Computer simulations in statistical physics
Homework 2: data analysis

Code of statistical analysis program

Analysis of data sets

- set 1
- set 2
- set 3
- set 4
- set 5
- set 6
- set 7
- set 8
- set 9

Code of statistical analysis program

```
#define PROGNAME "stats"
#define VERSION "1.4"
#define DATE  "06.11.2006"
#define AUTHOR "Nils Bluemer"

/* program stats (successor of statnew), computes average, error etc. */
/* expects input on stdin in 1st column */
/* compile with cc -lm -o stats stats.c */

#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#define BUFSIZE 100
#define NUMHIST 40
#define MAXDATA 100001
#define MAXKORR 1000
#define MIN(a,b) (a<b?a:b)
```

```
void histogram ()
{
  double data[MAXDATA];
  double hist[NUMHIST];
  char buf[BUFSIZE];
  int i,n,numdata;
  double min, max, x;

  numdata=0;
  do {
    if (fgets(buf,BUFSIZE,stdin)!=NULL){
      numdata++;
      sscanf(buf,"%lf",&data[numdata]);
/*        printf("Nr %d: %f\n",nr,data[numdata]); */
    }
  } while (feof(stdin)==0);
/*   printf ("stat/histogram: read %d lines\n",numdata); */
  if (numdata>MAXDATA) error ("too many data points");
  if (numdata<2) error ("not enough data");
  min = data[1];
  max = data[1];
```

```
  for (i=2;i<=numdata;i++){
    if (data[i]<min) min=data[i];
    if (data[i]>max) max = data[i];
  }
/*    printf ("min: %lf, max: %lf\n",min,max); */
  for (i=0;i<NUMHIST;i++) hist[i]==0.0;
  for (i=1;i<=numdata;i++){
    x = NUMHIST/(max-min)*(data[i]-min)*0.999999;
    hist[(int)floor(x)] += 1.0*NUMHIST/((max-min)*numdata);
/*        printf("x: %lf\n",x); */
  }
  for (i=0;i<NUMHIST;i++)
    printf ("%8.6lf   %8.6lf\n",(i+0.5)/NUMHIST*(max-min)+min,
hist[i]);

}
```

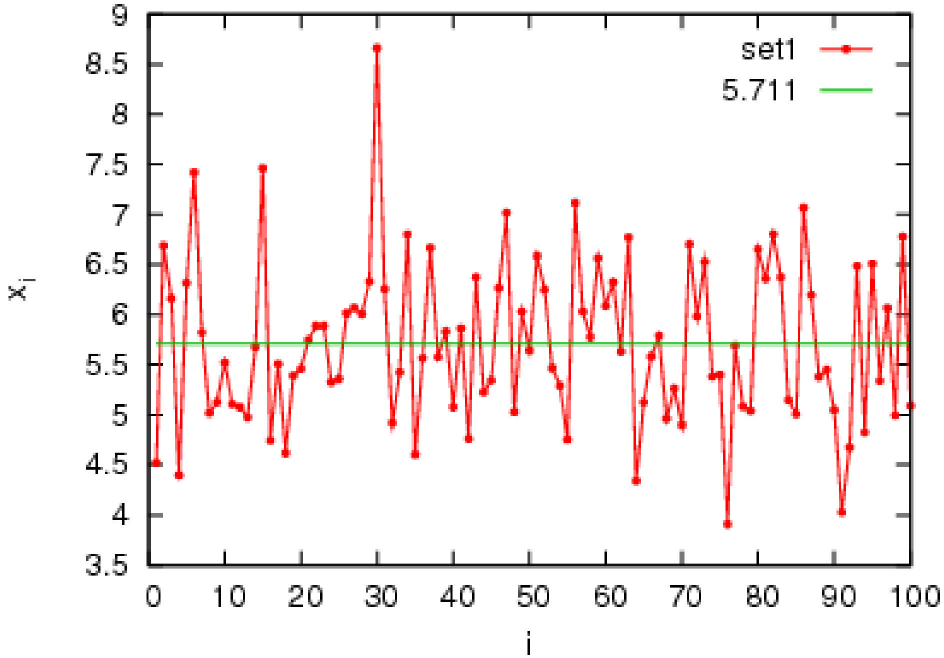
```
void average(char form){
  double data[MAXDATA];
  double korr[MAXDATA];
  char buf[BUFSIZE];
  int i,n,numdata,numkorr;
  double sum, sqsum,nsum,av, var,korrtime,trans;

  numdata=0;
  sum=0.0;
  sqsum=0.0;
  nsum=0;
  do {
    if (fgets(buf,BUFSIZE,stdin)!=NULL){
      numdata++;
      sscanf(buf,"%lf",&data[numdata]);
      sum +=data[numdata];
      sqsum += data[numdata]*data[numdata];
      nsum +=numdata*data[numdata];
    }
  } while (feof(stdin)==0);
```

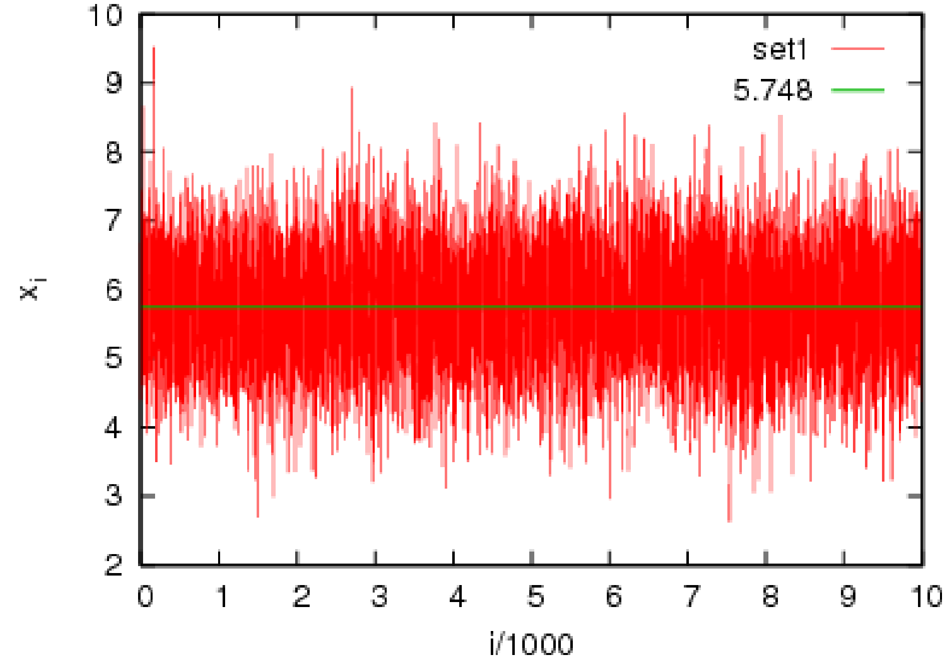
```
if (numdata>MAXDATA) error ("too many data points");
if (numdata<2) error ("not enough data");
av=sum/numdata;
var=(sqsum-numdata*av*av)/(numdata-1);
/* compute transient: slope of best linear fit on data[n] */
/* a = (<xy>-<x><y>)/(<x^2>-<x>^2), here: x=numdata,
y=data[numdata] */
trans=(nsum/numdata-0.5*(numdata+1)*av)/
  ((numdata+.5)*(numdata+1)/3-0.25*(numdata+1)*(numdata+1));
if (form=='l')
  printf("Average:  %10.8g   variance:  %10.8g   error:
%10.8g\n",av,var,sqrt(var/numdata));

numkorr=numdata/3;

korr[0]=1.0;
if (form=='c'){
  printf("# Autocorrelation function:  (i,c(i))\n");
    printf ("%4d %10lf\n",0,korr[0]);
}
```

```
for (i=1;i<=numkorr;i++){
  korr[i]=0.0;
  for (n=1;n<=numdata-i;n++)
    korr[i]+=(data[n]-av)*(data[n+i]-av);
  korr[i]=(korr[i]/(var*(numdata-i))+1.0/numdata)/
    ((1-1.0/numdata)*(1-1.0/numdata));
  if (form=='c')
    printf ("%4d %10lf\n",i,korr[i]);
}
korrtime=1;
n =1;
while ((korr[n]>0)&&(n<=numkorr)){
  korrtime += 2*korr[n];
  n++;
}
if (form=='l')
  printf ("Korrelation time:  %10.8g   corrected error:  %10.8g
transient:  %10.8g\n",
   korrtime, sqrt(var/(numdata-1))*sqrt(korrtime),trans);
```

