Computational Methods (PHYS 2030)

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Schedule: Lecture: MWF 11:30-12:30 (CLH M)

Website: http://www.yorku.ca/cberge/2030W2018.html

York University
Winter 2018
Lecture 31

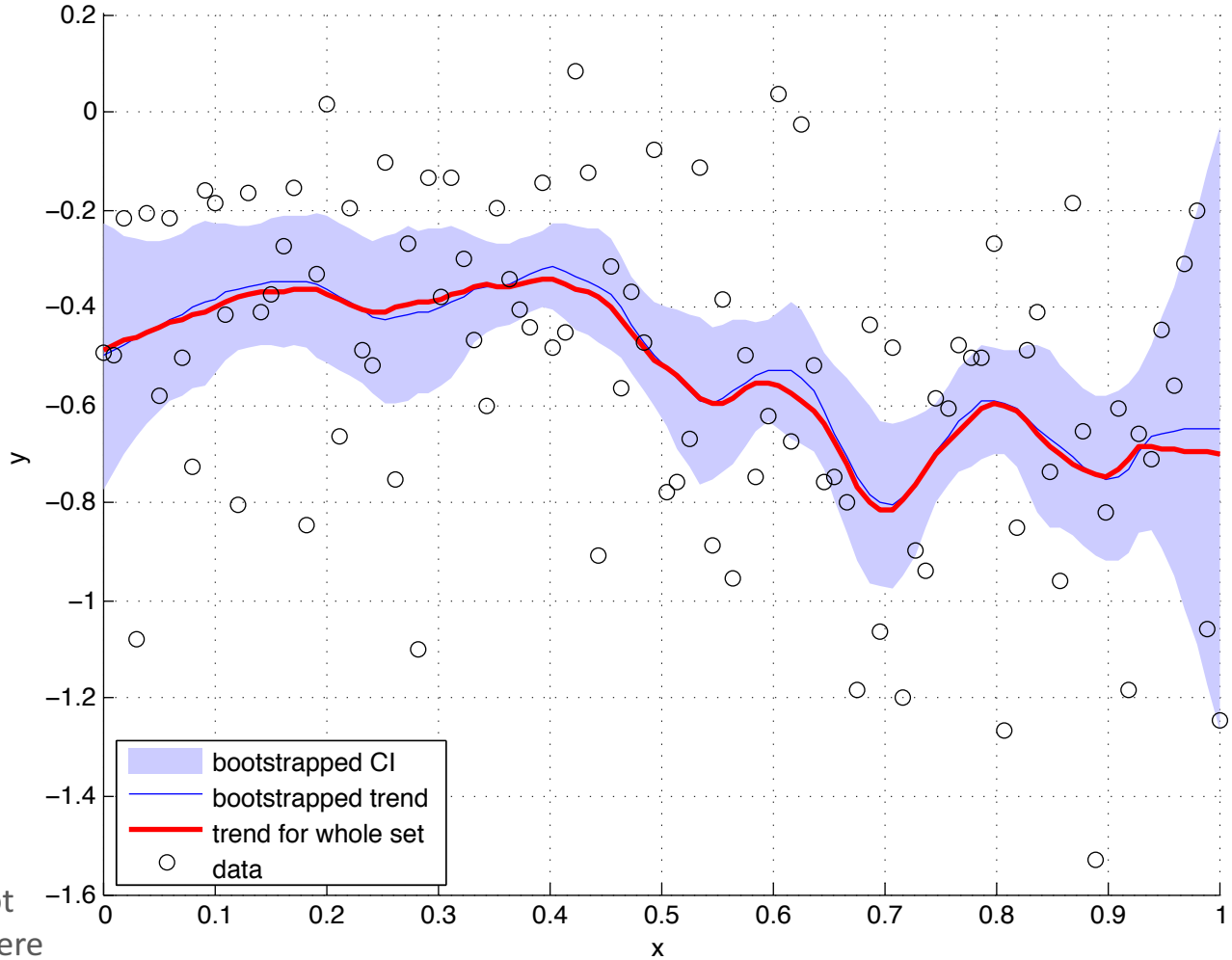
```
% ### EXresampleLoess.m ###
clear;
% ----------------------------
N= 100;     % # of points for fit (over interval [min(x) max(x)])
xR= [0 1];  % range of x-values
scaleN= 0.3;    % scale factor for noise
alpha= 0.17;     % loess fit parameter (between 0 and 1)
order= 1;        % order of polynomial for fit
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
% ---------------------------------------------------
x= linspace(min(xR),max(xR),N); % determine fit x-values
polyS= ceil(10*rand(1));   % randomly determine polynomial order
Pv= 2*rand(polyS,1)-1;  % polynomial coefficients
y= polyval(Pv,x)+ rand(1)*sin(2*pi*x)+ scaleN*randn(N,1)'; % pseudo-random 'data'
N= numel(x);   % total number of points
% ---
% loess fit to ENTIRE data set
xFit= linspace(min(xR),max(xR),N); % can 'resample' if desired (i.e., need not have xFit=x)
yFitW= loess(x,y,xFit,alpha,order,[],1,0,0.1);   % loess fit via external function
% ------------
% Resampling: regression on randomly chosen subsets of the data
for nn=1:M
    temp= randperm(N);              % create randomresampling index
    tINDX= temp(1:ceil(range*N));   % trim to subset of specified size
    temp2(nn,:)= loess(x(tINDX),y(tINDX),xFit,alpha,order,[],1,0,0.1);
end
yFitBS= mean(temp2);
errBS= std(temp2);
% ---
% visualize
figure(1); clf; hold on; grid on;
boundedline(xFit,yFitBS,2*errBS,'b');   % trend from bootstrapping
%plot(xFit,yFitBS,'b-','LineWidth',2);    % without boundedline.m, uncomment these lines
%plot(xFit,yFitBS-2*errBS,'b-'); plot(xFit,yFitBS+2*errBS,'b-'); % 95% CIs for bootstrapped trend
plot(xFit,yFitW,'r-','LineWidth',2);    % trend for whole data set
plot(x,y,'ko');
xlabel('x'); ylabel('y');
legend('resampled CI','mean resampled trend','trend to whole set','data','Location','SouthWest');
```

