

Research Article



Leveraging Python for Potentiometric Titrations: An AI-Enhanced Approach to Hydrochloric Acid Detection

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Received: 12 August 2026

Revised: 28 September 2026

Accepted: 29 September 2026

Published Online: 29 September 2026

Citation

S. Vunguturi, Leveraging python for potentiometric titrations: an AI-enhanced approach to hydrochloric acid detection, *Journal of Smart Sensors and Computing*, 2026, 2(3), 26214, <https://doi.org/10.64189/ssc.26214>.

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Abstract

Potentiometric titration is a classical analytical method for determining the concentration of acids and bases with high precision. Traditional titration techniques, however, often require manual interpretation of titration curves, which may introduce errors and limit reproducibility. This study presents an AI-enhanced approach to hydrochloric acid (HCl) detection through potentiometric titration using Python-based automation and machine learning. The system integrates automated data acquisition, preprocessing, and curve fitting to identify equivalence points with greater accuracy. By applying regression models and anomaly detection algorithms, the proposed framework reduces subjectivity and improves consistency in endpoint determination. Experimental trials using standard NaOH titrants demonstrated that the AI-assisted approach achieved higher precision in detecting HCl concentrations compared to traditional manual methods. The Python framework also provides visualization tools and real-time feedback, enabling a user-friendly interface for laboratory and educational settings. This study highlights the potential of combining artificial intelligence and classical analytical chemistry to advance modern titration practices.

Keywords: Potentiometric titration; Hydrochloric acid detection; Python automation; Artificial intelligence; Chemometrics; Machine learning in chemistry.

1. Introduction

Potentiometric titrations represent a fundamental analytical procedure that relies on monitoring changes in electrode potential throughout the course of a titration. These titrations typically employ either a pH-sensitive or a redox electrode to accurately determine the equivalence point of the reaction.^[1] The underlying principle is governed by the Nernst equation, which defines the relationship between electrode potential and the activity or concentration of ions involved in the system.^[2] As the titrant is progressively added to the analyte solution, the electrode potential undergoes measurable variations until a distinct shift occurs at the equivalence point, where the stoichiometric ratio between analyte and titrant is achieved.^[3] This method is particularly valuable in acid–base and redox titrations, where the electromotive force (EMF) of the electrochemical cell is continuously monitored. The standard setup typically consists of a potentiometer, a reference electrode, and an indicator electrode. The reference electrode provides a stable half-cell potential independent of the sample composition, while the indicator electrode responds to changes in ion concentration during the titration.^[4] For acid–base titrations, the saturated calomel electrode is frequently working as a reference due to its stability and reproducibility. The wide applicability of potentiometric titrations extends across several industrial sectors. In chemical manufacturing, they are used to ensure precise concentrations of acids and bases during production. The pharmaceutical industry applies them for drug formulation and quality control, while the food and beverage sector utilize them for pH monitoring to maintain product safety and consistency. Environmental

monitoring relies on potentiometric titration for assessing water quality and waste treatment processes. In addition, the oil and gas industry employs this technique to supervise acidizing and refining operations, whereas metal finishing industries apply it for processes such as pickling and electroplating. Cosmetics manufacturing also benefits from potentiometric titrations to regulate product pH, ensuring consumer safety. Furthermore, their role in research and education remains indispensable, as they serve as a robust teaching and analytical tool across laboratories.^[5,6] Despite its advantages, traditional potentiometric titration often depends on manual endpoint determination, which is susceptible to operator bias and inconsistency. Recent developments highlight the potential of computational approaches to improve reproducibility and accuracy.^[7] Specifically, Python programming offers a versatile platform for automating titration analysis. Its integration with scientific libraries such as NumPy and visualization tools like Matplotlib enables efficient simulation and precise curve analysis.^[8,9] The adoption of artificial intelligence (AI) techniques further enhances the robustness of endpoint detection and data interpretation, reducing human error and enabling real-time automation. This study proposes a Python-driven, AI-assisted framework for potentiometric titration with a focus on the determination of hydrochloric acid (HCl) concentration. By combining classical potentiometric methods with modern computational approaches, the work demonstrates an efficient, accurate, and reproducible strategy suitable for applications in analytical chemistry, industrial process monitoring, environmental analysis, and quality assurance, Figs. 1 and 2.^[10]