Set 1

Trace and averages

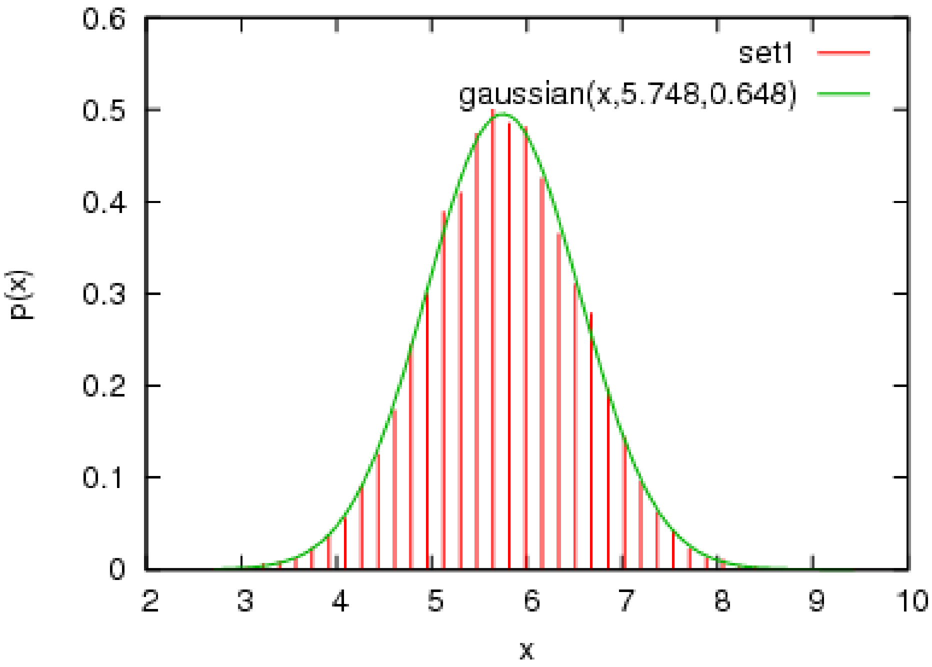


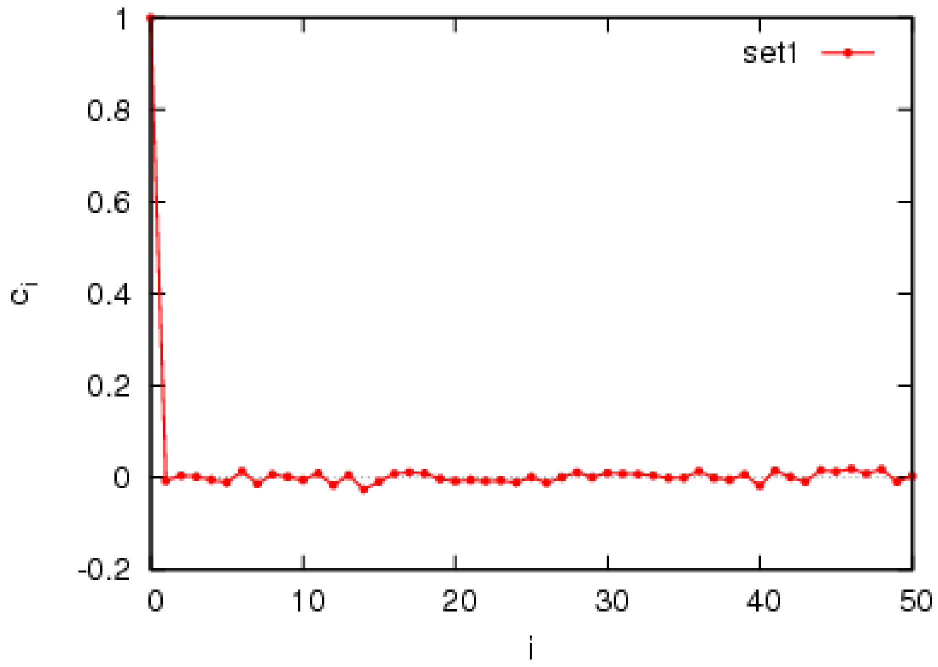


Estimates of mean / initial error analysis

- $\langle x \rangle \approx 5.748 \pm 0.008$ `(naive estimate)`
- `no transient`
- `autocorrelation?`

Histogram, autocorrelation function, full error estimate

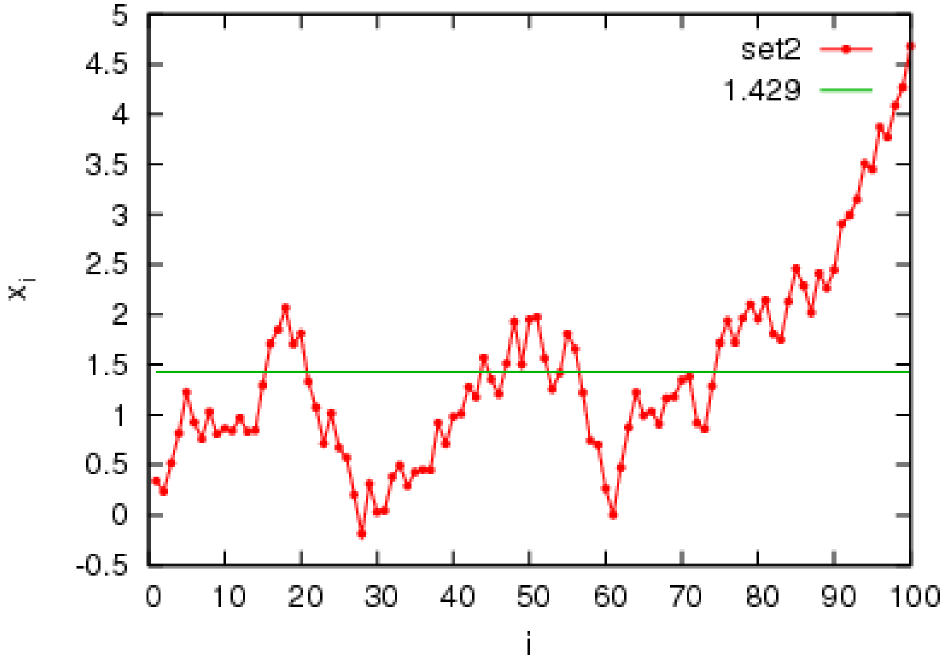


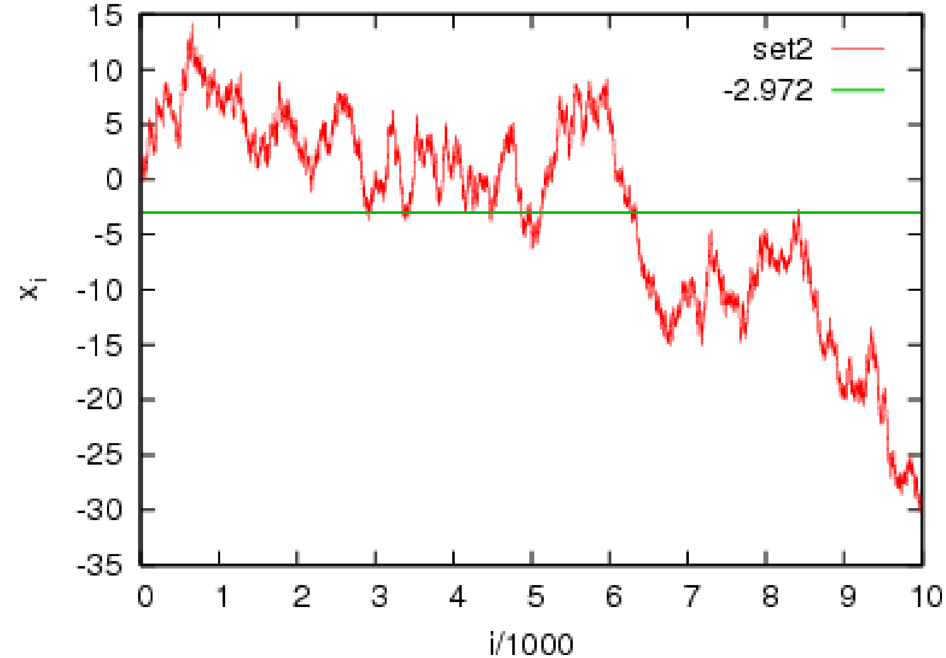


- `gaussian distribution of ''measurements'' - width` $\sqrt{0.648}$
- `no autocorrelation` $(\tau = 1.0)$
- `final error estimate:` $\langle x \rangle \approx 5.748 \pm 0.008$
- `true distribution: gaussian, mean 5.740, variance 0.650`

Set 2

Trace and averages

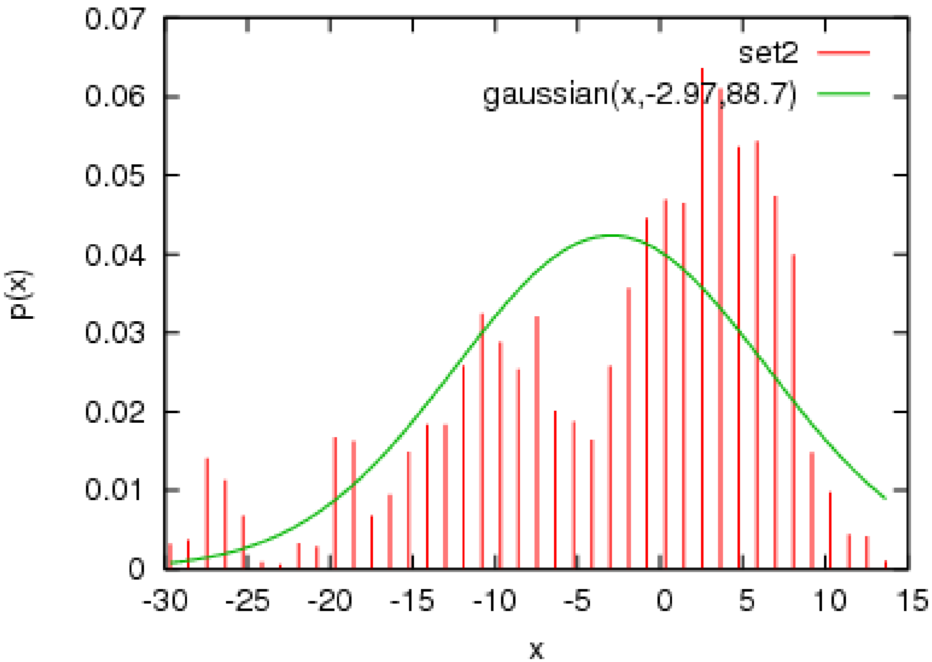


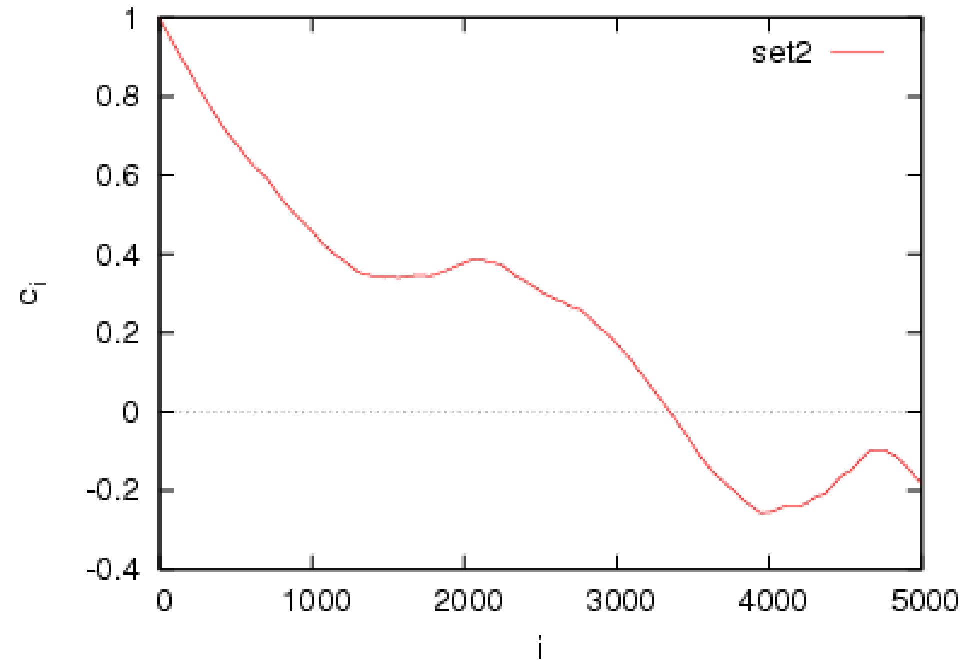


Estimates of mean / initial error analysis

- $\langle x \rangle \approx -2.972 \pm 0.094$ `(naive estimate)`
- `transient?`
- `long autocorrelation: of order of run length!`

