THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 13: PCA, LDA, QDA for Spectra and Images

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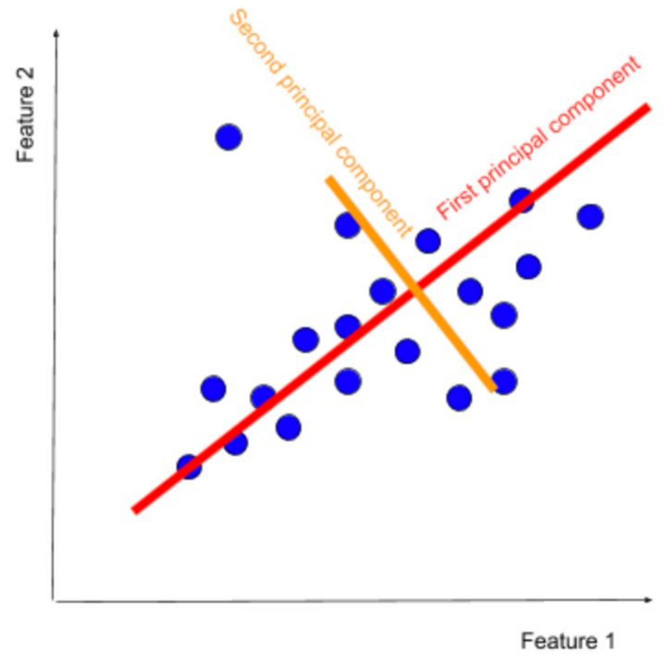
Principal Component Analysis

PCA: orthogonal transformation converting possibly correlated variables into linearly uncorrelated *principal components*

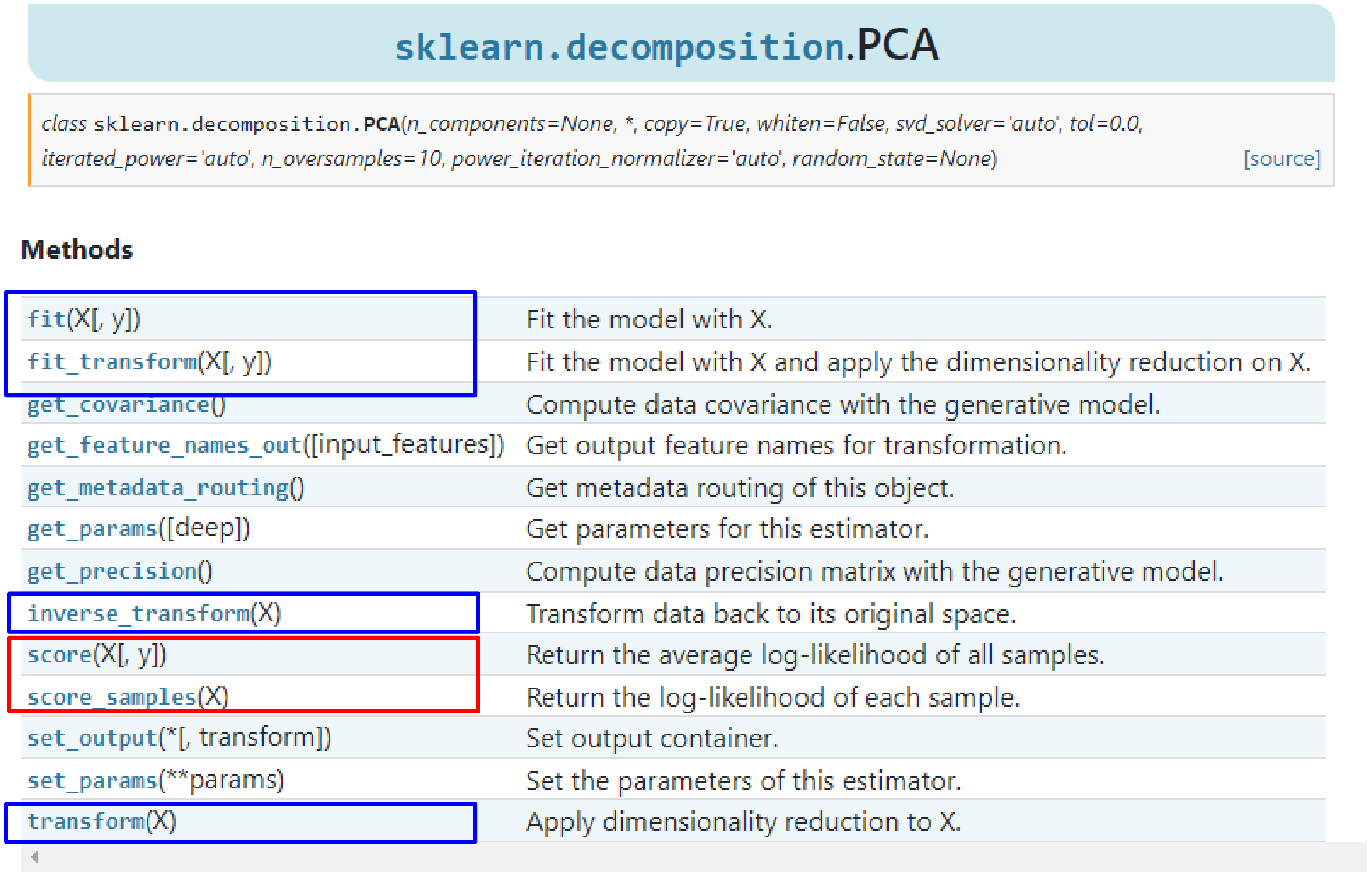
- PCA transforms the data such that the greatest variance by any projection lies on the first coordinate
- The first PC retains the greatest amount of variation in the sample. The k^{th} PC retains the k^{th} greatest fraction of the variation in the sample.
- The k^{th} largest eigenvalue of the correlation matrix C is the variance in the sample along the k^{th} PC
- Reveals internal structure that best explains variance in the dataset

The least-squares view: PCs are a series of linear least squares fits to a sample, each orthogonal to all previous ones



https://medium.com/@kayalgen/principal-component-analysis-pca-for-machine-learning-89db6cb63e4

PCA in scikit-learn



sklearn.decomposition.PCA

class sklearn.decomposition.**PCA**(*n_components=None*, ***, *copy=True*, *whiten=False*, *svd_solver='auto'*, *tol=0.0*, *iterated_power='auto'*, *n_oversamples=10*, *power_iteration_normalizer='auto'*, *random_state=None*) [source]

Methods

`fit`(X[, y])	Fit the model with X.
`fit_transform`(X[, y])	Fit the model with X and apply the dimensionality reduction on X.
`get_covariance`()	Compute data covariance with the generative model.
`get_feature_names_out`([input_features])	Get output feature names for transformation.
`get_metadata_routing`()	Get metadata routing of this object.
`get_params`([deep])	Get parameters for this estimator.
`get_precision`()	Compute data precision matrix with the generative model.
`inverse_transform`(X)	Transform data back to its original space.
`score`(X[, y])	Return the average log-likelihood of all samples.
`score_samples`(X)	Return the log-likelihood of each sample.
`set_output`(*[, transform])	Set output container.
`set_params`(**params)	Set the parameters of this estimator.
`transform`(X)	Apply dimensionality reduction to X.

- In scikit-learn, PCA is implemented as **probabilistic model**: can estimate the likelihood of data based on the amount of variance it explains.
- **Incremental PCA:** add partial_fit method
- **SparsePCA:** introduce sparsity in decomposition

