galleani, P. Tavella, "Dynamic Allan variance" , IEEE Trans UFFC, vol. 56, no. 3, March 2009, pp450-464

Simulation results : Bump

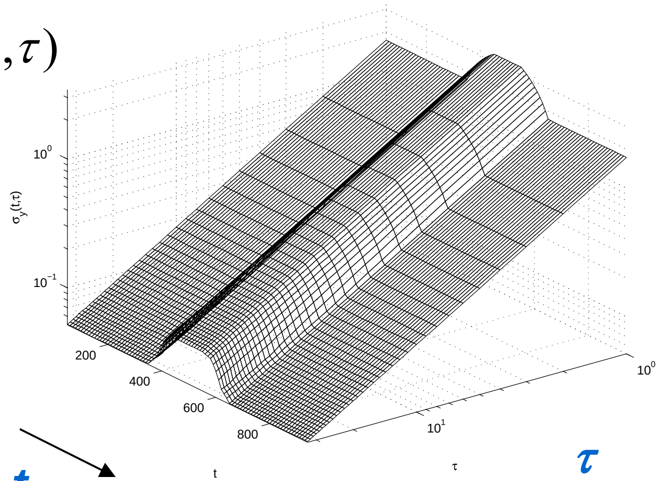


t



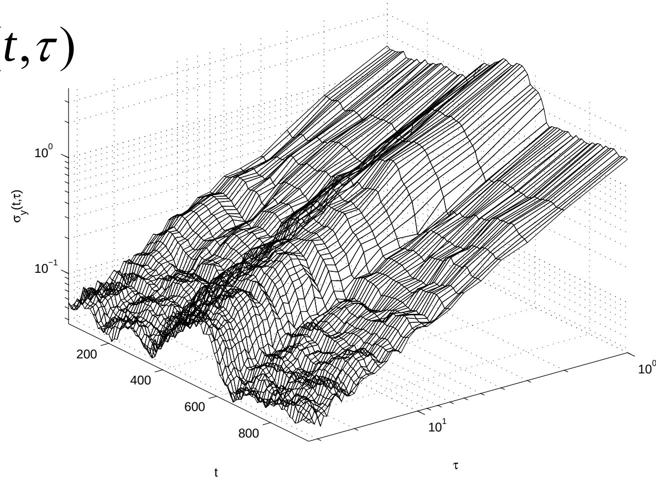
τ

$\sigma_y(t,\tau)$



t τ

$\hat{\sigma}_y(t,\tau)$



The Dynamic Allan variance

Discrete time formulation from the phase samples $x[n]$

$$\sigma^2{}_y[n,k] = \frac{1}{2k^2\tau_0{}^2}\frac{1}{Nw-2k}\sum_{m=n-Nw/2+k}^{n+Nw/2-k-1} E\left[\left(x_N[m+k]-2x_N[m]+x_N[m-k]\right)^2\right]$$

where:

- Nw is the window length
- x_N is the phase signal in the window Nw
- τ_0 is the sampling time

