National Technical University of Athens
School of Applied Mathematical and Physical Sciences

Mathematical Modelling in Modern Technologies and Finance

# Analysis of Rough Surfaces with Network Theory

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# Outline

1. Introduction – Motivation
2. From rough surfaces to networks (Height similarity method)
3. Applications of the method and results
4. Summary and Conclusion
5. Future work

# Motivation

**Technological** : roughness affects several surface properties (adhesion, catalysis, friction, wetting, conductivity, wave scattering, …) and is of increased importance in nanotechnology since the surface to volume increases on nanoscale.

**Theoretical** : A rough surface is a complex system (a hierarchical synergy of order and randomness in many scales) whose evolution is a non-equilibrium process.

The characterization of the static and dynamic aspects of a rough surface is crucial and with open issues.

For example: 1. Characterization of the degree of order of a surface morphology since the conventional approaches (Fourier transform and correlation functions) have shortcomings

2. Roughness evolution not obeying to scaling hypothesis

New approach: Network theory

# Previous Litterature

A relevant problem: from time series to networks

- The visibility criterion with all the points as nodes and links between points with visibility (Lacasa et al. [2008] ,  Yang et al. [2009], Luque et al. [2009]).
- The phase space reconstruction with the phase space points as nodes and links between the neighbouring points (Xu et al. [2008], Gao and Jin [2009], Marwan et al. [2009]).
- A partition of time series values into bins with the bins of the partition as nodes and links between bins with one step time correlations (Shirazi et al. [2009]).

# Roughness characterization

## Vertical roughness

Height distribution function

second moment: Rms value (surface width) sigma or w (99% of surface is included in a zone with width 6w)

## Spatial roughness

Fractal self-affine surfaces (stochastic, invariant under anisotropic scaling)

Correlation length $\xi$

For $r>\xi$ , surface points become uncorrelated and rms value saturates.

Roughness exponent  $0<\alpha<1$ (d=2-a)

It gives the relative contribution of high frequency fluctuations to the total roughness.

# Roughness characterization

**Mounded surfaces**

Rms (vertical roughness)

Correlation length

Period (selected wavelength)

Deviation from periodicity (order parameter, Fourier transform)

# Network theory – statistical measures

$$k_i = \sum_{j \in \mathcal{N}} a_{ij}$$

$$P(k)$$

$$L = \frac{1}{N(N-1)} \sum_{i,j \in \mathcal{N},\ i \neq j} d_{ij}$$

$$C = \langle c \rangle = \frac{1}{N} \sum_{i \in \mathcal{N}} c_i,\ \ c_i = \frac{2e_i}{k_i(k_i - 1)},\ \ 0 \leq C \leq 1$$

$$E = \frac{1}{N(N-1)} \sum_{i,j \in \mathcal{N},\ i \neq j} \epsilon_{ij},\ \ \epsilon_{ij} = \frac{1}{d_{ij}}$$

# Graph theory – network models

Random graph: $G^{ER}_{N,K},\ G^{ER}_{N,p}$

$$\langle k \rangle = p(N-1),\ P(k) = e^{-\langle k \rangle} \frac{\langle k \rangle^k}{k!}$$

$$C = p,\ L \sim \frac{\ln N}{\ln \langle k \rangle}$$

Ring lattice: N nodes connected to K neighbours

$$P(k) = \begin{cases} N, & \text{for } \ k_i = K \\ 0, & \text{otherwise} \end{cases}$$

$$C = \frac{3(K-2)}{4(K-1)} \sim 3/4,\ L = \frac{N}{2K}$$

# Height Similarity Method (HS method) (1/2)

Transforms rough surfaces to networks

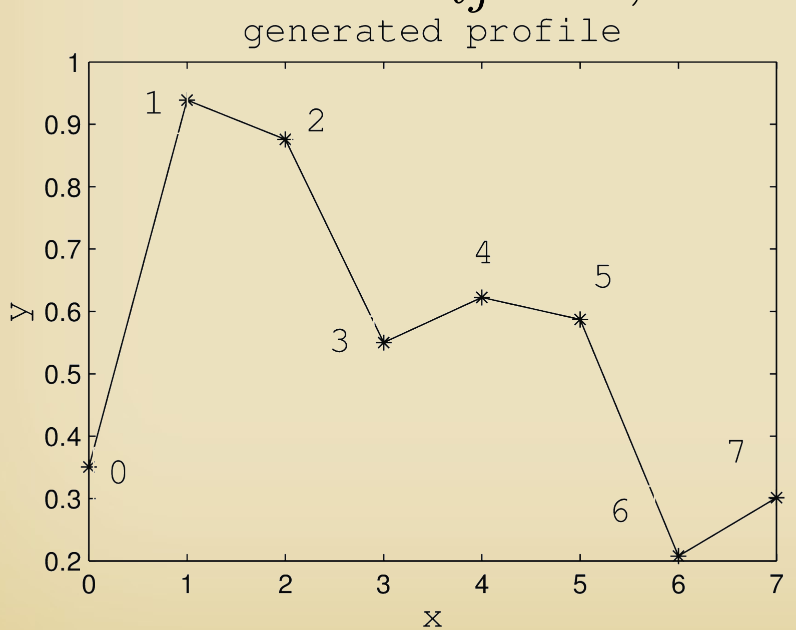
Input: Surface data $h(x_i)$ $i=1,\ldots,N$

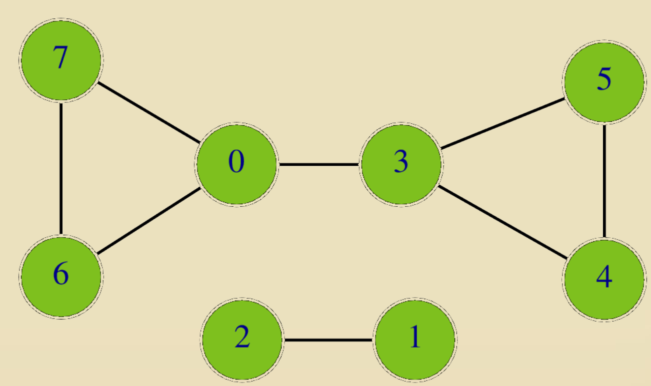
Output: a network

- nodes: N points of the profile
- links: height similarity criterion

$$\text{if} \quad p(i,j) = e^{-|y_i - y_j|} > p_{thres}$$

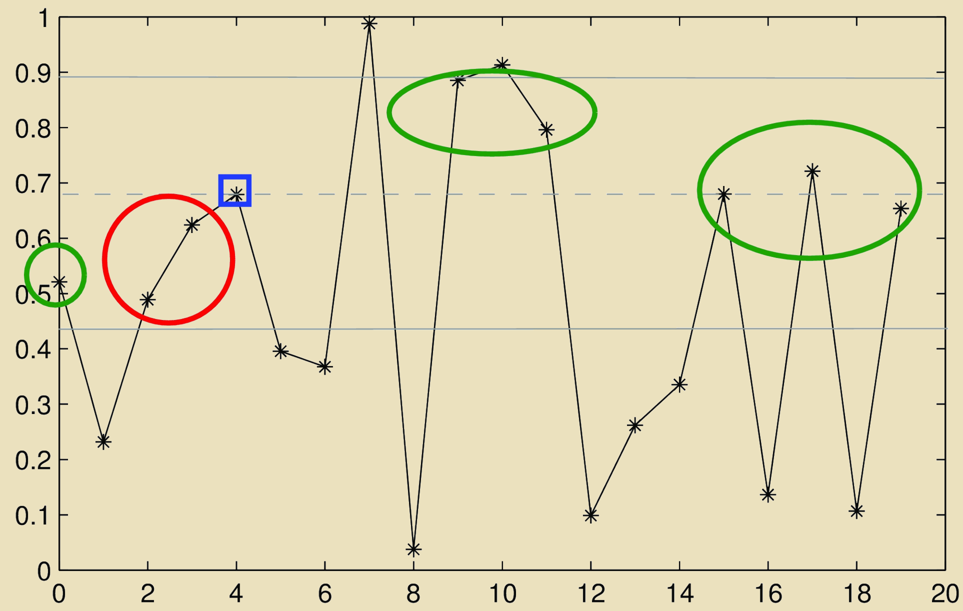
$$\text{then} \quad a_{ij} = 1, \; \text{otherwise} \quad a_{ij} = 0, \quad \forall\, i \neq j$$