Note: This subsampling method **does not use replacement** (i.e., a given data point can appear once at most in a resampled set)

EXresampleLoess.m

```
scaleN= 0.3;     % scale factor for noise
alpha= 0.17;      % loess fit parameter (between 0 and 1)
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
```

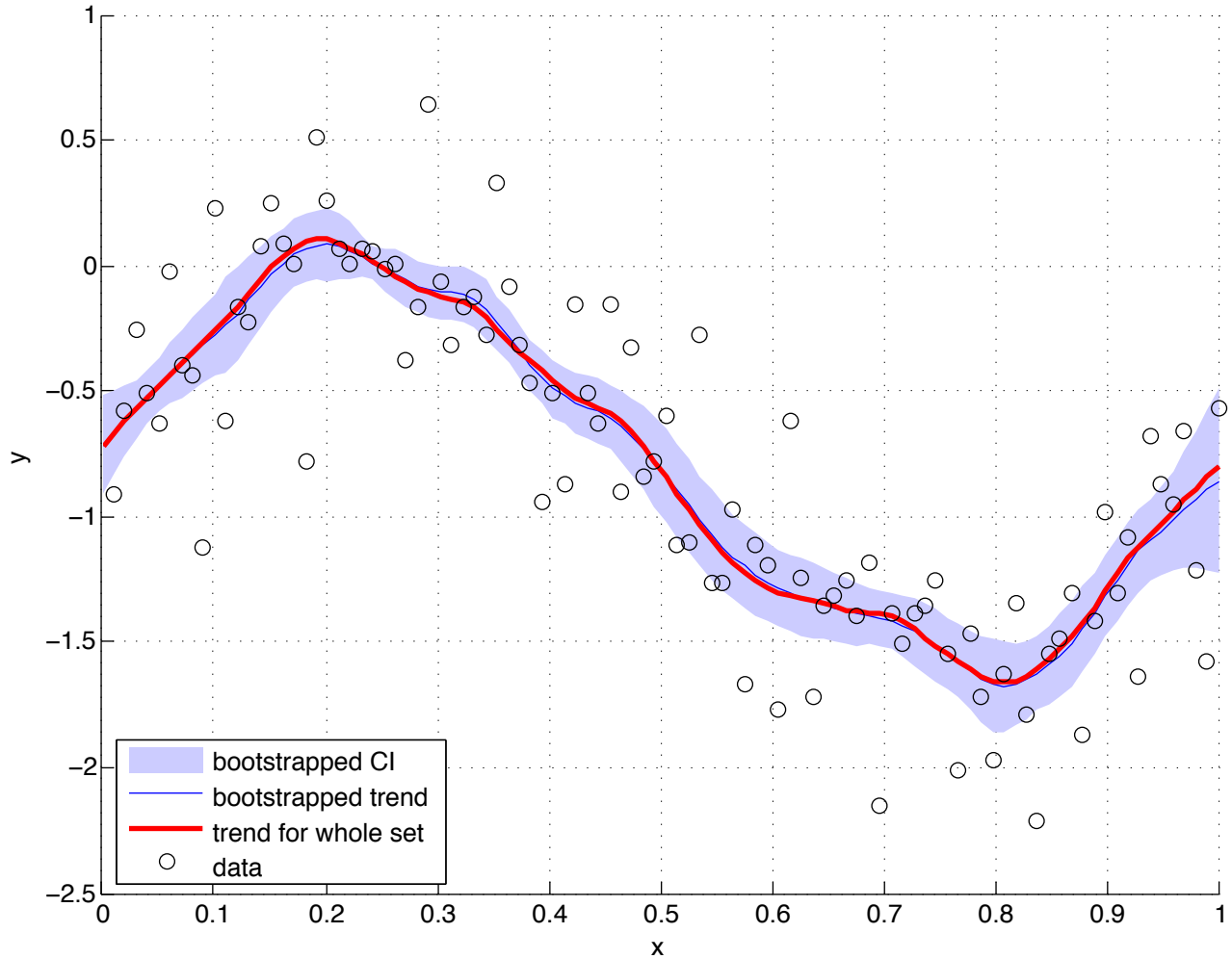
Very useful idea here: *We can determine uncertainty associated with our trends!*



Note: We are not bootstrapping here (strictly speaking)

