Assignment 2 - Numerical Linear Algebra

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Abstract

We derive linear and polynomial regression in subsets of $\mathbb{R}$ and discuss the condition number of the associated matrices, numerical algorithms for the SVD and QR factorization are built and used on an efficiency analysis of the 3 methods to do linear or polynomial regression, stability of these algorirths is discussed.

Contents

1. Introduction

Given $D \subset \mathbb{R}^2$, a dataset, approximating this set through a *continuous* $f : \mathbb{R} \to \mathbb{R}$ is a very important problem in statistics, we will derive the 2 most important and most used methods to do this: linear and polynomial regression. Both are based on the least squares minimization problem. We will also discuss the conditioning number of the problems shown. A computational approach to regression is shown as well. We discuss how the condition number changes when the matrix is QR or SVD decomposed, and the algorithms for such decompositions are built.

2. Norms and Problems

A **norm** is a way to quantify *size* on a vector space. A norm is a class of functions that satisfy some properties, which we define below:

Definition 2.1: (Norm) Given E a vector space over a field $\mathbb{K}$, a **norm** is a function $\|\cdot\| : E \to \mathbb{R}$ that satisfies:

- $\|x\| > 0_E, \forall x \in E^*$, and $\|x\| = 0_E \Leftrightarrow x = 0_E$
- $\|x + y\| \le \|x\| + \|y\|$
- $\|\varphi x\| = |\varphi| \|x\|, \forall \varphi \in \mathbb{K}$

Throughout this document we will use the most famous class of norms, the p-norms defined below:

Definition 2.2: (p-norm) Given $p \in \mathbb{R}$, the **p-norm** of $x \in \mathbb{C}^m$ is:

$$\|x\|_p = \left(\sum_{i=1}^{m} |x_i|^p \right)^{\frac{1}{p}} \qquad\qquad 1$$

Some famous cases are:

$$\|x\|_1 = \sum_{i=1}^{m} |x_i|$$

$$\|x\|_2 = \left(\sum_{i=1}^{m} |x_i|^2 \right)^{\frac{1}{2}} \qquad\qquad 2$$

$$\|x\|_\infty = \max_{1 \le i \le m} |x_i|$$

Now we proceed with the main topic of this section, the condition number of a problem. It is useful to see a problem as a function $f : X \to Y$ from a *normed* vector space X of data and a space Y of solutions, f is not always a well-behaved continuous function, which is why we are interested in **well-conditioned** problems and not in **ill-conditioned** problems.

Definition 2.3: (Well-Conditioned Problem) A problem $f : X \to Y$ is *well-conditioned* at $x_0 \in X \Leftrightarrow \forall \varepsilon > 0, \exists \delta > 0 \mid \|x - x_0\| < \delta \Rightarrow f(x) - \|f(x_0)\| < \varepsilon$.

This means that small perturbations in x lead to small changes in $f(x)$, a problem is **ill-conditioned** if $f(x)$ can suffer huge changes with small changes in x.

We usually say f is well-conditioned if it is well-conditioned $\forall x \in X$. If there is at least one x_i in which the problem is ill-conditioned, then we can use that whole problem is ill-conditioned.

2.1. The Condition number of a problem

Condition numbers are a tool to quantify how well/ill conditioned a problem is:

Definition 2.1.1: (Absolute Conditioning Number) Let δx be a small pertubation of x, so $\delta f = f(x + \delta x) - f(x)$. The **absolute** conditioning number of f is:

$$\hat{\kappa} = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|\delta f\|}{\|\delta x\|} \qquad\qquad 3$$

The limit of the supremum can be seen as the supremum of all *infinitesimal* perturbations, so this can be rewritten as:

$$\hat{\kappa} = \sup_{\delta x} \frac{\|\delta f\|}{\|\delta x\|} \qquad\qquad 4$$

If f is differentiable, we can evaluate the abs.conditioning number using its derivative. If J is the matrix whose $i \times j$ entry is the derivative $\frac{\partial f_i}{\partial x_j}$ (jacobian of f), then we know that $\delta f \approx J(x)\delta x$, with equality in the limit $\|\delta x\| \to 0$. So the absolute conditioning number of f becomes:

$$\hat{\kappa} = \|J(x)\| \qquad\qquad 5$$

2.2. The Relative Condition Number

When, instead of analyzing the whole set X of data, we are interested in *relative* changes, we use the **relative condition number:**

Definition 2.2.1: (Relative Condition Number) Given $f : X \to Y$ a problem, the *relative condition number* $\kappa(x)$ at $x \in X$ is:

$$\kappa(x) = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \left(\frac{\|\delta f\|}{\|f(x)\|} \right) \cdot \left(\frac{\|\delta x\|}{\|x\|} \right)^{-1} \qquad\qquad 6$$

Or, as we did in Definition 2.1.1, assuming that δf and δx are infinitesimal:

$$\kappa(x) = \sup_{\delta x} \left(\frac{\|\delta f\|}{\|f(x)\|} \right) \cdot \left(\frac{\|\delta x\|}{\|x\|} \right)^{-1} \qquad\qquad 7$$

If f is differentiable:

$$\kappa(x) = (\|J(x)\|) \cdot \left(\frac{\|f(x)\|}{\|x\|} \right)^{-1} \qquad\qquad 8$$

Relative condition numbers are more useful than absolute conditioning numbers because the **floating point arithmetic** used in many computers produces *relative* errors, the latter is not a highlight of this discussion.

Here are some examples of the definitions above:

Example 2.2.1.: Consider the problem of obtaining the scalar $\frac{x}{2}$ from $x \in \mathbb{R}$. The function $f(x) = \frac{x}{2}$ is differentiablle, so by eq. (8):

$$\kappa(x) = (\|J\|) \cdot \left(\frac{\|f(x)\|}{\|x\|} \right)^{-1} = \left(\frac{1}{2} \right) \cdot \left(\frac{\frac{x}{2}}{x} \right)^{-1} = 1. \qquad\qquad 9$$

This problem is well-conditioned (κ is small).

Example 2.2.2.: Consider the problem of computing the scalar $x_1 - x_2$ from $(x_1, x_2) \in \mathbb{R}^2$ (Use the ∞-norm in $\mathbb{R}^2$ for simplicity). The function associated is differentiable and the jacobian is:

$$J = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 1 & -1 \end{bmatrix} \qquad 10$$

With $\|J\|_\infty = 2$, so the condition number is:

$$\kappa = (\|J\|_\infty) \cdot \left(\frac{\|f(x)\|}{\|x\|} \right)^{-1} = \frac{2}{|x_1 - x_2| \cdot \max\{|x_1|, |x_2|\}} \qquad 11$$

This problem can be ill-conditioned if $|x_1 - x_2| \approx 0$ (κ gets huge), and well-conditioned otherwise

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2.3. Condition Number of Matrices

We will deduce the conditioning number of a matrix from the conditioning number of *matrix-vector* multiplication:

Consider the problem of obtaining Ax given $A \in \mathbb{C}^{m \times n}$. We will calculate the relative condition number with respect to perturbations on x. Directly from Definition 2.2.1, we have:

$$\kappa = \sup_{\delta x} \frac{\|A(x + \delta x) - Ax\|}{\|Ax\|} \cdot \left(\frac{\|\delta x\|}{\|x\|} \right)^{-1} = \sup_{\delta x} \frac{\|A\delta x\|}{\|\delta x\|} \cdot \left(\frac{\|Ax\|}{\|x\|} \right)^{-1} \qquad 12$$

Since $\sup_{\forall x} \frac{\|A\delta x\|}{\|\delta x\|} = \|A\|$, we have:

$$\kappa = \|A\| \cdot \frac{\|x\|}{\|Ax\|} \qquad 13$$

This is a precise formula as a function of (A, x).

The following theorem will be useful in a near future:

Theorem 2.3.1: $\forall x \in \mathbb{C}^n, A \in \mathbb{C}^{n \times n}, \det(A) \neq 0$, the following holds:

$$\frac{\|x\|}{\|Ax\|} \leq \|A^{-1}\| \qquad 14$$

Proof: Since $\|AB\| \leq \|A\|\|B\|$, we have:

$$\|AA^{-1}x\| \leq \|Ax\|\|A^{-1}\| \Leftrightarrow \frac{\|x\|}{\|Ax\|} \leq \|A^{-1}\| \qquad 15$$

$\square$

So using this in eq. (13), we can write:

$$\kappa \leq \|A\| \cdot \|A^{-1}\| \qquad 16$$

Or:

$$\kappa = \alpha \|A\| \cdot \|A^{-1}\| \qquad\qquad 17$$

With

$$\alpha = \frac{\|x\|}{\|Ax\|} \cdot \left(\|A^{-1}\|\right)^{-1} \qquad\qquad 18$$

From Theorem 2.3.1, we can choose x to make $\alpha = 1$, and therefore $\kappa = \|A\| \cdot \|A^{-1}\|$.

Consider now the problem of calculating $A^{-1}b$ given $A \in \mathbb{C}^{n \times n}$. This is mathematically identical to the problem we just analyzed, so the following theorem has already been proven:

> **Theorem 2.3.2**: Let $A \in \mathbb{C}^{n \times n}, \det(A) \neq 0$, and consider the problem of computing b, from $Ax = b$, by perturbating x. Then the following holds:
>
> $$\kappa = \|A\|\frac{\|x\|}{\|b\|} \leq \|A\| \cdot \|A^{-1}\| \qquad\qquad 19$$
>
> Where κ is the condition number of the problem.

Proof: Read from eq. (12) to eq. (18). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ □

Finally, $\|A\| \cdot \|A^{-1}\|$ is so useful it has a name: **the condition number of A** (relative to the norm $\|\cdot\|$)

If A is singular, $\kappa(A) = \infty$. Notice that if $\|\cdot\| = \|\cdot\|_2$, then $\|A\| = \sigma_1$ and $\|A^{-1}\| = \frac{1}{\sigma_m}$, so:

$$\kappa(A) = \frac{\sigma_1}{\sigma_m} \qquad\qquad 20$$

This is the condition number of A with respect to the 2-norm, which is the most used norm in practice. The condition number of a matrix is a measure of how sensitive the solution of a system of equations is to perturbations in the data. A large condition number indicates that the matrix is ill-conditioned, meaning that small changes in the input can lead to large changes in the output.

3. Linear Regression (1a)

Given the dataset:

$$D := \left\{ t_i = \frac{i}{m} \right\}, i = 0, 1, ..., m \in \mathbb{R} \qquad\qquad 21$$

of equally spaced points , linear regression consists of finding the best *line* $f(t) = \alpha + \beta t$ that approximates the points $(t_i, b_i) \in \mathbb{R}^2$, where b_i are arbitrary.

Approximating 2 points in $\mathbb{R}^2$ by a line is trivial, now approximating more points is a task that requires linear algebra. To see this, we will analyze the following example to build intuition for the general case:
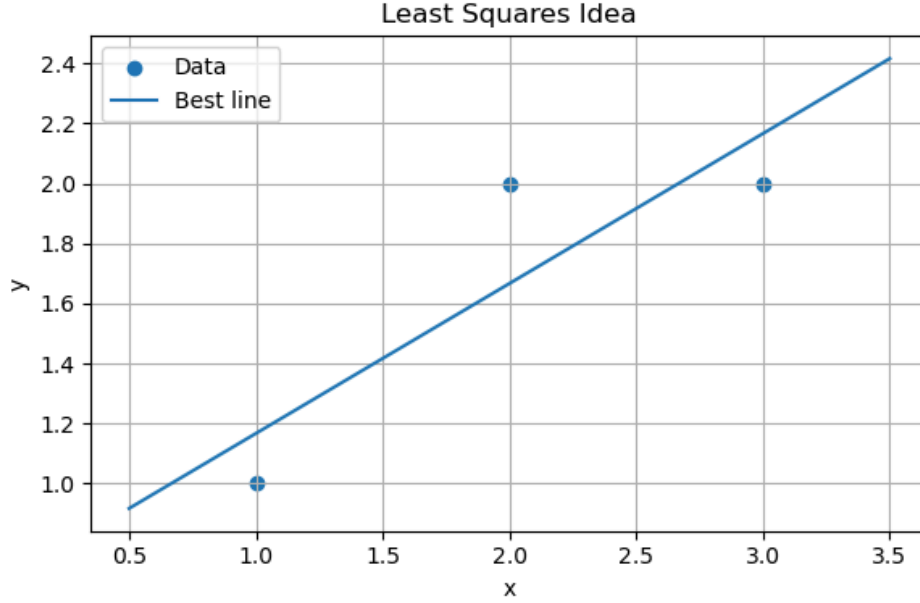
Figure 1: A good approximation for the 3 points shown

Figure 1 is a glimpse onto what we are about to produce.

Given the points $(1,1), (2,2), (3,2) \in \mathbb{R}^2$, we have $(t_1, b_1) = (1,1), (t_2, b_2) = (2,2), (t_3, b_3) = (3,2)$ we would like a *line* $f(t) = y(t) = \alpha + \beta t$ that best approximates (t_i, b_i). In other words, since we know that the line does not pass through all 3 points, we would like to find the *closest* line to **each point** of the dataset D. So the system:

$$f(1) = \alpha + \beta = 1$$
$$f(2) = \alpha + 2\beta = 2 \qquad\qquad 22$$
$$f(3) = \alpha + 3\beta = 2$$

Which is:

$$\underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}}_{A} \cdot \underbrace{\begin{bmatrix} \alpha \\ \beta \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}}_{b} \qquad\qquad 23$$

Clearly has no solution. But it has a *closest solution* which we can find through **minimizing** the errors produced by this approximation.

