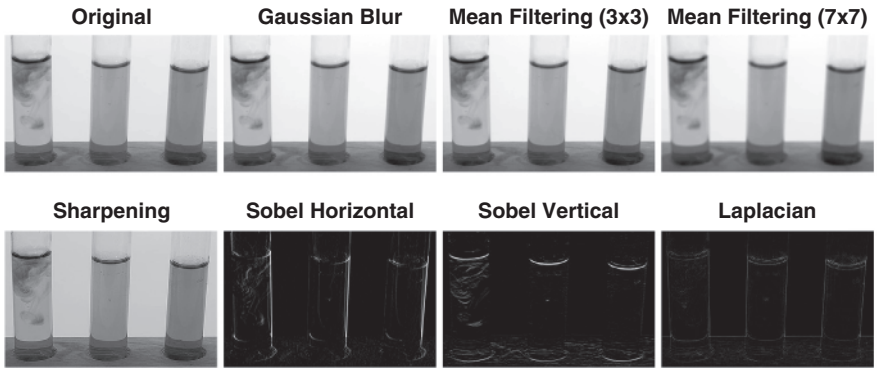

Figure 1.14 Exemplar demonstrations of the effect of using the convolutional filters described in Figure 1.13 on the output image.

From color spaces and their interconversions to photography hardware, color arrays, and all the valuable manipulations thereof, this combined software and hardware approach to understanding computer vision leaves us well-placed to consider the illustrative chemistry case studies below. Considering the broader topic of ML, we learn that, with computer vision, it is as much about the choice of machine as it is about any of the underlying software that comes front of mind with a term like ML.

1.3 Computer Vision and Machine Learning in Chemistry

Given that, at the time of writing, the applications of computer vision in catalysis itself remain sparse, the examples below include catalysis and phenomena that, while not directly related to catalysis, represent analytical challenges that will likely be relevant to future applications in the field.

1.3.1 Single Image Applications

1.3.1.1 High-throughput Digital Fingerprinting of Drug-like Compound Libraries

In 2011, Hodder and coworkers combined the hardware and software needed to build a system for assessing the quality of a library of drug-like compounds solvated in dimethyl sulfoxide (DMSO) [15]. Their system exemplified several key features that make computer vision valuable to chemistry and, potentially, catalysis. The team's use of a telecentric lens system was key to enabling distortion-free imaging of an entire well plate without optical distortion of parallax errors leading to unequal imaging of central versus outer wells. A telecentric lens is a specialized type of optical lens designed to have constant magnification regardless of the distance between the lens and the object being imaged. This unique characteristic is achieved by ensuring that the chief rays (rays passing through the center of the aperture) are parallel to the optical axis in either object space, image space, or both.

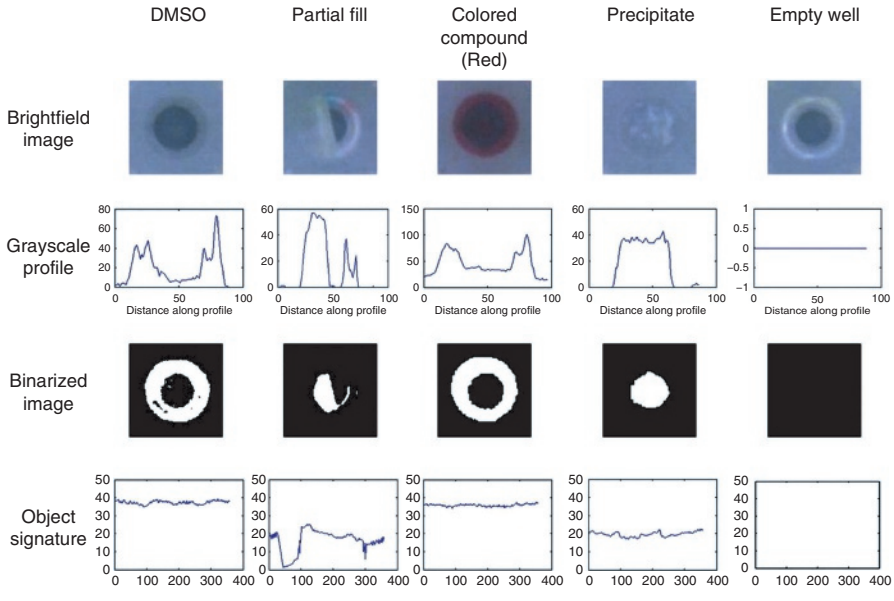

Figure 1.15 Use of grayscale profiling and binary image thresholding to characterize solubility behavior of a drug-like compound library. Reproduced with permission from [15]/SAGE.

From a chemical perspective, the solvation screening of the available compound library involved colored compounds, colorless compounds, soluble and precipitous insoluble candidates, as well as empty wells and solvent-only wells for calibration. With such a range of physicochemical behaviors, a range of visible "artifacts" could be captured and processed with computer vision. Using the grayscale lightness histogram distribution from a single well image, it was possible to create a binary black and white image to visually exaggerate the homo- or heterogeneity of the DMSO-solvated sample. The team used a combination of visible and infrared imaging in order to more fully distinguish visibly similar wells, especially in cases where colored compounds masked underlying precipitates. From here, a unique compound "signature" (the details of which are not clear from or not disclosed in the publication), providing a digital fingerprint with which that compound could be stored in a database containing all computer vision outputs (Figure 1.15).