Histogram, autocorrelation function, full error estimate



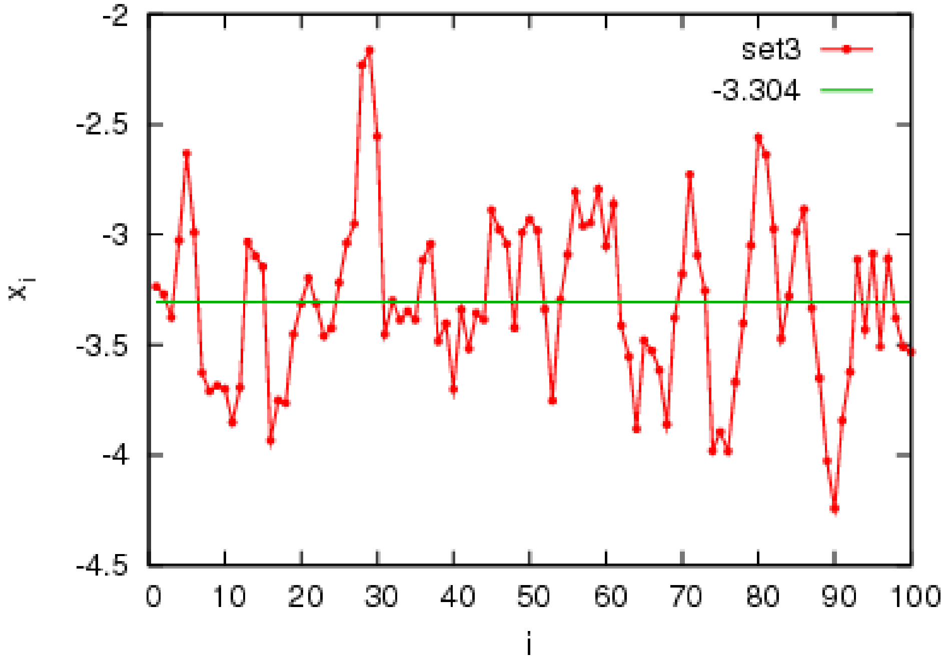


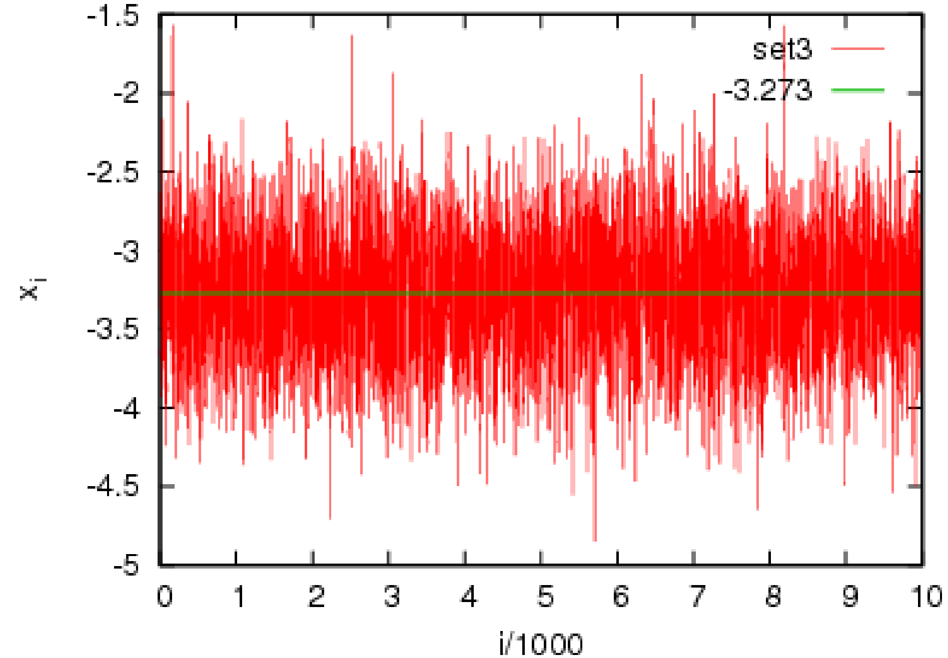
- nongaussian distribution of ‘‘measurements’’
- strong autocorrelation ($\tau = 2797$ for $N = 10000$)
- final error estimate: $\langle x \rangle \approx -2.97 \pm 4.98$

- true distribution: gaussian (from random walk), mean 0, non-uniform variance $\sigma(X_k) = k$

Set 3

Trace and averages

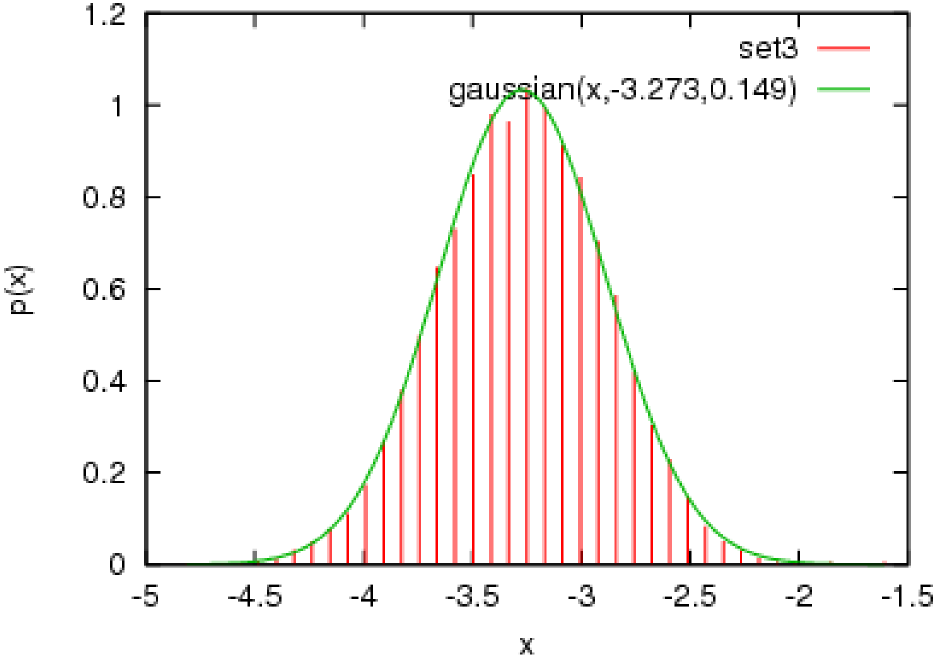


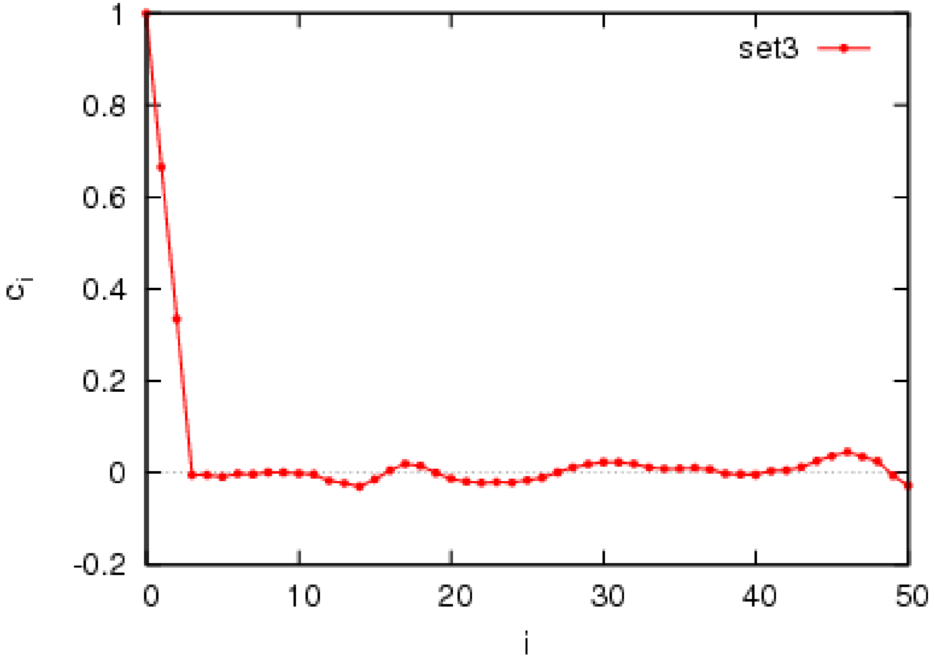


Estimates of mean / initial error analysis

- $\langle x \rangle \approx -3.273 \pm 0.004$ `(naive estimate)`
- `no transient`
- `short-time autocorrelation?`

