

BAYESIAN MODELLING TO PREDICT PROPERTY SPECTRUM**Technical Field**

[0001] The present disclosure relates to the use of Bayesian modeling to predict a property spectrum associated with a chemical.

Background

[0002] Spectroscopy is the field of study that measures and interprets electromagnetic spectra that result from the interaction between electromagnetic radiation and matter as a function of the wavelength or frequency of the radiation. Spectroscopy has applications in many fields, such as medicine, physics, chemistry, and astronomy.

[0003] Chemical producers may use process monitoring equipment in plants to make decisions. The sensors associated with the equipment may use simple physical property inputs (e.g., dielectric constant or electrical conductivity) to make binary measurements and then turn on pumps to alter a tank level or chemical reaction. Sensors can also use spectroscopies or chromatographies to monitor chemistry and physics, such as concentration, catalyst efficiency, etc.

Summary of the Disclosure

[0004] The present disclosure relates to the use of Bayesian modeling to predict a property spectrum associated with a chemical. Measurement of a property associated with a chemical can be initiated over a range of frequencies or wavelengths. As used herein, “a property associated with a chemical” can include any of a property of a chemical reaction, a property of a chemical product, a property of a catalyst, and a property of a reactant. Data collected from the measurement can be modeled recursively, via Bayesian modeling, to an expected property spectrum thereby yielding a predicted property spectrum before completion of the measurement over all of the range of frequencies or wavelengths. A peak in the predicted property spectrum can be predicted and a probability of the peak can be calculated recursively before completion of the measurement over all of the range of frequencies or wavelengths. The measurement can be stopped before completion thereof over all of the range of frequencies or wavelengths in response to the probability being greater than a threshold value.

[0005] Embodiments described herein can allow simple sensors, such as those that measure dielectric constant or conductivity, to be used to monitor chemistry and can allow more complicated sensors to be used to make more accurate decisions faster without input from an experienced user. Such techniques can be useful to predict a peak of the property spectrum without having to measure all points of the property spectrum, thereby saving time and expense. Such techniques can be useful to make decisions (automated or otherwise) in a chemical plant process.

[0006] The above summary of the present disclosure is not intended to describe each disclosed embodiment or every implementation of the present disclosure. The description that follows more particularly exemplifies illustrative embodiments. In several places throughout the application, guidance is provided through lists of examples, which examples can be used in various combinations. In each instance, the recited list serves only as a representative group and should not be interpreted as an exclusive list.

Brief Description of the Drawings

[0007] Figure 1 is a prior art graph of a property spectrum.

[0008] Figure 2A is a graph of a posterior predicted property spectra density after measurement of a property associated with a chemical at two data points.

[0009] Figure 2B is a graph of a posterior predicted property spectra density after measurement of the property at twenty data points.

[0010] Figure 2C is a graph of a posterior predicted property spectra density after measurement of the property at thirty data points.

[0011] Figure 3A is an Arrhenius plot of the glass transition of a chemical based on a measurement of a property spectrum of the chemical.

[0012] Figure 3B is a graph of time to collect each data point for the measurement associated with Figure 3A.

[0013] Figure 4 is a block diagram of a system for Bayesian modeling to predict a property spectrum.

[0014] Figure 5 is a block diagram illustrating an example of a method for Bayesian modeling to predict a property spectrum.

[0015] Figure 6 is a block diagram of a machine within which a set of instructions, for causing the machine to perform various methodologies discussed herein, can be executed.

Detailed Description

[0016] The present disclosure relates to the use of **Bayesian** modeling to predict a property spectrum associated with a chemical. Examples of a property spectrum include a spectrogram, spectrograph, thermogram, etc. Spectroscopy can be used to measure and interpret the property spectrum. Examples of spectroscopy include dielectric spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, ultraviolet-visible (UV-vis) spectroscopy, and Fourier-transform infrared (FTIR) spectroscopy, among others.

[0017] Dielectric spectroscopy, which is a type of impedance spectroscopy, measures the dielectric properties of a medium as a function of frequency based on the interaction of an external field with the electric dipole moment of a sample. Dielectric spectroscopy can be used to measure permittivity and/or impedance. Dielectric spectroscopy can be used to investigate the quality of coatings and to detect the presence of corrosion. For heterogeneous mixtures like suspensions, impedance spectroscopy can be used to monitor the particle sedimentation process. One example of dielectric spectroscopy is broadband dielectric spectroscopy (BDS), which covers a broad frequency range (e.g., from microhertz to gigahertz).

[0018] NMR resonance spectroscopy is a chemical analysis technique to observe local magnetic fields around atomic nuclei. A sample is placed in a magnetic field and an NMR signal is produced by excitation of nuclei with radio waves into nuclear magnetic resonance, which is detected with radio receivers. The intramolecular magnetic field around an atom in a molecule changes the resonance frequency, thus giving access to details of the electronic structure of a molecule. NMR spectroscopy can be used to identify monomolecular organic compounds and functional groups because the fields are highly characteristic to individual compounds.