1.3.1.2 Segmentation and Parallel Analysis of Nerve Agents

In 2018, Anslyn and Marcotte reported the use of photographic methods to measure fluorescence from self-propagating cascades used to amplify the signal and thus optically detect ions of various nerve agents (Figure 1.16) [16]. While the measurement of fluorescence for such purposes typically requires sophisticated, capital-intensive methods like fluorescence microscopy, UV-vis spectroscopy, and X-ray photoelectron spectroscopy, a demand for a more accessible and field-deployable technique was required in this case. To this end, a smartphone was used as the optical detector of fluorescence for samples housed in an opaque stage built from black toy building blocks.

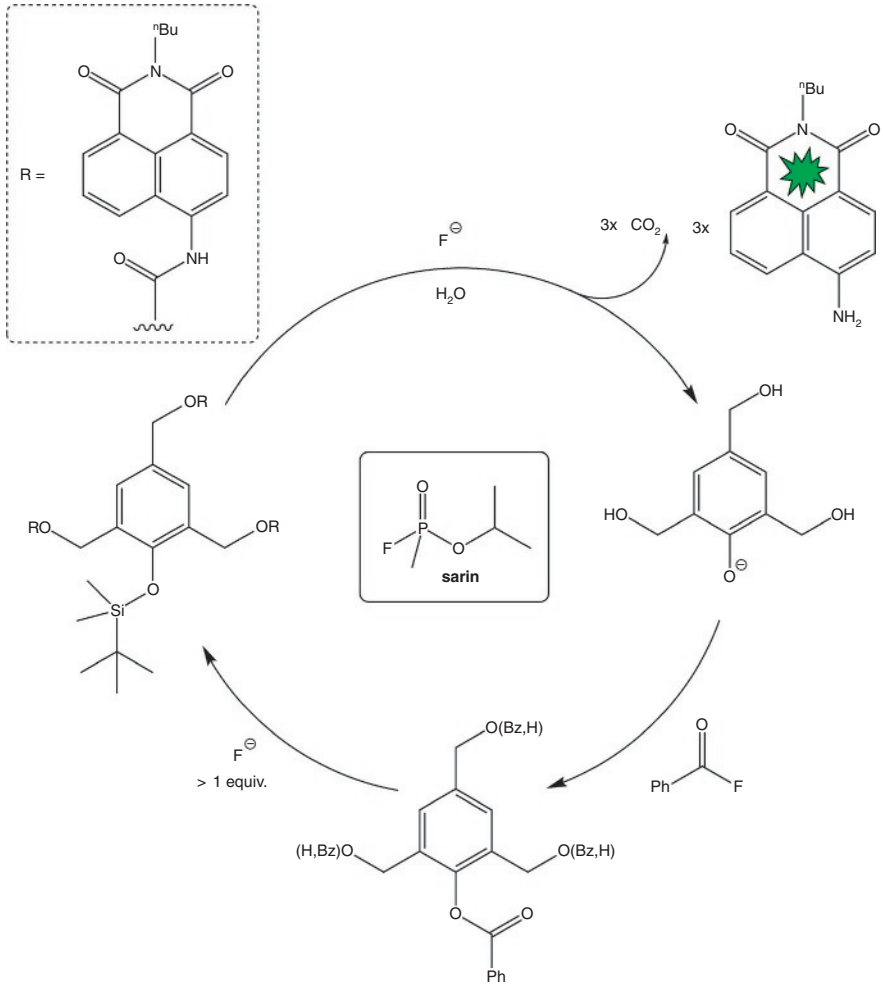

Figure 1.16 A simplified overview of one of two fluorescence amplification cascades used to generate samples amenable to high-throughput imaging of fluorescent samples via a computer vision approach. Adapted from [16].

Two elements of this work are important from a computer vision perspective, and both appear in Figure 1.17. First, the team employed the xyY color space, closely related to the above-mentioned XYZ color space (see Section 2.1.2). In doing so, the team used the *chromaticity* components, x and y, separate from the lighting-focused luminosity parameter, Y, to find the representative color of each sample well. In relation to the above-mentioned computer vision analytics and algorithms, the representative chromaticity of each sample was calculated based on the median pixel distribution within a given sample's color histogram for components x and y. By discounting the luminosity component, it was envisaged that the method would remain robust to changes in mobile phones used, owing to the inevitable variation in camera sensors when moving from one device to another. Plotting calibration samples on the xy-plane, the team interpolated the concentration of unknown nerve