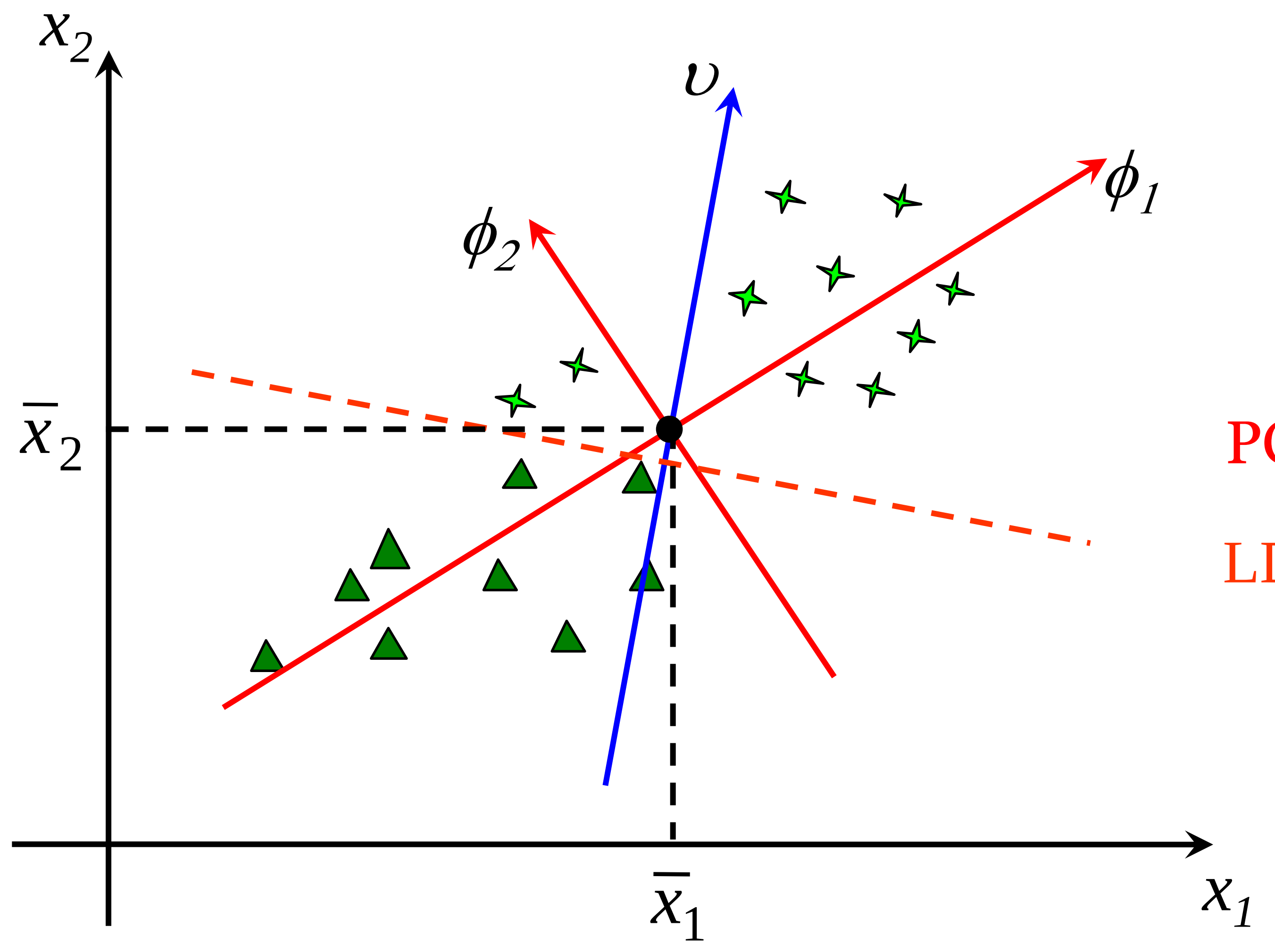
$$(U^*, V^*) = \underset{U,V}{\arg\min}\ \frac{1}{2}||X - UV||_{\text{Fro}}^2 + \alpha||V||_{1,1}$$
$$\text{subject to } ||U_k||_2 <= 1 \text{ for all } 0 \leq k < n_{components}$$

- … and there is always more (dictionary methods, etc)

Linear Discriminant Analysis

- Linear Discriminant Analysis, or simply LDA, is a feature extraction technique that has been used successfully in many statistical pattern recognition problems.
- LDA is often called Fisher Discriminant Analysis (FDA).
- The primary purpose of LDA is to separate samples of distinct groups by transforming then to a space which maximises their between-class separability while minimising their within-class variability.
- It assumes implicitly that the true covariance matrices of each class are equal because the same within-class scatter matrix is used for all the classes considered.
- If we remove this assumption, we get Quadratic Discriminant Analysis

Geometric Idea of LDA



PCA: (ϕ_1, ϕ_2)

LDA: υ

LDA Steps

1. Compute the d-dimensional mean vectors.
2. Compute the scatter matrices
3. Compute the eigenvectors and corresponding eigenvalues for the scatter matrices.
4. Sort the eigenvalues and choose those with the largest eigenvalues to form a $d \times k$ dimensional matrix
5. Transform the samples onto the new subspace.

LDA Method

- Let the between-class scatter matrix S_b be defined as

$$S_b = \sum_{i=1}^{g} N_i (\bar{x}_i - \bar{x})(\bar{x}_i - \bar{x})^T$$

- and the within-class scatter matrix S_w be defined as

$$S_w = \sum_{i=1}^{g} (N_i - 1) S_i = \sum_{i=1}^{g} \sum_{j=1}^{N_i} (x_{i,j} - \bar{x}_i)(x_{i,j} - \bar{x}_i)^T$$

- where $x_{i,j}$ is an n-dimensional data point j from class p_i, N_i is the number of training examples from class p_i, and g is the total number of classes or groups.

LDA Method

- The sample mean, sample covariance, and grand mean vector are given respectively by:

$$\bar{x}_i = \frac{1}{N_i} \sum_{j=1}^{N_i} x_{i,j}$$

$$S_i = \frac{1}{(N_i - 1)} \sum_{j=1}^{N_i} (x_{i,j} - \bar{x}_i)(x_{i,j} - \bar{x}_i)^T$$

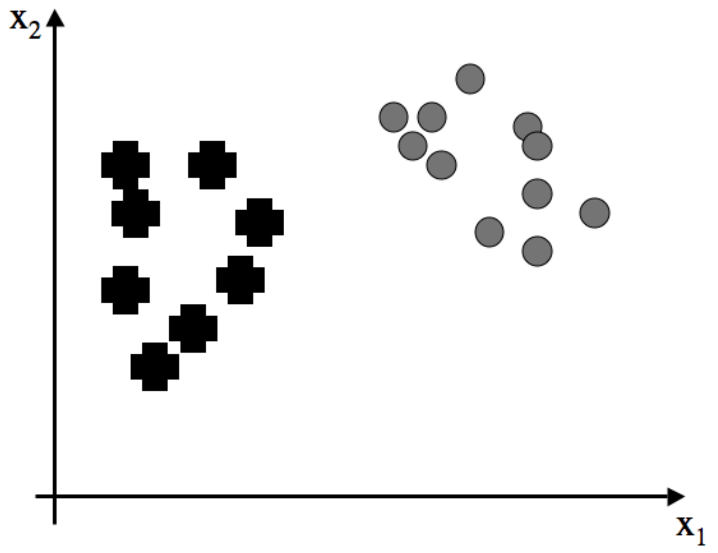
$$\bar{x} = \frac{1}{N} \sum_{i=1}^{g} N_i \bar{x}_i = \frac{1}{N} \sum_{i=1}^{g} \sum_{j=1}^{N_i} x_{i,j}$$

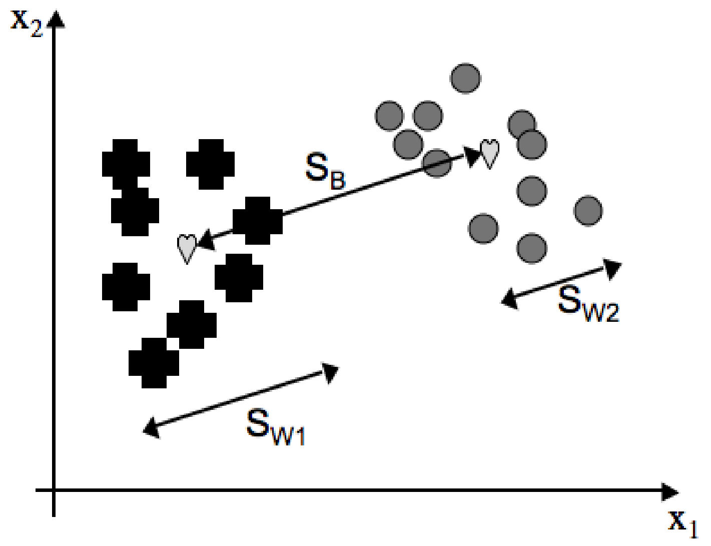
$$N = N_1 + N_2 + \ldots + N_g$$

LDA Method

The objective of LDA is to find a projection matrix P_{lda} that maximises the ratio of the determinant of S_b to the determinant of S_w (Fisher's criterion) as:

$$P_{lda} = \arg\max_{P} \frac{\left| P^T S_b P \right|}{\left| P^T S_w P \right|}$$