[0019] UV-vis spectroscopy, which is a type of absorption spectroscopy, involves shining a monochromatic beam of light at a sample and measuring how much of that beam is absorbed by the sample. This process is repeated at different wavelengths of light to obtain a spectrum. UV-vis spectroscopy can be used in analytical chemistry for quantitative determination of diverse analytes, highly conjugated organic compounds, and biological macromolecules.

[0020] FTIR spectroscopy, which is a type of absorption spectroscopy, is a technique used to obtain an infrared spectrum of absorption or emission of a solid, liquid, or gas by collecting high resolution spectral data over a wide spectral range. As opposed to UV-vis spectroscopy, FTIR spectroscopy involves shining a beam containing many frequencies of light at once and measuring how much of that beam is absorbed by the sample. In FTIR spectroscopy, each data point is collected using a different combination of frequencies generated by shining a broadband light source into a configuration of mirrors (a Michelson interferometer), where one of the mirrors is moved by a motor to generate wave interference (periodically blocked wavelengths). A Fourier transform is used to convert the raw data into a spectrum by converting displacement of the mirror into wavenumbers. FTIR spectroscopy can be used to obtain spectra from compounds as they are separated by gas chromatograph. FTIR spectroscopy can be used to determine water content in thin plastic and composite parts.

[0021] Figure 1 is a prior art graph of a property spectrum. The property spectrum illustrated in Figure 1 is generically representative of a property spectrum obtained, for example, from dielectric spectroscopy. The lower horizontal axis indicates the frequency 104 in Hertz (Hz) over which the data points in the graph were collected. The upper horizontal axis indicates the time required to collect a single data point at each frequency. The units for time are generally seconds, although milliseconds (ms) and microseconds (μ s) are labeled on the upper horizontal axis. Both the upper and lower horizontal axes are presented logarithmically. The vertical axis indicates a value of the measured property 102, which in this example is dielectric loss.

[0022] As indicated on the graph, data points are generally collected in order from those at higher frequencies to those at lower frequencies. It takes less time to capture data points at higher frequencies than lower frequencies. Some spectroscopic analytical techniques require tens of minutes in order to collect a single spectra. For example, each data point in BDS uses at minimum a full sine wave at the frequency of interest. On a logarithmic horizontal axis, the time becomes exponentially longer at lower frequencies.

[0023] The spectrum includes a peak 105 near a middle of the measurement range. In many spectroscopic techniques, the position and height of the peaks 105 are used to make decisions or track concentrations in a process. In BDS, the position of a peak 105 is directly related to the speed of a rotating dipole. This rotation speed can be related to the viscosity or

temperature of the system, the size of the dipole, and the interactions of the dipole with its surrounding environment. The size of the peak 105 is related to the concentration of the dipole, and thus will reduce due to chemical changes (e.g., reacting away) or physical changes (e.g., crystallization of the dipole preventing rotation) in the system. Some previous approaches may use the position and size of a peak 105 to track processes via BDS, but only for very slow processes (e.g., $\sim 10^5$ seconds per data point). This is because a full BDS spectrum takes tens of minutes to collect, and thus any chemistry occurring faster than this would not be observable.

[0024] Arguably, the points on the left portion of the graph that were collected last may not have been necessary, particularly if the goal was to determine the peak 105 of the spectrum. Furthermore, the points on the left side of the graph required the most time to determine and are therefore the costliest to obtain. In chemical processing, wasted time is expensive.

[0025] At least one embodiment described herein addresses the above and other deficiencies by measuring only an initial portion (e.g., the first few seconds; only a portion of the range of frequencies or wavelengths intended to be measured) of a property spectrum and then predicting where the peak 105 will occur. Although dielectric spectroscopy, and particularly BDS, is used as an example herein, embodiments are not limited to a particular spectroscopic technique.

[0026] Some previous approaches may use databases of modeled spectra to predict the behavior of a new, unknown sample. The use of Bayes' Theorem to model complicated spectra according to some previous approaches may take tens of minutes at best. Furthermore, such approaches are not aimed at stopping the measurement early, but instead are aimed at modeling all of the data once captured. Such previous approaches are not used in real time as the data is captured for analysis, prediction, and decision making.

[0027] As used herein, the singular forms "a", "an", and "the" include singular and plural referents unless the content clearly dictates otherwise. For example, "predicting a peak" means "predicting one or more peaks". Furthermore, the word "may" is used throughout this application in a permissive sense (i.e., having the potential to, being able to), not in a mandatory sense (i.e., must). The term "include," and derivations thereof, mean "including, but not limited to." The term "coupled" means directly or indirectly connected and, unless stated otherwise, can include a wireless connection.

