



Computational Colour
and Spectral Imaging

“Advanced Colour and Spectral Imaging”

Chapter 5: Spectral estimation

Javier Hernández-Andrés and Eva M. Valero
javierha@ugr.es **valerob@ugr.es**
Colour Imaging Lab (colorimaginglab.ugr.es)



**UNIVERSIDAD
DE GRANADA**

Departamento de Óptica, Facultad de Ciencias,
Universidad de Granada, 18071-Granada (SPAIN)

1. How are the spectral curves we are dealing with?

- Reflectances, Illuminants, Color Signals

2. Dimensionality reduction

- Principal Component Analysis (PCA)
- Independent Component Analysis (ICA)
- Non-linear approaches of PCA and ICA (not in this course)
- Alternative methods for dimensionality reduction: NNMF
- Multidimensional scaling (not in this course)

3. Algorithms for spectral estimation

- Matrix notation
- Linear models
- Regression models
- Neural Network Model (not in this course)
- Others methods

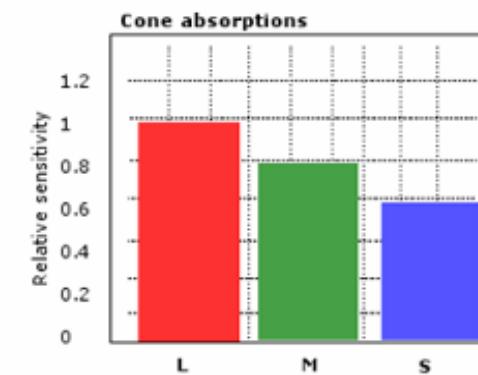
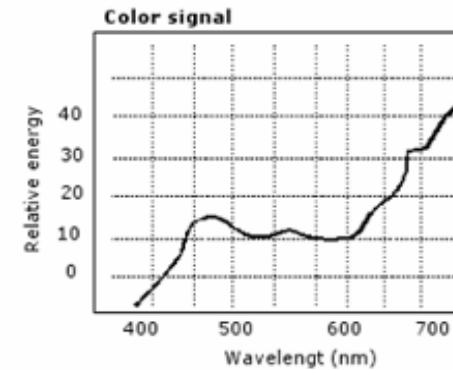
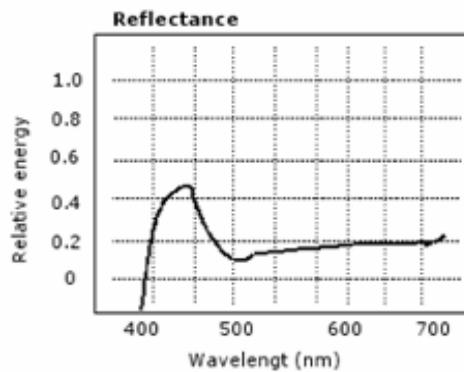
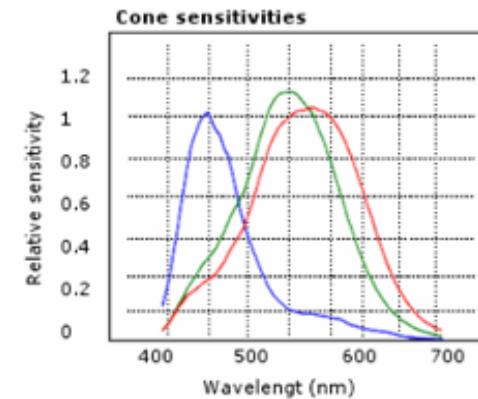
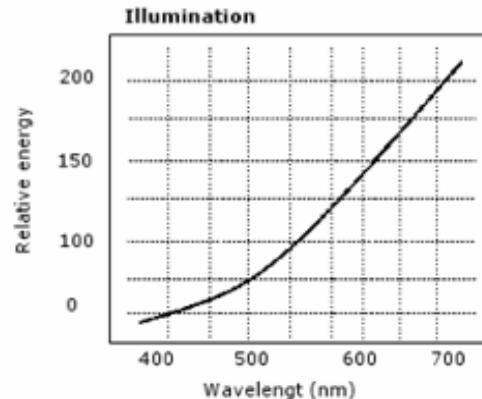
4. Selection of samples

