993SM - Laboratory of Computational Physics week VIII November 14, 2025

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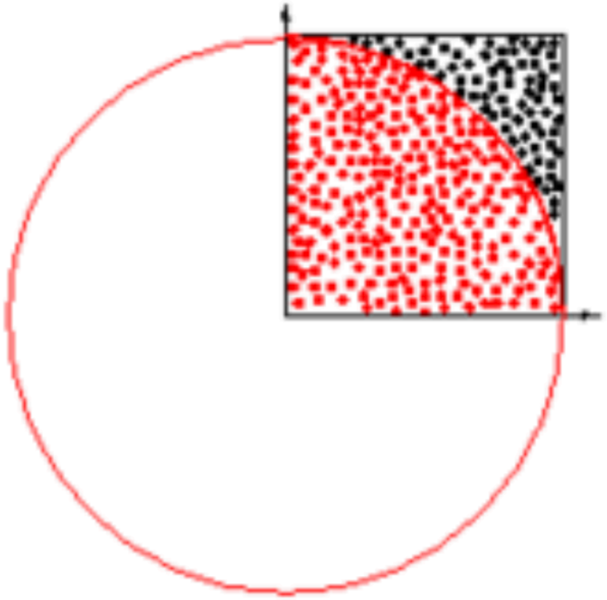
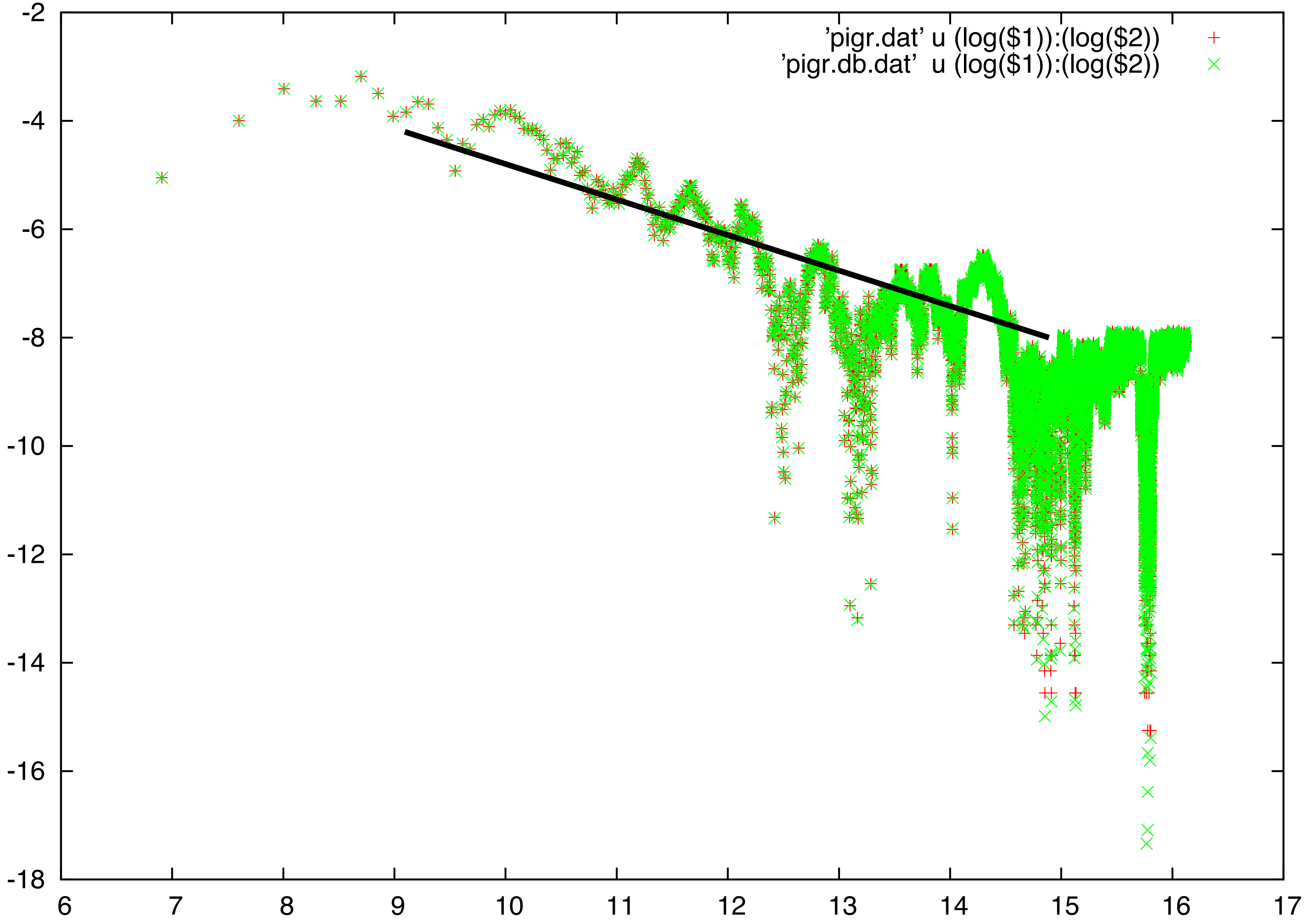
Behaviour of the error and efficiency in acceptance-rejection Monte Carlo method for integration

1. Monte Carlo method: acceptance-rejection

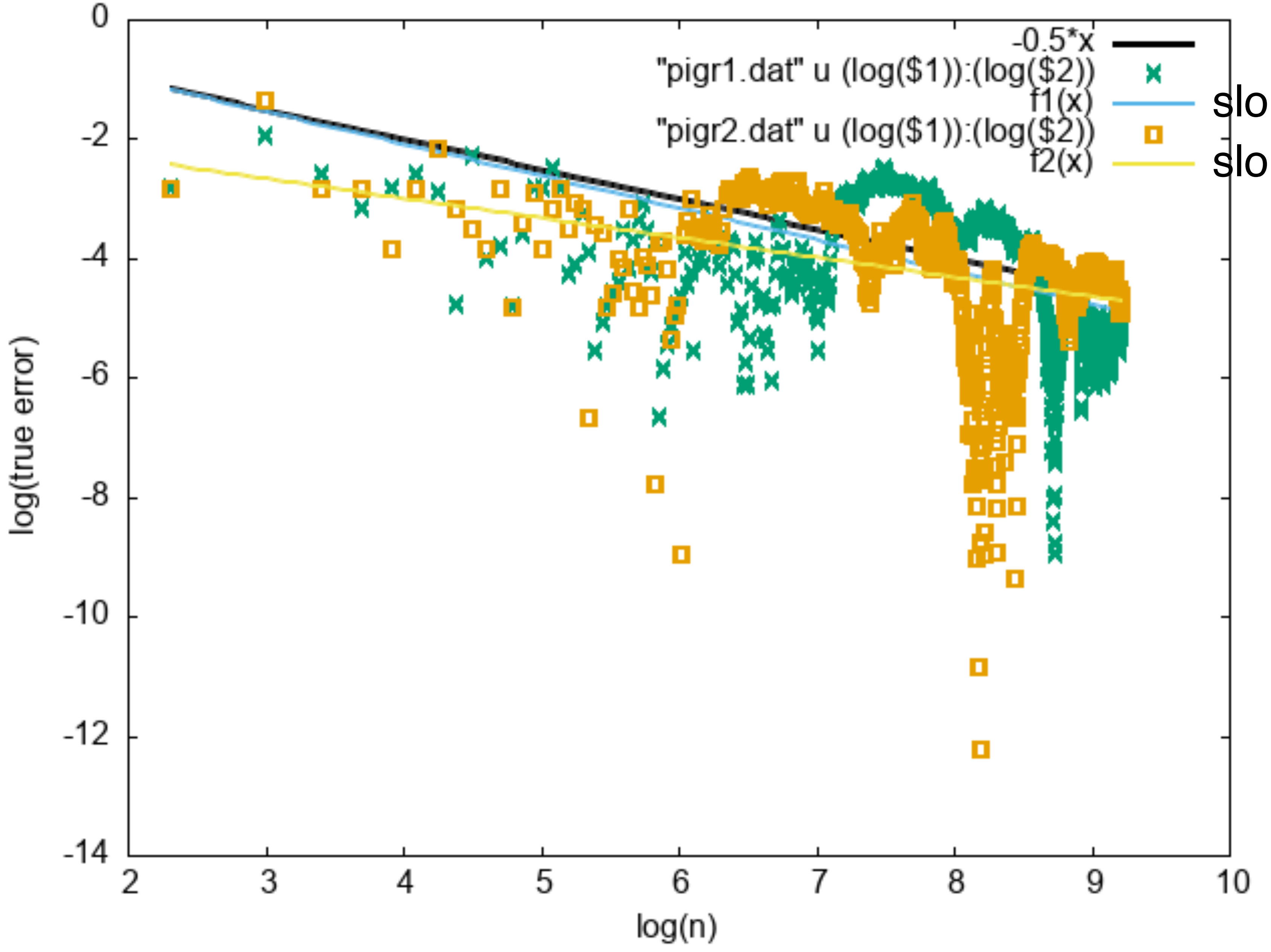
Using the acceptance-rejection method, calculate $I = \int_0^1 \sqrt{1-x^2}dx$ (notice that $\pi = 4I$). The numerical estimate of the integral is $F_n = \frac{n_s}{n}$ where n_s is the number of points under the curve $f(x) = \sqrt{1-x^2}$, and n the total number of points generated. An example is given in `pi.f90`. Estimate the error associated, i.e. the difference between F_n and the true value. Discuss the dependence of the error on n.
(*Notice that many points are needed to see the $n^{-1/2}$ behavior, which can be hidden by stochastic fluctuations; it is easier to see it by averaging over many results (obtained from random numbers sequences with different seeds)*)



error(MC)~1/$\sqrt{N}$ => see log(error) vs. log(N)