[0028] As will be appreciated, elements shown in the various embodiments herein can be added, exchanged, and/or eliminated so as to provide a number of additional embodiments of the present disclosure. In addition, as will be appreciated, the proportion and the relative scale of the elements provided in the figures are intended to illustrate certain embodiments of the present invention and should not be taken in a limiting sense.

[0029] The figures herein follow a numbering convention in which the first digit or digits correspond to the drawing figure number and the remaining digits identify an element or component in the drawing. Similar elements or components between different figures may be identified by the use of similar digits. For example, 438 may reference element “38” in Figure 4, and a similar element may be referenced as 638 in Figure 6. Analogous elements between different figures may be referenced with a hyphen and extra numeral or letter. See, for example, elements 208-1, 208-2, and 208-3 in Figures 2A, 2B, and 2C respectively. Such analogous elements may be generally referenced without the hyphen and extra numeral or letter. For example, elements 208-1, 208-2, and 208-3 may be collectively referenced as 208. As will be appreciated, elements shown in the various embodiments herein can be added, exchanged, and/or eliminated so as to provide a number of additional embodiments. In addition, as will be appreciated, the proportion and the relative scale of the elements provided in the figures are intended to illustrate certain embodiments of the present invention and should not be taken in a limiting sense.

[0030] Figure 2A is a graph of posterior predicted property spectra density 216 after measurement of a property 202 of a chemical at two data points 214. The lower horizontal axis indicates the frequency 204 on a logarithmic scale in Hz over which the data points in the graph were collected or were intended to be collected (e.g., from 10 mHz (“-2”) to 6 MHz (“6”)). The unfilled dots 212 represent predicted data that has not yet been observed, which may be referred to as all data. The filled dots 214 represent observed or measured data. In Figure 2A there are two filled dots 214 starting on the right side of the horizontal axis at the relatively higher frequency 204 (e.g., approximately 1 MHz in this example). The upper horizontal axis is the same as the lower horizontal axis. The left vertical axis indicates a value of the measured property 202, which in this example is dielectric loss. The right vertical axis is the same as the left vertical axis. The posterior predicted property spectra density 216 is illustrated as a plurality of predictions where the line darkness is weighted by the probability (more probable predictions

are darker). There are so many that they cannot be seen individually. The darker shading represents a greater concentration of predicted property spectra 216, the lighter shading represents a lesser concentration of predicted property spectra 216. There are a few very faint individual predicted property spectra 216 that are visible rising above the darker and lighter shaded areas. In the examples of Figures 2A-2C, data is collected at -49.0 degrees Celsius.

[0031] The additional plot on top labeled “density” illustrates kernel density estimations of priors 218 (solid line) and posteriors 220 (dashed line). The top density plot represents the probability of the horizontal location of the predicted peak 206. The additional plot on the right, labeled “density” illustrates kernel density estimations of priors 218 (solid line) and posteriors 220 (dashed line). The right density plot represents the probability of the vertical height of the predicted peak 206. The priors 218 represent a prior probability and the posteriors 220 represent a posterior probability as described in more detail below.

[0032] Bayesian modeling can be used to predict a spectrographic peak 206 before all of the data 212 has been collected. If the confidence in the peak 206 is acceptable (within a threshold value), the program terminates data collection and then uses the probable peak 206 to make a decision regarding the state of the process. More specifically, the position 208 and/or height 210 of the peak 206 can be predicted using Bayesian modeling.

[0033] Bayesian modeling is a method of statistical inference in which Bayes’ theorem is used to update the probability for a hypothesis as more data becomes available. Bayesian modeling may be useful in the dynamic analyses of a sequence of data, such as measurement of a property spectrum associated with a chemical over a range of frequencies or wavelengths. Bayesian modeling derives a posterior probability 220 as a consequence of two antecedents: a prior probability 218 and a likelihood function derived from a statistical model for the observed data. The posterior probability 220 can be computed according to Bayes’ theorem:

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

where H stands for any hypothesis whose probability may be affected by data. P(H) is the prior probability 218, which is the estimate of the probability of the hypothesis H before data E 214 is observed. Observed data E 214 is the data that is observed and used to compute the probability. P(H | E) is the posterior probability 220, which is the probability of any hypothesis H being correct given observed data E 214. P(E | H) is the probability of observing data E given prior

hypothesis H, which is referred to as the likelihood. P(E) is the marginal likelihood, which is a likelihood function representing the probability of generating observed data from a prior.