$$|y_i - y_j| < -\ln p_{thres}$$

# Height Similarity Method (HS method) (2/2)




$$k_i = k_{i,local} + k_{i,nonlocal}, \quad \text{for } i = 1, ..., N$$

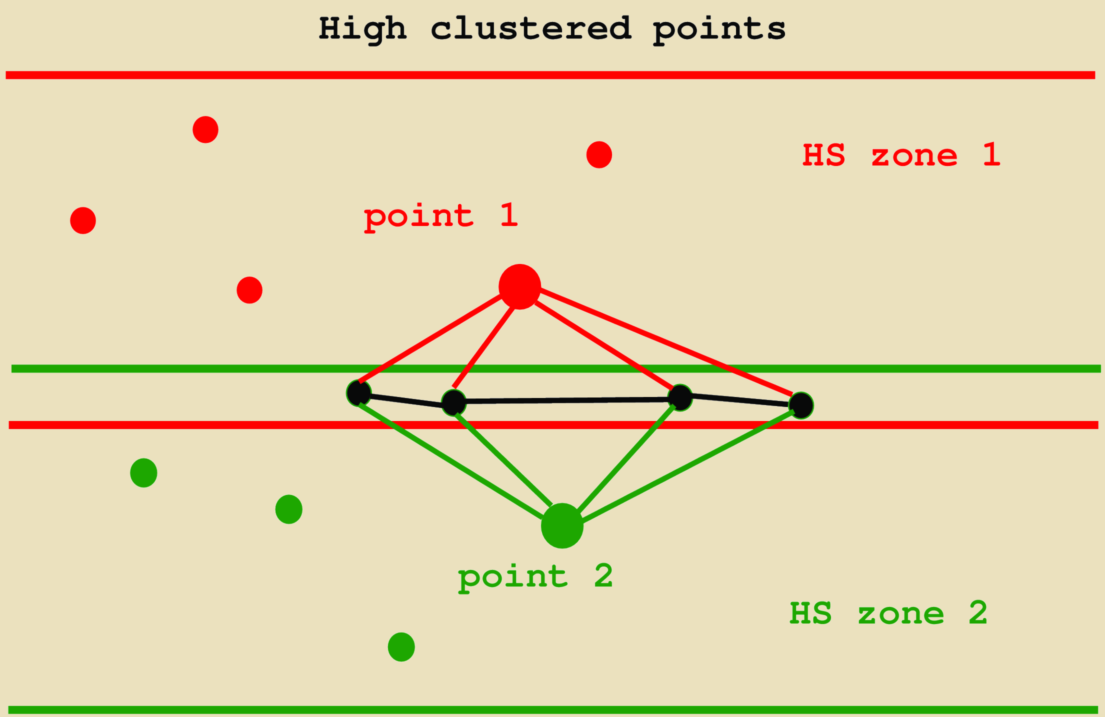
$$[h(min), h(min) + (-\ln p_{thres})]$$

boundary points

$$[(h(max) - (-\ln p_{thres}), h(max)]$$

# HS method – properties

- Highly clustered nets
- Long average shortest path length




$$l(p_1 \to p_2) = \frac{dh}{-ln(p_{thres})}$$

# Proof: C ~ ¾ (points uniformly distributed)

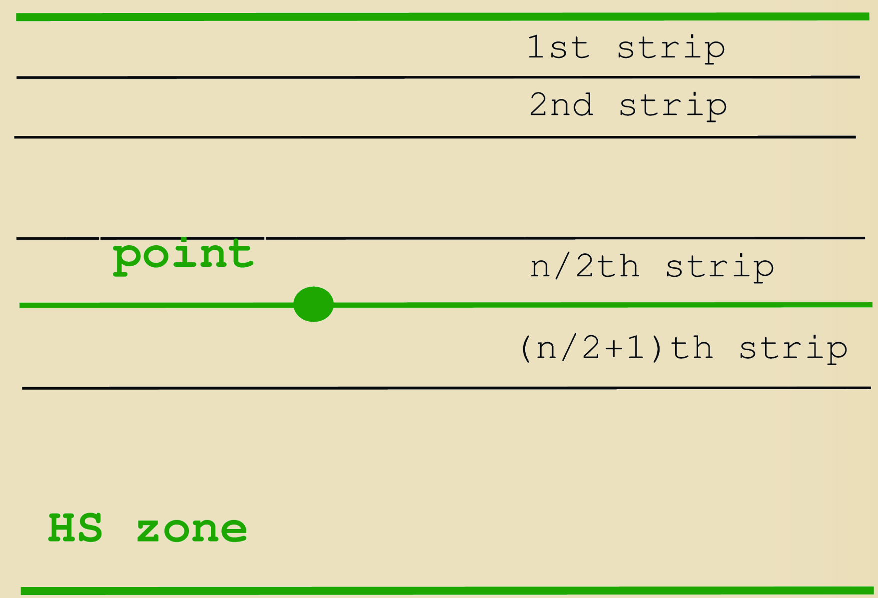
$$1st \quad \frac{k}{n} \longrightarrow \frac{k}{2} + \frac{k}{n}$$

$$2nd \quad \frac{k}{n} \longrightarrow \frac{k}{2} + 2\frac{k}{n}$$

$$jth \quad \frac{k}{n} \longrightarrow \frac{k}{2} + j\frac{k}{n}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$\frac{n}{2}th \quad \frac{k}{n} \longrightarrow \frac{k}{2} + \frac{n}{2}\frac{k}{n} = k$$



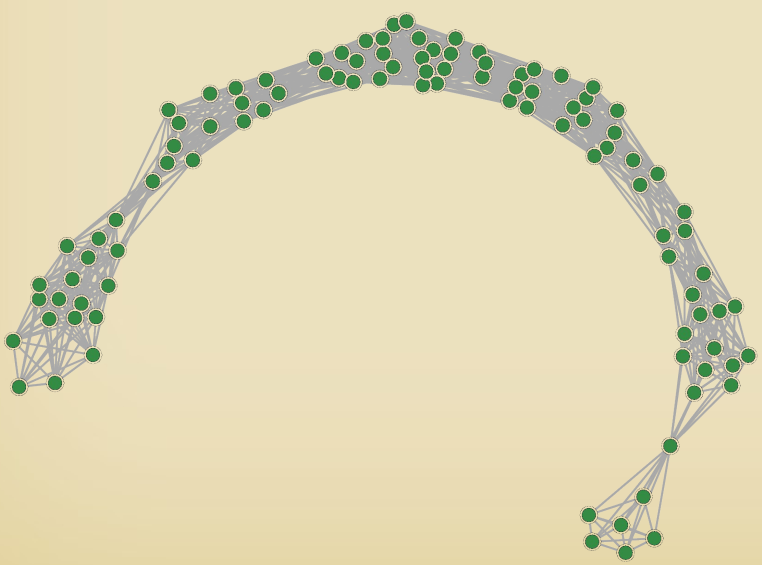

$$2e_i = 2\sum_{j=1}^{n/2} \frac{k}{n}\left(\frac{k}{2} + j\frac{k}{n}\right) = \frac{3}{4}k^2, \ n \rightarrow \infty$$

$$c_i = \frac{2e_i}{k(k-1)} \simeq 0.75$$

# Applications to Rough Surfaces

1. Extreme cases
   a. White noise
   b. Fully periodic surfaces
      i. Square pulse
      ii. Triangular pulse
      iii. Harmonic wave
2. Fractal self-affine surfaces
3. Mounded Surfaces
   a. fully periodic
   b. deviations from periodicity (position, height, width)

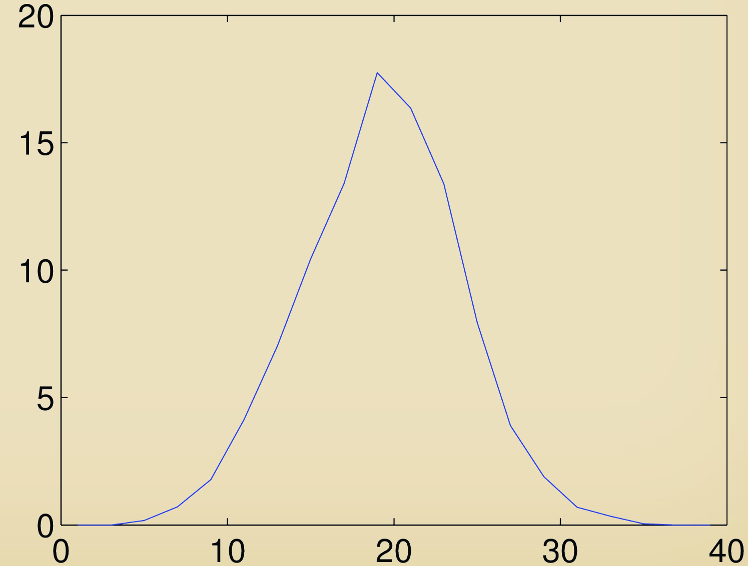
# 1-a. White noise (1/3)

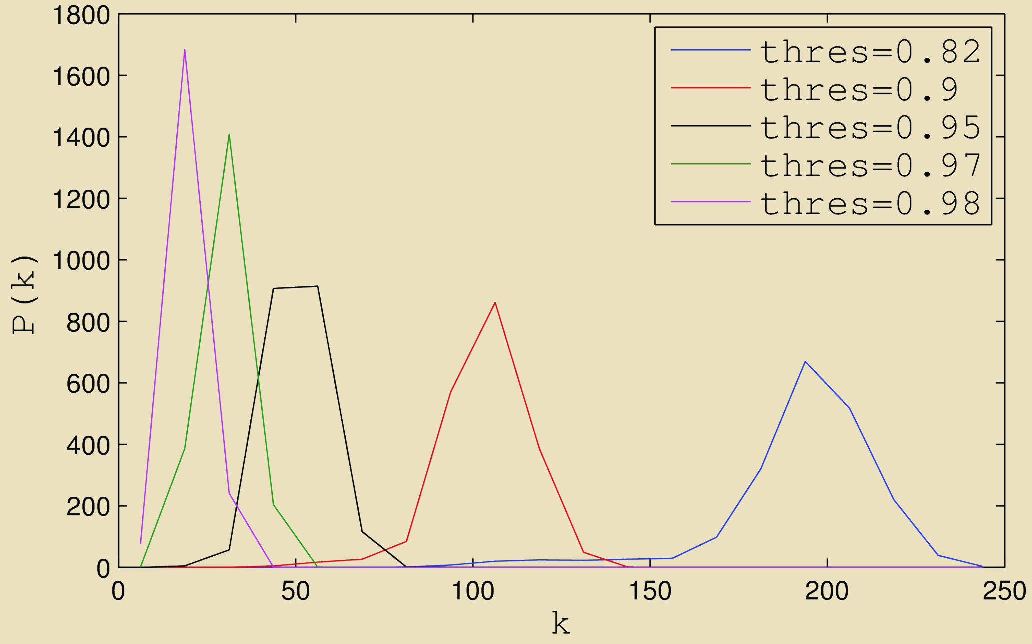
$$k_{i,local} \sim 0$$

Poisson d.d

$$\langle k \rangle = \frac{-2 \ln p_{thres}}{A} N$$



# 1-a. White noise (2/3)




$$A,\ p_{thres} \nearrow \quad \Rightarrow \quad \langle k \rangle \searrow,\ C \searrow\ (s.e.),\ L \nearrow$$

$C \sim 0.75$ (points uniformly distributed)

