Math 541 - Numerical Analysis

Population Growth and Planets Examples

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Yeast Population

Yeast Population: Suppose that a yeast population is given by the following table.

t (hr)	p	t (hr)	p	t (hr)	p
0	0.95	7	8.1	14	26.1
1	1.4	8	10.1	15	28.1
2	1.9	9	12.6	16	29.8
3	2.5	10	15.5	17	31.1
4	3.4	11	18.4	18	32.1
5	4.6	12	21.2	19	32.9
6	6.2	13	23.9	20	33.4

We combine a number of numerical methods to approximate when this population is ***growing most rapidly***.

Growth of Yeast 1

Growth of Yeast: To find the growth rate of the yeast, we convert the discrete data into derivatives from the population data.

The easiest method is the ***two point central difference*** ($\mathcal{O}\left(h^2\right)$).

For data p_i at time t_i, we approximate the derivative at the midpoint between two successive times:

$$g(s_i) = p'(s_i) \approx \frac{p(t_{i+1}) - p(t_i)}{t_{i+1} - t_i}, \qquad \text{where} \quad s_i = \frac{t_{i+1} + t_i}{2}.$$

```
function [t2d,g2pd] = der2pt(td,pd)
%Computes central difference between 2 pts
N = length(td);
for i=1:N-1
    t2d(i) = (td(i)+td(i+1))/2;
    g2pd(i) = (pd(i+1)-pd(i))/(td(i+1)-td(i));
end
end
```


Growth of Yeast 2

Growth of Yeast: The program converts the population data into growth data.

t (hr)	$g(t)$	t (hr)	$g(t)$	t (hr)	$g(t)$
0.5	0.45	7.5	2	14.5	2
1.5	0.5	8.5	2.5	15.5	1.7
2.5	0.6	9.5	2.9	16.5	1.3
3.5	0.9	10.5	2.9	17.5	1
4.5	1.2	11.5	2.8	18.5	0.8
5.5	1.6	12.5	2.7	19.5	0.5
6.5	1.9	13.5	2.2		

We use our **least squares techniques** to fit ***polynomials*** through these approximations, and the ***polynomials*** are easily ***differentiated*** to find the ***maximum growth rate***.

Growth of Yeast–Polynomial Fit

Two point central difference approximations to the ***derivative*** are fit with ***polynomials*** for with the ***least squares techniques***.

Quadratic fit with $SSE = 1.4893$,

$$g(t) = -0.02636t^2 + 0.5519t - 0.3839.$$

Cubic fit with $SSE = 1.2431$,

$$g(t) = -0.0007469t^3 - 0.003951t^2 + 0.3724t - 0.08254.$$

Quartic fit with $SSE = 0.2038$,

$$g(t) = 0.0003108t^4 - 0.01318t^3 + 0.1562t^2 - 0.3438t - 0.6501.$$

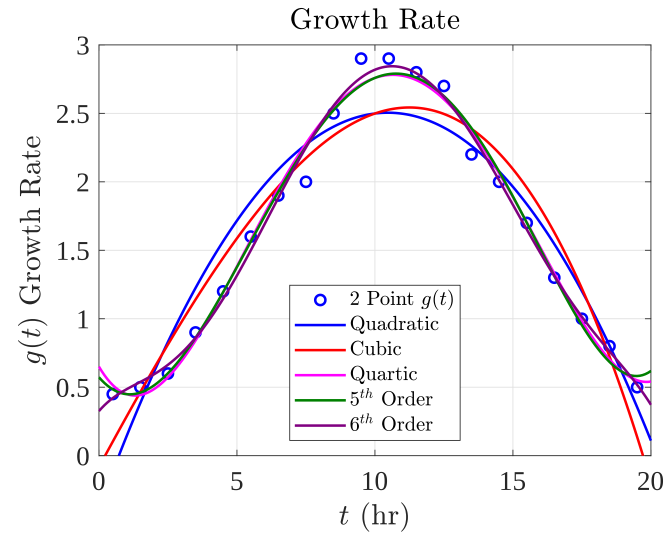
5^{th}***-Order fit*** with $SSE = 0.1957$,

$$g(t) = 0.000005636t^5 + 0.00002903t^4 - 0.008159t^3 + 0.1183t^2 - 0.2337t + 0.5727.$$

6^{th}***-Order fit*** with $SSE = 0.1422$,

$$g(t) = -3.029\times10^{-6}t^6+1.874\times10^{-4}t^5-0.004112t^4+0.03632t^3-0.1076t^2+0.2345t+0.3257.$$

Growth of Yeast–Polynomial Fit



Growth of Yeast 3

Growth of Yeast: We developed higher order differentiation techniques, including the ***best three point differences*** for approximating the ***derivative*** $(\mathcal{O}(h^3))$ through the yeast data:

```
function g3pd = der3pt(td,pd)
%Computes best 3 pt derivative for evenly spaced ...
    time data
N = length(pd);
h = td(2)-td(1);
for i=1:N
    if (i==1)
        g3pd(1) = 1/(2*h)*(-3*pd(1)+4*pd(2)-pd(3));
    elseif (i==N)
        g3pd(N) = ...
            1/(2*h)*(pd(N-2)-4*pd(N-1)+3*pd(N));
    else
        g3pd(i) = 1/(2*h)*(-pd(i-1)+pd(i+1));
    end
end
```