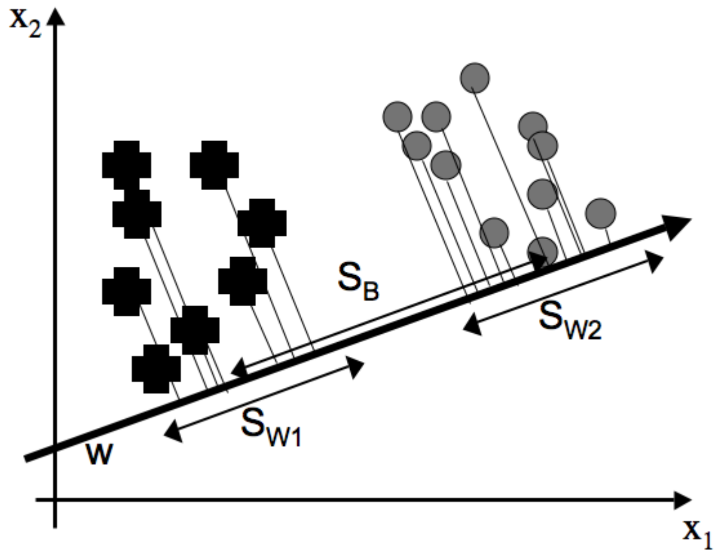




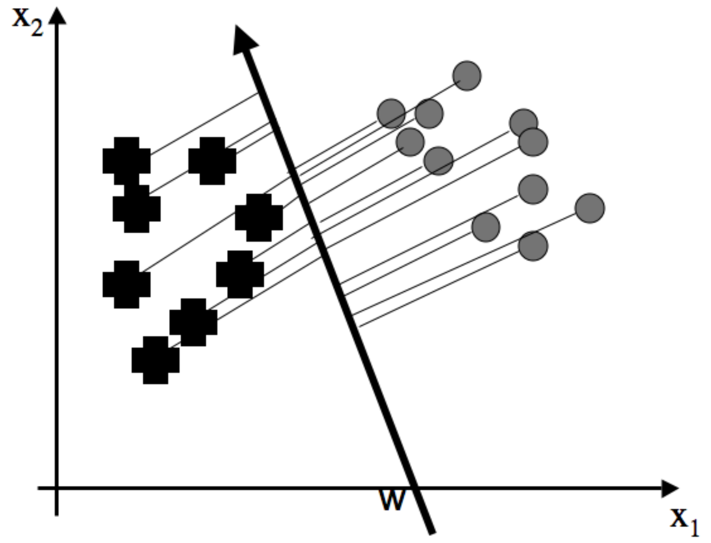
From Intelligent Data Analysis and Probabilistic Inference by Longin Jan Latecki Temple University

LDA Method

- So Fisher's criterion tries to find the projection that:
  - Maximises the variance of the class means
  - Minimises the variance of the individual classes



Good projection

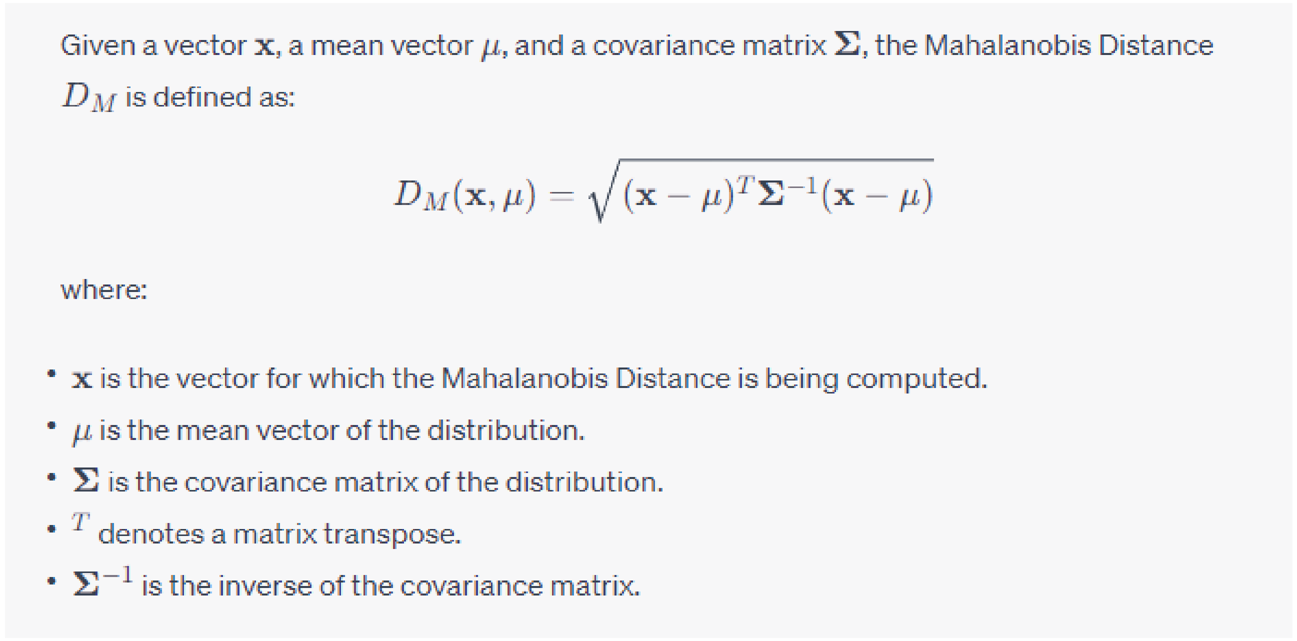


Bad projection

From Intelligent Data Analysis and Probabilistic Inference by Longin Jan Latecki Temple University

Classification using LDA

- The LDA is an axis projection.
- Once the projection is found all the data points can be transformed to the new axis system along with the class means and covariances.
- Allocation of a new point to a class can be done using a distance measure such as the Mahalanobis distance.



Given a vector $\mathbf{x}$, a mean vector μ, and a covariance matrix $\mathbf{\Sigma}$, the Mahalanobis Distance D_M is defined as:

$$D_M(\mathbf{x}, \mu) = \sqrt{(\mathbf{x} - \mu)^T \mathbf{\Sigma}^{-1} (\mathbf{x} - \mu)}$$

where:

- $\mathbf{x}$ is the vector for which the Mahalanobis Distance is being computed.
- μ is the mean vector of the distribution.
- $\mathbf{\Sigma}$ is the covariance matrix of the distribution.
- ^{T} denotes a matrix transpose.
- $\mathbf{\Sigma}^{-1}$ is the inverse of the covariance matrix.

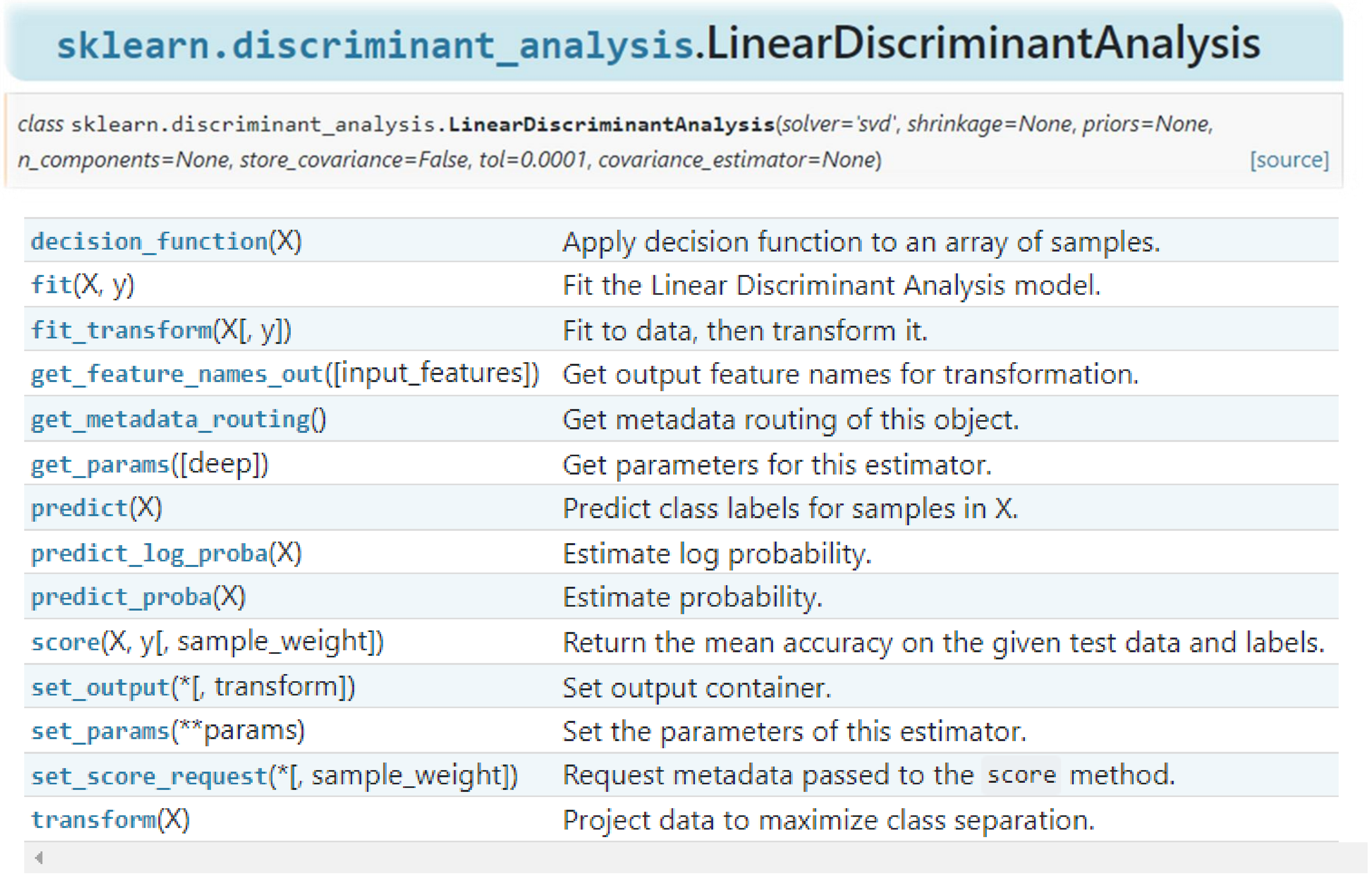
From Intelligent Data Analysis and Probabilistic Inference by Longin Jan Latecki Temple University

LDA vs. PCA

- LDA is supervised ML method, PCA is unsupervised method

- LDA seeks directions that are efficient for *discriminating* data whereas PCA seeks directions that are efficient for *representing* data.

