

Output Regulation Based on Object Detection and High Gain Observers in Liquid Handling Robots

Regulación de la salida basada en detección de objetos y observadores de alta ganancia en robots de manipulación de líquidos

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Recibido 22/05/2026, aceptado 30/06/2026, publicado 01/07/2026.



Abstract

Liquid Handling Robots have acquired a significant role in modern laboratories due to their capabilities to automate pipetting and dispensing liquids with high precision and repeatability. Additionally, advances in artificial intelligence have contributed to research areas such as biology or material science, generating sophisticated systems to conduct complex assays. This paper presents an overview of the impact of artificial intelligence techniques and Liquid Handling Robots in applications related to sample preparation, such as cell culturing, microscopy, and in vivo experimentation. In this context, the paper proposes object identification of common labware to support liquid handling tasks. The detection system is based on the ResNet-50 classifier and YOLO v2 detector. The information provided by the detector is used for trajectory planning of a robotic system. To minimize the tracking position error, is proposed a control scheme based on High-Gain observer and Output Regulation, where the trajectories are considered as unmodeled reference signals.

Index terms: liquid handling robot, deep learning, object identification, output regulation, labware recognition, high-gain observer.

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Resumen

Los robots de manipulación de líquidos han adquirido un papel relevante en los laboratorios modernos gracias a su capacidad para automatizar el pipeteo y la dispensación de líquidos con alta precisión y repetibilidad. Asimismo, los avances en inteligencia artificial han contribuido a áreas de investigación como la biología y la ciencia de materiales, dando lugar a sistemas sofisticados para realizar ensayos complejos. Este artículo presenta una visión general del impacto de las técnicas de inteligencia artificial y los robots de manipulación de líquidos en aplicaciones relacionadas con la preparación de muestras, tales como el cultivo celular, la microscopía y la experimentación ‘in vivo’. En este contexto, se propone la identificación de objetos — específicamente material de laboratorio común— para facilitar las tareas de manipulación de líquidos. El sistema de detección se basa en el clasificador ResNet-50 y el detector YOLO v2. La información proporcionada por el detector se utiliza para la planificación de trayectorias de un sistema robótico. Con el fin de minimizar el error de seguimiento de posición, se propone un esquema de control basado en un observador de alta ganancia y regulación de salida, donde las trayectorias se consideran señales de referencia no modeladas.

Palabras clave: robot de manipulación de líquidos, aprendizaje profundo, identificación de objetos, regulación de salida, reconocimiento de material de laboratorio, observador de alta ganancia.

I. INTRODUCTION

Traditional laboratory environments can involve time-consuming manual tasks such as sample handling, pipetting, or data analysis, which are highly susceptible to human errors. Above, have been addressed by automating repetitive tasks through the integration of robotic systems, due to their inherent characteristics of repeatability and accuracy. Consequently, robotics plays a crucial role in the development of industries relative to chemistry, biology, pharmacology, and materials science, which are characterized by complex processes such as the handling of hazardous chemicals, handling of pathogenic organisms, the carrying out numerous assays or process steps, and the need of frequent measurements over extended periods. The complexity involved in discovering new molecules, materials, or systems, coupled with advances in machine learning and artificial intelligence, have led to the idea of expanding the concept of automation to autonomy. In this context, Self-Driving Laboratories (SDL) integrate artificial intelligence models and fully automated systems in a closed-loop, enabling them to make decisions about conducting experiments based on previous acquired experimental data [1], [2].

One industry with a high demand for the development of new technologies is the pharmaceutical, where the potential of SDL offers robust platforms capable to accelerating and optimizing the formulations of therapeutic proteins and vaccines to contribute to human health [3]. The performance of an SDL in the fields of protein engineering and synthetic biology is described in [4], where the design of new proteins can be derived from an intelligent agent learning about protein sequence-function relationships. This agent sends the designed proteins to a fully robotic system to conduct experimental tests, and results provide feedback to enhance the agent's capabilities and optimize the process. Living organisms are complex systems that cannot be easily controlled, making processes related to engineering biological organisms potentially benefit from an approach based on autonomy, allowing humans to set goals and receive the results of the assays. However, the level of autonomy in these processes depends on advances and access to new technologies in fields such as electrical and mechanical engineering, informatics, and even the manufacturing of new materials [5]. Similarly, a platform was developed in [6] to automate the discovering of relationship between genes and their functions, in molecular biology, facilitating collaboration with researchers. More recently, in [7], an SDL based on active learning with a liquid handling robot is applied to enable data-driven development in the field of nanomedicine. Discoveries in the pharmaceutical industry are conditioned and constrained by economic factors, as the development of treatments for diseases can be costly and time-consuming [8]. High costs are often associated with assays that involve testing large libraries of compounds, which can range from tens to millions of samples. Furthermore, retesting experiments is necessary to reduce the likelihood of false positives. It is important to note that these systems demonstrate the potential of applying artificial intelligence techniques to generate hypotheses, design and execute experiments to test hypotheses, analyze, and interpret results to make decisions [9]. Then, the combination of robotics and artificial intelligence plays a fundamental role in reducing costs and accelerating processes as drug discovery [8].

