Fitting Linear Relationships

File: `Ch21_DataFitting.m`

Fitting linear relationships to experimental data is one of the basic tools for laboratory data analysis. This script demonstrates a simple approach using Matlab.

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Data

The sample data comes from Example 21.5 of Seborg, et al. The first column is the biological oxygen demand (BOD) and the second column is solids concentration (mg/liter) for a series of daily samples of the effluent of a waste water treatment plant.

```
data = [ ...
    17.7    1380;
    23.6    1458;
    13.2    1322;
    25.2    1448;
    13.1    1334;
    27.8    1485;
    29.8    1503;
     9.0    1540;
    14.3    1341;
    26.0    1448;
    23.2    1426;
    22.8    1417;
    20.4    1384;
    17.5    1380;
    18.4    1396;
    16.8    1345;
    13.8    1349;
    19.4    1398;
    24.7    1426;
    16.8    1361;
    14.9    1347;
    27.6    1476;
    26.1    1454;
    20.0    1393;
    22.9    1427;
    22.4    1431;
    19.6    1405;
    31.5    1521;
    19.9    1409;
```

```
    20.3    1392];
```

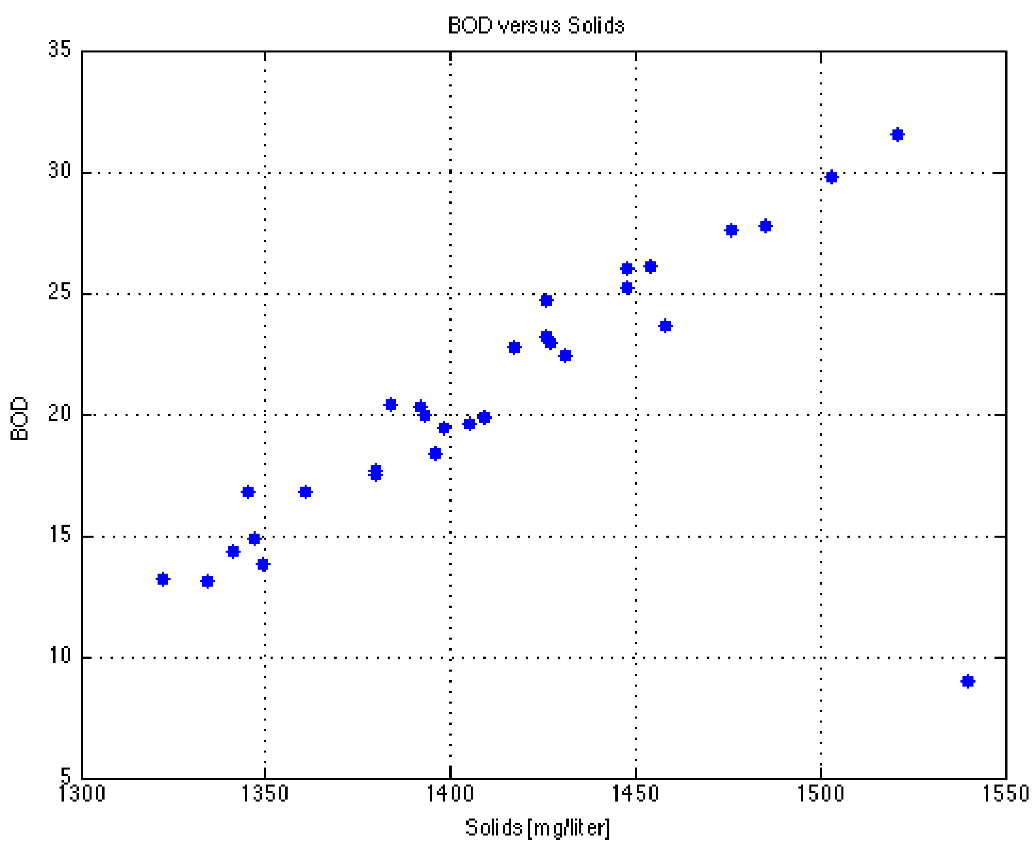
Preliminary data exploration

Our expectation is that BOD ought to be related to the dissolved solids. We'll assume that a linear relationship exists of the form

```
[BOD] = alpha*[solids] + beta
```

where alpha and beta are to be determined from the data. Our first step is to examine the data to see if this is a plausible model.