# 1-a. White noise (3/3)

## Comparison with random graphs, ring lattice

$$C_{random} = p = \frac{\langle k \rangle}{N-1}$$

$$L_{random} = \frac{\ln N}{\ln \langle k \rangle}$$

$$C_{ring} = \frac{3(K-2)}{4(K-1)}$$

$$L_{ring} = \frac{N}{2K}$$

$$P(k)_{random} \; Poisson$$

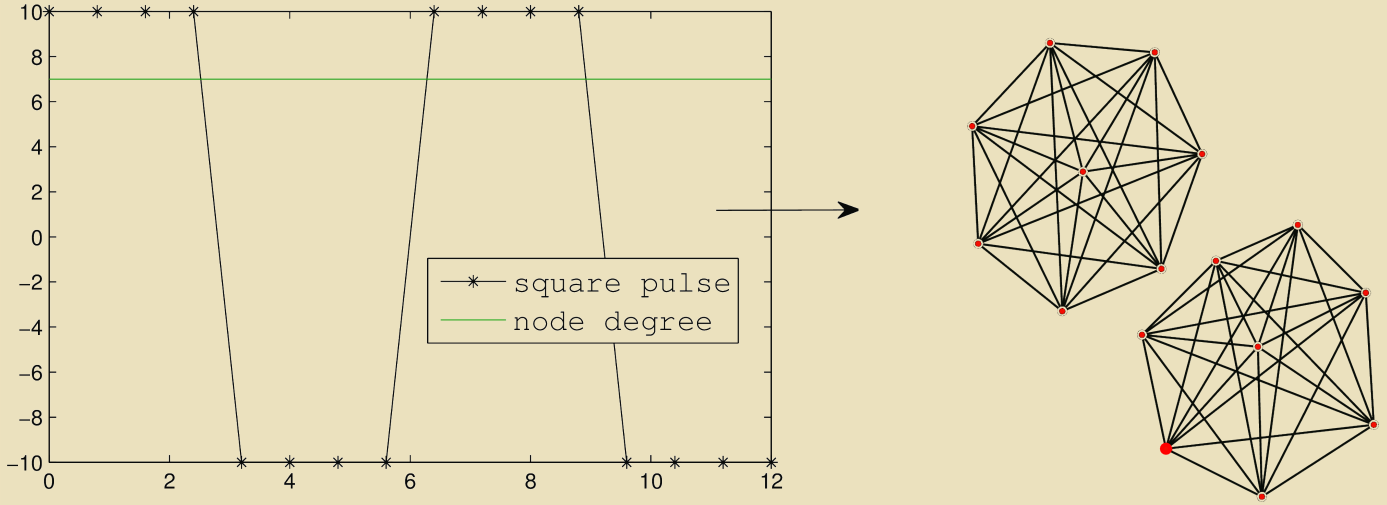
$$P(k)_{ring} \; deltafunction$$

$$C_{random} \ll C \sim C_{ring}$$

$$L_{random} < L \sim L_{ring}$$

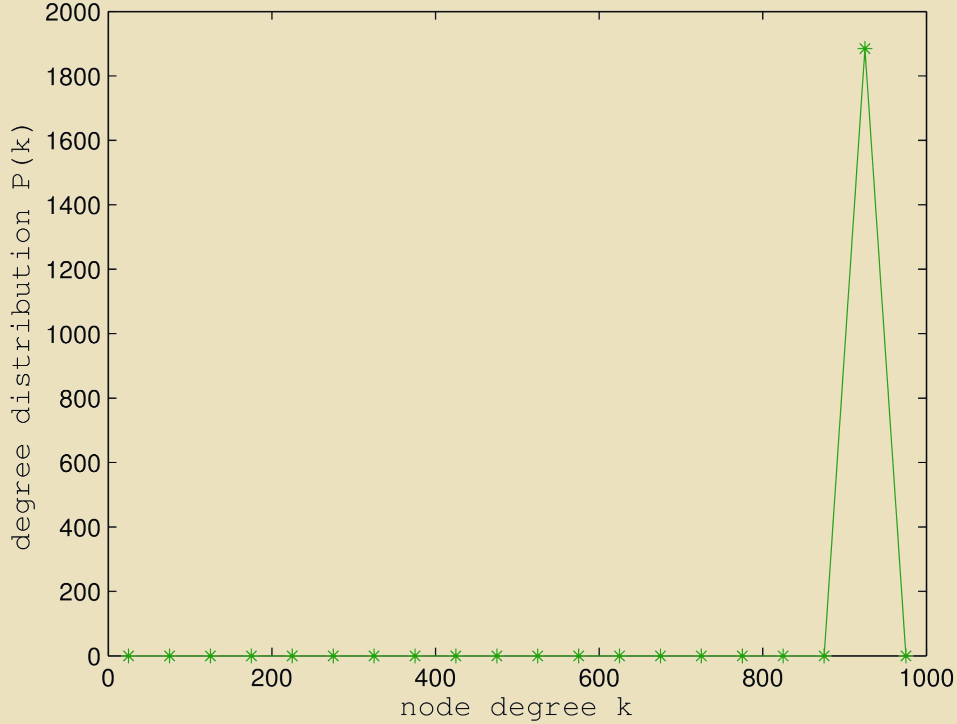
$$P(k) \; Poisson$$

# 1-b-i. Square pulse (1/2)




$$k_i = \frac{N}{2} - 1,\ c_i = 1,\ l_i = 1,\ \forall i \in N,\ L\ diverges$$

# 1-b-i. Square pulse (2/2)

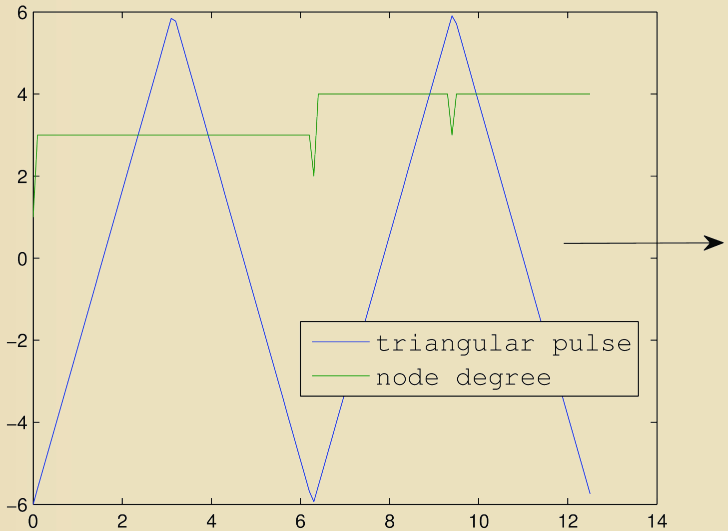


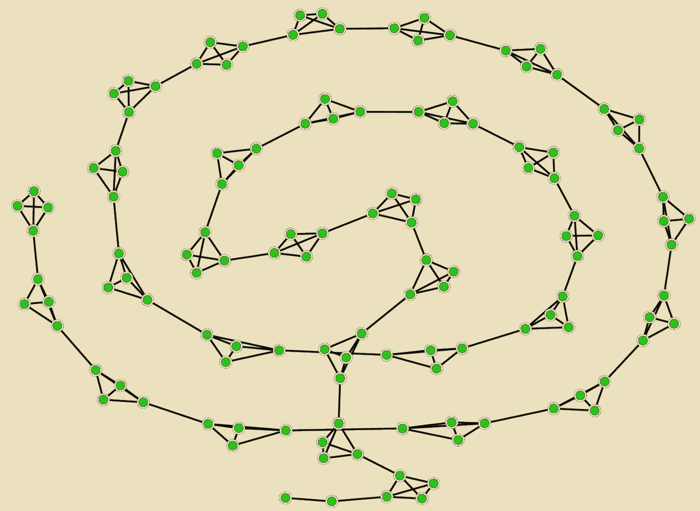

$$P(k) = \begin{cases} N, & \text{for} \;\; k = \frac{N}{2} - 1 \\ 0, & \text{otherwise} \end{cases}$$

(delta function)

type I peak: comes from points in same height zone

# 1-b-ii. Triangular pulse (1/2)



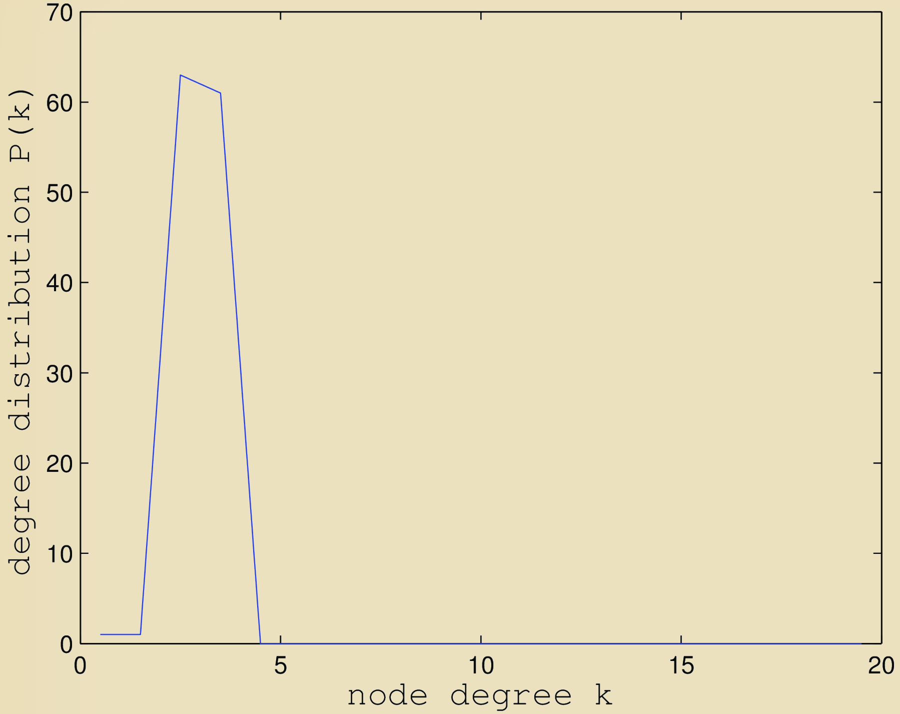



$$k_i = 2m(k_{i,local} + 1) - 1, \ \forall i \in N$$

$$k_{i,local} \sim \frac{T}{2A}$$

$$C \sim 0.75$$

# 1-b-ii. Triangular pulse (2/2)




$$C \sim C_{ring}, \;\; L < L_{ring}$$

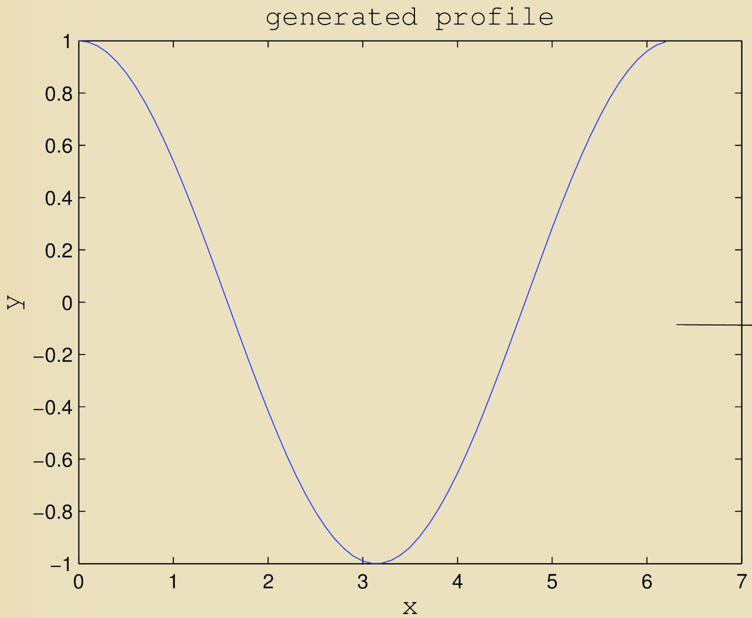
$$P(k) = \begin{cases} N, & \text{for} \;\; k = k_i \\ 0, & \text{otherwise} \end{cases}$$

(delta function)