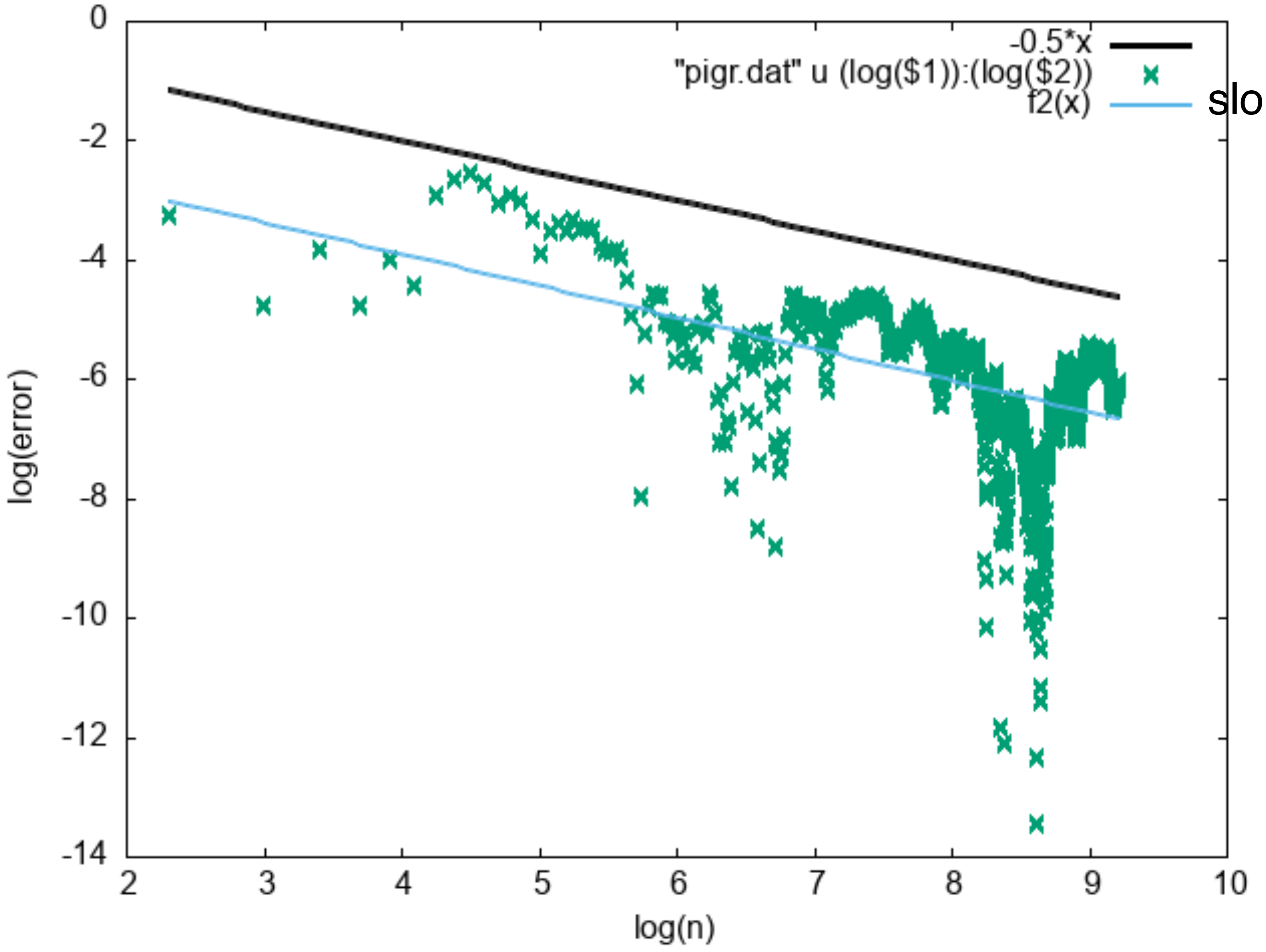
different seeds



slope -0.54

slope -0.33

average over 20 different seeds



slope -0.52

Extension to the hypersphere

VOLUME OF HYPERSPHERE

$$V_n = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)}$$

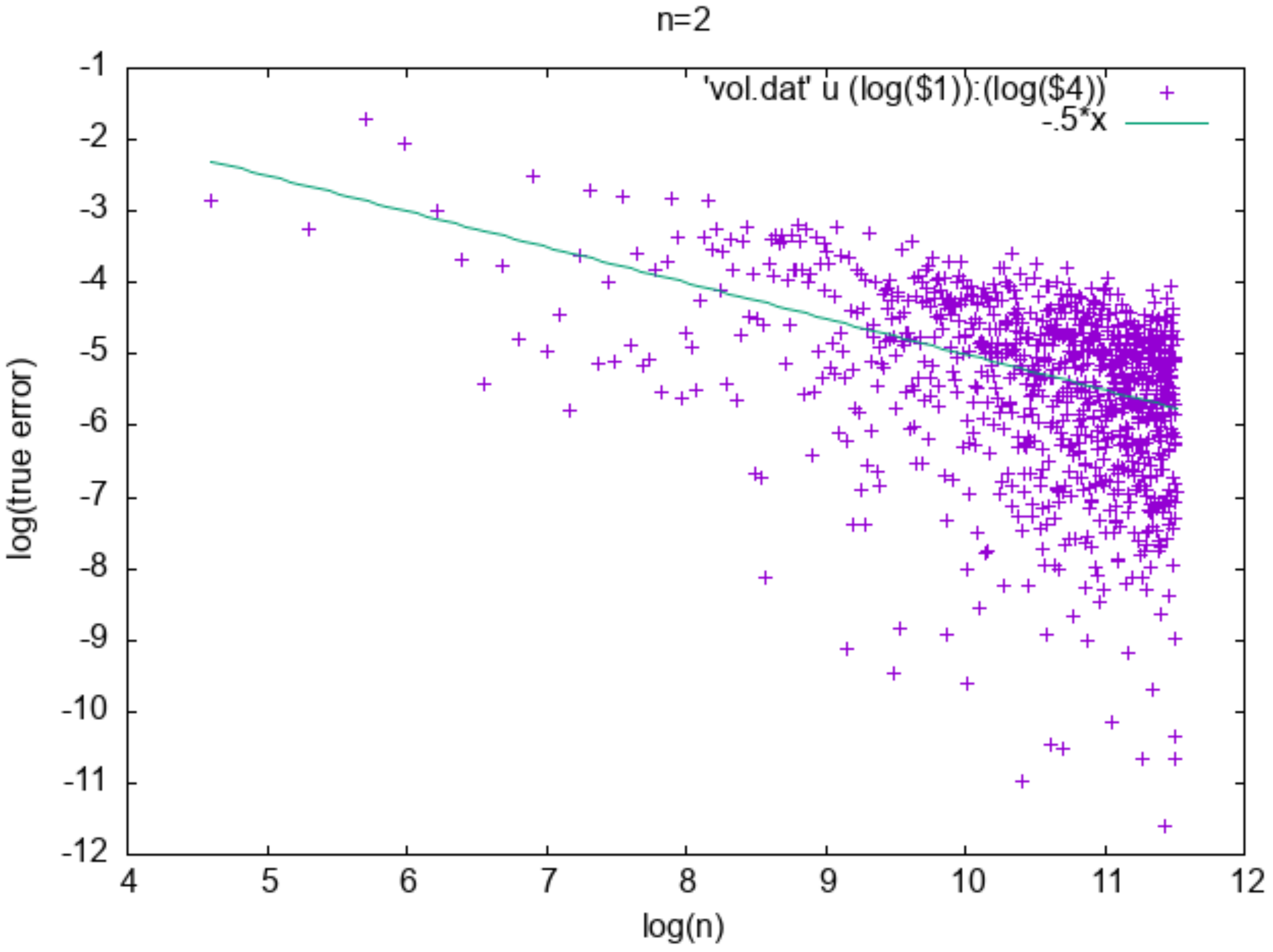
$$\Gamma(1/2) = \sqrt{\pi}; \Gamma(1) = 1; \Gamma(x+1) = x\Gamma(x)$$

$$V_{n+2} = 2\pi V_n/(n+2)$$

Numero di dimensioni *n*	Ipervolume $V_n(r)$	Misura ipersuperficiale $S_n(r)$	Valore numerico $V_n(1)$	Valore numerico $S_n(1)$
1	$2r$	2	2,000.000.000	2,000.000.000
2	πr^2	$2\pi r$	3,141.592.654	6,283.185.307
3	$\frac{4}{3}\pi r^3$	$4\pi r^2$	4,188.790.205	12,566.370.614
4	$\frac{1}{2}\pi^2 r^4$	$2\pi^2 r^3$	4,934.802.201	19,739.208.802
5	$\frac{8}{15}\pi^2 r^5$	$\frac{8}{3}\pi^2 r^4$	5,263.789.014	26,318.945.070
19	$\frac{1.024}{654.729.075}\pi^9 r^{19}$	$\frac{1.024}{34.459.425}\pi^9 r^{18}$	0,046.621.601	0,885.810.420
20	$\frac{1}{3.628.800}\pi^{10} r^{20}$	$\frac{1}{181.440}\pi^{10} r^{19}$	0,025.806.891	0,516.137.828