Robotics provides benefits to facilitate the implementation of reproducible protocols, ensure consistency across experiments, and enhance the reliability of research. Additionally, a precise control over experimental parameters and conditions enables researchers to explore biologicals phenomena, conduct large-scale screening studies, and accelerate hypothesis testing. As can be observed, a wide range of laboratory workflows involve the handling of small volumes of liquid solutions, where liquid handling robots (LHRs) are a fundamental component in laboratory automation for executing pipetting and dispensing tasks. LHRs provide systems with an efficient means of handling small volumes of liquid solutions, precisely dispensing reagents, conducting complex assays, facilitating high throughput screening, and performing large-scale liquid handling reactions automatically. These platforms have demonstrated their potential to minimize hands-on time, maximize experiment scale, increase reproducibility, reduce sample contamination, minimize wastage of expensive reagents, and manage experimental complexity, being a useful tool in drug discovery, genomics, and clinical research [10]. In this context, liquid Handling Robots have emerged as indispensable and modern tools in

laboratory settings, providing researchers with a different approach to develop experiments and assays, offering an alternative to manual liquid handling, alleviating researchers from tedious, tireless, and potential errors associated with repetitive manual tasks. Beyond the cost, LHRs have significantly improved the reproducibility of experiments and assays [11] including cell microinjection [12], DNA extraction [13], [14], yeast spot assay [15], nucleic acid testing [16], or shot gun proteomic analysis [17]. Due to its current relevance, in [18] is provided a detailed analysis of the use of LHRs for solvent extraction techniques, which are not only applied in molecular biology, but also in pharmacokinetics or toxicology. Additionally, authors also present an update of several types of robots and their applications in solvent extraction where LHRs offer advantages over manual procedures, especially when is necessary to analyze large number of samples in a short period of time. LHRs can be equipped with a variety of components, depending on the specific needs of an experiment. For instance, in protein and organism evolution experiments, necessary devices may include pipettes (which could have multiple channels), pipette tips, robotic grippers, sterilization stations, and plates. However, the cost of automation varies depending on the flexibility required for handling different types of samples. Moreover, with the evolving requirements in research and education, the development of open-source platforms has gained significant importance, enabling greater flexibility in robot programming and the sharing of protocols [19].

4 It is clear that LHRs have contributed to the development of research areas related to pathogen discovery due to their capabilities to execute complex liquid handling protocols with high levels of accuracy and consistency, even surpassing human performance in many cases. These capabilities can be further improved by incorporating artificial intelligence and machine learning techniques to develop intelligent controls, monitoring tasks to detect anomalies, and implementing corrective actions when necessary. In addition, deep learning brings to LHRs capabilities to operate and adapt them to diverse experimental conditions, by leveraging that neural networks learn from large volumes of data. Deep learning allows robots to autonomously optimize their performance, adapt to dynamic environments, and even discover novel strategies for liquid manipulation. The autonomy of a robotic system in laboratory settings or within an SDL lies in the capacity to make decisions based on the knowledge of its environment. The potential of deep learning has carried out a trend toward developing applications focused on reducing the duration of assays, in any of their stages, particularly those that are repetitive or require high precision, such as sample preparation. Above can be achieved by integrating convolutional neural networks (CNN) for labware identification, allowing a LHR to distinguish between sample and black wells and perform monitoring tasks [20]. Similarly, [21] presents the adaptation of a commercial robotic manipulator for liquid handling, as well as the labware recognition based on classifiers for motion planning purposes, thus avoiding reprogramming the robot. Object detection using convolutional neural networks has been demonstrated to be a robust tool for recognizing labware, identifying the color of liquids, and estimating liquid levels in pipette tips [17]. Moreover, convolutional networks are useful for tackling with complex classification problems, such as the identification of internal viscous dissipation in dispensing tasks [22].

As previously mentioned, researchers deal with large-step and complex protocols, which, in conjunction with the lack of standardization, can lead to a loss of flexibility. This situation can make it challenging to execute different protocols or integrate new components, requiring a considerable amount of time for programming. To address this issue, the implementation of a Hierarchical Task Network can increase the flexibility of LHRs [23]. On the other hand, strategies based on Bayesian optimization allow the evaluation of experiments based on the analysis of captured images that provide data about the growing of cells in regenerative medicine [24]. Previous literature highlights the importance of liquid handling in a variety of complex processes, where LHRs and artificial intelligence combined with advancements in hardware and software, represent an alternative to exploit a wide range of applications, which accelerate discoveries in different research areas. This paper explores the object detection of common labware to support liquid handling tasks. The detection system is based on the ResNet-50 classifier and YOLO v2 detector. The information provided by the detector is used for trajectory planning of a robotic system. To minimize the position error and ensure the asymptotic tracking, is proposed a control scheme based on High-Gain observer and Output Regulation, where the

trajectories are considered as unmodeled reference signals. This capability can enhance the performance of liquid handling tasks and increase overall efficiency.

