## AM205 HW1. Data fitting. Solution

## P1. Polynomial approximation of the gamma function

(a) We consider finding a polynomial $g(x)=\sum_{k=0}^{4} p_{k} x^{k}$ that fits the data points $(\mathrm{j}, \Gamma(\mathrm{j}))$ for $j=1,2,3,4,6$. Since here are a small number of data points, we can use the Vandermonde matrix to find the coefficients of the interpolating polynomial $g(x)=\sum_{k=0}^{4} g_{k} x^{k}$. The linear system is

$$
\left[\begin{array}{ccccc}
1 & 1 & 1 & 1 & 1  \tag{1}\\
1 & 2 & 4 & 8 & 16 \\
1 & 3 & 9 & 27 & 81 \\
1 & 4 & 16 & 64 & 256 \\
1 & 6 & 36 & 216 & 1296
\end{array}\right]\left[\begin{array}{l}
g_{0} \\
g_{1} \\
g_{2} \\
g_{3} \\
g_{4}
\end{array}\right]=\left[\begin{array}{c}
1 \\
1 \\
2 \\
6 \\
120
\end{array}\right]
$$

The program gamma p1_gamma.py solves this system, and shows that the coefficients are $g_{0}=17.8, g_{1}=-34.917, g_{2}=24.458, g_{3}=-7.0833, g_{4}=0.74167$
(b) We now consider finding a polynomial $p(x)=\sum_{k=0}^{4} p_{k} x^{k}$ that fits the transformed data points $(\mathrm{j}, \log (\mathrm{j}))$ for $\mathrm{j}=1,2,3,4,6$. The coefficients are given by

$$
\left[\begin{array}{ccccc}
1 & 1 & 1 & 1 & 1  \tag{2}\\
1 & 2 & 4 & 8 & 16 \\
1 & 3 & 9 & 27 & 81 \\
1 & 4 & 16 & 64 & 256 \\
1 & 6 & 36 & 216 & 1296
\end{array}\right]\left[\begin{array}{l}
p_{0} \\
p_{1} \\
p_{2} \\
p_{3} \\
p_{4}
\end{array}\right]=\left[\begin{array}{c}
\log 1 \\
\log 1 \\
\log 2 \\
\log 6 \\
\log 120
\end{array}\right]
$$

We get the coefficients as $p_{0}=1.1274, p_{1}=-1.8725, p_{2}=0.848, p_{3}=-0.10902, p_{4}=$ 0.006107
(c) The plots of three functions and relative errors are as follows


(d) Maximum relative error: 0.69894 for $g(x), 0.027223$ for $h(x)$. The more accurate approximation is $h(x)$.

## P2. Error bounds with Lagrange polynomials

(a) and (b) The following figure shows the Lagrange polynomial $p_{3}(x)$ over the true function $f(x)$ using a slightly modified version of the in-class code example. Running the code, the infinity norm of the error is approximately 6.04238 .

(c) The difference between $\mathrm{f}(\mathrm{x})$ and and the interpolating polynomial $p_{n-1}(x)$ can be expressed as

$$
\begin{equation*}
f(x)-p_{n-1}(x)=\frac{f^{(n)}(\theta)}{n!} \prod_{i=1}^{n}\left(x-x_{i}\right) \tag{3}
\end{equation*}
$$

where $\theta$ is a specific value within the interval from -1 to 1 . To obtain a bound on $\| f-$ $p_{n-1} \|_{\infty}$, we consider the magnitude of the terms on the right hand side. Since the $x_{i}$ are at the roots of the $n$-th Chebyshev polynomial $T_{n}(x)$, it follows that the product is a scalar multiple of this polynomial

$$
\begin{equation*}
\prod_{i=1}^{n}\left(x-x_{i}\right)=\lambda T_{n}(x) \tag{4}
\end{equation*}
$$

where $\lambda$ is some scaling constant. The coefficient in front of $x^{n}$ on the left hand side is 1 . Using properties of Chebyshev polynomials, the coefficient of $x^{n}$ in $T_{n}(x)$ is $2^{n-1}$. Hence $\lambda=2^{-(n-1)}$. The Chebyshev polynomials satisfy $\left|T_{n}(x)\right| \leq 1$ for $x \in[-1,1]$ and hence

$$
\begin{equation*}
\left|\prod_{i=1}^{n}\left(x-x_{i}\right)\right| \leq \frac{1}{2^{n-1}} \tag{5}
\end{equation*}
$$

for $x \in[-1,1]$.