- The directions that are discarded by PCA might be exactly the directions that are necessary for distinguishing between groups.

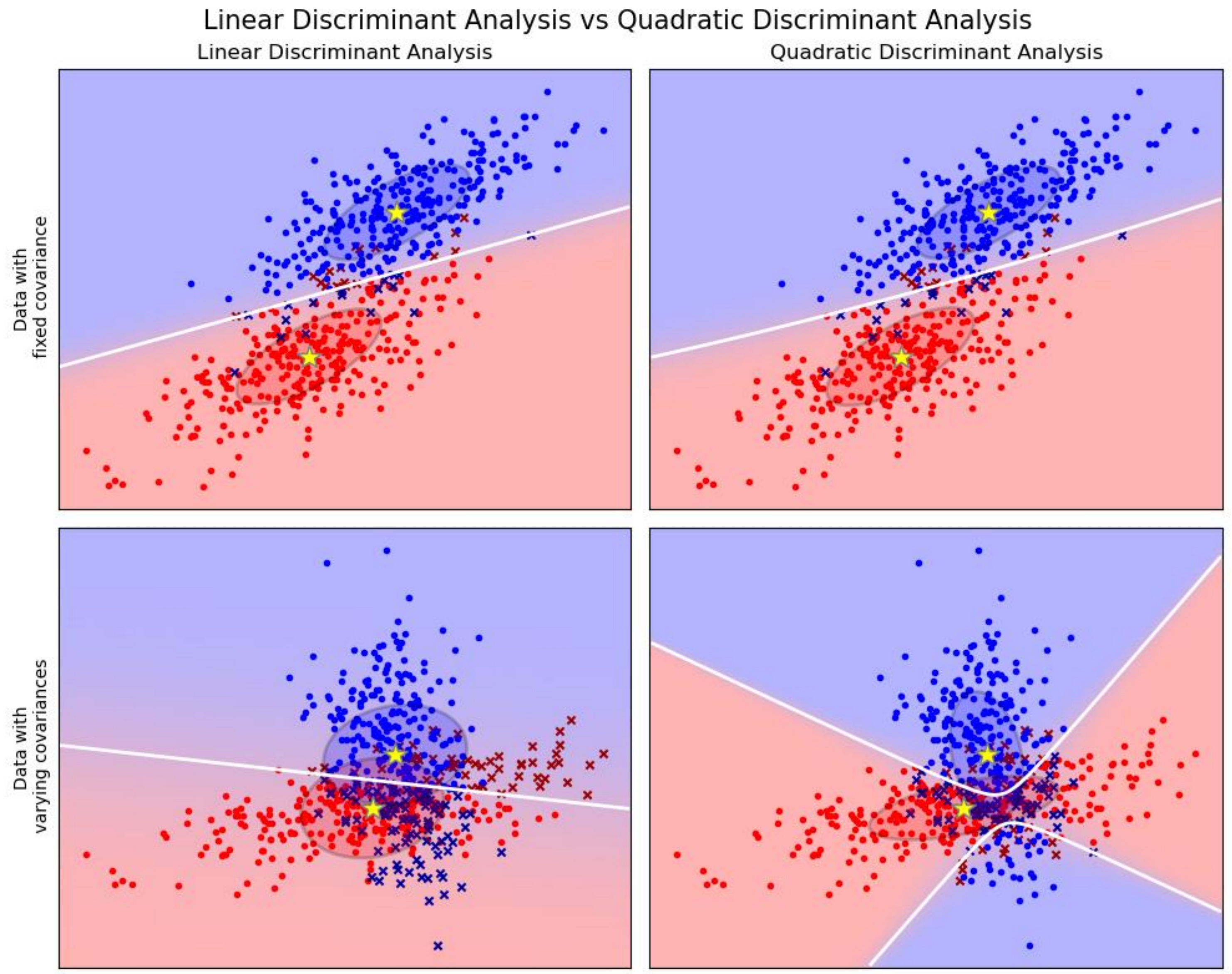


sklearn.discriminant_analysis.LinearDiscriminantAnalysis

class sklearn.discriminant_analysis.**LinearDiscriminantAnalysis**(*solver='svd', shrinkage=None, priors=None, n_components=None, store_covariance=False, tol=0.0001, covariance_estimator=None*) [source]

decision_function(X)	Apply decision function to an array of samples.
fit(X, y)	Fit the Linear Discriminant Analysis model.
fit_transform(X[, y])	Fit to data, then transform it.
get_feature_names_out([input_features])	Get output feature names for transformation.
get_metadata_routing()	Get metadata routing of this object.
get_params([deep])	Get parameters for this estimator.
predict(X)	Predict class labels for samples in X.
predict_log_proba(X)	Estimate log probability.
predict_proba(X)	Estimate probability.
score(X, y[, sample_weight])	Return the mean accuracy on the given test data and labels.
set_output(*[, transform])	Set output container.
set_params(**params)	Set the parameters of this estimator.
set_score_request(*[, sample_weight])	Request metadata passed to the `score` method.
transform(X)	Project data to maximize class separation.

Quadratic Discriminant Analysis



https://scikit-learn.org/stable/modules/lda_qda.html#lda-qda

LDA vs. QDA

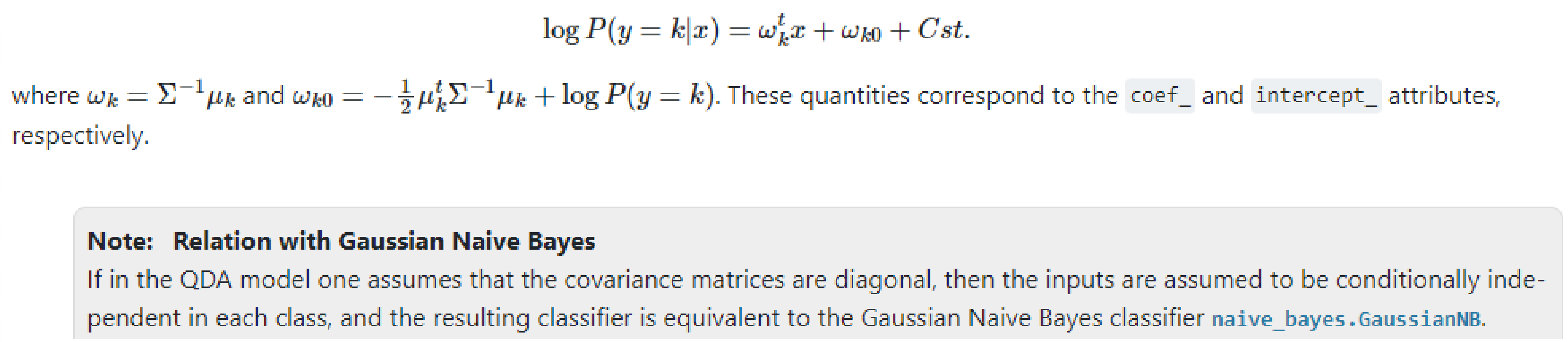
Bayesian classification framework:

$$P(y=k|x) = \frac{P(x|y=k)P(y=k)}{P(x)} = \frac{P(x|y=k)P(y=k)}{\sum_l P(x|y=l)\cdot P(y=l)}$$

QDA approximation:

$$P(x|y=k) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_k)^t \Sigma_k^{-1}(x-\mu_k)\right)$$

LDA is a special case of QDA, where the Gaussians for each class are assumed to share the same covariance matrix: $\Sigma_k = \Sigma$. If so



$$\log P(y=k|x) = \omega_k^t x + \omega_{k0} + Cst.$$

where $\omega_k = \Sigma^{-1}\mu_k$ and $\omega_{k0} = -\frac{1}{2}\mu_k^t\Sigma^{-1}\mu_k + \log P(y=k)$. These quantities correspond to the `coef_` and `intercept_` attributes, respectively.