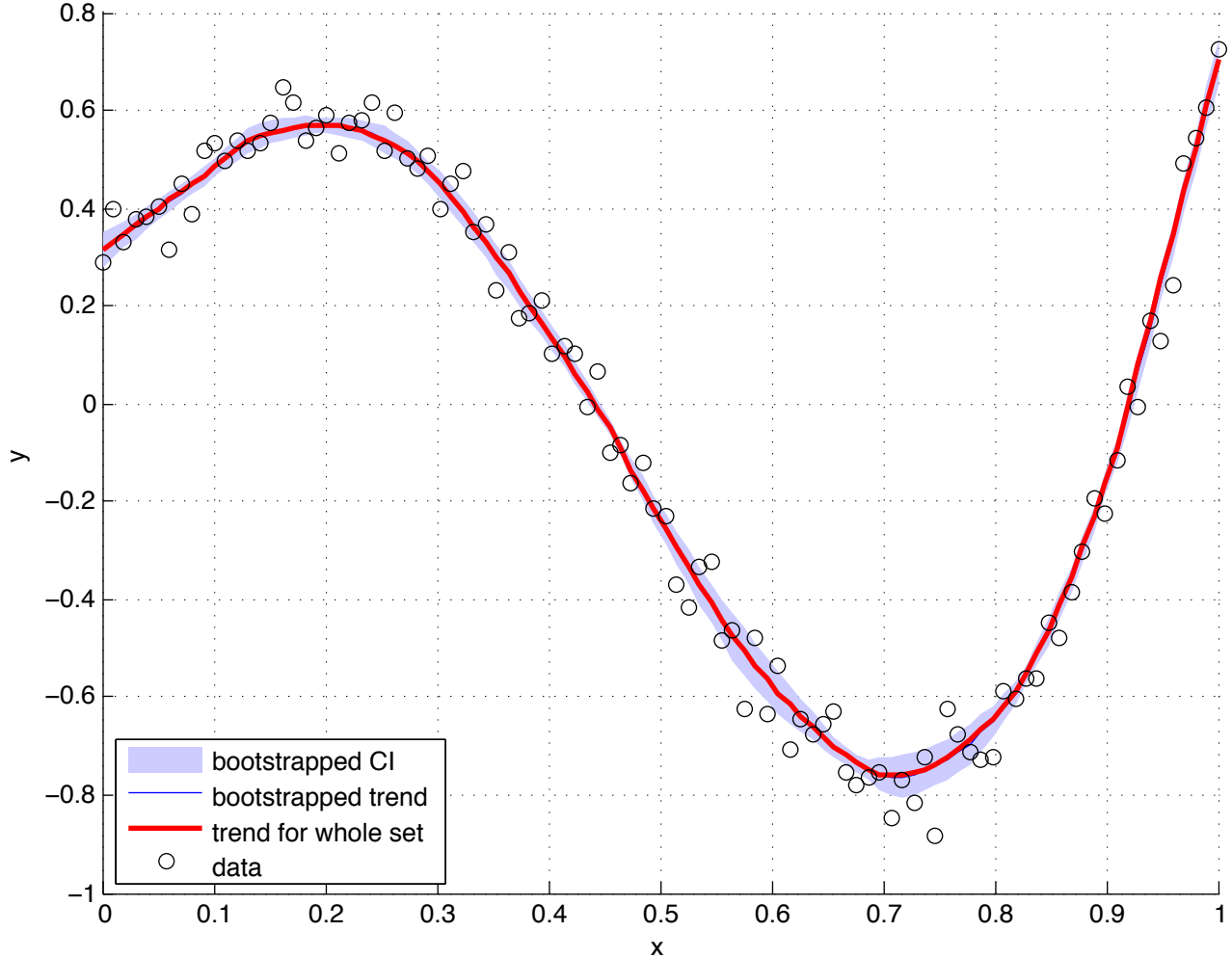
EXresampleLoess.m

```
scaleN= 0.3;     % scale factor for noise
alpha= 0.17;      % loess fit parameter (between 0 and 1)
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
```



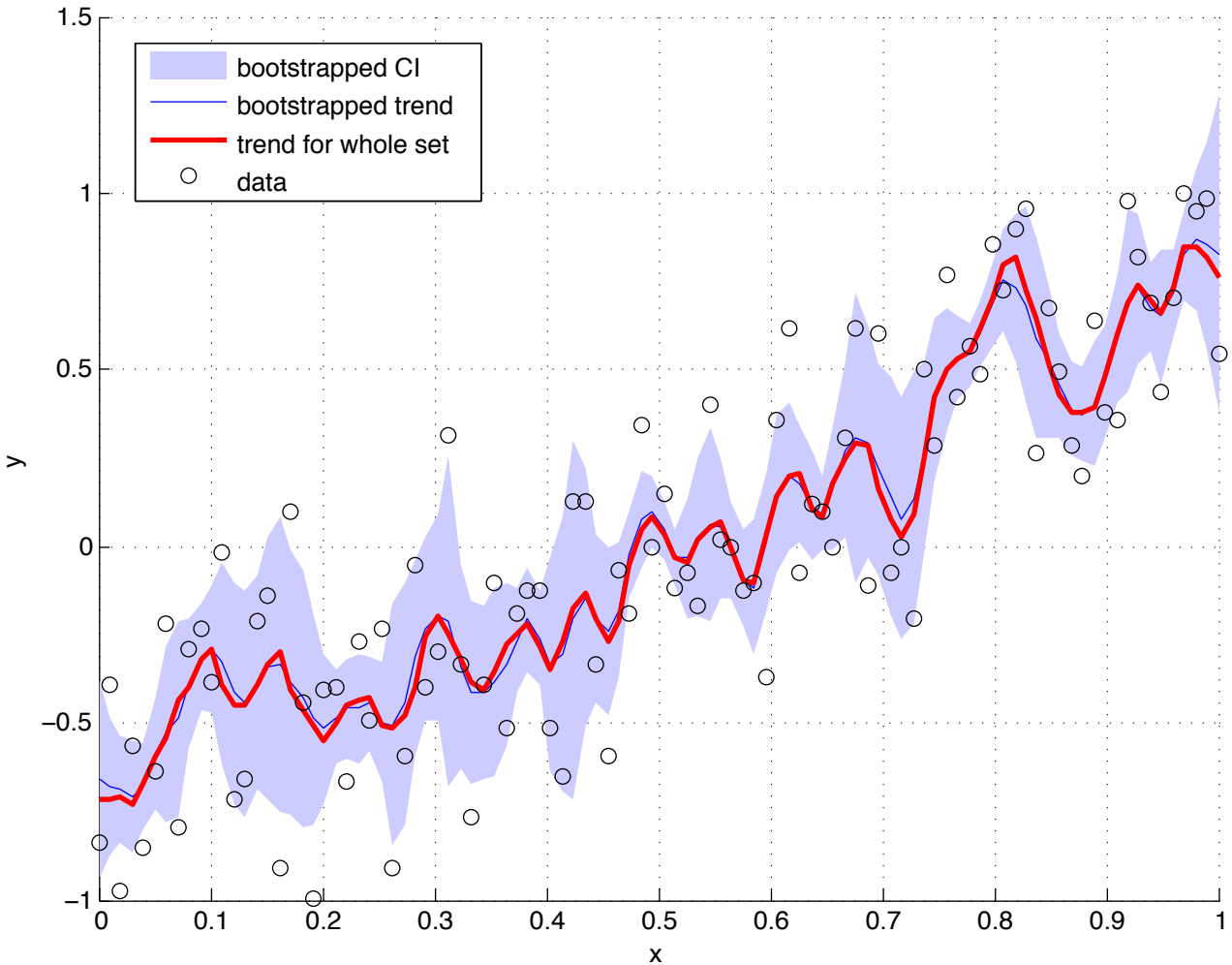
EXresampleLoess.m

```
scaleN= 0.05;     % scale factor for noise
alpha= 0.17;      % loess fit parameter (between 0 and 1)
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
```