[0034] In some embodiments, the property spectrum can be modeled via the Havriliak-Negami equation, which was developed for empirically modeling polymer rheological data:

$$\epsilon^* = \epsilon_\infty + \sum \frac{\Delta\epsilon}{(1 + (j\omega\tau)^a)^b}$$

where ϵ^* is the permittivity, ω is the angular frequency, and j is $\sqrt{-1}$. ϵ_∞ , τ , $\Delta\epsilon$, a , and b are empirically derived constants for each individual peak. ϵ_∞ is the permittivity at the high frequency limit, τ is the characteristic relaxation time of the medium, $\Delta\epsilon = \epsilon_s - \epsilon_\infty$, where ϵ_s is the static, low frequency permittivity, a and b describe the asymmetry and broadness of the corresponding spectra. The empirically derived constants are each related to a specific property of interest. Table 1 includes empirical values from the Havriliak-Negami equation, what they relate to in the system, and justification for the priors.

Table 1

Empirical Value from the Havriliak-Negami Equation	Relates to	Typical Values for Priors	Justification for Priors
τ	Rotational speed of the dipole, referred to as the relaxation time	1 nanosecond – 10 minutes, normally distributed on a log scale.	Constrains the peak to the measurement range.
$\Delta\epsilon$	Concentration of free-to-rotate dipoles	0 – 40, weighted to values less than 1.	This covers the range from zero to pure water but skews toward hydrocarbons.
a	Breadth of the peak due to the imperfect uniformity of real-world dipoles of different types (e.g. polymer molecular weight distribution (MWD))	0 – 1, uniformly distributed.	Defined by the equation.
b	Breadth of the peak due to the imperfect uniformity of real-world dipoles of different types (e.g. polymer MWD)	0 – 1, uniformly distributed.	Defined by the equation.

ϵ_{∞}	Polarizability of the electron cloud of the dipole	0 – 3, normally distributed.	This covers materials of interest.
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[0035] The existing data can be modeled to the Havriliak-Negami equation using Bayes’ Theorem. The model provides a statistical probability that the peak location (τ) and size ($\Delta\epsilon$) are any given value, which in turn gives the operator measurable confidence in the general location of the peak. The constants a , b , and ϵ_{∞} are used to find the other two values but are otherwise not used, so it is not imperative that they are correct. The probable location of the peak can be used to make a decision based on prior knowledge about the expected position of the peak given the particulars of the chemistry/physics being monitored. For example, the catalyst might be deactivating and more should be added to the reactor. As another example, the viscosity could be increasing, which could lead to fouling, and thus the temperature should be adjusted accordingly. Other variables that may be adjusted based on the probable location of the peak include catalyst concentrations, reactant concentrations, product concentrations, pressure, mixing conditions, etc. The entire automated modeling then repeats itself, giving readings every several seconds with a computational cost well within the specifications of a laptop computer.

[0036] Using Bayesian modeling (inference), the probability $P(H | E)$ for any given model to the data can be calculated. The distribution of all weighted probabilities can be used to calculate a posterior histogram 220, for example, to predict the position of the peak 206-1. The Bayesian model can be used to model data as it is collected in real time as each additional data point is collected. The model may use earlier measurements to optimize the priors $P(H)$ and calculate the posterior prediction via a considered likelihood given the current data and adjusted priors accordingly. The model does not require user input during any part of the analysis. After collecting only two data points 214, the confidence in the peak location 208-1 and peak height 210-1 is very low as represented by the broad range of the posterior plots 220 illustrated by the dashed lines in the density plots. This indicates that more data points 214 need to be observed.

[0037] In each iteration, Bayesian modeling can make many predictions and calculate the probability of each prediction being correct with respect to possible predictions (e.g., all possible predictions). The predictions are not random, but are based on priors. Each prediction includes a respective prediction for the empirical variables (e.g., ϵ_{∞} , τ , $\Delta\epsilon$, a , and b). The predictions can be weighted by the probability. Each variable can be plotted against its probability to provide a

histogram centered on the predictions that are in the realm of the correct result. Neither an exactly correct prediction nor more correct predictions than incorrect predictions are necessary because predictions that are relatively more correct are weighted more heavily than predictions that are relatively less correct. A kernel density estimation can change a bar graph-type histogram into a smooth curve, such as is illustrated in Figures 2A-2C in the top and right graphs (labeled “density”). Statistical methods (e.g., mean, median, standard deviation, etc.) can be applied to the histogram to determine the most likely value for a respective variable.

[0038] Figure 2B is a graph of a posterior predicted property spectra density 216 after measurement of the property 202 at twenty data points 214. In Figure 2B there are twenty filled dots 214 starting on the right side of the horizontal axis at the relatively higher frequencies 204. The posterior predicted property spectra density 216 is illustrated as a plurality of predictions. As compared to Figure 2A, the density of posterior predicted property spectra 216 is much narrower with only a few individual stray posterior spectra being visible. However, as compared to Figure 2A, the width of the posterior distributions 220 are still unacceptably large and the confidence is not within the user-defined preset threshold value. Although indicating an increased confidence in the prediction, more data points 214 should be observed.