Let $x^* \neq x$ be a solution to the system. And let the error produced by approximating the points through a line be $e = Ax - b$. Minimizing the error requires a *norm*, which is defined

$$e_1^2 + e_2^2 + e_3^2 \qquad\qquad 24$$

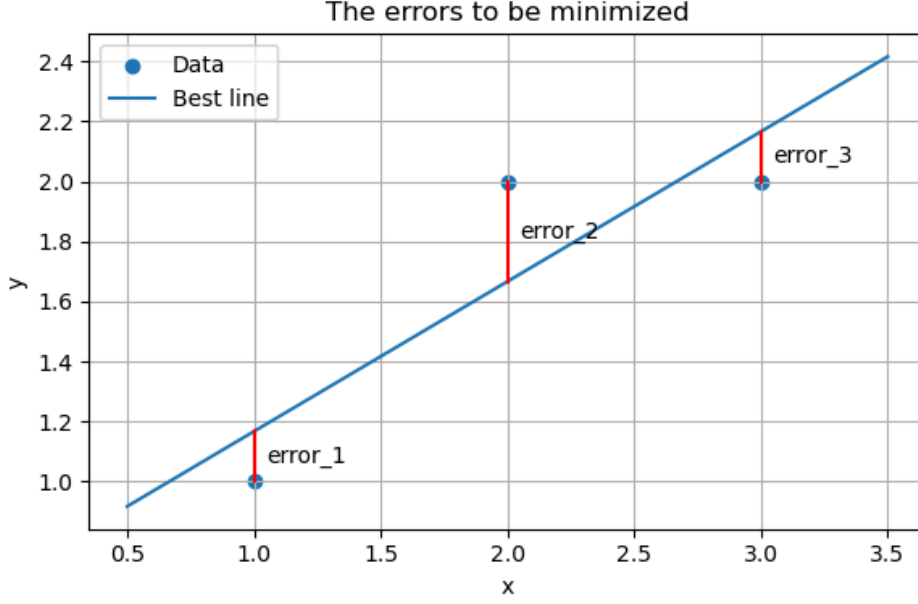Is what we want to minimize, where e_i is the error (distance) from the ith point to the line:

Figure 2: The errors (distances)

So we will project b into $C(A)$, giving us the closest solution, and the least squares solutions is when $\hat{x}$ minimizes $\|Ax - b\|^2$, this occurs when the residual $e = Ax - b$ is orthogonal to $C(A)$. Since $N(A^*) \perp C(A)$ and the dimensions sum up the left dimension of the matrix. so by the well-known projection formula, we have:

$$A^*A\hat{x} = A^*b$$

$$= \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$= \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 5 \\ 11 \end{bmatrix}$$

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So the system to find $\hat{x} = \begin{bmatrix} \hat{\alpha}, \hat{\beta} \end{bmatrix}$ becomes:

$$3\alpha + 5\beta = 5$$
$$6\alpha + 14\beta = 11$$

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Notice that with the *errors* e_i^2 as:

$$e_1^2 = (f(t_1) - b_1)^2 = (f(1) - 1)^2 = (\alpha + \beta - 1)^2$$
$$e_2^2 = (f(t_2) - b_2)^2 = (f(2) - 2)^2 = (\alpha + 2\beta - 2)^2$$
$$e_3^2 = (f(t_3) - b_2)^2 = (f(3) - 2)^2 = (\alpha + 3\beta - 2)^2$$

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This is consistent with what we see in Figure 2. Notice that eq. (26) is *precisely* what is obtained after using partial derivatives to minimize the erros sum as a function of (α, β):

$$f(\alpha, \beta) = (\alpha + \beta - 1)^2 + (\alpha + 2\beta - 2)^2 + (\alpha + 3\beta - 2)^2$$
$$= 3\alpha^2 + 14\beta^2 + 12\alpha\beta - 10\alpha - 22\beta + 9,$$

$$\frac{\partial f}{\partial \alpha} = \frac{\partial f}{\partial \beta} = 0 \Leftrightarrow 6\alpha + 12d - 10 = 28\beta + 12\alpha - 22 = 0 \Leftrightarrow \begin{cases} 3c + 6d = 11 \\ 6c + 14d = 11 \end{cases}$$

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This new system has a solution in $\hat{\alpha} = \frac{2}{3}, \hat{\beta} = \frac{1}{2}$, so the equation of the optimal line, obtained through *linear regression* (or least squares) is:

$$y(t) = \frac{2}{3} + \frac{1}{2}t. \qquad\qquad 29$$

If we have $n > 3$ points to approximate with linear regression, the reasoning is analogous:

Going back to D in eq. (21) , we want to find the extended system as we did in eq. (26), so let:

$$f(t) = \alpha + \beta t \qquad\qquad 30$$

Be the linear regression line, for $D = \left\{(0, b_0), \left(\frac{1}{m}, b_1\right), ..., (1, b_m)\right\}$. The system is:

$$f\left(\frac{0}{m} = 0\right) = b_0 = \alpha,$$
$$f\left(\frac{1}{m}\right) = b_1 = \alpha + \frac{\beta}{m},$$
$$f\left(\frac{2}{m}\right) = b_2 = \alpha + \frac{2}{m}\beta \qquad\qquad 31$$
$$...$$
$$f\left(\frac{m}{m} = 1\right) = b_m = \alpha + \beta$$

Or:

$$\underbrace{\begin{bmatrix} 1 & 0 \\ 1 & \frac{1}{m} \\ \vdots & \vdots \\ 1 & 1 \end{bmatrix}}_{A} \cdot \underbrace{\begin{bmatrix} \alpha \\ \beta \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} b_0 \\ \vdots \\ b_m \end{bmatrix}}_{b} \qquad\qquad 32$$

Projecting into $C(A)$, we have:

$$A^*Ax = A^*b$$

$$= \begin{bmatrix} 1 & 1 & ... & 1 \\ 0 & \frac{1}{m} & ... & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 1 & \frac{1}{m} \\ \vdots & \vdots \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} m+1 & \frac{m+1}{2} \\ \frac{m+1}{2} & \frac{(m+1)(2m+2)}{6m} \end{bmatrix} \cdot \begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix} \qquad\qquad 33$$

$$= \begin{bmatrix} 1 & 1 & ... & 1 \\ 0 & \frac{1}{m} & ... & 1 \end{bmatrix} \cdot \begin{bmatrix} b_0 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} b_0 + b_2 + ... + b_m \\ \frac{1}{m}[b_1 + 2b_2 + ... + (m-1)b_{m-1} + b_m] \end{bmatrix}$$

So the system to find the optimal vector $\begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix}$ is:

$$\begin{bmatrix} m+1 & \frac{m+1}{2} \\ \frac{m+1}{2} & \frac{(m+1)(2m+2)}{6m} \end{bmatrix} \cdot \begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix} = \begin{bmatrix} b_0 + b_1 + ... + b_m \\ \frac{1}{m}[b_1 + 2b_2 + ... + (m-1)b_{m-1} + b_m] \end{bmatrix} \qquad\qquad 34$$

Or, as a function of t_i, b_i and m:

$$\underbrace{\begin{bmatrix} m+1 & \sum_{i=1}^{m} t_i \\ \sum_{i=1}^{m} t_i & \sum_{i=1}^{m} t_i^2 \end{bmatrix}}_{\hat{A}} \cdot \begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{m} b_i \\ \sum_{i=1}^{m} \frac{i}{m} \cdot b_i \end{bmatrix} \qquad\qquad 35$$

This provides the optimal vector $\hat{x}$ that minimizes the least squares error, which is the solution to the linear regression problem.

4. How the condition number of A changes (1b)

We are interested in the condition number of $\hat{A} = A^{*}A$ shown in eq. (34). We will analyze how the condition number of $\hat{A}$ changes with respect to perturbations on m, the number of points in the dataset. A computational approach is appropriate.

Here is a python code that numerically calculates many values of $\kappa\left(\hat{A}_{m}\right)$ as a function of m:

```python
import numpy as np
import matplotlib.pyplot as plt

def cond_number(m):

    """
    This function computes the condition number of the matrix A(m) in the 2-
    norm. The matrix A is defined.

    Args:
        m (float): parameter for the matrix A(m)
    Returns:
        float: condition number of A(m)
    Raises:
        ZeroDivisionError: if m = 0
        np.linalg.LinAlgError: if A(m) is not invertible
    """

    A = np.array([
        [m + 1,          (m + 1) / 2],
        [(m + 1) / 2,  (m + 1)**2 / (3 * m)]
    ])
    A_inv = np.linalg.inv(A)
    return np.linalg.norm(A, 2) * np.linalg.norm(A_inv, 2)

M = float(input("Enter maximum m (M > 0): "))
N = int(input("Enter number of sample points: ")) #however the user wants to
plot

m_vals = np.linspace(0, M, N)
conds  = []

for m in m_vals:
    try:
        conds.append(cond_number(m))
    except (ZeroDivisionError, np.linalg.LinAlgError):
        conds.append(np.inf) #if it is not invertible
```

```
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37  plt.figure()
38  plt.plot(m_vals, conds)
39  plt.xlabel('m')
40  plt.ylabel('Condition number $κ(A^* A)$')
41  plt.title('Condition number of $A^* A(m)$')
42  plt.grid(True)
43  plt.tight_layout()
44  plt.show()
```
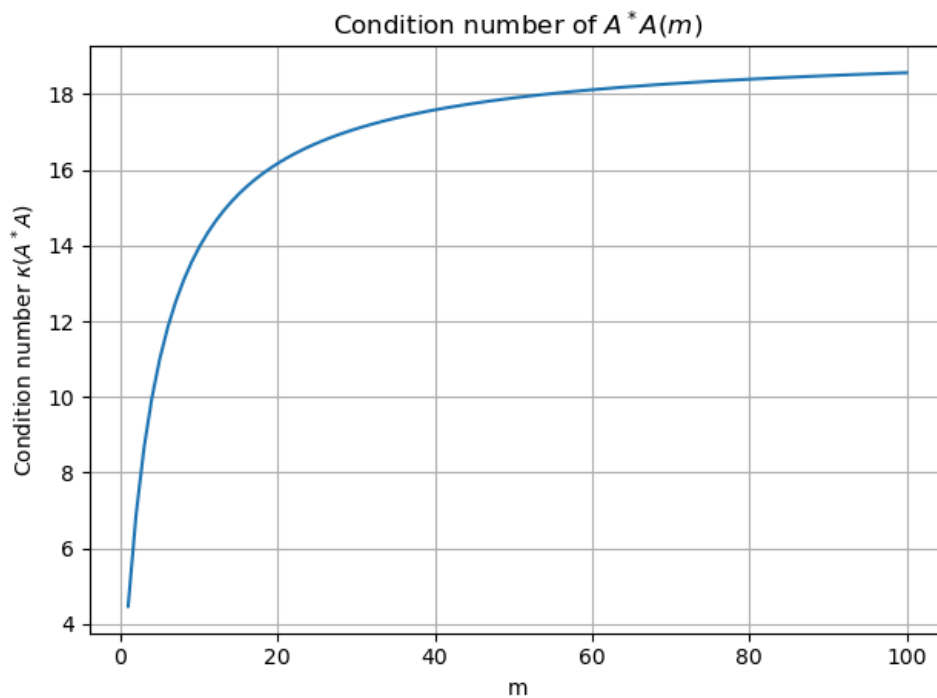
Good visualizations of this are:

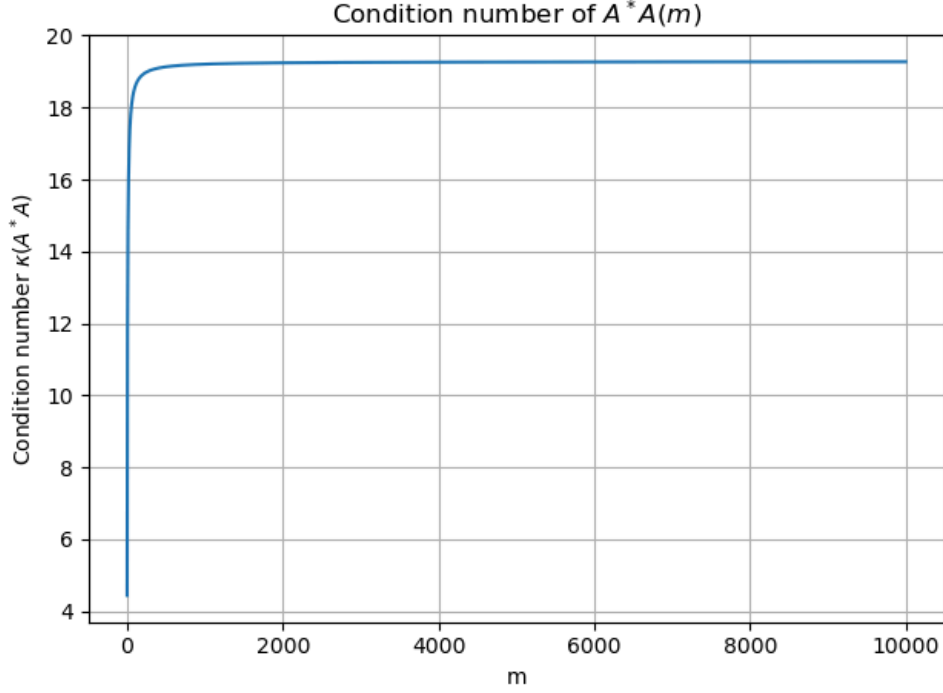Figure 3: Condition number of $\hat{A}$ over $[0, 100]$