Histogram, autocorrelation function, full error estimate

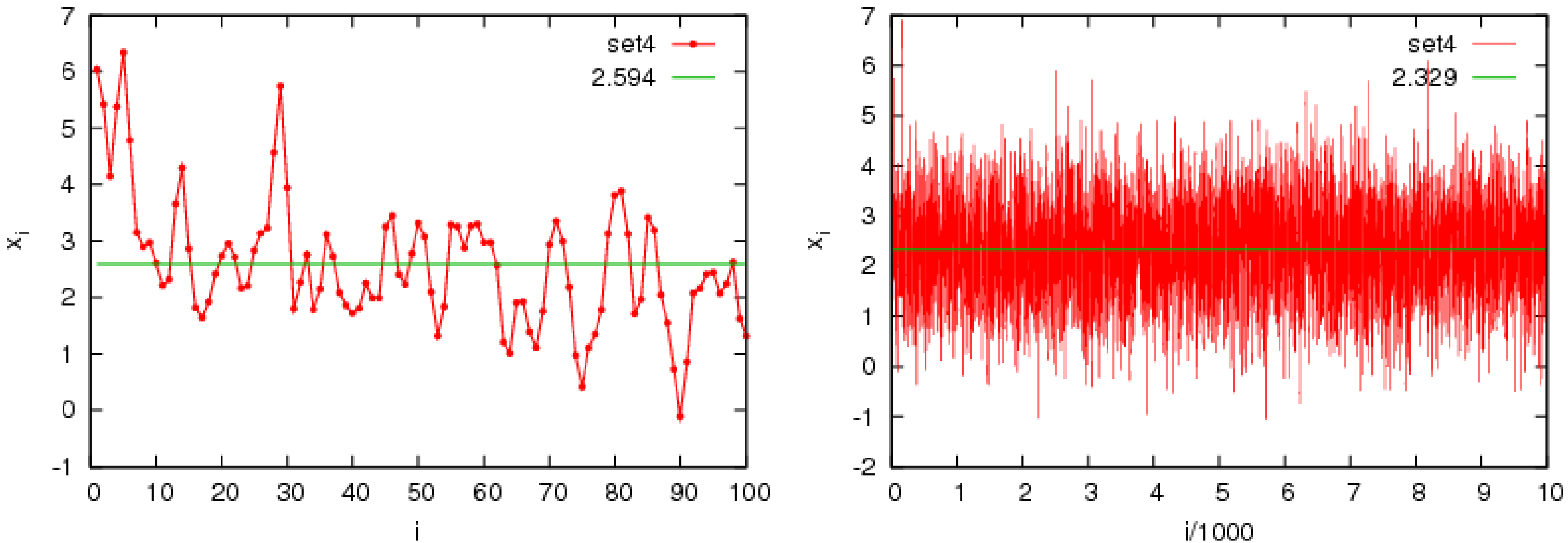




- gaussian distribution of ‘‘measurements’’ - width $\sqrt{0.149}$
- finite autocorrelation ($\tau = 3.0$)
- final error estimate: $\langle x \rangle \approx -3.273 \pm 0.007$
- true distribution: gaussian, mean -3.28, variance 0.15

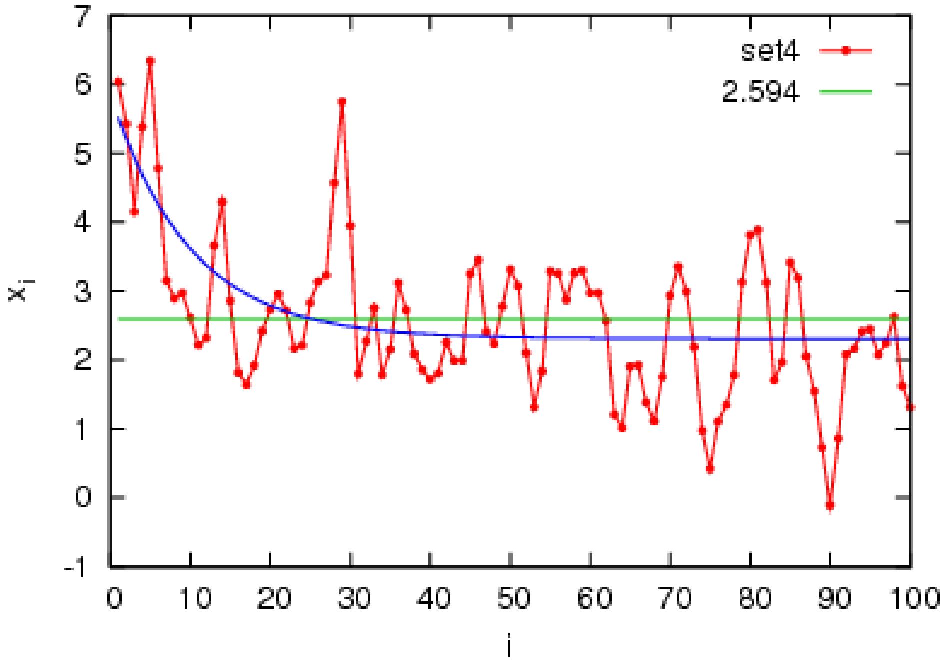
Set 4

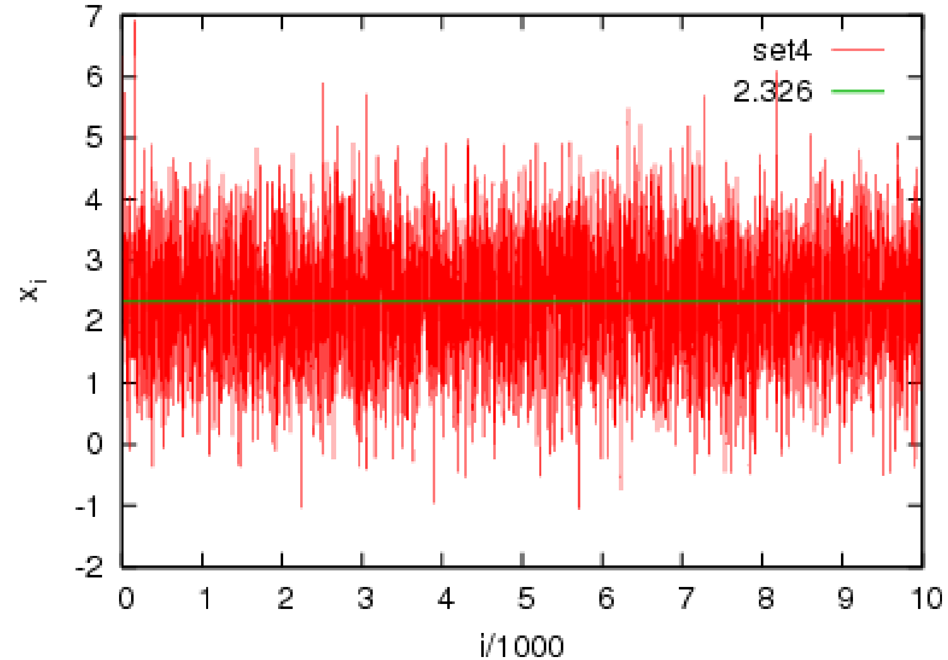
Trace and averages



Estimates of mean / initial error analysis

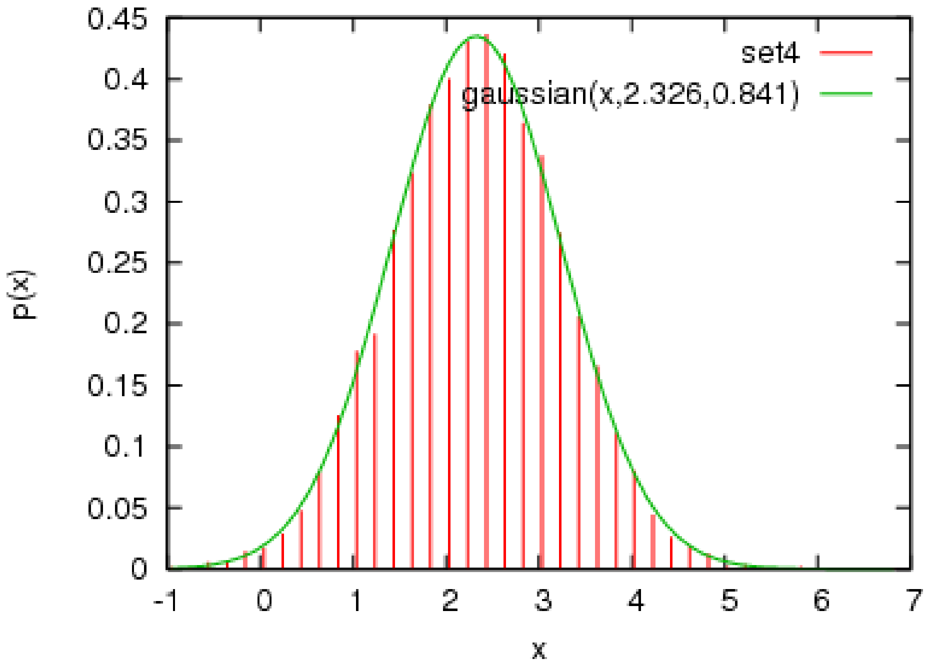
- $\langle x \rangle \approx 2.329 \pm 0.009$ `(naive estimate)`

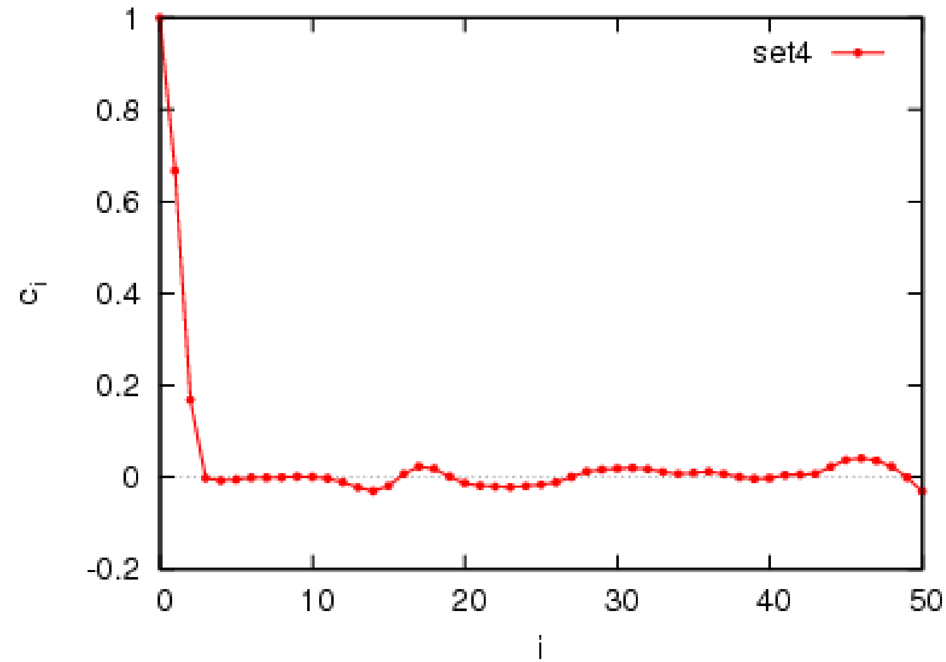




- $\langle x \rangle \approx 2.329 \pm 0.009$ `(naive estimate)`
- `transient, remove first 100 points` $\rightsquigarrow$ $\langle x \rangle \approx 2.326 \pm 0.009$
- `some autocorrelation?`

