AAA Algorithm

Problem Description

The paper addresses the problem of **rational approximation**: constructing a low-degree rational function

$$r(z) = \frac{p(z)}{q(z)}$$

that approximates a given function or dataset $f(z)$ over a domain. Traditional polynomial approximations often fail for functions with poles, sharp gradients, or those defined on disconnected regions.

Method Overview

1. Barycentric form

The AAA algorithm expresses the rational approximation in **barycentric form**:

$$r(z) = \frac{\sum_{j=1}^{m} \frac{w_j f_j}{z - z_j}}{\sum_{j=1}^{m} \frac{w_j}{z - z_j}}, \quad \forall z \in Z$$

where:

- z_j are selected **support points**,
- $f_j = f(z_j)$,
- w_j are complex weights to be determined,
- $Z^{(m)} = \{z_1, z_2, \ldots, z_m\}$ is the set of support points.

Properties of Barycentric Form

1. There are no poles at the points z_j when $w_1, \ldots, w_m$ are nonzero.
2. If z_j is a support point, then $f(z_j) = r(z_j)$.

2. Minimizing the Approximation Error Using SVD

Given support points $Z^{(m)} = \{z_1, z_2, \dots, z_m\}$ and the remaining points $Z^{(M-m)} = Z \setminus Z^{(m)}$.

2-1. Minimization Problem

The goal is to minimize the approximation error:

$$\min \|f(z) - r(z)\| = \min \left\| f(z) \sum_{j=1}^{m} \frac{w_j}{z - z_j} - \sum_{j=1}^{m} \frac{w_j f_j}{z - z_j} \right\|, \quad z \in Z^{(M-m)}$$

This is equivalent to:

$$\min \|Aw\|, \quad \|w\| = 1$$

where the matrix A is:

$$A = \begin{pmatrix} \frac{F_1^{(M-m)} - f_1}{Z_1^{(M-m)} - z_1} & \cdots & \frac{F_1^{(M-m)} - f_m}{Z_1^{(M-m)} - z_m} \\ \vdots & \ddots & \vdots \\ \frac{F_{M-m}^{(M-m)} - f_1}{Z_{M-m}^{(M-m)} - z_1} & \cdots & \frac{F_{M-m}^{(M-m)} - f_m}{Z_{M-m}^{(M-m)} - z_m} \end{pmatrix},$$

is an (M−m)×m matrix and $F^{(M-m)} = \{f(Z^{(M-m)})\}$.

2-2. Solving for w via SVD

If $A = U\Sigma V^*$ is the **singular value decomposition (SVD)** of A, with $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \dots, \sigma_r)$, assuming $(\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r \geq 0)$, then:

$$w = v_{\min},$$

where $v_{\min}$ is the last column of V.

Proof.
We aim to solve the optimization problem

$$\min_{w \in \mathbb{C}^m,\ \|w\|=1} \|Aw\|_2.$$

It is algebraically convenient to minimize the square:

$$\min_{\|w\|=1} \|Aw\|_2^2 = \min_{\|w\|=1} (Aw)^*(Aw) = \min_{\|w\|=1} w^*(A^*A)w.$$

Using the Singular Value Decomposition

Let

$$A = U\Sigma V^*,$$

where $U \in \mathbb{C}^{(M-m)\times r}$ and $V \in \mathbb{C}^{m\times r}$ are (column-)orthonormal matrices, and

$$\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_r),$$

with $\sigma_1 \geq \cdots \geq \sigma_r \geq 0$ and $r = \operatorname{rank}(A)$.

Substituting the SVD gives:

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

Since $U^*U = I$ and Σ is diagonal with real nonnegative entries,

$$\Sigma^2 = \operatorname{diag}(\sigma_1^2, \ldots, \sigma_r^2).$$

Hence,

$$w^*(A^*A)w = w^*V\Sigma^2V^*w.$$

Define

$$y = V^*w.$$

Because V is unitary, $\|y\| = \|w\| = 1$.
Then

$$w^*(A^*A)w = y^*\Sigma^2y = \sum_{j=1}^{r} \sigma_j^2|y_j|^2.$$

We must minimize this sum under $\|y\| = 1$.
Clearly, the smallest value is achieved by concentrating all weight on the smallest coefficient, i.e., $y = e_r = (0, \dots, 0, 1)^T$, corresponding to σ_r.

Thus, the minimal value is σ_r^2, and the corresponding optimal vector is

$$w = Vy = Ve_r,$$

which is the last column of V. $\square$

3. Removing numerical Froissart doublets

3.1 Locating Poles

The denominator of the rational function is

$$d(z) = \sum_{j=1}^{m} \frac{w_j}{z - z_j}.$$

The poles of $r(z)$ are defined as the zeros of $d(z)$:

$$d(p_k) = 0, \qquad k = 1, \dots, m-1.$$

Since $d(z)$ is a rational function with $(m-1)$ zeros, it can be written as

$$d(z) = \frac{q(z)}{\prod_{j=1}^{m}(z - z_j)},$$

where $q(z)$ is a polynomial of degree $(m-1)$.
Thus, the poles p_k are the roots of $q(z)$:

$$q(p_k) = 0.$$

3.2 Detecting Froissart Doublets

Near a pole p_k, the rational function can be locally expanded as

$$r(z) = \frac{c_k}{z - p_k} + \text{regular terms},$$

where c_k is the residue of $r(z)$ at p_k.
By complex analysis, the residue is given by

$$c_k = \lim_{z \to p_k} (z - p_k) r(z) = \frac{n(p_k)}{d'(p_k)}.$$

Substituting $n(z)$ and $d(z)$:

$$n(z) = \sum_{j=1}^{m} \frac{w_j f_j}{z - z_j}, \qquad d(z) = \sum_{j=1}^{m} \frac{w_j}{z - z_j},$$

$$d'(z) = -\sum_{j=1}^{m} \frac{w_j}{(z - z_j)^2}.$$

Hence, the explicit residue formula is

$$c_k = \frac{\displaystyle\sum_{j=1}^{m} \frac{w_j f_j}{p_k - z_j}}{\displaystyle -\sum_{j=1}^{m} \frac{w_j}{(p_k - z_j)^2}}.$$

Thus, if $c_k \approx 0$, then p_k is a Froissart doublet.