II. METHODS AND MATERIALS

The integration of the deep learning models into LHRs is a promising approach to achieving autonomy in these systems. This work proposes the recognition of common labware used in liquid handling tasks, which is achieved through two main stages: classification and real time detection. Classification is based on a residual network (ResNet), while the real-time detection uses the you-only-look-once (YOLO v2) object detector. Fig. 1 shows the workflow for object detection process.

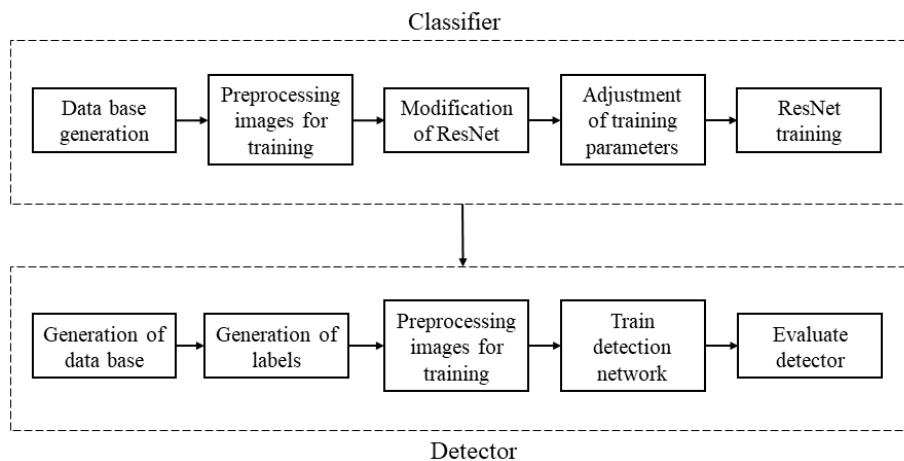


Fig. 1. Block diagram for object identification process.

The labware of interest is a pipette, a 3d printed rack for reagents, a 3d printed test tube rack, pipette tips, open tube, and closed tube (Fig. 2).

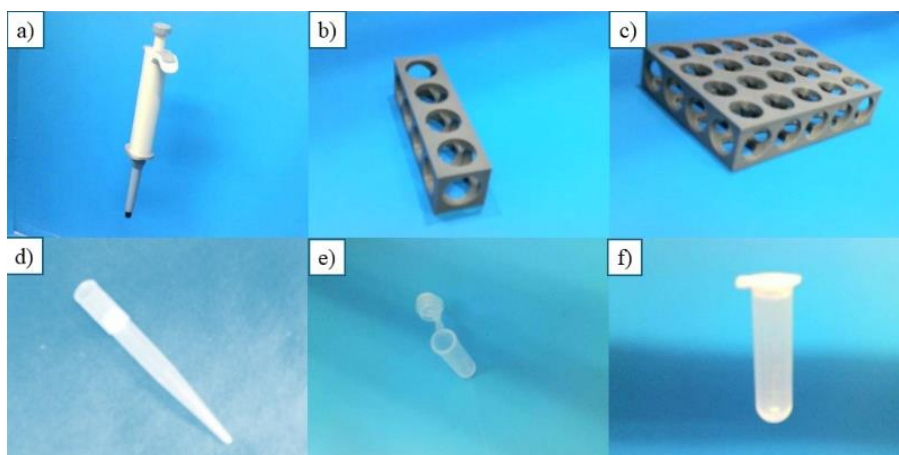


Fig. 2. Labware to identify. a) pipette, b) 3d printed rack for reagents, c) 3d printed test tube rack, d) pipette tip, e) open tube and f) closed tube.

A. Clasification

ResNet-50 employs residual connections to overcome the limitations of traditional deep learning architectures. This architecture comprises 50 layers, allowing the creation of complex models with a high level of accuracy. The first step for labware recognition involves generating a dataset with images of the objects of interest (Fig. 2), images were captured at a resolution of 640×480 dpi. The dataset is then resized to fit the network input size of 224×224×3, ensuring that the data input and the network dimensions are consistent. Deep Network Designer toolbox of Matlab® is used to retrain the ResNet-50 network. Above requires replacing the existing network head, which includes the blocks associated to the fully connected layer, the Softmax layer, and the Classification output layer, with similar blocks configured according to the classes on the new dataset. The initial learn rate for training was set to 0.01. As seen in Fig. 3, an accuracy of 98.1% was achieved with the dataset and training parameters.

