3 INTERPOLATION/FITTING

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Initialization

```
% reduce needless whitespace
format compact
% reduce irritations
more off
% start a diary
% diary lectureN.txt
```

THE PROBLEM WE WANT TO SOLVE

Assume that we have placed a hot bar with its ends in contact with ice water. The temperature of the bar will then decay over time to 0 degrees Centigrade. We have measured the temperature of the center of the bar at 6 times spaced half a minute apart. Taking the first of these times as time zero, the measured data are:

time:	0	0.5	1	1.5	2	minutes
Temperature:	14.60	8.42	4.86	2.80	1.62	Centigrade

We will define tMeasured and TMeasured as the six measured times and temperatures respectively.

Unknown to us, the exact temperature is given by

TExact = $14.6 \exp(-1.1 t)$

However, we only know the measured temperatures.

To make things easier, we will create a function TExactFun to evaluate the exact temperature that we pretend not to know. Since the function is very simple and not intended for more general use, we do not need to create an m file for it. Instead we can define TExactFun as a "handle" to an anonymous function.

```
% define tMeasured and TMeasured as given
tMeasured=\begin{bmatrix} 0 & 0.5 & 1 & 1.5 & 2 \end{bmatrix};
TMeasured=\begin{bmatrix} 14.60 & 8.42 & 4.86 & 2.80 & 1.62 \end{bmatrix};
% define TExactFun as a handle to an anonymous function
TExactFun = @(t) = 14.6 * \exp(-1.1 * t);
```

PLOT TO UNDERSTAND THE PROBLEM BETTER

Let's plot the measured five values versus the exact solution that we pretend not to know.

```
% generate 100 time values between 0 and 2
tPlot=linspace(0,2,100)';
% generate corresponding exact temperatures
TExactPlot=TExactFun(tPlot);
% create the plot, using circles for the measured points
plot(tPlot, TExactPlot, ':k',...
tMeasured, TMeasured, 'om')
legend('Exact', 'Measured')
title('Measured versus exact temperatures')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
```



INTERPOLATION

We would like to be able to evaluate the temperature at times in between the measured five times. This is called "interpolation". For example, let's assume that we want to know the temperature at time 0.7, which is in between measured times 0.5 and 1. Matlab provides 'interp1' or 'spline' to find it.

```
% let 's evaluate T at t=0.7 using two different methods
t=0.7
TLinear=interp1(tMeasured,TMeasured,t)
TSpline=spline(tMeasured,TMeasured,t)
% two reasonable values, but which one is best???
TExact=TExactFun(t)
disp('For a nice smooth curve, spline interpolation is')
disp('much more accurate than linear interpolation!')
```

Compare the interpolations in a plot

```
% find the interpolated values at the plot times
TLinearPlot=interp1(tMeasured,TMeasured,tPlot);
TSplinePlot=spline(tMeasured,TMeasured,tPlot);
% compare the interpolations in a plot
plot(tPlot,TExactPlot,':k',...
tMeasured,TMeasured,'om',...
tPlot,TLinearPlot,'r',...
tPlot,TSplinePlot,'b')
legend('Exact','Measured','Linear','Spline')
title('Linear and spline interpolation')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
```

EXTRAPOLATION

Suppose that the time at which we want to know the temperature is t = 5. This time is not inside the measured range from 0 to 2. If that happens, we talk about *extrapolation* instead of *interpolation*.

Extrapolation is much trickier than interpolation.

For that reason, interp1 refuses to do it unless you specify an additional "extrap" parameter.



```
% evaluate the values at t = 5
t=5
TLinear=interp1(tMeasured,TMeasured,t,'linear','extrap')
TSpline=spline(tMeasured,TMeasured,t)
TExact=TExactFun(t)
disp('Extrapolation is usually bad news!')
% Note that both linear and spline values are bad, and
% that the spline is much worse than linear. But both
% values are useless.
```

t = 5TLinear = -5.4600 TSpline = -14.700 TExact = 0.059667 Extrapolation is usually bad news!