Histogram, autocorrelation function, full error estimate

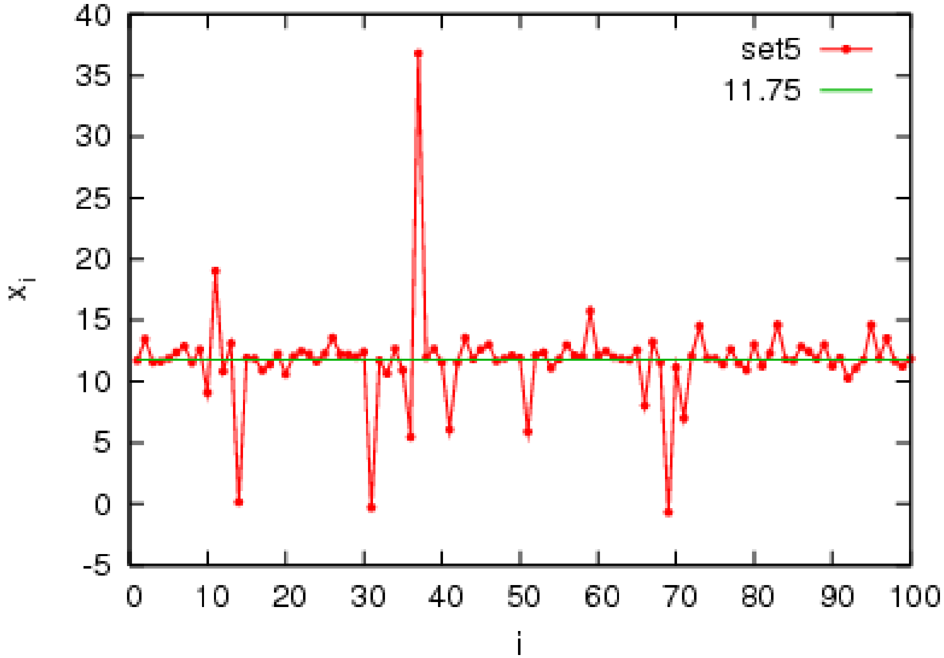


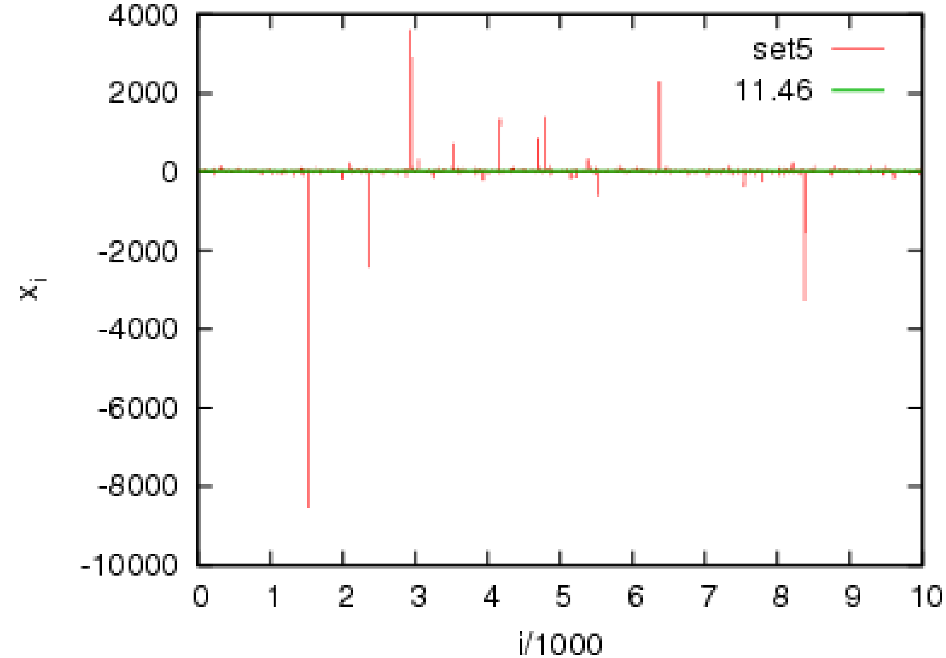


- gaussian distribution of ‘‘measurements’’ - width $\sqrt{0.841}$
- finite autocorrelation ($\tau = 2.67$)
- final error estimate: $\langle x \rangle \approx 2.326 \pm 0.015$
- true distribution: gaussian, mean 2.310, variance 0.85

Set 5

Trace and averages

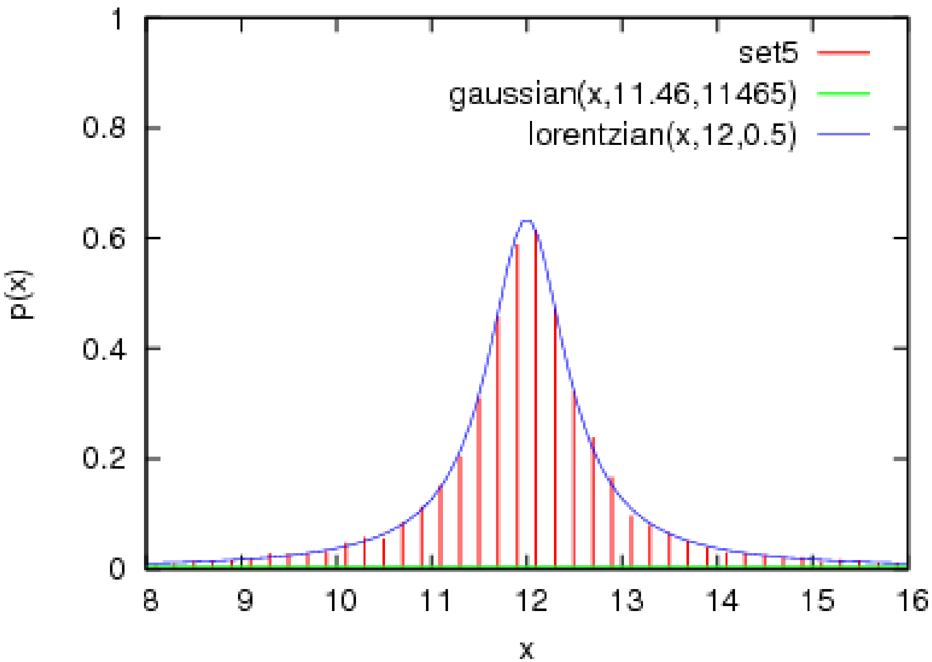


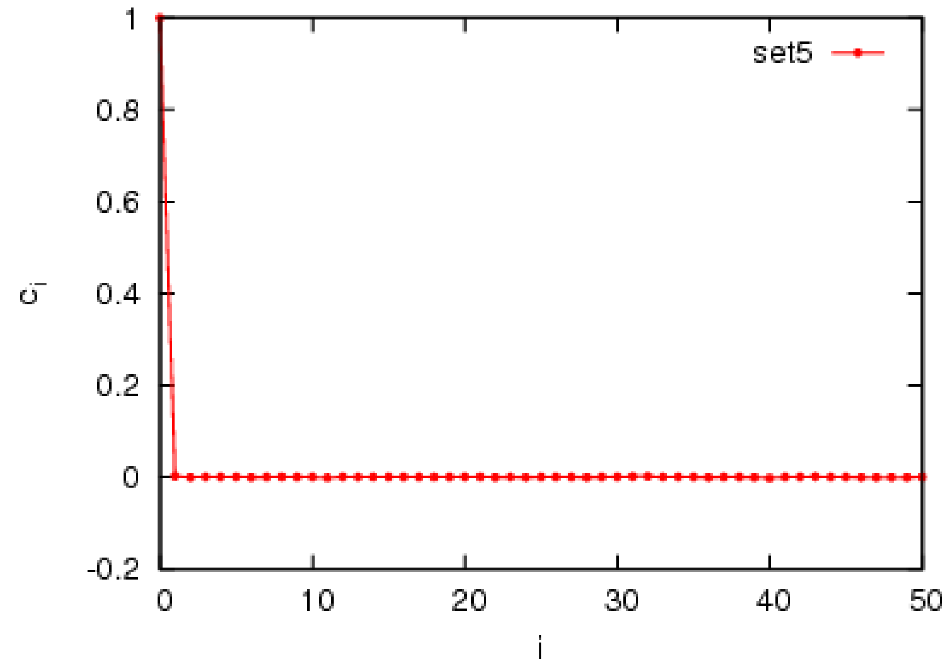


Estimates of mean / initial error analysis

- $\langle x \rangle \approx 11.46 \pm 1.08$ (naive estimate)
- no transient
- no autocorrelation
- variance estimate increases with length of set!