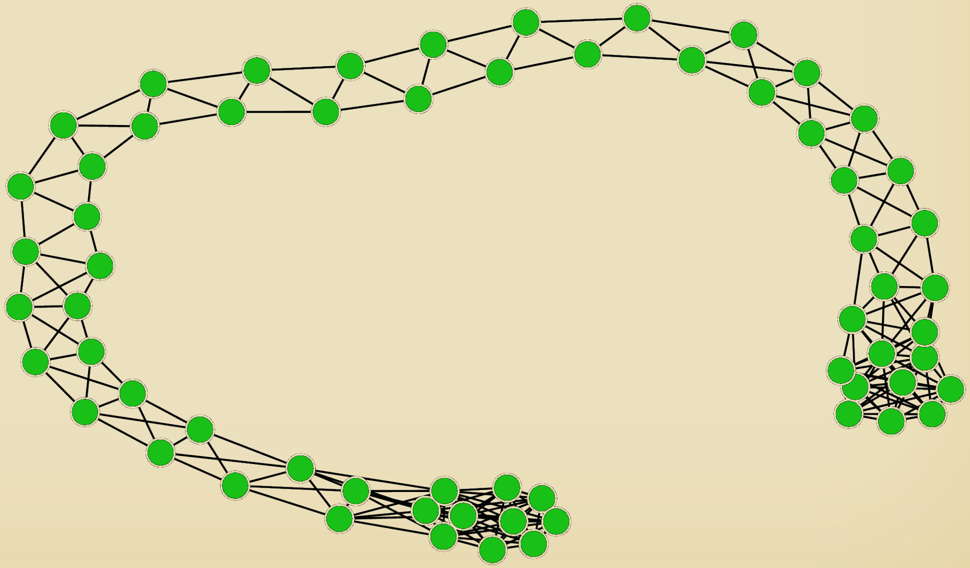
$$A, \; p_{thres} \nearrow \quad \Rightarrow \quad \langle k \rangle \searrow, \; C \searrow \;, \; L \nearrow$$

type II peak: comes from points in different height zones

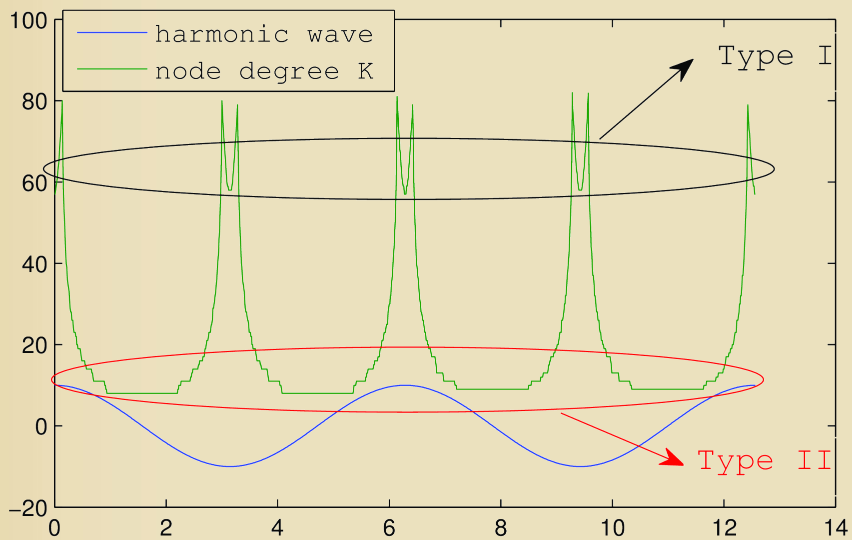
# 1-b-iii. Harmonic wave (1/3)