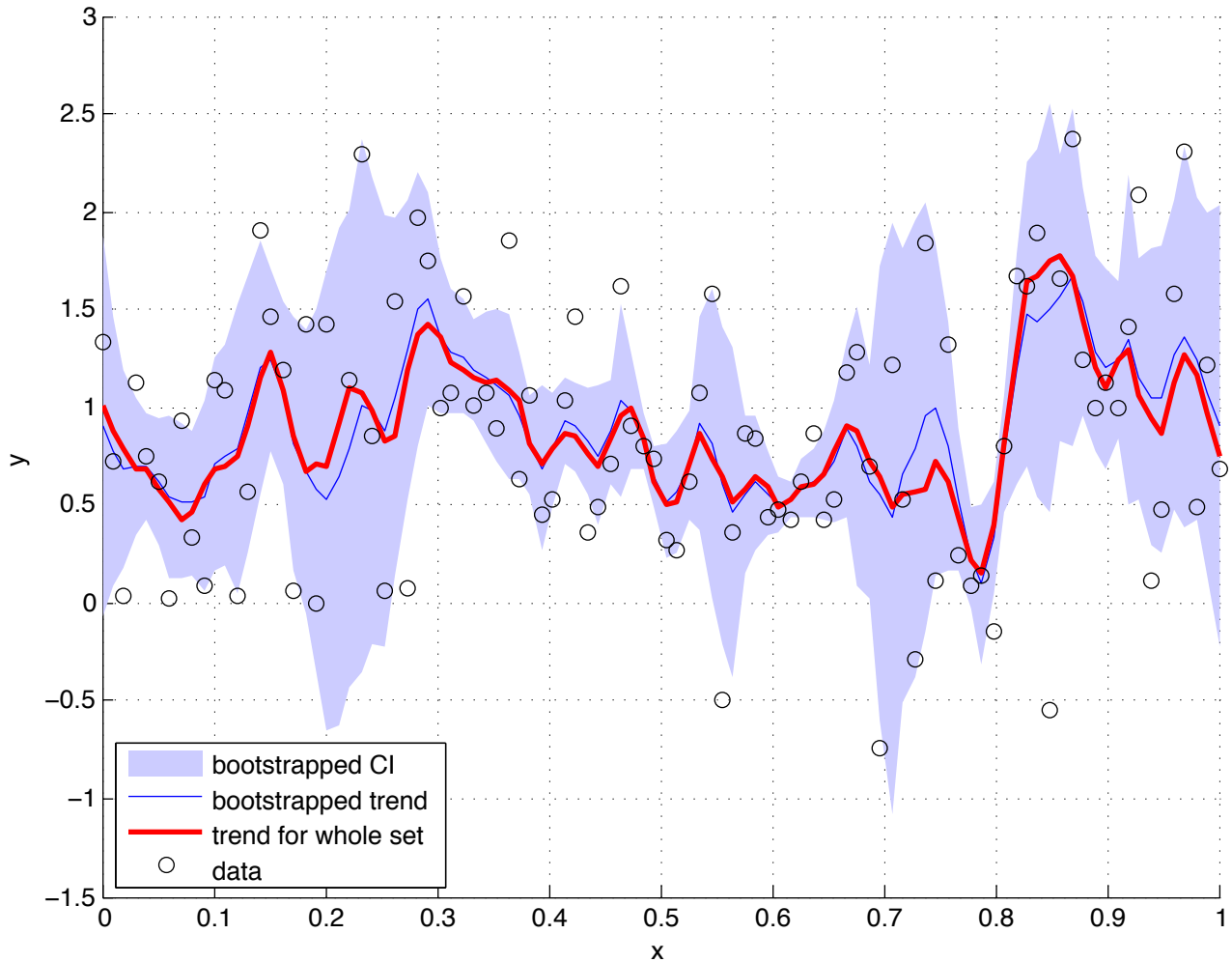
EXresampleLoess.m

```
scaleN= 0.3;     % scale factor for noise
alpha= 0.07;      % loess fit parameter (between 0 and 1)
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
```