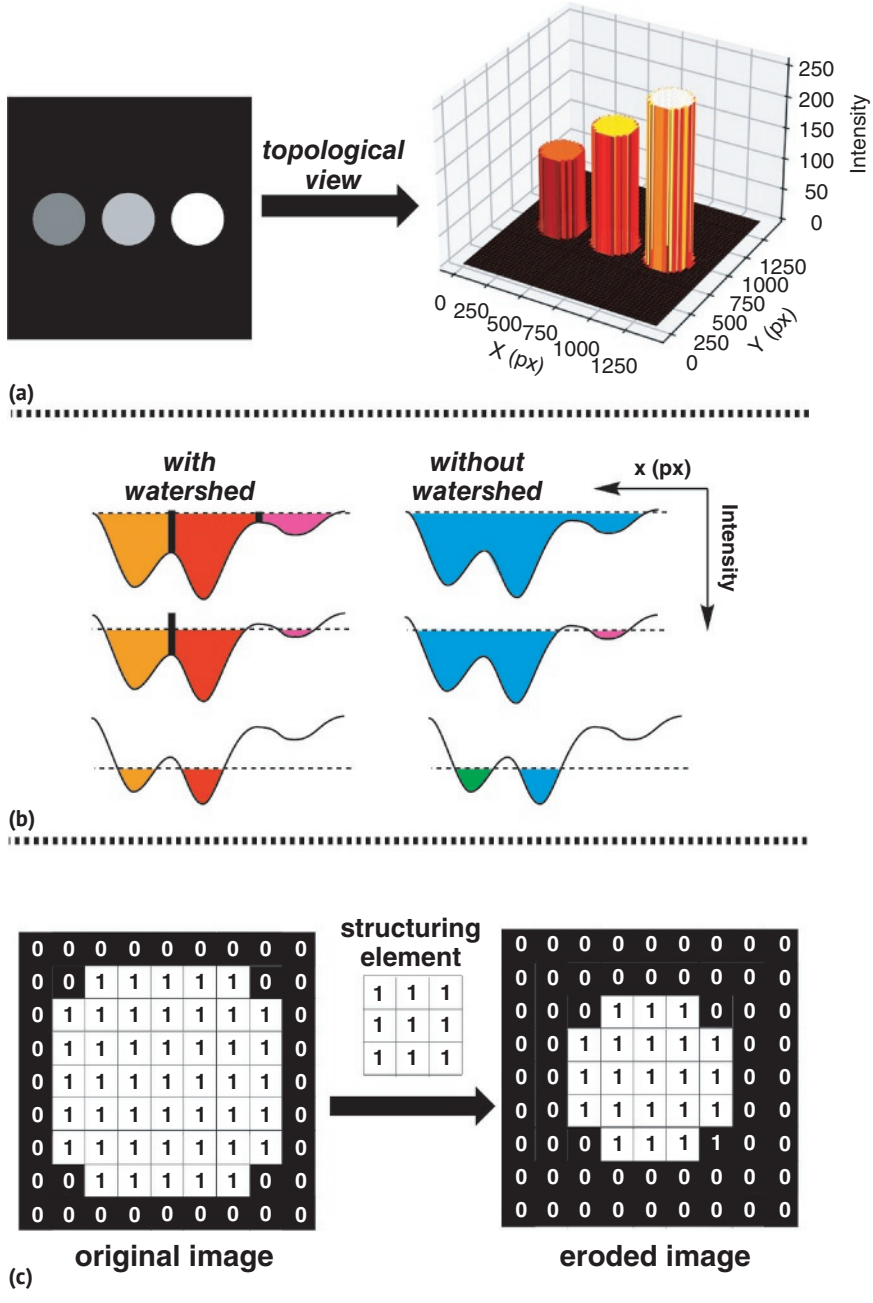

Figure 1.17 (a) Top: a demonstration of how grayscale values on an image can be viewed as a topological relief. (b) Middle: a one-dimensional pixel representation of filling the topological relief, where the bold black "dams" represent the identified watershed segments between local minima. (c) Bottom: an illustration of the morphological erosion technique employed in the second part of the computer vision algorithm by Anslyn's team.