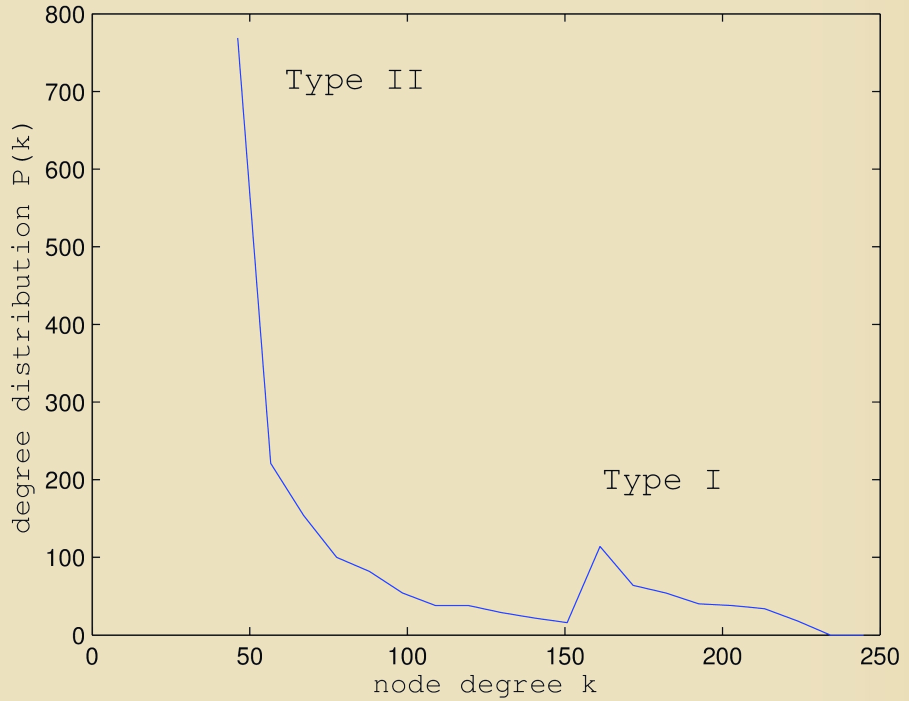



$$y(x) = A \cdot \cos(\omega x + \phi)$$



# 1-b-iii. Harmonic wave (2/3)

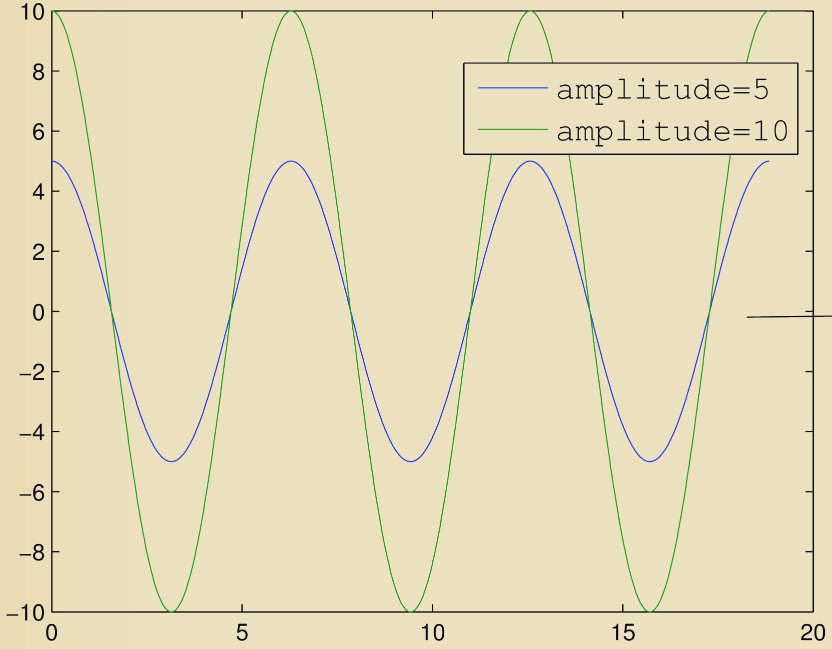


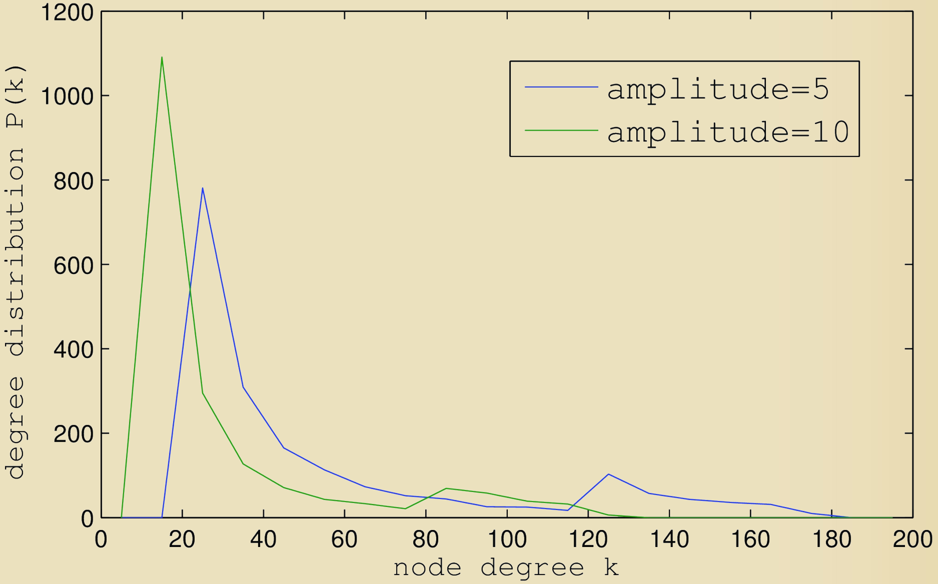




type I peak: comes maxima & minima

type II peak: comes from almost linear slopes

# 1-b-iii. Harmonic wave (3/3)

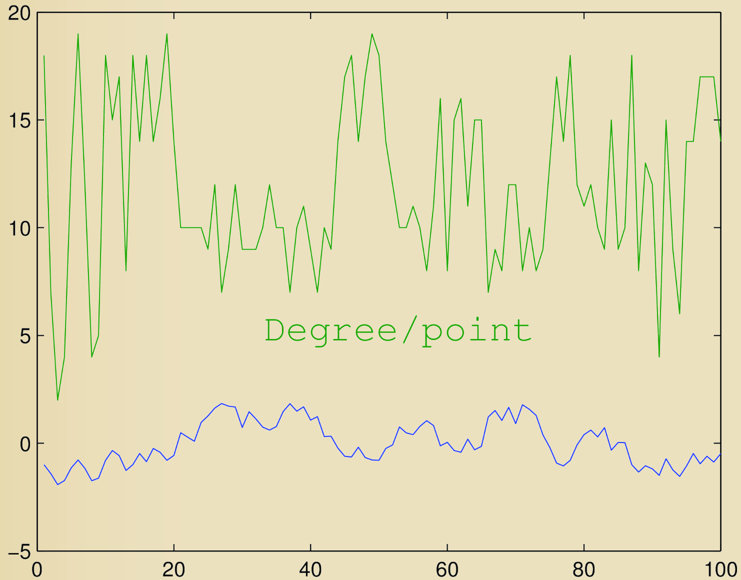


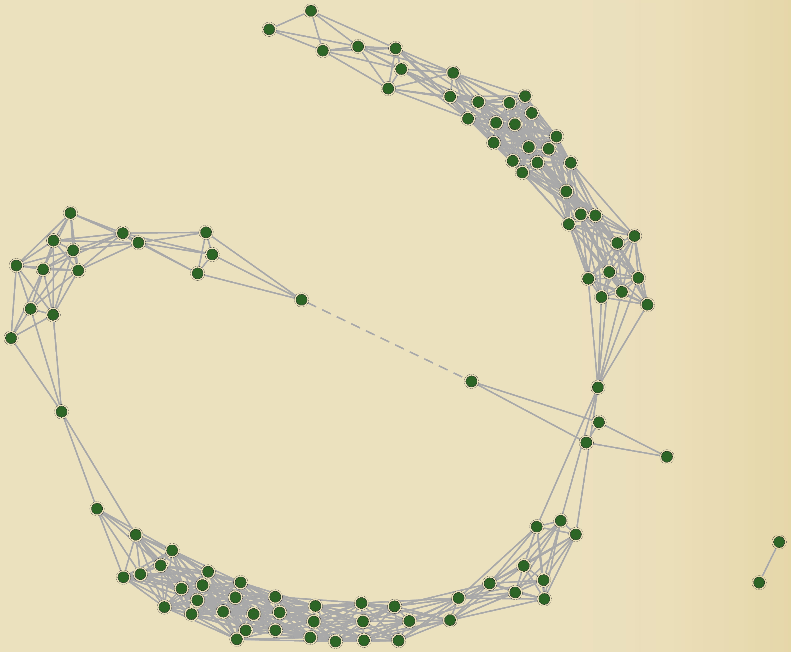



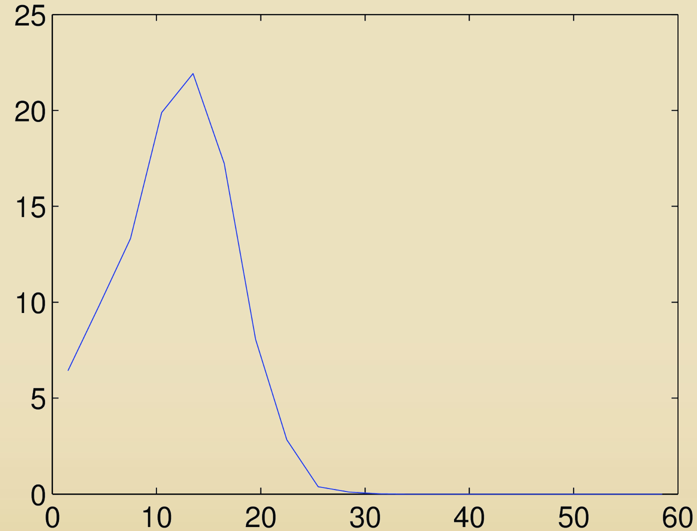

$$A,\ p_{thres} \nearrow \quad \Rightarrow \quad \langle k \rangle \searrow,\ C \searrow\ ,\ L \nearrow$$

# 2. Fractal self-affine surfaces (1/7)

type I peak: comes from the same (or similar) height zones.

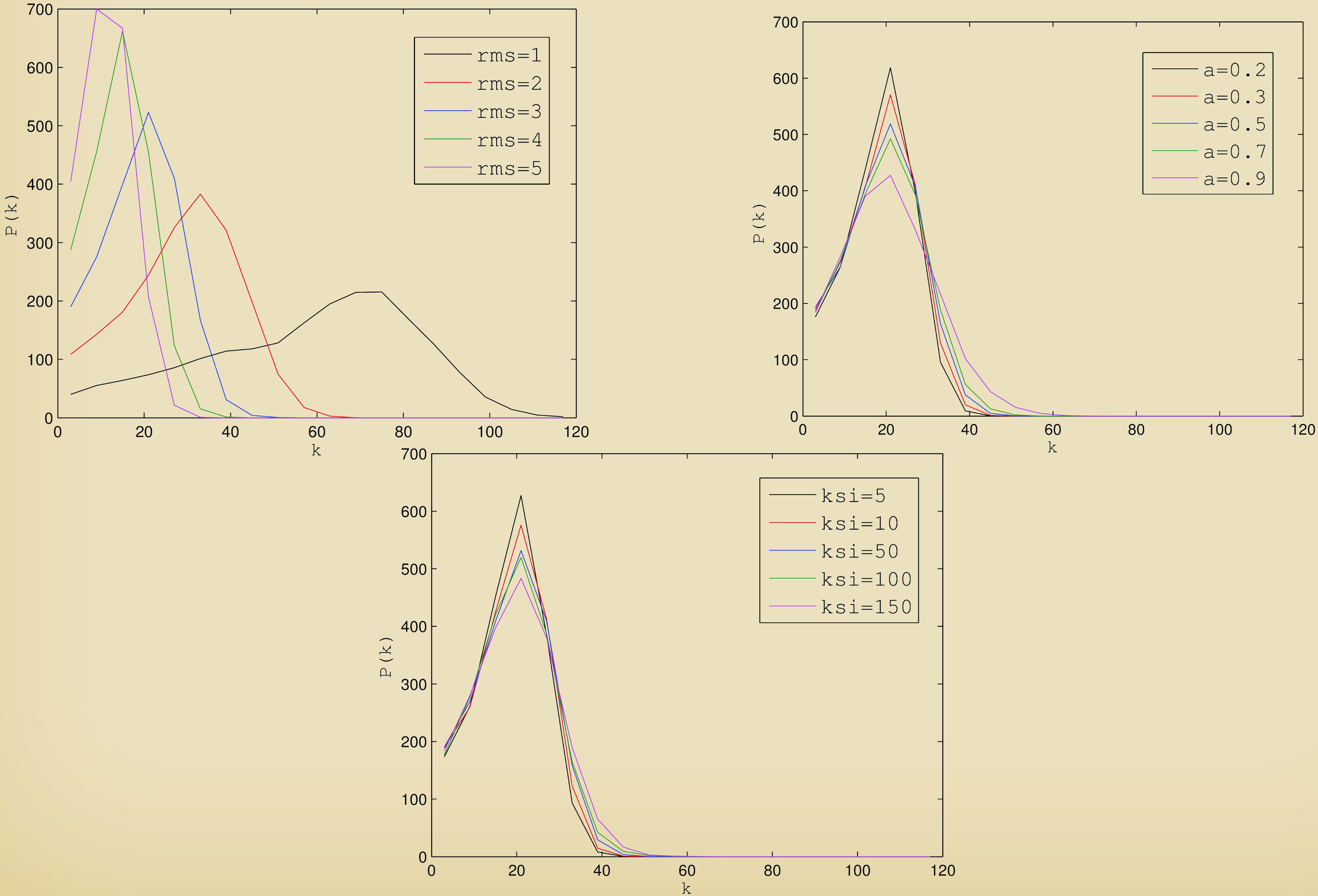




# 2. Fractal self-affine surfaces (2/7)

## Impact of rms, ksi, a on P(k)



# 2. Fractal self-affine surfaces (3/7)

Impact of rms, ksi, a on P(k)

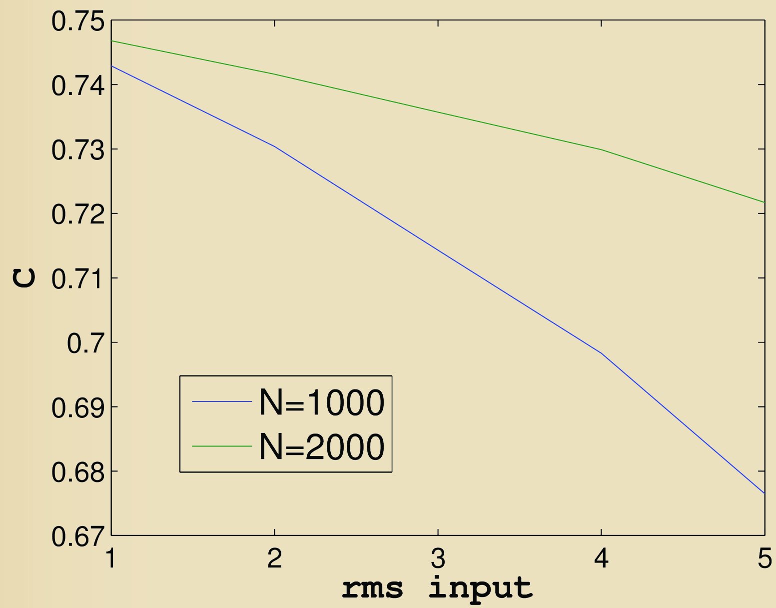
$rms \nearrow \quad \Rightarrow \quad$ P(k): shifts to lower k's, increament of peak

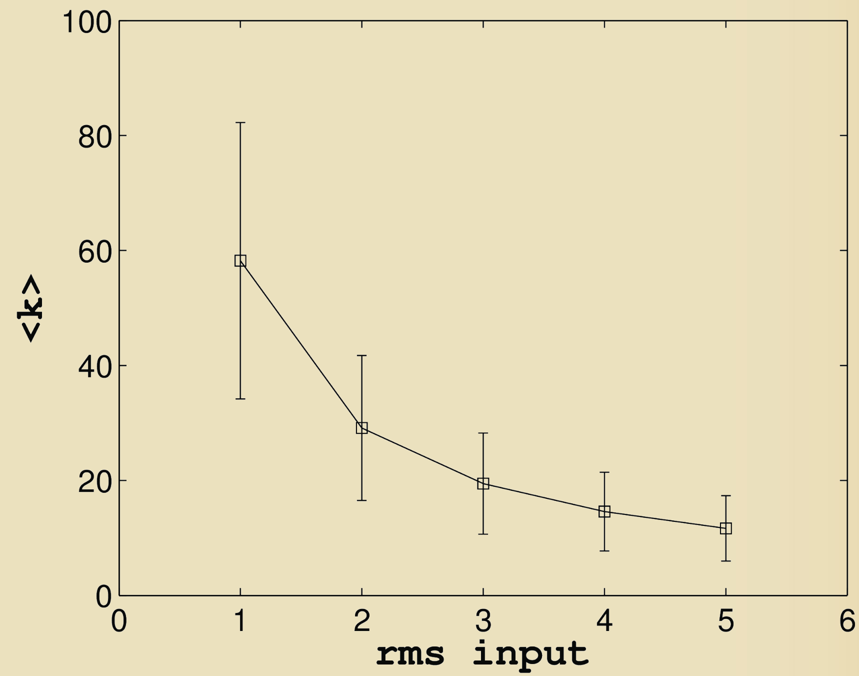
$ksi,\ \alpha \nearrow \quad \Rightarrow$ P(k): enhancement of high k's, lowering of peak