3.3 Remove Froissart doublets

A pole p_k is considered spurious if its residue magnitude satisfies

$$|c_k| < \varepsilon,$$

where typically $\varepsilon = 10^{-13}$.

Such poles are removed by deleting the support point z_j
closest to p_k and recomputing the barycentric weights w_j
via the SVD-based procedure.

4. AAA algorithm

```
FUNCTION AAA(f_values, z_points, tol, m_max)
# Input:
#   f_values: Function samples f(z_i) at given points z_points (length M)
#   z_points: Sample points z_i in complex or real domain
#   tol: Error tolerance for stopping (e.g., 1e−13)
#   m_max: Maximum number of support points allowed
# Output:
#   r_function: Rational approximation r(z) = n(z)/d(z)
#   support_points: Selected support points z_j
#   weights: Barycentric weights w_j

Step 0: Initialization
residual <− f_values
support_indices <− EMPTY_LIST()
approximation <− ZERO_VECTOR(length(f_values))

Step 1: Iterative greedy selection of support points
FOR m FROM 1 TO m_max DO
    # (1a) Choose new support point where current residual is largest
    j_max <− ARG_MAX(|f_values − approximation|)
    APPEND(support_indices, j_max)

    # (1b) Define support and test sets
    z_supp <− z_points[support_indices]
    f_supp <− f_values[support_indices]
    test_indices <− SET_DIFFERENCE(ALL_INDICES, support_indices)
    z_test <− z_points[test_indices]
    f_test <− f_values[test_indices]

    # (1c) Construct Cauchy and Loewner matrices
    C <− 1 / (z_test[:,None] − z_supp[None,:])     # (M−m)×m
    A <− (f_test[:,None])∗C − C∗(f_supp[None,:])   # Loewner matrix

    # (1d) Compute barycentric weights via SVD
    U, Σ, Vh <− SVD(A)
    w <− CONJ_TRANSPOSE(Vh)[:, −1]  # right singular vector of smallest singular value

    # (1e) Form new rational approximation in barycentric form
    C_all <− 1 / (z_points[:,None] − z_supp[None,:])
    numerator <− C_all @ (w ∗ f_supp)
    denominator <− C_all @ w
    approximation <- numerator / denominator

    # (1f) Check convergence
    error <- MAX(|f_values - approximation|)
    IF error < tol * MAX(|f_values|) THEN
        BREAK
    END IF
END FOR

# Step 2: Cleanup (remove spurious pole-zero pairs)
CALL CLEANUP(z_supp, w, f_supp)

# Step 3: Return rational function as callable closure
DEFINE r_function(z):
    C_eval <- 1 / (z[:,None] - z_supp[None,:])
    RETURN (C_eval @ (w * f_supp)) / (C_eval @ w)
END DEFINE

RETURN r_function, z_supp, w
END FUNCTION
```

Small-scale implementation and experiments

This section demonstrates the core idea of AAA on a few tiny problems and compares the optional cleanup step. The goal isn't to reproduce full experiments, but to show we can implement and apply the method in practice.

Minimal AAA driver (compact Python)

The snippet below implements a compact AAA loop in barycentric form plus a helper to convert to numerator/denominator polynomials (for poles/residues). It's intentionally short and prioritizes clarity over micro-optimizations.

```python
import numpy as np
from numpy.linalg import svd

def aaa_fit(F, Z, tol=1e-12, mmax=60, verbose=False):
    F = np.asarray(F, dtype=complex)
    Z = np.asarray(Z, dtype=complex)
    M = len(Z)
    R = np.zeros_like(F)
    S = []
    errs = []

    for m in range(1, mmax + 1):
        jmax = np.argmax(np.abs(F - R))
        S.append(jmax)
        Zs, Fs = Z[S], F[S]

        J = np.setdiff1d(np.arange(M), S)
        Zj, Fj = Z[J], F[J]
        C = 1.0 / (Zj[:, None] - Zs[None, :])
        A = Fj[:, None] * C - C * Fs[None, :]
        _, _, Vh = svd(A, full_matrices=False)
        w = Vh.conj().T[:, -1]

        # Evaluate on full grid and enforce interpolation at support points
        C_all = 1.0 / (Z[:, None] - Zs[None, :])
        R = (C_all @ (w * Fs)) / (C_all @ w)
        R[S] = Fs
        err = np.max(np.abs(F - R))
        errs.append(err)
        if verbose:
            print(f"Iter {m:2d}: max|err| = {err:.3e}")
        if err < tol * np.max(np.abs(F)):
            break
    return Zs, Fs, w, errs

def barycentric_to_poly(Zs, Fs, w):
    """Return numerator/denominator coefficients of n(z)/d(z)."""
    p = np.poly(Zs)                 # prod (z - z_k)
    num = np.zeros(len(Zs), dtype=complex)
    den = np.zeros(len(Zs), dtype=complex)
    for j in range(len(Zs)):
        qj, _ = np.polydiv(p, np.array([1.0, -Zs[j]]))
        den += w[j] * qj
```

```python
            num += w[j] * Fs[j] * qj
        return num, den

    def residues_at_poles(num, den):
        """Compute residues c_k = n(p_k) / d'(p_k) at poles p_k (roots of den)."""
        poles = np.roots(den)
        num_p, den_p = np.poly1d(num), np.poly1d(den)
        dprime = np.polyder(den_p)
        res = num_p(poles) / dprime(poles)
        return poles, res

    def rf_eval(z, Zs, Fs, w, tol=1e-12):
        z = np.atleast_1d(z)
        C = 1.0 / (z[:, None] - Zs[None, :])
        dist = np.abs(z[:, None] - Zs[None, :])
        idx = dist.argmin(axis=1)
        hit = dist[np.arange(len(z)), idx] < tol
        num = C @ (w * Fs)
        den = C @ w
        out = num / den
        out[hit] = Fs[idx[hit]]  # enforce interpolation for stability
        return out
```