5. Selection of filters (or LEDs)

6. Influence of noise

1. How are the spectral curves we are dealing with?

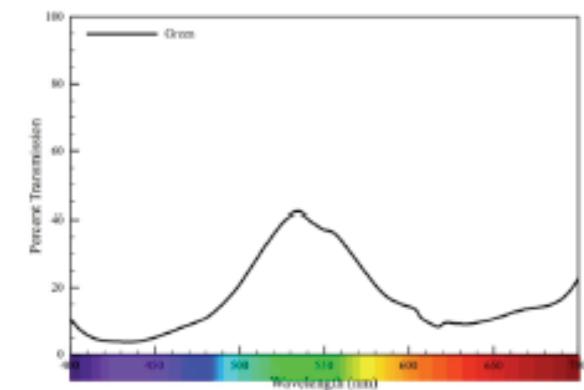
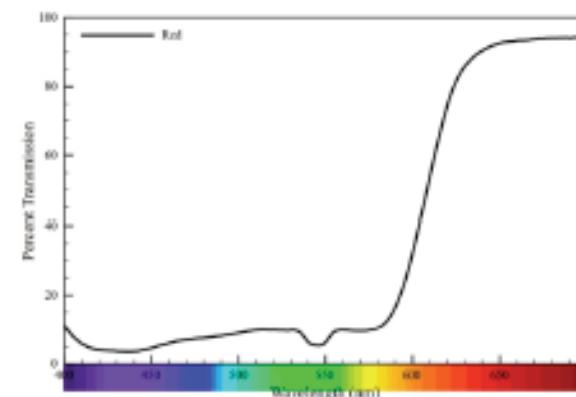
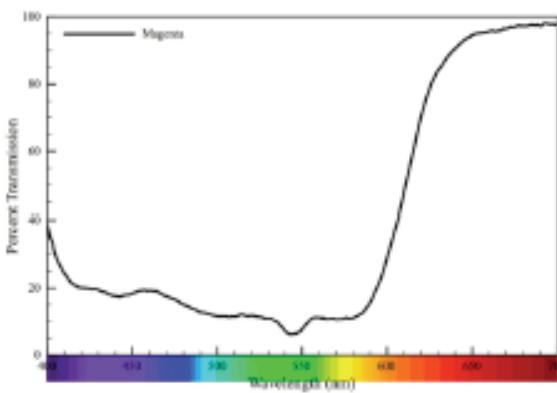
- Reflectances, Illuminants, Color Signals



1. How are the spectral curves we are dealing with?

- Reflectances

Fraction of light reflected by a surface: as a function of wavelength.

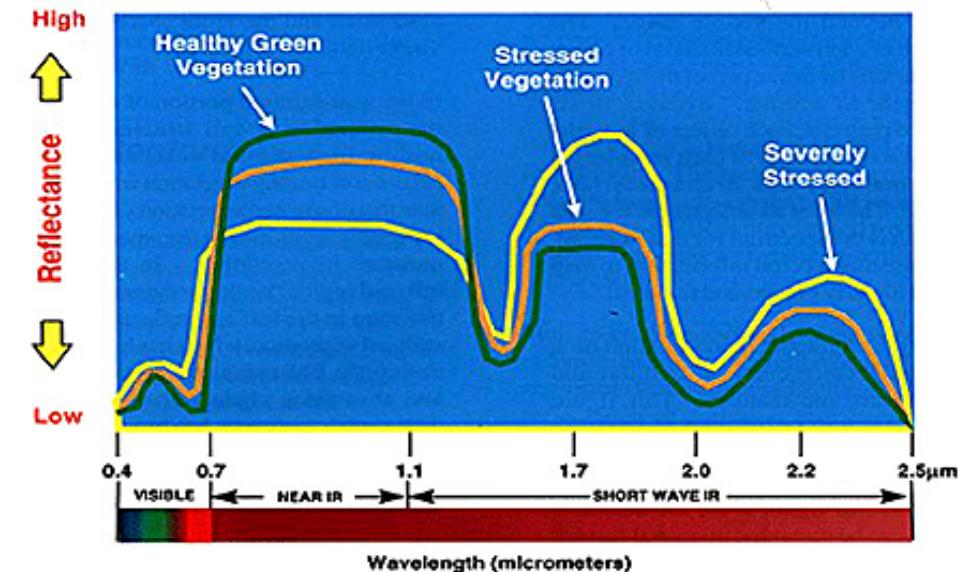
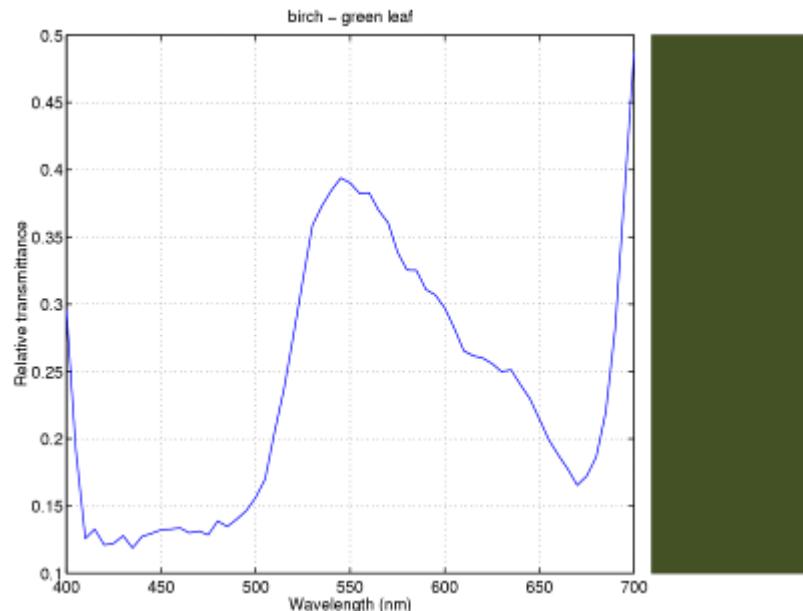


How we could describe them from a mathematical or statistical point of view?