$$N = 2000,\ p_{thres} = 0.95,\ runs = 100,\ rms = 3,\ \xi = 50,\ \alpha = 0.5$$

# 2. Fractal self-affine surfaces (4/7)

## Impact of rms on <k>, C, L



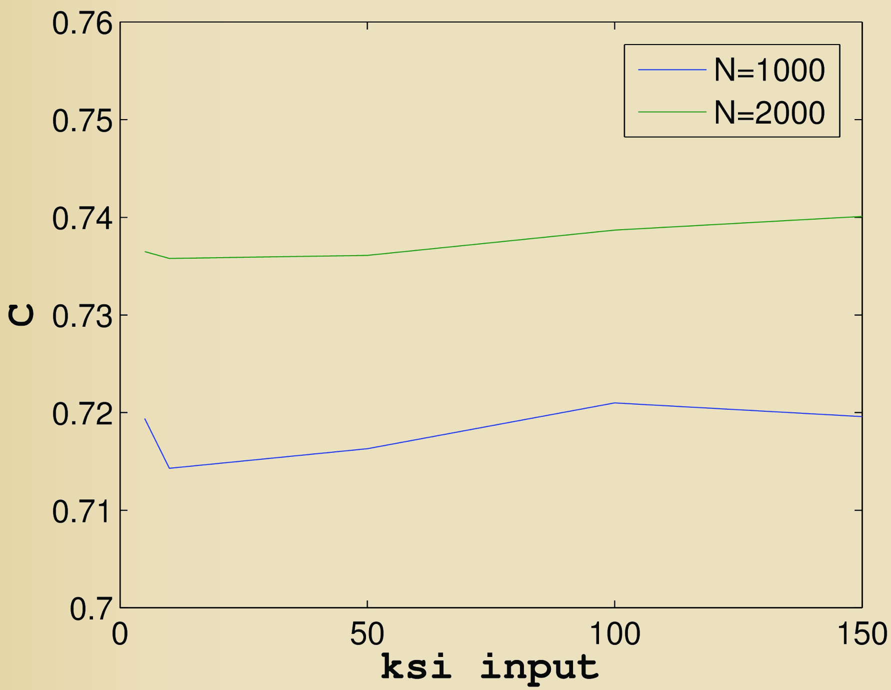



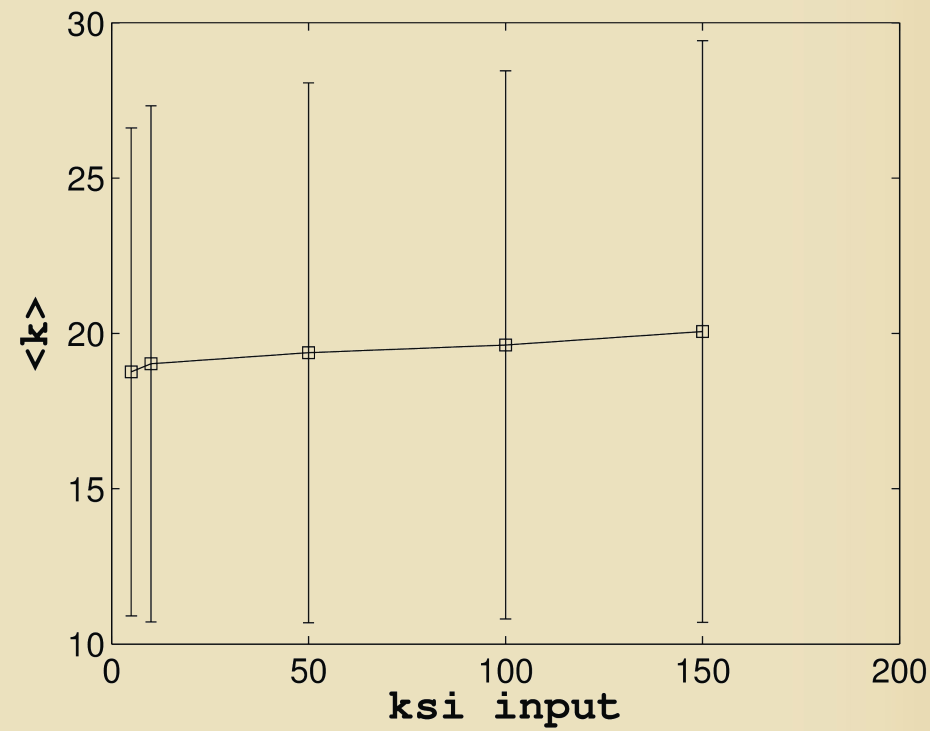

$$rms \nearrow \quad \Rightarrow \quad \langle k \rangle \searrow,\ C \searrow,\ \text{L diverges}$$

$$N = 2000,\ p_{thres} = 0.95,\ runs = 100,\ rms = 3,\ \xi = 10,\ \alpha = 0.5$$

# 2. Fractal self-affine surfaces (5/7)

## Impact of ξ on <k>, C, L




$ksi \nearrow \quad \Rightarrow \quad \langle k \rangle \nearrow (s.e.),\ C \searrow (s.e.),$ for $\xi = 100 \Rightarrow \ maxC$

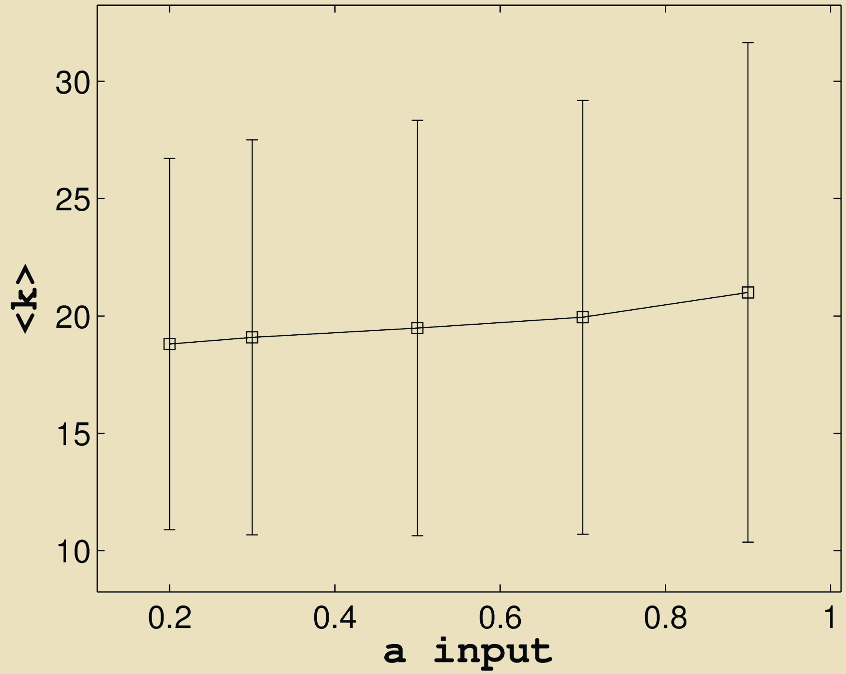
L diverges

for $\xi = 10 \Rightarrow \ minC$

$N = 2000,\ p_{thres} = 0.95,\ runs = 100,\ rms = 3,\ \xi = 10,\ \alpha = 0.5$

# 2. Fractal self-affine surfaces (6/7)

## Impact of α on <k>, P(k)



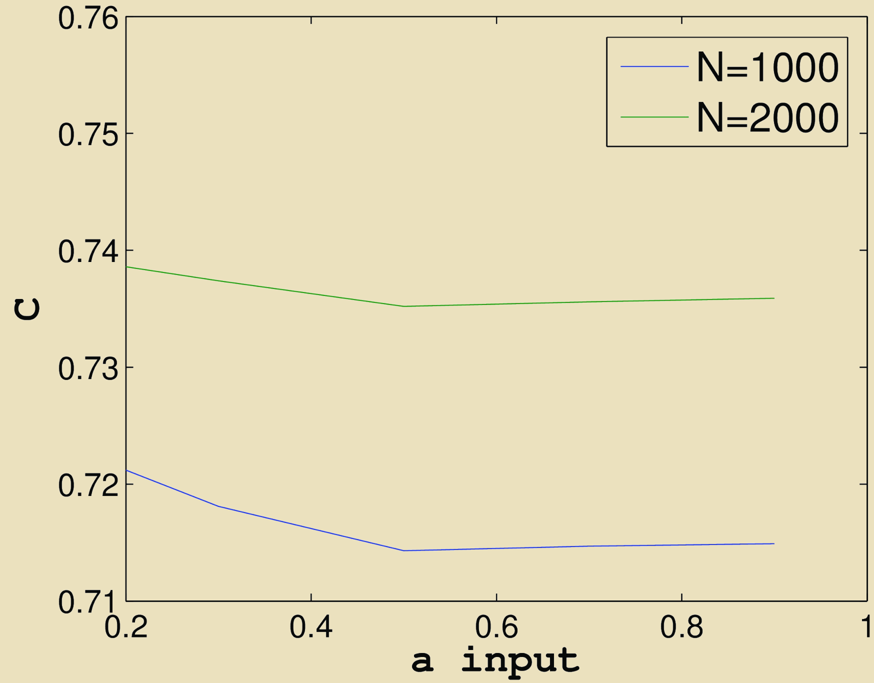

$$\alpha \nearrow \quad \Rightarrow \quad \langle k \rangle \nearrow (s.e.),\ k_{local} \nearrow$$