Histogram, autocorrelation function, full error estimate

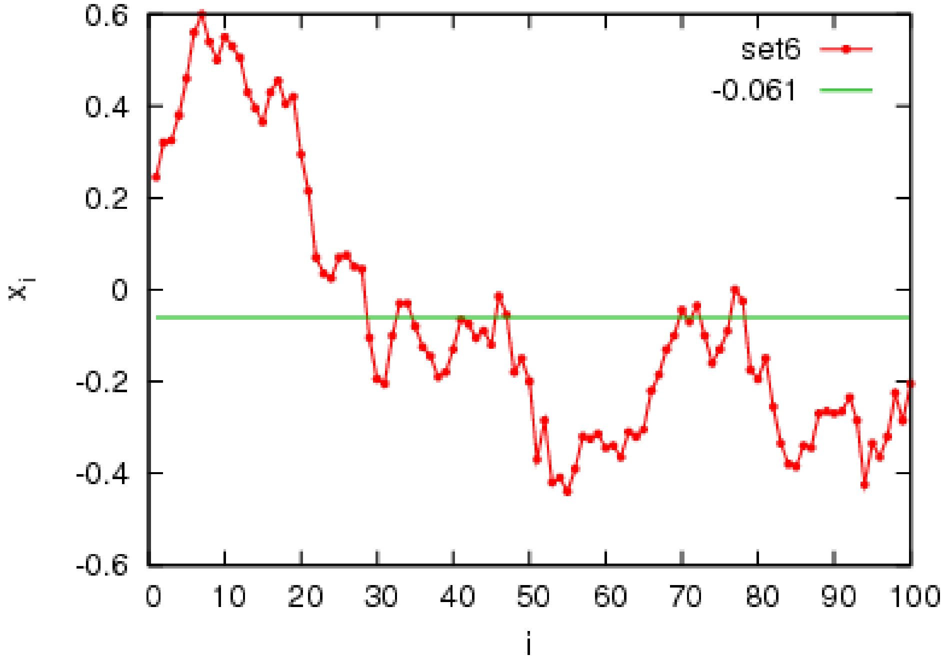


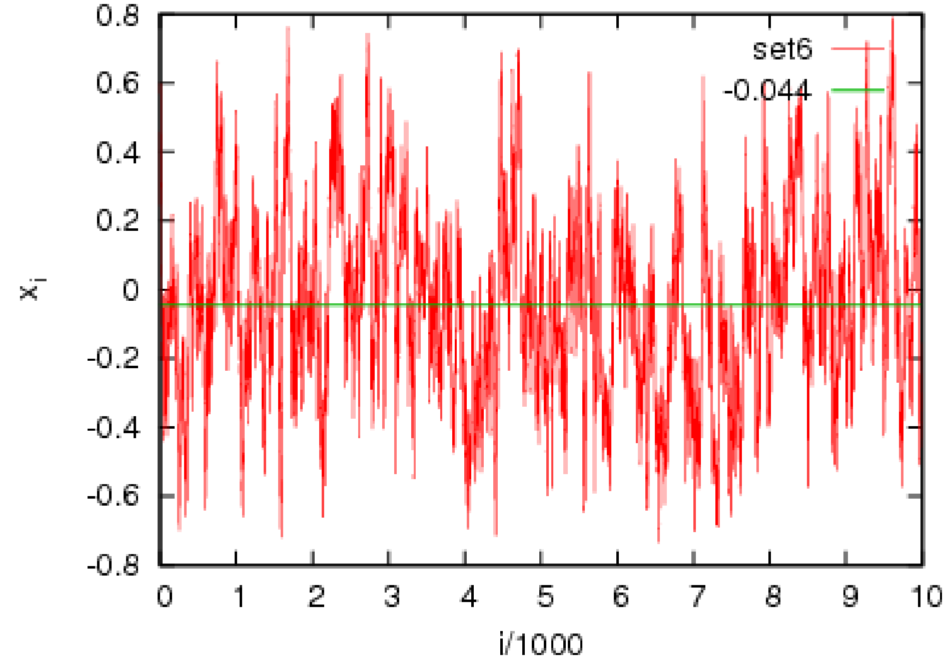


- `strongly nongaussian distribution of ‘‘measurements’’: lorentzian`
- `no autocorrelation` $(\tau = 1.0)$
- `no finite variance, still ‘‘consistent’’ statistics`
- `true distribution:` `lorentzian, median 12, ‘‘width’’ 0.5`

Set 6

Trace and averages

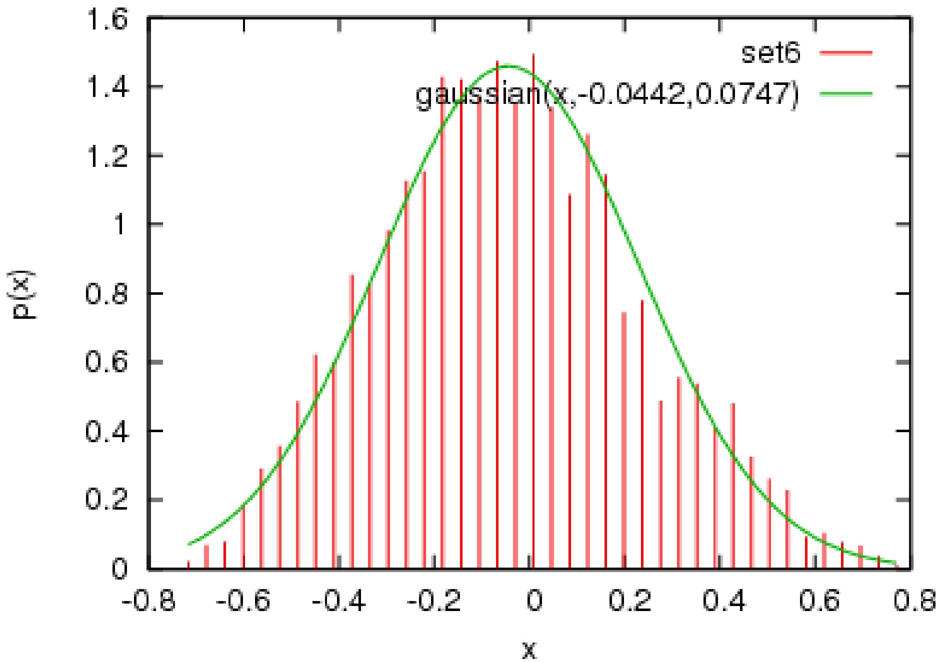


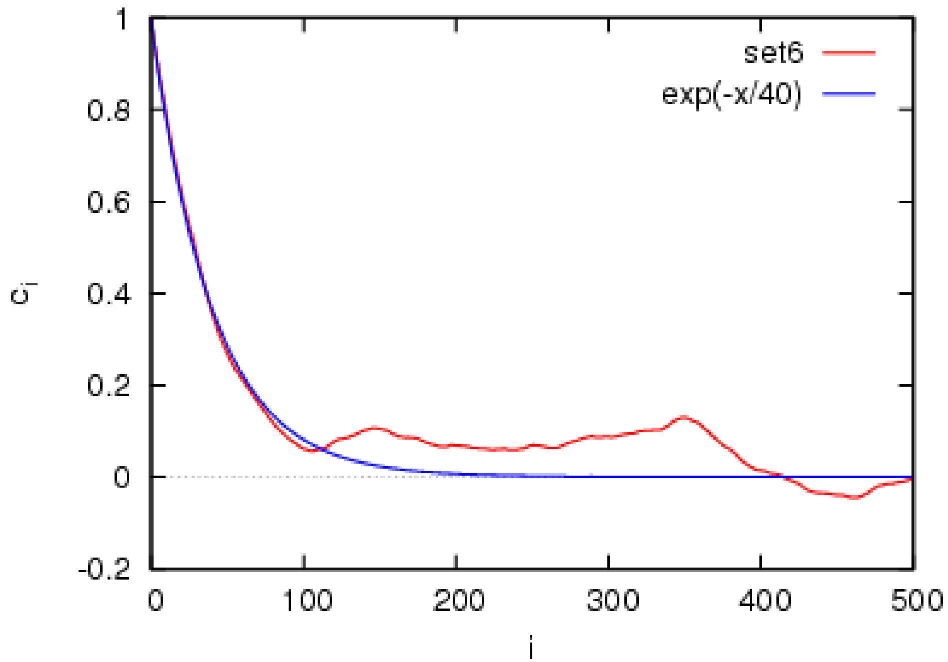


Estimates of mean / initial error analysis

- $\langle x \rangle \approx -0.044 \pm 0.003$ `(naive estimate)`
- `transient?`
- `long autocorrelation`

Histogram, autocorrelation function, full error estimate

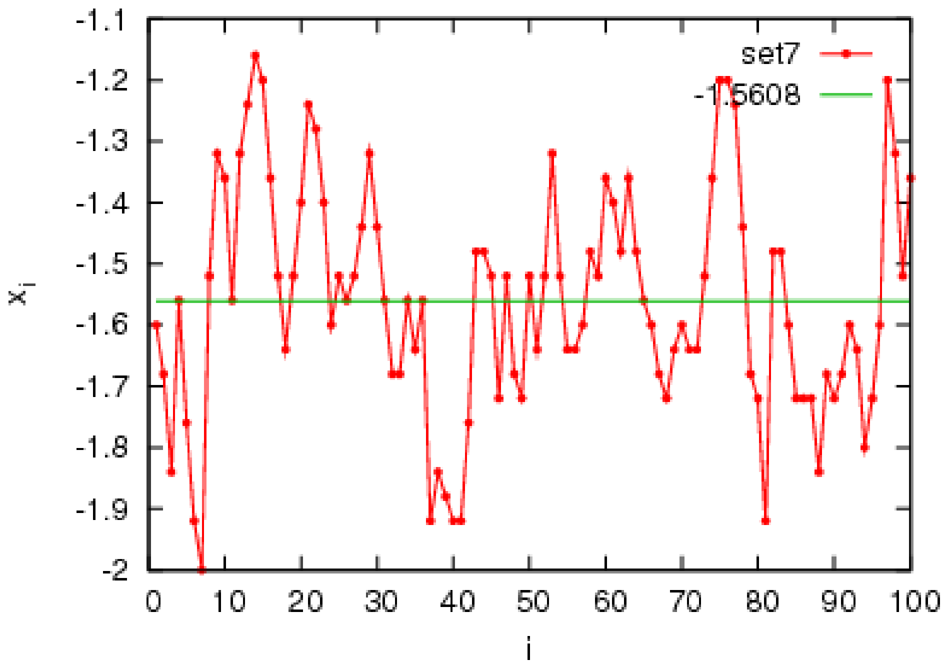


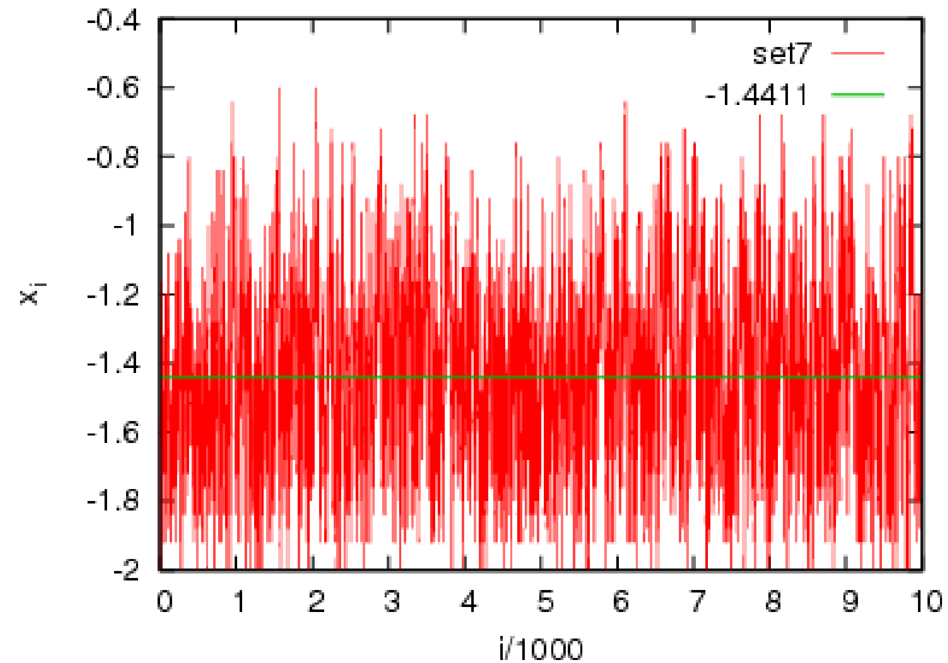


- essentially gaussian distribution of ‘‘measurements’’ – width $\sqrt{0.075}$
- strong autocorrelation ($\tau = 119$)
- final error estimate: $\langle x \rangle \approx -0.044 \pm 0.030$
- true distribution: magnetization in 20x20 2D Ising model (kT/J=2.6), mean 0