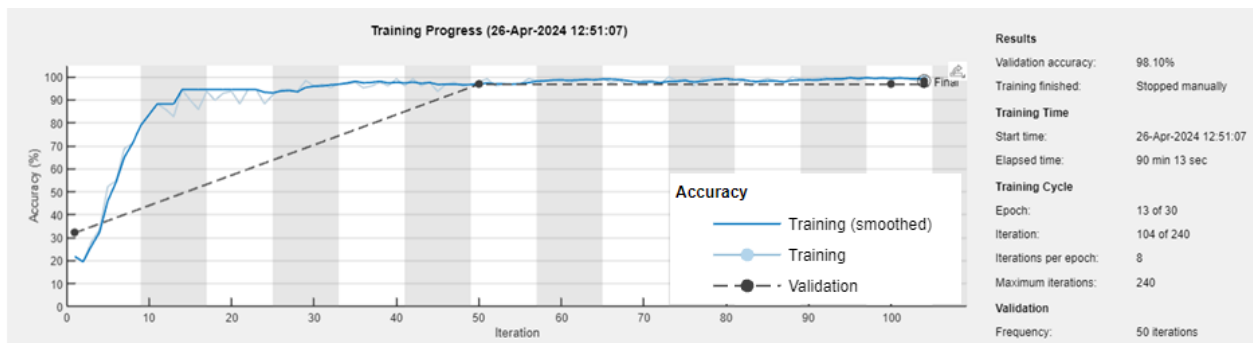


Fig. 3. Accuracy of the retrained ResNet-50 network.

B. Object detection

YOLO v2 is a fast and efficient method for detecting objects in images and videos. The model employs a deep convolutional neural network (CNN) to extract features from an input image, allowing it to predict multiple bounding boxes and class probabilities in a single forward pass. This approach makes YOLO v2 suitable for real-time applications. In labware recognition, a new dataset is generated for training. This dataset contains captured images of the objects of interest, which are different from the images used in the classifier. This new dataset is used to generate the labels of each object, and they are used to train the YOLO v2 network. If necessary, each image may need to be resized to ensure consistency with the input layer size of the network. The preprocessing step consists of splitting the dataset into 60% of the images for training, 10% for validation and 30% for testing.

C. Control scheme base don high-gain observer

In this paper the Liquid Handling Robot is a cartesian robot as can be seen in Fig. 4. To control the cartesian robot is proposed a control scheme based on output regulation and a high-gain observer [25]. The controller is graphically described in the block diagram of Fig. 5.

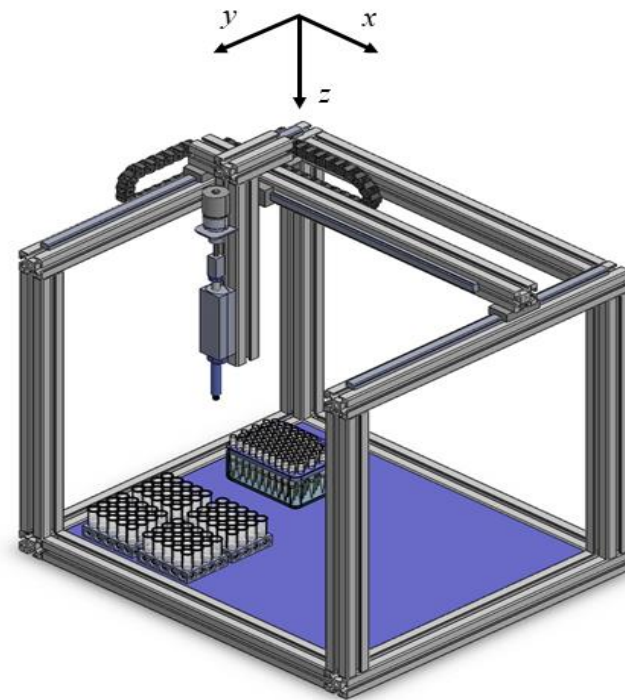


Fig. 4. Prototype of a Liquid Handling robot based on a cartesian robot.

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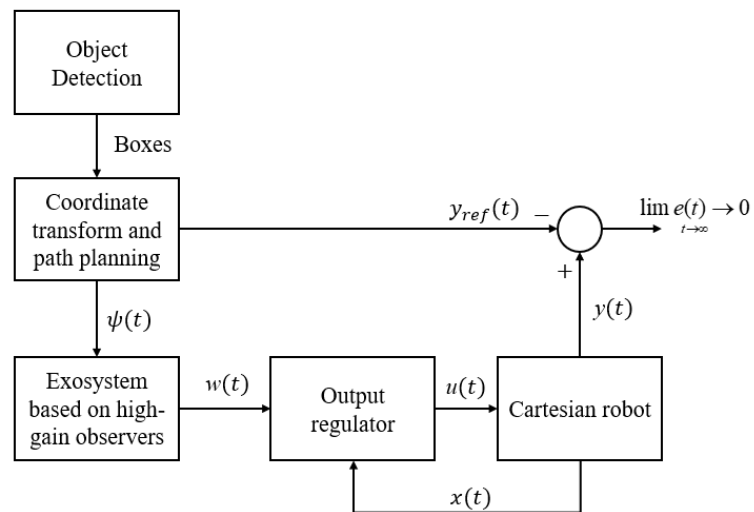


Fig. 5. Block diagram of the proposed controller.