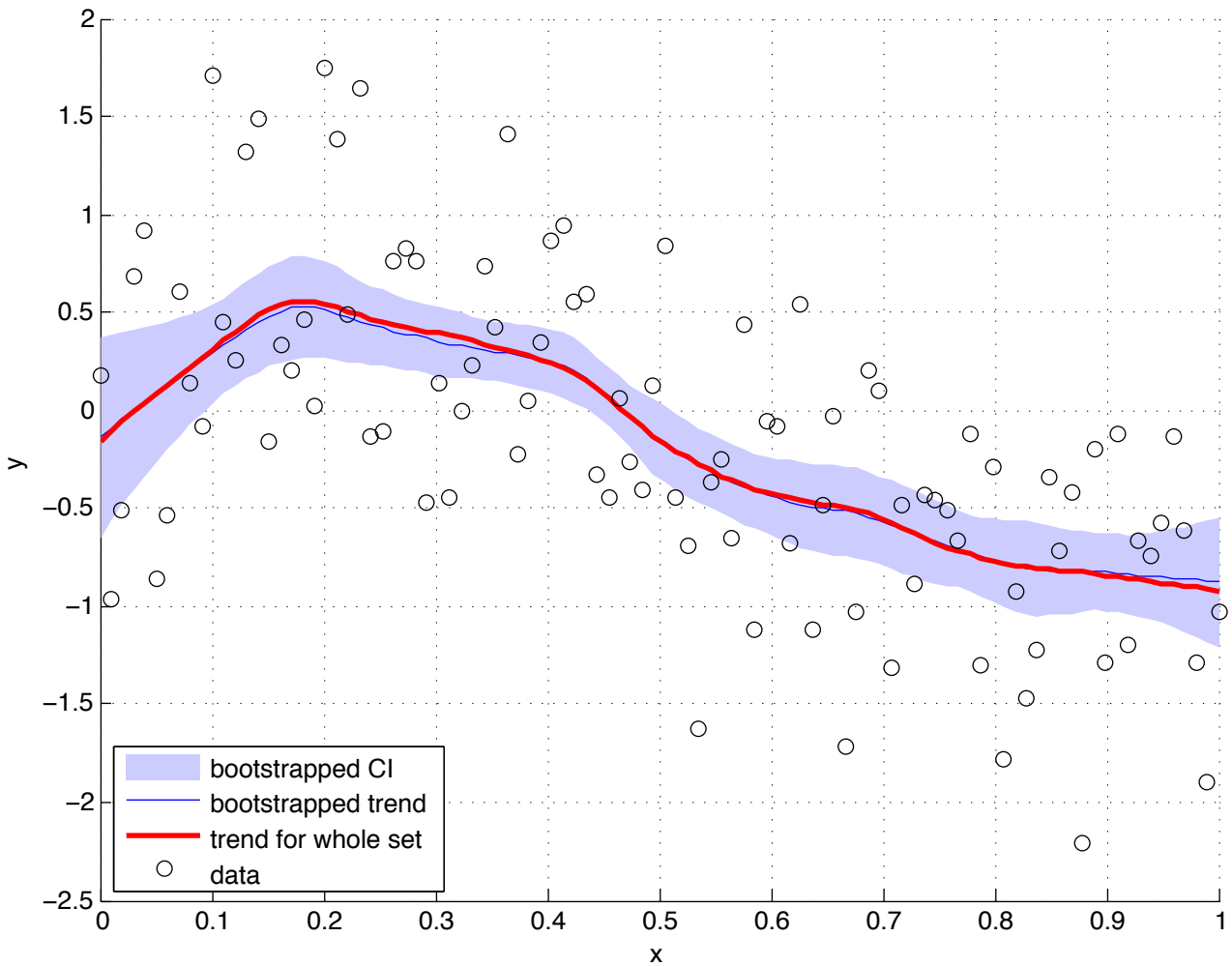
EXresampleLoess.m

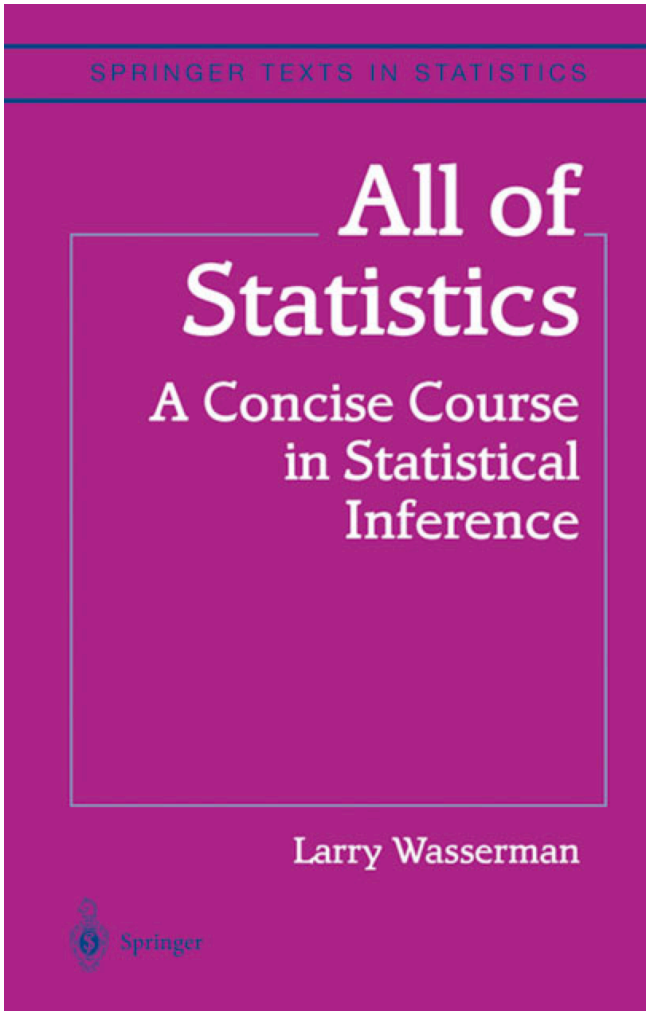
```
scaleN= 0.6;     % scale factor for noise
alpha= 0.07;      % loess fit parameter (between 0 and 1)
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
```



EXresampleLoess.m

```
scaleN= 0.6;     % scale factor for noise
alpha= 0.3;      % loess fit parameter (between 0 and 1)
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
```





9

The Bootstrap

The bootstrap is a nonparametric method for estimating standard errors and computing confidence intervals. Let

$$T_n = g(X_1, \ldots, X_n)$$

be a **statistic**, that is, any function of the data. Suppose we want to know $\mathbb{V}_F(T_n)$, the variance of T_n. We have written $\mathbb{V}_F$ to emphasize that the variance usually depends on the unknown distribution function F. For example, if $T_n = n^{-1}\sum_{i=1}^n X_i$ then $\mathbb{V}_F(T_n) = \sigma^2/n$ where $\sigma^2 = \int (x-\mu)^2 dF(x)$ and $\mu = \int x dF(x)$. The bootstrap idea has two parts. First we estimate $\mathbb{V}_F(T_n)$ with $\mathbb{V}_{\widehat{F}_n}(T_n)$. Thus, for $T_n = n^{-1}\sum_{i=1}^n X_i$ we have $\mathbb{V}_{\widehat{F}_n}(T_n) = \widehat{\sigma}^2/n$ where $\widehat{\sigma}^2 = n^{-1}\sum_{i=1}^n (X_i - \overline{X}_n)$. However, in more complicated cases we cannot write down a simple formula for $\mathbb{V}_{\widehat{F}_n}(T_n)$. This leads us to the second step which is to approximate $\mathbb{V}_{\widehat{F}_n}(T_n)$ using simulation. Before proceeding, let us discuss the idea of simulation.