Note: Relation with Gaussian Naive Bayes
If in the QDA model one assumes that the covariance matrices are diagonal, then the inputs are assumed to be conditionally independent in each class, and the resulting classifier is equivalent to the Gaussian Naive Bayes classifier `naive_bayes.GaussianNB`.

https://scikit-learn.org/stable/modules/lda_qda.html#lda-qda

Spectroscopic Imaging

Scanning probe microscopy:

- Force-distance curve measurements
- Current-voltage measurements
- Piezoresponse force/electrochemical strain spectroscopy

Electron microscopy:

- Electron Energy Loss Spectroscopy

Optical microscopy:

- Hyperspectral imaging
- Time resolved measurements

Mass-spectrometry:

- Secondary ion MS imaging

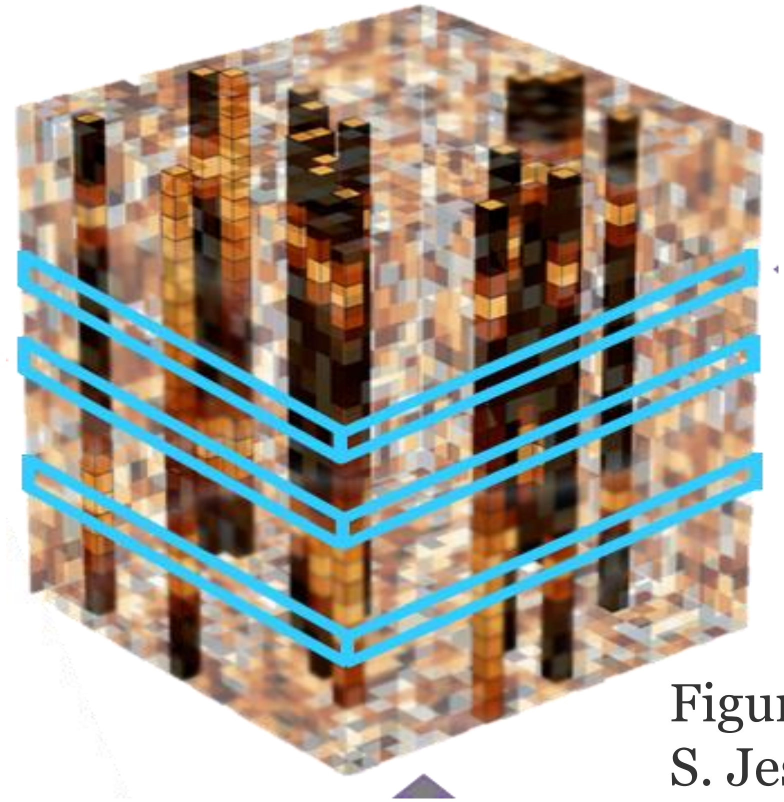
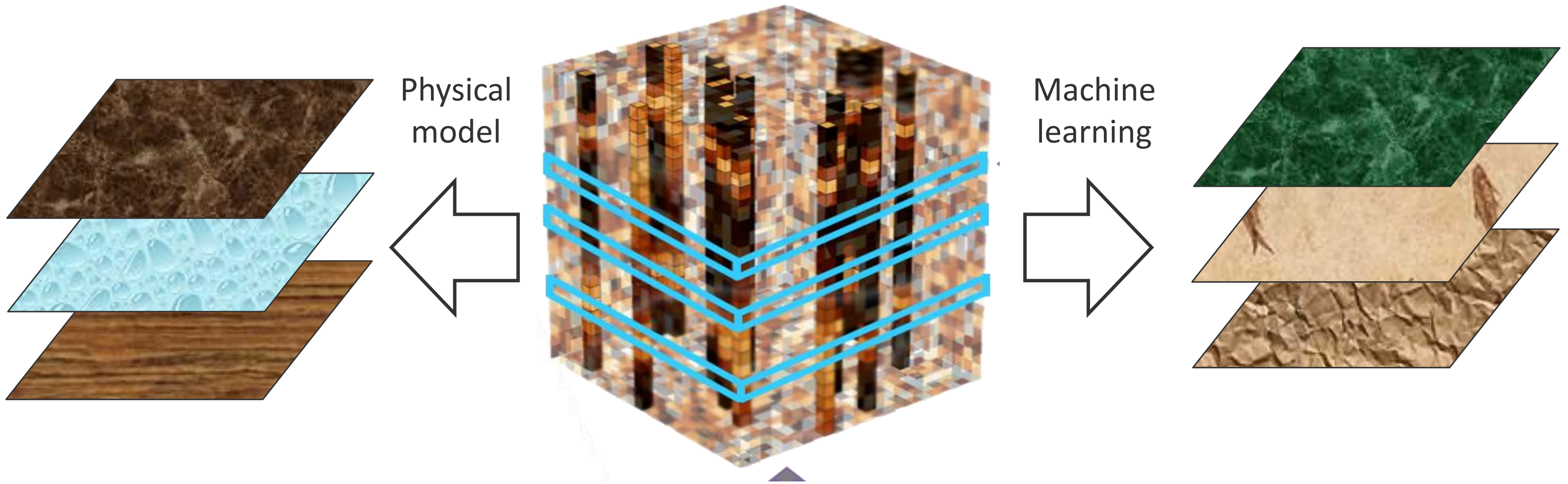


Figure by S. Jesse

In many cases, measured signal can be represented or approximated as a linear combination of signals. However, their functional forms are generally unknown

Very important: convolution with resolution function is also mixing

Physics vs. ML based analysis



- If we have physical model, we can extract relevant parameters from data
- Imperfect model: epistemic uncertainty
- Noisy data: aleatoric uncertainty
- Analysis results do not depend on sampling of data in *x*,*y*

- If we don't have physical model, we can learn intrinsic structure of data
- **Unsupervised learning:** based on data only
  - But not really (definition of distance)
  - Analysis can depend on sampling of data
- **Supervised learning:** based on prior examples
  - Out of distribution shifts

Physics-informed ML: Combines strengths (and limitations) of both

General linear unmixing

$$S(\mathbf{x}, \mathbf{R}) = \sum_i a_i(\mathbf{x})\, w_i(\mathbf{R}) + \mathrm{N}$$

We start with:

- $\mathbf{x}$ is the spatial variable, x = (x,y)
- R is the (vector) parameter variable

Overall, for MxM image and P point in spectra, we have M^2P data points

We aim to get:

- $a_i(\mathbf{x})$ are loading maps
- $w_i(\mathbf{R})$ are endmembers/eigenvectors
- N is noise

Overall, we can have (maximum) P loading maps of M^2 size. However, not all of them will have useful information