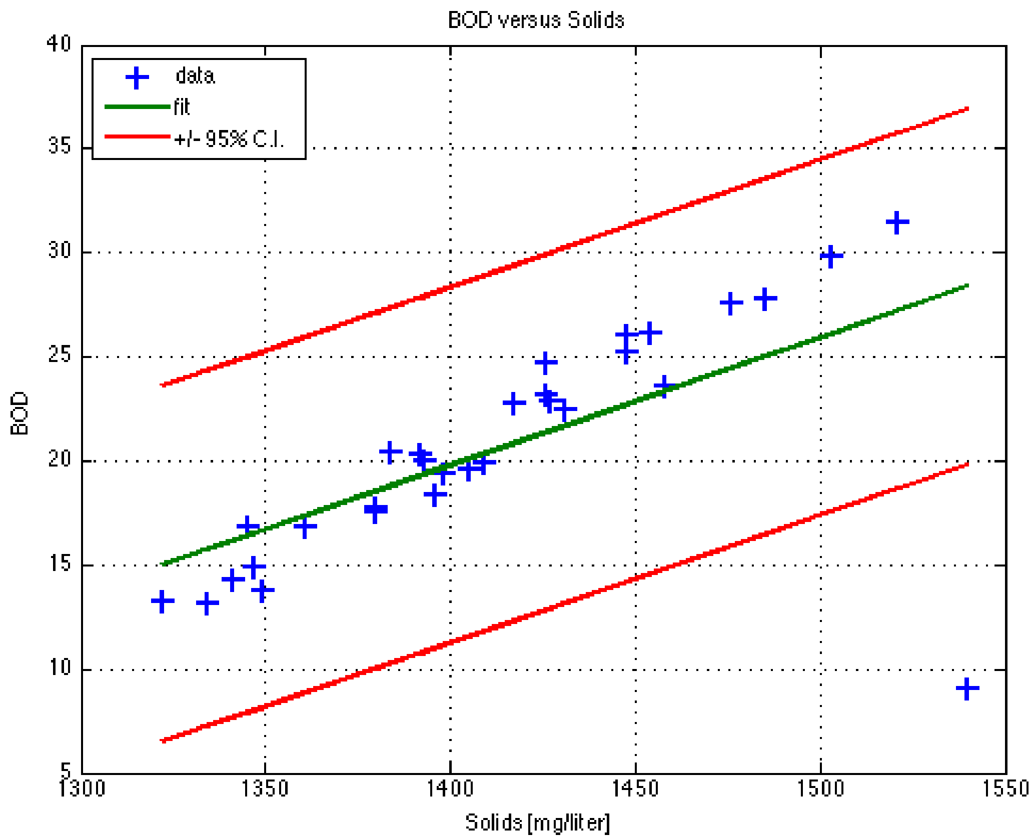
```
BOD = data(:,1);
solids = data(:,2);
N = length(BOD);

figure(1); clf;
plot(solids,BOD,'.','Markersize',20);
xlabel('Solids [mg/liter]');
ylabel('BOD');
title('BOD versus Solids');
grid;
```



Model fitting

Our initial conclusion is that the data appears consistent with a linear relationship, though there is at least one point that may be an outlier. Let's first do a least squares fit using all of the data.