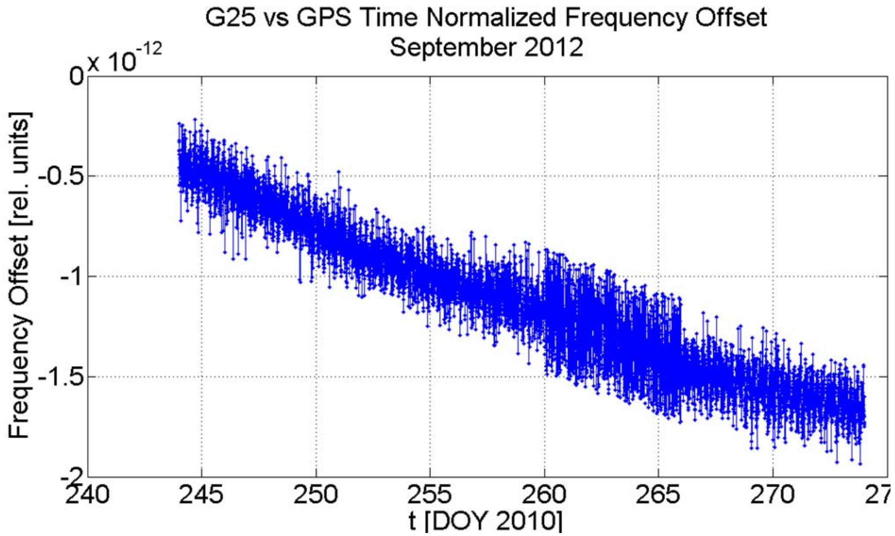
the DAVAR estimator

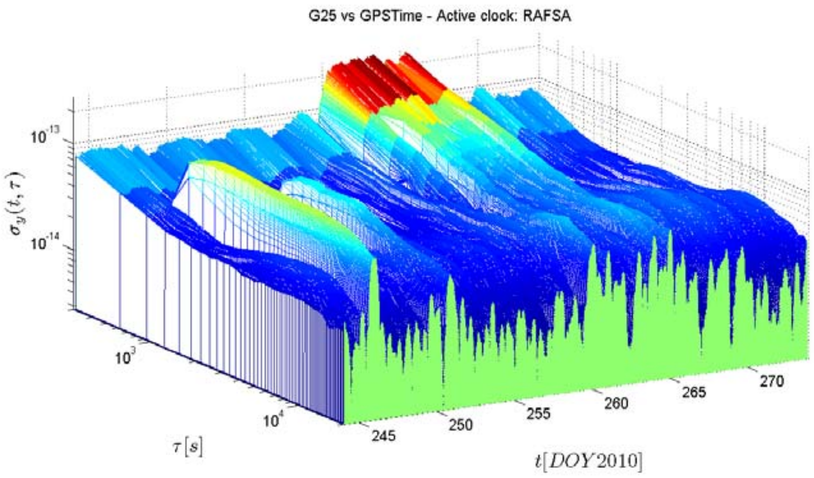
has no expectation value E because we have one realization only

L. Galleani, P. Tavella, "Dynamic Allan variance" , IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, UFFC, vol. 56, no. 3, March 2009, pp450-464

L. Galleani, P. Tavella, "The Dynamic Allan Variance V: Recent Advances in Dynamic Stability Analysis", EEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. 63, No. 4, Pag 624 - 635, April 2016