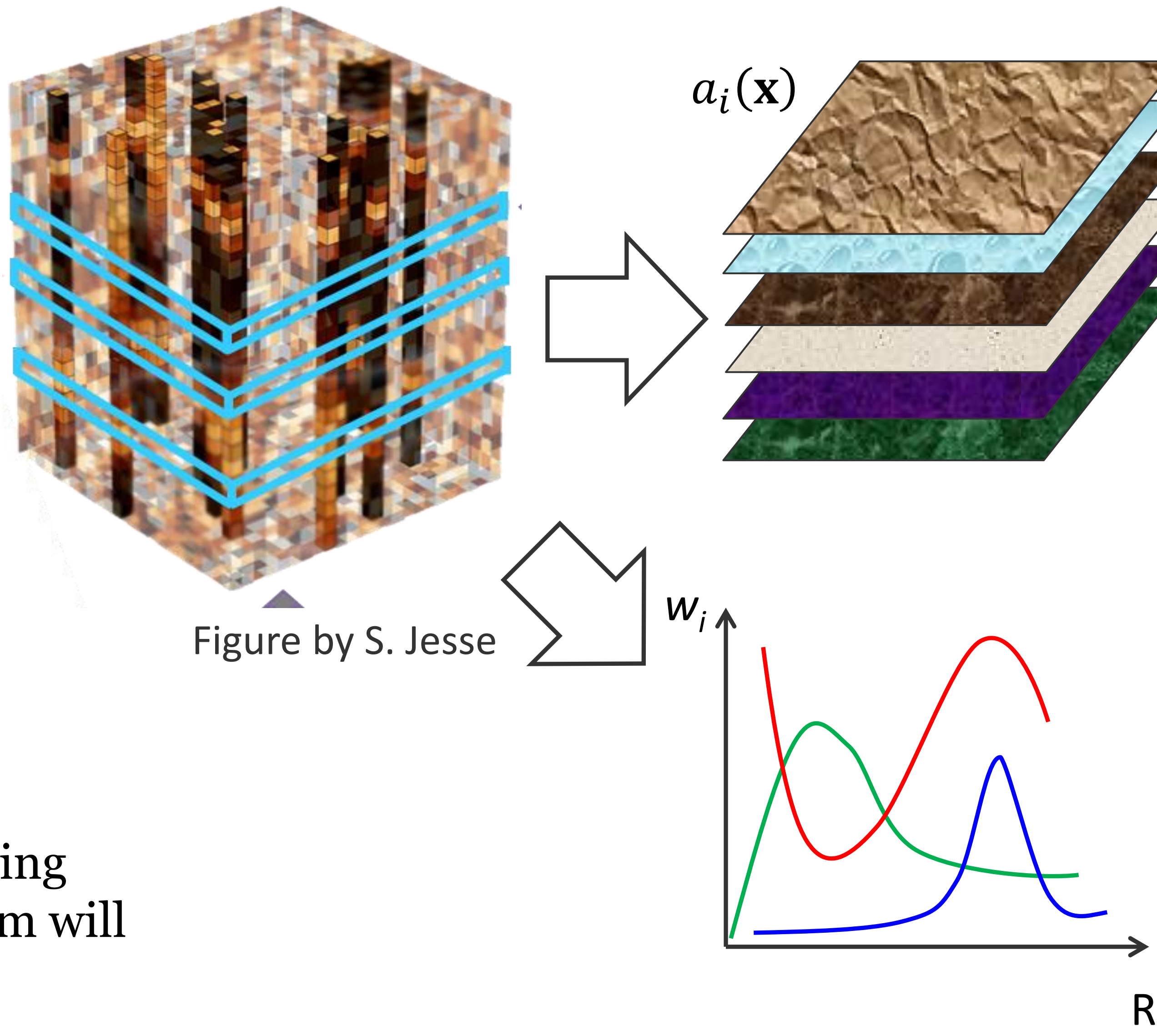
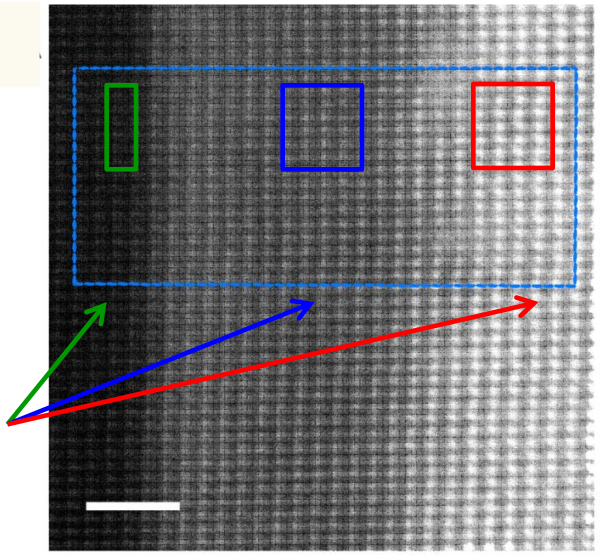


Figure by S. Jesse

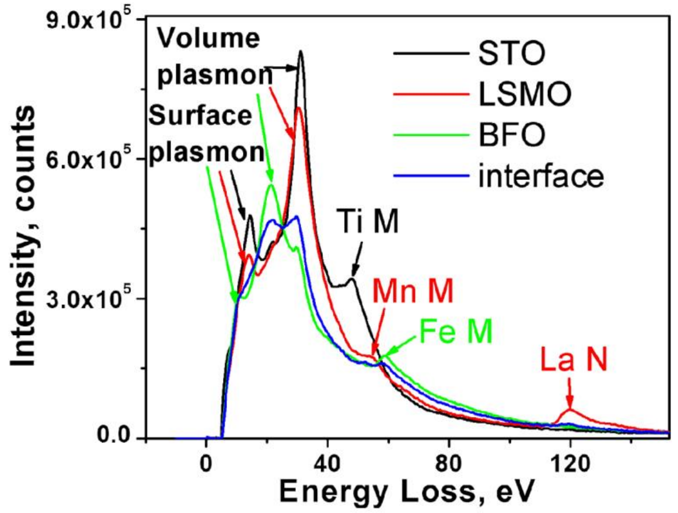
Multiple Linear Regression

Linear mixing $S(\mathbf{x},\mathbf{R}) = \sum_i \boxed{a_i(\mathbf{x})}\, w_i(\mathbf{R})$ +N but $w_i(\mathbf{R})$ are **known**

STEM of STO/LSMO/BFO interface



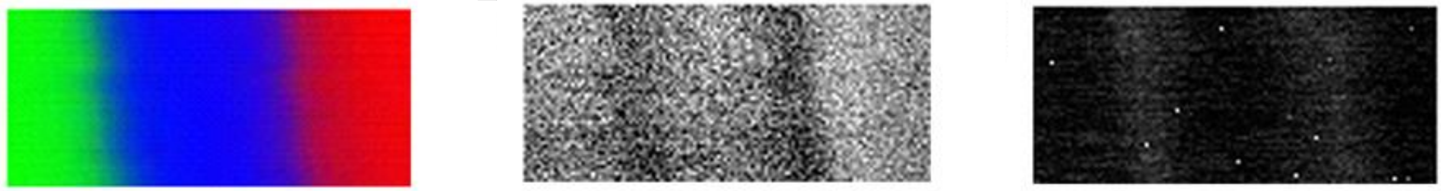
Low-loss EELS spectra of three components



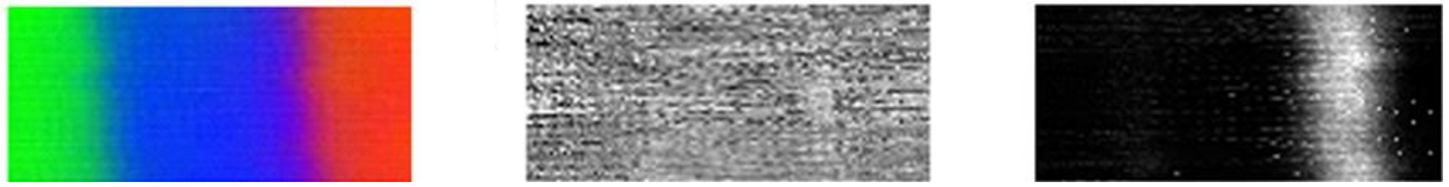
A.Y. Borisevich et al, *Suppression of Octahedral Tilts and Associated Changes in Electronic Properties at Epitaxial Oxide Heterostructure Interfaces*, Phys. Rev. Lett. **105**, 087204 (2010).