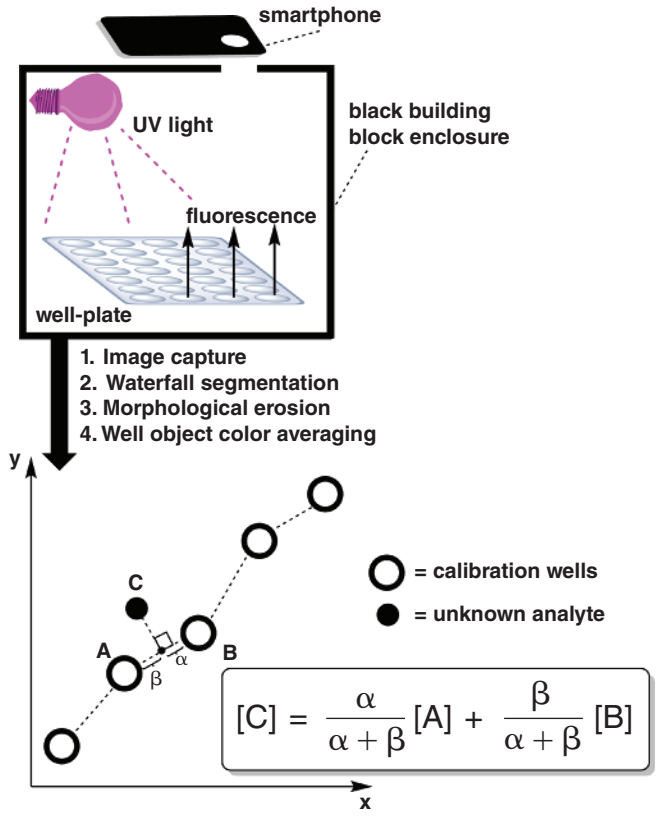

Figure 1.18 Top: A representation of the photographic hardware and staging used for the fluorescent imaging of nerve agents. Bottom: The resulting statistical framework, built around the xy-plane of the xyY color space, through which unknown sample concentrations could be estimated from the extracted xy-color parameters of calibration wells.

agent samples by using a piecewise linear regression approach. Here, Euclidean distances (i.e., lines between two points) were calculated for every adjacent pair of data points. Unknown sample concentrations were then estimated according to the equation embedded in Figure 1.18.

Yet, beyond the application of color theory and simple statistical analysis to produce a field-deployable method, it is how the individual samples on the 96-well plate were identified that merits further illustrative discussion. To this end, the team applied the so-called *waterfall* algorithm (Figure 1.17a,b) to segment one well from another and thus automatically optimize the selection of pixels used for the above-mentioned calculation of median chromaticity in each case. The waterfall algorithm is a refinement of the watershed algorithm, treating the grayscale image as a topographic surface, where the pixel values represent elevation. It simulates the process of water flooding from the lowest points (local minima), progressively filling up basins, and defining boundaries at points where water from different

basins would meet (Figure 1.17b). This method effectively segments the image into distinct regions based on the topography of the intensity landscape. However, as noted by Anslyn and Marcotte, the watershed algorithm can be sensitive to noise and over-segmentation, creating too many small regions. The waterfall algorithm addresses this issue by iteratively merging regions based on certain criteria, such as similarity in intensity or connectivity, to produce more meaningful and less fragmented segments. Essentially, the waterfall algorithm enhances the watershed method by introducing a post-processing step that reduces over-segmentation, leading to more coherent and robust image segmentation outcomes. The overall practical impact of this transformation is to shrink the object whose remaining pixels are then used for further analysis (Figure 1.17c). One can imagine such methods being applied to the analysis of high-throughput catalyst screening samples.

1.3.1.3 Neural Networks for Identifying Glassware

While case-specific edge detection, object recognition, and segmentation approaches are established aplenty in computer vision, the identification of myriad variations on chemistry glassware and its multiphase contents represents a notable challenge in chemistry-focused computer vision applications. In 2020, the Eppel and Aspuru-Guzik groups collaboratively released an approach to this problem, and in so doing provided an ideal exemplar of using CNNs in chemistry-centered computer vision [17].

CNNs are a class of deep learning models specifically designed for and trained on tasks involving image analysis and computer vision. They are inspired by the organization of the animal visual cortex, where individual neurons respond to stimuli only in their receptive fields, allowing for hierarchical feature extraction. In CNNs, convolutional layers perform feature extraction by applying a set of learnable filters (kernels) to input training images, first discussed in Section 2.2.3 (Figures 1.13 and 1.14). These filters detect various features such as edges, textures, and patterns, preserving spatial relationships through weight sharing and parameter sharing. Pooling layers then down sample the feature maps, reducing computational complexity and helping the network become more robust to translation and distortion invariance. Through multiple convolutional and pooling layers followed by fully connected layers, CNNs can learn hierarchical representations of visual data, enabling them to perform the likes of the object and chemical phase detection tasks reported by the Eppel and Aspuru-Guzik groups. The fundamental connectivity of a deep neural network and the distinct elements of CNNs are shown in Figure 1.19.

Using a labeled library of 2187 images of reaction vessels containing different colors and phases of material, the team employed several different CNNs to investigate how best to segment the reaction vessel from the material within. It is worth noting that the image library used for training in this case was relatively small, especially compared to available training libraries like ImageNet, which, at the time of writing, contains over 14 million openly available training images [18]. Among the methods tested was the R-Mask CNN approach [19]. An R-mask CNN (region-based mask convolutional neural network) is a type of CNN architecture specifically designed for semantic segmentation tasks in computer vision. It combines the