The change in instability is easily detected



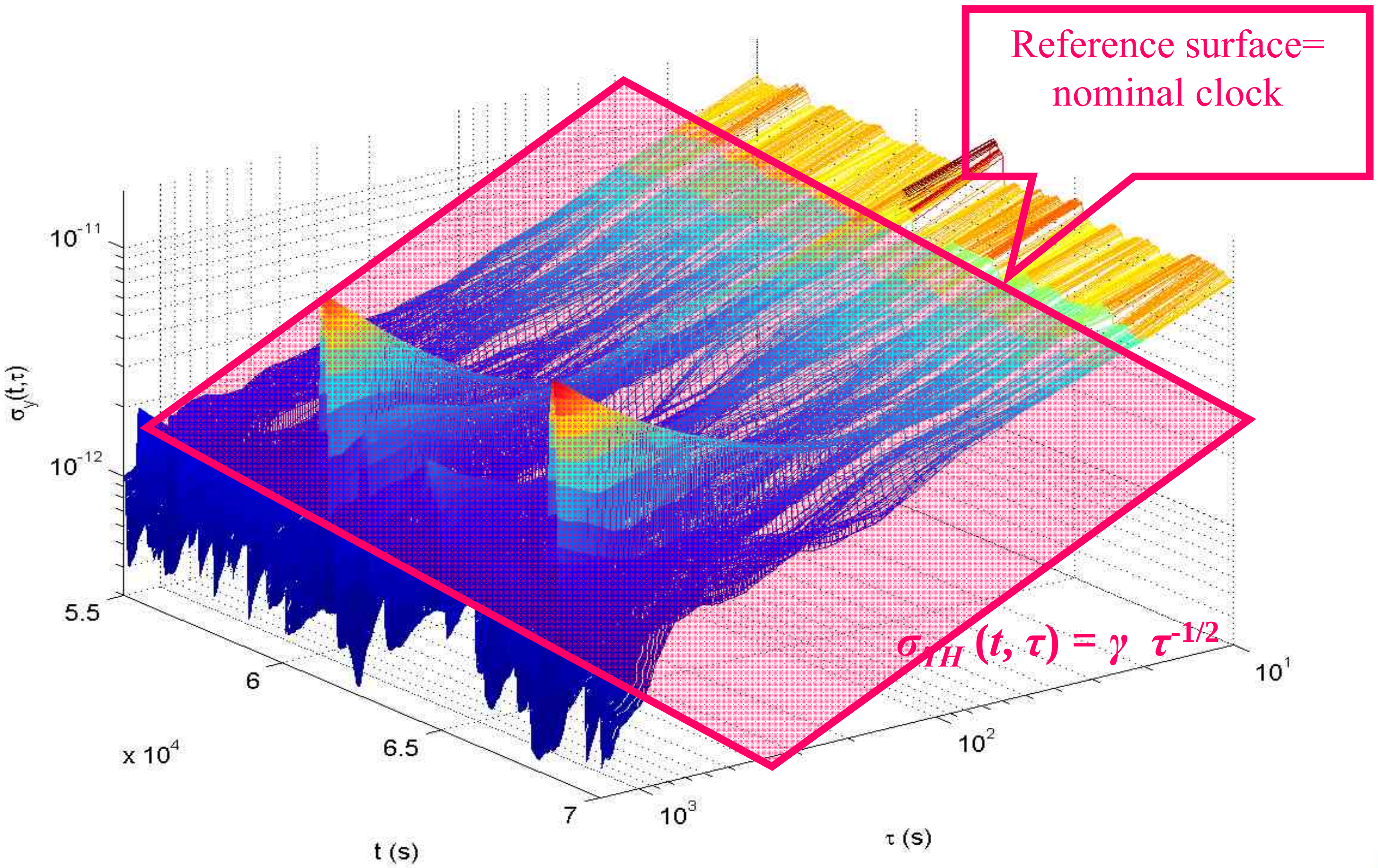


Free Matlab implementation, http://www.inrim.it/res/tf/allan.shtml