Fit coefficient map **residuals map** **χ2 map**

“Chemistry”:
35 to 125 eV



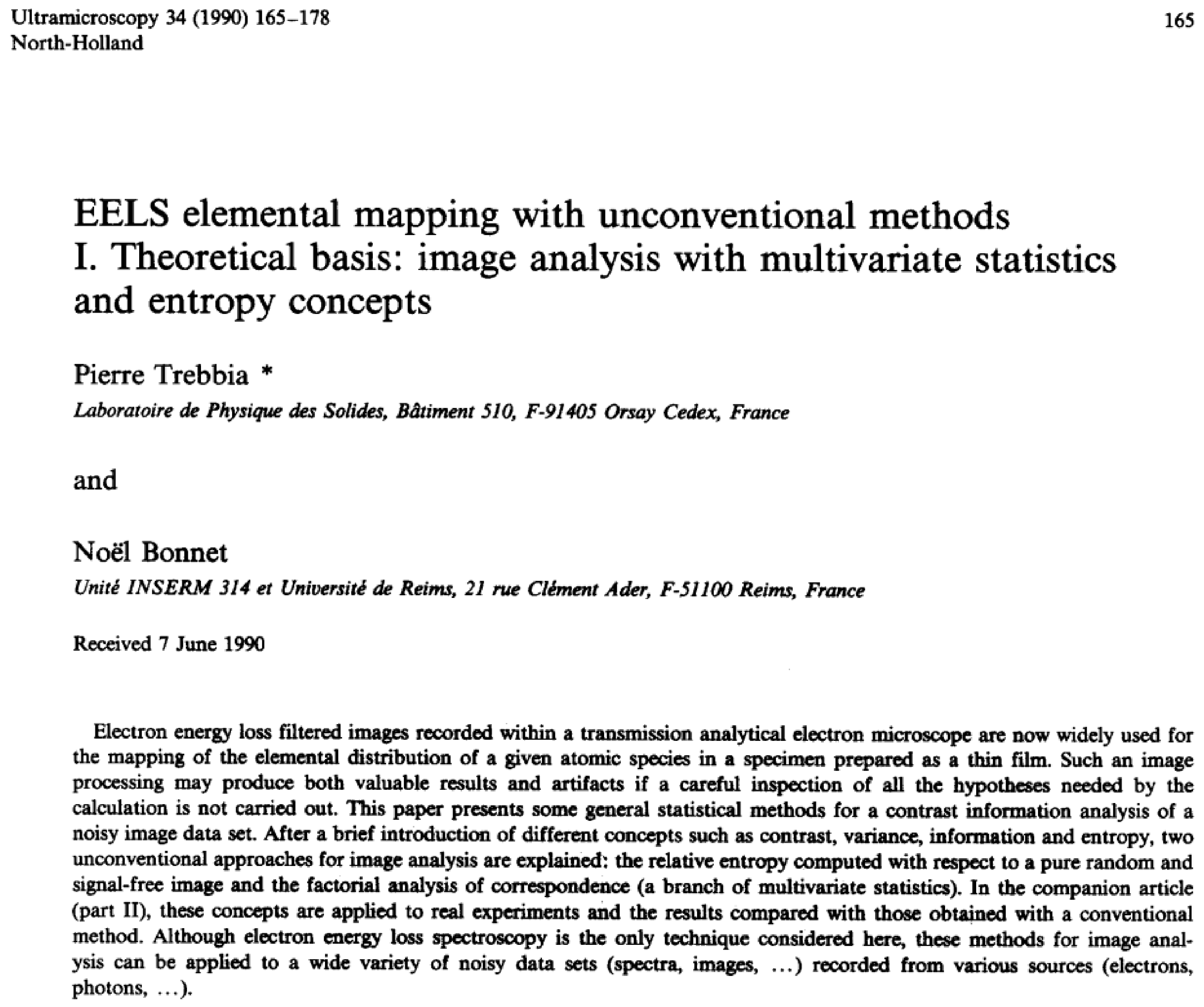
“Plasmons”
5 to 35 eV



Principal Component Analysis

$$S(\mathbf{x},\mathbf{R}) = \sum_i a_i(\mathbf{x})\, w_i(\mathbf{R})$$

- In PCA, the eigenvectors $w_i(\mathbf{R})$ are orthonormal and are arranged such that corresponding eigenvalues are placed in descending order by variance
- Can be used to separate “real data” from “noise” – but needs cut-off/selection criteria
- PCA eigenvectors generally do not have defined physical meaning
- PCA is a starting point for many other unmixing methods



Ultramicroscopy 34 (1990) 165–178
North-Holland

EELS elemental mapping with unconventional methods
I. Theoretical basis: image analysis with multivariate statistics and entropy concepts

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Received 7 June 1990

Electron energy loss filtered images recorded within a transmission analytical electron microscope are now widely used for the mapping of the elemental distribution of a given atomic species in a specimen prepared as a thin film. Such an image processing may produce both valuable results and artifacts if a careful inspection of all the hypotheses needed by the calculation is not carried out. This paper presents some general statistical methods for a contrast information analysis of a noisy image data set. After a brief introduction of different concepts such as contrast, variance, information and entropy, two unconventional approaches for image analysis are explained: the relative entropy computed with respect to a pure random and signal-free image and the factorial analysis of correspondence (a branch of multivariate statistics). In the companion article (part II), these concepts are applied to real experiments and the results compared with those obtained with a conventional method. Although electron energy loss spectroscopy is the only technique considered here, these methods for image analysis can be applied to a wide variety of noisy data sets (spectra, images, ...) recorded from various sources (electrons, photons, ...).

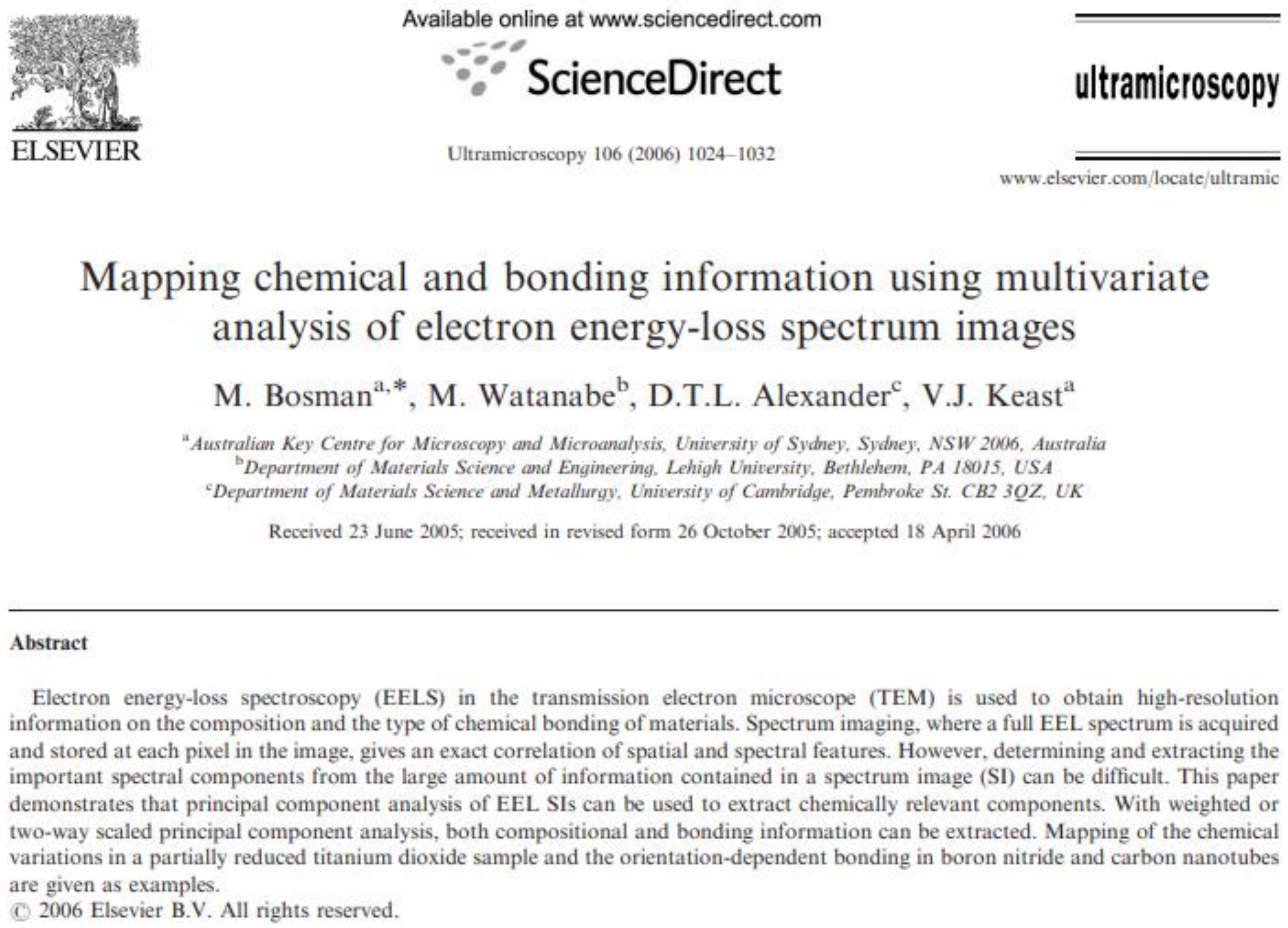
Why historical papers matter:

1. Often contain elementary introductions
2. Deep insights into principles
3. Surprisingly prescient predictions
4. Comparison with the present: see the big picture

““Those who cannot remember the past are condemned to repeat it.”

George Santayana,
The Life of Reason, 1905

KNOXVILLE



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Ultramicroscopy 106 (2006) 1024–1032

www.elsevier.com/locate/ultramic

Mapping chemical and bonding information using multivariate analysis of electron energy-loss spectrum images