[0039] Figure 2C is a graph of a posterior predicted property spectra density 216 after measurement of the property 202 at thirty data points 214. In Figure 2C there are thirty filled dots 214 starting on the right side of the horizontal axis at the relatively higher frequency 204. The posterior predicted property spectra density 216 is illustrated as a plurality of predictions. As compared to Figure 2B, the concentration of predicted property spectra 216 is much narrower with essentially zero individual stray posterior spectra being visible. The predicted peak 206-3 is much easier to identify due to the greater concentration of predicted property spectra 216. As compared to Figure 2B, the width of the posteriors 220 has decreased significantly, indicating an increased confidence in the prediction. This confidence is now within the user-defined preset threshold value and indicates that no more datapoints 214 need to be observed and the measurement may terminate early.

[0040] Figure 3A is an Arrhenius plot of a glass transition of a chemical based on a measurement of a property spectrum of the chemical. The lower horizontal axis indicates the inverse of temperature. The values 4.1 to 4.7 are shown, where the units are inverse of degrees in Kelvin times 1000 ($1000 \cdot K^{-1}$). The upper horizontal axis indicates the temperature in degrees

Celsius. The vertical axis indicates a value of the characteristic relaxation time (rate) on a logarithmic scale. In this example, the vertical axis represents the property being measured via dielectric spectroscopy, represented as τ . The Vogel-Fulcher-Tammann (VFT) equation correlates rate and temperature:

$$\tau(T) = Ae^{\frac{-B}{T-T_v}}$$

where k is the temperature-dependent rate, T is the absolute temperature, and A , B , and T_v are empirical constants. In some experiments, $T_v = 0$. In this case, the VFT equation becomes the Arrhenius equation, where B equals $E_a \cdot R^{-1}$ (E_a is the activation energy, R is the universal gas constant, and A is the Arrhenius preexponential factor). The slope of the Arrhenius plot can therefore be used to find the activation energy. The plot can be extrapolated back to the vertical axis to obtain a value of the pre-exponential factor. The data points are plotted as dots with error bars to indicate uncertainty in the values, which in most cases is the user-defined preset threshold value from the Bayesian inference of the partial spectrum from the terminated measurement. The number of data points (including uncertainty) needed to acquire a good prediction of the values of the VFT or Arrhenius equations may also be determined by a continuous Bayesian inference model.

[0041] Figure 3B is a graph of time to collect each data point for the measurement associated with Figure 3A. The horizontal axis indicates temperature in degrees Celsius. The vertical axis indicates measurement time in minutes. The data points are plotted as dots representing the time it took to complete each measurement. The time to collect the full spectrum from 10 mHz to 1 MHz is indicated by the dashed line 322, which is about 25 minutes. However, according to at least one embodiment, the Arrhenius plot illustrated in Figure 3A can be predicted without measuring the full spectrum indicated by all of the data points in the plot of Figure 3B. In one measurement, the time used to acquire data and predict the plot of Figure 3A was seven times shorter than acquiring the full spectrum. Given the same amount of time, a researcher with the benefit of the present disclosure could acquire the same amount of data with one instrument as another without the benefit of this disclosure would with seven instruments.

[0042] Figure 4 is a block diagram of a system for Bayesian modeling to predict a property spectrum. The system can include a sensor 432 configured to measure a property associated with a chemical 430. Examples of the sensor 432 include a spectroscope, a concentration sensitive detector, a molecular weight sensitive detector, a composition sensitive

detector, or combinations thereof. Examples of concentration sensitive detectors include UV absorption, differential refractometer or refractive index detectors, infrared absorption, and density detectors. Examples of molecular weight sensitive detectors include low angle light scattering detectors and multiangle light scattering detectors. Examples of the analytical characterization methods include size-exclusion chromatography, liquid chromatography, gas chromatography, thermal gradient chromatography, calorimetry, rheology, optical spectroscopy, mass spectroscopy, viscometry, particle sizing, and nuclear magnetic resonance spectroscopy. The sensor 432 can be configured to generate series data 434 from sensing the property over a range of frequencies or wavelengths.

[0043] The system can include a controller 436 coupled to the sensor 432 and to other equipment that can control the chemical 430. The other equipment can be a control system for temperature, introduction of chemicals, and the like. The controller 436 can include a processor 438 and memory resources 440 storing instructions executable by the processor 438 to cause the controller 436 to perform the functions described herein. An example of the controller 436 is described in more detail with respect to Figure 6. The controller 436 can be configured to initiate measurement by the sensor 432 of a property associated with the chemical 430 over a range of frequencies or wavelengths. The controller 436 can receive signals indicative of the data 434 representing the property associated with the chemical 430 from the sensor 432.