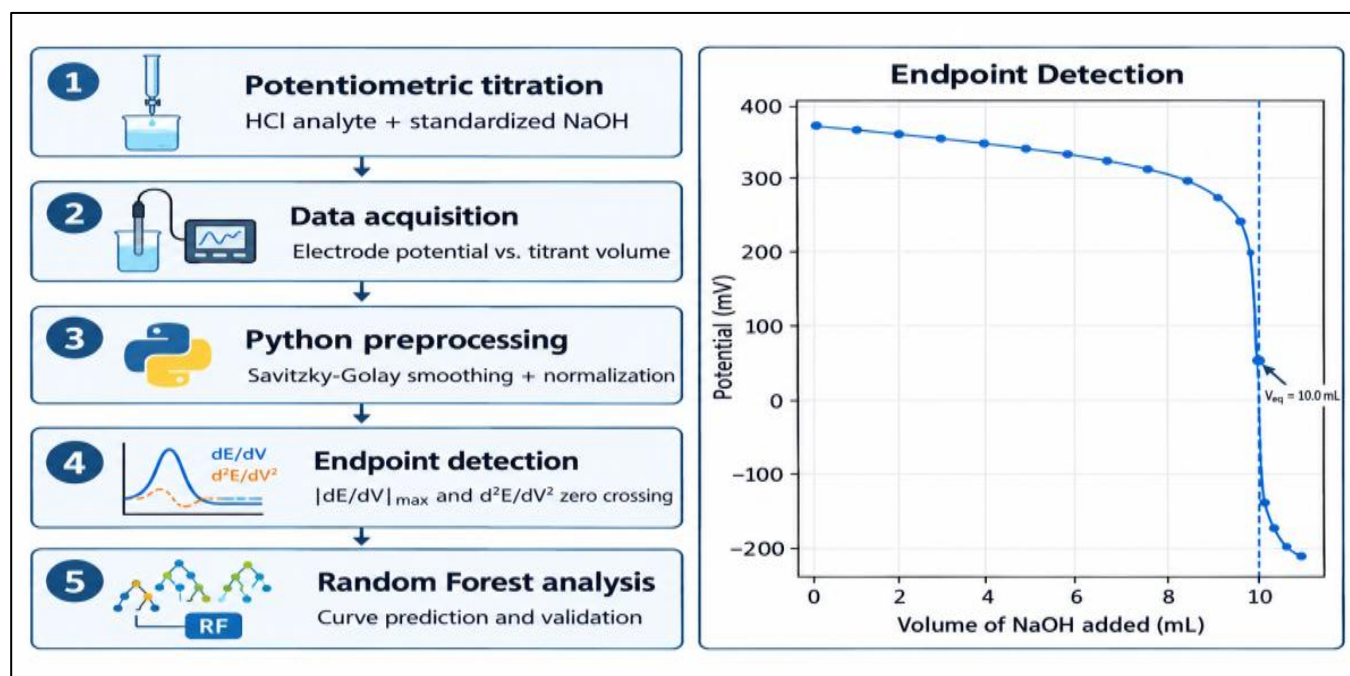


Fig. 1: AI-enhanced potentiometric titration using Python.

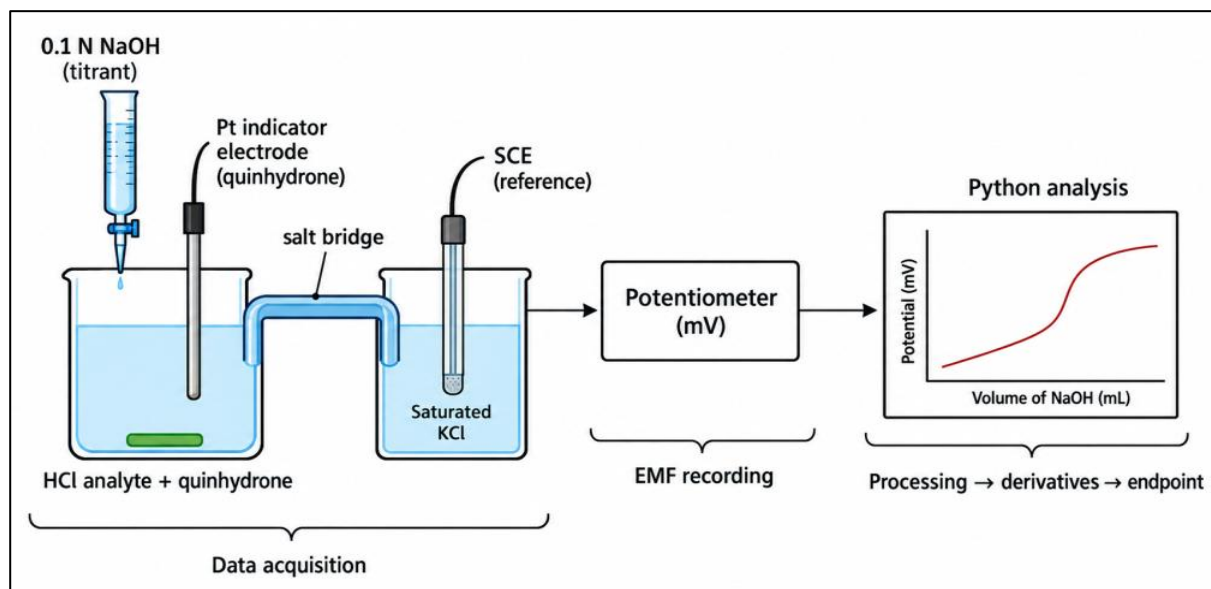


Fig. 2: Workflow of AI-enhanced potentiometric titration using Python.

2. Materials and methods

2.1 Chemicals and reagents

Standardized hydrochloric acid (HCl) and sodium hydroxide (NaOH) solutions were prepared and used as the analyte and titrant, respectively. Deionized water was employed for solution preparation and dilution to ensure accuracy. All reagents were of analytical grade.

2.2 Instrumentation

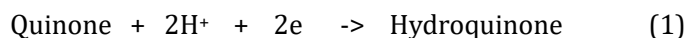
The experimental setup consisted of:

- A digital potentiometer connected to a pH electrode (glass electrode) and a reference electrode (saturated calomel electrode).
- A magnetic stirrer to maintain uniform mixing during titration.
- A burette (50 mL) for controlled addition of NaOH titrant.
- A computer system with Python environment for real-time data acquisition and processing.

2.2.1 Potentiometric titrations: HCl against standard NaOH

2.2.1.1 Principle

The electrochemical cell configuration uses a saturated calomel electrode (SCE; $E^0 = 0.242$ V) as the reference electrode and a quinhydrone/platinum electrode as the indicator electrode. The quinhydrone system consists of quinone and hydroquinone in a 1:1 molar ratio and establishes reversible redox equilibrium at the platinum surface in the presence of hydrogen ions.



This electrode exhibits reversibility with respect to hydronium (H_3O^+) ions in the solution. The reduction potential for this system is defined by the following Nernst equation:

$$E_{\text{Q/QH}_2} = E_{\text{Q/QH}_2}^0 - 0.0591\text{pH} \quad (2)$$

The electrochemical cell is built by way of combining the saturated calomel electrode (SCE) with the quinhydrone electrode (QE). The SCE provides a stable reference potential, whereas the quinhydrone/platinum electrode responds to changes in hydrogen-ion activity. In routine potentiometric measurements, the electrodes are treated as reference and indicator electrodes rather than being assigned fixed anode/cathode roles, because the measurement is made under essentially zero current. The measured cell potential is expressed as the indicator-electrode potential relative to the reference electrode.