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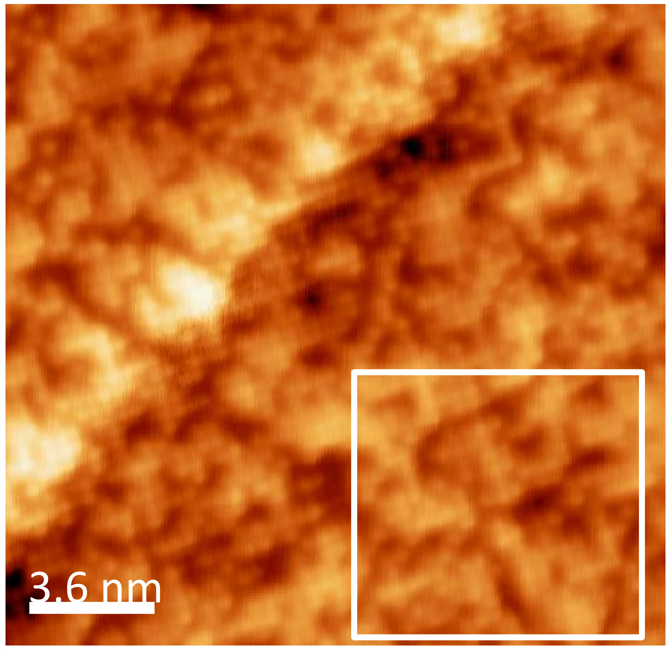
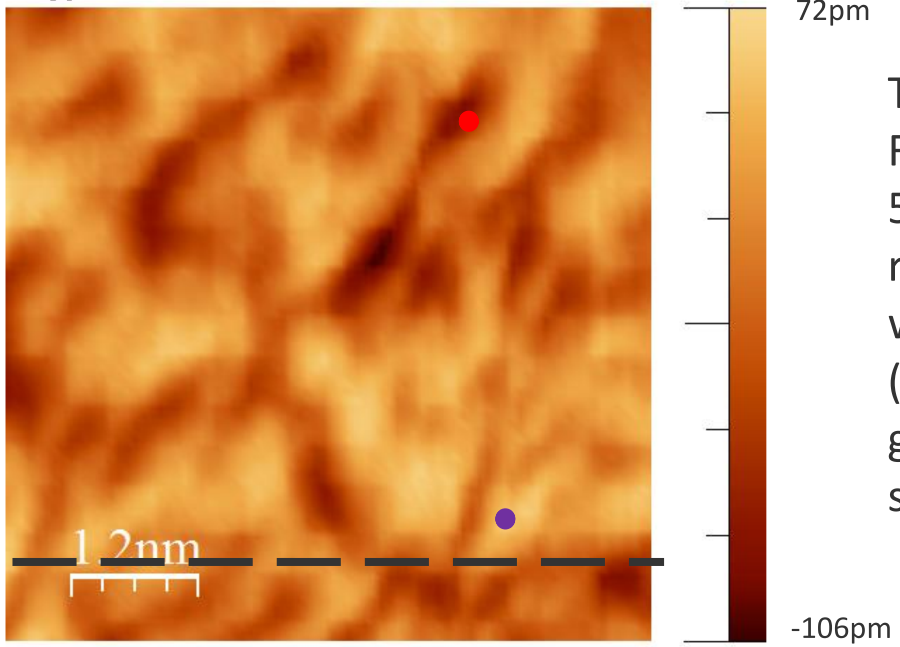
Abstract

Electron energy-loss spectroscopy (EELS) in the transmission electron microscope (TEM) is used to obtain high-resolution information on the composition and the type of chemical bonding of materials. Spectrum imaging, where a full EEL spectrum is acquired and stored at each pixel in the image, gives an exact correlation of spatial and spectral features. However, determining and extracting the important spectral components from the large amount of information contained in a spectrum image (SI) can be difficult. This paper demonstrates that principal component analysis of EEL SIs can be used to extract chemically relevant components. With weighted or two-way scaled principal component analysis, both compositional and bonding information can be extracted. Mapping of the chemical variations in a partially reduced titanium dioxide sample and the orientation-dependent bonding in boron nitride and carbon nanotubes are given as examples.

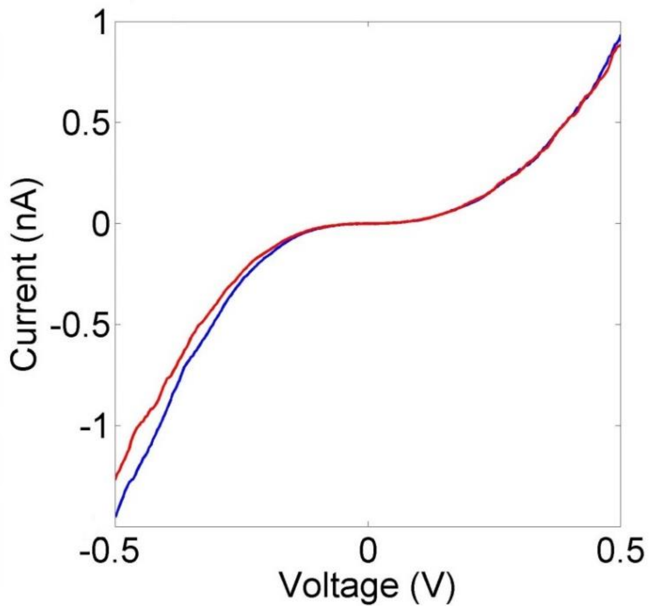
Why did the PCA on EELS started to grow in 2005 – 2010?

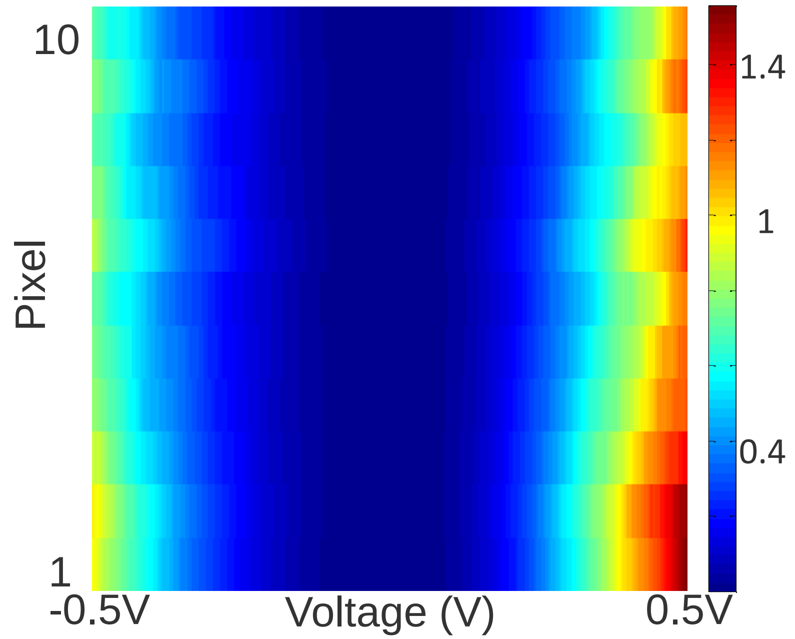
Grain boundary by STM





Topographical STM of FeSeTe, T = 82K 15x15nm^2, 50mV, 100pA, white rectangle represents area where CITS was performed; (b) CITS 80x80 pixel graphical average of the spectrographic data.





M. Ziatdinov, A. Maksov, L. Li, A. Sefat, P. Maksymovych, and S.V. Kalinin, *Deep data mining in a real space: Separation of intertwined electronic responses in a lightly-doped* $BaFe_2As_2$, Nanotechnology **27**, 475706 (2016).

Eigenvectors and loadings

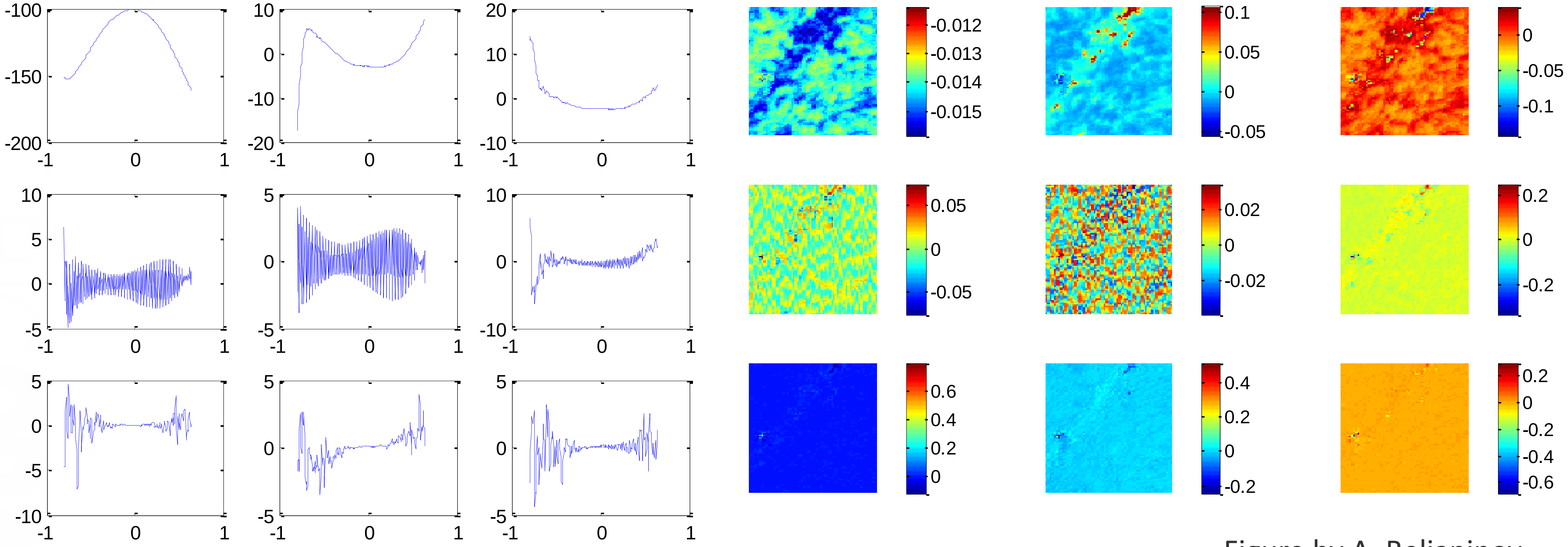


Figure by A. Belianinov