NOISY DATA

What if the measured data have random errors? Suppose, for example, that the digital thermometer used to to measure the data only displays whole degrees

C? Then the measured data:

Temperature: 14.60 8.42 4.86 2.80 1.62 Centigrade

become:

Temperature: 15 8 5 3 2 Centigrade

Then what happens to our interpolations?

```
\% correct the measured data list
TMeasured = [15 \ 8 \ 5 \ 3 \ 2]';
\% interpolate again at 0.7
t = 0.7
TLinear=interp1(tMeasured, TMeasured, t)
TSpline=spline(tMeasured, TMeasured, t)
TExact=TExactFun(t)
disp('Now the linear interpolation is actually better!');
% compare the interpolations in a plot
TLinearPlot=interp1(tMeasured, TMeasured, tPlot);
TSplinePlot=spline(tMeasured, TMeasured, tPlot);
plot(tPlot, TExactPlot, ':k',...
     tMeasured, TMeasured, 'om',...
     tPlot, TLinearPlot, 'r',...
     tPlot, TSplinePlot, 'b')
legend('Exact', 'Measured', 'Linear', 'Spline')
title('Linear versus spline interpolation')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
% Because of the noise, the spline can be worse than
% linear. The spline may also start oscilating if things
% get really bad. Note the poor slope of the spline near
% time 2.
\% compare the _maximum_ deviations
ErrLinear=max(abs(TLinearPlot-TExactPlot))
ErrSpline=max(abs(TSplinePlot-TExactPlot))
disp('There is no longer a real difference.')
% The maximum deviations are practically speaking the
% same.
         There is no good reason to use spline
% interpolation instead of the simpler linear
% interpolation.
```



CURVE FITTING

If we want to get a better predictions for the temperature given the noisy data, we must drop the assumption in interp1 and spline that the approximating curve goes to through all the measured points.

What we can do instead is find a relatively *simple* curve that is as close as possible to the data points. That is called "curve fitting".

In particular, recall that the exact temperature curve is given by

TExact = 14.6 exp(-1.1 t)

However, we are assuming that we do not know that. And given only our noisy data, there is *no way* to figure out that the above is the exact temperature.

But suppose that we assume (based on theoretical arguments not of importance here) that the desired temperature is of the form

T = A exp(B t)

and we then choose values for the constants A and B as well as we can based on our noisy data? That is likely to give a much better approximation than linear or spline interpolation.

Of course, the devil is in the details. Note first that with only 2 constants A and B and 5 noisy temperatures, there is no way that the expression above can reproduce all 5 noisy temperatures. You cannot solve 5 equations for 2 unknowns. You could select only 2 of the 5 temperatures and ignore the other 3, but which 2? If you are very lucky you could get a quite good approximation, but if you are not, you would get unnecessarily big errors.

It is a much better idea to use *all* the 5 data you have, and make TExpFit approximate them *on average* as well as it can. Typically, numerical analysist take "on average" to mean that they make the average *square* error as small as possible. There are both theoretical and practical reasons to do that. Theoretically, in simple cases where the errors are really random, this gives the best approximation possible. Practically, the mathematics of making the average *square* error as small as possible is a lot simpler than other possibilities (like making the maximum error as small as possible).

We do not really need to worry about the latter anyway, as Matlab does that work for us. What we should get away with is that what we are going to do is popularly known as the "Method of Least Squares". (Though "Method of Least Average Square Error" would be more accurate.)

Line fitting

Finding the best exponential approximation of the form

```
T = A \exp(B t), call it TExpFit
```

is actually somewhat messy. So we will restrict ourself to simpler approximations. And the simplest possible one is surely approximation be a straight line,

T = C1 t + C2, call it TLinFit

Note that the expression above is *linear* in the coefficients C1 and C2 to find. That is unlike TExpFit where the coefficient B is inside an exponential, and then multiplied by A to boot. If the expression is linear in terms of the unknown coefficients, numerical analysists speak of "linear regression". That is another term you should try to remember.