P(k): enhancement of high k's, lowering of peak

$$N = 2000,\ p_{thres} = 0.95,\ runs = 100,\ rms = 3,\ \xi = 10,\ \alpha = 0.5$$

# 2. Fractal self-affine surfaces (7/7)

## Impact of α on C, L



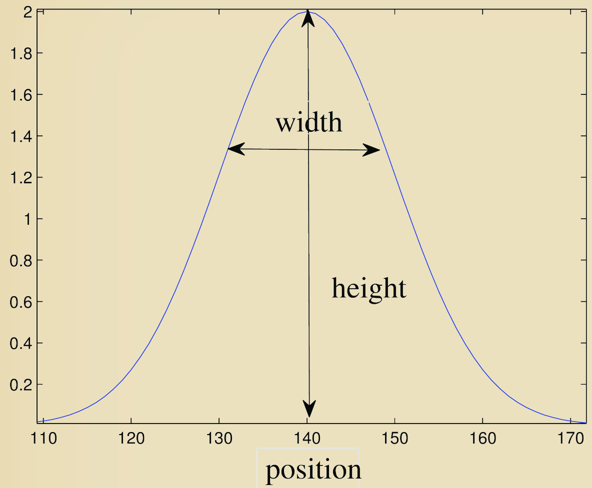

$C \searrow (s.e.)$ for $\alpha \in [0.2, 0..5]$

$C \searrow (n.e.)$ for $\alpha \in [0.5, 0..9]$

L diverges

$N = 2000,\ p_{thres} = 0.95,\ runs = 100,\ rms = 3,\ \xi = 10,\ \alpha = 0.5$

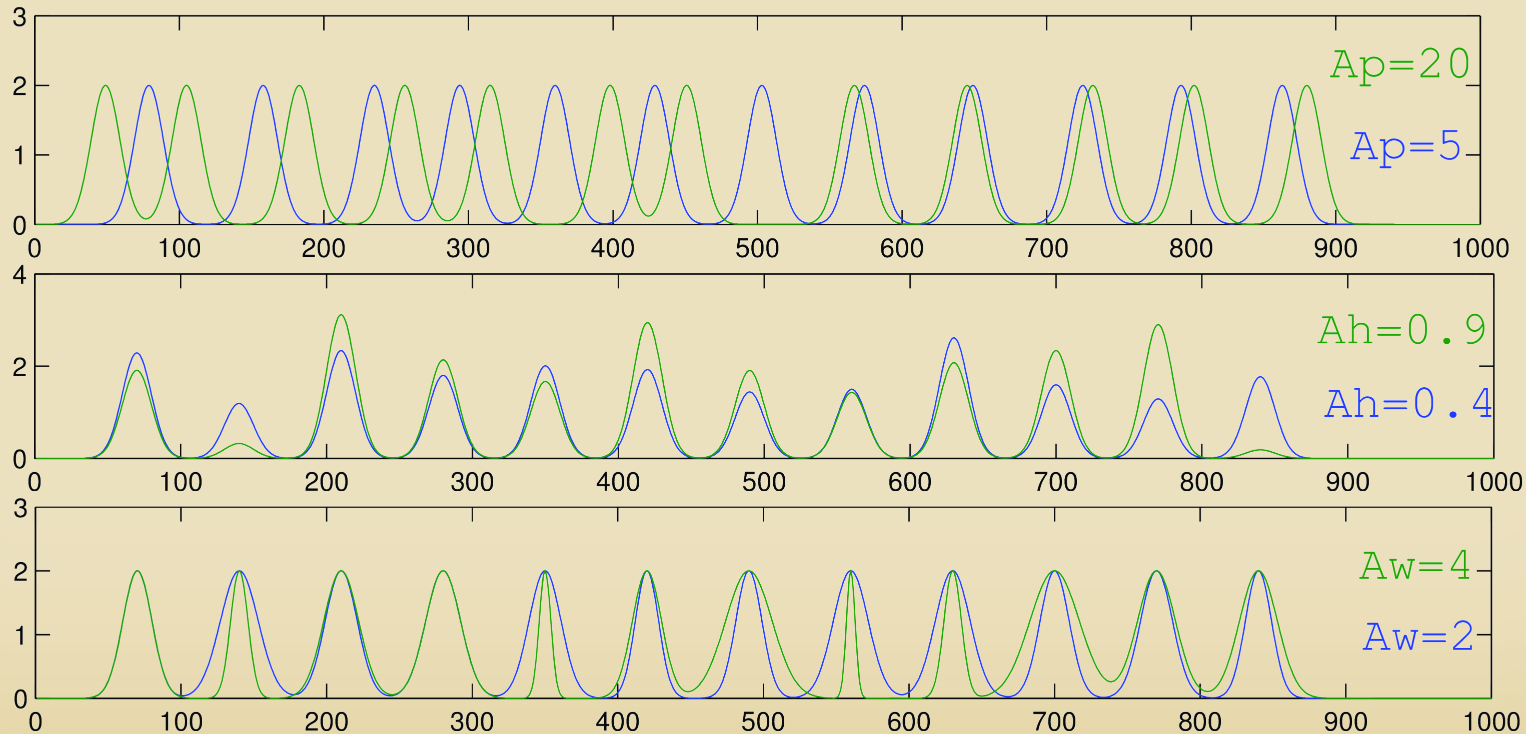
# 3. Mounded surfaces (1/5)



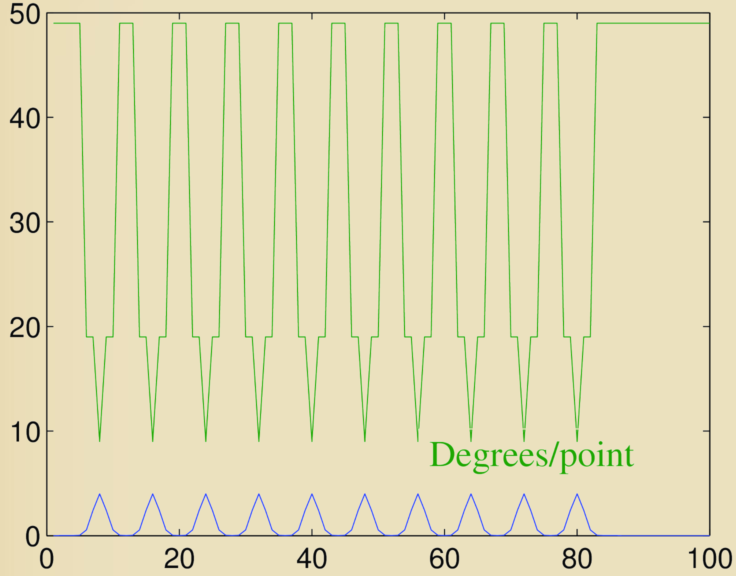

$$d_i(dev) = d_i(per) + A_p \times \eta_i, \ \forall \text{ peak } i$$

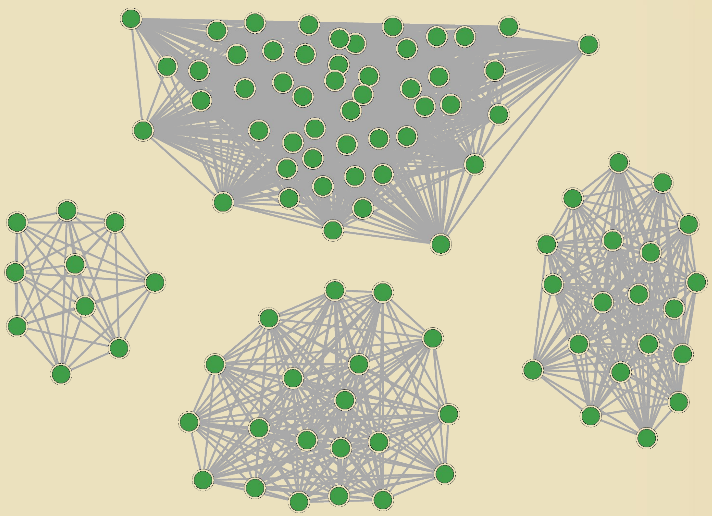
$$h_i(dev) = h(per) + A_h \times \eta_i$$

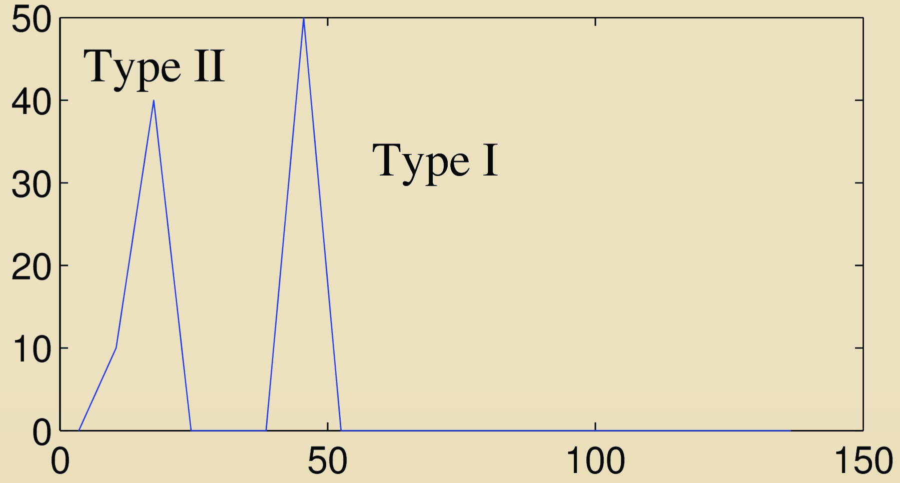
$$w_i(dev) = w(per) + A_h \times \eta_i$$



# 3. Mounded surfaces (2/5)

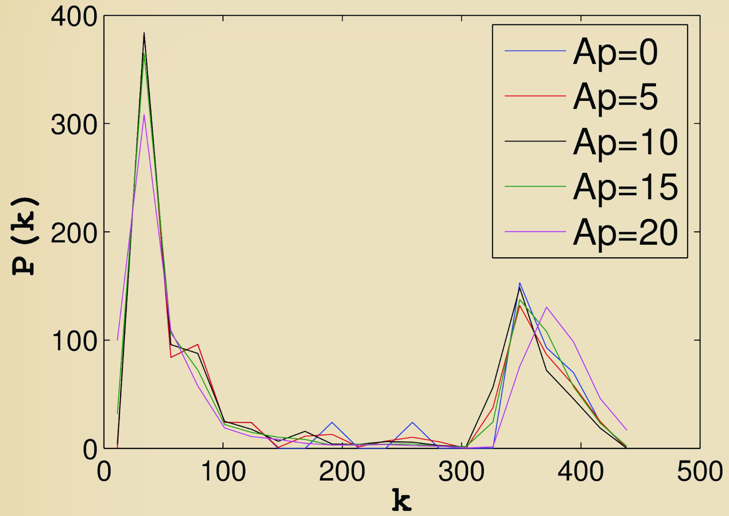


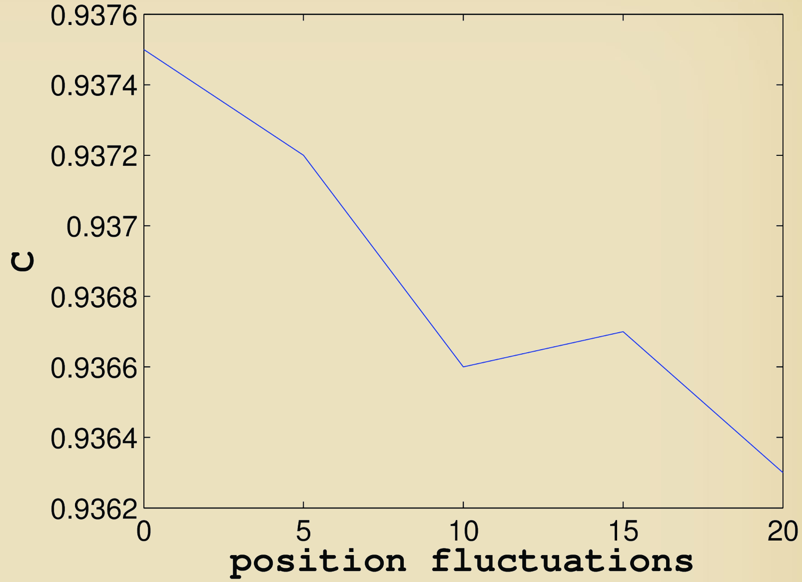



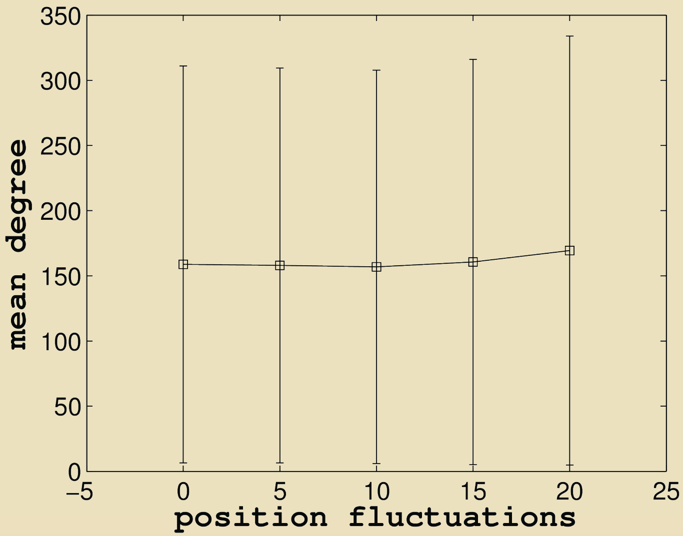



$$N = 100,\ runs = 100,\ p_{thres} = 0.9,\ d_i(per) = 8,\ h_i(per) = 4,\ w_i(per) = 1$$