[0044] The controller 436 can be configured to recursively model the data 434 to an expected property spectrum 444 using Bayesian modeling 442 before completion of the measurement over all of the range of frequencies or wavelengths. In some embodiments, the expected property spectrum can be based on the collected data 434 and other data collected before the measurement for an analogous chemical. In some embodiments, the expected property spectrum can be based on the collected data 434 and empirical modeling of the property spectrum 444 (e.g., based on the Havriliak-Negami equation). The controller 436 can be configured to model data 434 to the expected property spectrum 444 after the measurement at each frequency or wavelength at which the measurement has been conducted.

[0045] The controller 436 can be configured to recursively predict a peak 406 in the property spectrum 444 and calculate a probability 446 of the peak according to the data before completion of the measurement over all of the range of frequencies or wavelengths. The controller 436 can be configured to cause the sensor 432 to stop 450 the measurement before

completion thereof over all of the range of frequencies or wavelengths in response to the probability 446 being greater than a threshold value 448.

[0046] The controller 436 can be configured to output an indication of the predicted peak 406. Although not specifically illustrated, the indication can be output to a display and displayed to a user. In some embodiments, the output can be provided to the other equipment in order to facilitate the taking of further actions based on the predicted peak 406. The controller 436 can be configured to adjust 452 a reaction condition for the chemical 430 based on the probability 446 of the predicted peak 406 being greater than the threshold value 448. Examples of reaction conditions include catalyst concentrations, reactant concentrations, product concentrations, temperature, pressure, mixing conditions, etc. The output can be provided to a plant control room and the measurement/modeling can be repeated. The measurement can be stopped early, and a new sample or parameter can be measured.

[0047] Figure 5 is a block diagram illustrating an example of a method for Bayesian modeling to predict a property spectrum. The method may be performed, in some examples, using a computing system such as those described with respect to Figure 4. The method can be performed by processing logic that can include hardware (e.g., processing device, circuitry, dedicated logic, programmable logic, microcode, hardware of a device, integrated circuit, etc.), software (e.g., instructions run or executed on a processing device), or a combination thereof. In some embodiments, the method is performed by or using the controller 436 shown in Figure 4. Although shown in a particular sequence or order, unless otherwise specified, the order of the processes can be modified. Thus, the illustrated embodiments should be understood only as examples, and the illustrated processes can be performed in a different order, and some processes can be performed in parallel. Additionally, one or more processes can be omitted in various embodiments. Thus, not all processes are required in every embodiment. Other process flows are possible.

[0048] As illustrated at 560, the method can include initiating a measurement of a property associated with a chemical over a range of frequencies or wavelengths. The measurement can be initiated automatically or manually. Initiating the measurement can include initiating a series of measurements to be made at each of several discrete frequencies or wavelengths within the range of frequencies or wavelengths.

[0049] At 562, the method can include recursively modeling data collected from the measurement to an expected property spectrum using Bayesian modeling thereby yielding a predicted property spectrum before completion of the measurement over all of the range of frequencies. In some embodiments, recursively modeling data means that after the measurement at each frequency or wavelength at which the measurement has been conducted, the observed data is modeled to the expected property spectrum. In some embodiments, recursively modeling data means that after the measurement at each of a subset of frequencies or wavelengths at which the measurement has been conducted, the observed data is modeled to the expected property spectrum. This modeling is recursive because it repeats after each measurement or each subset of measurements.

[0050] At 564, the method can include recursively predicting a peak in the property spectrum and calculating a probability of the peak according to the data before completion of the measurement over all of the range of frequencies or wavelengths. Recursively predicting the peak can include predicting a plurality of peaks at each frequency or wavelength at which the measurement has been conducted. Recursively calculating the probability can include calculating a standard deviation of the plurality of peaks at each frequency or wavelength at which the measurement has been conducted. Predicting the peak can include predicting a magnitude of the predicted peak and a frequency or wavelength at which the predicted peak occurs.

[0051] At 566, the method can include stopping the measurement before completion thereof over all of the range of frequencies or wavelengths in response to the probability being greater than a threshold value. The measurement can be stopped manually or automatically. Stopping the measurement can mean that the property is measured at less than all of the discrete frequencies or wavelengths covering only a portion of the range of frequencies or wavelengths.

[0052] Although not specifically illustrated in Figure 5, the method can include starting a new measurement of a property associated with a different chemical after stopping the previous measurement. As such, the method can advantageously expedite operations in a chemical process by increasing the efficiency of measurements and decreasing the time required to complete them. The method can include initiating a new measurement of a property associated with the new chemical over the range of frequencies or wavelengths without completing the

measurement of the property associated with the previous chemical over the entire range of frequencies or wavelengths.