The trajectories for $x_{ref}(t)$ and $y_{ref}(t)$ are considered as unmodeled reference signals for each independent joint of the two-degree-of-freedom cartesian robot [26]. Furthermore, considering gravity acting in the z robot axis results in simple kinematics and dynamics model for the X-Y motion. Thus, the dynamics is given by Eq. (1):

$$\begin{bmatrix} m_1 + m_2 & 0 \\ 0 & m_2 \end{bmatrix} \begin{bmatrix} \ddot{q}_1 \\ \ddot{q}_2 \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad (1)$$

The state space representation leads to:

$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \\ \dot{x}_4(t) \end{bmatrix} = \begin{bmatrix} x_2 \\ f_1(x(t), u(t)) \\ x_4 \\ f_2(x(t), u(t)) \end{bmatrix}, \quad (2)$$

with:

$$\begin{bmatrix} f_1(x(t), u(t)) \\ f_2(x(t), u(t)) \end{bmatrix} = [D(x(t))]^{(-1)} [u(t)] \quad (3)$$

Thus, by defined the control law as $u(t) = K(x(t) - \Pi w(t)) + \Gamma w(t)$, the condition for output regulation rest on the linear matrix equations described as $\Pi S = A\Pi + B\Gamma$ and $C\Pi = Q_{ref}$ with solution for Π and Γ . To this, the linear counterpart is obtained by linearizing the system (2) around the origin, i.e. $\dot{x}(t) = Ax(t) + Bu(t)$, additionally consider x_1 and x_3 as the output to be regulated.

The joint trajectories of the actuators $\psi(t)$ (exogenous dynamic model) can be considered as the output of a non-existent dynamical model, and the High-Gain Observer described by the set of equation (4) can be used to estimate the state and output of such a system, resulting [25]:

$$\begin{aligned} \dot{w}(t) &= Sw(t) + S_H \psi(t), \\ y_{ref} &= Q_{ref} w(t), \end{aligned} \quad (4)$$

subjected to the solution of the system of equations (5) [25]:

$$\begin{aligned} \Pi(S + S_H Q_w) &= A\Pi + B\Gamma + P, \\ C\Pi &= Q_{ref}, \end{aligned} \quad (5)$$

By considering $A = \begin{bmatrix} m_1 + m_2 & 0 \\ 0 & m_2 \end{bmatrix}; B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}; C = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}; Q_{ref} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$.

According to [25], and by assuming $\rho = 2$, the block matrices S_H and S for $\alpha_1 = \alpha_2 = 1$, and $\varepsilon = 0.02$ are:

$$S_H = \begin{bmatrix} 100 & 0 \\ 2500 & 0 \\ 0 & 100 \\ 0 & 2500 \end{bmatrix} \text{ and } S = \begin{bmatrix} -100 & 1 & 0 & 0 \\ -2500 & 0 & 0 & 0 \\ 0 & 0 & -100 & 1 \\ 0 & 0 & -2500 & 0 \end{bmatrix}$$

The linear mappings are computed by the equation (5) which leads to:

$$\Pi = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } \Gamma = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

can be easily verified that the gain: $K = \begin{bmatrix} 22.4849 & -13.9878 & 7.2044 & -1.3438 \\ 2.1375 & -0.40 & 13.3867 & -5.3859 \end{bmatrix}$,

can be used to stabilize the pair (A, B).

III. RESULTS

Fig. 6 presents the results of the classifier based on the ResNet-50 network. The data shows that classifier achieves a class score of 93% for the reagent rack, which is the lowest score among the classes. This score can be attributed to its similar characteristics to the test tube rack. In contrast, for the tip and tube rack a score of 100% is obtained.