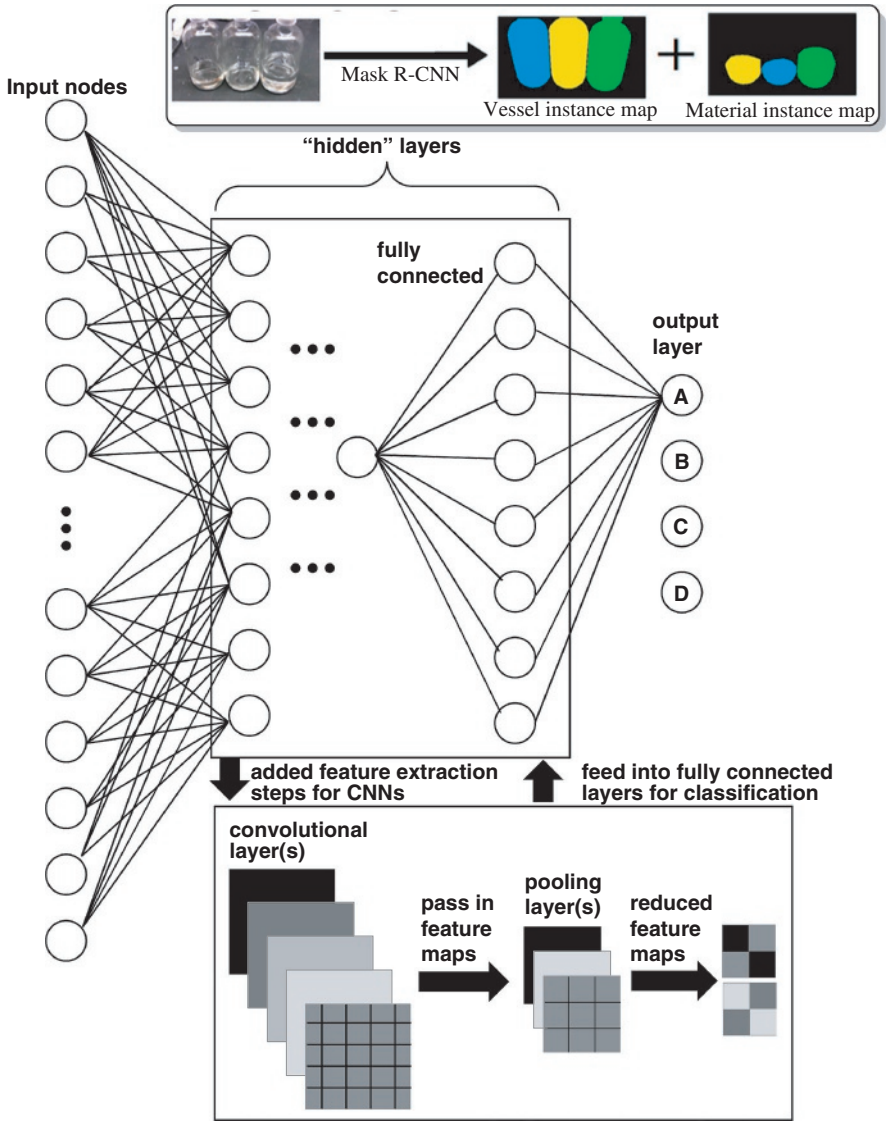

Figure 1.19 An overview of deep neural networks and the layers through which CNNs represent a strategic architecture for the analysis of grid-like or image-based input data. Inset: An example of the output segmentation of liquid from the vessel, published by Aspuru-Guzik. Reproduced with permission from [17]/American Chemical Society.

strengths of region-based convolutional neural networks (R-CNNs), which are adept at object localization, and mask-based CNNs, which excel at pixel-level segmentation. In R-Mask CNNs, the network first generates region proposals using techniques like selective search or region proposal networks (RPNs). Then, for each region proposal, the network simultaneously predicts the class label and generates a binary mask indicating the object's presence at the pixel level. This allows for accurate object detection and precise segmentation in images, making R-Mask CNNs

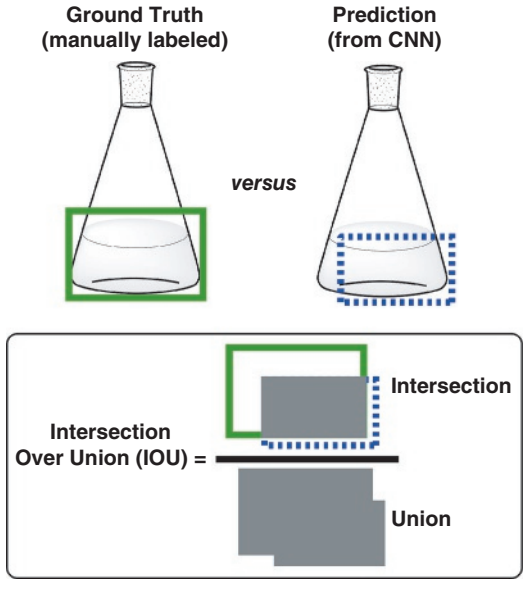

Figure 1.20 A visual representation of the IOU evaluation metric is applied to understanding CNN performance versus human-labeled definitions of object detection.

particularly suitable for tasks such as instance segmentation, where distinguishing between individual object instances is crucial.