[0053] Although not specifically illustrated in Figure 5, the method can include outputting an indication of the predicted peak. The indication of the predicted peak can be a graphical representation, an indication of a value of the height of the peak, and/or an indication of the location of the peak, as described herein. The indication can be provided to a human operator and/or to other hardware components of a system in order to facilitate taking further actions based on the peak. For example, the method can further include adjusting reaction conditions based on the predicted peak. The adjustment can be manual or automatic. As another example, the method can further include adjusting a temperature for the chemical reaction based on the predicted peak.

[0054] Figure 6 is a block diagram of a machine 670 within which a set of instructions 680, for causing the machine 670 to perform various methodologies discussed herein, can be executed. Although not required for one or more embodiments of the present disclosure, the machine 670 can be connected (e.g., networked) to other machines in a LAN, an intranet, an extranet, and/or the Internet. The machine 670 can operate in the capacity of a server or a client machine in client-server network environment, as a peer machine in a peer-to-peer (or distributed) network environment, or as a server or a client machine in a cloud computing infrastructure or environment.

[0055] The machine 670 can be a personal computer (PC), a tablet PC, a set-top box (STB), a Personal Digital Assistant (PDA), a cellular telephone, a web appliance, a server, a network router, a switch or bridge, or any machine capable of executing a set of instructions (sequential or otherwise) that specify actions to be taken by that machine. Further, while a single machine 670 is illustrated, the term “machine” shall also be taken to include any collection of machines that individually or jointly execute a set (or multiple sets) of instructions to perform any one or more of the methodologies discussed herein.

[0056] The example machine 670 includes a processing device 638, a main memory 640 (e.g., read-only memory (ROM), flash memory, dynamic random access memory (DRAM) such as synchronous DRAM (SDRAM) or Rambus DRAM (RDRAM), etc.), a static memory 674 (e.g., flash memory, static random access memory (SRAM), etc.), and a data storage system 676, which communicate with each other via a bus 682.

[0057] The processing device 638 represents one or more general-purpose processing devices such as a microprocessor, a central processing unit (CPU), or the like. More particularly, the processing device can be a complex instruction set computing (CISC) microprocessor, reduced instruction set computing (RISC) microprocessor, very long instruction word (VLIW) microprocessor, or a processor implementing other instruction sets, or processors implementing a combination of instruction sets. The processing device 638 can also be one or more special-purpose processing devices such as an application specific integrated circuit (ASIC), a field programmable gate array (FPGA), a digital signal processor (DSP), network processor, or the like. The processing device 638 is configured to execute instructions 680 for performing the operations and steps discussed herein. The machine 670 can further include a network interface device 672 to communicate over the network 684.

[0058] The data storage system 676 can include a machine-readable storage medium 678 (also known as a computer-readable medium) on which is stored one or more sets of instructions 680 or software embodying any one or more of the methodologies or functions described herein. The instructions 680 can also reside, completely or at least partially, within the main memory 640 and/or within the processing device 638 during execution thereof by the machine 670, the main memory 640 and the processing device 638 also constituting machine-readable storage media.

[0059] In at least one embodiment, the instructions 680 include instructions to implement functionality described herein, such as that corresponding to the controller 436 of Figure 4. While the machine-readable storage medium 678 is shown in an example embodiment to be a single medium, the term “machine-readable storage medium” should be taken to include a single medium or multiple media that store the one or more sets of instructions. The term “machine-readable storage medium” shall also be taken to include any medium that is capable of storing or encoding a set of instructions for execution by the machine and that cause the machine to perform any one or more of the methodologies of the present disclosure. The term “machine-readable storage medium” shall accordingly be taken to include, but not be limited to, solid-state memories, optical media, and magnetic media.

[0060] Although specific embodiments have been described above, these embodiments are not intended to limit the scope of the present disclosure, even where only a single embodiment is described with respect to a particular feature. Examples of features provided in

the disclosure are intended to be illustrative rather than restrictive unless stated otherwise. The above description is intended to cover such alternatives, modifications, and equivalents as would be apparent to a person skilled in the art having the benefit of this disclosure.

[0061] The scope of the present disclosure includes any feature or combination of features disclosed herein (either explicitly or implicitly), or any generalization thereof, whether or not it mitigates any or all of the problems addressed herein. Various advantages of the present disclosure have been described herein, but embodiments may provide some, all, or none of such advantages, or may provide other advantages.

[0062] In the foregoing Detailed Description, some features are grouped together in a single embodiment for the purpose of streamlining the disclosure. This method of disclosure is not to be interpreted as reflecting an intention that the disclosed embodiments of the present disclosure have to use more features than are expressly recited in each claim. Rather, as the following claims reflect, inventive subject matter lies in less than all features of a single disclosed embodiment. Thus, the following claims are hereby incorporated into the Detailed Description, with each claim standing on its own as a separate embodiment.