# 3b. Mounded surfaces (3/5)



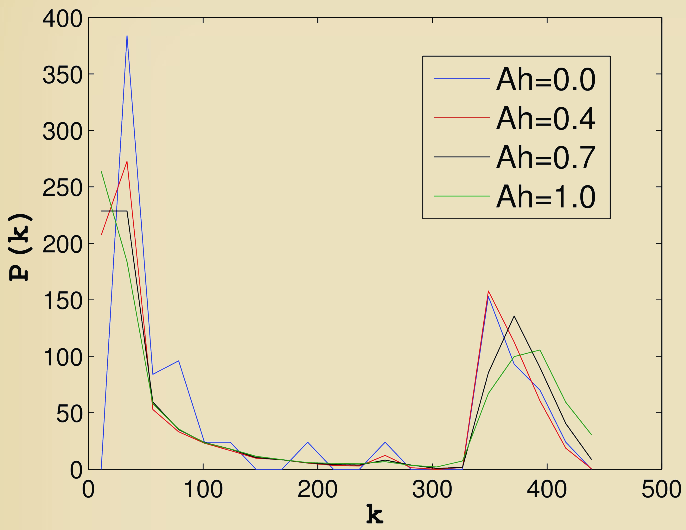



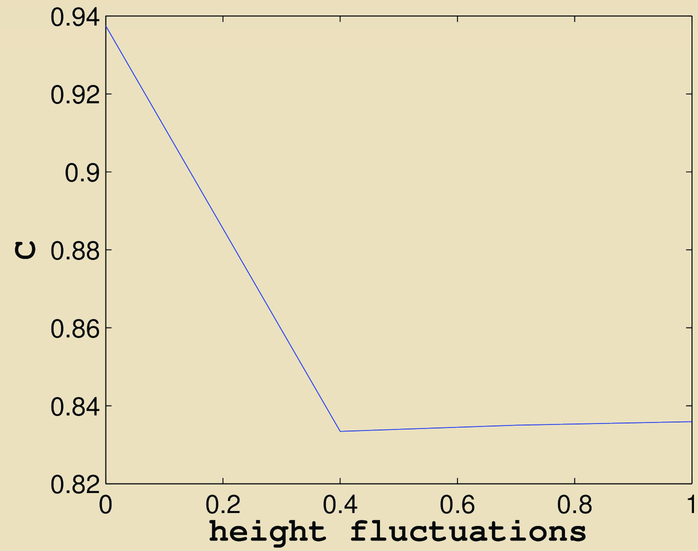

$N = 1000,\ p_{thres} = 0.95,\ runs = 100$

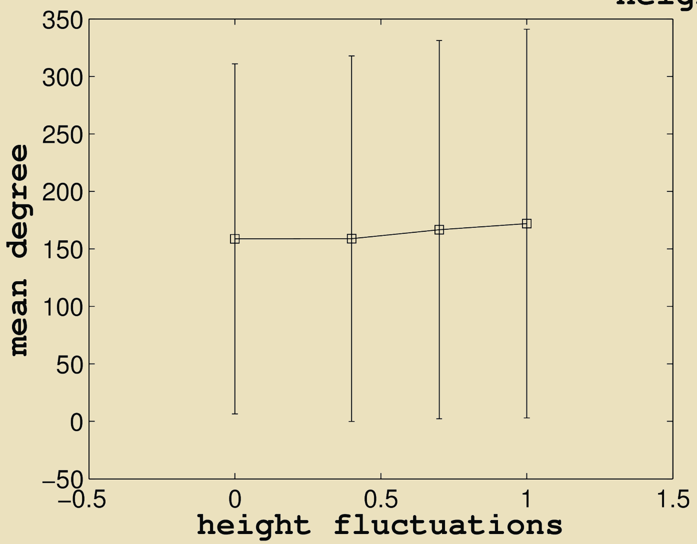
$d_i(per) = 70,\ h_i(per) = 2,\ w_i(per) = 10$

position fluctuations

# 3b. Mounded surfaces (4/5)



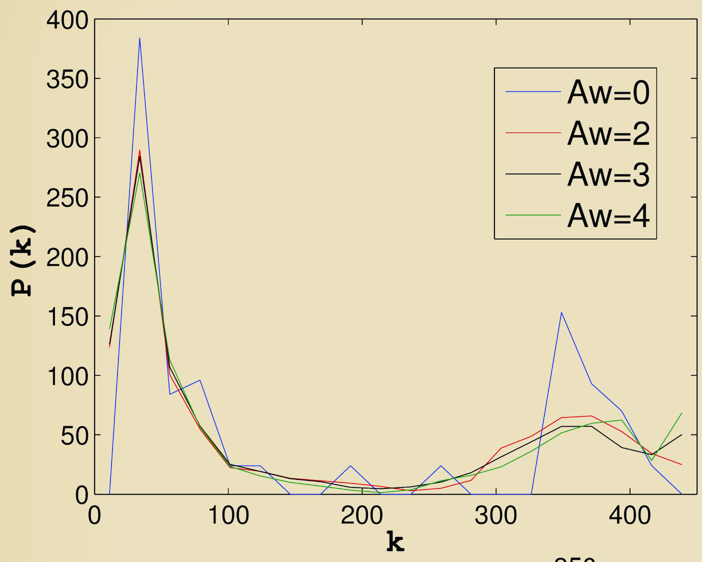



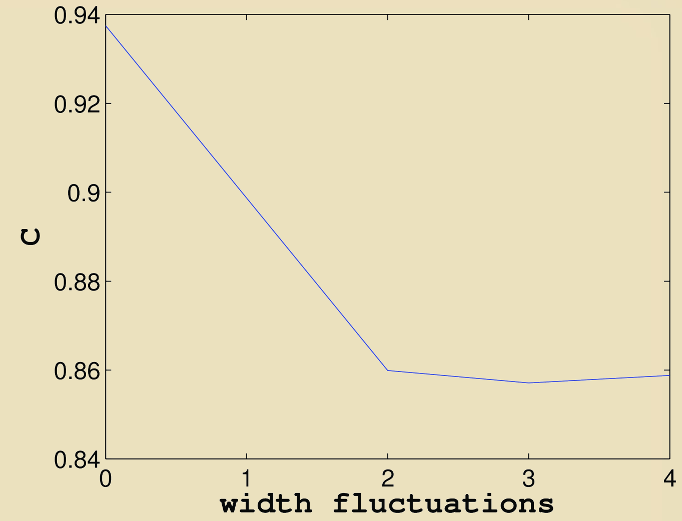

$N = 1000,\ p_{thres} = 0.95,\ runs = 100$

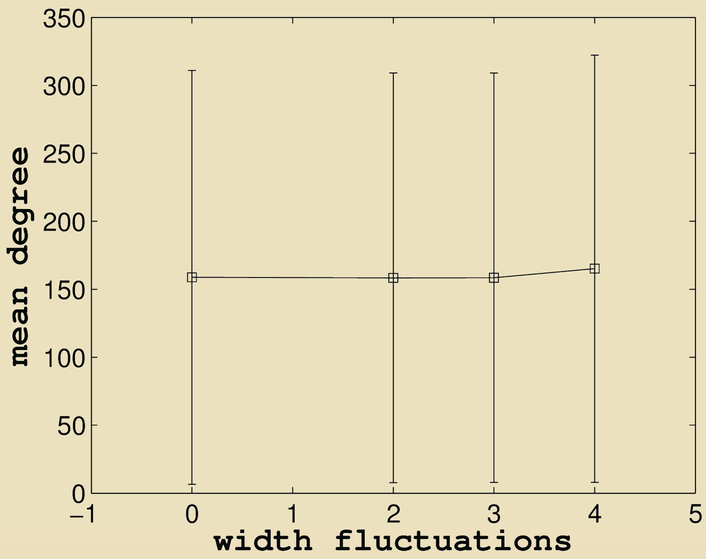
height fluctuations

$d_i(per) = 70,\ h_i(per) = 2,\ w_i(per) = 10$

# 3b. Mounded surfaces (5/5)




$N = 1000,\ p_{thres} = 0.95,\ runs = 100$

width fluctuations

$d_i(per) = 70,\ h_i(per) = 2,\ w_i(per) = 10$

# Summary and Conclusion (1/2)

- **Motivation**: alternative approaches to roughness characterization are needed
- **Aim**: investigate the structure of rough surfaces through complex network theory (<k>, P(k), C, L)
- **Idea**: transform a rough surface into a network through height similarity method
- **Application**: random, fully periodic, fractal self-affine, mounded rough surfaces
- **HS method**: Highly clustered networks with long average path length, boundary points

# Summary and Conclusion (2/2)

- <k>: analytical estimation for white noise, square, triangular pulse
- P(k): sensitive to surface periodicity
- Fully periodic: type I or type II or both
- White noise: Poisson d.d
- Fractal self-affine: rms affects P(k)
- Mounded surfaces: type I, II affected by deviations from periodicity
- C ~ 0.75 (white noise, triangular pulse)
- L: I will come back hopefully with a theoretical prediction for the average path length.

# Things for future consideration

- Estimation of more network statistical measures (efficiency E in cases where L diverges)
- Extension of the method to include the spatial distance, transformation to geographical models
- Examination of real experimental surfaces, comparison with the conventional methods for roughness analysis

Thank you very much!