Based on the chosen scoring systems of the CNNs applied, it was found that segmentation between the vessel and a solid or liquid material inside was higher scoring than more granular segmentation of multiphase systems (e.g., liquid vs. foam). Indeed, this point helps exemplify a broader point of importance when considering CNNs and ML for image analysis. CNNs can make various types of errors in predictions, such as false positives (where the model incorrectly identifies a pattern or feature as present) and false negatives (where the model fails to identify a pattern or feature that is present). These errors are manifested in predicted values versus actual values, often expressed as metrics like mean squared error (MSE) or root mean squared error (RMSE). In the Eppel and Aspuru-Guzik study [17], the more CNN-focused evaluation metric known as intersection over union (IOU) was applied (Figure 1.20). The roots of errors in CNNs can include the likes of overfitting, which occurs when the CNN model learns noise or irrelevant details from the training data, leading to poor generalization of new data. Conversely, if the CNN model is too simple, it may not capture the complexity of the chemical data, leading to high bias and systematic errors. Additionally, errors can arise if the training data (in this case, labeled images) contains noise, mislabeled samples, deliberate adversarial manipulation [20], or is not representative of the broader chemical space. Having said this, if errors themselves can be quantified, they can be used as an additional model parameter to help improve CNN performance [21].

Such single image-based applications of computer vision are far more broadly precedented than is detailed here [7, 22–24]. However, going beyond images into the domain of video analysis represents a relatively more opportune and underdeveloped area for catalysis and ML. This brings us to the final application-focused section of this chapter.

1.3.2 Video Analysis Applications

When we move from analyzing static images to dynamic video data, we build in the dimension of time, opening ML opportunities in time series analysis for reaction monitoring, mechanistic analysis, and a more characteristic level of problem diagnosis than is possible from single image inputs.

1.3.2.1 Phase Separation and Partition Coefficients

An emerging area of time-resolved computer vision for chemical interests in analyzing the dynamic nature of biphasic mixtures used in separation and purification strategies [25–27]. From a catalysis perspective, such efforts are of potentially high value in processes like metal scavenging during post-catalytic reaction clean-up [28].

An illustrative example of such analysis, revealing several key features of computer vision methodology in a chemistry context, was reported by Kapur's team and industrial collaborators in 2023 [25]. Here, the team set up a monochrome camera to capture grayscale video frames over time (1 FPS) and used these data to analyze layer heights in biphasic mixtures. The chemical composition of the mixtures was designed to represent common aqueous/organic liquid–liquid combinations, generating visibly separate layers over a range of time periods or, in extreme cases, generating stable emulsions that never settle into a visible bilayer. A key feature employed in the early steps of the algorithms included a low-pass filter to smooth (or blur) the raw grayscale image frame to remove high-frequency noise prior to more in-depth analysis. More specifically, the primary purpose of the low-pass finite impulse response (FIR) filter used is to allow low-frequency components of a signal to pass through while reducing the amplitude of the high-frequency components [29]. The FIR filter processes the input grayscale image by performing a convolutional operation similar to the one introduced in Section 2.2.3 (Figures 1.13 and 1.14). When you apply this filter to a grayscale image, each pixel in the output image is the average of the corresponding pixel in the input image and its neighbors. The output image appears smoother because the high-frequency components (sharp edges and noise) are reduced. Fine details and sharp transitions are blurred. While fine details are smoothed out, the overall structure and low-frequency components of the image (such as larger regions and gradual transitions) will be preserved.

With the use of the FIR filter, the team was then able to provide a rare example of using the first, second, and third derivatives of the smoothed grayscale image frame to help extract the sediment and cream phase fronts. These derivatives, with respect to pixel coordinates, provide important information about the changes in intensity values and highlight edges in the image via abrupt changes in intensity. High values of the first derivative, therefore, indicate the presence of edges. The magnitude of the gradient gives the strength of the edge, and the direction of the gradient indicates the orientation of the edge. The second derivative of a grayscale image measures the rate of change of the first derivative and provides information about the curvature of the intensity surface. Points where the second derivative changes sign indicate potential edges. These so-called zero-crossings are used in edge detection problems, as exemplified in Kapur's time-resolved detection of bilayers. The same second derivative can enhance the edges detected by the first derivative, making them more prominent.