Growth of Yeast 4

Growth of Yeast: The program converts the population data into growth data using the ***best three point derivative approximations***.

t (hr)	$g(p)$	t (hr)	$g(p)$	t (hr)	$g(p)$
0	0.425	7	1.95	14	2.1
1	0.475	8	2.25	15	1.85
2	0.55	9	2.7	16	1.5
3	0.75	10	2.9	17	1.15
4	1.05	11	2.85	18	0.9
5	1.4	12	2.75	19	0.65
6	1.75	13	2.45	20	0.35

Again our **least squares techniques** fit ***polynomials*** through these approximations, and the ***polynomials*** are easily ***differentiated*** to find the ***maximum growth rate***.

Growth of Yeast–Polynomial Fit

Best three point difference approximations to the ***derivative*** are fit with ***polynomials*** for with the ***least squares techniques***.

Quadratic fit with $SSE = 1.7112$,

$$g(t) = -0.02436t^2 + 0.5073t - 0.1837.$$

Cubic fit with $SSE = 1.3826$,

$$g(t) = -0.0007263t^3 - 0.002572t^2 + 0.3372t + 0.06466.$$

Quartic fit with $SSE = 0.1680$,

$$g(t) = 0.0002688t^4 - 0.01148t^3 + 0.1336t^2 - 0.2350t + 0.5112.$$

5^{th}***-Order fit*** with $SSE = 0.1614$,

$$g(t) = 0.000003878t^5 + 0.00007488t^4 - 0.008067t^3 + 0.1088t^2 - 0.1705t + 0.4825.$$

6^{th}***-Order fit*** with $SSE = 0.07863$,

$$g(t) = -2.712\times10^{-6}t^6 + 1.666\times10^{-4}t^5 - 0.003595t^4 + 0.03024t^3 - 0.07332t^2 + 0.1488t + 0.4006.$$

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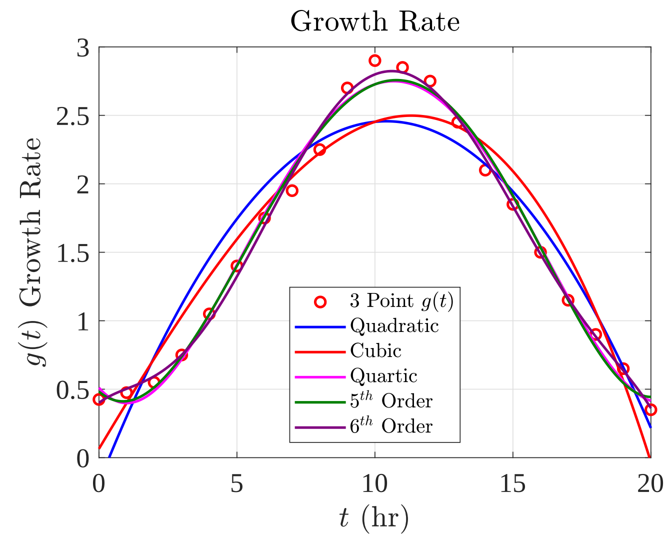
Growth of Yeast–Polynomial Fit



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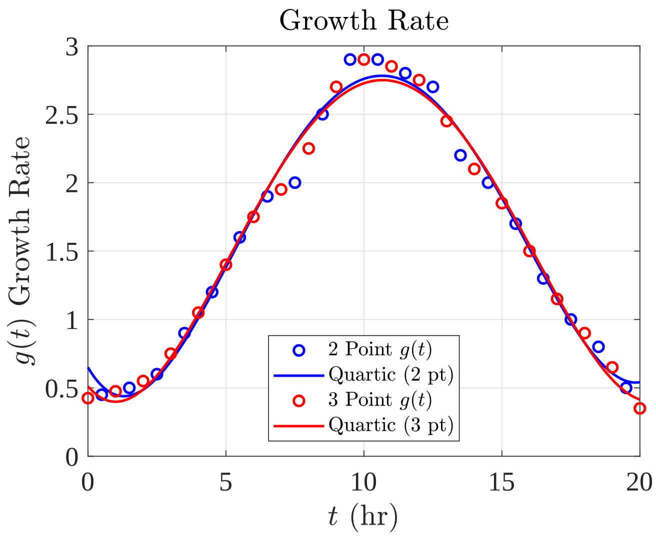
Growth of Yeast–Polynomial Fit



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Maximum Growth of Yeast

Maximum Growth of Yeast: The best nonlinear fitting model to the data is given by:

$$p(t) = \frac{34.9786}{1 + 34.1387e^{-0.32995t}},$$

which has a maximum growth rate of

$$p'(t_{max}) = 2.8853 \qquad \text{at} \quad t_{max} = 10.6998.$$

Below is a Table of the Maximum growth rates computed from the n^{th} order polynomial approximations of the growth rates.