Now consider the $n$-th derivative of $f$, which is given by

$$
\begin{equation*}
f^{(n)}(\theta)=(-4)^{n} e^{-4 \theta}+(3)^{n} e^{3 \theta} \tag{6}
\end{equation*}
$$

The maximum value of $|f(n)(\theta)|$ can occur at two places: (i) at an internal maximum, or (ii) at one of the end points of the interval, $\theta= \pm 1$. Consider case (i) first. If $n$ is odd, then

$$
\begin{equation*}
f^{(n+1)}(\theta)=4^{n+1} e^{-4 \theta}+3^{n+1} e^{3 \theta} \tag{7}
\end{equation*}
$$

and since both terms are positive, there is no value of $\theta$ where $f^{n+1}(\theta)=0$. If $n$ is even, then

$$
\begin{equation*}
f^{(n+1)}(\theta)=-4^{n+1} e^{-4 \theta}+3^{n+1} e^{3 \theta} \tag{8}
\end{equation*}
$$

Setting $f^{n+1}(\theta)=0$ gives

$$
\begin{equation*}
4^{n+1} e^{-4 \theta}=3^{n+1} e^{3 \theta} \tag{9}
\end{equation*}
$$

and hence $(4 / 3)^{n+1}=e^{7 \theta}$, so

$$
\begin{equation*}
\theta=\frac{(n+1) \log (4 / 3)}{7} \tag{10}
\end{equation*}
$$

is a single solution. However, since

$$
\begin{equation*}
f^{(n+2)}(\theta)=\left|(-4)^{n+2} e^{-4 \theta}+2^{n+2} e^{2 \theta}\right|>0 \tag{11}
\end{equation*}
$$

it follows that this must be a minimum of $f(n)$. Since $f(n)>0$, it must be a minimum of $\left|f^{(n)}\right|$ also. Hence, for all values of $n$ there is no possibility that the maximum of $\left|f^{(n)}\right|$ occurs in the interior of the interval. Thus the only remaining possibilities are at the endpoints. Since the factor of $(-3)^{n}$ grows more rapidly in magnitude, the maximum will occur at $\theta=-1$, and hence

$$
\begin{equation*}
\left|f^{(n)}(\theta)\right| \leq\left|(-4)^{n} e^{4}+3^{n} e^{-3}\right| \tag{12}
\end{equation*}
$$

Combining the results from above equations establishes that

$$
\begin{equation*}
\left\|f-p_{n-1}\right\|_{\infty} \leq \frac{\left|(-4)^{n} e^{4}+3^{n} e^{-3}\right|}{n!2^{n-1}} \tag{13}
\end{equation*}
$$

(d) There are many ways to find better control points, and this problem illustrates that while the Chebyshev points are a good set of points at which to interpolate a general unknown function, they are usually not optimal for a specific function. One simple method is to examine where the maximum interpolation error is achieved. This is happens near $x=-1$. Hence if we move the first control point to the left, it will result in a better approximation of $f(x)$ within this region. In this case, we shift the first control point by -0.02 , which leads to an infinity norm of 5.16790 . The following are the fitting plots after changing tha control points and the corresponding errors.