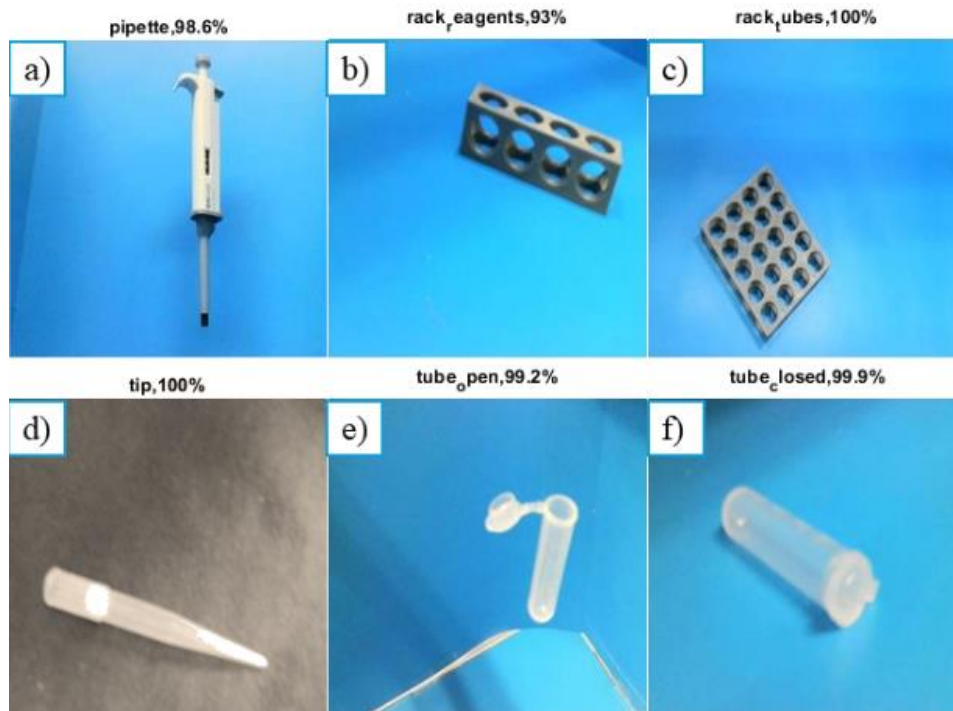


Fig. 6. Results for labware classification: a) pipette, b) 3d printed rack for reagents, c) 3d printed test tube rack, d) pipette tip, e) open tube and f) closed tube.

Finally, the network is evaluated using the trained detector. The results of object recognition using YOLO v2 are presented in Fig. 7, highlighting its effectiveness in detecting the labware objects.

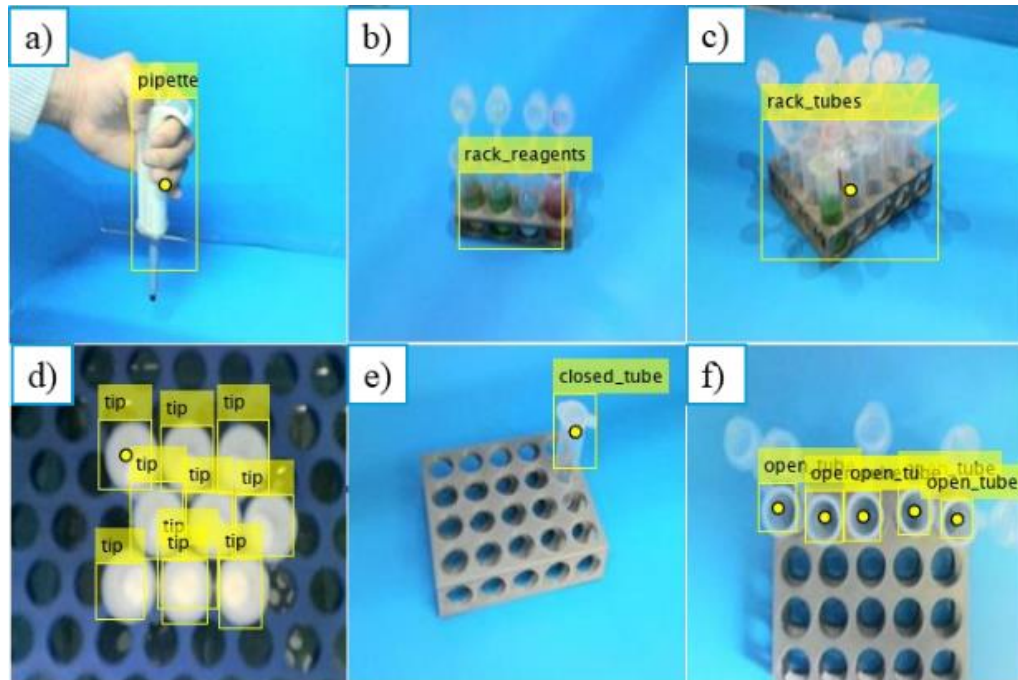


Fig. 7. Results for labware recognition: a) pipette, b) 3d printed rack for reagents, c) 3d printed test tube rack, d) pipette tip, e) open tube and f) closed tube.

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The principal idea is to impose an unmodeled trajectory by a set of points in the X-Y plane, as depicted in Fig. 8. Then, object detection is carried out with the corresponding transformation of coordinates from image space to Cartesian. Once the transformation is achieved, path planning for point-to-point motion is proposed. Open tubes indicate the viapoints, in Fig. 8 the path is graphically depicted. From the X-Y workspace path, the joint trajectories of the actuators are obtained, i.e. $x_{ref}(t)$ and $y_{ref}(t)$ as can be observed in Fig. 9.