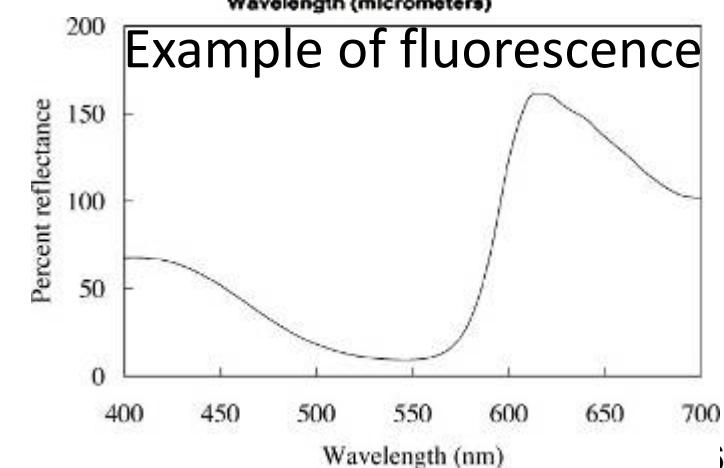
1. How are the spectral curves we are dealing with?

- Reflectances

-Usually reflectances are quite smooth functions.

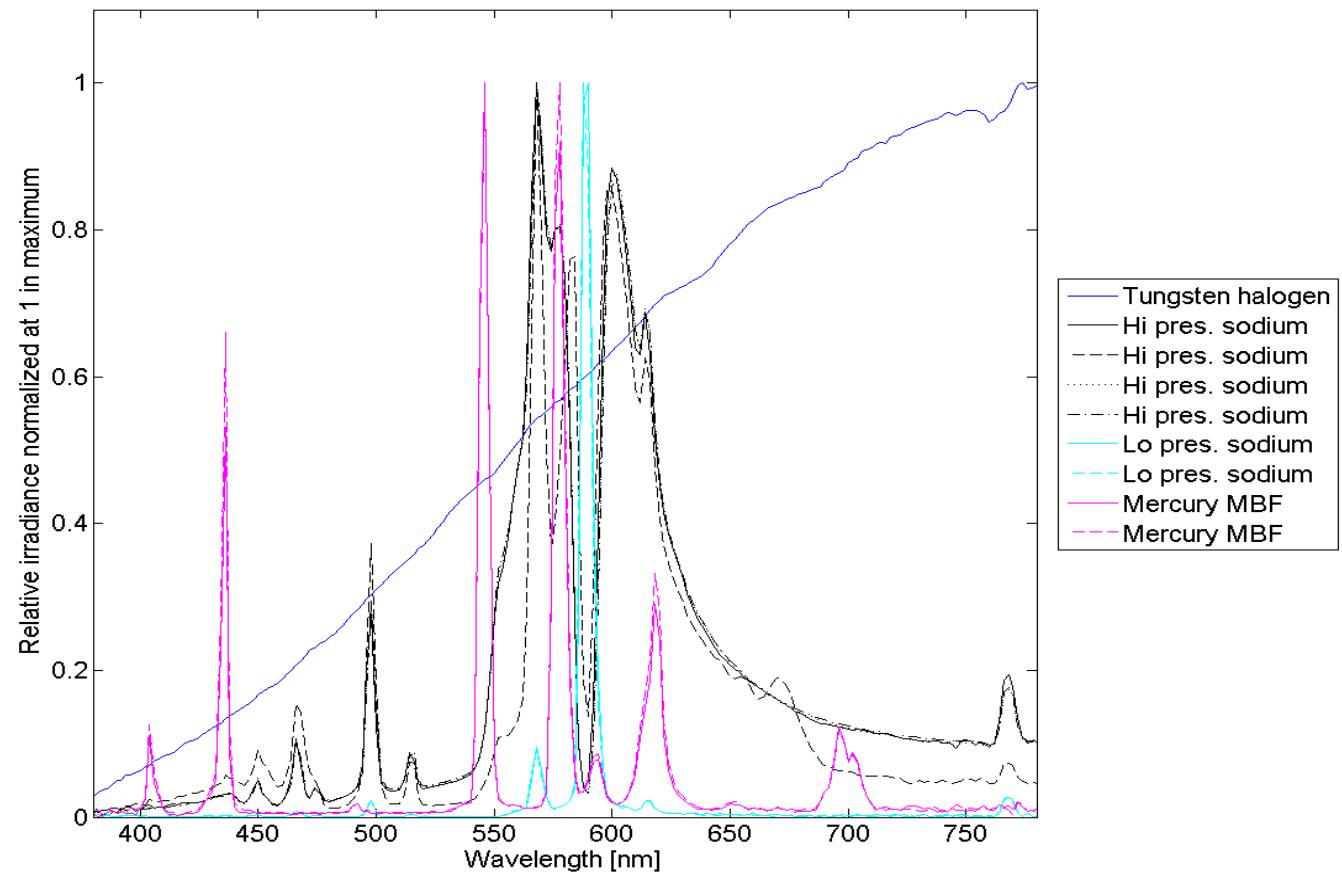


-But subject to measurement artifacts (watch especially the ends of the spectrum!)