Cell representation: -Cell representation: SCE | saturated KCl || H^+ -containing analyte,



Cell Reactions: -

Reference electrode: saturated calomel electrode (stable reference potential)

Indicator electrode: $\text{Q} + 2\text{H}^+ + 2\text{e}^- \rightarrow \text{QH}_2$ at the Pt surface

$$E_{\text{cell}} = E_{\text{indicator}} - E_{\text{reference}} \quad (4)$$

$$E_{\text{cell}} = (0.6996 - 0.0591 \text{ pH}) - 0.242 \text{ V}$$

$$E_{\text{cell}} = 0.4576 - 0.0591 \text{ pH}$$

Thus, the measured cell potential changes systematically with pH.

During titration, incremental addition of NaOH consumes H^+ and changes the pH of the analyte. The quinhydrone/platinum indicator responds to this change, and the measured cell potential changes accordingly. The titration curve is obtained by plotting cell potential against NaOH volume. For the strong acid-strong base system studied here, the equivalence region is identified at the inflection point, corresponding to the

maximum absolute slope and the zero crossing of the second derivative. During the titration process, the incremental addition of sodium hydroxide (NaOH) base to the acidic analyte solution causes a decrease in the concentration of H^+ ions within the half-cell containing the quinhydrone electrode. This change in pH directly affects the potential of the quinhydrone electrode. Consequently, the measured electromotive force (EMF) of the entire electrochemical cell exhibits a corresponding decrease. These EMF values are recorded, and a titration curve is generated by plotting the cell potential against the volume of titrant added. The endpoint of the titration is identified from the inflection point on this curve, and the concentration of the unknown acid solution is calculated based on this endpoint. The potentiometric titration curve is generated from the series of cell potential measurements taken throughout the reaction.

Apparatus Required: The following apparatus are required:

- Potentiometer
- saturated calomel electrode (SCE)
- platinum indicator electrode
- beakers
- burette
- pipette
- magnetic stirrer (or stir bar)
- salt bridge (e.g., KNO_3 or KCl in agar)

Chemicals Required: The following solutions are required:

- Analyte: The unknown acid solution
- Titrant: 0.1 N (N/10) Sodium Hydroxide (NaOH)
- Quinhydrone solid (Quinone and Hydroquinone 1: 1)
- Saturated KCl solution (for the SCE, if not pre-filled)

2. Methodology

2.1 PART-A: Preparation oxalic acid solution

Accurately weigh the required quantity of oxalic acid crystals in a clean, dry weighing bottle. Transfer the sample into a 100 mL standard volumetric flask using a funnel. Add a small amount of distilled water and swirl the flask until the crystals dissolve completely. Then, carefully dilute the solution with distilled water up to the calibration mark and mix well to obtain a homogeneous standard solution.

Calculation of Normality:

The normality of the prepared oxalic acid solution can be determined from the weight of oxalic acid taken:

$$\text{Normality (N)} = \frac{\text{Weight of oxalic acid (g)} \times 1000}{\text{Equivalent weight of oxalic acid} \times \text{Volume of solution (mL)}}$$

Molecular weight of oxalic acid dihydrate ($C_2H_2O_4 \cdot 2H_2O$) = 126 g/mol

Since oxalic acid is a diprotic acid, Equivalent weight = $\frac{126}{2}$ = 63 g

2.2 PART-B: Standardization of NaOH solution

Fill a clean burette with approximately N/10 sodium hydroxide solution. Using a pipette, transfer 20 mL of the prepared standard oxalic acid solution into a conical flask. Add a few drops of phenolphthalein indicator to the flask. Titrate the oxalic acid solution against sodium hydroxide until the solution changes from colourless to a faint pink end point. Record the burette readings, and calculate the exact normality of the NaOH solution from the titration data.

2.3 PART-C: Estimation of hydrochloric acid in the test solution

Prepare the HCl test solution by dilution with deionized water to the required volume. Pipette 20 mL of the HCl solution into a clean 100 mL beaker, add a small amount of quinhydrone, and immerse the platinum indicator electrode. In a separate beaker, place the saturated calomel reference electrode in saturated KCl solution. Connect the reference and indicator half-cells through a salt bridge and connect the electrodes to the potentiometer. Record the cell potential in mV after each NaOH addition.

Cell arrangement: SCE (reference) | saturated KCl || HCl analyte + quinhydrone | Pt (indicator)

Switch on the instrument and set it to the millivolt (mV) mode using the mV/current selector. The display will show the cell potential in millivolts. Adjust the initial reading as required. Begin titration by adding sodium hydroxide solution from the burette in 1 mL portions to the acid solution, stirring after each addition, and record the corresponding EMF values. Continue the process until a sudden change in EMF is observed, indicating that the equivalence region is being approached. Beyond this point, take 6–8 additional readings at 1 mL intervals.

For greater accuracy, repeat the titration with 0.1 mL increments in the endpoint region. Plot E versus NaOH volume, then calculate the absolute first derivative $|dE/dV|$ and the second derivative d^2E/dV^2 . The equivalence point is assigned to the maximum $|dE/dV|$ and confirmed by the zero crossing of d^2E/dV^2 .

2.4 Data acquisition

The supplied experimental dataset contains 30 electrode-potential observations collected during incremental addition of NaOH, with finer 0.1 mL spacing around the equivalence region. For the revised quantitative analysis, the 30 experimental observations in Table 1 were used directly. The original manuscript also described the generation and merging of synthetic datasets; however, the number, generation parameters, and complete synthetic records were not available in the supplied manuscript. Therefore, synthetic observations were not included in the revised model-validation results,

Table 1: Electrode potential and differential values during potentiometric titration with NaOH.