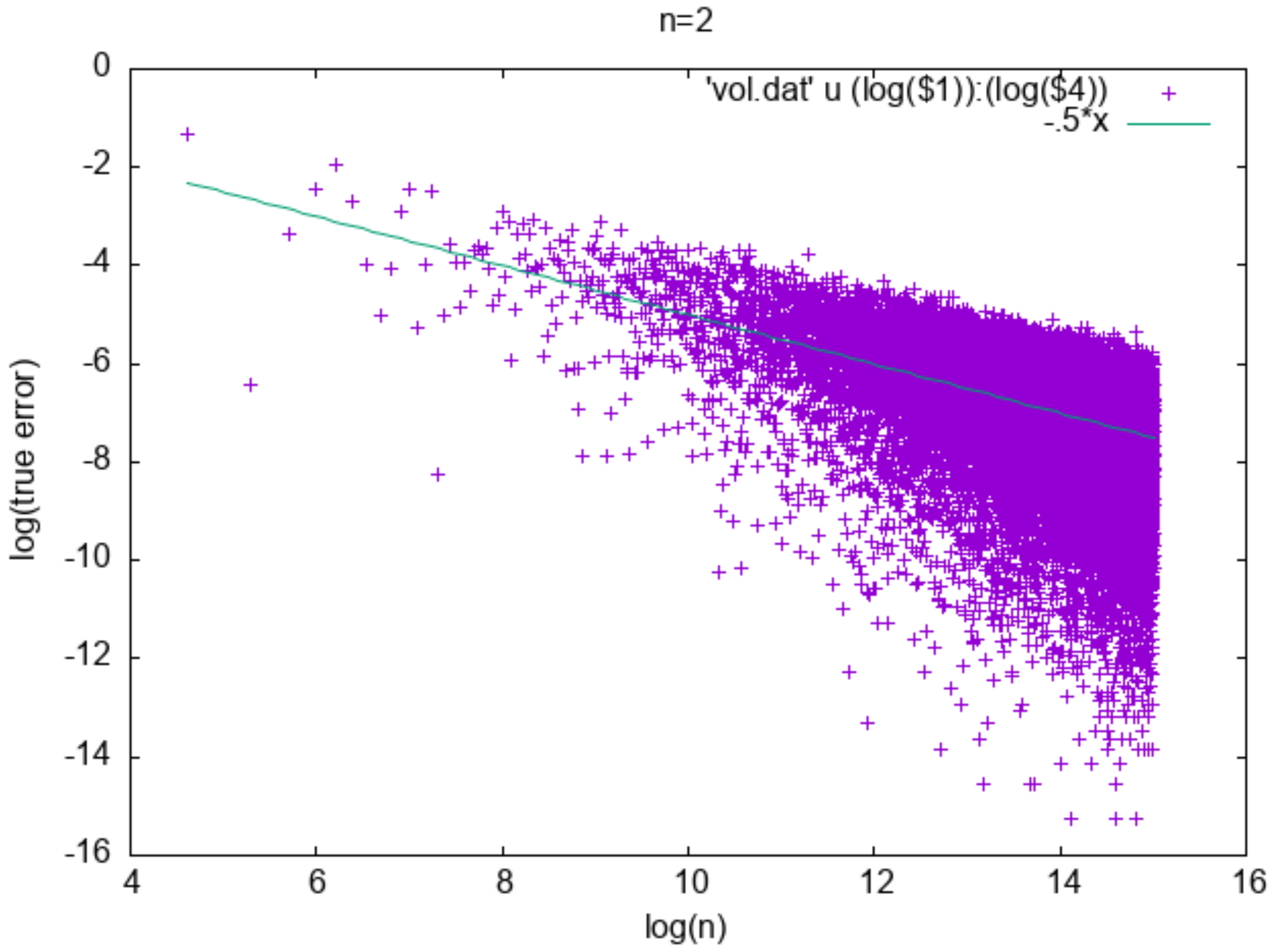
10000 punti - runs non correlati per diversi n (dimensione)

```
n=2:
area cerchio (con r=1) numerico e esatto:   3.14256001 vs. 3.14159274
```



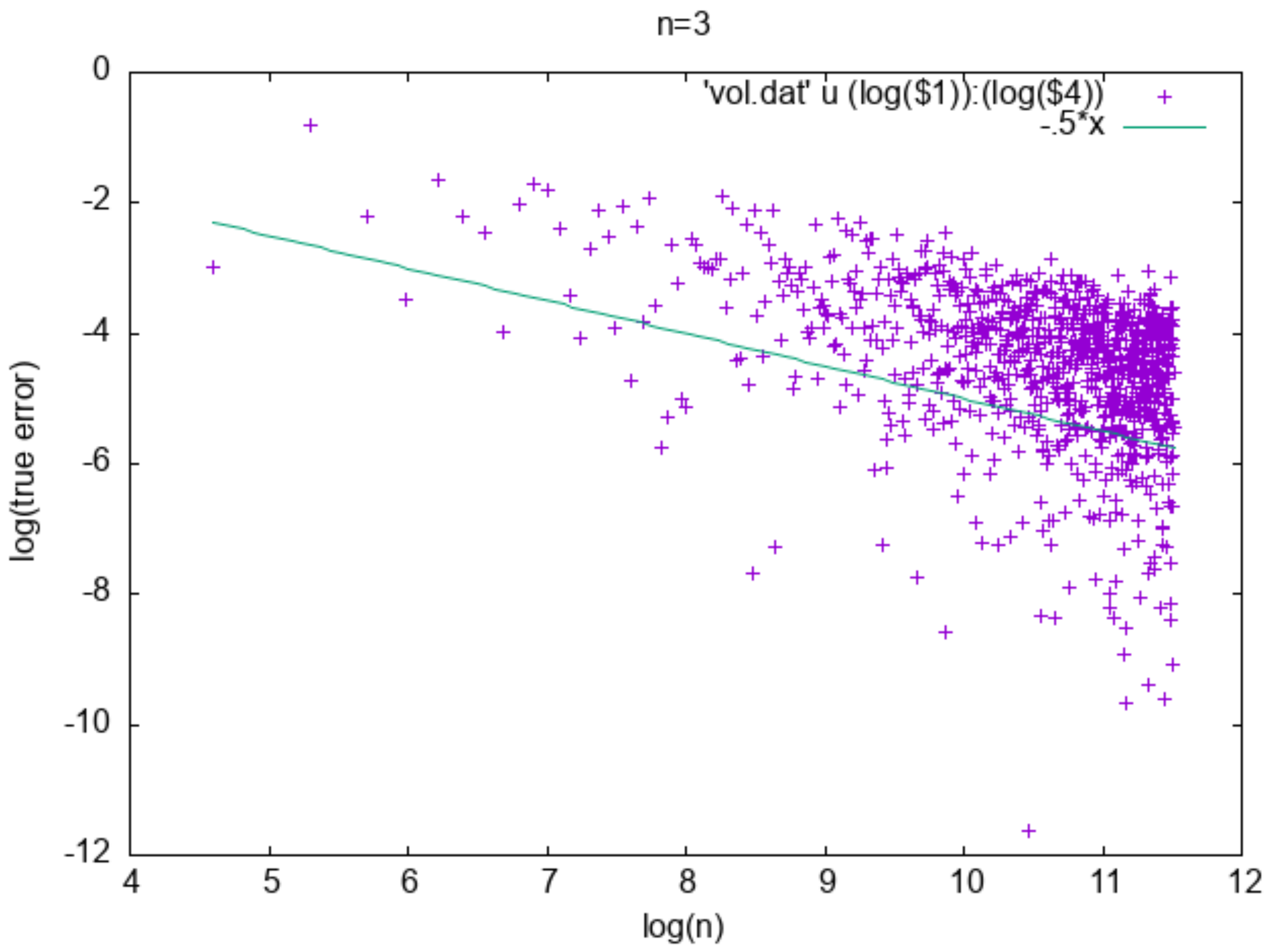
100000 punti - runs non correlati per diversi n (dimensione)

```
n=2:
area cerchio (con r=1) numerico e esatto:   3.14256001 vs. 3.14159274
```



100000 punti - runs non correlati per diversi n (dimensione)

```
n=3
volume sfera (con r=1) numerico e esatto:   4.19895983 vs 4.18879080
```