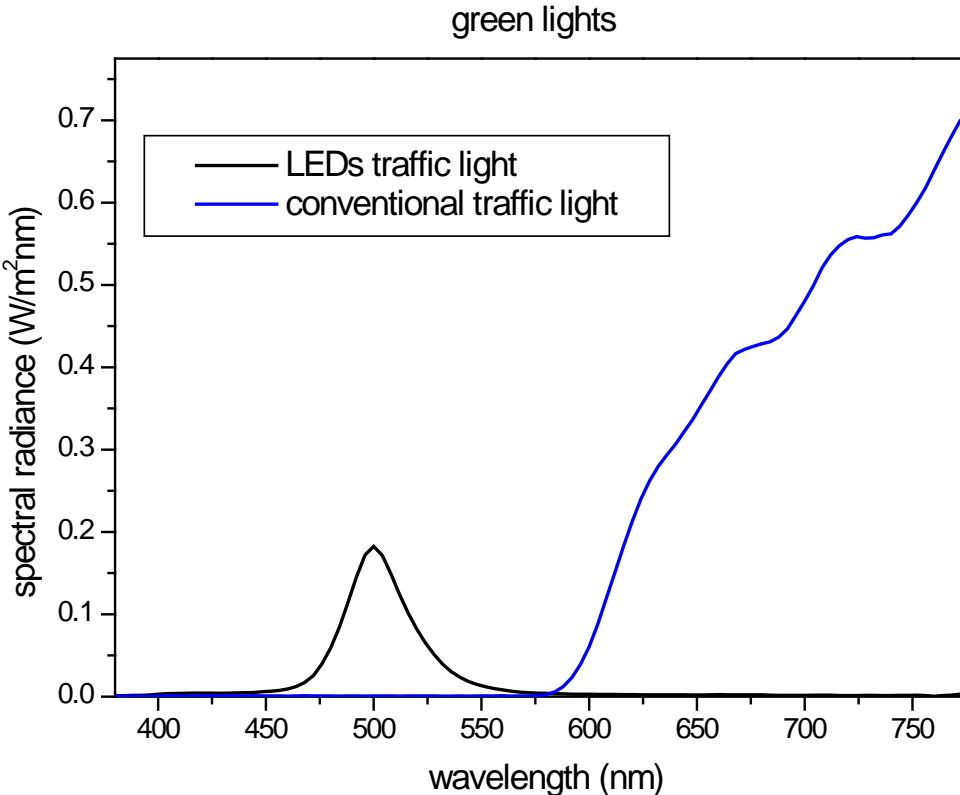
1. How are the spectral curves we are dealing with?

- Illuminants, sources of light
 - Sources of light. Characterized by their SPDs (spectral power distributions).