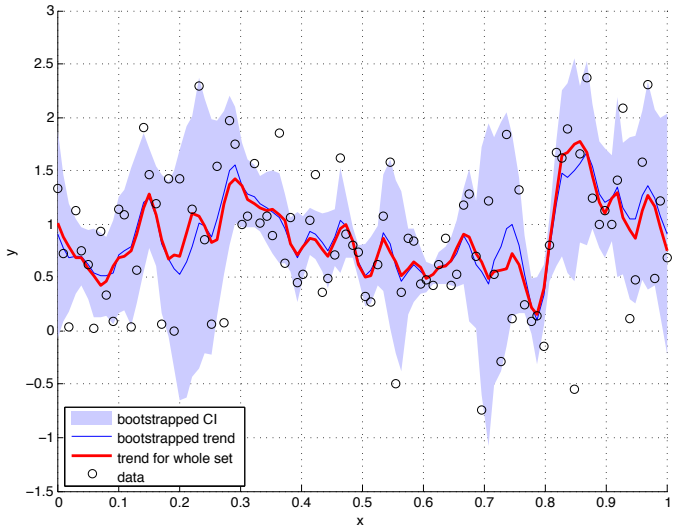
“ There is another method for computing standard errors called the jackknife... It is less computationally expensive than the bootstrap but it is less general... However, unlike the bootstrap, the jackknife does not produce consistent estimates of standard error of sample quantiles.”

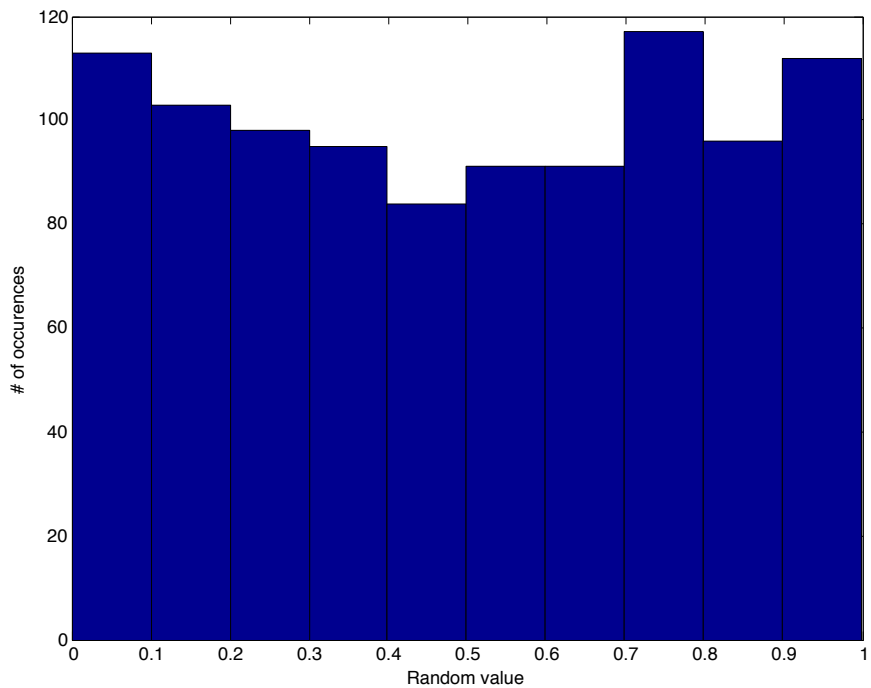
```
% ### EXresampleLoess2.m ###
 clear;
% ------------------------------
N= 100;     % # of points for fit (over interval [min(x) max(x)])
xR= [0 1];  % range of x-values
scaleN= 0.3;    % scale factor for noise
alpha= 0.17;     % loess fit parameter (between 0 and 1)
order= 1;        % order of polynomial for fit
M= 20;  % # of resamples
range= 2/3; % range to vary span over [0,1]
replace= 1; % use replacement? [0-no, 1-yes]
% ---------------------------------------------------
x= linspace(min(xR),max(xR),N); % determine fit x-values
polyS= ceil(10*rand(1));   % randomly determine polynomial order
Pv= 2*rand(polyS,1)-1;  % polynomial coefficients
y= polyval(Pv,x)+ rand(1)*sin(2*pi*x)+ scaleN*randn(N,1)'; % pseudo-random 'data'
N= numel(x);   % total number of points
% ---
% loess fit to ENTIRE data set
xFit= linspace(min(xR),max(xR),N); % can 'resample' if desired (i.e., need not have xFit=x)
yFitW= loess(x,y,xFit,alpha,order,[],1,0,0.1);   % loess fit via external function
% ------------
% Resampling: regression on randomly chosen subsets of the data
for nn=1:M
    % create randomresampling index
    if replace==0
        temp= randperm(N);  % each entry is unique
    elseif replace==1
        temp= floor(N*rand(1,N))+1;  % allow for possible repeated values
    end
    tINDX= temp(1:ceil(range*N));   % trim to subset of specified size
    temp2(nn,:)= loess(x(tINDX),y(tINDX),xFit,alpha,order,[],1,0,0.1);
end
yFitBS= mean(temp2);
errBS= std(temp2);
% ---
% visualize
figure(1); clf; hold on; grid on;
boundedline(xFit,yFitBS,2*errBS,'b');   % trend from bootstrapping
%plot(xFit,yFitBS,'b-','LineWidth',2);    % without boundedline.m, uncomment these lines
%plot(xFit,yFitBS-2*errBS,'b-'); plot(xFit,yFitBS+2*errBS,'b-'); % 95% CIs for bootstrapped trend
plot(xFit,yFitW,'r-','LineWidth',2);    % trend for whole data set
plot(x,y,'ko');
xlabel('x'); ylabel('y');
legend('resampled CI','mean resampled trend','trend to whole set','data','Location','SouthWest');
```

