or nature. Therefore, for a correct qualitative analysis and quantitative analysis, it is extremely important to correctly separate the peaks originating from the different components in the peak detection process.

CITATION LIST

PATENT LITERATURE

[0005]

Patent Literature 1: JP 2013-171014 A

Patent Literature 2: JP 2017-083441 A

SUMMARY

[0006]

Various techniques or algorithms have conventionally been used in order to separate the peaks overlapping each other on a chromatogram or spectrum and detect each individual peak. However, those conventionally and commonly used peak detection methods require various parameters and conditions to be set before the execution of the peak detection or peak separation. Inappropriate setting of those parameters and conditions leads to an inappropriate peak detection or peak separation. Consequently, an important peak may be missed, a peak which actually is not a peak may be incorrectly detected as a peak, or the peak area may significantly deviate from the actual value.

[0007]

Depending on the peak detection method, an operator may need to make a judgment and manually give instructions for appropriate separation of the peaks. When such a technique is used, the analysis result may possibly vary depending on the individual operator, making it

difficult to ensure the reliability or reproducibility of the result. Furthermore, the amount of burden on the operator is significantly large.

[0008]

A peak which appears to be a single peak on a chromatogram is not always a peak originating from a single component; it may contain an additional component different from the target component. Accordingly, a peak-purity determination process for determining whether or not a given peak is a pure peak originating from a single component has conventionally been performed in some cases (see Patent Literature 1). Although such a peak-purity determination process does not require separating the overlapping peaks, it is necessary to perform peak detection under various parameters and conditions in order to determine whether an apparently single peak has originated from a single component or multiple components. This causes a problem similar to the previously described problem concerning the peak separation.

[0009]

The present disclosure has been developed to solve such a problem. Its objective is to provide a peak analyzing method which can satisfactory separate the overlapping peaks or determine the purity of a single peak observed on a chromatogram, spectrum or similar signal waveform, without requiring a significant amount of work for the complex setting of the parameters and manual instructions, as well as a waveform processing device employing the same method.

[0010]

In a first aspect, the present disclosure provides a peak analyzing method using a computer to

process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters, and to separate overlapping peaks observed in a second signal waveform representing a relationship between the second parameter and the signal intensity into a plurality of individual peaks originating from different factors based on signal patterns observed in a dimension of the first parameter, wherein the peak analyzing method executes:

a singular value decomposition step configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition;

a transformation matrix acquisition step configured to estimate characteristic orientations within a space spanned by the plurality of basis vectors by performing a geometric analysis on a trajectory defined by the plurality of weighting vectors in an SVD projection space whose number of dimensions is equal to the lowered rank given by a singular value decomposition process, and to determine a transformation matrix containing relevant information of the characteristic orientations; and

a peak separation step configured to deconvolute signal waveforms in the first matrix of the dimension of the first parameter by the transformation matrix, and to separate peaks in the second signal waveform in the second matrix by the transformation matrix.

[0011]

In a second aspect, the present disclosure provides a peak analyzing method using a computer to process three-dimensional data obtained by acquiring a series of first signal

waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters, and to determine a purity of a peak observed in a second signal waveform representing a relationship between the second parameter and the signal intensity, wherein the peak analyzing method executes:

a singular value decomposition step configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition; and

a component number estimation step configured to estimate the number of components contributing to the peak from a behavior of a trajectory in an SVD projection space whose number of dimensions is equal to the lowered rank, and which is described by the plurality of weighting vectors.

[0012]

In a third aspect, the present disclosure provides a waveform processing device configured to process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters, and to separate overlapping peaks observed in a second signal waveform representing a relationship between the second parameter and the signal intensity into a plurality of individual peaks originating from different factors based on signal patterns observed in a dimension of the first parameter, the waveform processing device comprising:

a singular value decomposition processor configured to perform singular value

decomposition on an input matrix representing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter and a second matrix expressing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition;

a transformation matrix acquirer configured to estimate characteristic orientations within a space spanned by the plurality of basis vectors by performing a geometric analysis on a trajectory defined by the plurality of weighting vectors in an SVD projection space whose number of dimensions is equal to the lowered rank given by a singular value decomposition process, and to determine a transformation matrix containing relevant information of the characteristic orientations; and

a peak separation calculator configured to deconvolute signal waveforms in the first matrix of the dimension of the first parameter by the transformation matrix, and to separate peaks in the second signal waveform in the second matrix by the transformation matrix.