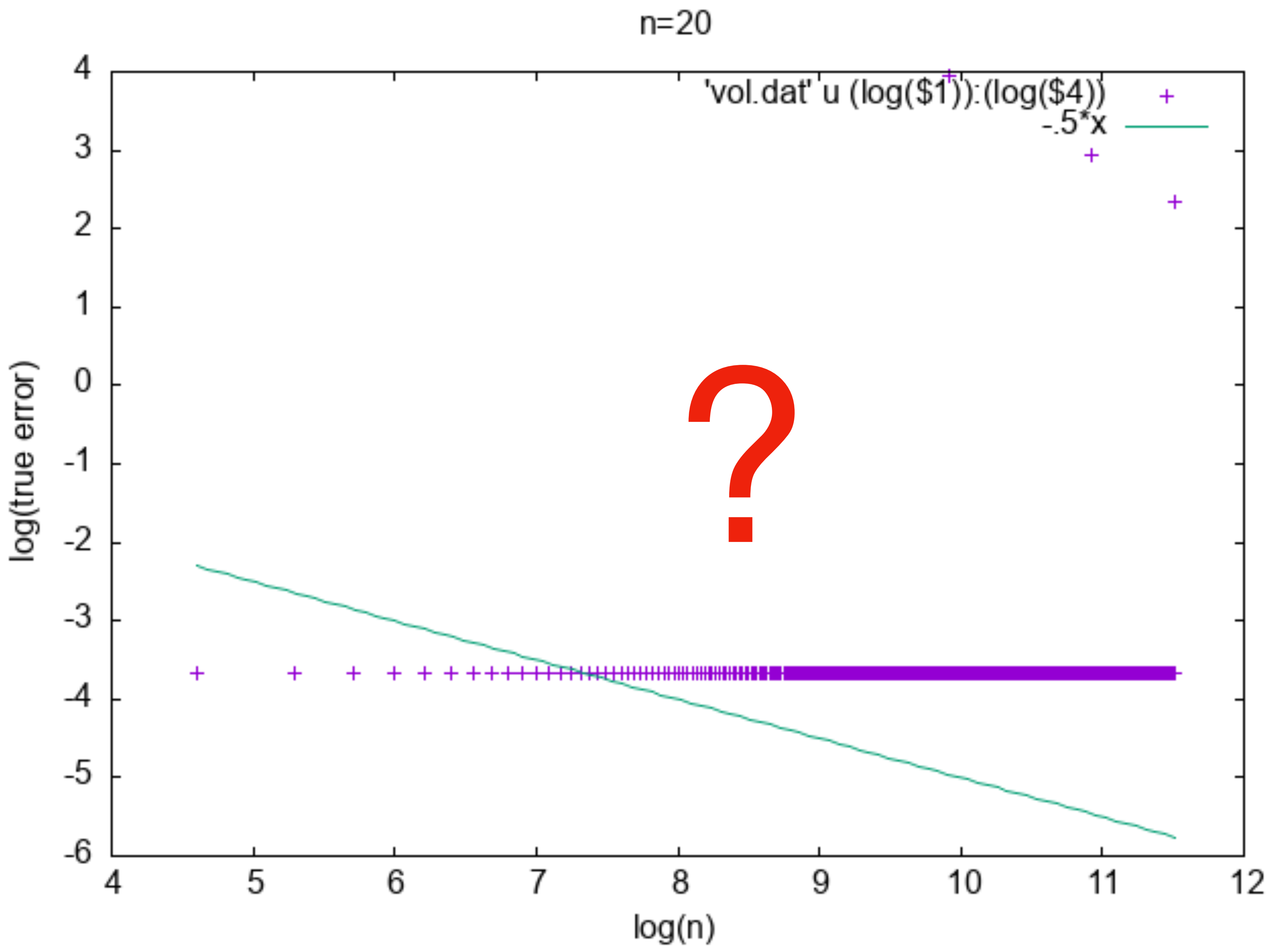
100000 punti - runs non correlati per diversi n (dimensione)

dim	V calc	V vero
10	2.82624006	2.55016422
12	1.43359995	1.33526301
15	0.327679992	0.381443381
16	0.655359983	0.235330686

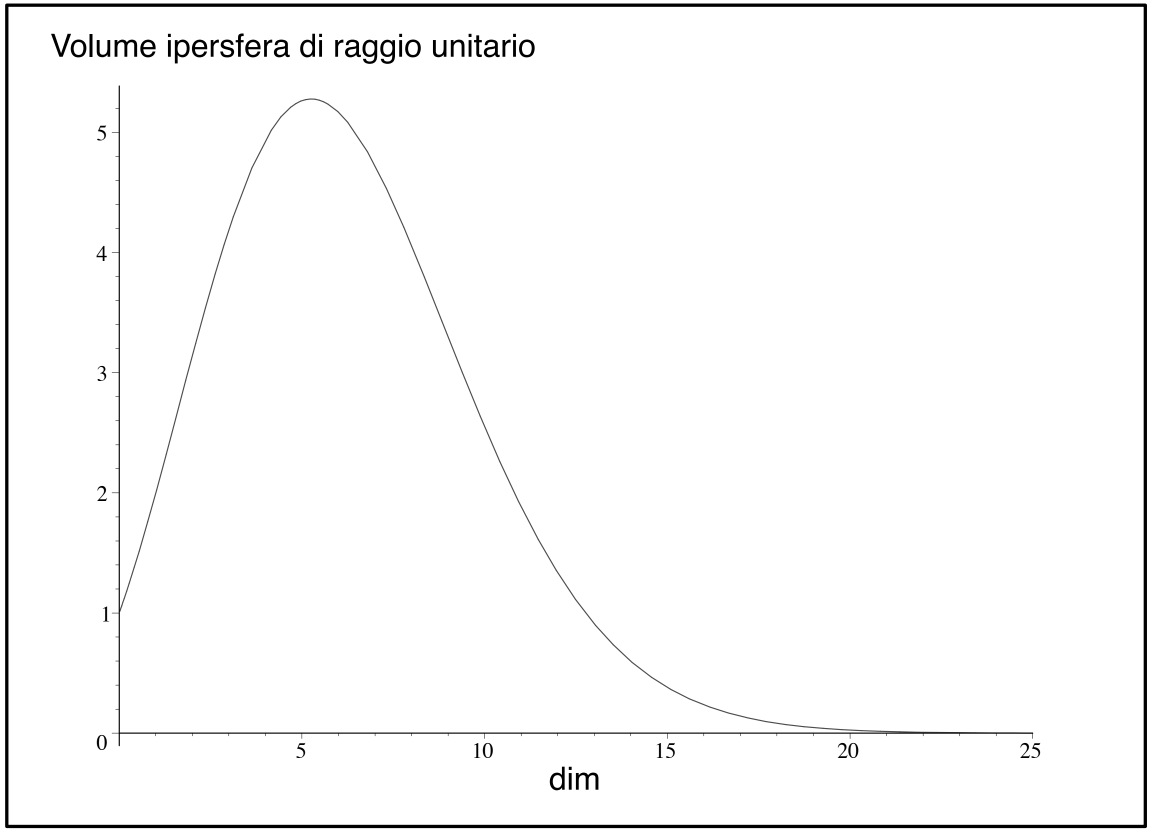
perché il risultato peggiora con il crescere della dimensione?

100000 punti - runs non correlati per diversi n (dimensione)

```
volume sfera numerico e esatto:    0.00000000        2.58068983E-02
```



il volume dell'ipersfera ha un andamento non monotono con la dimensione



crescendo con la dimensione, gli "spigoli vuoti" dell'ipercubo dov'è iscritta l'ipersfera pesano molto!
quindi di fatto si rifiutano molti dei punti generati
e il metodo accettazione-rifiuto diventa molto inefficiente!

Efficiency in importance sampling Monte Carlo method for integration

2. **Monte Carlo method:**
generic sample mean and importance sampling

(a) Write a code to compute the numerical estimate F_n of $I = \int_0^1 e^{-x^2} dx = \frac{\sqrt{\pi}}{2} erf(1) \approx 0.746824$ with the MC *sample mean* method using a set $\{x_i\}$ of n random points uniformly distributed in [0,1]:

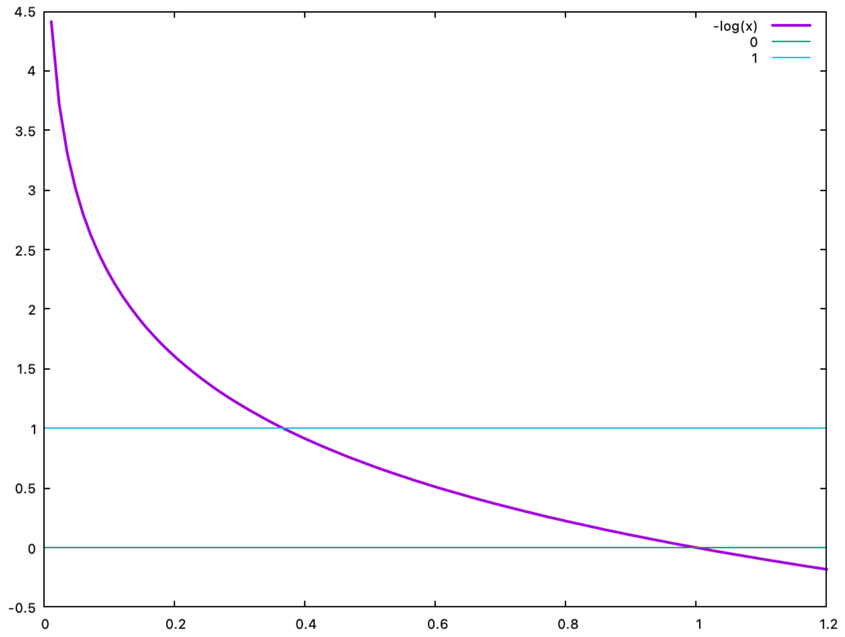
$$F_n = \frac{1}{n} \sum_{i=1}^{n} f(x_i)$$

(b) Write a code (a different one, or, better, a unique code with an option) to compute F_n using the *importance sampling* with a set $\{x_i\}$ of points generated according to the distribution $p(x) = Ae^{-x}$ (*Notice that* erf *is an intrinsic fortran function; useful to compare the numerical result with the true value*). Remind that in the *importance sampling* approach:

$$\int_a^b f(x)dx = \left\langle \frac{f(x)}{p(x)} \right\rangle \int_a^b p(x)dx \approx \frac{1}{n} \sum_{i=1}^{n} \frac{f(x_i)}{p(x_i)} \int_a^b p(x)dx = F_n$$

with $p(x)$ which approximates the behaviour of $f(x)$, and the average is calculated over the random points $\{x_i\}$ with distribution $p(x)$.