Figure 4: Condition number of $\hat{A}$ over $[0, 10000]$

Figure 3 and Figure 4 show us that apparently $\kappa\left(\hat{A}_m\right)$ converges to a real number. We will evaluate this hypothesis below:

Using $\|\cdot\|_2$, the condition number of $\hat{A}$ is:

$$\kappa\left(\hat{A}\right) = \left\|\hat{A}\right\|_2 \cdot \left\|\hat{A}^{-1}\right\|_2 = \frac{\sigma_1}{\sigma_m} \qquad 36$$

Singular Values are better explored in Section 10.2. Now we calculate the singular values of $\hat{A}$, which are the square roots of the eigenvalues of $\hat{A}$ (see Theorem 10.2.2). So we have:

$$\det\left(\hat{A} - \lambda I\right) = 0 \Leftrightarrow \det\left(\begin{bmatrix} m+1-\lambda & \frac{m+1}{2} \\ \frac{m+1}{2} & \frac{(m+1)(2m+1)}{6m} - \lambda \end{bmatrix}\right) = 0$$

$$\Leftrightarrow (m+1-\lambda)\left[\frac{(m+1)(2m+1)}{6m} - \lambda\right] - \left(\frac{m+1}{2}\right)^2 = 0 \qquad 37$$

$$\Leftrightarrow \lambda^2 - \frac{(m+1)(8m+1)}{6m}\lambda + \frac{(m+1)^2(m+2)}{12m} = 0$$

$$\Leftrightarrow \lambda = \frac{m+1}{12m}\left[(8m+1) \pm \sqrt{52m^2 - 8m + 1}\right]$$

And the singular values are:

$$\sigma_1 = \sqrt{\lambda_1} = \sqrt{\frac{m+1}{12m}\left[(8m+1) + \sqrt{52m^2 - 8m + 1}\right]},$$

$$\sigma_2 = \sqrt{\lambda_2} = \sqrt{\frac{m+1}{12m}\left[(8m+1) - \sqrt{52m^2 - 8m + 1}\right]} \qquad 38$$

This gives:

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$$\kappa\left(\hat{A}\right) = \frac{\sigma_1}{\sigma_m} = \frac{\sqrt{\frac{m+1}{12m}\left[(8m+1) + \sqrt{52m^2 - 8m + 1}\right]}}{\sqrt{\frac{m+1}{12m}\left[(8m+1) - \sqrt{52m^2 - 8m + 1}\right]}}$$

$$= \sqrt{\frac{(8m+1) + \sqrt{52m^2 - 8m + 1}}{(8m+1) - \sqrt{52m^2 - 8m + 1}}}$$

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And the limit as $m \to \infty$:

$$\lim_{m \to \infty} \kappa\left(\hat{A}\right) = \lim_{m \to \infty} \sqrt{\frac{(8m+1) + \sqrt{52m^2 - 8m + 1}}{(8m+1) - \sqrt{52m^2 - 8m + 1}}}$$

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Multiplying by the conjugate of the denominator and ignoring the square root (it is irelevant for the limit):

$$= \lim_{m \to \infty} \left[\frac{(8m+1) + \sqrt{52m^2 - 8m + 1}}{(8m+1) - \sqrt{52m^2 - 8m + 1}} \cdot \frac{(8m+1) + \sqrt{52m^2 - 8m + 1}}{(8m+1) + \sqrt{52m^2 - 8m + 1}}\right]$$

$$= \lim_{m \to \infty} \frac{\left((8m+1) + \sqrt{52m^2 - 8m + 1}\right)^2}{(8m+1)^2 - 52m^2 - 8m + 1}$$

$$= \lim_{m \to \infty} \frac{(8m+1)^2 + 2(8m+1)\sqrt{52m^2 - 8m + 1} + (52m^2 - 8m + 1)}{(8m+1)^2 - (52m^2 - 8m + 1)}$$

$$= \lim_{m \to \infty} \frac{64m^2 + 16m + 1 + (16m+1)\sqrt{52m^2 - 8m + 1} + 52m^2 - 8m + 1}{64m^2 + 16m + 1 - 52m^2 + 8m - 1}$$

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Regretting having ignored the square root, and putting it back, we have:

$$= \lim_{m \to \infty} \sqrt{\frac{\left((8m+1) + \sqrt{52m^2 - 8m + 1}\right)^2}{12m^2 + 24m}}$$

$$= \lim_{m \to \infty} \frac{(8m+1) + \sqrt{52m^2 - 8m + 1}}{\sqrt{12m^2 + 24m}}$$

$$= \lim_{m \to \infty} \frac{8m + 1 + m\sqrt{52 - \frac{8}{m} + \frac{1}{m^2}}}{m\sqrt{12 + \frac{24}{m}}}$$

$$= \lim_{m \to \infty} \frac{m\left(8 + \frac{1}{m} + \sqrt{52 - \frac{8}{m} + \frac{1}{m^2}}\right)}{m\sqrt{12 + \frac{24}{m}}}$$

$$= \lim_{m \to \infty} \frac{8 + \frac{1}{m} + \sqrt{52 - \frac{8}{m} + \frac{1}{m^2}}}{\sqrt{12 + \frac{24}{m}}}$$

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And finally:

$$\lim_{m \to \infty} \kappa\left(\hat{A}_m\right) = \frac{8 + \sqrt{52}}{\sqrt{12}} = \frac{4 + \sqrt{13}}{\sqrt{3}}$$

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A very good visualization of this is:

Figure 5: The purple line is the limit and the red is the function eq. (39)

Figure 5 shows the function approaching the limit. One could say that this problem is well conditioned, for $\kappa\left(\hat{A}\right)_m < \frac{4+\sqrt{13}}{\sqrt{3}}, \forall m > 0$, and $\frac{4+\sqrt{13}}{\sqrt{3}}$ is not a very big number. We will not go deep into the discussion of how well-condition this problem is, but we can say that the condition number of A is not a problem for the linear regression algorithm.

5. Polynomial Regression (1c)

In this section we will discuss what changes when we decide to use **polynomials** instead of **lines** to approximate our dataset:

$$f(t) = \alpha + \beta t \rightarrow p(t) = \varphi_0 + \varphi_1 t + ... + \varphi_n t^n \tag{44}$$

From a first perspective, it seems way more efficient to describe a dataset with many variables then to do so with a simple line $\alpha + \beta t$, so let's use the same dataset $S := \left\{(t_i, b_i), t_i = \frac{i}{m}\right\}, i = 0, 1, ..., m$. Where b_i is arbitrary. As we did in Section 3, finding the new system to be solved gives us:

$$p(t_0 = 0) = b_0 = \varphi_0,$$

$$p\left(t_1 = \frac{1}{m}\right) = b_1 = \varphi_0 + \varphi_1 \frac{1}{m} + ... + \varphi_n \left(\frac{1}{m}\right)^n$$

$$p\left(t_2 = \frac{2}{m}\right) = b_2 = \varphi_0 + \varphi_1 \frac{2}{m} + \varphi_2 \left(\frac{2}{m}\right)^2 + ... + \varphi_n \left(\frac{2}{m}\right)^n \tag{45}$$

$$\vdots$$

$$p(t_m = 1) = b_m = \varphi_0 + ... + \varphi_n$$

Or:

$$
\underbrace{\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & \frac{1}{m} & \left(\frac{1}{m}\right)^2 & \dots & \left(\frac{1}{m}\right)^n \\ 1 & \frac{2}{m} & \left(\frac{2}{m}\right)^2 & \dots & \left(\frac{2}{m}\right)^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix}}_{A_{m+1 \times n+1}} \cdot \underbrace{\begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_n \end{bmatrix}}_{\Phi_{n+1 \times 1}} = \underbrace{\begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}}_{b_{m+1 \times 1}}
\qquad 46
$$

Projecting into $C(A)$:

$$
A^* A \hat{\Phi} = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 0 & \frac{1}{m} & \frac{2}{m} & \dots & 1 \\ 0 & \left(\frac{1}{m}\right)^2 & \left(\frac{2}{m}\right)^2 & \dots & 1 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & \left(\frac{1}{m}\right)^n & \left(\frac{2}{m}\right)^n & \dots & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & \frac{1}{m} & \left(\frac{1}{m}\right)^2 & \dots & \left(\frac{1}{m}\right)^n \\ 1 & \frac{2}{m} & \left(\frac{2}{m}\right)^2 & \dots & \left(\frac{2}{m}\right)^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix} \cdot \begin{bmatrix} \widehat{\varphi_0} \\ \widehat{\varphi_1} \\ \widehat{\varphi_2} \\ \vdots \\ \widehat{\varphi_n} \end{bmatrix}
$$

$$
= \begin{bmatrix} m+1 & \sum_{i=1}^{m} \frac{i}{m} & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^2 & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^n \\ \sum_{i=1}^{m} \frac{i}{m} & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^2 & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^3 & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+1} \\ \sum_{i=1}^{m} \left(\frac{i}{m}\right)^2 & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^3 & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^4 & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^{m} \left(\frac{i}{m}\right)^n & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+1} & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+2} & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{2n} \end{bmatrix} \cdot \begin{bmatrix} \widehat{\varphi_0} \\ \widehat{\varphi_1} \\ \widehat{\varphi_2} \\ \vdots \\ \widehat{\varphi_n} \end{bmatrix}
\qquad 47
$$

$$
= \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 0 & \frac{1}{m} & \frac{2}{m} & \dots & 1 \\ 0 & \left(\frac{1}{m}\right)^2 & \left(\frac{2}{m}\right)^2 & \dots & 1 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & \left(\frac{1}{m}\right)^n & \left(\frac{2}{m}\right)^n & \dots & 1 \end{bmatrix} \cdot \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^{m} b_i \\ \sum_{i=0}^{m} \frac{i b_i}{m} \\ \sum_{i=0}^{m} \left(\frac{i}{m}\right)^2 m \\ \vdots \\ \sum_{i=0}^{m} \left(\frac{i}{m}\right)^n b_i \end{bmatrix}
$$

So the system to be solved is:

$$
\underbrace{\begin{bmatrix} m+1 & \sum_{i=1}^{m} \frac{i}{m} & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^n \\ \sum_{i=1}^{m} \frac{i}{m} & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^2 & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+1} \\ \sum_{i=1}^{m} \left(\frac{i}{m}\right)^2 & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^3 & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+2} \\ \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^{m} \left(\frac{i}{m}\right)^n & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{n+1} & \dots & \sum_{i=1}^{m} \left(\frac{i}{m}\right)^{2n} \end{bmatrix}}_{\hat{A}} \cdot \begin{bmatrix} \widehat{\varphi_0} \\ \widehat{\varphi_1} \\ \widehat{\varphi_2} \\ \vdots \\ \widehat{\varphi_n} \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^{m} b_i \\ \sum_{i=0}^{m} \frac{i b_i}{m} \\ \sum_{i=0}^{m} \left(\frac{i}{m}\right)^2 m \\ \vdots \\ \sum_{i=0}^{m} \left(\frac{i}{m}\right)^n b_i \end{bmatrix}
\qquad 48
$$

This gives the optimal vector $\hat{\Phi}$ that solves the least squares problem. We will use computational methods to analyze this system in some of the next sections.

6. Computing the polynomial regression matrix, given (m,n) (1d)

Here is a python function that calculates the polynomial regression matrix $\hat{A} = A^* A$ from eq. (48), given the dimensions (m, n):

```Python
1   import numpy as np
2
```

```
3   def poly_ls(m, n):

4

5       """
6       Builds the (n+1) x (n+1) matrix A^T A for least-squares polynomial fitting.

7

8       Args:
9           m (int): number of subintervals (m >= 0)
10          n (int): polynomial degree (n >= 0)
11      Returns:
12          np.ndarray: shape (n+1, n+1) Gram matrix
13      Raises:
14          ValueError: if m or n is negative or not integer
15      """

16

17      if not isinstance(m, int) or not isinstance(n, int):
18          raise ValueError("m and n must be integers")
19      if m < 0 or n < 0:
20          raise ValueError("m and n must be non-negative")

21

22      x = np.linspace(0, 1, m+1) #sample space

23

24      A = np.zeros((n+1, n+1), dtype=float) #intializes 0 matrix to be filled
25      np.set_printoptions(precision=3, suppress=True)
26      for j in range(n+1): #THIS IS NOT A, IT IS A^* A
27          for k in range(n+1):
28              A[j, k] = np.sum(x**(j + k)) #fills each entry

29

30      return A

31

32  for m, n in [(1, 1), (2, 2), (2, 3)]: #trivial examples
33      M = poly_ls(m, n)
34      print(f"m = {m}, n = {n}:")
35      print(M, end="\n\n")
```

Some simple cases are:

$$\hat{A}(1,1) = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\hat{A}(2,2) = \begin{bmatrix} 3 & 1.5 & 1.25 \\ 1.5 & 1.25 & 1.125 \\ 1.25 & 1.125 & 1.062 \end{bmatrix}$$

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$$\hat{A}(2,3) = \begin{bmatrix} 3 & 1.5 & 1.25 & 1.125 \\ 1.5 & 1.25 & 1.125 & 1.062 \\ 1.25 & 1.125 & 1.062 & 1.031 \\ 1.125 & 1.062 & 1.031 & 1.016 \end{bmatrix}$$

7. How Perturbations Affect The Condition Number (1e)

Still on polynomial regression, in this section we analyze what happens to $\kappa(\hat{A})$, when $\hat{A}$ is perturbated with $m = 100$ and $n = 1, ..., 20$.