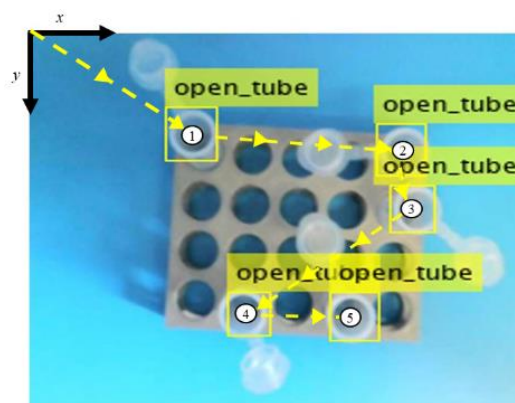


Fig. 8. Desire path in X-Y plane.

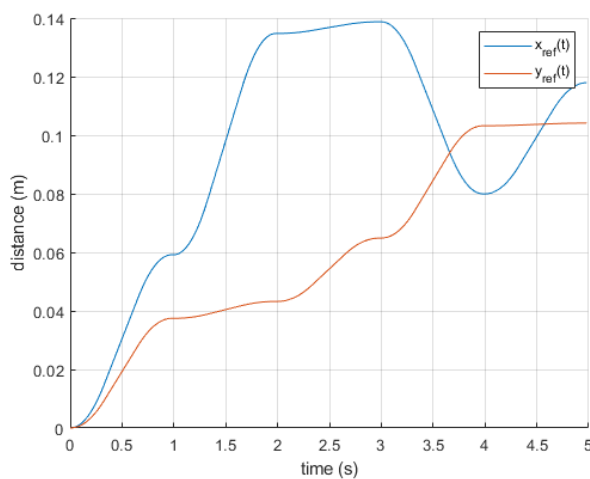


Fig. 9. Desired trajectories for x and y coordinates.

The results of the controller for the tracking of $x_{ref}(t)$ and $y_{ref}(t)$ are shown in Fig. 10.

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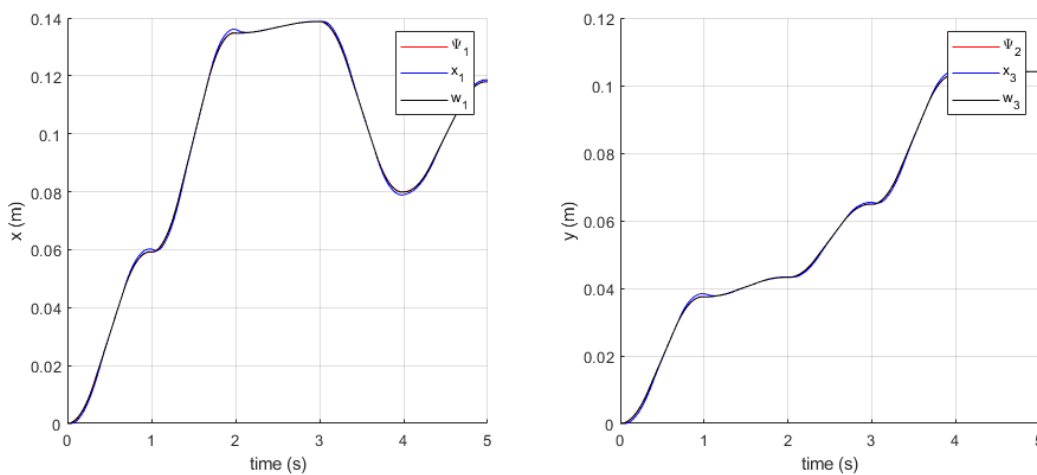


Fig. 10. Tracking results for x and y coordinates.

Additionally, tracking errors for x and y coordinates are given in Fig. 11. The corresponding control signals are depicted in Fig. 12 for simulation system.