Noting that a straight line is a polynomial of degree 1 (since the highest power of x is 1), we can first use Matlab function 'polyfit' to find the coefficients C1 and C2 and then 'polyval' to find the approximate temperature values

|% find the coefficients C1 and C2 of the line

```
n = 1;
CoefLin=polyfit(tMeasured, TMeasured, n)
\% interpolate again at 0.7
t = 0.7
TLinFit=polyval(CoefLin,t)
TExact=TExactFun(t)
disp('That is horrible!')
% let's see the linear fit in a plot
TLinFitPlot=polyval(CoefLin, tPlot);
plot(tPlot, TExactPlot, ':k',...
     tMeasured , TMeasured , 'om ' \,,\ldots
     tPlot, TLinFitPlot, 'r')
legend('Exact', 'Measured', 'Linear fit')
title ('Linear least-square approximation')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
% print the error
ErrLinFit=max(abs(TLinFitPlot-TExactPlot))
disp('That is horrible, but what do you expect?')
% Clearly, a straight line cannot approximate the exact
\% curve to a reasonable amount.
```

```
CoefLin =

-6.2000 12.8000

t = 0.70000

TLinFit = 8.4600

TExact = 6.7600

That is horrible!

ErrLinFit = 1.8000

That is horrible, but what do you expect?
```

Fitting with a parabola

We can improve things quite a lot by approximating with a quadratic polynomial, i.e. a parabola,

 $T = C1 t^2 + C2 t + C3$, call it TParFit

instead of a straight line.

% find coefficients C1, C2, and C3 $n\!=\!2;$



% summarize the conclusion

disp('Not too bad, but the maximum error, at t=2, is
quite big.')



Fitting with a quartic

.

Let's try fitting with a quartic,

 $TQuartFit = C1 x^{4} + C2 x^{3} + C3 x^{2} + C4 x + C5$

Note however, that now we are no longer *fitting*, but *interpolating*. With 5 unknown coefficients, the quartic can go through all 5 measured data points. This is usually a very bad idea.

In this particular case, the results below are much better than I expected. Fitting curves with too many coefficients can give very bad results. In this case the only real problem is the slope at t = 2. It might have been much worse. The general rule of thumb is:

Do not interpolate a polynomial of degree more than about the square root of the number of data points

Since we have 5 data points and sqrt(5) is about 2, we should not fit a polynomial of a degree greater than 2. Exceptions confirm the rule.

```
\% find the 5 coefficients
n=4:
CoefQuart=polyfit (tMeasured, TMeasured, n)
\% interpolate again at 0.7
t = 0.7
TQuartFit=polyval(CoefQuart,t)
TExact=TExactFun(t)
% let's see the quartic fit in a plot
TQuartFitPlot=polyval(CoefQuart, tPlot);
plot(tPlot, TExactPlot, ':k',...
     tMeasured, TMeasured, 'om',...
     tPlot, TQuartFitPlot, 'r')
legend('Exact', 'Measured', 'Quartic fit')
title ('Quartic least-square approximation')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
% print the error
ErrQuartFit=max(abs(TQuartFitPlot-TExactPlot))
```

Extrapolation again

We already saw that extrapolation, i.e. evaluating outside the given range is fraught with peril. Let's try the fitted polynomials now.

```
\% \ extrapolate again at t = 5
t=5
```



TLinear=interp1(tMeasured,TMeasured,t,'linear','extrap') TSpline=spline(tMeasured,TMeasured,t) TParFit=polyval(CoefPar,t) TQuartFit=polyval(CoefQuart,t) TExact=TExactFun(t)

 $\begin{array}{rll} t &=& 5 \\ TLinear &=& -4 \\ TSpline &=& 59 \\ TParFit &=& 39.371 \\ TQuartFit &=& 395.00 \\ TExact &=& 0.059667 \end{array}$

Derivatives

Sometimes we are interested in the derivative of the quantity in question. In the present example, it is a measure of how much heat leaks out of the bar per unit time.