Volume of NaOH added (mL)	Electrode Potential (mV)	ΔE (mV)	$ \Delta E/\Delta V $ (mV/mL)
0	381	0	0
1	376	-5	5
2	373	-3	3
3	369	-4	4
4	362	-7	7
5	357	-5	5
6	351	-6	6
7	342	-9	9
8	331	-11	11
9	312	-19	19
9.1	310	-2	20
9.2	307	-3	30
9.3	303	-4	40
9.4	300	-3	30
9.5	295	-5	50
9.6	288	-7	70
9.7	281	-7	70
9.8	270	-11	110
9.9	253	-17	170
10	44	-209	2090
10.1	-164	-208	2080
10.2	-181	-17	170
10.3	-192	-11	110
10.4	-199	-7	70
10.5	-205	-6	60
10.6	-209	-4	40
10.7	-213	-4	40
10.8	-216	-3	30
10.9	-219	-3	30
11	-221	-2	20

ensuring that all reported calculations are traceable to the experimental values shown in Table 1. The recorded values were imported into the Python workflow for preprocessing, differentiation, regression, and endpoint analysis. The revised potentiometric titration curve (Fig. 3) shows a gradual decrease in electrode potential followed by a sharp transition between 9.9 and 10.1 mL NaOH. The inflection region is centered at approximately 10.0 mL. This value is consistent with the derivative calculations and with the stoichiometric calculation for a 20.0 mL aliquot of 0.050 N HCl titrated with 0.100 N NaOH. The first derivative was calculated from successive potential and volume differences and plotted as an absolute value so that the peak points upward. The largest absolute slope occurs at approximately 10.0 mL, (Fig-4) identifying the equivalence region. The scale is expressed directly in mV/mL; the maximum observed derivative is approximately 2.09×10^3 mV/mL before smoothing. The plotted smoothed derivative is lower because the Savitzky–Golay filter reduces the influence of the abrupt experimental transition. The second

derivative was calculated from the smoothed potential curve. The zero crossing occurs at approximately 10.0mL, coinciding with the inflection region identified from the first derivative. The revised plot uses direct mV/mL² units rather than an artificial 10^{17} scale.

Estimated equivalence point (from maximum $|dE/dV|$ and d^2E/dV^2 zero crossing): $V_{eq} \approx 10.00$ mL
 Calculated HCl normality: $N_{HCl} = (N_{NaOH} \times V_{NaOH}) / V_{HCl} = (0.100 \text{ N} \times 10.00 \text{ mL}) / 20.00 \text{ mL} = 0.050\text{N}$.

$$NHCl = \frac{0.10 \times 11.0 \text{ mL}}{20.0 \text{ mL}}$$

These calculations are based directly on the 20 mL HCl aliquot, 0.1 N NaOH titrant, and the experimental potential values reported in Table 1. The revised endpoint is therefore determined from the supplied dataset rather than from the previously reported 11.0 mL value (Fig-5).

2.5 Data processing and preprocessing

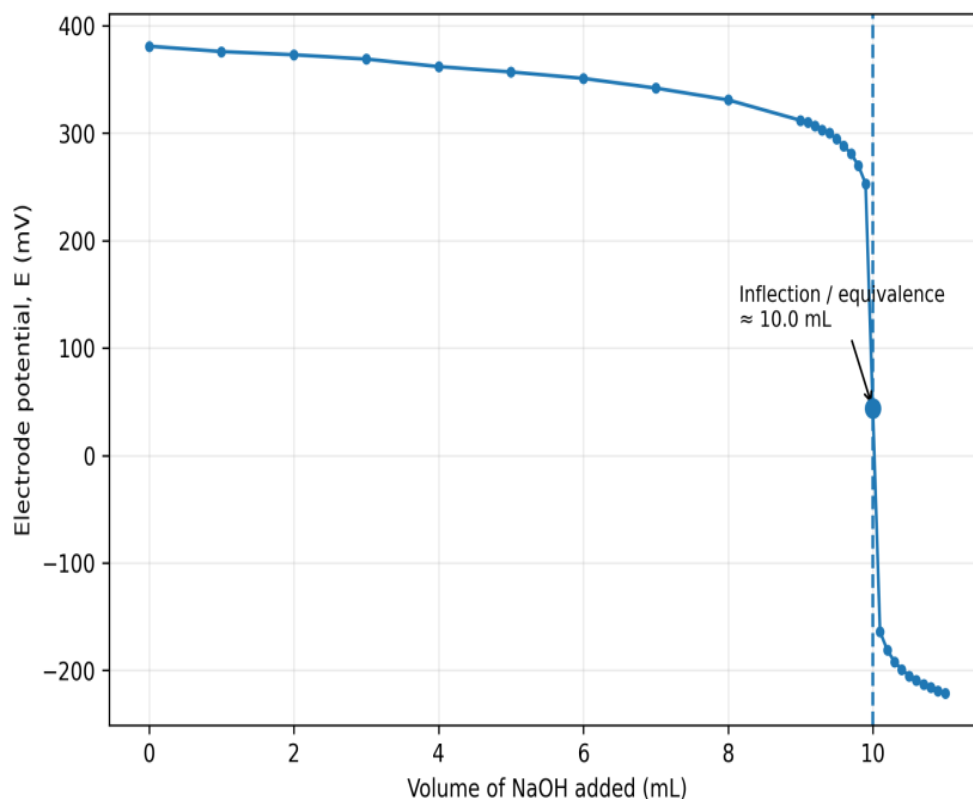


Fig. 3: Titration curve of electrode potential (mV) versus NaOH volume (mL).

To ensure high accuracy and reproducibility in endpoint detection, raw electrode potential data were subjected to multiple preprocessing steps prior to computational and machine learning analysis (Table 2).^[11,12]

i. **Noise reduction**

The raw potential data were smoothed using a Savitzky–Golay filter with a seven-point window and

second-order polynomial, selected for the revised analysis to suppress high-frequency fluctuations while preserving the sharp transition near the equivalence region.

ii. **Normalization**

For machine-learning input, the potential values were normalized using Min–Max scaling. Derivative