## P3. Condition number of a matrix

(a) Throughout this problem, $\|\cdot\|$ is taken to mean the Euclidean norm. The first two parts of this problem can be solved using diagonal matrices only. Consider first

$$
B=\left[\begin{array}{ll}
2 & 0  \tag{14}\\
0 & 1
\end{array}\right], \quad C=\left[\begin{array}{ll}
1 & 0 \\
0 & 2
\end{array}\right]
$$

Then $\|B\|=2,\left\|B^{-1}\right\|=1$ and hence $\kappa(B)=2$. Similarly, $\kappa(C)=2$. Adding the two matrices together gives

$$
B+C=\left[\begin{array}{ll}
3 & 0  \tag{15}\\
0 & 3
\end{array}\right]=3 I
$$

and hence $\kappa(B+C)=\|3 I\|\left\|\frac{1}{3} I\right\|=3 \times \frac{1}{3}=1$. For these choices of matrices, $\kappa(B+C)<$ $\kappa(B)+\kappa(C)$.
(b) If

$$
B=\left[\begin{array}{ll}
4 & 0  \tag{16}\\
0 & 2
\end{array}\right], \quad C=\left[\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right]
$$

then $\kappa(B)=2$. Similarly, $\kappa(C)=1$. Adding the two matrices together gives

$$
B+C=\left[\begin{array}{ll}
5 & 0  \tag{17}\\
0 & 1
\end{array}\right]
$$

and hence $\kappa(B+C)=5$. For these choices of matrices, $\kappa(B+C)>\kappa(B)+\kappa(C)$.
(c)

$$
\kappa(\alpha A)=\|\alpha A\| \times\left\|(\alpha A)^{-1}\right\|=\|\alpha A\| \times\left\|\frac{1}{\alpha} A^{-1}\right\|=\|\alpha\| \times\left\|\frac{1}{\alpha}\right\| \times\|A\| \times\left\|A^{-1}\right\|
$$

$$
\begin{gathered}
\kappa(\alpha A)=\|A\| \times\left\|A^{-1}\right\|=\kappa(A) \\
\|Q A\|=\sup _{x \neq 0} \frac{\|Q A x\|}{\|x\|} .
\end{gathered}
$$

But, multiplying by an orthogonal matrix $Q$ does not change the 2-norm. Therefore,

$$
\sup _{\mathrm{x} \neq 0} \frac{\|Q A x\|}{\|x\|}=\sup _{\mathrm{x} \neq 0} \frac{\|A x\|}{\|x\|}=\|A\| .
$$

One can also show this by

$$
\|Q A x\|=\sqrt{\langle Q A x, Q A x\rangle}=\sqrt{\left\langle A x, Q^{T} Q A x\right\rangle}=\sqrt{\langle A x, A x\rangle}=\|A x\|
$$

Similary, one may also find

$$
\left\|(Q A)^{-1}\right\|=\left\|A^{-1}\right\|
$$

Finally,

$$
\kappa(Q A)=\|Q A\| \times\left\|(Q A)^{-1}\right\|=\|A\| \times\left\|A^{-1}\right\|=\kappa(A)
$$

## P4. Periodic cubic splines

(a)

$$
s_{x}(t)= \begin{cases}6 t-2 t^{3} & 0 \leq t<1 \\ -4+18 t-12 t^{2}+2 t^{3} & 1 \leq t<2 \\ -4+18 t-12 t^{2}+2 t^{3} & 2 \leq t<3 \\ 104-90 t+24 t^{2}-2 t^{3} & 3 \leq t \leq 4\end{cases}
$$

(b)

(c)

$$
s_{y}(t)=\frac{1}{2} s_{x}(t+1)= \begin{cases}3(t+1)-(t+1)^{3} & 0 \leq t<1 \\ -2+9(t+1)-6(t+1)^{2}+(t+1)^{3} & 1 \leq t<2 \\ -2+9(t+1)-6(t+1)^{2}+(t+1)^{3} & 2 \leq t<3 \\ 52-45(t+1)+12(t+1)^{2}-(t+1)^{3} & 3 \leq t \leq 4\end{cases}
$$

simplifies to

$$
s_{y}(t)= \begin{cases}2-3 t^{2}-t^{3} & 0 \leq t<1 \\ 2-3 t^{2}+t^{3} & 1 \leq t<2 \\ 2-3 t^{2}+t^{3} & 2 \leq t<3 \\ 18-24 t+9 t^{2}-t^{3} & 3 \leq t \leq 4\end{cases}
$$


(d)


The estimated $\pi$ value is 3.05000 .