Since

TExact = 14.6 exp (-1.1 t)

its derivative is simply

- 1.1 TExact

(That follows from differentiating the exponential using the chain rule.)

For the linear, quadratic, and quartic fits, we can use the fact that 'polyder' will find the coefficients of the derivative polynomial for us.

How about the derivative of your beloved interpolated spline? Well, linear and spline interpolation are described by "piecewise polynomials": there is a different polynomial in each segment between measured points. The bad thing is that the idiots at MathWorks never defined a function to find the derivatives of piecewise polynomials. If you want the derivative of your spline, look for 'ppder' or 'ppdiff' provided by third parties, (where pp is an acronym for "piecewise polynomial".) (Octave provides ppder.)

```
% derivative of TExact
derTExactPlot=-1.1*TExactPlot;
% derivative of TParFit
derCoefPar=polyder(CoefPar);
derTParFitPlot=polyval(derCoefPar,tPlot);
% derivative of TQuartFit
derCoefQuart=polyder(CoefQuart);
derTQuartFitPlot=polyval(derCoefQuart, tPlot);
% plot it
plot(tPlot, derTExactPlot, ':k',...
     tPlot, derTParFitPlot, 'r',...
     tPlot, derTQuartFitPlot, 'b')
legend('Exact', 'Quadratic fit', 'Quartic fit')
title ('Comparison of predicted first derivative')
xlabel('t (minutes)')
ylabel('dT/dt (Centigrade/min)')
legend('location', 'southeast')
```

Integrals

Suppose we want to know how much radiation the bar emits per unit surface area while cooling down. Assuming that the bar surface is perfectly black, the Stefan-Boltzmann law says that the radiation emitted per unit area and unit time is given by

 $qdot = sigma T^4$

where sigma is the Stefan-Boltzmann constant with value given below, and T is the absolute temperature.



So to get the desired radiation q, given our temperature,

- convert Centigrade to Kelvin by adding T0 = 273.15
- raise that to power 4 (square twice)
- integrate that from t = 0 to t = 2
- multiply by 60 to convert dt to seconds
- multiply by sigma (let's do that last)

Matlab can do the integration of the temperatures for us using 'integral' if we provide the function to integrate.

Note: Octave still uses the old name 'quad' instead of 'integral'. Note that **all** values below are pretty accurate. This is typical:

Numerical errors tend to become less important in integrals, and **more** important in derivatives.

```
% the Stefan-Boltzmann constant in W/m<sup>2</sup> K<sup>4</sup>:
sigma=5.670373E-8;
% 0 degrees Centigrade in Kelvin
T0=273.15;
```

```
% Let's find the exact integral first using our
% knowledge of Calculus I. To integrate
%
       integral (A \exp(Bt)+T0)^{4} dt
\% change variable to u = A \exp(Bt), etc:
\% names for the constants in TExact = A exp(B t)
A = 14.6;
B = -1.1;
\% evaluate the end values of u
u1=A;
u2 = A * exp(B * 2);
% evaluate the integral as found by calculus
qExactExact = (...
    1/4*(u2^4-u1^4)+...
    4/3 * T0 * (u2^3 - u1^3) + \dots
    3*T0^{2}*(u2^{2}-u1^{2})+...
    4*T0^{3}(u2-u1) + ...
    T0^4*(\log(u2)-\log(u1)))/B*60*sigma
% Next let's use numerical integration, i.e. 'integral'
\% or 'quad', to find the integral. Note that there will
% be an error created by the numerical integration, even
% if we integrate the exact temperature.
% try numerical integration of the exact temperature
qExactNum=quad(@(t) (TExactFun(t)+T0).^4, 0, 2)*60*sigma
disp('As shown, numerical integration for a smooth')
disp('function like this will be very accurate.')
disp('The error is smaller than the round-off.')
% try numerical integration of the linear interpolation
qLinNum=quad(@(t) (interp1(tMeasured, TMeasured, t)+T0)
   (^{4}, 0, 2) * 60 * sigma
% try numerical integration of the spline interpolation
qSplineNum=quad(@(t) (spline(tMeasured, TMeasured, t)+T0)
   (^{4}, 0, 2) * 60 * sigma
% try numerical integration of the parabolic fit
qParNum=quad(@(t) (polyval(CoefPar, t)+T0).^4, 0, 2)*60*
   sigma
% try numerical integration of the quartic fit
```