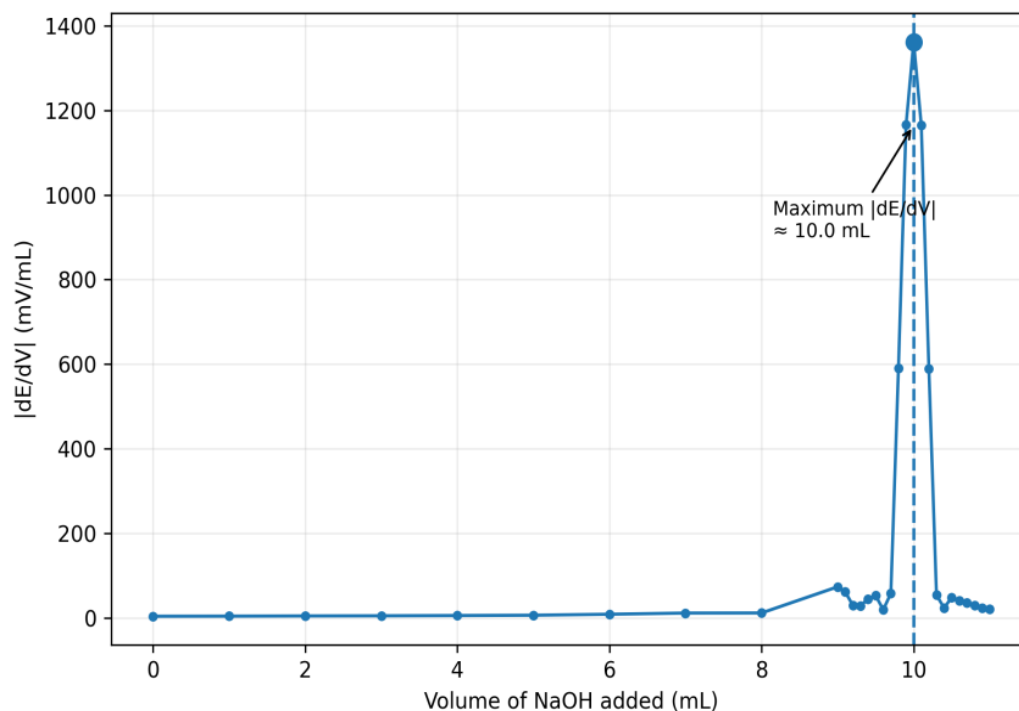


Fig. 4: Absolute first derivative, $|dE/dV|$ (mV/mL), versus NaOH volume (mL).

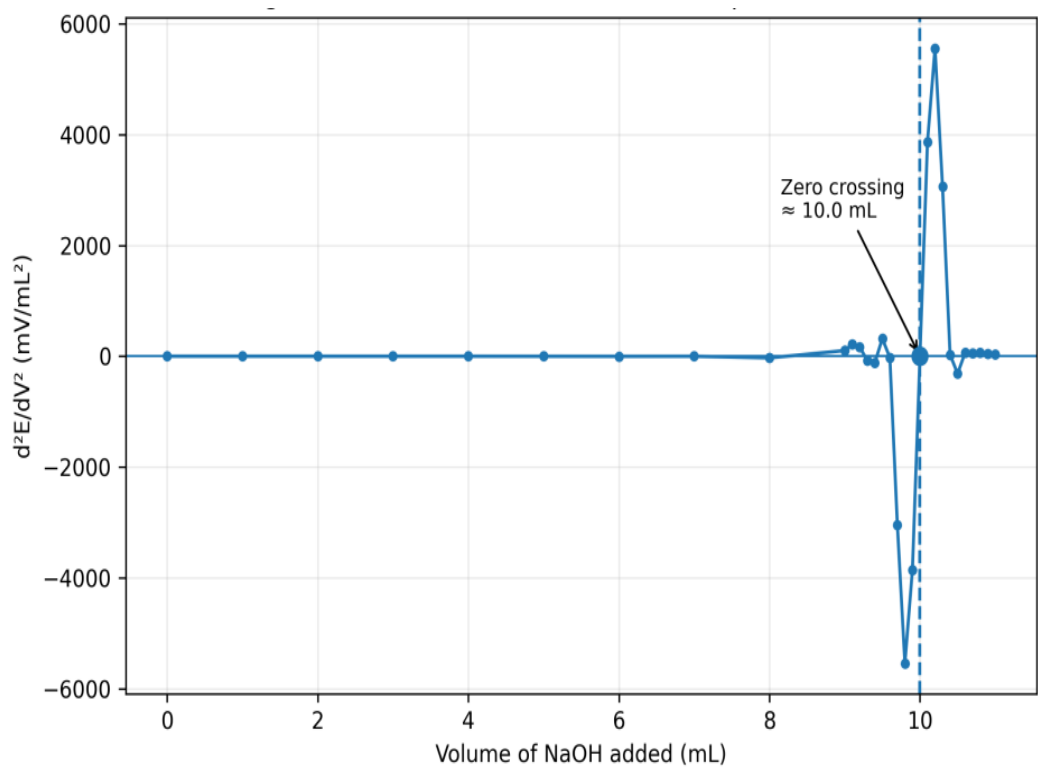


Fig. 5: Second derivative, d^2E/dV^2 (mV/mL²), versus NaOH volume (mL).

Table 2: Preprocessing methods and outcomes for titration data.

Preprocessing Step	Method Applied	Purpose	Outcome
Noise Reduction	Savitzky–Golay Filter	Remove random fluctuations	Smooth, continuous titration curve
Normalization	Min–Max scaling (0–1)	Reduce inter-trial variability	Standardized potential scale
Feature Extraction	Numerical differentiation ($\Delta E/\Delta V, \Delta^2 E/\Delta V^2$)	Identify slope & inflection	Equivalence point localization

plots were calculated in physical units from the unnormalized potential values so that the reported slopes retain the unit’s mV/mL and mV/mL².

iii. **Feature extraction**

From the smoothed and normalized data, key features were extracted for endpoint determination, including Electrode potential slope ($\Delta E/\Delta V$), First derivative profile to highlight sharp potential changes Second derivative profile to detect inflection points at the equivalence point

2.6 Computational framework

Python 3.11 served as the primary programming platform. NumPy and SciPy were used for numerical calculations, Pandas for tabular data handling, Matplotlib for visualization, and scikit-learn for Random Forest regression and validation.^[13] The computational workflow consisted of: (1) importing the recorded volume–potential pairs; (2) checking volume order and units; (3) Savitzky–Golay smoothing; (4) calculation of $|dE/dV|$ and d^2E/dV^2 ; (5) localization of the equivalence region; (6) fitting a Random Forest regression model to

electrode potential as a function of titrant volume; and (7) evaluation on a held-out validation subset.