1. How are the spectral curves we are dealing with?

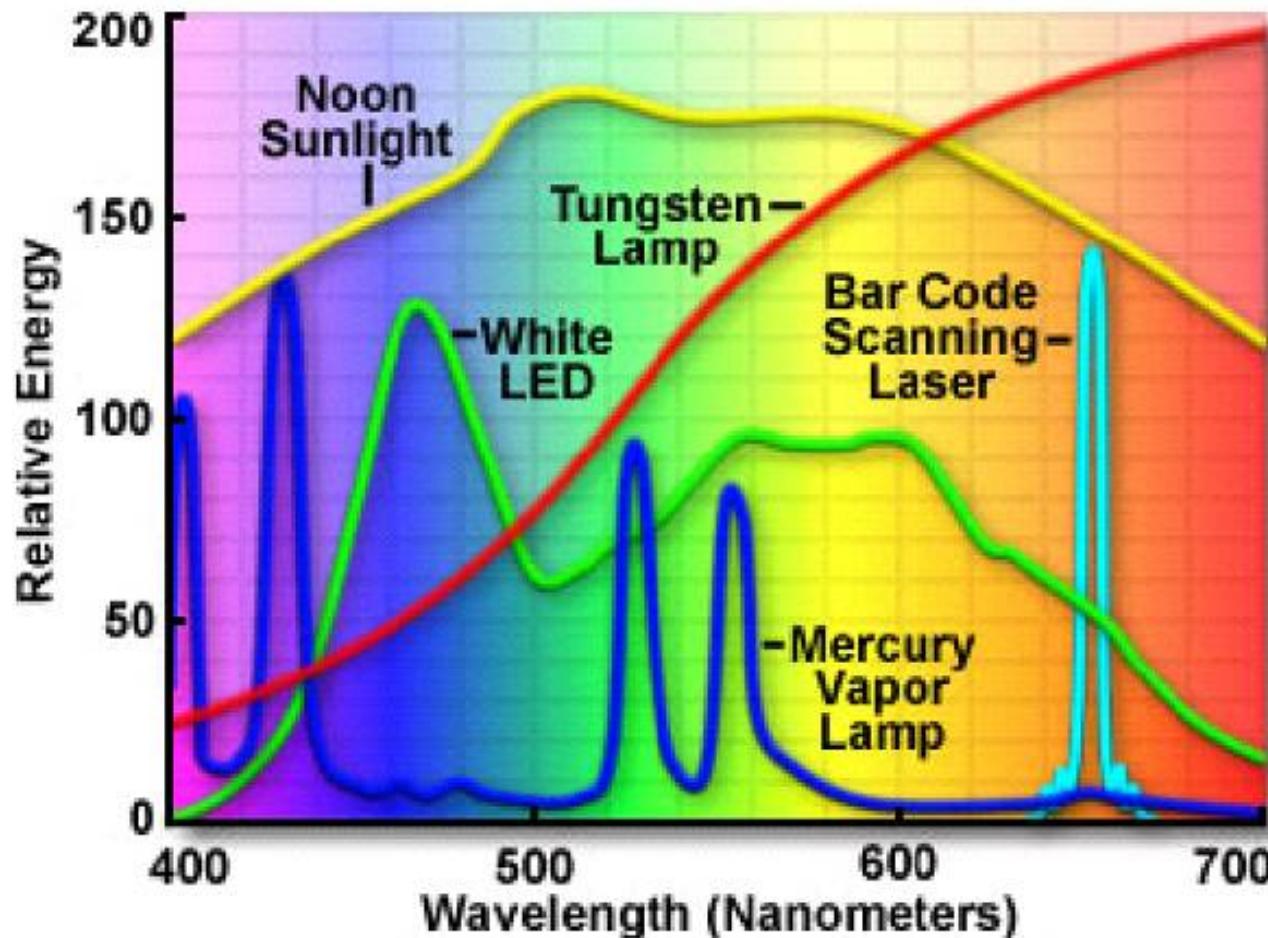
- Illuminants, sources of light



Artificial light sources: low or high pressure sodium (street lamps), incandescence (old traffic light), LEDs (new traffic lights, cars, etc.), tungsten-halogen lights (car lights), xenon lights (car lights, etc.)

1. How are the spectral curves we are dealing with?

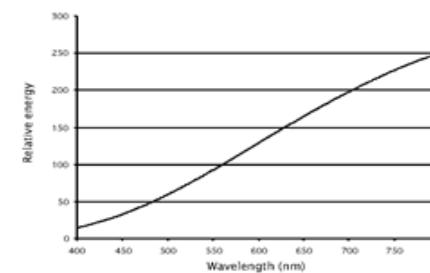
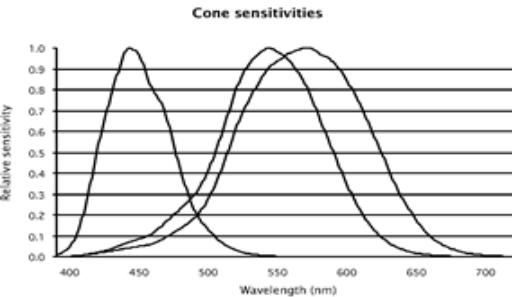
- Illuminants, sources of light



1. How are the spectral curves we are dealing with?

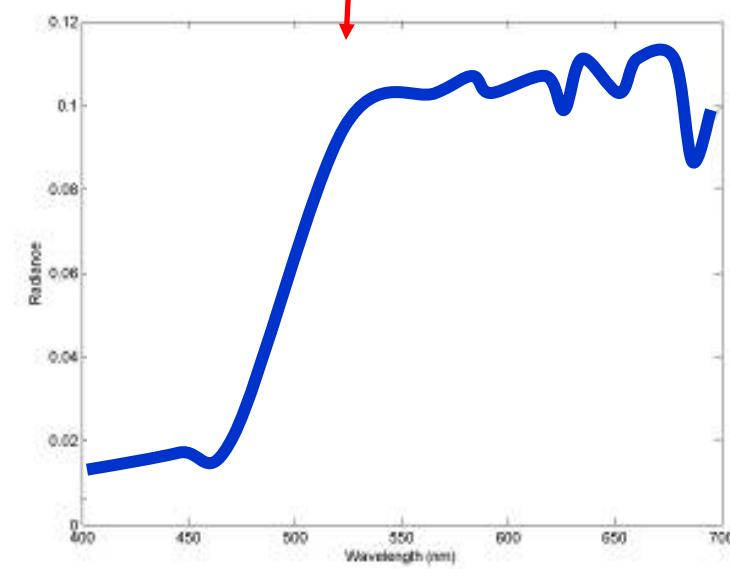
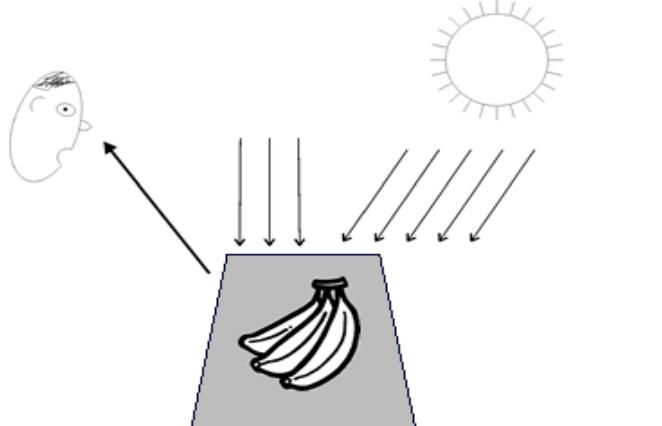
- Color signals

$$C_\lambda = E_\lambda R_\lambda$$



Cone signal
(Relative)