Punto di attenzione:
servono punti con distribuzione esponenziale tra 0 e 1 :
è possibile limitare il numero random
con distribuzione uniforme in ingresso
alla subroutine expdev(rnd)



exponential variate $0 \le rnd < 1 \Rightarrow x = -\ln(rnd)$ results in $x > 0$

hence $0 < x < 1 \Rightarrow \frac{1}{e} < rnd < 1$

but since $0 \le rnd < 1 => rnd' = \frac{1}{e} + \left(1 - \frac{1}{e}\right) * rnd$ results in $\frac{1}{e} \le rnd' < 1$

Efficiency and correlations in generating gaussian deviates with Metropolis Monte Carlo method

Random numbers with gaussian distribution: Metropolis algorithm

Here we use the Metropolis algorithm to generate points with the distribution $P(x) = e^{-x^2/(2\sigma^2)}$. The algorithm is implemented for instance in the code `gauss_metropolis.f90`. We consider $\sigma = 1$, but the suggestion is to write the code for a generic σ.

The Metropolis algorithm

$p(x)$ is given.

If the "walker" is at position x_i and we wish to generate x_{i+1}, we can implement this choice of $T(x_i \to x_j)$ by the following steps:

1. Choose a trial position $x_{\text{trial}} = x_i + \delta_i$, where δ_i is a random number in the interval $[-\delta, \delta]$.
2. Calculate $w = p(x_{\text{trial}})/p(x_i)$.
3. If $w \geq 1$, accept the change and let $x_{i+1} = x_{\text{trial}}$.
   else
4. If $w < 1$, generate a random number r.
5. If $r \leq w$, accept the change and let $x_{i+1} = x_{\text{trial}}$.
6. If the trial change is not accepted, then let $x_{i+1} = x_i$.

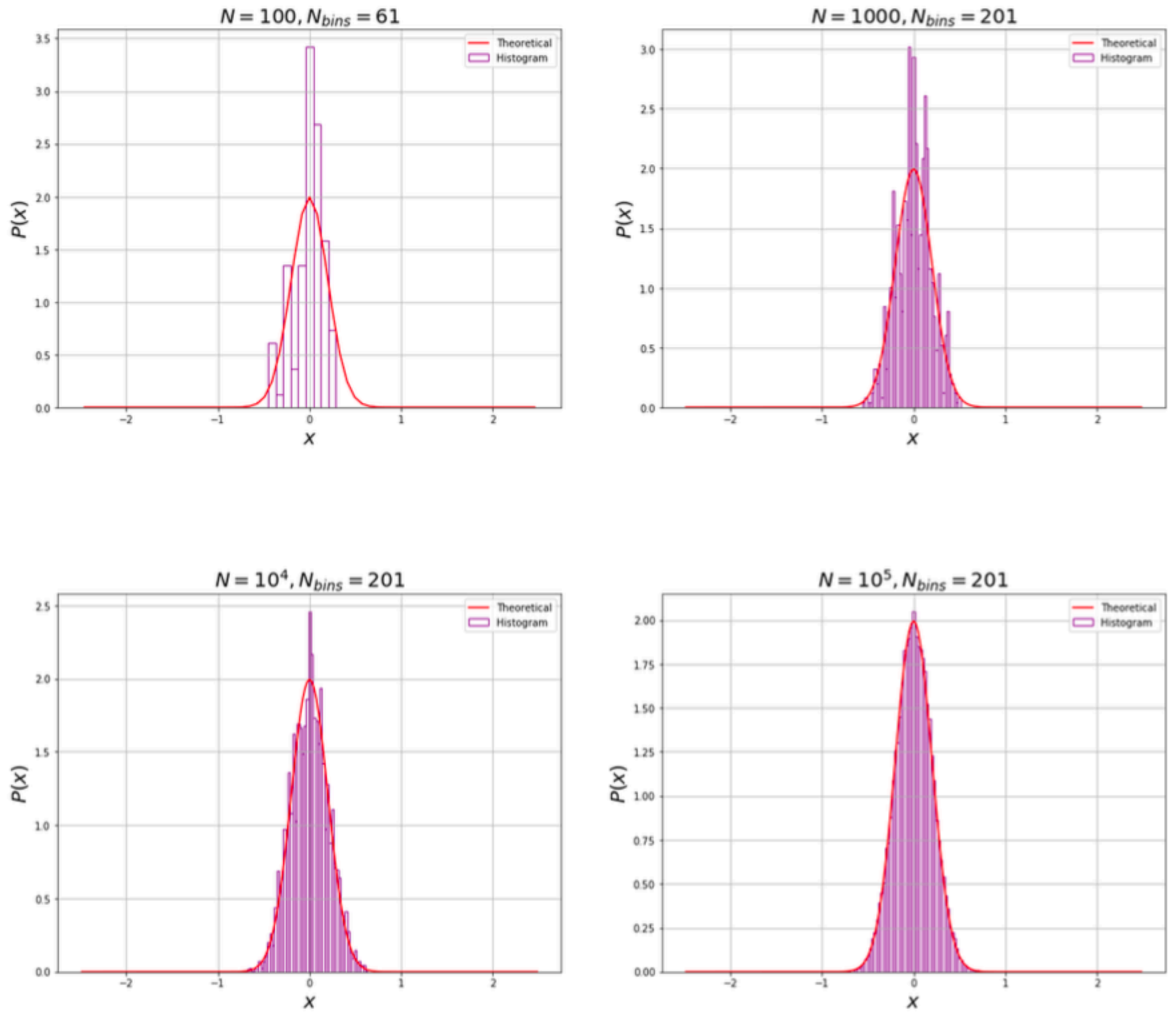
The algorithm from 1) to 6) has to be repeated until the distribution $p(x)$ of the points $\{x_i\}$ is reached.

Some issues:

- how to choose x_0 ?
  Convenient to start from a maximum
- how to choose δ ?
  (if too small, most trial steps accepted, but the walker moves too slowly; if too large, only a few trial steps are accepted...)
  A good compromise is a choice accepting from ~ 1/3 to ~1/2 of the trial steps
- equilibration is necessary (how many steps?)
  A possible criterion based on error estimate

(a)

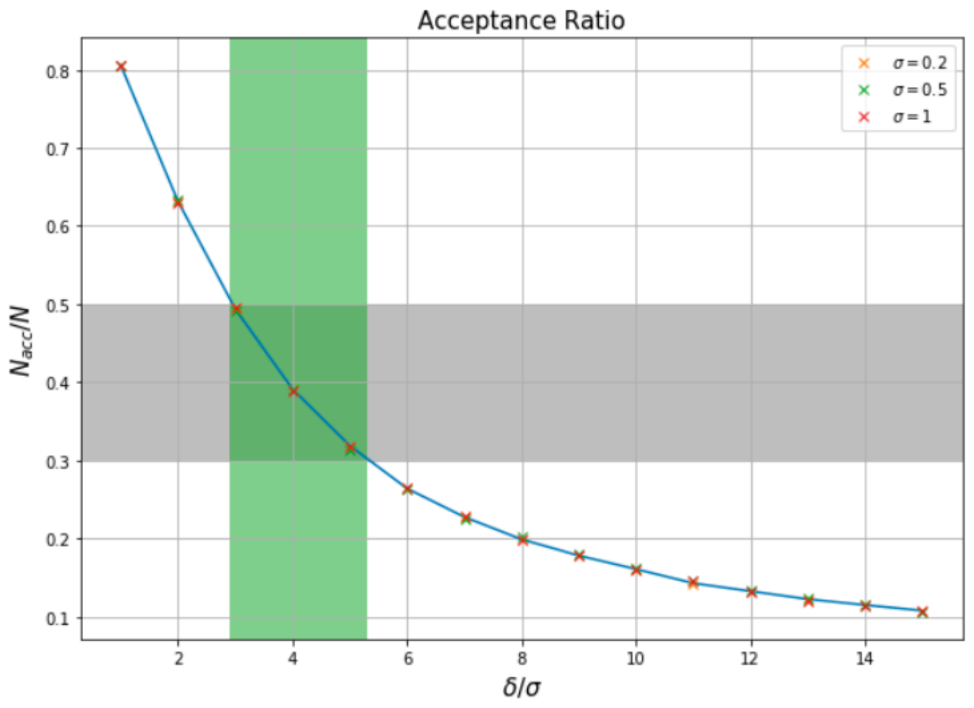
Si considera $x_0 = 0$, $\sigma = 0.2$ e $\delta = 5\sigma$



Per $N \sim 10^4, 10^5$ si ha un un buon accordo fra la distribuzione teorica e quella ottenuta numericamente con l'algoritmo Metropolis

(b)

Si fissa $N = 10^5$ e si studia l'acceptance ratio al variare di δ, fissato σ, ovvero in funzione del rapporto δ/σ