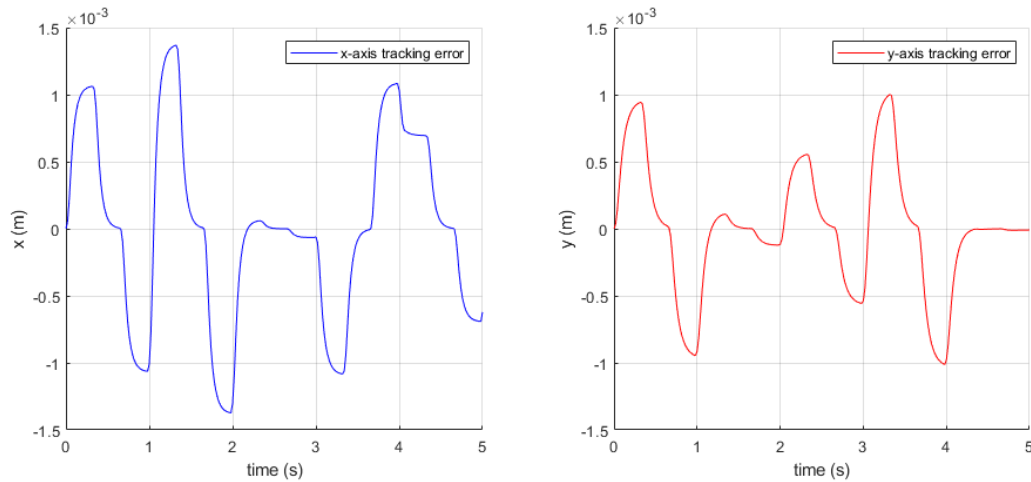


Fig. 11. Tracking error for x and y coordinates.

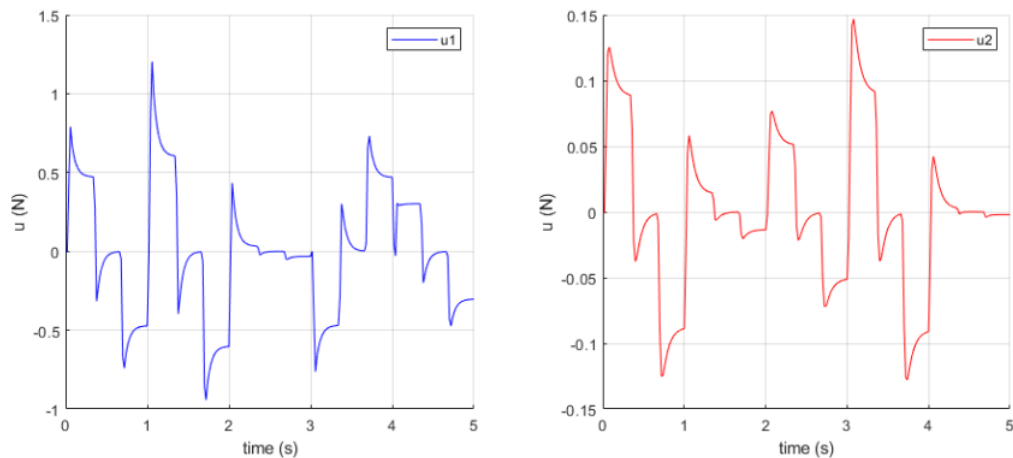


Fig. 12. Control signal for x and y actuators.

IV. CONCLUSIONS

The development of artificial intelligence has represented significant advances in experimentation and data analysis in different research fields, wherein robotics, automation systems, and artificial intelligence have converged to open new possibilities, enhancing capabilities such as efficiency, precision, and acceleration of discoveries. Deep learning has become in an effective technology that can provide a degree of autonomy to those automation systems with potential applications in fields as biology and pharmacology, which are relevant in public health. However, due to the complexity of experiments, deep learning faces challenges such as the lack of sufficient data for training or the lack of standardized assay protocols. Additionally, robotic systems have emerged as an essential tool in laboratory automation,

particularly in liquid handling routines, wherein LHRs have demonstrated their capabilities in terms of repeatability, precision, and time reduction in tasks such as liquid metering, aspirating, addition, dispensing, mixing, positioning, or cleaning.

Traditionally, robots are programmed to execute a program with the routines of an assay but could exist the probability of a programming error as well as complications derived from the variability inherent in laboratory workflows, then deep learning can represent a useful tool for real-time monitoring of a LHR routine. For above, in this work were trained a ResNet-50 network and the YOLO v2 detector for recognition of common labware. The training results showed that detector can recognize with an accuracy of 93% to 100% the labware of interest. Information acquired from detector were used in the control based on the output regulation theory and high gain observers ensuring the asymptotic tracking of unmodeled reference signals.

CRedit (Contributor Roles Taxonomy)

Authors' contributions: Conceptualization: RTH, JAMC; Methodology: RTH, THC; Software: BAJF, ESCM; Investigation: RTH, THC; Writing-original draft: RTH, ESCM; Writing-review and editing: BAJF, JAMC, ESCM; Supervision: RTH, JAMC; Formal analysis: RTH, JAMC; Project administration: RTH; Funding acquisition: BAJF.

Funding: The authors declare that no external funding was received

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries may be directed to the corresponding author.

Acknowledgments: The authors acknowledge the Instituto Politécnico Nacional for supporting this work through SIP Project IND-2026-0339 and the Secretaría de Ciencia, Humanidades, Tecnología e Innovación for supporting this work through Project CIR/0059/2022 under the Investigadoras e Investigadores por México program.

Conflicts of Interest: The authors declare no conflicts of interest.

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