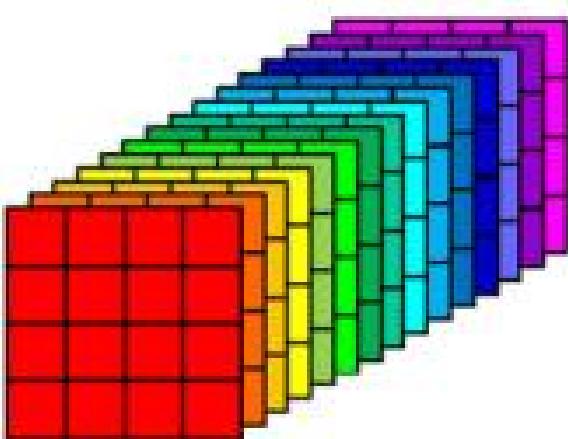
L	M	S
1.00000	0.65890	0.00011



How many samples do we need to recover the spectrum of a color signal, an illuminant or a reflectance?

- What is the required accuracy in the recovery?
- Are the samples equispaced?
- Are the samples just mathematical samples o samples obtained with real sensors?
- Real sensors: narrow or wide band?
- Shannon-Whittaker's theorem?
- Fourier Transform? High frequencies or low frequencies?
- Are the samples valid for all the color signals spectra, the illuminant spectra and the reflectance spectra? Are they universal or should be application-dependent?
- Can we take advantage of the correlation among spectral curves?

Spectral images



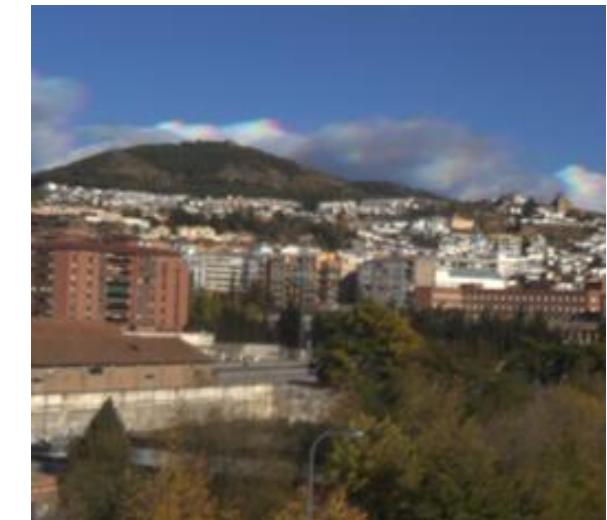
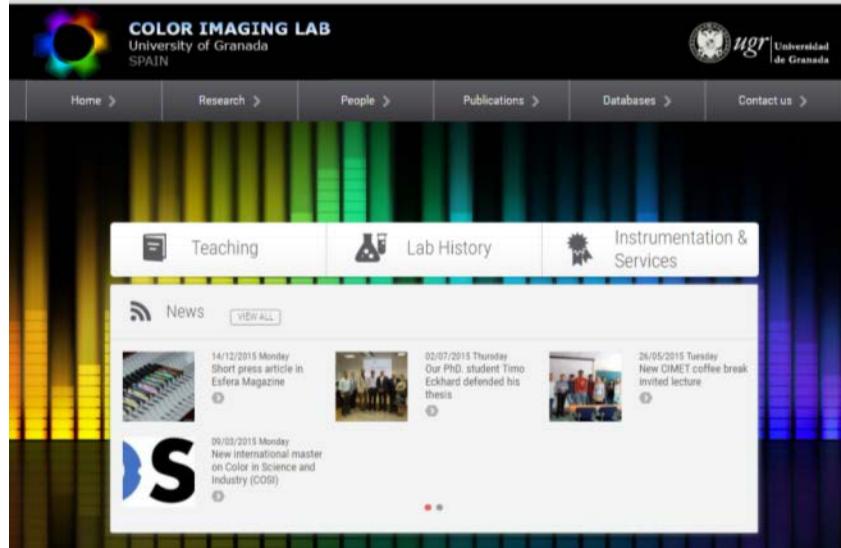
K-band
Multispectral image

Number of channels / bands	Name
1	Monochrome
3	RGB or trichromatic
From 4 to 9	Multispectral
From 10 to 100	Hyperspectral
More than 100	Ultraspectral

MEMORY REQUIREMENTS OF IMAGES

Image size	256x256	512x512	1024x1024
gray-level image	65 kB	262 kB	1 MB
color (RGB-) image	196 kB	786 kB	3 MB
spectral, 5 nm resol(61sam)	4 MB	16 MB	64 MB

UGR Hyperspectral Image database



UGR Hyperspectral Image database:

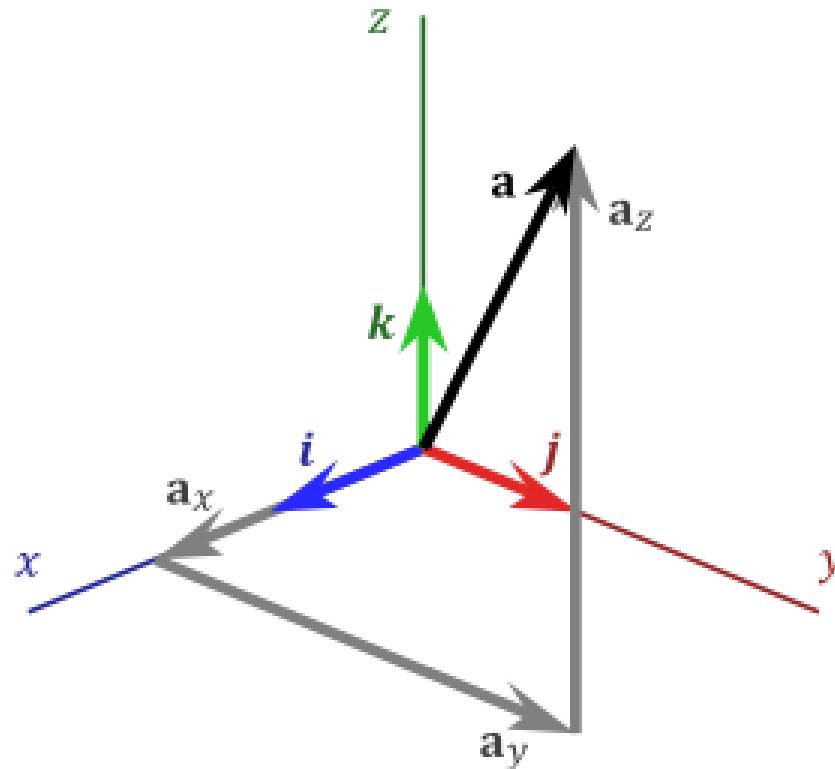
- 14 hyperspectral reflectance factor images.
- acquired using a volumetric Bragg-grating based hyperspectral imager: (camera V-EOS by Photon etc) .
- spatial resolution: most of **1000 × 900 pixels**.
- spectral range: from **400 nm to 1000 nm in 10 nm (61 channels)**.
- Image format: TIFF, 16 bits per channel
- **Image sizes: around 155M per image.**
- To get the hyperspectral data in the range of [0,1], we need to normalize it by 2^{16} after reading it from the tiff file.
For example in Matlab, we can use the following command to read out a $1000 \times 900 \times 61$ data matrix in range [0,1] with single precision: `im = imread('scene1_sp.tiff')/216`

2. Dimensionality reduction

- Principal Component Analysis (PCA)
- Independent Component Analysis (ICA)
- Non-linear approaches of PCA and ICA (not in this course)
- Alternative methods for dimensionality reduction: NNMF
- Multidimensional scaling (not in this course)

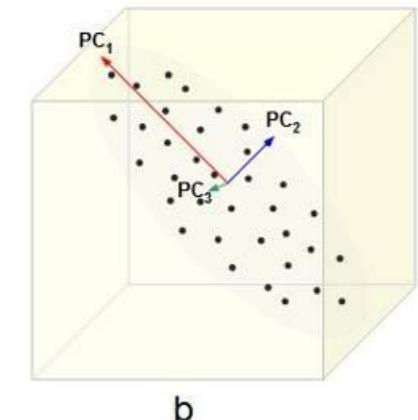
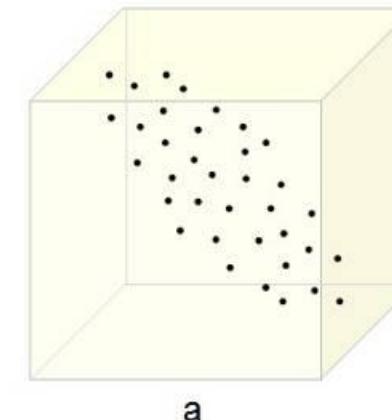
2. Dimensionality reduction: Principal Component Analysis

In a 3D space we need 3 numbers to specify any vector



$$\mathbf{a} = a_x \hat{\mathbf{i}} + a_y \hat{\mathbf{j}} + a_z \hat{\mathbf{k}}$$

$$\hat{\mathbf{i}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad ; \quad \hat{\mathbf{j}} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad ; \quad \hat{\mathbf{k}} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



2. Dimensionality reduction: Principal Component Analysis

In a **n multidimensional** space we need **n numbers** to specify any spectrum

$$r(\lambda) = \sum_{k=1}^n a_k V_k(\lambda)$$

a_k coefficients

$V_k(\lambda)$ vectors (canonical base)

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$r(\lambda) = (3, 1, 6, -2, \dots, 5)$$

$$r(\lambda) = 3 \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix} + 1 \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix} + 6 \cdot \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \dots \\ 0 \end{pmatrix} - 2 \cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \dots \\ 0 \end{pmatrix} + \dots + 5 \cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dots \\ 1 \end{pmatrix}$$

2. Dimensionality reduction: Principal Component Analysis

In a **n multidimensional** space we need **n numbers** to specify any spectrum

$$r(\lambda) = \sum_{k=1}^n a_k V_k(\lambda)$$

a_k coefficients
 $V_k(\lambda)$ vectors

a_k are the projections of $r(\lambda)$ over $V_k(\lambda)$

$$a_k = \langle r(\lambda) | V_k(\lambda) \rangle = r(\lambda) \bullet V_k(\lambda)$$

inner product
(or scalar product or dot product)

$$r(\lambda) = \sum_{k=1}^n \langle r(\lambda) | V_k(\lambda) \rangle V_k(\lambda)$$

Could we truncate this sum without loosing accuracy?