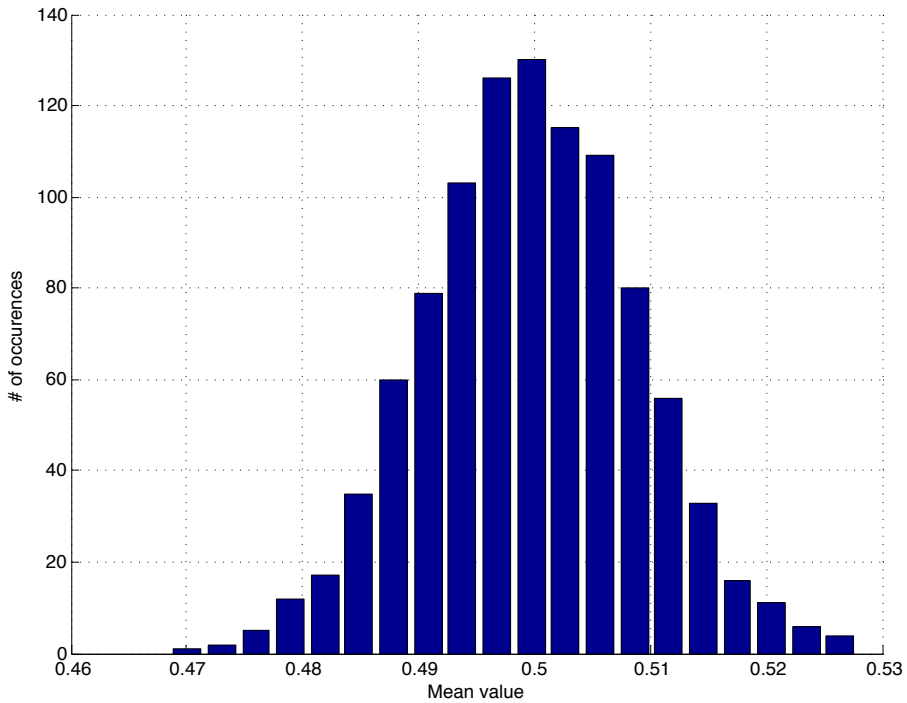
Note: This version **does allow for replacement** (i.e., if `replace= 1` and `range= 1`, then this would be *bootstrapping*)

Be careful!

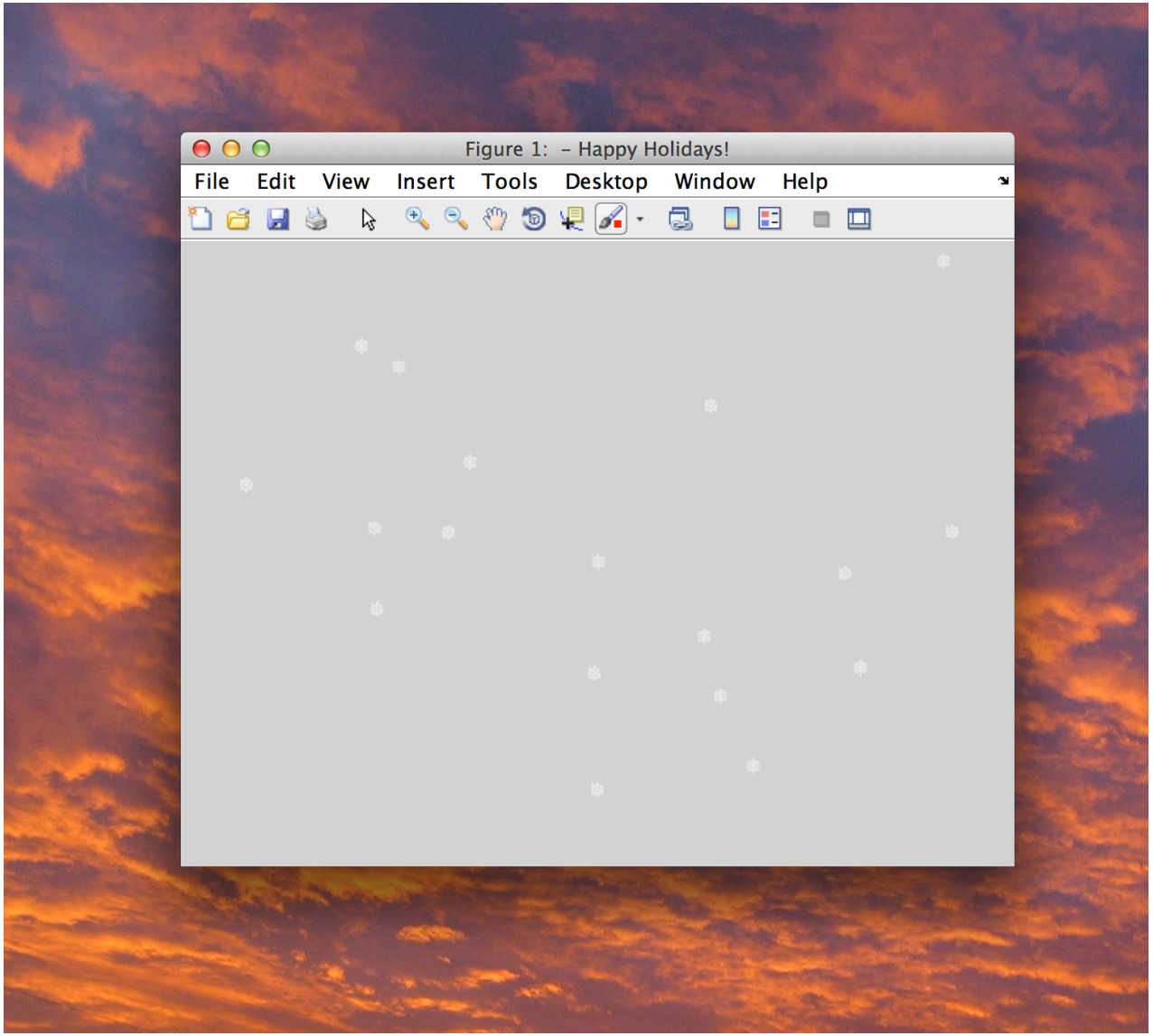
→ A normal distribution doesn't necessarily tell you where an individual measurement lies, but the mean value across a set of measurements (i.e., what happens for compiling across REPEATED measurements)