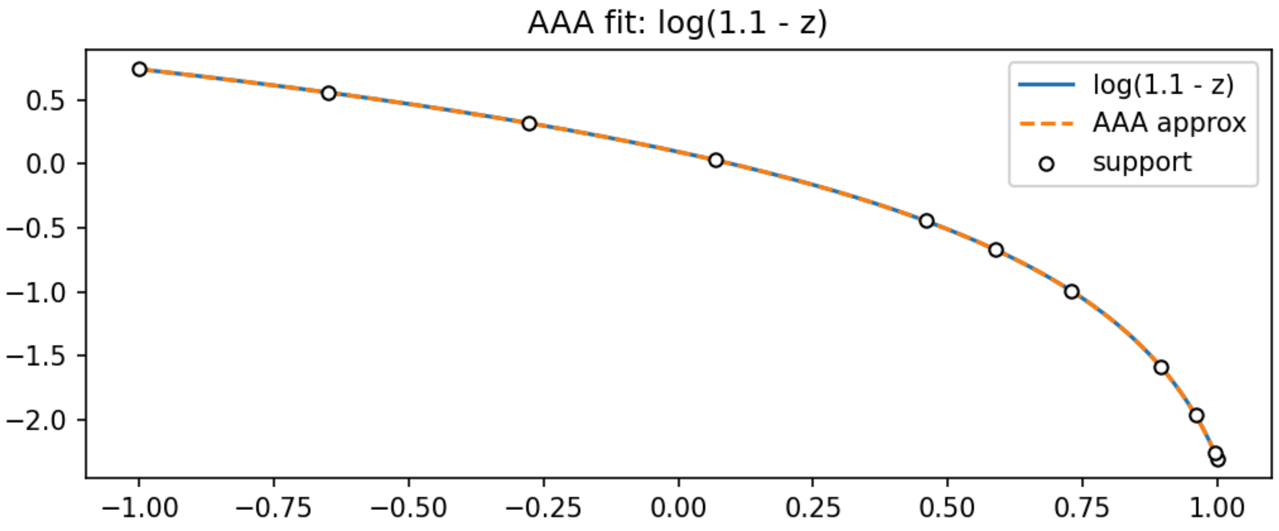
Experiment 1: Real-valued benchmarks on [–1, 1] and [–10, 10]

```
# log(1.1 - z) on [-1,1]
Z1 = np.linspace(-1, 1, 400)
F1 = np.log(1.1 - Z1)
Zs1, Fs1, w1, _ = aaa_fit(F1, Z1, tol=1e-12)
zz1 = np.linspace(-1, 1, 800)
err1 = np.max(np.abs(np.log(1.1 - zz1) - rf_eval(zz1, Zs1, Fs1, w1)))
print(f"log(1.1 - z): support points = {len(Zs1)}, max|error| ≈ {err1:.3e}")

# |1/x| on [-1,1] (avoid 0 exactly for the reference curve)
Z2 = np.linspace(-1, 1, 400)
Z2[np.isclose(Z2, 0)] = 1e-12
F2 = np.abs(1.0 / Z2)
Zs2, Fs2, w2, _ = aaa_fit(F2, Z2, tol=1e-12)
zz2 = np.linspace(-1, 1, 800)
zz2[np.isclose(zz2, 0)] = 1e-12
err2 = np.max(np.abs(np.abs(1.0/zz2) - rf_eval(zz2, Zs2, Fs2, w2).real))
print(f"|1/x|: support points = {len(Zs2)}, max|error| (away from 0) ≈ {err2:.3e}")

# exp(z) on [-10,10]
Z3 = np.linspace(-10, 10, 400)
F3 = np.exp(Z3)
Zs3, Fs3, w3, _ = aaa_fit(F3, Z3, tol=1e-12)
zz3 = np.linspace(-10, 10, 800)
err3 = np.max(np.abs(np.exp(zz3) - rf_eval(zz3, Zs3, Fs3, w3).real))
print(f"exp(z): support points = {len(Zs3)}, max|error| ≈ {err3:.3e}")
```