CANVAS by NRL @ **https://goby.nrl.navy.mil/canvas/download/**

STABLE 32 Users: Upgrade to version 1.5

We insert a “threshold” surface to detect increase of instability



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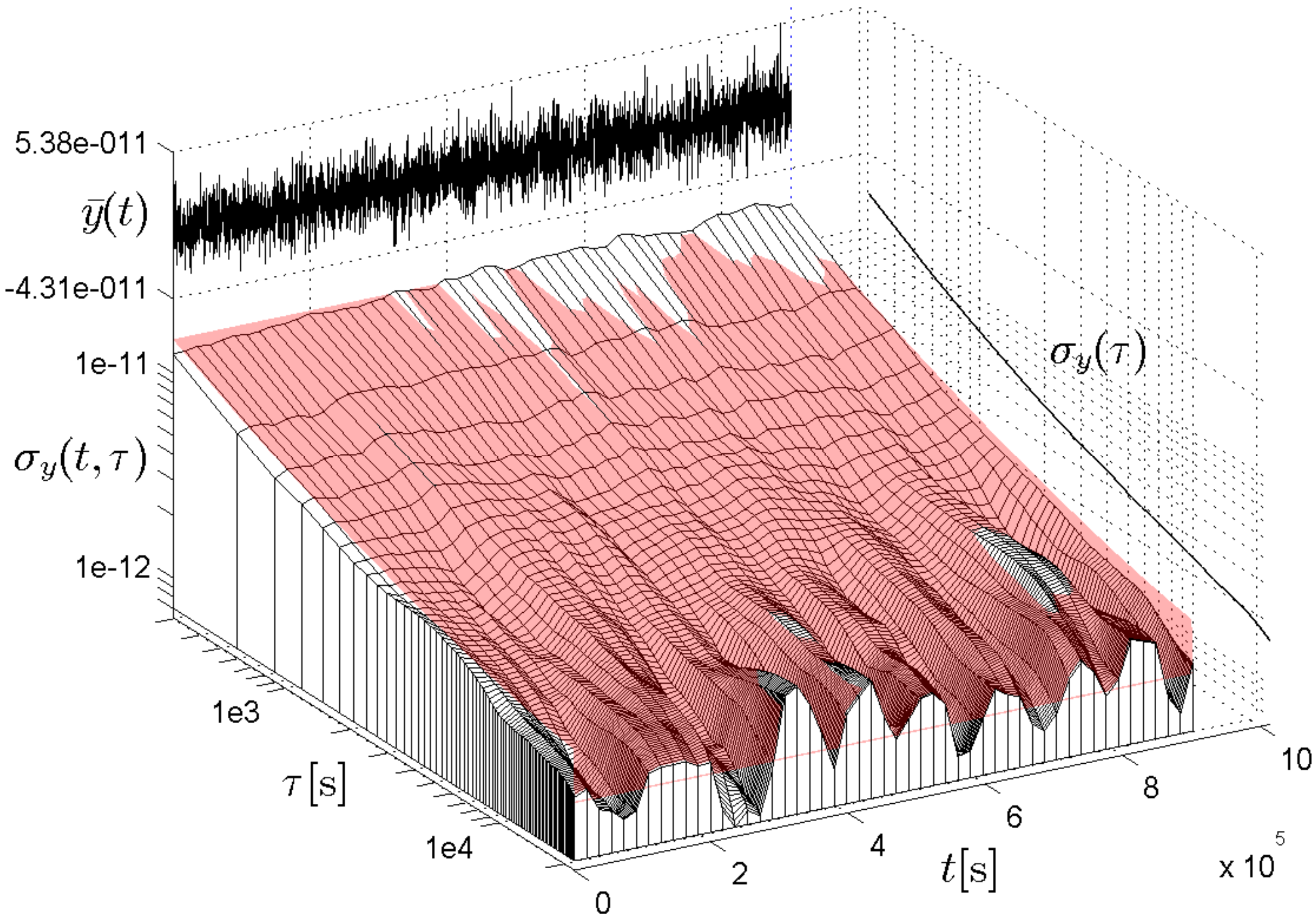
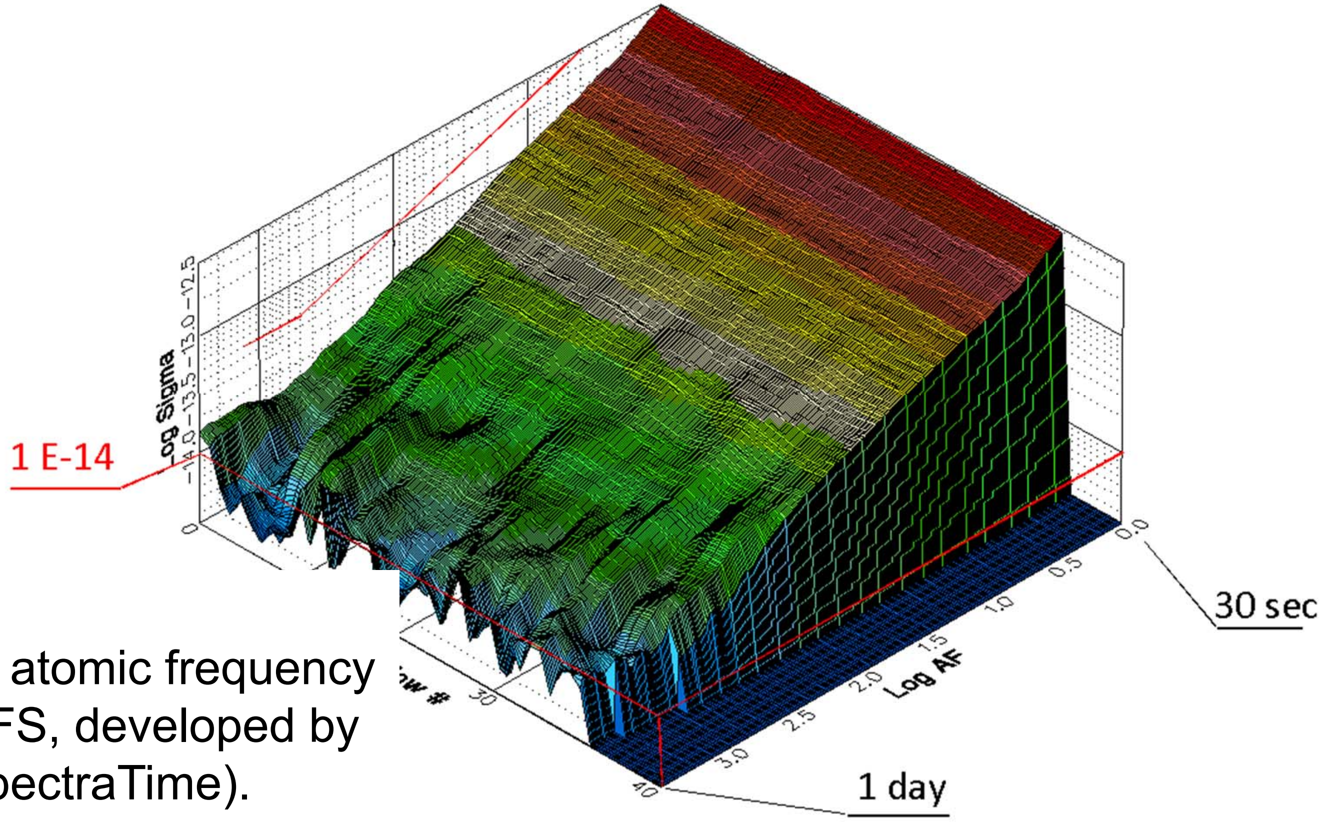
The threshold surface may reveal a noise increasing in time