Set 7

Trace and averages

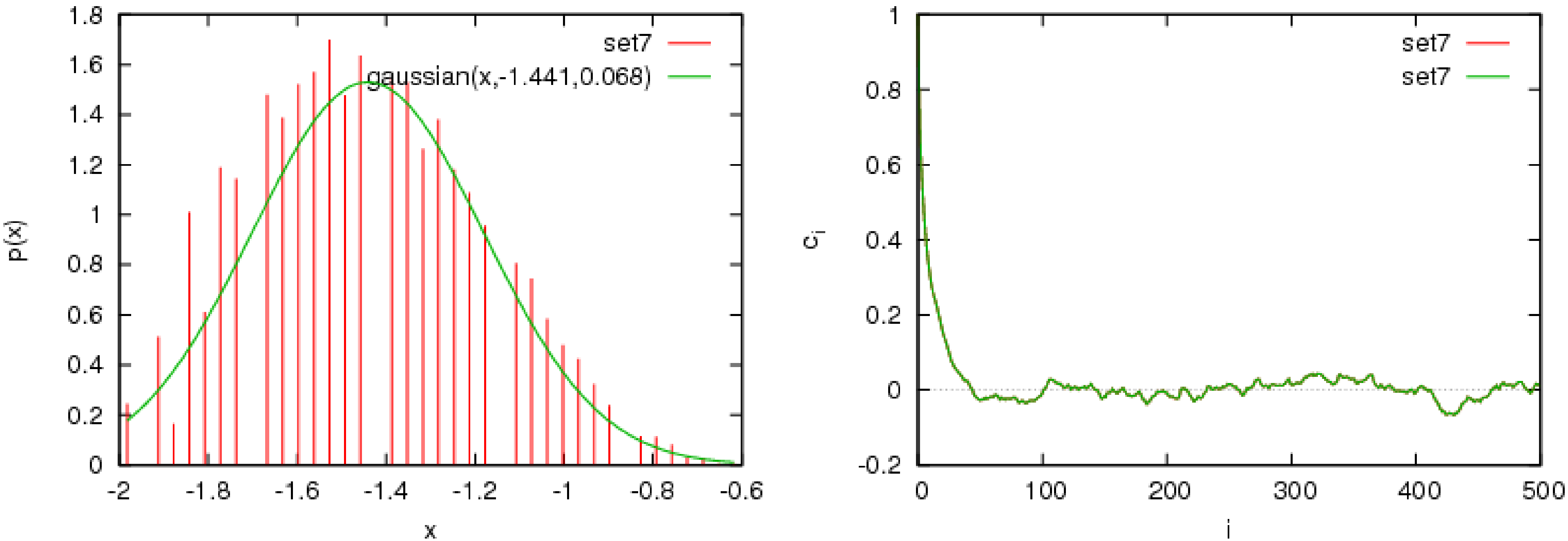




Estimates of mean / initial error analysis

- $\langle x \rangle \approx -1.441 \pm 0.003$ (naive estimate)
- no apparent transient
- significant autocorrelation

Histogram, autocorrelation function, full error estimate

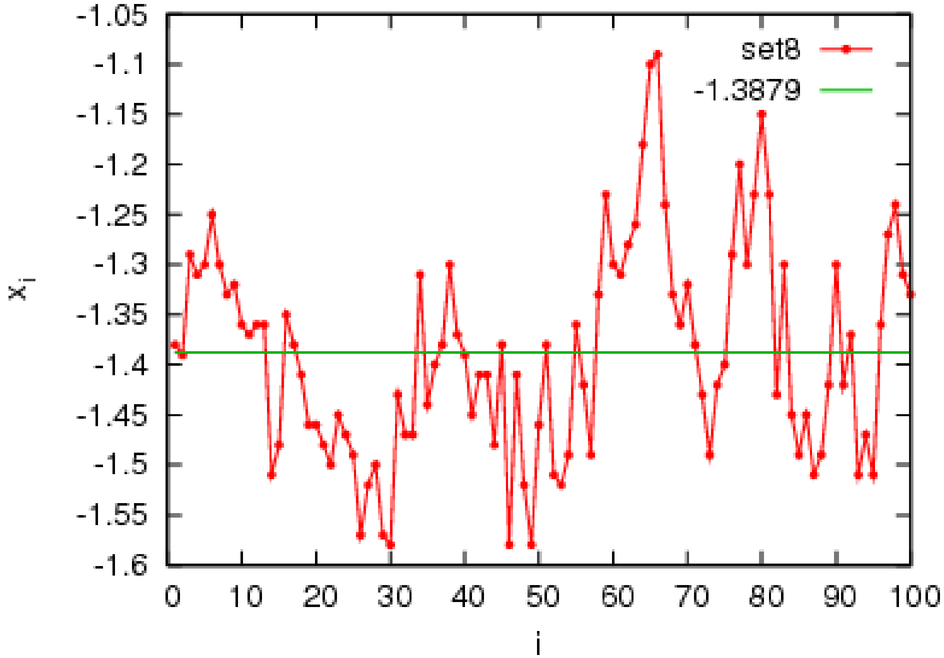


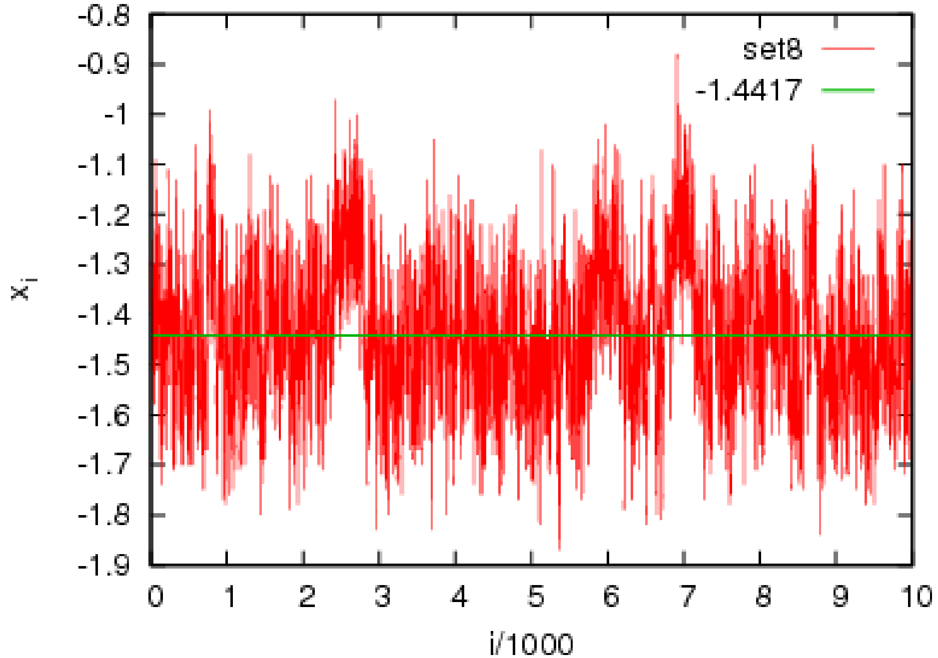
- essentially gaussian distribution of ''measurements'' – width $\sqrt{0.068}$, but with gaps -- why?
- autocorrelation ($\tau = 18$)
- final error estimate: $\langle x \rangle \approx -1.44 \pm 0.01$

- true distribution: energy/site in 10x10 Ising model (kT/J=2.27), more precise estimate: -1.4744 ± 0.00082

Set 8

Trace and averages

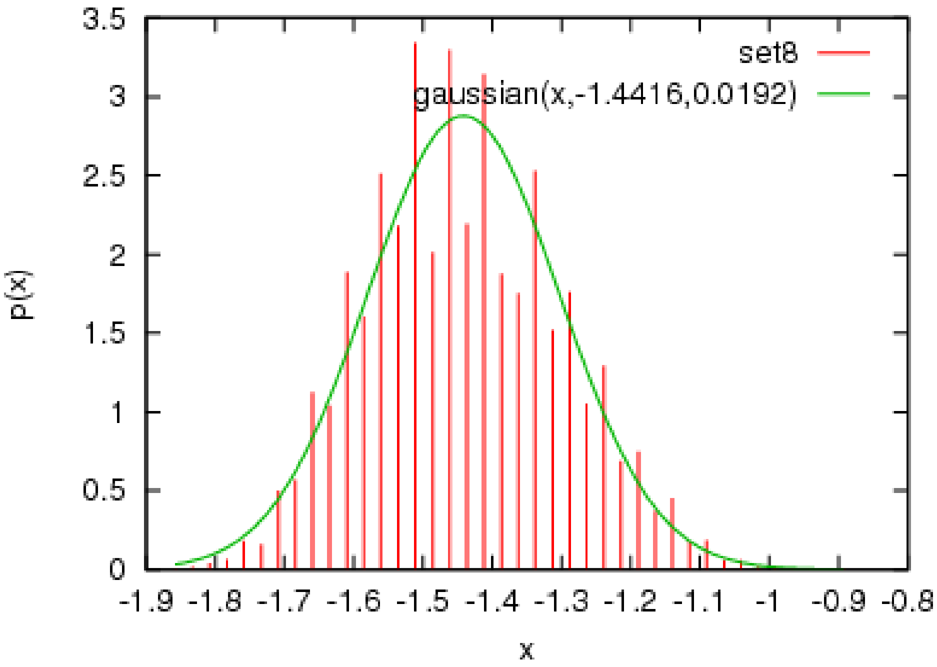


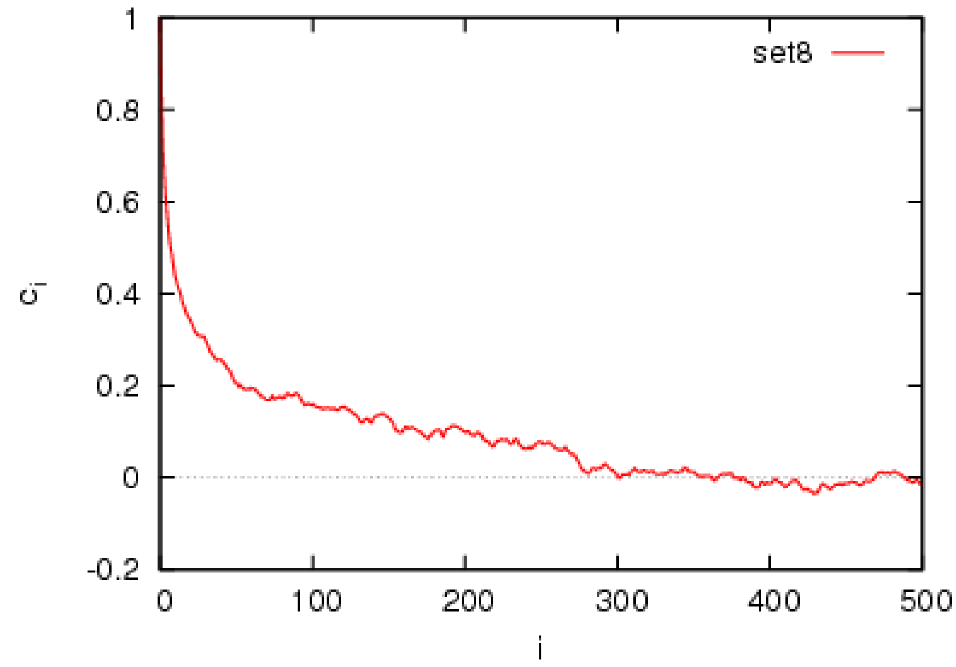


Estimates of mean / initial error analysis

- $\langle x \rangle \approx -1.441 \pm 0.001$ (naive estimate)
- no apparent transient
- significant autocorrelation