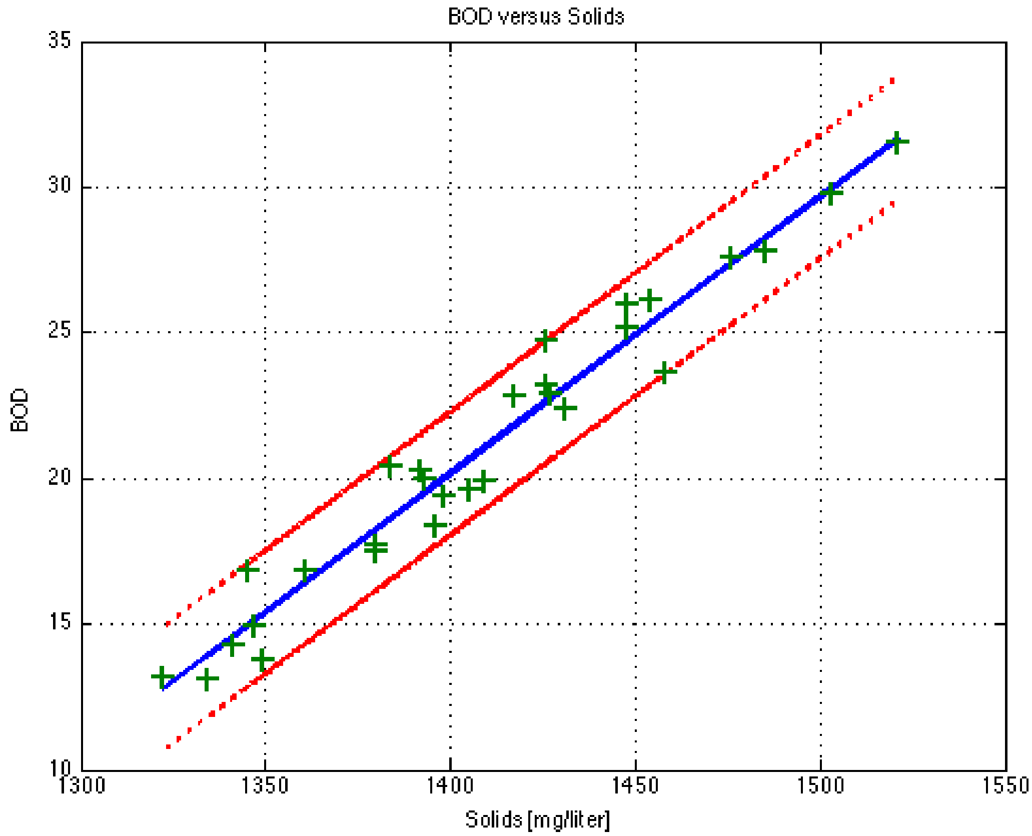
```
% create data matrix where the unknown parameters are stored in x such that
% Ax = b + e where are model/measurement errors and
%
%   x(1) : alpha
%   x(2) : beta

A = [solids ones(N,1)];
b = [BOD];

% least squares solution for x = [alpha;beta]
x = A\b;

% residuals
e = b - A*x;
s = std(e);
t95 = tinv(0.975,N-2);

plot(solids,BOD,'+', ...
     solids,A*x,'-', ...
     solids,A*x + t95*s, 'r-', ...
     solids,A*x - t95*s, 'r-', ...
     'Markersize',10,'Linewidth',2);

xlabel('Solids [mg/liter]');
ylabel('BOD');
title('BOD versus Solids');
legend('data','fit','+/- 95% C.I.','Location','NW');
grid;
```



Remove Outliers

Remove all points that lie outside of the 99% confidence interval

```
t99 = tinv(0.995,N-2);
idx = find(abs(e) < t99*s);

% data matrix
A = [solids(idx) ones(length(idx),1)];
b = [BOD(idx)];

% least squares solution
x = A\b;

% error bounds
e = b - A*x;
s = std(e);
t95 = tinv(0.025,N-2);

% plotting
plot(solids(idx),A*x,'-', ...
     solids(idx),A*x + t95*s, 'r:', ...
     solids(idx),A*x - t95*s, 'r:', ...
     solids(idx),BOD(idx),'+','Markersize',10,'Linewidth',2);
xlabel('Solids [mg/liter]');
ylabel('BOD');
title('BOD versus Solids');
grid;
```



error estimates

```
K = 1000;
xs = zeros(K,length(x));
n  = size(idx,1);

for k = 1:K

    ndx = idx(randsample(n,n,1));

    A = [solids(ndx) ones(n,1)];
    b = [BOD(ndx)];

    % least squares solution
    x = A\b;
    xs(k,:) = x';

end
```

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