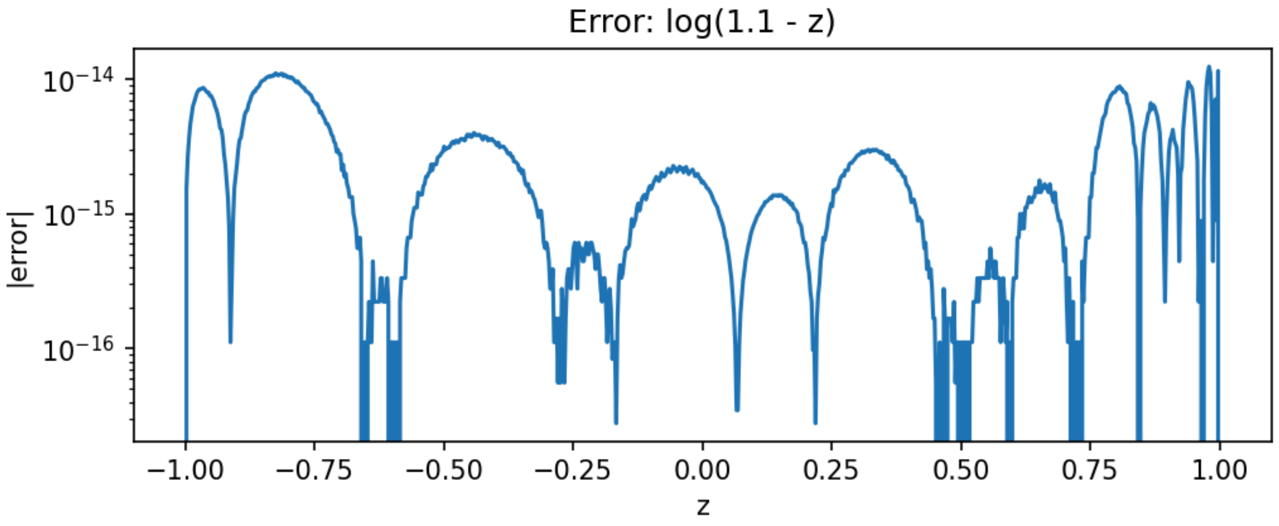
In our notebook runs, we observed representative support-point counts: log(1.1 – z): 11, |1/x|: 33, exp(z): 11. Errors are typically in the $10^{\{-12\}–10}\{-14\}$ range on these grids (except near the removable singularity at z = 0 for |1/x| where the reference itself diverges).

Corresponding figures:

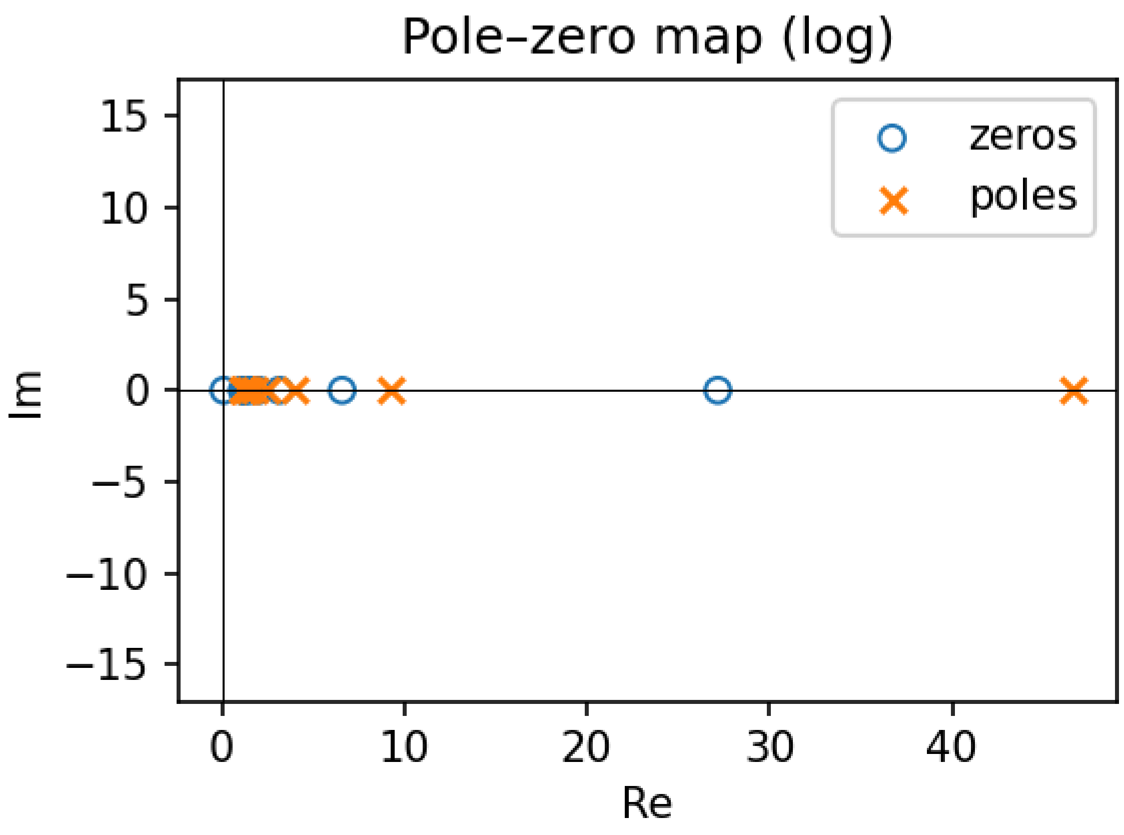
- log(1.1 – z):
  - Fit:



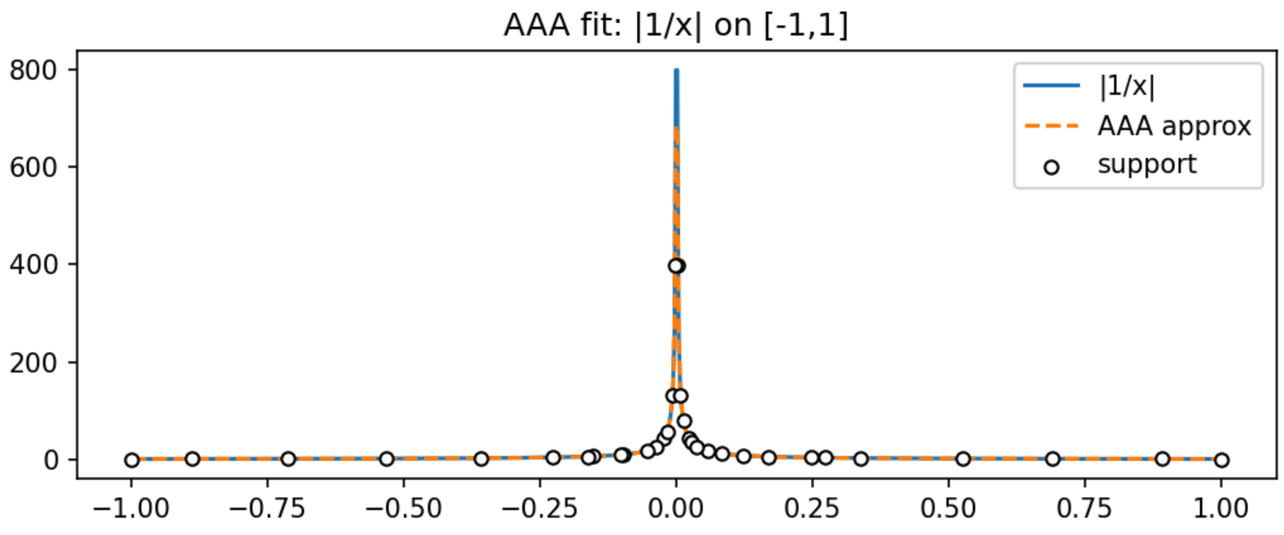
- Error:



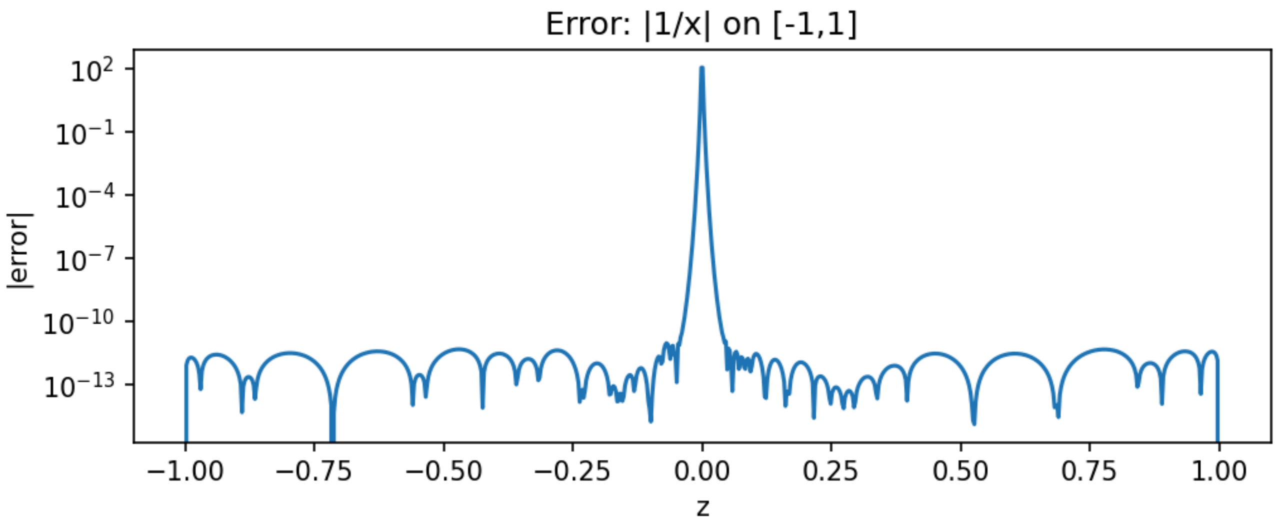
- Pole–zero map:



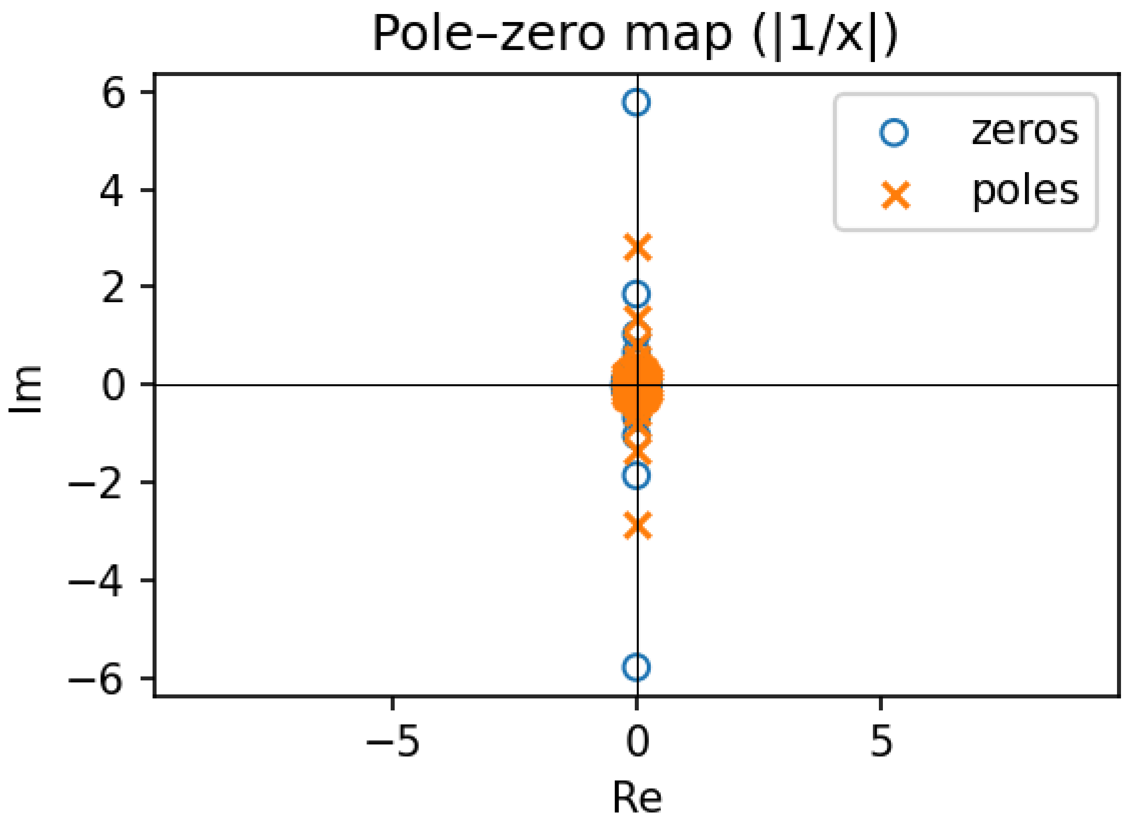
- |1/x| on [−1,1]:
  - Fit:



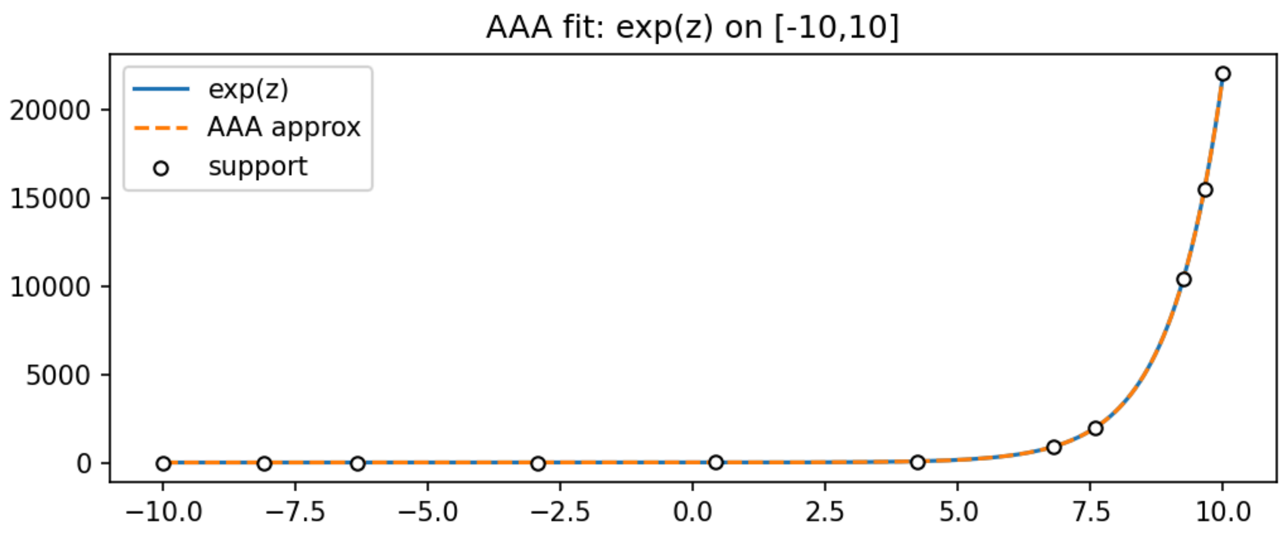
  - Error:



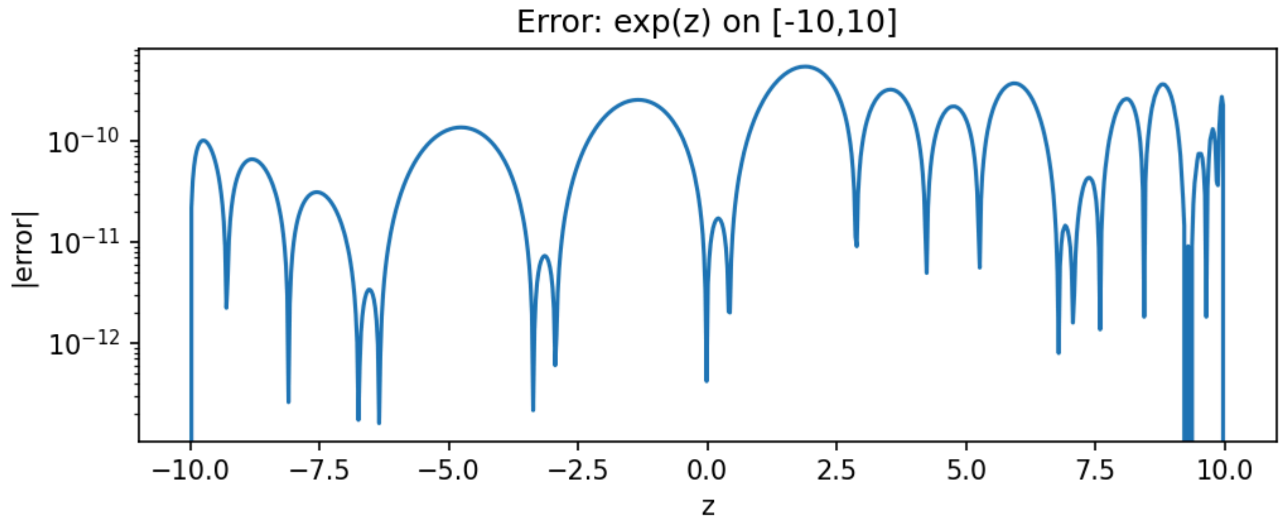
- Pole–zero map:



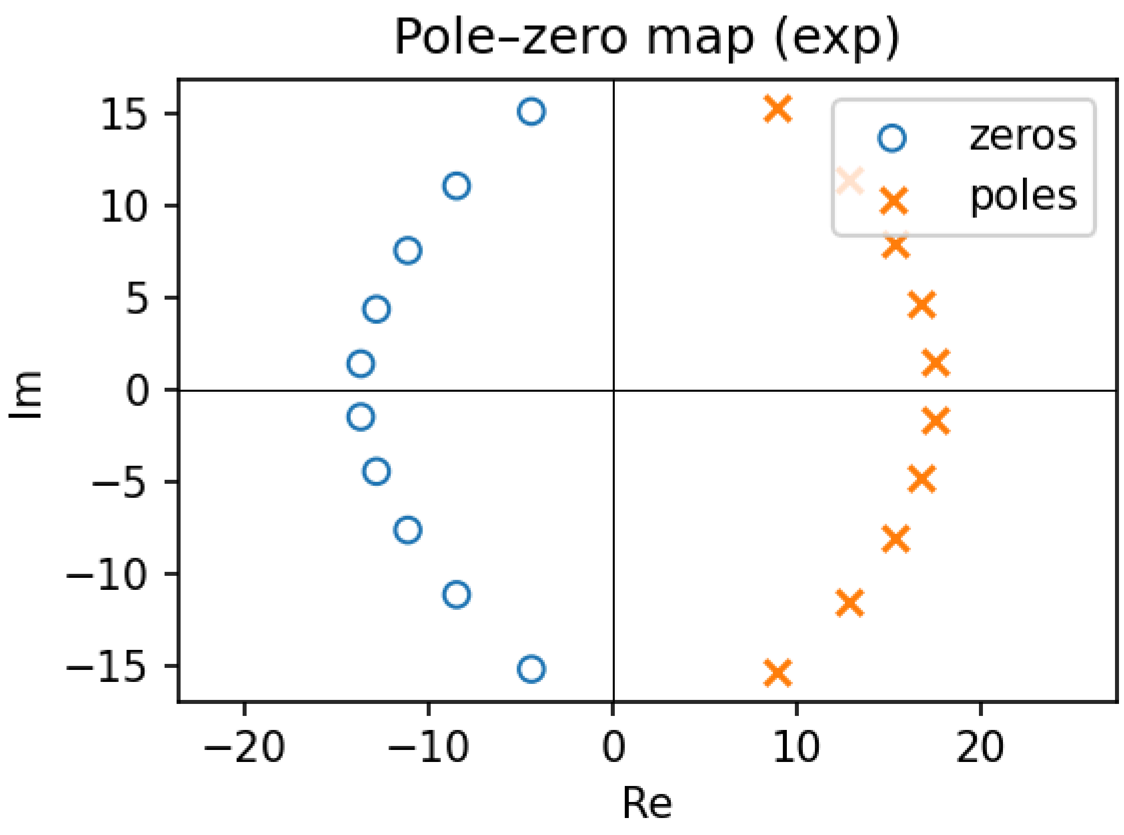
- exp(z) on [−10,10]:
  - Fit:



- Error:



- Pole–zero map:



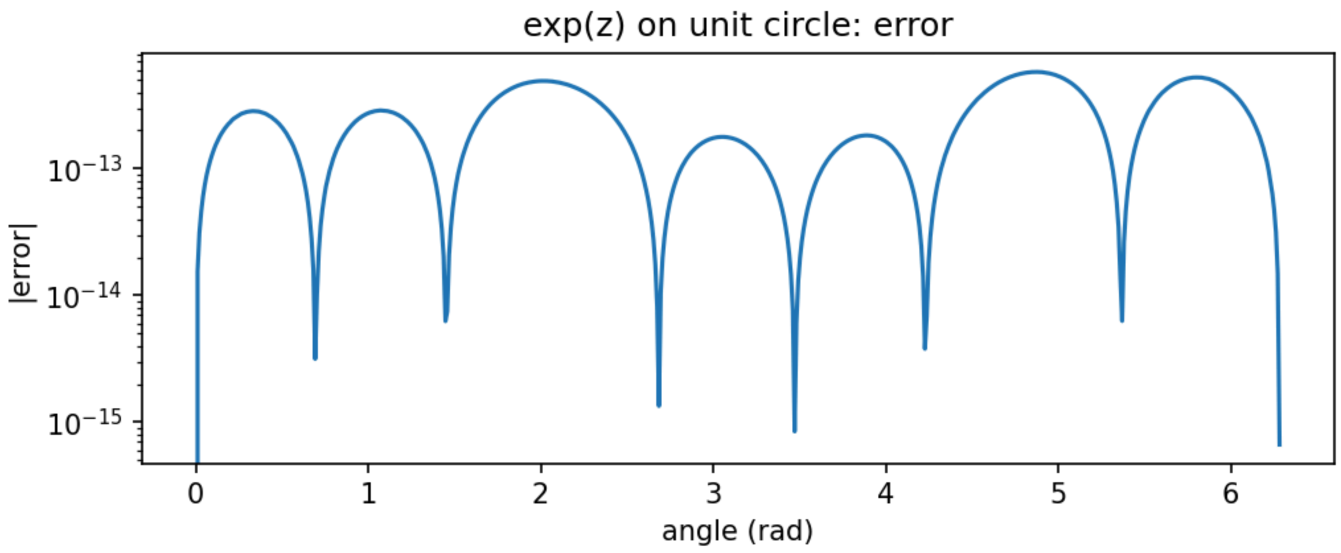
Experiment 2: exp(z) on the unit circle (complex domain)

We approximate f(z) = exp(z) sampled on the unit circle z = e^{iθ}. The same AAA machinery applies in the complex plane; evaluation and pole–zero extraction use the barycentric form and the polynomial conversion helper.