Histogram, autocorrelation function, full error estimate



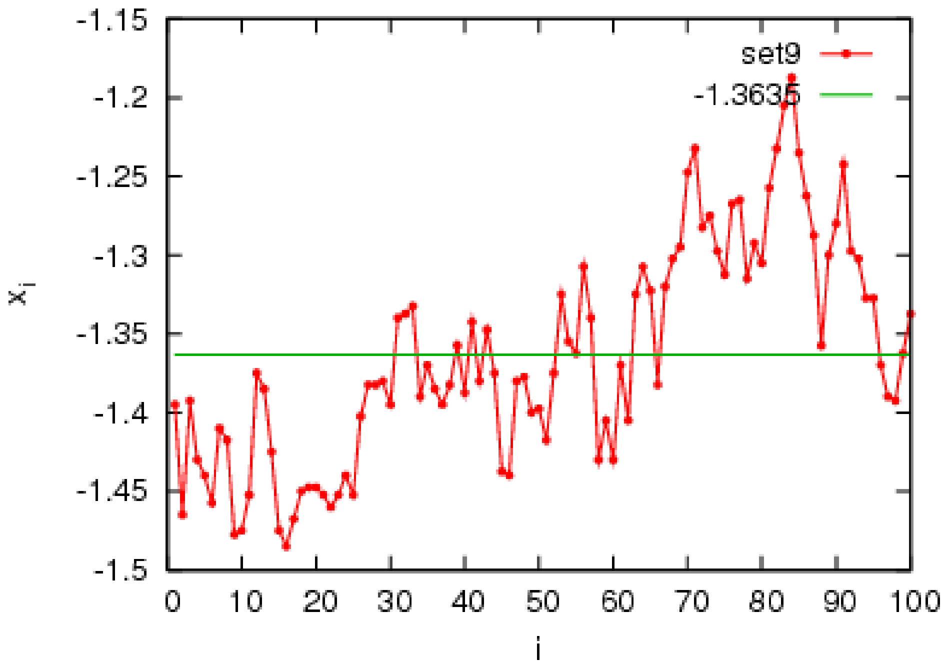


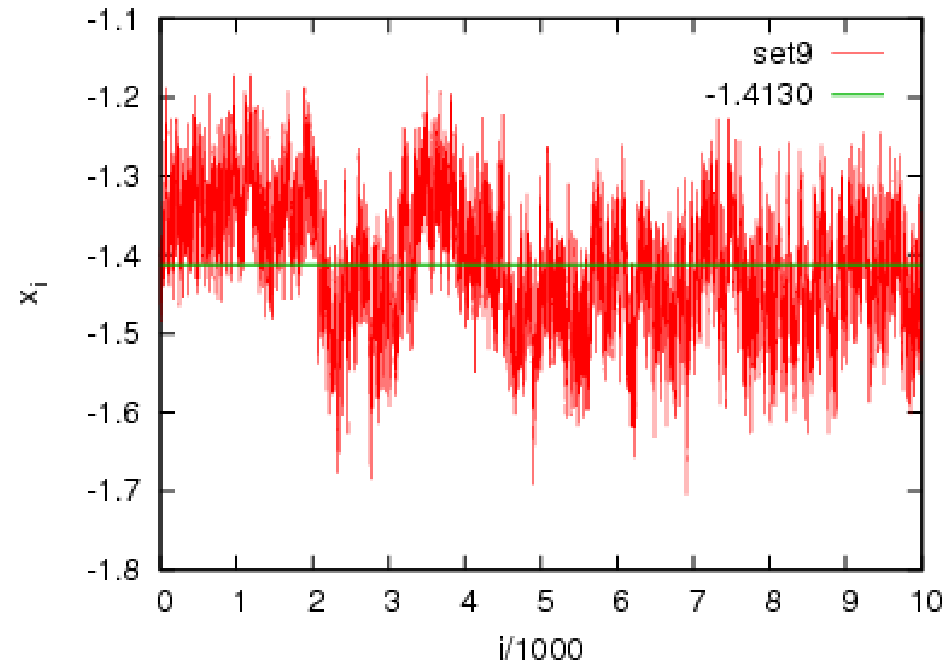
- essentially gaussian distribution of ''measurements'' – width $\sqrt{0.0192}$, now with less pronounced gaps -- why?
- strong autocorrelation ($\tau = 90$)
- final error estimate: $\langle x \rangle \approx -1.44 \pm 0.01$

- true distribution: energy/site in 20x20 Ising model (kT/J=2.27), more precise estimate: -1.4441 ± 0.00045

Set 9

Trace and averages

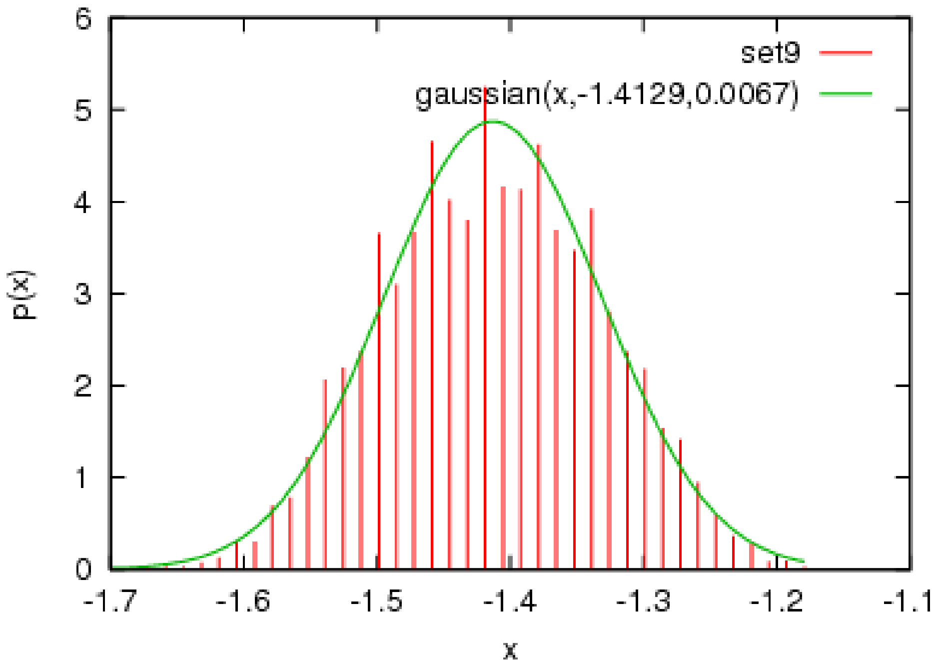


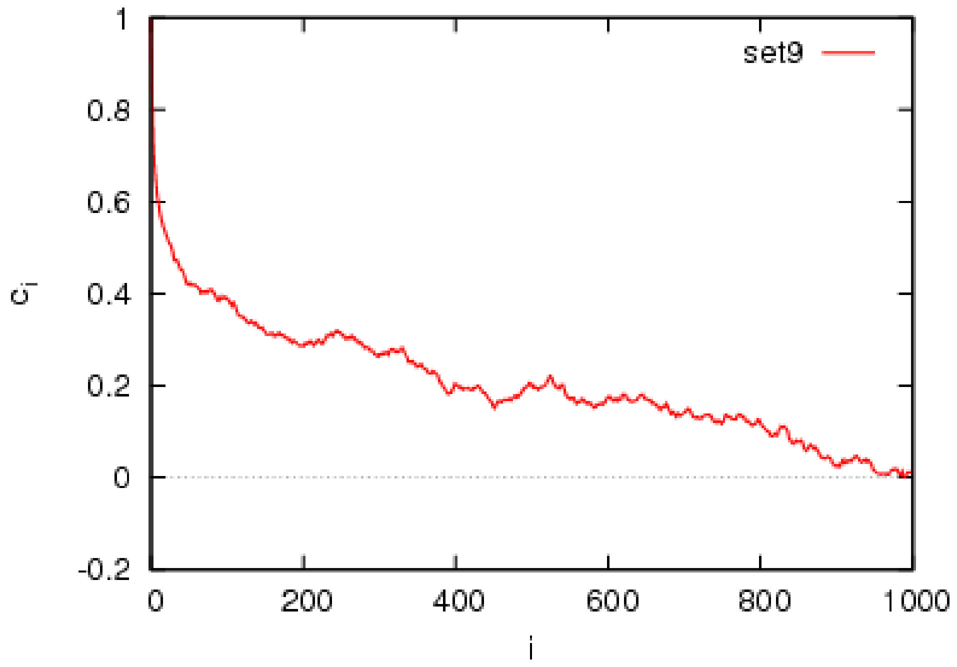


Estimates of mean / initial error analysis

- $\langle x \rangle \approx -1.413 \pm 0.001$ (naive estimate)
- transient?
- strong autocorrelation

Histogram, autocorrelation function, full error estimate





- essentially gaussian distribution of ‘‘measurements’’ – width $\sqrt{0.068}$, but with gaps -- why?
- strong autocorrelation ($\tau = 424$)
- final error estimate: $\langle x \rangle \approx -1.41 \pm 0.02$
- true distribution: energy/site in 40x40 Ising model (kT/J=2.27), more precise estimate: -1.4285 ± 0.00025