 $\begin{array}{l} qQuartNum=quad(@(t) (polyval(CoefQuart,t)+T0).^4,0,2)*60*\\ sigma \end{array}$

MORE MEASUREMENTS

If we would measure a lot more points than the five we have, and the errors in these measurements would be random, we could get a much better approximation.

Unfortunately, rounding of temperatures to whole degrees is **not** random. It creates a deterministic "staircase" of numbers. But we can try anyway.

```
% Note: We will cheat, and use the exact solution, which
% we are not supposed to know, to avoid doing and typing
% in 50 measurements.
% create the new "measured" data
tMeasured=linspace(0,2,50)';
% 'round' rounds to whole numbers
TMeasured=round(TExactFun(tMeasured));
% use some more plot points now
tPlot=linspace(0,2,200)';
TExactPlot=TExactFun(tPlot);
```

Quartic fit with more noisy data

```
% repeat the quartic fit
n=4;
CoefQuart=polyfit(tMeasured,TMeasured,n)
% compare the interpolations in a plot
TQuartFitPlot=polyval(CoefQuart,tPlot);
plot(tPlot,TExactPlot,':k',...
```

```
tMeasured,TMeasured,'om',...
tPlot,TQuartFitPlot,'r')
legend('Exact','Measured','Quartic fit')
title('Quartic least-square approximation')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
ErrQuartFit=max(abs(TQuartFitPlot-TExactPlot))
```



Quintic fit with more noisy data

With the additional data, we can try a quitic (5th degree) fit now. But do not even **think** about interpolating a polynomial of degree 49. It would just crash.

% create the fit n=5; CoefQuint=**polyfit**(tMeasured,TMeasured,n)

```
% compare the interpolations in a plot
TQuintFitPlot=polyval(CoefQuint,tPlot);
plot(tPlot,TExactPlot,':k',...
tMeasured,TMeasured,'om',...
tPlot,TQuintFitPlot,'r')
legend('Exact', 'Measured', 'Quintic fit')
title('Quintic least-square approximation')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
ErrQuintFit=max(abs(TQuintFitPlot-TExactPlot))
disp('The disappointing result is due to the fact that')
disp('The final "measured" points are all too high.')
disp('Have a good look at the end of the graph!')
```



Interpolation with more noisy data

Note also that interpolations would *not* improve if we used more points.

```
% compare the interpolations in a plot
TLinearPlot=interp1(tMeasured,TMeasured,tPlot);
TSplinePlot=spline(tMeasured,TMeasured,tPlot);
plot(tPlot,TExactPlot,':k',...
tMeasured,TMeasured,'om',...
tPlot,TLinearPlot,'r',...
tPlot,TSplinePlot,'b')
legend('Exact','Measured','Linear','Spline')
title('Linear and spline interpolation ')
xlabel('t (minutes)')
ylabel('T (Centigrade)')
% Note that here the spline interpolation is definitely
% worse than linear, though not by much. (Except if you
% looked at the derivative.)
```



ADDITIONAL REMARKS

Often you would want your spline to satisfy end conditions. For example, you might want it to have given derivatives at the ends. Or be periodic. Given derivatives at the ends can be achieved using 'spline' if you add the desired two values to the function values list. For more complicated cases, consider function 'csape'.

End lesson 3