We will run *poly_ls(m, n)* built in Section 6 for $m = 100$ and $n = 1, ..., 20$. Given the sad fact that polynomial rootfinding is not a well-conditioned problem, we will then numerically calculate the condition number of $\hat{A}$ for each output of *poly_ls(m, n)*. See the code:

```python
import numpy as np
import matplotlib.pyplot as plt

def format_scientific(x, sig=3):

    """
    Formats a number in scientific notation with a specified number of
    significant digits.

    Args:
        x (float): number to format
        sig (int): number of significant digits (default: 3)
    Returns:
        str: formatted string in scientific notation
    """

    if x == 0:
        return "0"
    exp = int(np.floor(np.log10(abs(x))))
    mant = x / 10**exp
    return f"{mant:.{sig}f} * 10^{exp}"

def compute_condition_numbers(m, max_n):

    """
    Returns a list of the condition numbers of the polynomial least-squares
    matrix A(m) for degrees n = 1 to max_n.

    Args:
        m (int): number of subintervals (m >= 0)
        max_n (int): maximum polynomial degree (max_n >= 0)
    Returns:
        list: condition numbers of A(m) for degrees n = 1 to max_n
    """

    conds = []
    for n in range(1, max_n + 1):
        A = poly_ls(m, n)
        sv = np.linalg.svd(A, compute_uv=False) #computes singular values
```

```
38          conds.append(sv[0] / sv[-1]) #condition number is the ratio of the
            largest to smallest singular value.
39      return conds
40
41  if __name__ == "__main__":
42      m = 100
43      max_n = 20
44
45      cond_nums = compute_condition_numbers(m, max_n)
46      n_values = np.arange(1, max_n + 1)
47
48      print(f"Condition numbers of A (m={m}) for degree n:")
49      for n, c in zip(n_values, cond_nums):
50          print(f"  n = {n:2d} → κ₂(A) = {format_scientific(c)}")
51
52      plt.figure()
53      plt.semilogy(n_values, cond_nums, marker="o", linestyle="-")
54      plt.xlabel("Polynomial degree $n$")
55      plt.ylabel("Condition number $\\kappa(A)$")
56      plt.title(f"Growth of Condition Number, $m={m}$")
57      plt.grid(True, which="both", ls="--")
58      plt.tight_layout()
59      plt.show()
```

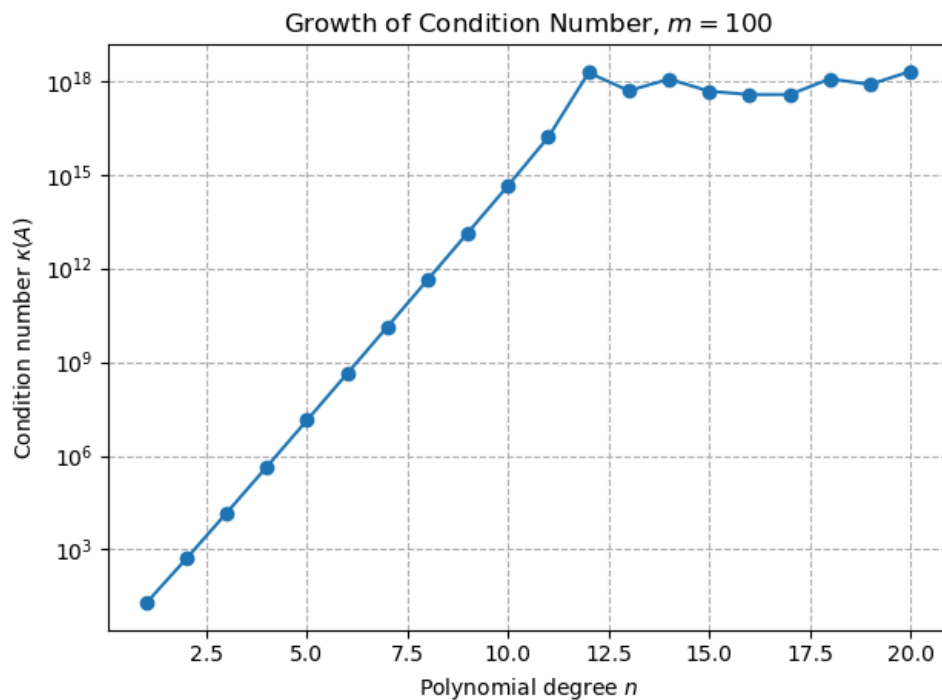A good plot of the growth of the condition number is:

Figure 6: Growth of the condition number of A(m) for polynomial regression

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Figure 6 Shows that with higher degrees of polynomials, $\kappa\left(\hat{A}_m\right)$ grows **exponentially**. This can make polynomial regression a **bad choice** for approximating datasets with many points. Which contradicts our initial assumption!

One could notice that the graph wiggles up and down at $12 \leq n \leq 20$. To understand this we must take into account that $\varepsilon_m \approx 2.22 \cdot 10^{-16}$, and at $n = 12$, $\kappa\left(\hat{A}\right)$ is already past 10^{16}. Notice as well that we are calculating on $\hat{A}$, not A, so:

$$\kappa\left(\hat{A} = A^*A\right) = \frac{\sigma_{\max(A^*A)}}{\sigma_{\min(A^*A)}} = \left(\frac{\sigma_{\max(A)}}{\sigma_{\min(A)}}\right)^2 = \kappa(A)^2 \qquad 50$$

Squaring $\kappa(A)$ pushes numbers past the IEEE 754 double precision quickly. So once the trye $\kappa\left(\hat{A} = A^*A\right)$ exceeds $\frac{1}{\varepsilon_m}$, the smallest singular value underflows to 0. So everything above that is **numerically indistinguishable**. So the line stops at $\approx 10^{16}$ and wiggles for a while.

8. Polynomial Regression with a Different Dataset

8.1. A Different Dataset

If we change $S := \left\{(t_i, b_i) \mid t_i = \frac{i}{m}, i = 0, 1, ..., m\right\}$ to $\hat{S} = \left\{(t_i, b_i) \mid t_i = \frac{i}{m} - \frac{1}{2}\right\}$, the polynomial regression becomes:

$$p\left(t_0 = 0 - \frac{1}{2}\right) = \varphi_0 + \varphi_1\left(-\frac{1}{2}\right) + ... + \varphi_n\left(-\frac{1}{2}\right)^n = b_0$$

$$p\left(t_1 = \frac{1}{m} - \frac{1}{2}\right) = \varphi_0 + \varphi_1\left(\frac{1}{m} - \frac{1}{2}\right) + \varphi_2\left(\frac{1}{m} - \frac{1}{2}\right)^2 + ... + \varphi_n\left(\frac{1}{m} - \frac{1}{2}\right)^n \qquad 51$$

$$\vdots$$

$$p\left(t_m = 1 - \frac{1}{2}\right) = \varphi_0 + \varphi_1\left(1 - \frac{1}{2}\right) + ... + \varphi_n\left(1 - \frac{1}{2}\right)^n$$

So:

$$\underbrace{\begin{bmatrix} 1 & -\frac{1}{2} & \left(-\frac{1}{2}\right)^2 & \cdots & \left(-\frac{1}{2}\right)^n \\ 1 & \left(\frac{1}{m} - \frac{1}{2}\right) & \left(\frac{1}{m} - \frac{1}{2}\right)^2 & \cdots & \left(\frac{1}{m} - \frac{1}{2}\right)^n \\ 1 & \left(\frac{2}{m} - \frac{1}{2}\right) & \left(\frac{2}{m} - \frac{1}{2}\right)^2 & \cdots & \left(\frac{2}{m} - \frac{1}{2}\right)^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \left(-\frac{1}{2}\right) & \left(-\frac{1}{2}\right)^2 & \cdots & \left(-\frac{1}{2}\right)^n \end{bmatrix}}_{A} \cdot \underbrace{\begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \vdots \\ \varphi_n \end{bmatrix}}_{\Phi} = \underbrace{\begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_m \end{bmatrix}}_{b} \qquad 52$$

Projecting onto $C(A)$:

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ -\frac{1}{2} & \left(\frac{1}{m} - \frac{1}{2}\right) & \left(\frac{2}{m} - \frac{1}{2}\right) & \cdots & -\frac{1}{2} \\ \left(-\frac{1}{2}\right)^2 & \left(\frac{1}{m}, -\frac{1}{2}\right)^2 & \left(\frac{2}{m} - \frac{1}{2}\right)^2 & \cdots & \left(-\frac{1}{2}\right)^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \left(-\frac{1}{2}\right)^n & \left(\frac{1}{m} - \frac{1}{2}\right)^n & \left(\frac{2}{m} - \frac{1}{2}\right)^n & \cdots & \left(-\frac{1}{2}\right)^n \end{bmatrix}}_{A^*} \cdot \underbrace{\begin{bmatrix} 1 & -\frac{1}{2} & \left(-\frac{1}{2}\right)^2 & \cdots & \left(-\frac{1}{2}\right)^n \\ 1 & \left(\frac{1}{m} - \frac{1}{2}\right) & \left(\frac{1}{m} - \frac{1}{2}\right)^2 & \cdots & \left(\frac{1}{m} - \frac{1}{2}\right)^n \\ 1 & \left(\frac{2}{m} - \frac{1}{2}\right) & \left(\frac{2}{m} - \frac{1}{2}\right)^2 & \cdots & \left(\frac{2}{m} - \frac{1}{2}\right)^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & -\frac{1}{2} & \left(-\frac{1}{2}\right)^2 & \cdots & \left(-\frac{1}{2}\right)^n \end{bmatrix}}_{A} \cdot \underbrace{\begin{bmatrix} \widehat{\varphi_0} \\ \widehat{\varphi_1} \\ \vdots \\ \widehat{\varphi_n} \end{bmatrix}}_{\hat{\Phi}} \quad 53$$

Notice that to calculate A^*A we can do:

$$(A^*A)_{ij} = \langle l_i^{A^*}, c_j^A \rangle = \langle c_i^A, c_j^A \rangle = \sum_{k=0}^{m} \left(\frac{k}{m} - \frac{1}{2} \right)^{i+j-2}$$

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So we have:

$$\begin{bmatrix} n+1 & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right) & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^2 & \cdots & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^n \\ \sum_{i=0}^{n}\frac{i}{m}-\frac{1}{2} & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^2 & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^3 & \cdots & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{n+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^n & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{n+1} & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{n+2} & \cdots & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{2n} \end{bmatrix} \cdot \begin{bmatrix} \widehat{\varphi}_0 \\ \widehat{\varphi}_1 \\ \vdots \\ \widehat{\varphi}_n \end{bmatrix}$$

55

And doing A^*b gives:

$$= \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ -\frac{1}{2} & \left(\frac{1}{m}-\frac{1}{2}\right) & \left(\frac{2}{m}-\frac{1}{2}\right) & \cdots & -\frac{1}{2} \\ \left(-\frac{1}{2}\right)^2 & \left(\frac{1}{m},-\frac{1}{2}\right)^2 & \left(\frac{2}{m}-\frac{1}{2}\right)^2 & \cdots & \left(-\frac{1}{2}\right)^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \left(-\frac{1}{2}\right)^n & \left(\frac{1}{m}-\frac{1}{2}\right)^n & \left(\frac{2}{m}-\frac{1}{2}\right)^n & \cdots & \left(-\frac{1}{2}\right)^n \end{bmatrix} \cdot \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^{n} b_i \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)b_i \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^2 b_i \\ \vdots \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^n b_i \end{bmatrix}$$

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So the system to be solved is:

$$\underbrace{\begin{bmatrix} m+1 & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right) & \cdots & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^n \\ \sum_{i=0}^{n}\frac{i}{m}-\frac{1}{2} & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^2 & \cdots & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{n+1} \\ \vdots & \vdots & \vdots & \vdots \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^n & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{n+1} & \cdots & \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^{2n} \end{bmatrix}}_{\hat{A}} \cdot \begin{bmatrix} \widehat{\varphi}_0 \\ \widehat{\varphi}_1 \\ \widehat{\varphi}_2 \\ \vdots \\ \widehat{\varphi}_n \end{bmatrix} = \cdot \begin{bmatrix} \sum_{i=0}^{n} b_i \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)b_i \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^2 b_i \\ \vdots \\ \sum_{i=0}^{n}\left(\frac{i}{m}-\frac{1}{2}\right)^n b_i \end{bmatrix}$$

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The following code calculates the new matrix $\hat{A}$ in eq. (57):

```Python
1   import numpy as np
2   import matplotlib.pyplot as plt
3
4   def poly_ls_2(m, n):
5
6       """
7       Builds the (n+1) x (n+1) matrix for least-squares polynomial fitting.
8
9       Args:
10          m (int): number of subintervals (m >= 0)
11          n (int): polynomial degree (n >= 0)
12      Returns:
13          np.ndarray: shape (n+1, n+1) Gram matrix
14      Raises:
15          ValueError: if m or n is negative or not integer
16      """
17
18      if not (isinstance(m, int) and isinstance(n, int)) or m < 0 or n < 0:
```

```
19             raise ValueError("m and n must be non-negative integers")
20
21     t = np.linspace(0, 1, m + 1) - 0.5
22     powers = t[:, None] ** np.arange(2 * n + 1)
23     col_sums = powers.sum(axis=0)
24     M = np.empty((n + 1, n + 1))
25     for i in range(n + 1):
26         for j in range(n + 1):
27             M[i, j] = col_sums[i + j] #fills each entry
28
29     return M
30
31 #examples:
32 m_1 = poly_ls_2(2, 1)
33 m_2 = poly_ls_2(2, 2)
34 m_3 = poly_ls_2(2, 3)
35 print("m = 2, n = 1:")
36 print(m_1)
37 print("\nm = 2, n = 2:")
38 print(m_2)
39 print("\nm = 2, n = 3:")
40 print(m_3)
```