Claims

What is claimed is:

1. A method, comprising:
initiating measurement of a property associated with a chemical over a range of frequencies or wavelengths;
recursively modeling data collected from the measurement to an expected property spectrum, via Bayesian modeling, thereby yielding a predicted property spectrum before completion of the measurement over all of the range of frequencies or wavelengths;
recursively predicting a peak in the predicted property spectrum and calculating a probability of the peak according to the data before completion of the measurement over all of the range of frequencies or wavelengths; and
stopping the measurement before completion thereof over all of the range of frequencies or wavelengths in response to the probability being greater than a threshold value.
2. The method of claim 1, wherein initiating the measurement comprises initiating a series of measurements to be made at each of a plurality of frequencies or wavelengths comprising the range of frequencies or wavelengths; and
wherein stopping the measurement before completion thereof comprises measuring the property at less than all of the plurality of frequencies or wavelengths covering only a portion of the range of frequencies or wavelengths.
3. The method of claim 1, further comprising initiating a new measurement of the property associated with a new chemical over the range of frequencies or wavelengths without completing the measurement of the property associated with the chemical over the entire range of frequencies or wavelengths.
4. The method of claim 1, comprising recursively modeling data and recursively predicting a peak after the measurement at each frequency or wavelength at which the measurement has been conducted.

5. The method of claim 1, further comprising outputting an indication of the predicted peak.
6. The method of claim 5, further comprising adjusting a reaction condition based on the predicted peak.
7. The method of claim 6, wherein the reaction condition comprises at least one of a group of reaction conditions comprising catalyst concentration, reactant concentration, product concentration, temperature, pressure, and mixing condition; and
wherein adjusting the reaction condition comprises manually adjusting the reaction condition.
8. The method of claim 1, wherein recursively predicting the peak comprises predicting a plurality of peaks at each frequency or wavelength at which the measurement has been conducted; and
wherein recursively calculating the probability comprises calculating a standard deviation of the plurality of peaks after probability density weighting thereof at each frequency or wavelength at which the measurement has been conducted.
9. The method of claim 1, wherein recursively predicting the peak comprises recursively predicting a magnitude of the peak and a frequency or wavelength at which the peak is predicted to occur.
10. A system, comprising:
a sensor configured to measure a property associated with a chemical; and
a controller coupled to the sensor and configured to:
initiate the measurement over a range of frequencies or wavelengths;
recursively model data collected from the measurement to an expected property spectrum, via Bayesian modeling, thereby yielding a predicted property spectrum before completion of the measurement over all of the range of frequencies or wavelengths;

recursively predict a peak in the predicted property spectra and calculate a probability of the peak according to the data before completion of the measurement over all of the range of frequencies or wavelengths; and

stop the measurement by the sensor before completion thereof over all of the range of frequencies or wavelengths in response to the probability being greater than a threshold value.

11. The system of claim 10, wherein the controller is further configured to output an indication of one or more of the predicted peak and the predicted property spectrum.
12. The system of claim 10, wherein the controller is further configured to adjust a reaction condition based on the predicted peak.
13. The system of claim 10, wherein the property associated with the chemical comprises a property of a chemical reaction, a property of a chemical product, a property of a catalyst, or a property of a reactant.
14. The system of claim 10, wherein to recursively model data, the controller is configured to predict the peak after the measurement at each frequency or wavelength at which the measurement has been conducted.
15. The system of claim 14, wherein the expected property spectrum is based on the collected data and data collected before the measurement for an analogous chemical.
16. The system of claim 14, wherein the expected property spectrum is based on the collected data and empirical modeling of the property spectrum.
17. A non-transitory machine-readable medium storing instructions executable by a processor to:
recursively model data collected from measurement of a property associated with a chemical over a range of frequencies or wavelengths to an expected property spectrum, via

Bayesian modeling, thereby yielding a predicted property spectrum before completion of the measurement over all of the range of frequencies or wavelengths;

 recursively predict a peak in the predicted property spectrum and calculate a probability of the peak according to the data before completion of the measurement over all of the range of frequencies or wavelengths; and

 output an indication of the predicted peak before completion of the measurement over all of the range of frequencies or wavelengths in response to the probability being greater than a threshold value.

18. The medium of claim 17, further comprising instructions to adjust a reaction condition based on the predicted peak.

19. The medium of claim 17, wherein the instructions to recursively predict a peak comprise instructions to recursively predict a plurality of peaks.

20. The medium of claim 17, further comprising instructions to initiate the measurement; and stop the measurement before completion of the thereof over all of the range of frequencies or wavelengths in response to the probability being greater than the threshold value.