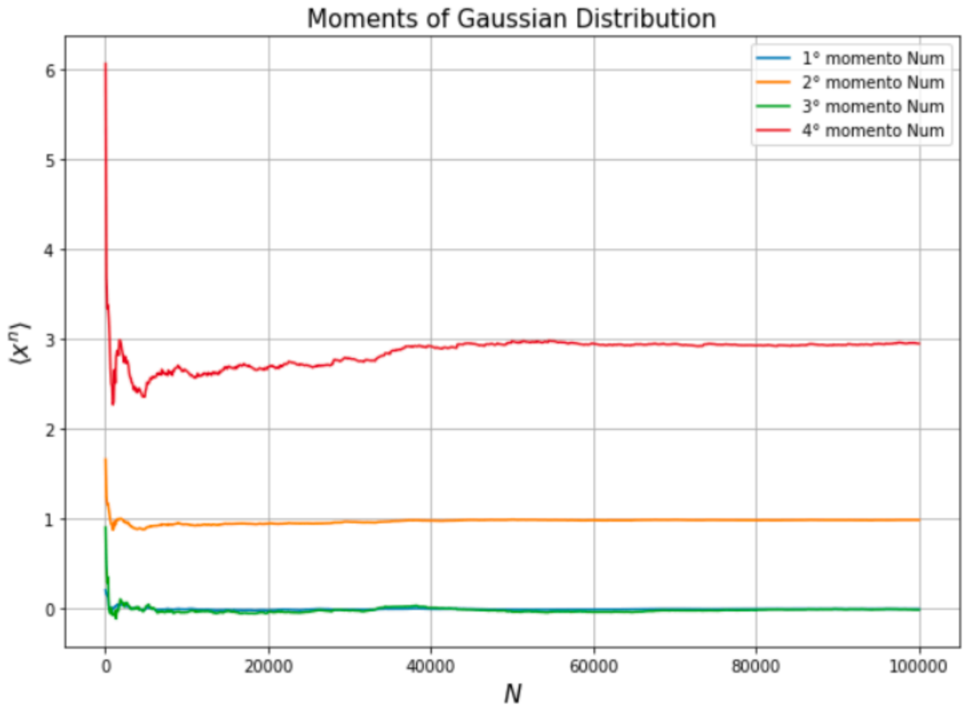


Per una distribuzione gaussiana con media μ e varianza σ si ha la seguente relazione per i momenti

$$\langle x^n \rangle = \begin{cases} (n-1)!! \cdot \sigma^n, & n \text{ even} \\ 0, & n \text{ odd} \end{cases} \tag{2}$$

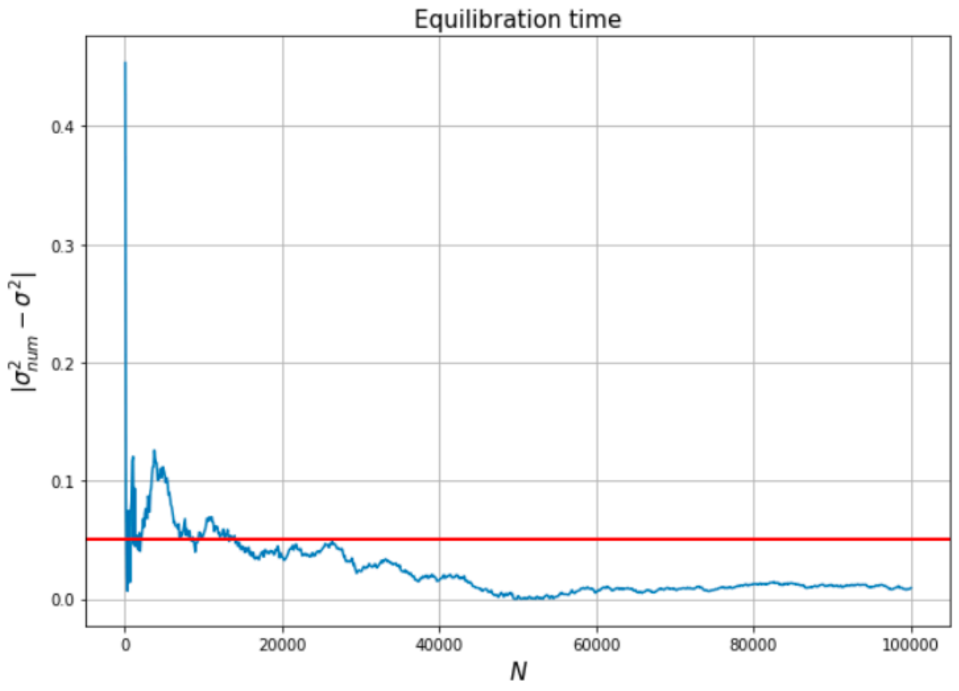
Si fissa $\mu = 0$, $\sigma = 1$ e $\delta = 5\sigma$ e si studiano i primi quattro momenti della distribuzione, dalla formula precedente si ottiene

$$\langle x \rangle = 0 \qquad \langle x^2 \rangle = 1 \qquad \langle x^3 \rangle = 0 \qquad \langle x^4 \rangle = 3 \tag{3}$$



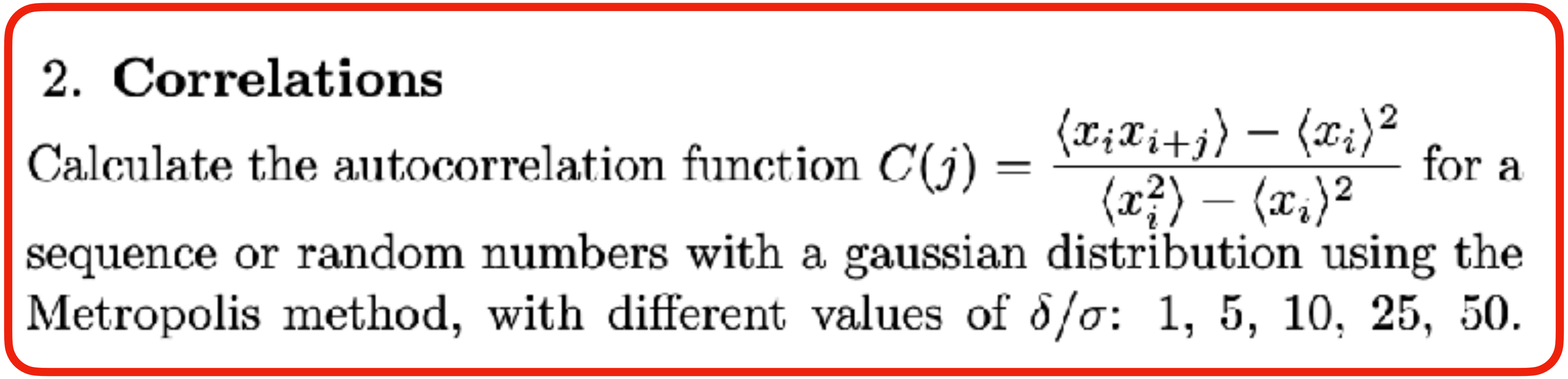
NOTA:
per momenti di ordine superiore convergenza più lenta!

In particolare si studia l'andamento della varianza stimata numericamente rispetto al valore teorico che può essere utilizzato per stimare l' equilibration time



Dal grafico di osserva che a partire da $N^* = 3 \cdot 10^4$ l'errore fra varianza teorica e numerica risulta minore del 5%, si può stimare dunque con N^* l'equilibration time

Correlations - Metropolis algorithm



2. Correlations

Calculate the autocorrelation function $C(j) = \dfrac{\langle x_i x_{i+j}\rangle - \langle x_i\rangle^2}{\langle x_i^2\rangle - \langle x_i\rangle^2}$ for a sequence or random numbers with a gaussian distribution using the Metropolis method, with different values of δ/σ: 1, 5, 10, 25, 50.

In gauss_metropolis.f90 , δ is defined as the full amplitude of the possible displacement:

```
xp = x + delta * (rnd-0.5_dp)
```

Correlations - Metropolis algorithm

Random number sequence generated with the Metropolis algorithm and different values of δ/σ