The examples are:

Example 8.1.1.:

$$M(2,1) = \begin{bmatrix} 3 & 0 \\ 0 & 0.5 \end{bmatrix}$$

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Example 8.1.2.:

$$M(2,2) = \begin{bmatrix} 3 & 0 & 0.5 \\ 0 & 0.5 & 0 \\ 0.5 & 0 & 0.125 \end{bmatrix}$$

59

Example 8.1.3.:

$$M(2,3) = \begin{bmatrix} 3 & 0 & 0.5 & 0 \\ 0 & 0.5 & 0 & 0.125 \\ 0.5 & 0 & 0.125 & 0 \\ 0 & 0.125 & 0 & 0.031 \end{bmatrix}$$

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8.2. How Conditioning changes (1f)

Here we will analyze how the condition number of $\hat{A}$ shown in the previous section changes with perturbations on the degree n. We will use the same method used in Section 7. $m = 100$ and $n = 1, ..., 20$. The following code is used:

```Python
1  import numpy as np
2  import matplotlib.pyplot as plt
```

```
 3
 4   def compute_condition_numbers_centered(m: int, max_n: int):
 5
 6       """
 7       Computes the condition numbers of the polynomial least-squares matrix M(m)
         for degrees n = 1 to max_n.
 8
 9       Args:
10           m (int): number of subintervals (m >= 0)
11           max_n (int): maximum polynomial degree (max_n >= 0)
12       Returns:
13           list: condition numbers of M(m) for degrees n = 1 to max_n
14       """
15
16       conds = []
17       for n in range(1, max_n + 1):
18           M  = poly_ls_2(m, n)
19           s  = np.linalg.svd(M, compute_uv=False) #computes singular values
20           conds.append(s[0] / s[-1]) #κ = σ_max / σ_min
21       return conds
22
23   m, max_n = 100, 20
24
25   cond_nums = compute_condition_numbers_centered(m, max_n)
26   n_values  = np.arange(1, max_n + 1)
27
28   print(f"Condition numbers at (m = {m})")
29   for n, κ in zip(n_values, cond_nums):
30       print(f"  n = {n:2d} → κ(G) = {format_scientific(κ)}")
31
32   plt.figure()
33   plt.semilogy(n_values, cond_nums, marker="o")
34   plt.xlabel("Polynomial degree $n$")
35   plt.ylabel(r"Condition number $\kappa_2(G)$")
36   plt.title(fr"Growth of $\kappa$, $m={m}$")
37   plt.grid(True, which="both", ls="--")
38   plt.tight_layout()
39   plt.show()
```
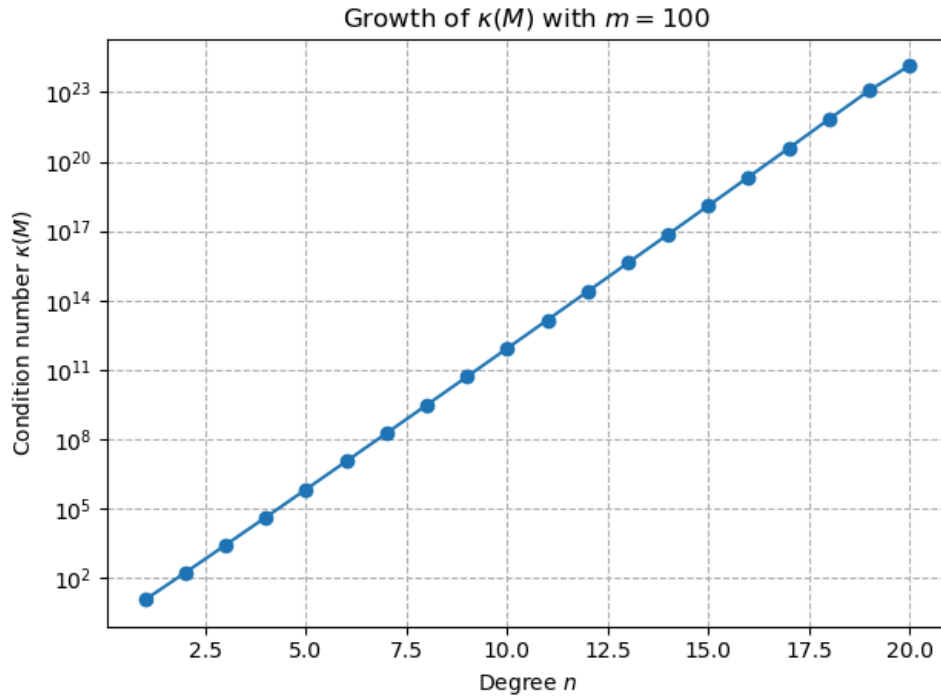
The expected output is:

Figure 7: Growth of the condition number of $\hat{A}$ with a new dataset

The weird behavior noticed in Figure 6 is not seen in Figure 7. This is due to the fact that the dataset has been scaled to be centered at 0, reducing the dynamic range in each column and preventing the singular values from the underflow zone (at least for $20 \geq n$)

9. Comparing the Condition Number

Here we graphically compare both condition numbers seen in Figure 6 and Figure 7. The following code is used:

```python
def compute_condition_numbers(m, max_n):

    """
    Compute k(A^* A).

    Each matrix A is constructed by
    poly_ls(m, n)

    Args:
        m (int): Number of subintervals in the sample grid t_i = i/m.
        max_n (int): Maximum polynomial degree to evaluate.

    Returns:
        list[float]: The list
        [ k(A_i^* A_i)) ],
        where k(A^* A) = k(A)^2 and κ is the 2-norm condition number.
    """

    conds = []
```

```python
20          for n in range(1, max_n + 1):
21              A = poly_ls(m, n)
22              sigma = np.linalg.svd(A, compute_uv=False)
23              κ2 = sigma[0] / sigma[-1]   #k_2(A)
24              conds.append(κ2 ** 2) #κ_2(A^* A) = κ_2(A)^2
25          return conds
26
27
28  def compute_condition_numbers_centered(m, max_n):
29
30          """
31          Compute k(M) for a centred / scaled polynomial basis.
32          Each matrix M is produced by poly_ls_2(m, n)
33
34          Args:
35              m (int): Number of subintervals in the sample grid t_i = i/m.
36              max_n (int): Maximum polynomial degree to evaluate.
37
38          Returns:
39              list[float]: The list
40              [ k(M_i) ] where
41              k is the 2-norm condition number of the centred design matrix.
42          """
43
44          conds = []
45          for n in range(1, max_n + 1):
46              M = poly_ls_2(m, n)
47              sigma = np.linalg.svd(M, compute_uv=False)
48              conds.append(sigma[0] / sigma[-1])
49          return conds
50
51
52  def plot_condition_numbers(m = 100, max_n = 20):
53
54          """
55          Plot the growth of condition numbers for raw and centred Vandermonde bases.
56
57          Args:
58              m (int, optional): Number of subintervals in the sample grid
59                  t_i = i/m. Defaults to 100.
60
61              max_n (int, optional): Maximum polynomial degree to display.
62                  Defaults to 20.
63
64          Returns:
65              None.  The function displays a semilog plot comparing
```

```
66              k(A^* A) (raw basis) and k(M) (centred / scaled basis).
67      """
68
69      n_vals = np.arange(1, max_n + 1)
70      κ_raw = compute_condition_numbers(m, max_n)
71      κ_centered = compute_condition_numbers_centered(m, max_n)
72
73      plt.figure(figsize=(7, 5))
74      plt.semilogy(
75          n_vals,
76          κ_raw,
77          marker="o",
78          linestyle="-",
79          linewidth=1.4,
80          markersize=5,
81          label=r"$\kappa(A^{\top}A)$ (raw basis)",
82      )
83      plt.semilogy(
84          n_vals,
85          κ_centered,
86          marker="s",
87          linestyle="--",
88          linewidth=1.4,
89          markersize=5,
90          label=r"$\kappa(M)$ (centred / scaled basis)",
91      )
92
93      plt.xlabel("Polynomial degree $n$")
94      plt.ylabel("Condition number")
95      plt.title(fr"Condition-number growth, $m={m}$")
96      plt.grid(True, which="both", ls=":", lw=0.7)
97      plt.legend()
98      plt.tight_layout()
99      plt.show()
100
101 plot_condition_numbers(m=100, max_n=20)
```
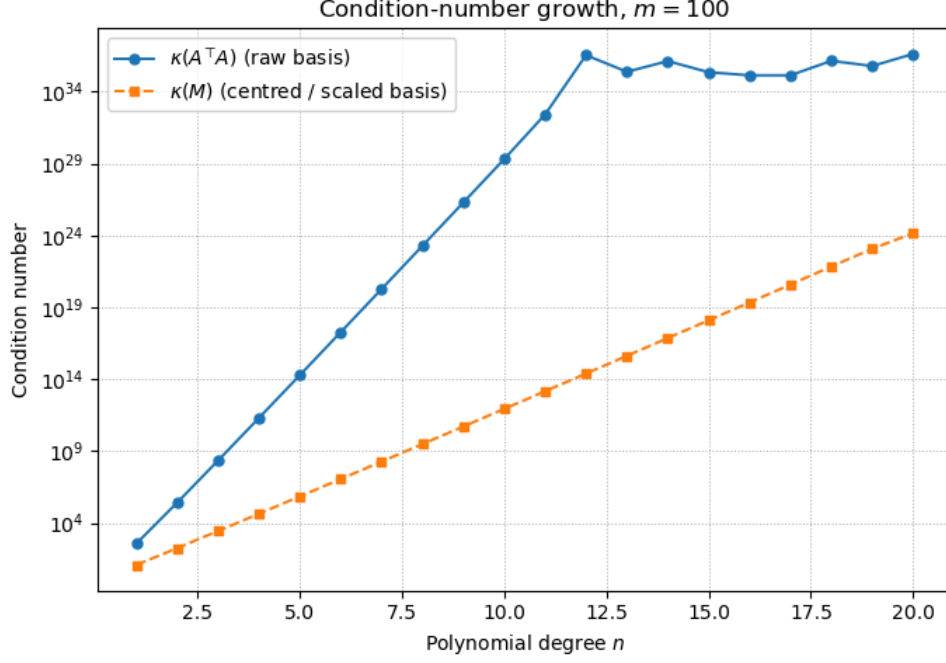
The expected output is the plot below:

Figure 8: A comparison of both datasets

Figure 8 confirms the hypothesis that the condition number of the non-centered dataset tends to produce bigger condition numbers.

10. Least Squares with QR and SVD decompositions

We have shown the solutions to the least squares problem $Ax = b$, but this problem could be solved with factorizations of A, such as the QR and SVD, in the following sections we will show these factorizations and use them to solve the least squares problem.

10.1. QR

The QR factorization of a full-rank $A \in \mathbb{C}^{m \times n}$, $m \geq n$ an consists of finding orthonormal vectors $q_1, ..., q_n$ such that $q_1, ..., q_i$ spans $a_1, ..., q_1$, where a_i is the ith-column of A. So we want:

$$\begin{aligned} \text{span}(a_1) &= \text{span}(q_1) \\ \text{span}(a_1, a_2) &= \text{span}(q_1, q_2) \\ &\vdots \\ \text{span}(a_1, ..., a_n) &= \text{span}(q_1, ..., q_n) \end{aligned}$$

61

This is equivalent to:

$$A = \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix} \cdot \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \vdots & \vdots \\ & & & r_{nn} \end{bmatrix}$$

62

Where $r_{ii} \neq 0$, because a_i will be expressed as a linear combination of q_i, and since the triangular matrix is invertible, q_i can be expressed as a linear combination of a_i. Therefore eq. (62) is:

$$a_1 = q_1 r_{11},$$
$$a_2 = r_{12} q_1 + r_{22} q_2,$$
$$\vdots$$
$$a_n = r_{1n} q_1 + r_{2n} q_2 + \dots + r_{nn} q_n.$$

<div align="right">63</div>

Or:

$$A = \hat{Q}\hat{R}$$

<div align="right">64</div>

Is the *reduced* QR decomposition of A.

The *full* QR decomposition of $A \in \mathbb{C}^{m \times n}$ not of full-rank is analogous to the reduced, but $|m - n|$ 0-columns are appended to $\hat{Q}$ to make it a unitary $m \times m$ matrix Q, and 0-rows are aded to $\hat{R}$ to make it a $m \times n$ still triangular matrix:
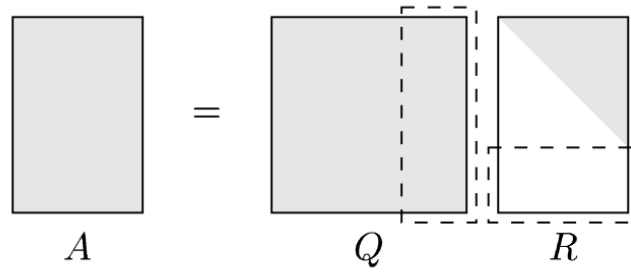

Figure 9: Full QR factorization

And the decomposition becomes:

$$A = QR$$

<div align="right">65</div>

Here are some examples:

Example 10.1.1.:

$$A = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

<div align="right">66</div>

This is a diagonal matrix, so its QR factorization is particularly simple:

$$Q = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, R = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

<div align="right">67</div>

With diagonal matrices, Q is the identity matrix and $R = A$.