## P5. Image reconstruction from low light

(a) Reconstruction of the regular-light photo 0927 from the three low-light photos 0258, 0646,0704 . Using fragments 0 and 1 for training, and fragments 2 and 3 for testing. The program p5_reconstruction.py implements the algorithm.

The fitted matrices are

$$
\begin{gathered}
F^{A}=\left[\begin{array}{lll}
0.01344 & 0.01344 & 0.01344 \\
0.04126 & 0.04126 & 0.04126 \\
0.05247 & 0.05247 & 0.05247
\end{array}\right] \\
F^{B}=\left[\begin{array}{lll}
-0.54727 & 0.34517 & -0.3521 \\
-1.34219 & 1.13862 & -0.20986 \\
-1.33221 & 0.21761 & 0.65449
\end{array}\right] \\
F^{C}=\left[\begin{array}{ccc}
1.57982 & -0.61108 & 0.40334 \\
0.07498 & 1.07357 & 0.2709 \\
0.08154 & -0.85494 & 2.11257
\end{array}\right] \\
\mathbf{p}_{\text {const }}=\left[\begin{array}{c}
4.54571 \\
-12.72907 \\
-5.966
\end{array}\right]
\end{gathered}
$$

The error for each fragment

$$
\begin{gathered}
S_{A B C}\left(K_{0}\right)=0.0598315 \\
S_{A B C}\left(K_{1}\right)=0.0719668 \\
S_{A B C}\left(K_{2}\right)=0.0795461 \\
S_{A B C}\left(K_{3}\right)=0.150443
\end{gathered}
$$


(b) Reconstruction of the regular-light photo 0927 from one low-light photo 0646. Using fragments 0 and 1 for training, and fragments 2 and 3 for testing.

$$
\begin{gathered}
F^{B}=\left[\begin{array}{ccc}
4.3031 & -3.56403 & 1.56626 \\
-1.11043 & 2.64979 & 0.97944 \\
-1.57174 & -4.69737 & 8.40347
\end{array}\right] \\
\mathbf{p}_{\text {const }}=\left[\begin{array}{l}
36.76942 \\
18.52413 \\
24.98479
\end{array}\right]
\end{gathered}
$$

The error for each fragment

$$
\begin{gathered}
S_{B}\left(K_{0}\right)=0.0845624 \\
S_{B}\left(K_{1}\right)=0.081768 \\
S_{B}\left(K_{2}\right)=0.106275 \\
S_{B}\left(K_{3}\right)=0.165774
\end{gathered}
$$


fragment 2
input 0646

fragment 3 input 0646

fragment 2 reconstructed 0927

fragment 3 reconstructed 0927

fragment 2 actual 0927

fragment 3 actual 0927
(c) The fitting error $S_{A B C}$ is smaller than $S_{B}$ for all fragments. The reconstructed fragments 2 and 3 from part (a) appear more similar to the actual images. Therefore, including more light levels improves the quality of the fit.

## P6. Determining hidden chemical sources

(a) The time derivative of $\rho_{c}$ is

$$
\begin{equation*}
\frac{\partial \rho_{c}}{\partial t}=\frac{x^{2}+y^{2}-4 b t}{16 \pi b^{2} t^{3}} \exp \left(-\frac{x^{2}+y^{2}}{4 b t}\right) \tag{18}
\end{equation*}
$$