- i. NumPy & SciPy: Provided optimized routines for numerical computation, including differentiation, regression, and error analysis.
- ii. Pandas: structured storage and manipulation of the 30 experimental titration observations used in the revised analysis.
- iii. Matplotlib & Seaborn: Used to generate titration curves, first/second derivative plots, and statistical visualizations. These visualizations ensured clear interpretation of the equivalence point.
- iv. Scikit-learn: Random Forest regression and validation using RMSE and R².

This computational design allowed automation, reproducibility, and scalability, making the framework suitable for both academic and industrial titration studies (Fig-6).

The computational framework was revised to distinguish endpoint localization from regression of electrode potential. Derivative-based analysis identifies the chemical equivalence region, while the Random

Forest model predicts electrode potential from titrant volume and provides an independent data-driven representation of the titration curve (Table-3). The first derivative, $|dE/dV|$, identifies the region of maximum potential change and the second derivative identifies the corresponding inflection by its zero crossing. Both derivative criteria identify an equivalence volume of approximately 10.0 mL in the supplied dataset.

Table 3: Computational tools and applications.

Library/Tool	Functionality	Application in titration analysis
NumPy & SciPy	Numerical methods, differentiation, regression	Data handling and curve fitting
Pandas	Data frames and tabular manipulation	Managing the 30 experimental titration observations
Matplotlib & Seaborn	Plotting and visualization	Graphical representation of titration curves and derivatives
Scikit-learn	Machine learning algorithms	Endpoint detection via regression modeling
Jupyter Notebook	Interactive coding and reporting	Reproducible analysis and real-time visualization

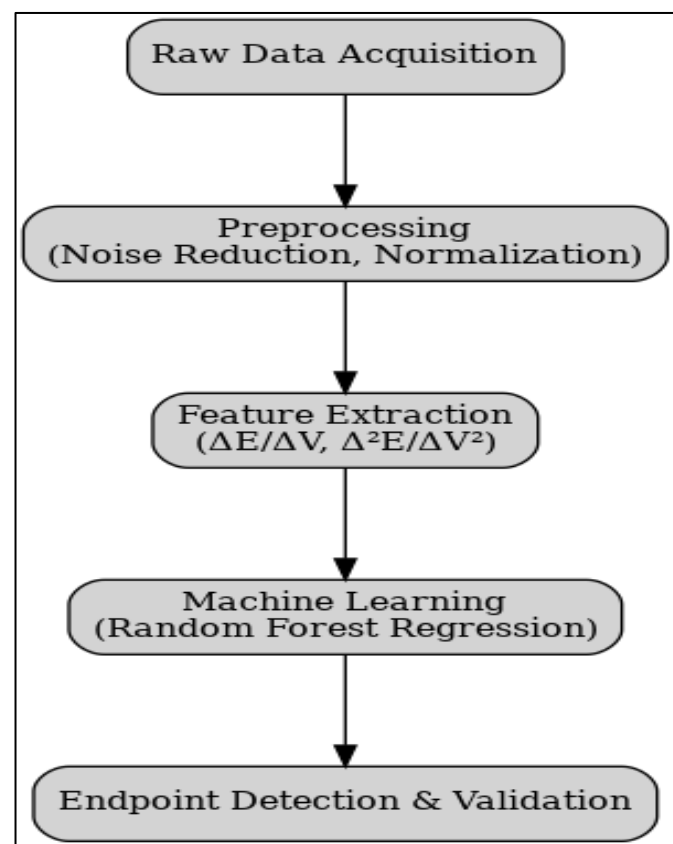


Fig. 6: Computational workflow from data acquisition through preprocessing, derivative-based endpoint localization, Random Forest regression, and validation.

2.7 Regression modelling

For the revised analysis, a Random Forest Regressor was fitted to the 30 experimental observations, using titrant volume as the predictor and electrode potential as the response. The model used 300 trees ($n_estimators = 300$), maximum tree depth of 8 ($max_depth = 8$), minimum samples per leaf of 1, and $random_state = 42$. An 80:20 random train/validation split was used. The model was evaluated only on the held-out observations and was not trained on the validation subset.^[14]

1. Derivative-based endpoint detection:

- The first derivative, $|dE/dV|$, identifies the point of maximum absolute slope. In the supplied data this occurs at approximately 10.0 mL.
- The second derivative, d^2E/dV^2 , identifies the inflection point through its zero crossing. The revised analysis places this crossing at approximately 10.0 mL.
- Both derivative criteria therefore identify an equivalence volume of approximately 10.0 mL, consistent with 20.0 mL of 0.050 N HCl titrated with 0.100 N NaOH.

2. Regression modelling:

- A Random Forest regression model was fitted only to the 30 experimental observations in Table 1. No synthetic observations were included in the revised validation analysis.
- The model was used to predict electrode potential from titrant volume. Endpoint localization remained a chemical/derivative-based step; the Random Forest curve was used as an independent data-driven representation rather than as a stand-alone chemical endpoint label.
- The fixed hyper parameters and 80:20 train/validation split provide a reproducible baseline for the supplied dataset; broader independent datasets are required before claims of generalizability can be made.

Fig. 7 compares the experimental electrode potentials with the Random Forest predictions. The model reproduces the major transition in the titration curve. A transition in the predicted curve occurs at approximately 9.95 mL, which is consistent with the derivative-based equivalence region of approximately 10.0 mL.