Example 10.1.2.:

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

<div align="right">68</div>

For this 3×2 matrix, we compute the reduced QR factorization:

$$\hat{Q} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}, \hat{R} = \begin{bmatrix} \sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix} \qquad 69$$

This is a reduced QR factorization where $\hat{Q}$ is 3×2. The full QR factorization would require extending $\hat{Q}$ to a 3×3 orthogonal matrix and adding a row of zeros to $\hat{R}$ as shown in Figure 9.

10.2. SVD

The *singular value decomposition* of a matrix is based on the fact that the image of the unit sphere under a $m \times n$ matrix is a **hyperellipse:**
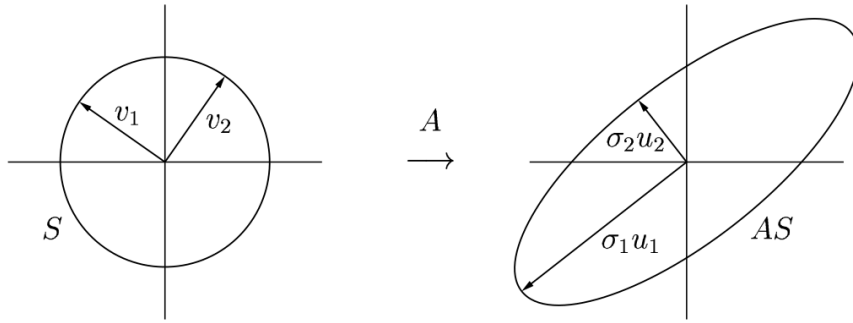

Figure 10: SVD of a 2×2 matrix

So the independent directions v_1, v_2 have been mapped to another set of orthogonal directions $\sigma_1 v_1, \sigma_2 v_2$, so with $S := \{v \in \mathbb{C}^n \mid \|v\| = 1\}$ as the unit ball, let's define:

Definition 10.2.1: (Singular Values) The n *singular values* σ_i of $A \in \mathbb{C}(m \times n)$ are the lengths of the n new axes of AS, written in non-crescent order $\sigma_1 \geq ... \geq \sigma_n$.

Definition 10.2.2: (Left Singular Vectors) The n **left** singular vectors of A are the unit vectors u_i laying in AS, oriented to correspond and number the singular values σ_i, respectively

Definition 10.2.3: (Right Singular Vectors) The **right** singular vectors of A are the v_i in S that are the preimages of $\sigma_i u_i \in AS$, such that $Av_i = \sigma_i u_i$

The equation $Av_i = \sigma_i u_i$ is equivalent to:

$$A \cdot \begin{bmatrix} v_1 & v_2 & ... & v_n \end{bmatrix} = \begin{bmatrix} \sigma_1 u_1 & \sigma_2 u_2 & ... & \sigma_n u_n \end{bmatrix} \qquad 70$$

Better:

$$A \cdot \begin{bmatrix} v_1 & v_2 & \ldots & v_n \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \ldots & u_n \end{bmatrix} \cdot \begin{bmatrix} \sigma_1 & 0 & \ldots & 0 \\ 0 & \sigma_2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & \sigma_n \end{bmatrix} \tag{71}$$

Or simple $AV = U\Sigma$, but since V has orthonormal columns:

$$A = U\Sigma V^* \tag{72}$$

The SVD is a very particular factorization for matrices, as the following theorem states:

Theorem 10.2.1: (Existence of SVD) *Every* matrix $A \in \mathbb{C}^{m \times n}$ has a singular value decomposition

Proof: We prove the existane by fixing the largest image of A and using induction on the dimension of A:

Let $\sigma_1 = \|A\|_2$. There must exist unitary vectors $u_1, v_1 \in \mathbb{C}^n$ such that $Av_1 = \sigma_1 u_1$, with $\|v_1\|_2 = \|u_1\|_2 = 1$. Let $\{v_j\}$ and $\{u_j\}$ be 2 orthonormal bases of $\mathbb{C}^n$. These column vectors form the unitary matrices V_1 and U_1. We will compute:

$$\Phi = U_1^* A V_1 \tag{73}$$

Notice that the first column of Φ is $U_1^* A v_1 = \sigma_1 U_1^* v_1 = \sigma_1 e_1$, since u_1 is the first column of U_1. So Φ looks like:

$$\Phi = \begin{bmatrix} \sigma_1 & w^* \\ 0 & B \end{bmatrix} \tag{74}$$

Where w^* is the rest of the first row, the action of A onto the remaining columns v_j. B acts on the subspace orthogonal to v_1.

We want $w = 0$, we can force this by using the norm. We know that:

$$\left\| \begin{bmatrix} \sigma_1 & w^* \\ 0 & B \end{bmatrix} \cdot \begin{bmatrix} \sigma_1 \\ w \end{bmatrix} \right\|_2 = \left\| \begin{bmatrix} \sigma_1^2 + w^*w \\ Bw \end{bmatrix} \right\|_2 = \sqrt{|\sigma_1^2 + w^*w|^2 + \|Bw\|_2^2} \tag{75}$$

And:

$$\sqrt{|\sigma_1^2 + w^*w|^2 + \|Bw\|_2^2} \geq \sigma_1^2 + w^*w \tag{76}$$

We also know:

$$\|\Phi\|_2 = \sup_{\|y\|=1} \|\Phi y\|_2 \tag{77}$$

For the specific $x = [\sigma_1, w]$ scaled to the unit ball, and knowing $\|\Phi\|_2 = \sigma_1$, we have:

$$\|\Phi\|_2 \geq \frac{\|\Phi x\|_2}{\|x\|_2} \geq \frac{\sigma_1^2 + w^*w}{\sqrt{\sigma_1^2 + w^*w}} = \sqrt{\sigma_1^2 + w^*w} \Leftrightarrow \sigma_1 \geq \sqrt{\sigma_1^2 + w^*w} \tag{78}$$

$$\Leftrightarrow \sigma_1^2 \geq \sigma_1^2 + w^*w \Leftrightarrow w^*w = 0 \Leftrightarrow w = 0.$$

If $m = 1$ or $n = 1$, we are done, If not, B has an SVD decomposition $B = U_2 \Sigma_2 V_2^*$ by the induction hypothesis, so from eq. (73) we have that the following is a SVD decomposition of A, completing the proof:

$$A = U_1 \begin{bmatrix} 1 & 0 \\ 0 & U_2 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & V_2 \end{bmatrix}^* V_1^* \qquad 79$$

$\square$

Is the SVD factorization of A. There are more about the SVD on computing U, Σ, V^*, as we will show below:

Theorem 10.2.2: $\forall A \in \mathbb{C}^{m \times n}$, the following holds:

- The eigenvalues of A^*A are the singular values *squared* of A, and the column-eigenvectors of A^*A form the matrix V.

- The eigenvalues of AA^* are the singular values *squared* of A, and the column-eigenvectors of AA^* form the matrix U.

Proof: Let $U\Sigma V^* = A$ be the SVD of A, then computing A^*A, knowing U, V are unitary matrices, we have:

$$A^*A = (U\Sigma V^*)^*(U\Sigma V^*) = V\Sigma^*U^*U\Sigma V^* = V\Sigma^*\Sigma V^* = V\Sigma^2 V^* \qquad 80$$

This is an *eigenvalue* decomposition of A^*A, where the eigenvalues are the entries of Σ^2, which are the singular values of A **squared**, and the eigenvectors are the columns of V.

For AA^*, we have:

$$AA^* = (U\Sigma V^*)(U\Sigma V^*)^* = U\Sigma V^*V\Sigma^*U^* = U\Sigma\Sigma^*U^* = U\Sigma^2 U^* \qquad 81$$

The reasoning here is analogous. So the proof is complete. $\square$

By Theorem 10.2.2, calculating the SVD of A has been reduced to calculating the eigenvalues and eigenvectors of A^*A and AA^*, here are some examples of singular value decompositions:

Example 10.2.1.: Consider $A = \begin{bmatrix} 3 & 2 \\ 2 & 3 \end{bmatrix}$. Computing the SVD:

First, find $A^*A = \begin{bmatrix} 13 & 12 \\ 12 & 13 \end{bmatrix}$ and calculate its eigenvalues: $\lambda_1 = 25, \lambda_2 = 1$

The singular values are $\sigma_1 = 5, \sigma_2 = 1$.

The right singular vectors (eigenvectors of A^*A): $V = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$

The left singular vectors (obtained from $Av_i = \sigma_i u_i$): $U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$

Therefore, the SVD is: $A = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} 5 & 0 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}^*$

Example 10.2.2.: Consider a non-square matrix $A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$. For this 2×3 matrix, for the SVD we do:

$$A^*A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix} \qquad 82$$

The eigenvalues of A^*A are $\lambda_1 = 3, \lambda_2 = 1, \lambda_3 = 0$, so the singular values are $\sigma_1 = \sqrt{3}, \sigma_2 = 1, \sigma_3 = 0$

The right singular vectors (eigenvectors of A^*A) are:

$$V = \begin{bmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{bmatrix} \qquad 83$$

And now for AA^*:

$$AA^* = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \qquad 84$$

The eigenvalues are $\lambda_1 = 3, \lambda_2 = 1$, so the singular values are $\sigma_1 = \sqrt{3}, \sigma_2 = 1$. The eigenvectors are:

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \qquad 85$$

Therefore, the full SVD is:

$$A = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{bmatrix}^* \qquad 86$$

10.3. Least Squares with QR and SVD

Here we will write code that solves the least squares problem usig the 2 factorizations shown in Section 10.1 and Section 10.2, as well as the ordinary approach to least squares shown in Section 3.

The following code has functions that solve the least squares problem using the QR and SVD decompositions, as well as through the normal approach shown in Section 3. A function to build the matrix A is also included. With a boolean parameter to alternate betweeen a centered $\left(t_i = \frac{i}{m}\right)$ or a non-centered $\left(t_i = \frac{i}{m} - \frac{1}{2}\right)$ dataset:

```Python
1   from numpy.linalg import qr, svd, solve, pinv, cond #easier
2
3   def ls_qr(A, b):
4
5       """
6       Solves the least squares problem Ax = b using QR decomposition.
7
8       Args:
9           A : system matrix
10          b : right-hand side vector
```

```python
11      Returns:
12          x : solution vector
13          y : fitted values (Ax)
14      """
15
16      Q, R = qr(A, mode='reduced')
17      x = solve(R, Q.T @ b)
18      y = A @ x
19
20      return x, y
21
22  def ls_svd(A, b):
23
24      """
25      Solves the least squares problem Ax = b using SVD decomposition.
26
27      Args:
28          A : system matrix
29          b : right-hand side vector
30      Returns:
31          x : solution vector
32          y : fitted values (Ax)
33      """
34
35      U, S, Vt = svd(A, full_matrices=False)
36
37      S_inv = np.zeros_like(S) #calculate the pseudo-inverse using SVD, x = V *
        S⁻¹ * U.T * b
38
39      tol = np.finfo(float).eps * max(A.shape) * S[0] #tolarance for singular
        values
40
41      for i in range(len(S)):
42          if S[i] > tol:
43              S_inv[i] = 1.0 / S[i] #inverts if above tolarance
44
45      x = (Vt.T @ np.diag(S_inv) @ U.T) @ b
46      y = A @ x
47
48      return x, y
49
50  def ls_normal(A, b):
51
52      """
53      Solves the least squares problem Ax = b using normal equations.
54
```

```
55      Args:
56          A : system matrix
57          b : right-hand side vector
58      Returns:
59          x : solution vector
60          y : fitted values (Ax)
61      """
62
63      ATA = A.T @ A
64      ATb = A.T @ b
65
66      x = solve(ATA, ATb)
67      y = A @ x
68
69      return x, y
70
71  def build_A_matrix(m, n, centralized=False):
72
73      """
74      Creates the matrix A for polynomial regression of degree n.
75
76      Args:
77          m (int): number of subintervals (m >= 0)
78          n (int): polynomial degree (n >= 0)
79          centralized (bool): if True, use centralized points
80      Returns:
81          A (np.ndarray): shape (m+1, n+1) matrix for polynomial regression
82          t (np.ndarray): array of points used to create the matrix
83      """
84
85      if centralized:
86          t = np.array([i/m - 1/2 for i in range(m+1)])
87      else:
88          t = np.array([i/m for i in range(m+1)])
89
90      A = np.zeros((m+1, n+1))
91
92      for i in range(n+1):
93          A[:, i] = t**i  #clever
94
95      return A, t
```