The $x$ derivative of $\rho_{c}$ is

$$
\begin{equation*}
\frac{\partial \rho_{c}}{\partial x}=\frac{-2 x}{16 \pi b^{2} t^{2}} \exp \left(-\frac{x^{2}+y^{2}}{4 b t}\right) \tag{19}
\end{equation*}
$$

and the second $x$ derivative is

$$
\begin{equation*}
\frac{\partial^{2} \rho_{c}}{\partial^{2} x}=\frac{x^{2}-2 b t}{16 \pi b^{3} t^{3}} \exp \left(-\frac{x^{2}+y^{2}}{4 b t}\right) \tag{20}
\end{equation*}
$$

By symmetry the second $y$ derivative is

$$
\begin{equation*}
\frac{\partial^{2} \rho_{c}}{\partial^{2} y}=\frac{y^{2}-2 b t}{16 \pi b^{3} t^{3}} \exp \left(-\frac{x^{2}+y^{2}}{4 b t}\right) \tag{21}
\end{equation*}
$$

and hence

$$
\begin{equation*}
\nabla^{2} \rho_{c}=\frac{x^{2}+y^{2}-4 b t}{16 \pi b^{3} t^{3}} \exp \left(-\frac{x^{2}+y^{2}}{4 b t}\right) \tag{22}
\end{equation*}
$$

(b) We now consider the case when $b=1$ and 49 point sources of chemicals are introduced at $t=0$ with different strengths, on a $7 \times 7$ regular lattice covering the coordinates $x=$ $-3,-2, \ldots, 3$ and $y=-3,-2, \ldots, 3$. The concentration satisfies

$$
\begin{equation*}
\rho(\mathbf{x}, t)=\sum_{k=0}^{48} \lambda_{k} \rho_{c}\left(\mathbf{x}-\mathbf{v}_{k}, t\right) \tag{23}
\end{equation*}
$$

where $\mathbf{v}_{k}$ is the $k$ th lattice site and $\lambda_{k}$ is the strength of the chemical introduced at that site. Two hundred measurements, $\rho_{M}\left(\mathbf{x}_{i}, t\right)$, at locations $\mathbf{x}_{i}$ and at $\mathrm{t}=4$ are provided. Estimating the concentrations can be viewed as a linear least squares problem, finding the $\lambda_{k}$ such that

$$
\begin{equation*}
S=\sum_{i=0}^{199}\left|\rho_{M}\left(\mathbf{x}_{i}, t\right)-\sum_{k=0}^{48} \lambda_{k} \rho_{c}\left(\mathbf{x}_{i}-\mathbf{v}_{k}, t\right)\right| \tag{24}
\end{equation*}
$$

Even though Eq. 24 is quite complicated and involves the the expression for $\rho_{c}$, the parameters $\lambda_{k}$ still enter linearly, and hence it can be solved using the linear least squares approach. The function part_b() in p6_diffusion.py computes the $\lambda_{k}$ and prints them. They are all positive, with a maximum value of approximately 24.
(c) Suppose that the measurements have some experimental error,so that the measured values $\widetilde{\rho}_{i}$ in the file are related to the true values $\rho_{i}$ according to

$$
\begin{equation*}
\widetilde{\rho}_{i}=\rho_{i}+e_{i} \tag{25}
\end{equation*}
$$

The function part_c() in p6_diffusion.py performs a sample of N computations of the $\lambda_{k}$ when each of the $\rho_{M}$ are perturbed by a small normally distributed shift with mean 0 and variance $10^{-8}$. The obtained standard deviations for the $\lambda_{k}$ at four lattice sites are: 22268 at $(0,0), 14034$ at $(1,1), 2868$ at $(2,2)$, and 117 at $(3,3)$. They show much larger variations than the actual $\lambda_{k}$ values that were measured in part (b). The largest errors are at the central $(0,0)$ lattice site, which is reasonable since it is furthest away from any of the measurements in the file, thus making it most difficult to estimate.
(d) A common mistake here is that the floating point values $\lambda_{k}$ are not rounded (e.g. using round ()) as requested but rather truncated (e.g. using int ()), which leads to incorrect images. The encoded message is "AM205"