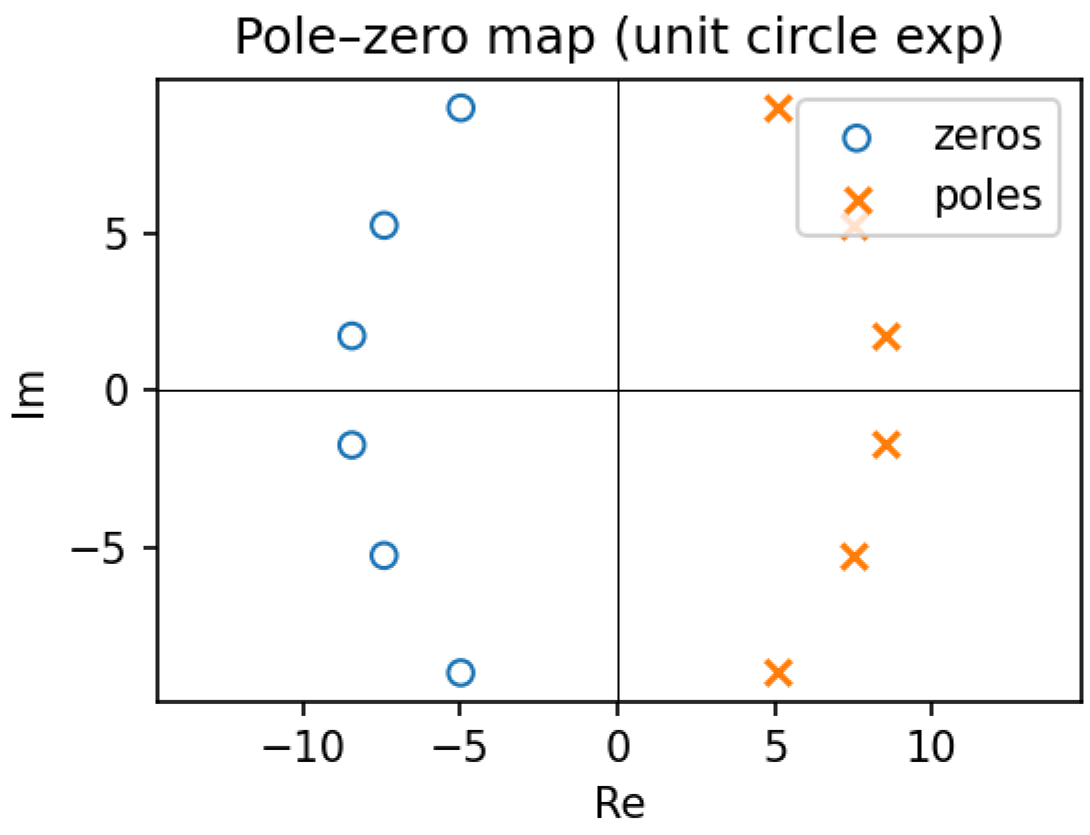
```
# Unit-circle complex example
theta = np.linspace(0, 2*np.pi, 200)
Zc = np.exp(1j * theta)
Fc = np.exp(Zc)

# Fit and validate
Zs_uc, Fs_uc, w_uc, _ = aaa_fit(Fc, Zc, tol=1e-12, mmax=80)
theta_t = np.linspace(0, 2*np.pi, 600)
Zt = np.exp(1j * theta_t)
F_true_uc = np.exp(Zt)
F_approx_uc = rf_eval(Zt, Zs_uc, Fs_uc, w_uc)
max_err = np.max(np.abs(F_true_uc - F_approx_uc))
print(f"Unit-circle exp(z): support points = {len(Zs_uc)}, max|error| ≈ {max_err:.3e}")

# Optional: pole-zero map via barycentric_to_poly
num_uc, den_uc = barycentric_to_poly(Zs_uc, Fs_uc, w_uc)
p_uc = np.roots(den_uc)
z_uc = np.roots(num_uc)
```

Corresponding figures:

- Error vs angle:



- Pole–zero map:



Summary and conclusion

Strengths

- High-accuracy, low-degree rational fits:
  Excels for functions analytic except at isolated poles or removable singularities.
  The same algorithm handles both real and complex domains seamlessly.
- Interpretability:
  Extraction of poles, zeros, and residues provides insight and diagnostic capability.
  The optional cleanup step enhances robustness when fits become aggressive.

Limitations and costs

- Computational cost: Each iteration builds a Loewner matrix (size roughly $(M - m) \times m)$ and performs an SVD; overall cost grows like $O(Mm^2)$ and can be noticeable for large M. Pole/zero extraction via polynomial conversion also grows in cost and can be ill-conditioned for very large m.
- A sufficiently rich yet not excessive sample grid is provided; AAA is data-driven and benefits from covering the domain uniformly and near difficult regions.

Possible improvements and extensions

- Employ randomized or truncated SVD for faster linear algebra.
- Use preconditioning or scaling to mitigate ill-conditioning.
- Parallelize or batch SVD computations for very large datasets.