10.4. Examples (2b)

We will use the functions defined on the previous sections to do regression on the following functions:

$$f(t) = \sin(t)$$
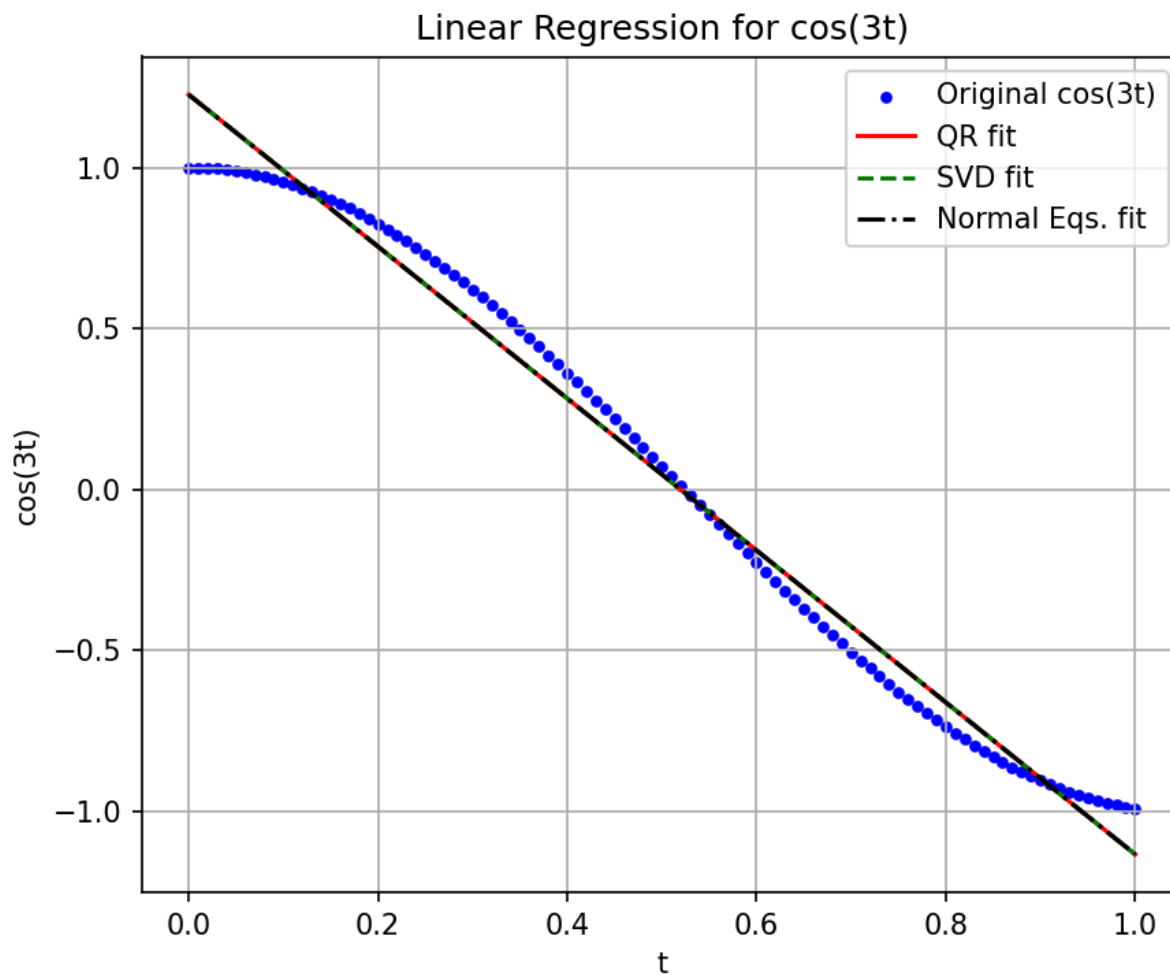$$g(t) = e^t$$
$$h(t) = \cos(3t)$$

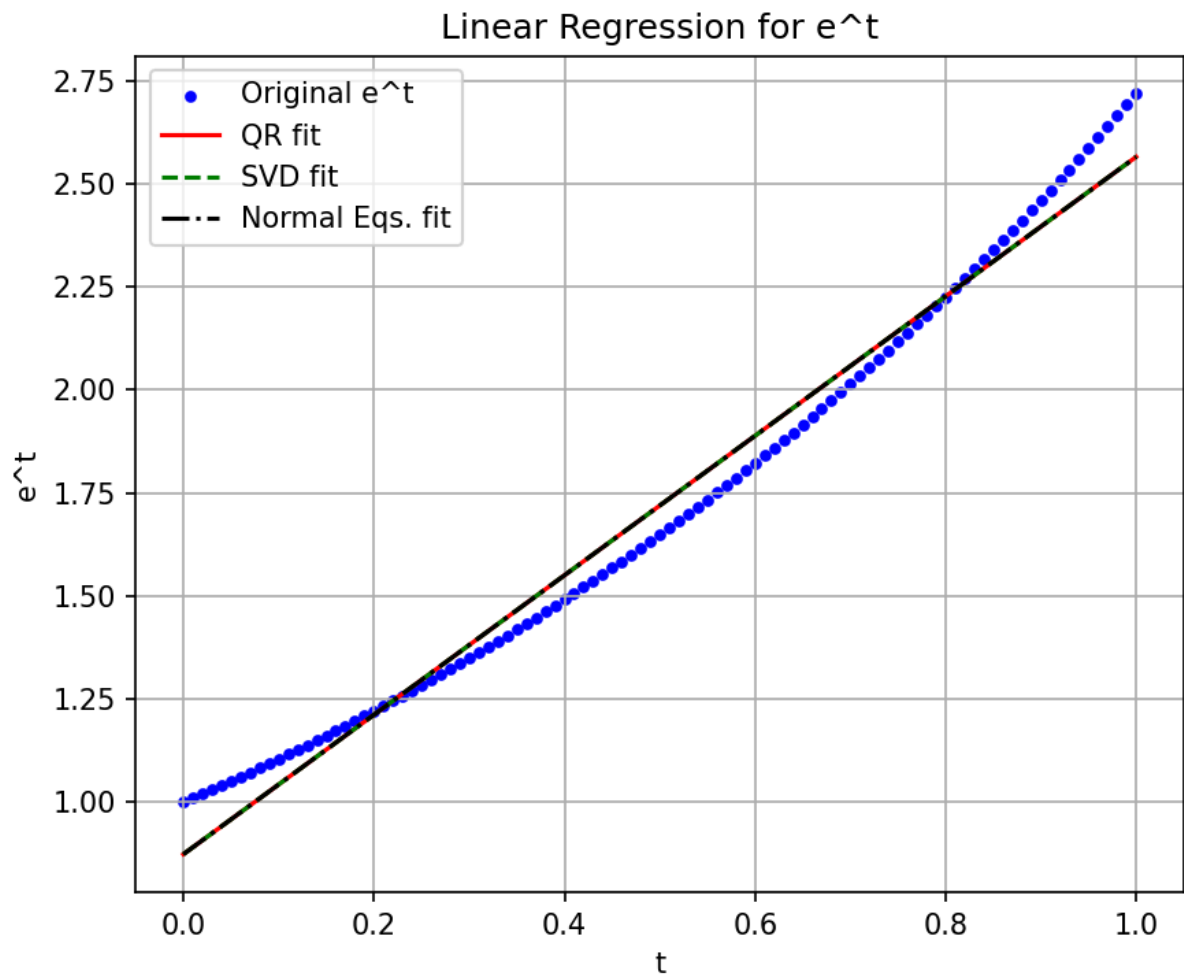The results are shown:

Figure 11: Linear regression on $\cos(t)$

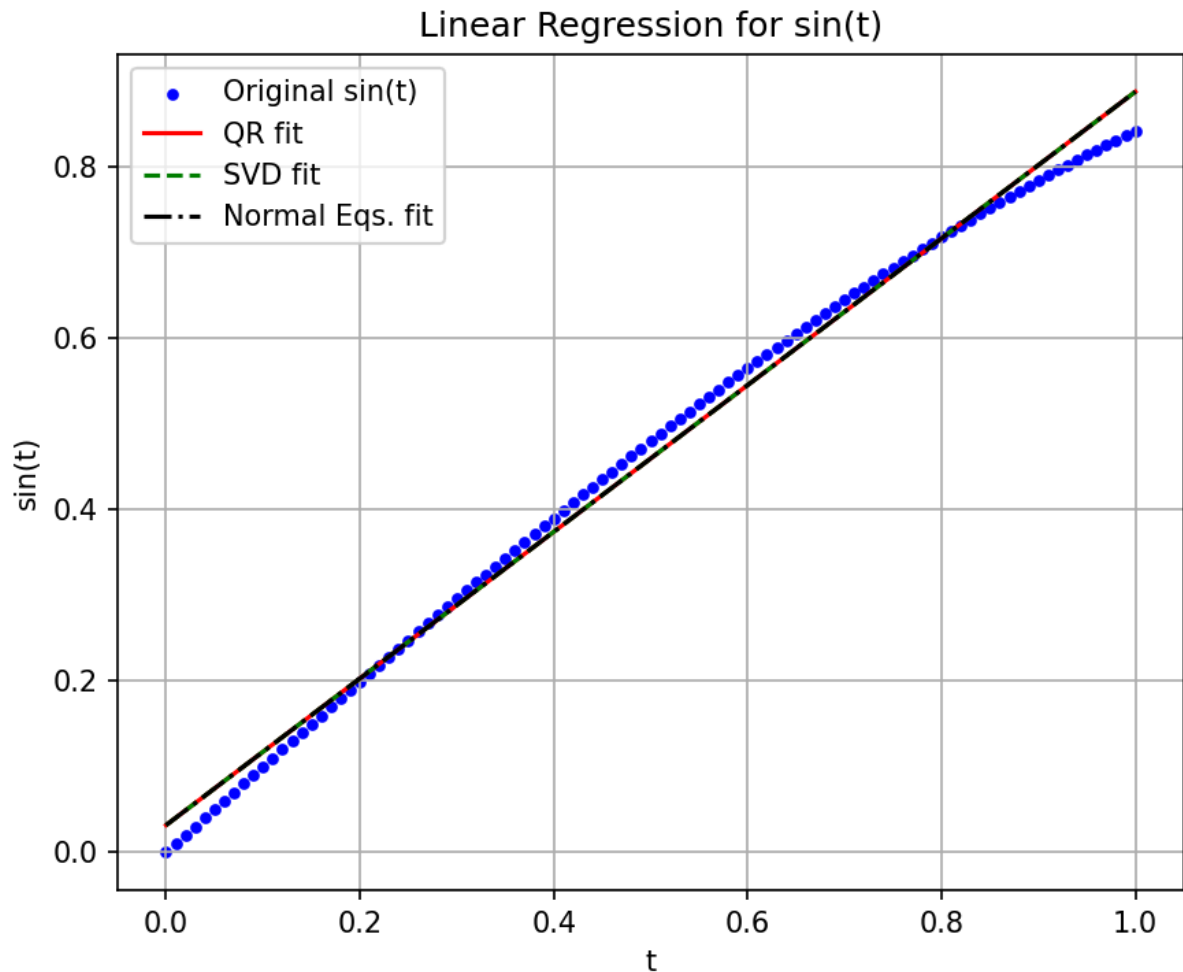Figure 12: Linear regression on e^t

Figure 13: Linear regression on $\sin(t)$

Plots Figure 11, Figure 12, Figure 13 shows us that all 3 methods result in the same line. This is expected, for we are using 100 equally sparse points on a small portion of the image of the functions.

10.5. How good are the approximations? (2c)

In Section 7, we have seen that polynomial regression is not a very well-conditioned problem, so here we will analyze the errors produced by such method. We use what has been done in the previous section.