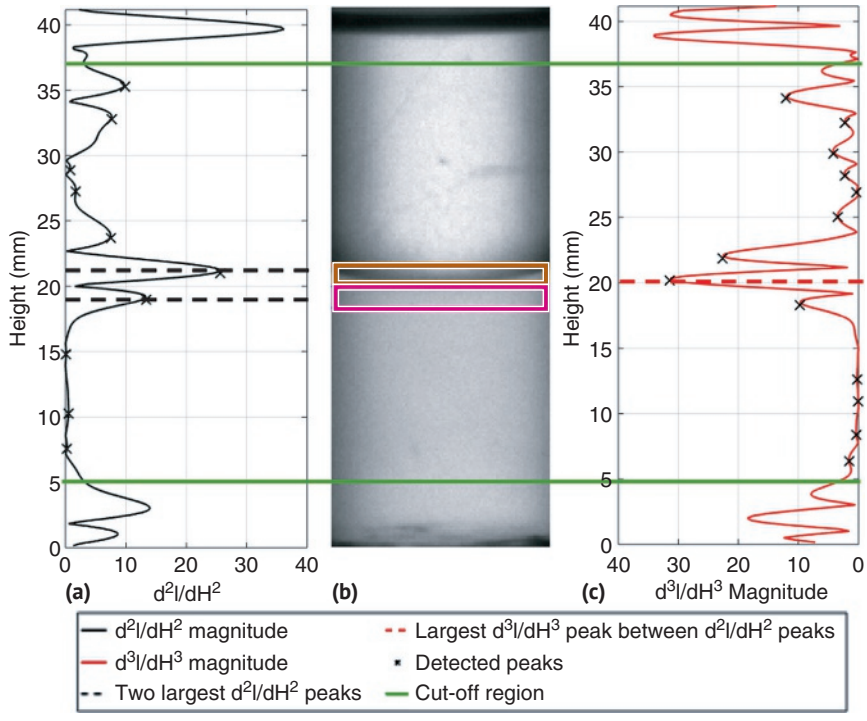

Figure 1.21 From Ref. [25], second (left) and third (right) derivative plots of grayscale gradient across the central image of a biphasic mixture. In the image, the bound boxes represent regions identified by the second derivative. The intersection of these areas is highlighted by a peak in the third derivative. [58]/Elsevier/CC BY 4.0.

The more rarely applied third derivative of the grayscale image measures the rate of change of the second derivative. While it is less commonly used in basic image processing tasks, it provides information about higher-order changes in intensity. Points where the third derivative changes sign can indicate inflection points in the intensity profile (Figure 1.21). In this case, Kapur was able to use the second derivative of the final video frame to locate positions near the interface within each of the two layers. The third derivative provided the reassuring location of the interface, between the positions found by the second derivatives of the top and bottom layers.

Each derivative order provides different levels of detail and can be used for various image processing tasks, from basic edge detection to more complex feature extraction and analysis. Consistent with earlier discussion on high-throughput methods, Kapur's team also made limited but promising attempts to use their method of monitoring phase separation dynamics in high-throughout developing a rig on which multiple biphasic samples could be mixed before being recorded using the monochrome camera chosen by the team. In relation to the introductory discussion on photography, it is worth noting that the monochrome camera is grayscale by its nature, without intermediate conversion of any RGB data to a linearized grayscale format. In other words, no Bayer (or other RGB) filter is applied before the incoming light is focused on the image sensor. Such cameras can be useful when higher sensitivity is needed, while color information is not.

1.3.2.2 Reaction Kinetics

From reaction monitoring [30] to solubility testing [31] and chemical networking [32], the use of video as an input data source for kinetic analysis via computer vision and ML is, at the time of writing, a growing trend.

In this author's team's efforts to develop time-resolved computer vision for reaction monitoring, including applications in catalysis, a necessary challenge in time series analysis presented itself. Namely, to understand the level of agreement between highly time-resolved imaging data from videos of reaction bulk and comparatively more sparse time series data collected from samples taken from the same reaction mixture for offline, more molecularly specific analyses (e.g., NMR, HPLC). In doing so, a ML approach was required such that any probable correlations between imaging and more established analytics could be determined without necessarily assuming whether any resulting model should be linear or otherwise.

To this end, mutual information (M.I.) analysis, based on Claude Shannon's pioneering quantification of information theory, became a natural choice [33, 34]. Here, entropy is used as the measure of the uncertainty associated with a random variable. The more uncertain we are, the more we lack information, where information is the capacity to reduce uncertainty. If a data source has a lowprobability value, the event carries more "surprisal" than when the source data has high probability. Overall, M.I. is a measure of the mutual dependence between two variables. It quantifies the amount of information obtained about one variable through the other, thus serving as a powerful tool for identifying correlations in time series datasets. Mathematically, M.I. I(X;Y) between two variables, X and Y is defined according to Eq. (1.19):

$$\begin{aligned} I(X;Y) &= -\sum_{x\in X}\sum_{y\in Y} P(x,y)\ .\ log_2\left[\frac{P(x,y)}{P(x)\ .\ P(y)}\right] \\ &= P(x,y)\ .\ \{\ log_2[P(x,y)] - log_2[P(x)\ .\ P(y)\ ]\} \end{aligned} \tag{1.19}$$

where $P(x,y)$ is the joint probability distribution of X and Y, and $P(x)$ and $P(y)$ are the marginal probability distributions of X and Y, respectively. A higher M.I. value indicates a stronger dependency between the variables, making it especially useful in analyzing the relationships and dependencies within multiple time series datasets. By capturing both linear and non-linear relationships, M.I. provide a more comprehensive measure compared to traditional correlation coefficients. Some non-mathematical intuition for the M.I. approach is provided in Figure 1.22.

One way to estimate marginal probability is the histogram approach (Figure 1.21a and Eq. 1.20). The marginal probabilities to be summed are then the frequency counts falling within each histogram bin divided by the total number of samples (i.e., elements in the time series array).

$$P(x_i) = \frac{no.\ elements\ in\ bin}{total\ no.\ elements\ in\ series} \tag{1.20}$$

If there are 10 histogram bins, the i ranges from 1 to 10. The process repeats for the number of supposedly independent features to be compared. After calculating the entropy for each feature, one can then look to understand the information available in one feature when another feature is given. This is where joint entropy (Eq. 1.21) comes in.