[0013]

In a fourth aspect, the present disclosure provides a waveform processing device configured to process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters, and to determine a purity of a peak observed in a second signal waveform representing a relationship between the second parameter and the signal intensity, the waveform processing device comprising:

a singular value decomposition processor configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter

and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition; and

a component number estimator configured to estimate a number of components contributing to the peak from a behavior of a trajectory in an SVD projection space whose number of dimensions is equal to the lowered rank, and which is described by the plurality of weighting vectors.

[0014]

The "SVD projection space" is a low-dimensional space defined by a few basis vectors obtained by performing a singular value decomposition (SVD) analysis on an input matrix expressing three-dimensional data to be processed.

[0015]

In any of the previously described modes of the peak analyzing method and waveform processing device according to the present disclosure, for example, the first parameter may be wavelength or mass-to-charge ratio, with the first signal waveform being a waveform spectrum (or wavenumber spectrum) or mass spectrum, while the second parameter may be time, with the second signal waveform being a chromatogram. The different factors may be different components contained in a sample.

[0016]

Three-dimensional data which show a signal intensity for each combination of one parameter value in the first parameter and one parameter value in the second parameter can be expressed in the form of a matrix. If the contribution of noise is negligible, the rank of this matrix equals the number of components contained in the three-dimensional data. If the

contribution of the noise is sufficiently small, the distribution of the singular values acquired by the singular value decomposition normally includes comparatively high values the number of which equals the number of components, while the other values due to the contribution of the noise are close to zero. Therefore, it is possible to estimate the number of components. Accordingly, in one mode of the peak analyzing method and waveform processing device according to the present disclosure, the number of components contributing to three-dimensional data is estimated from the distribution of the singular values determined for an input matrix expressing the three-dimensional data. In another mode of the peak analyzing method and waveform processing device according to the present disclosure, low rank approximation of the input matrix (three-dimensional data) is performed so that the number of vectors retained after the singular value decomposition equals the estimated number of components. If random noise is present in the three-dimensional data, the noise will be reduced (removed) by the low rank approximation.

[0017]

The low rank approximation of the matrix yields a low rank approximate matrix expressed in the form of a product of the first matrix and the second matrix. The weighting vectors which correspond to the columns in the second matrix shows a characteristic behavior in the SVD projection space whose number of dimensions equals the rank of the low rank approximate matrix. As a specific example, consider the case where two peaks originating from two components on the time axis have their respective base portions overlapping each other. If those peaks are observed with the passage of time, a period of time in which only the first peak is present initially appears, followed by a period of time in which the first and second peaks overlap each other, which is further followed by a period of time in which only the second peak is present. The weighting vector in the SVD projection space describes a characteristic trajectory corresponding to the three periods of time: During the period of time

in which only the first peak is present, as well as during the period of time in which only the second peak is present, the weighting vectors form a line in a characteristic direction corresponding to the first signal waveform of a single component which corresponds to the peak that is present. Accordingly, in the transformation matrix acquisition step, a geometric analysis is performed on the trajectory to estimate a plurality of characteristic orientation vectors based on the directions of the sections of the trajectory which respectively correspond to those periods of time. A transformation matrix is defined from the set of characteristic orientation vectors. Using this transformation matrix, a set of data in which the peaks are separated can be obtained from each of the first and second matrices.

[0018]

In one mode of the peak analyzing method and peak processing device according to the present disclosure, the task of separating peaks overlapping each other on a chromatogram or spectrum to extract information for each individual peak, or the task of accurately determining whether or not an apparently single peak has originated from a single component, can be performed without requiring the setting of complex parameters for the peak detection, peak separation or peak-purity determination, or without requiring a user to make a judgment or perform manual operations. Consequently, an efficient and highly accurate peak separation, peak-purity determination and peak detection can be achieved.

BRIEF DESCRIPTION OF DRAWINGS

[0019]

Fig. 1 is a schematic configuration diagram of one embodiment of an LC system employing a waveform processing device according to the present invention.

Fig. 2 is a flowchart showing the procedure of a peak separation process in the LC system according to the present embodiment.