The following code plots the errors:

```python
1   m = 100
2   t = np.linspace(0, 1, m+1)
3
4   function_data = [(res['name'], res['values']) for res in results] #data here
5
6   max_degree = 15
7   all_errors = {name: {'qr': [], 'svd': [], 'normal': []} for name, _ in
    function_data}
8   all_cond_numbers = []
9
```

```python
10  for n in range(1, max_degree + 1):
11      print(f"\nPolynomial degree: {n}")
12
13      A, _ = build_A_matrix(m, n) #matrix for regression
14      cond_num = cond(A)
15      all_cond_numbers.append(cond_num)
16      print(f"Condition number of A: {format_scientific(cond_num)}")
17
18      for name, values in function_data: #forall funcs, solve using all methods
19          try:
20              x_qr, y_qr = ls_qr(A, values)
21              error_qr = np.linalg.norm(y_qr - values)
22              all_errors[name]['qr'].append(error_qr)
23          except Exception as e:
24              print(f"Error with QR for {name}, degree {n}: {e}")
25              all_errors[name]['qr'].append(np.nan)
26
27          try:
28              x_svd, y_svd = ls_svd(A, values)
29              error_svd = np.linalg.norm(y_svd - values)
30              all_errors[name]['svd'].append(error_svd)
31          except Exception as e:
32              print(f"Error with SVD for {name}, degree {n}: {e}")
33              all_errors[name]['svd'].append(np.nan)
34
35          try:
36              x_normal, y_normal = ls_normal(A, values)
37              error_normal = np.linalg.norm(y_normal - values)
38              all_errors[name]['normal'].append(error_normal)
39          except Exception as e:
40              print(f"Error with Normal Equations for {name}, degree {n}: {e}")
41              all_errors[name]['normal'].append(np.nan)
42
43          #show errors
44          print(f"{name} - Errors: QR: {format_scientific(all_errors[name]['qr']
              [-1])}, "
45              f"SVD: {format_scientific(all_errors[name]['svd'][-1])}, "
46              f"Normal: {format_scientific(all_errors[name]['normal'][-1])}")
47
48  degrees = list(range(1, max_degree + 1))
49
50  for name, _ in function_data:
51      plt.figure(figsize=(6, 5), dpi=150)
52      plt.semilogy(degrees, all_errors[name]['qr'],      'ro-', label='QR')
53      plt.semilogy(degrees, all_errors[name]['svd'],     'gs-', label='SVD')
```

```
54    plt.semilogy(degrees, all_errors[name]['normal'], 'bx-', label='Normal
      Eqs.')
55
56    plt.title(f'Error vs. Polynomial Degree for {name}')
57    plt.xlabel('Polynomial degree $n$')
58    plt.ylabel('Residual error (log scale)')
59    plt.grid(True, which='both', ls=':')
60    plt.legend()
61    plt.tight_layout()
62    plt.show()
63
64 plt.figure(figsize=(6, 5), dpi=150)
65 plt.semilogy(degrees, all_cond_numbers, 'mo-')
66 plt.xlabel('Polynomial degree $n$')
67 plt.ylabel('Condition number (log scale)')
68 plt.title('Condition Number vs. Polynomial Degree')
69 plt.grid(True, which='both', ls=':')
70 plt.tight_layout()
71 plt.show()
```
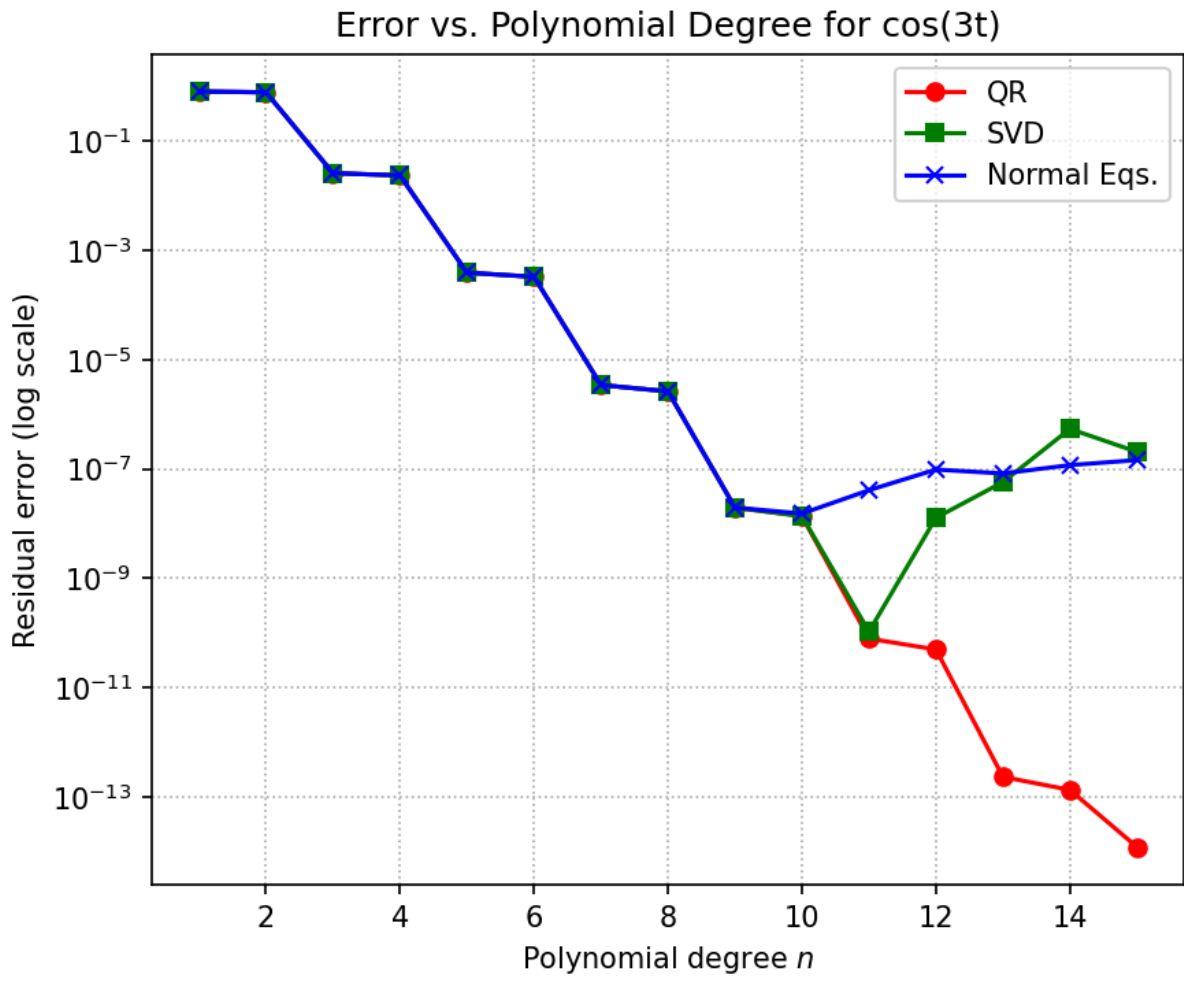
The expected output are the plots:
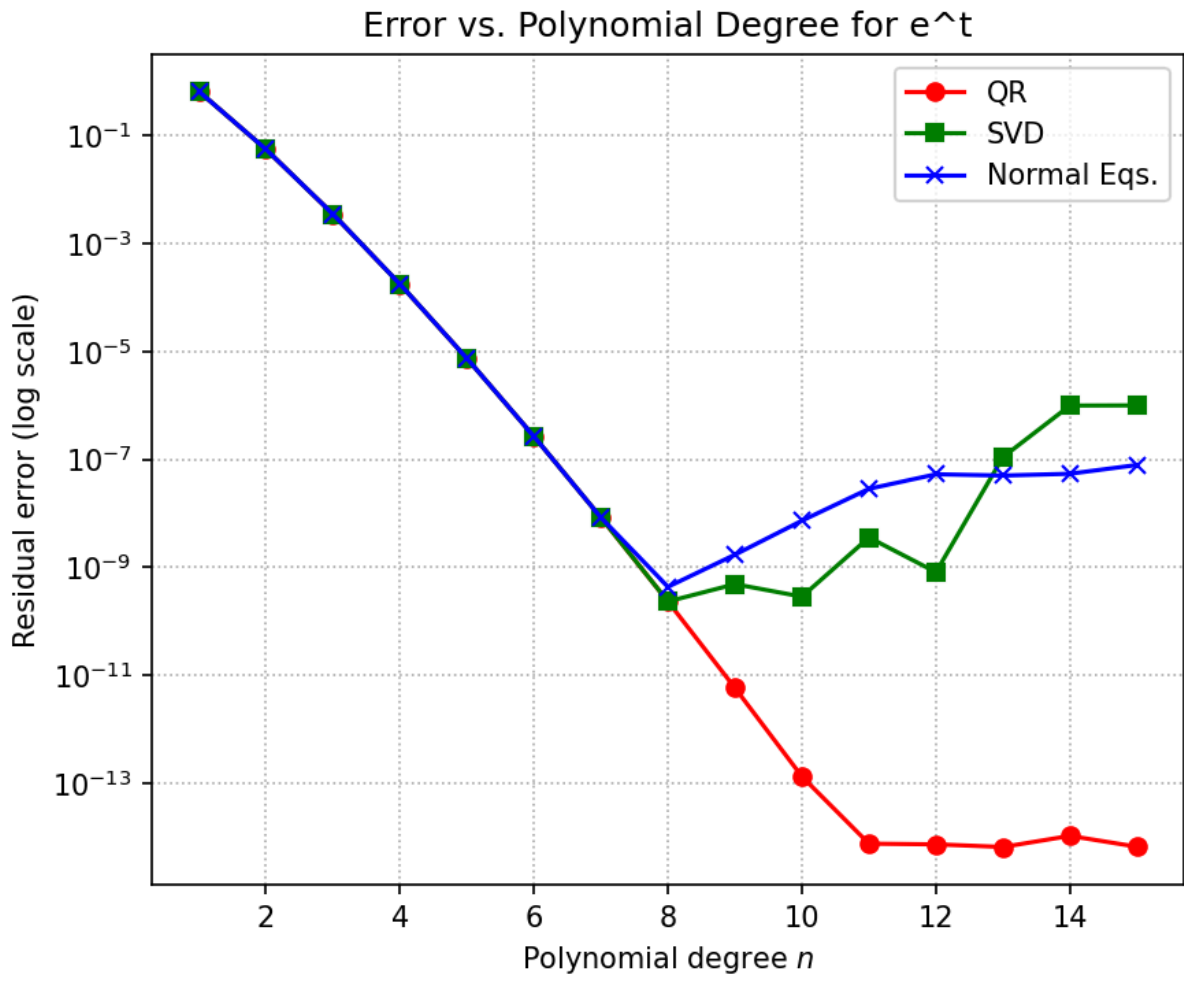
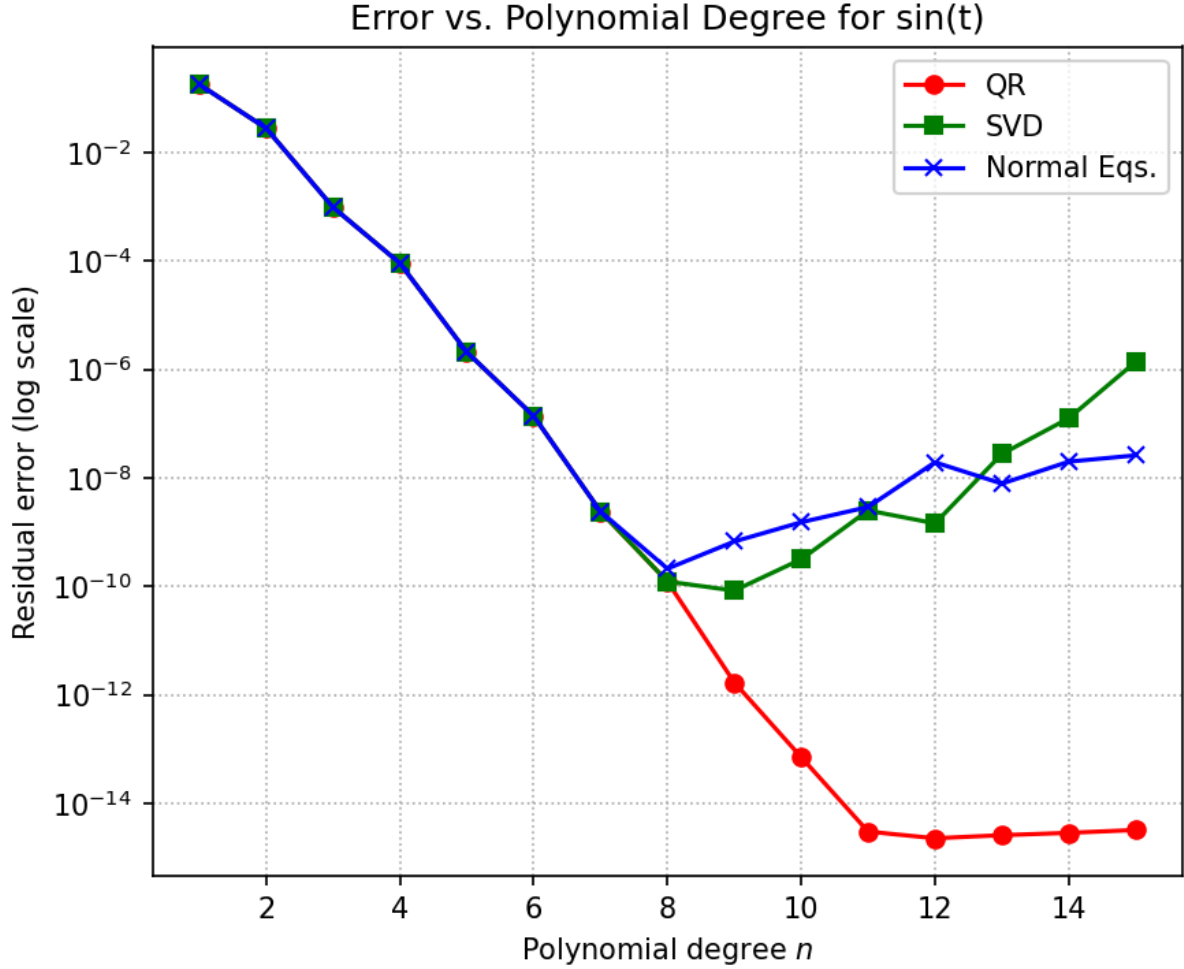Figure 14: Error on $\cos(3t)$

Figure 15: Error on e^t

Figure 16: Error on $\sin(t)$

We know that the functions e^t and $\sin(t)$ are crescent on $[0, 1]$ and shifted up, so the linear model would require higher degree to better describe this curve.

- **Normal System:** The error falls considerably until $\approx 10^{-8}$, which is expected. Since the condition numbr is squared, it climbs sooner than the 2 other approaches.

- **SVD:** After $\approx n = 8$ it starts climbing, due to the loss of significance from the ill-conditioned Vandermonde Matrix (huge condition number due to a big n). We see that the normal system of equations climbs sooner than the SVD, due to the difference in magnitude of the condition numbers

- **QR:** Climbs all the way down until machine precision, which is expected from the QR factorization.

Now the function $\cos(3t)$ behaves differently. Expanding it on the Taylor Series:

$$\cos(3t) = 1 - \frac{(3t)^2}{2!} + \frac{(3t)^4}{4!} - \frac{(3t)^6}{6!} + \dots \qquad 88$$

Only *even* powers appear. So when the degree increases from an odd φ to the next odd $\varphi + 1$, no even power is added. The expansion gains a term that has zero coefficient, as a consequence, the error does not improve. This explains the nearly horizontal parts between consecutive degrees.