3. Validation:

- The held-out validation observations were compared with their Random Forest predictions.
- Using an 80:20 split (24 training and 6 validation observations), the revised model produced an RMSE of 11.49 mV and $R^2 = 0.9977$ on the validation subset.
- These metrics quantify prediction of electrode potential, not direct prediction of equivalence volume. Therefore, they are not interpreted as independent evidence that the chemical endpoint

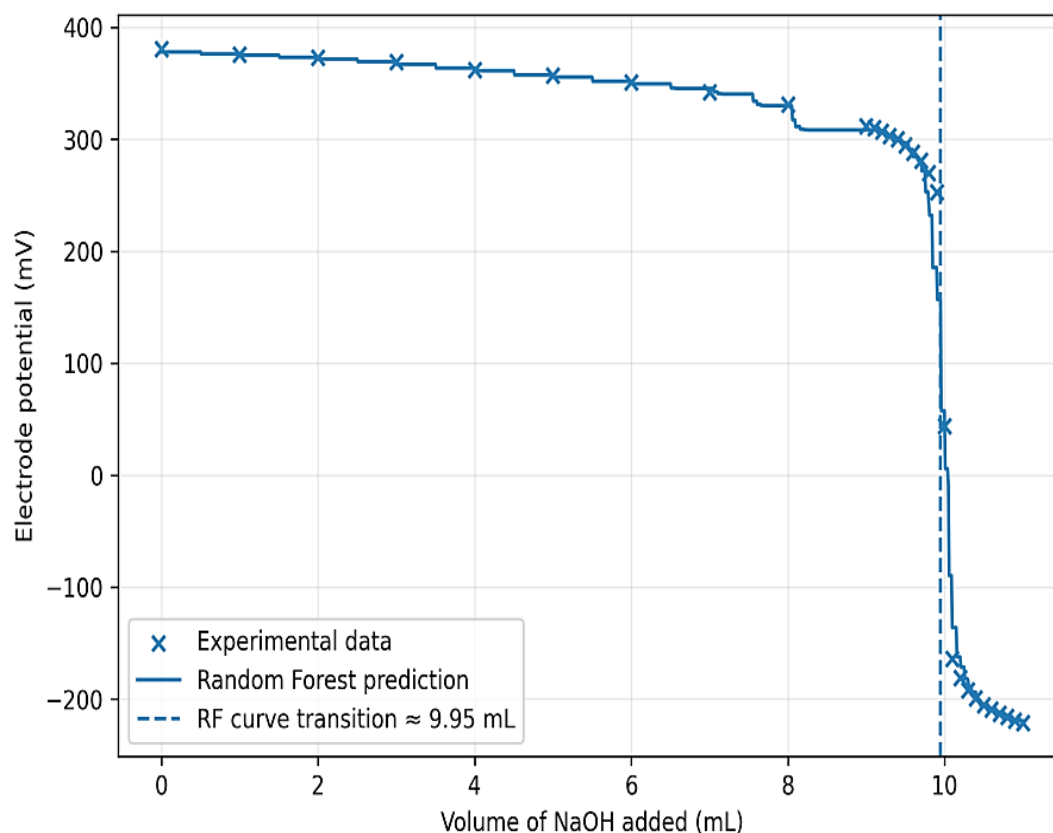


Fig. 7: Random Forest regression of electrode potential as a function of NaOH volume.

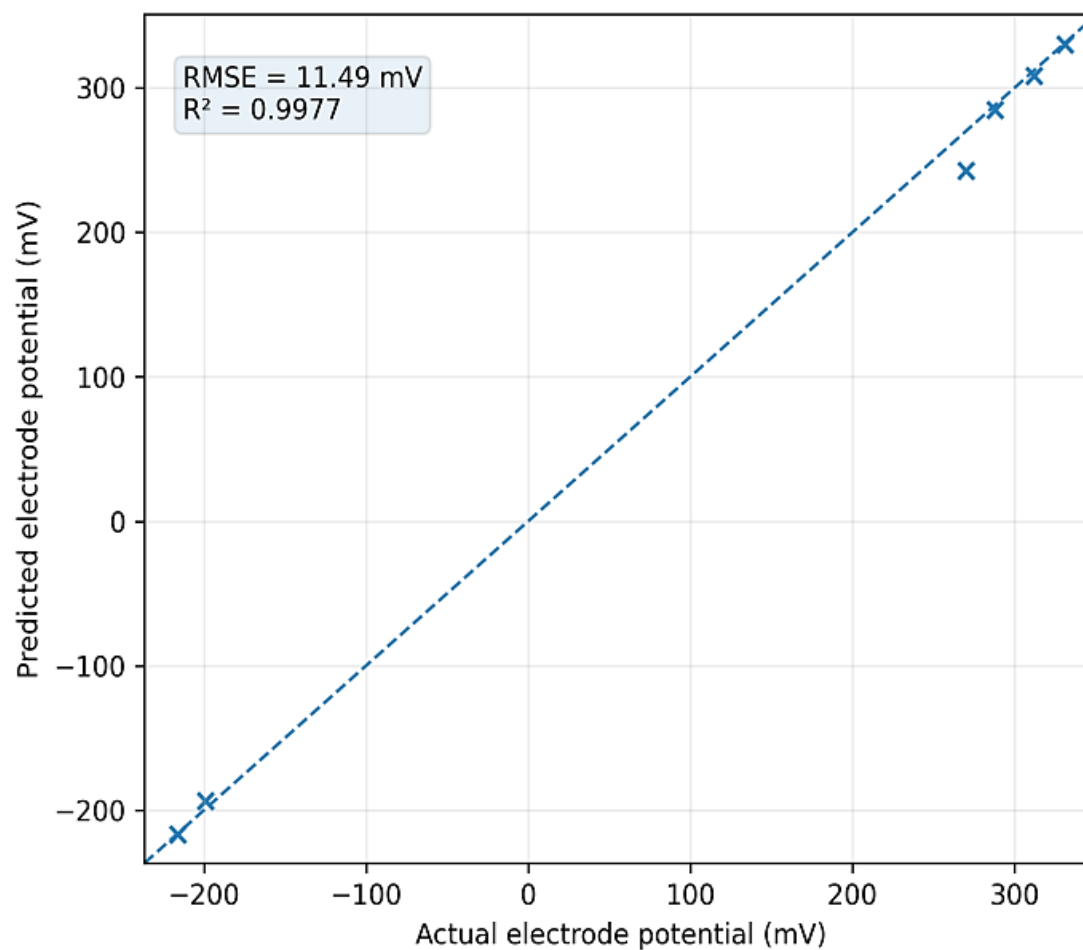


Fig. 8: Validation of Random Forest electrode-potential predictions.