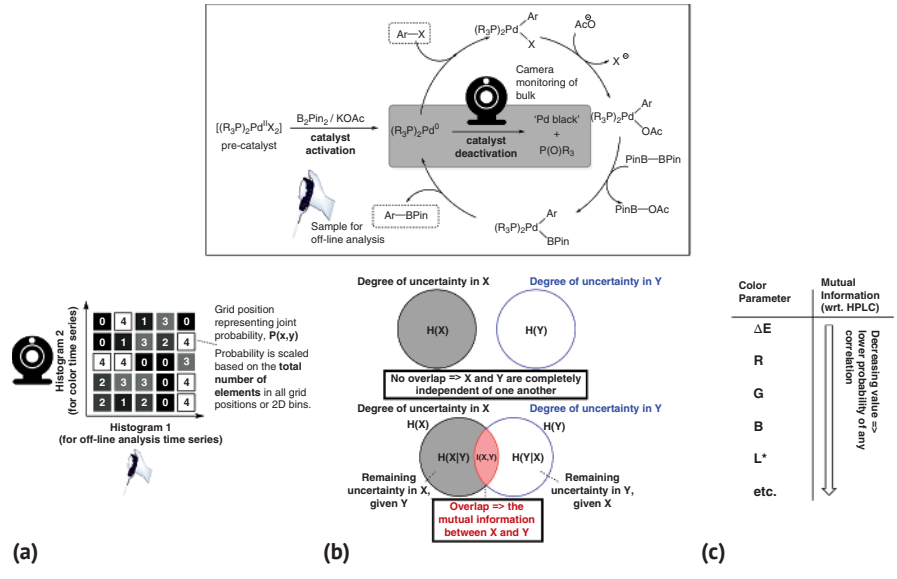

Figure 1.22 Top: A mechanistic representation of the Miyaura borylation, highlighting processes and analytes for which a combined monitoring approach employing cameras and HPLC analysis was employed. (a) A histogram approach to working out joint probabilities of occurrences from the independent computer vision and time series datasets. (b) A Venn diagrammatic overview of calculating M.I., I(X;Y). Part C: The practical output of a table showing a ranked order of color parameters that are decreasingly likely to correlate – linearly or otherwise – with the ground truth concentration data from HPLC.

The joint entropy of discrete random variables X and Y is the entropy of their pairing, H(X;Y). By the same chord, we now need to consider joint probability, $P(x_i, y_i)$, instead of marginal probability.

$$H(X,Y) = -\sum_{x \in X} \sum_{y \in Y} P(x,y) \; . \; log_2 [P(x,y)] \tag{1.21}$$

As a means of building intuition, (X,Y) could represent the position of a chess piece. X stores the row position, Y stores the column position. The entropy of the row of the piece and the entropy of the column of the piece come together to represent the entropy of the position of the piece. To estimate the joint probabilities, we can use 2D instead of 1D histograms. Each 1D histogram composing the 2D histogram can come from two "independent" features (Eq. 1.22).

$$P(x,y) = \frac{no.\ elements\ in\ 2D\ grid\ position}{total\ no.\ elements\ in\ the\ 2D\ grid} \tag{1.22}$$

Taking all of this toward an understanding of the M.I. held between two features or variables requires a Venn diagram visualization of the entropies thus far formulated (Figure 1.20). In reading these Venn diagrams:

- As overlap increases, the amount of shared information between X and Y increases. It does NOT mean there is any additional transfer of information between X and Y.

- When the M.I. is expressed using a *comma* between X and Y, it assumes the sizes of X and Y are the same. It also assumes we are only considering two features, X and Y. For example, X could be an array of HPLC samples over time. Y could be the subset of color data at the same time points as HPLC samples, making arrays X and Y the same size.
- The use of a semicolon is more general (e.g., for conditional M.I. involving more than two features). The semicolon denotes everything that is to be measured (left) given everything known (right).

Using this approach, it has been possible to rank order 10+ color parameters, collected and calculated with computer vision methods, in terms of their likely correlation with offline measures of product concentration by NMR and HPLC. Applications include the determination of reaction progress for the above-mentioned tracking of successful versus compromised Pd-catalyzed borylations [30], large-scale S_NAr reactions [10], and solid-phase peptide synthesis [35].

1.4 Summary and Conclusion

From a chemist's perspective, the field of computer vision is one of intriguing contradictions. On the one hand, it is a rapidly maturing field, with otherworldly applications developed for self-driving cars, factory robotics, drones and satellites, and cybersecurity. On the other hand, such sophisticated developments are surprising when they are compared to the relative infancy of computer vision applied to chemical analysis. This point is further emphasized when considering the near absence of any literature attending ML, computer vision, and catalysis.

In this chapter, we have considered selected illustrative examples of cameras being used to capture various visually characterizable chemical phenomena. Whether via single image or video, the availability of the singularly large datasets represented by arrays of pixels represents inordinate opportunities for the application and development of chemically intelligent ML applications.

Fueled by the wealth of transferable ML architectures and ever-increasing computing power available, it is envisaged that an increased number of video-focused computer vision applications will be realized for catalysis and computer vision. In the context of ML, the case studies shared show that, in the field of computer vision, much of the learning has as much to do with the machine (or camera) you choose as it does with the algorithms we more commonly associate with the term "machine learning."

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