n	$t2_{max}$	$g2_{max}$	$t3_{max}$	$g3_{max}$
2	10.4685	2.5047	10.4111	2.4569
3	11.2475	2.5428	11.3147	2.4982
4	10.6511	2.7813	10.6782	2.7496
5	10.7621	2.7902	10.7776	2.7572
6	10.6183	2.8441	10.6113	2.8231

where $(t2_{max}, g2_{max})$ is the time and value of the ***2 point derivative*** maximum growth rate, and $(t3_{max}, g3_{max})$ is the time and value of the ***3 point derivative*** maximum growth rate.

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BIC and AIC

BIC and AIC: We apply the Bayesian and Akaike Information Criteria to the polynomial fits to the growth calculations using the ***2 point*** and ***3 point derivative*** formula.

The polynomial of order n has $k = n + 1$ parameters. The Table below shows the sum of square errors, the information criteria for all the fits made.

k	SSE2	BIC2	AIC2	SSE3	BIC3	AIC3
3	1.489	-42.961	10.809	1.711	-48.120	12.942
4	1.243	-43.579	9.195	1.383	-53.348	10.463
5	0.204	-76.750	-24.971	0.168	-100.771	-31.796
6	0.196	-74.564	-23.781	0.161	-101.643	-30.643
7	0.142	-77.959	-28.172	0.0786	-116.904	-43.742

This Table suggests that the 6^{th} order polynomial with the best fitting ***3 point derivative*** formula gives the best estimate of the growth rate, which is consistent with the studies performed.

Planets Example

This problem examines ***Kepler's Third Law***.

We use the ***power law*** to determine the ***period of orbit*** about the **sun** for all ***planets*** given information about some of the planets.

Let d be the mean distance $\times 10^6$ km from the sun and p be the period of orbit in (Earth) days about the sun.

Planet	Distance d	Period p
Mercury	57.9	87.96
Earth	149.6	365.25
Jupiter	778.3	4337
Neptune	4497	60200

Allometric Model

We seek an ***Allometric model*** of the form:

$$p = kd^a.$$

By taking ***logarithms***, we have:

$$\ln(p) = \ln(k) + a\ln(d),$$

which is ***linear*** in the logarithms of the data.

Below is the Table of the ***logarithms of the data***.

Planet	$\ln(d)$	$\ln(p)$
Mercury	4.058717	4.476882
Earth	5.007965	5.900582
Jupiter	6.657112	8.374938
Neptune	8.411166	11.005428

Direct Linear Least Squares

The logarithmic model is:

$$\ln(p) = \ln(k) + a\ln(d),$$

so if $P_i = \ln(p_i)$, $D_i = \ln(d_i)$, and $K = \ln(k)$, the **Linear Least Squares model**, $P = K + a\,D$, satisfies the error:

$$E(K, a) = \sum_{i=0}^{n} [(K + a\,D_i) - P_i]^2$$

This is minimized for data set $(D_i, P_i), i = 0, ..., 3$.

Earlier we saw an easy formulation without matrices:

Define the averages

$$\bar{D} = \frac{1}{4}\sum_{i=0}^{3} D_i \quad \text{and} \quad \bar{P} = \frac{1}{4}\sum_{i=0}^{3} P_i.$$

The best fitting slope and intercept are

$$a = \frac{\sum_{i=0}^{3}(D_i - \bar{D})P_i}{\sum_{i=0}^{3}(D_i - \bar{D})^2} \quad \text{and} \quad K = \bar{P} - a\bar{D}.$$

Direct Linear Least Squares

The ***Allometric model*** is:

$$p = k\,d^a.$$

The averages ($\ln(d_i)$ and $\ln(p_i)$) are

$$\bar{D} = \frac{1}{4}\sum_{i=0}^{3} D_i = 6.03374 \qquad \text{and} \qquad \bar{P} = \frac{1}{4}\sum_{i=0}^{3} P_i = 7.43946.$$

The best fitting slope is

$$\begin{aligned} a &= \frac{\sum_{i=0}^{3}(D_i - \bar{D})P_i}{\sum_{i=0}^{3}(D_i - \bar{D})^2} \\ &= \frac{(4.05872 - \bar{D})4.47688 + (5.00797 - \bar{D})5.90058 + (6.65711 - \bar{D})8.37494 + (8.41117 - \bar{D})11.00543}{(4.05872 - \bar{D})^2 + (5.00797 - \bar{D})^2 + (6.65711 - \bar{D})^2 + (8.41117 - \bar{D})^2} \\ &= 1.50001. \end{aligned}$$

The best intercept is

$$\ln(k) = K = \bar{P} - a\bar{D} = 7.43946 - 1.50001(6.03374) = -1.61124,$$

so $k = 0.199639$, giving ***Kepler's Law***:

$$p = 0.199639 d^{1.5}.$$