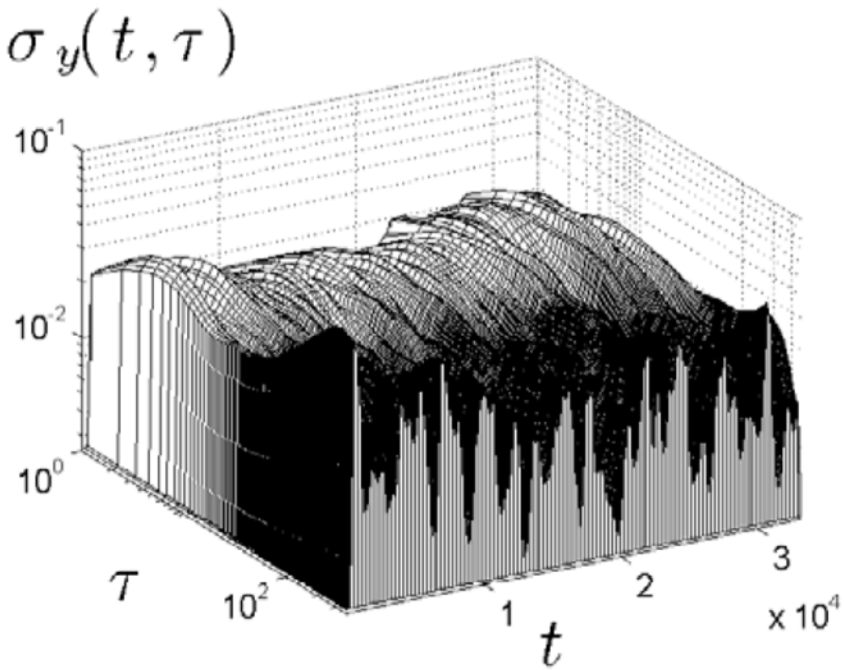
Demonstrating stationarity



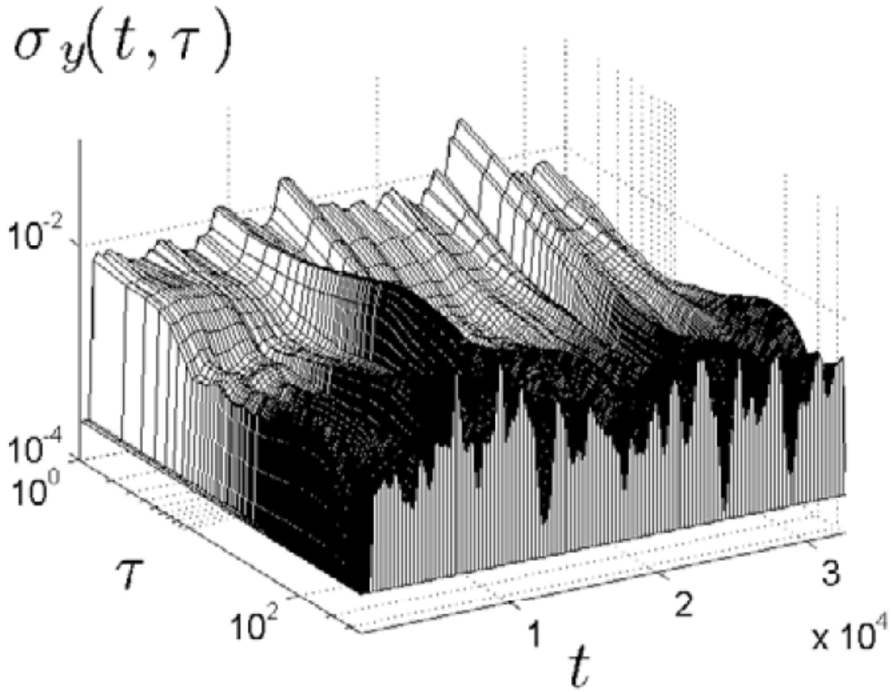
DADEV
of a new space Rubidium atomic frequency standard, the Robust-RAFS, developed by Orolia Switzerland SA (SpectraTime).
The clock manufacturer demonstrates to the customer that the Robust-RAFS follows the specifications throughout the entire performance test.

(courtesy of Fabien Droz)

Application to cardiology



DADEV of the heart interbeat rate for a normal patient



DADEV of the heart interbeat rate for a patient suffering from CHF (congestive heart failure)

courtesy of Ricardo Hernández-Pérez

R. Hernández-Pérez, L. Guzmán-Vargas, I. Reyes-Ramírez, and F. Angulo-Brown, .Evolution in time and scales of the stability of heart interbeat rate,.Europhysics Letters, vol. 92, no. 6, Dec. 2010.

What we learnt

1. The instability of time varying quantities may be highly impacting

2. Instability may be estimated by appropriate tools mathematical models including noises can be written

3. Models allow estimation, prediction, simulation, control

4. The behaviour may change due to ageing, failures, ve[illegible]ing… These changes are to be detected (rapidly) and the model is be dynamically updated

5. How many other statistical tools are useful in Metrology?

Thank you for your attention

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