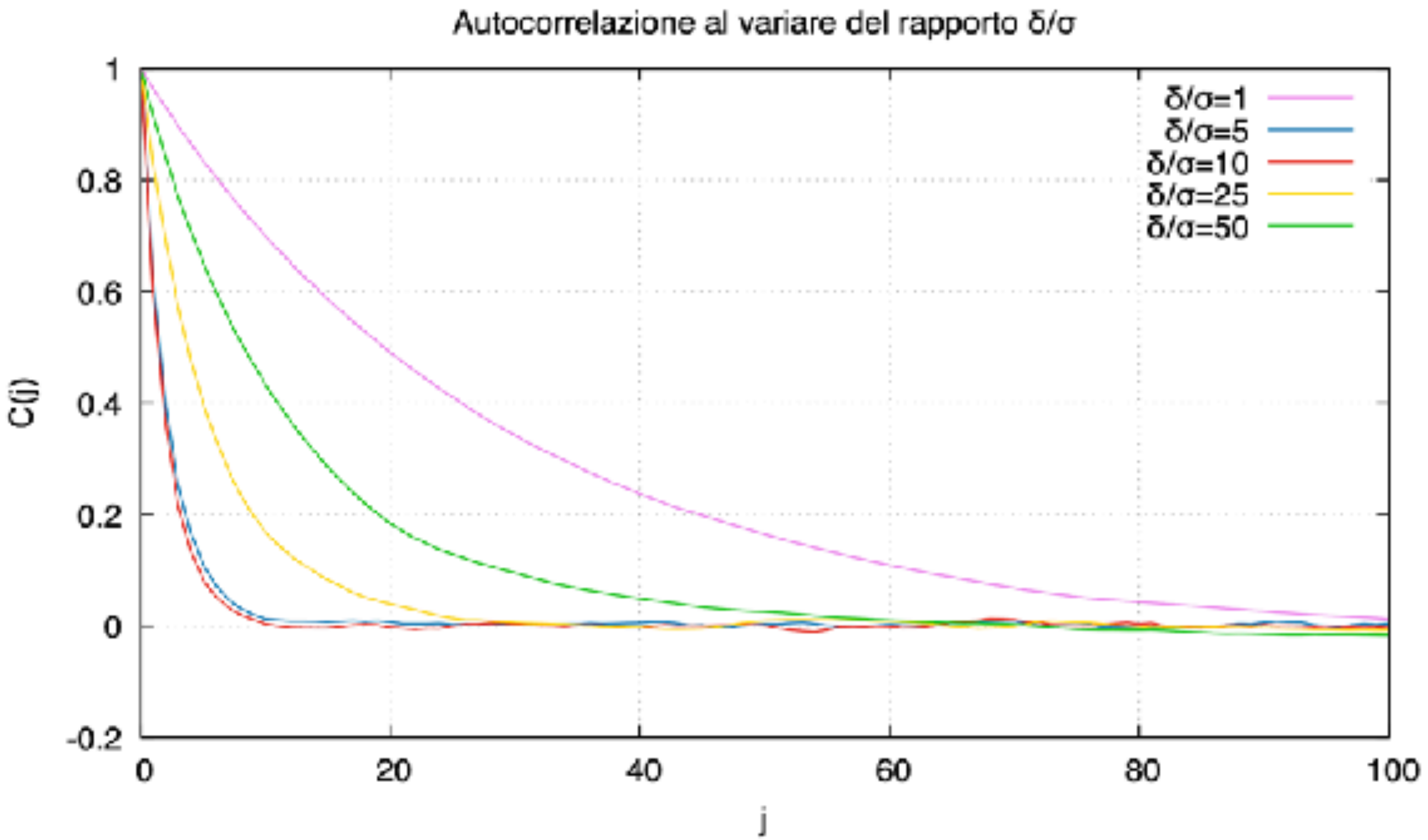
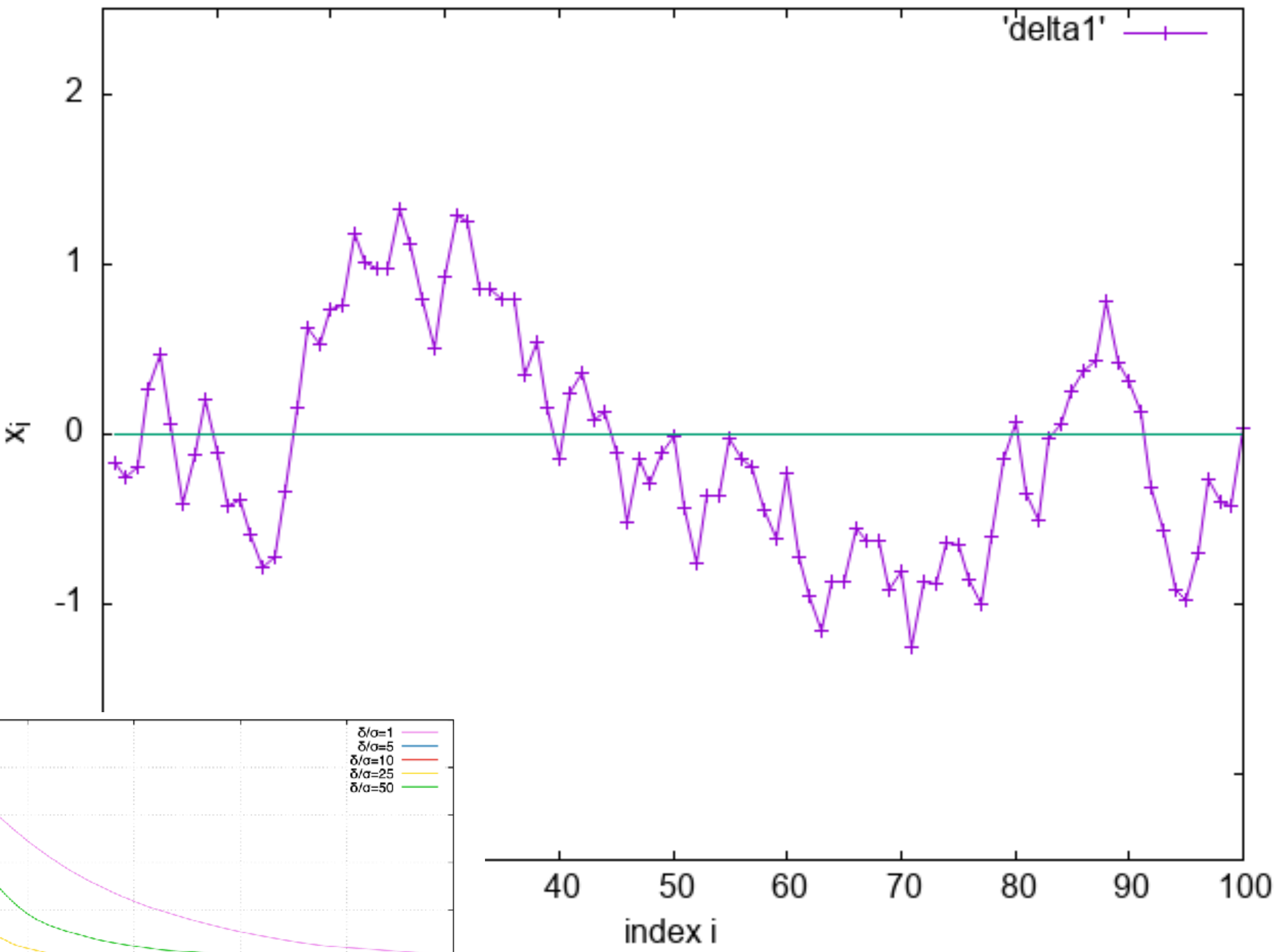
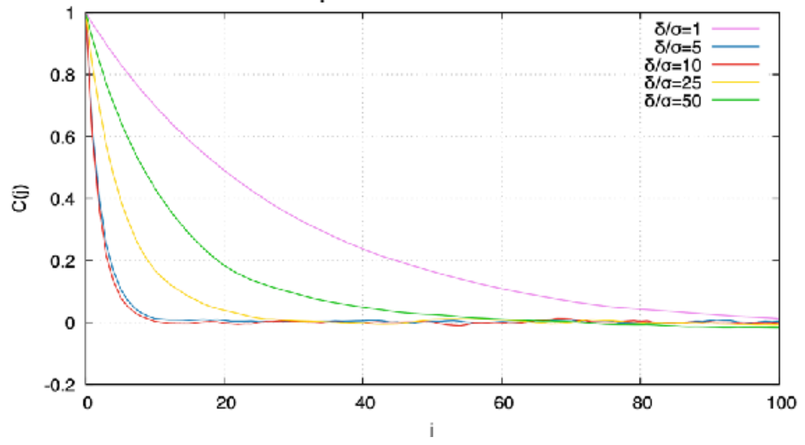


Figura 11: Andamento della funzione di autocorrelazione tra i punti generati con l'algoritmo Metropolis al variare di alcuni valori del parametro δ/σ