Table 4: Revised endpoint localization and Random Forest validation metrics

Method	Predicted Endpoint (mL)	Theoretical Endpoint (mL)	Error (%)	RMSE (mV)	R ²
First Derivative dE/dV	10.00	10.00	0.0	–	–
Second Derivative d ² E/dV ²	10.00	10.00	0.0	–	–
Random Forest Regression	9.95	10.00	0.5	11.49	0.9977

Note: RMSE and R² refer to held-out electrode-potential prediction, not to the chemical endpoint volume.

itself has an RMSE of 0.65 mL or 0.65 mV.

Fig. 8 compares predicted and actual electrode potentials for the held-out validation observations. The model achieved RMSE = 11.49 mV and R² = 0.9977. The revised interpretation distinguishes predictive accuracy for electrode potential from the chemical endpoint identified by derivative analysis (Table-4).^[15,16]

3. Results and discussion

3.1 Potentiometric titration behaviour

The electrode potential decreased as NaOH was added, with a sharp transition between 9.9 and 10.1 mL. The response is consistent with the expected strong acid–strong base titration behaviour of the HCl/NaOH system.

3.2 Derivative analysis for endpoint detection

The absolute first derivative showed its maximum at approximately 10.0 mL, while the second derivative crossed zero in the same region. These two independent numerical criteria therefore locate the equivalence region at approximately 10.0 mL.

3.3 Data preprocessing and computational efficiency

Savitzky–Golay smoothing (seven-point, second-order polynomial) reduced local fluctuations while preserving the sharp transition. The derivative calculations were performed in physical units, avoiding the numerical scaling artefacts present in the previous figures. The workflow therefore makes the relationship between raw data, preprocessing, endpoint detection, and machine-learning regression explicit.^[17]

3.4 Machine learning integration and validation

The revised Random Forest model was evaluated on the 30 experimental observations using an 80:20 train/validation split. The model predicted electrode potential with RMSE = 11.49 mV and R² = 0.9977 on the held-out observations. The predicted curve showed a transition at approximately 9.95 mL, consistent with the derivative-based equivalence region of approximately 10.0 mL. These results support the use of machine learning as a curve-modelling component, while the chemical endpoint remains anchored to the inflection-point analysis.

3.5 Comparative accuracy

Table 4 compares endpoint localization from the two derivative criteria with the Random Forest curve transition. The derivative methods provide the direct chemical endpoint criterion, whereas the Random Forest model provides a data-driven prediction of electrode potential.^[18] Because only one 30-observation experimental titration is available in the supplied dataset, the present results should be considered a proof-of-concept rather than a general performance benchmark.

3.6 Summary of findings

The major observations and results obtained from this study are outlined below:

- The potentiometric titration curve (Fig. 3) displayed a sharp potential transition around 10.0 mL of NaOH.
- The absolute first derivative and second derivative (Figs. 4–5) independently localized the equivalence region at approximately 10.0 mL.
- Savitzky–Golay filtering reduced local fluctuations while preserving the transition, and derivative calculations were reported in physically meaningful units.
- The Python-based framework automated data handling, preprocessing, derivative analysis, and Random Forest regression.
- The revised Random Forest analysis, based on 30 experimental observations and an 80:20 split, yielded RMSE = 11.49 mV and R² = 0.9977 for held-out electrode-potential prediction. The model is not presented as a direct substitute for chemical endpoint criteria.

Overall, the revised analysis demonstrates a traceable computational workflow for potentiometric titration and provides a reproducible baseline for future studies involving larger numbers of independent titrations.

4. Conclusion

The revised study demonstrates a Python-assisted workflow for potentiometric titration of HCl with standardized NaOH. The equivalence region in the supplied experimental dataset was identified at approximately 10.0 mL from the maximum absolute first derivative and the zero crossing of the second derivative. A Random Forest regression model provided an independent prediction of electrode potential, with RMSE = 11.49 mV and R² = 0.9977 on a held-out validation

subset. The results support the feasibility of integrating numerical analysis and machine learning into potentiometric titration workflows, but they do not establish universal superiority over conventional titration methods. The principal limitations are the small dataset (30 observations from the supplied experimental titration), the absence of independent experimental replicates in the supplied file, and the lack of a fully documented synthetic-data generation set. Generalization to weak acids, polyprotic systems, multivalent analytes, asymmetric curves, different electrode systems, and other experimental conditions require additional datasets and independent validation. The proposed framework should therefore be regarded as a proof-of-concept computational approach. Future work should include multiple independent titrations, replicate measurements, documented synthetic-data generation where used, and externally validated machine-learning models before deployment in routine analytical laboratories.

CRediT Author Contribution Statement

Shanthi Vunguturi: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing. The author has read and approved the final version of the manuscript for publication and agrees to be accountable for all aspects of the work, ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved.

Funding Statement

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Data Availability Statement

The experimental dataset used for the revised quantitative analysis is provided in [Table 1](#) of this manuscript. The revised analysis used the 30 experimental observations reported there; no external dataset was required.

Conflict of Interest

There is no conflict of interest.

Use of AI Disclosure Statement

During preparation of the revised manuscript, generative AI assistance was used for language editing, organization of the response to reviewers, and refinement of graphical/text presentation. The author reviewed the manuscript and remains responsible for the scientific content, data interpretation, and final submitted version.

Supporting Information

Not applicable.

Study Limitations

The present analysis is based on a single supplied experimental titration comprising 30 observations. Independent experimental replicates, larger datasets, and systematic testing across different acid/base strengths and electrode configurations are required to establish reproducibility and generalizability. The Random Forest results reported here quantify electrode-potential prediction and should not be interpreted as a universal endpoint-prediction accuracy estimate.

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