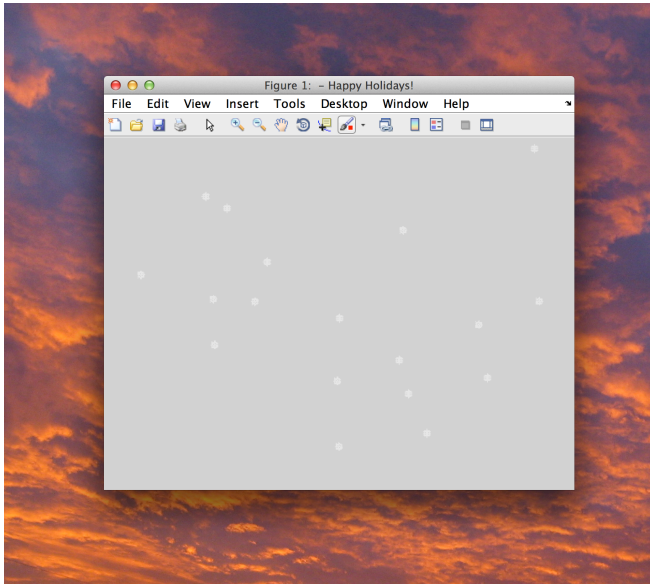
Bonus: Falling snowflakes



`letitsnow.m`

(http://www.mathworks.com/matlabcentral/fileexchange/34349-let-it-snow--falling-snow-on-every-figure-/content/letitsnow.m)

[snippet of the code to illustrate how random numbers are factored in]

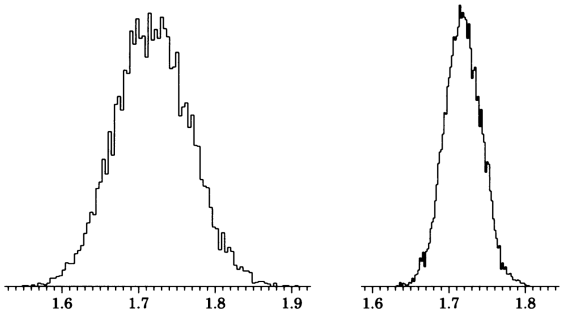



```
% - For snowflakes -
num_snowflakes = 120;
snowflakes_size = 11;
snowflakes_color = sf_color.*[1 1 1];
height_range = 3;

snow_timer = timer('TimerFcn', @updateSnow_Callback_nest,...
    'ExecutionMode','fixedRate',...
    'Period', 1./fps, 'BusyMode', 'queue');

% Position of snowflakes
snowflakes_x = rand(1, num_snowflakes);

snowflakes_y = rand(1, num_snowflakes);
snowflakes_y = (snowflakes_y .* height_range.^3).^(1/3)+1;
snowflakes_pos = [snowflakes_x; snowflakes_y];

% Velocity of snowflakes
snowflakes_v = rand(1, num_snowflakes).*0.1 + 0.1;  % (distance per second)
snowflakes_theta = (rand(1, num_snowflakes).*60 + 240).*pi/180;
snowflakes_vel = [snowflakes_v.*cos(snowflakes_theta);
snowflakes_v.*sin(snowflakes_theta)];
```

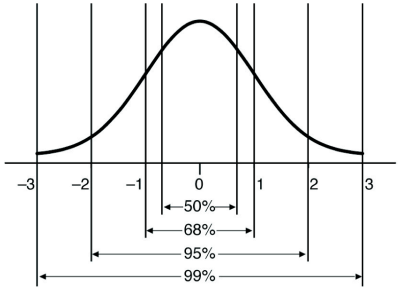
Post-class exercises

- Fiddle around with the random # generator codes (i.e., the ones that don't explicitly make use of `rand.m` or `rand.m`). Can you get something reasonable working?

- Modify `EXintegrateMC1.m` so to recreate these types of normal distributions

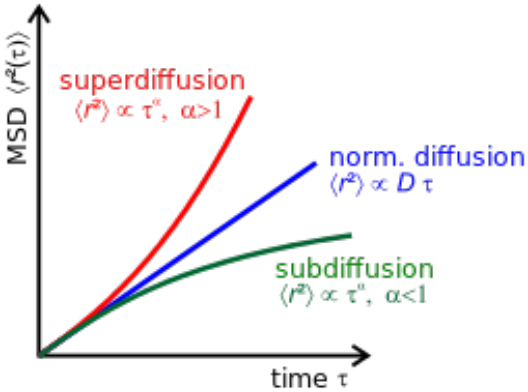


- Create a normally distributed set of numbers and verify the relationship between the area and associated STD



- Can you modify the random walker codes (1-D or 2-D) in some fashion to create 'anomalous diffusion' conditions?

- What is the connection between the MSD for an ensemble of random walkers and the STD of a normal distribution?



- What difference does 'with' or 'without replacement' make when resampling? How does such depend upon sample size?