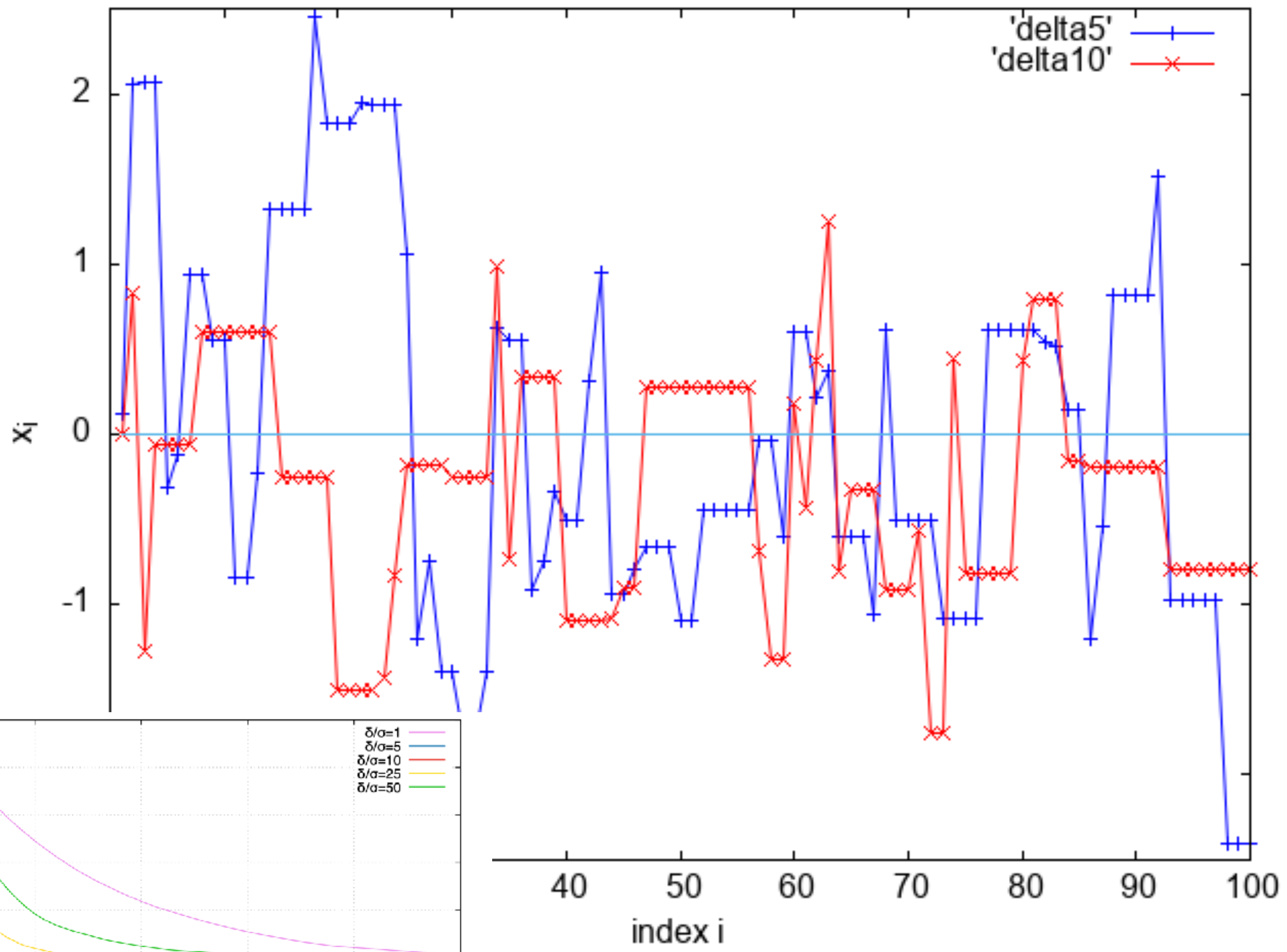
for values of the parameter δ/σ that are too low (< 5) or too high (> 10) the autocorrelation function decays very slowly: to effectively generate random numbers that are not correlated with each other it is therefore necessary to choose a ratio δ/σ such that 5 ≤ δ/σ ≤ 10, which corresponds to the acceptance ratio range between ≈ 1/3 and ≈ 1/3

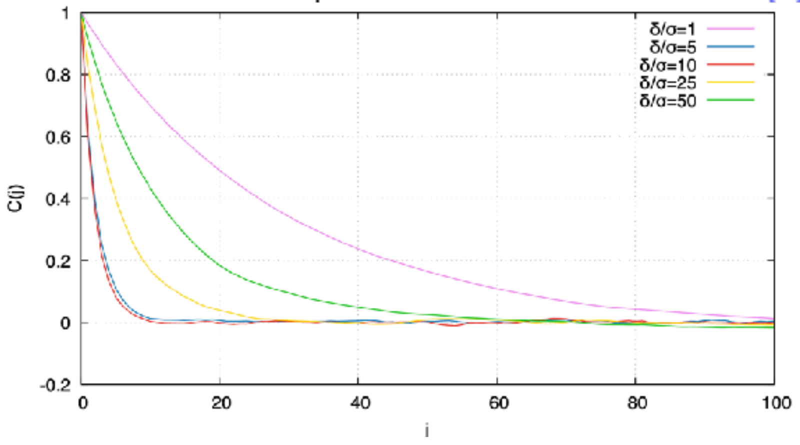


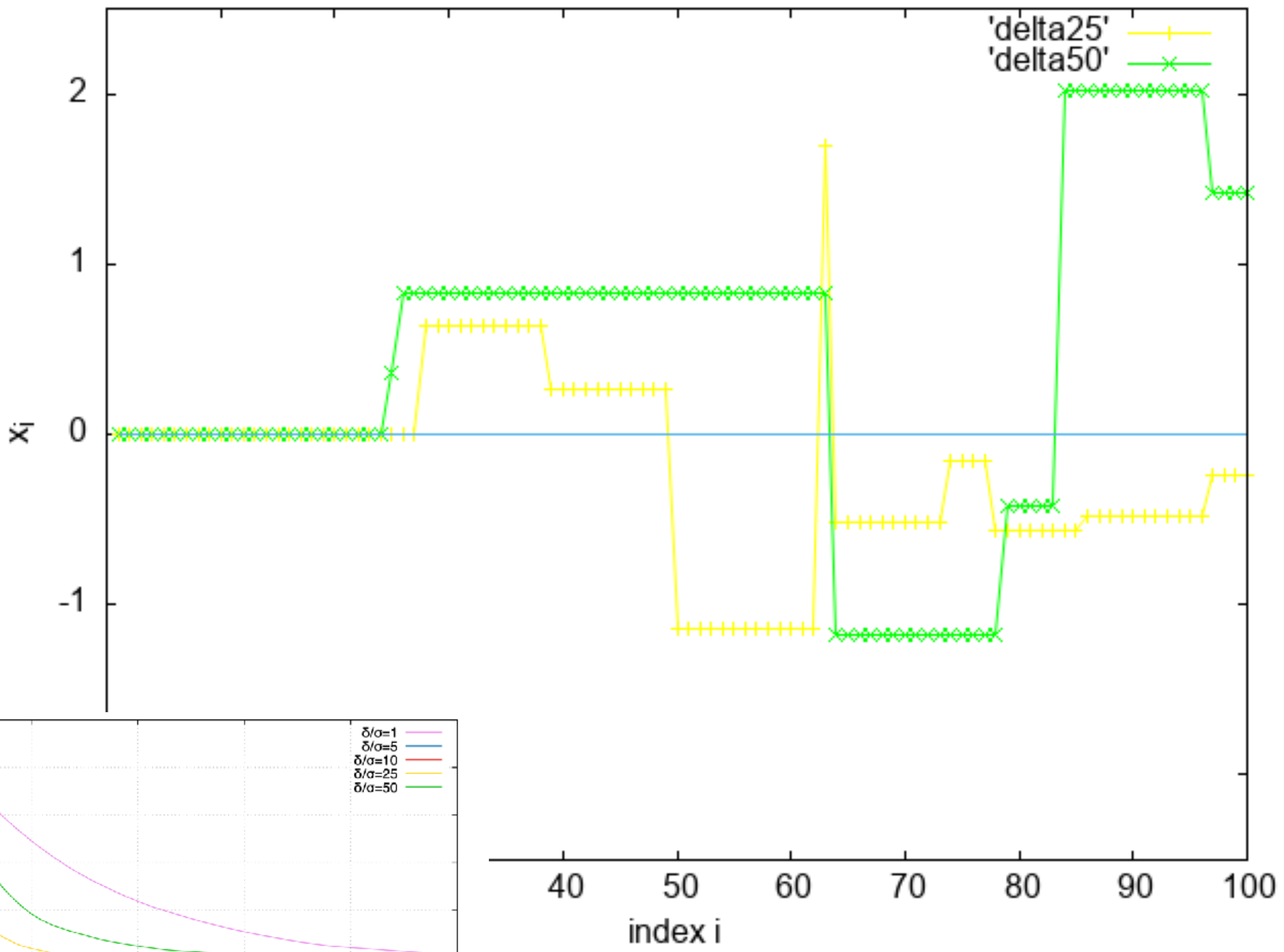
'delta1'
2
1
0
-1
x_i
40
50
60
70
80
90
100
index i

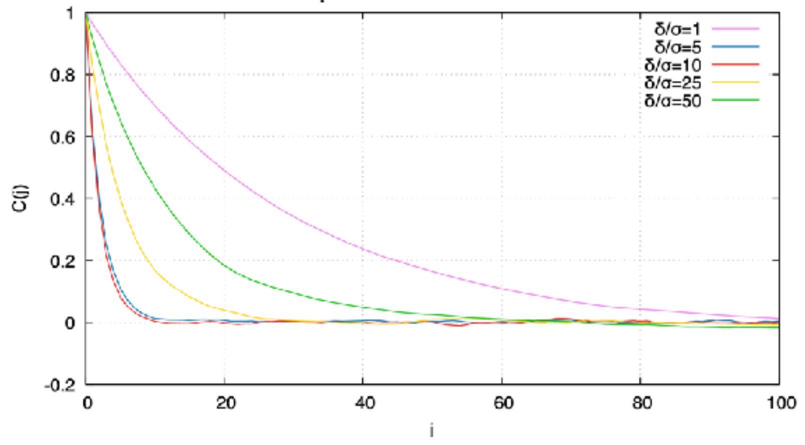


δ/σ=1
δ/σ=5
δ/σ=10
δ/σ=25
δ/σ=50
C(j)
1
0.8
0.6
0.4
0.2
0
-0.2
0
20
40
60
80
100
i


'delta5'
'delta10'
x_i
2
1
0
-1
40
50
60
70
80
90
100
index i


δ/σ=1
δ/σ=5
δ/σ=10
δ/σ=25
δ/σ=50
C(i)
1
0.8
0.6
0.4
0.2
0
-0.2
0
20
40
60
80
100
i


'delta25'
'delta50'
2
1
0
-1
x_i
40
50
60
70
80
90
100
index i


δ/σ=1
δ/σ=5
δ/σ=10
δ/σ=25
δ/σ=50
C(j)
1
0.8
0.6
0.4
0.2
0
-0.2
0
20
40
60
80
100
i