2. Dimensionality reduction: Principal Component Analysis

In a **n multidimensional** space we need **n numbers** to specify any spectrum

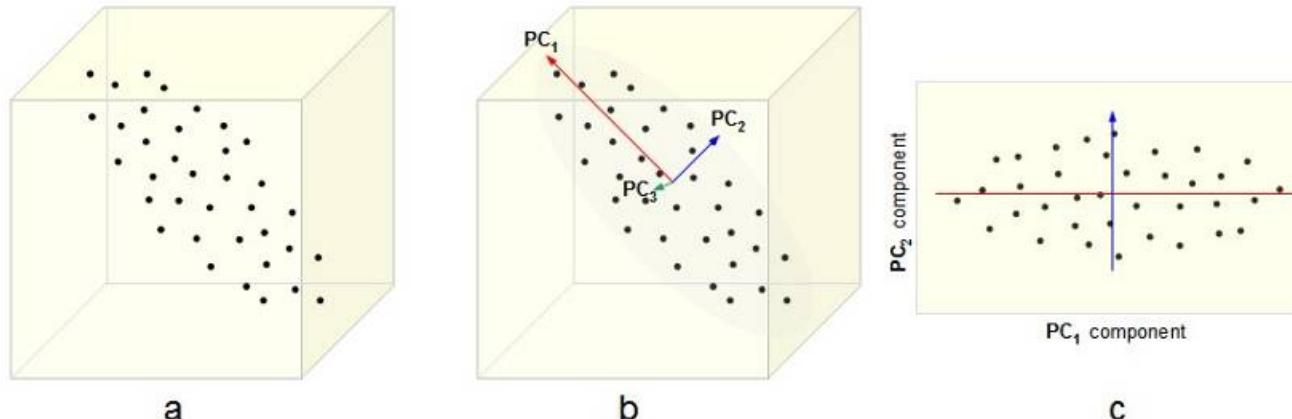
Could we truncate this sum without loosing accuracy?
How many? Which ones?

$$r(\lambda) = \sum_{k=1}^n a_k V_k(\lambda)$$

One UGR Hyperspectral Image database:

- spatial resolution: **1000 × 900 pixels**.
- spectral range: from **400 nm to 1000 nm in 10 nm (61 channels)**.
- **image sizes: around 155M per image**.
- if only 8 eigenvectors are needed (we must confirm) the size of the compressed image will $155\text{MB} * (8/61) = 20 \text{ MB}$

2. Dimensionality reduction: Principal Component Analysis



Lengths and orientation of the axes: **eigenvalues and eigenvectors (covariance matrix YY^t)**

- Idea:
 - Given data points in d-dimensional space, project into lower dimensional space while preserving as much information as possible
 - In particular, choose projection that minimizes the squared error in reconstructing original data

2. Dimensionality reduction: Principal Component Analysis

PCA [1] is a technique used to reduce dimensionality of suitable datasets. This means that if a vector or a set of vectors \mathbf{X} is included in one subspace of \mathbb{R}^N , “we” can identify its principal components and **express it in that subspace with a suitable basis and a given number of components.**

This will necessarily involve loosing some information contained in the vector’s data, but if the dimensionality reduction is appropriate, then it will not be relevant or important information.

[1] Jolliffe, I.T. Principal Component Analysis. 2nd Edition.
Springer, 2002.

2. Dimensionality reduction: Principal Component Analysis

- Thus, eigenvectors and eigenvalues will be the basis of PCA
- Several methods to solve the PCA problem
 - Singular Value Decomposition (SVD)
 - Eigenvector of the covariance matrix:

Find some orthonormal matrix \mathbf{P} where $\mathbf{Y} = \mathbf{P}\mathbf{X}$ such that $\mathbf{C_Y} \equiv \frac{1}{n-1}\mathbf{Y}\mathbf{Y}^T$ is diagonalized. The rows of \mathbf{P} are the *principal components* of \mathbf{X} .

2. Dimensionality reduction: Principal Component Analysis

Singular Value Decomposition (SVD)

(Remember slides from Chapter 3)

The calculation of the eigenvalues and eigenvectors involves a SVD of the covariance matrix \mathbf{C}_Y and a diagonalization procedure. So we will find a matrix \mathbf{P} , orthonormal (this means $\mathbf{P}\mathbf{P}^t$ gives the unity matrix as a result), and the matrix \mathbf{Y} would be the result of projecting \mathbf{P} onto the data set \mathbf{X} . The eigenvectors will be given by the rows of \mathbf{P} , and the eigenvalues by the coefficients of the diagonalized matrix \mathbf{D} . We have to find a matrix \mathbf{A} which allows us to express the covariance matrix as $\mathbf{P}\mathbf{A}\mathbf{P}^t$

2. Dimensionality reduction: Principal Component Analysis

Singular Value Decomposition (SVD)

(Remember slides from Chapter 3)

Usually, the diagonal matrix is sorted by coefficient value in descending order, establishing a priority ranking for the eigenvectors as a function of the degree of variance of the data that they are able to cover.

$$\mathbf{Y} = \mathbf{P}\mathbf{X}$$

$$\mathbf{C}_y = (\mathbf{Y}\mathbf{Y}^T)/(n-1)$$

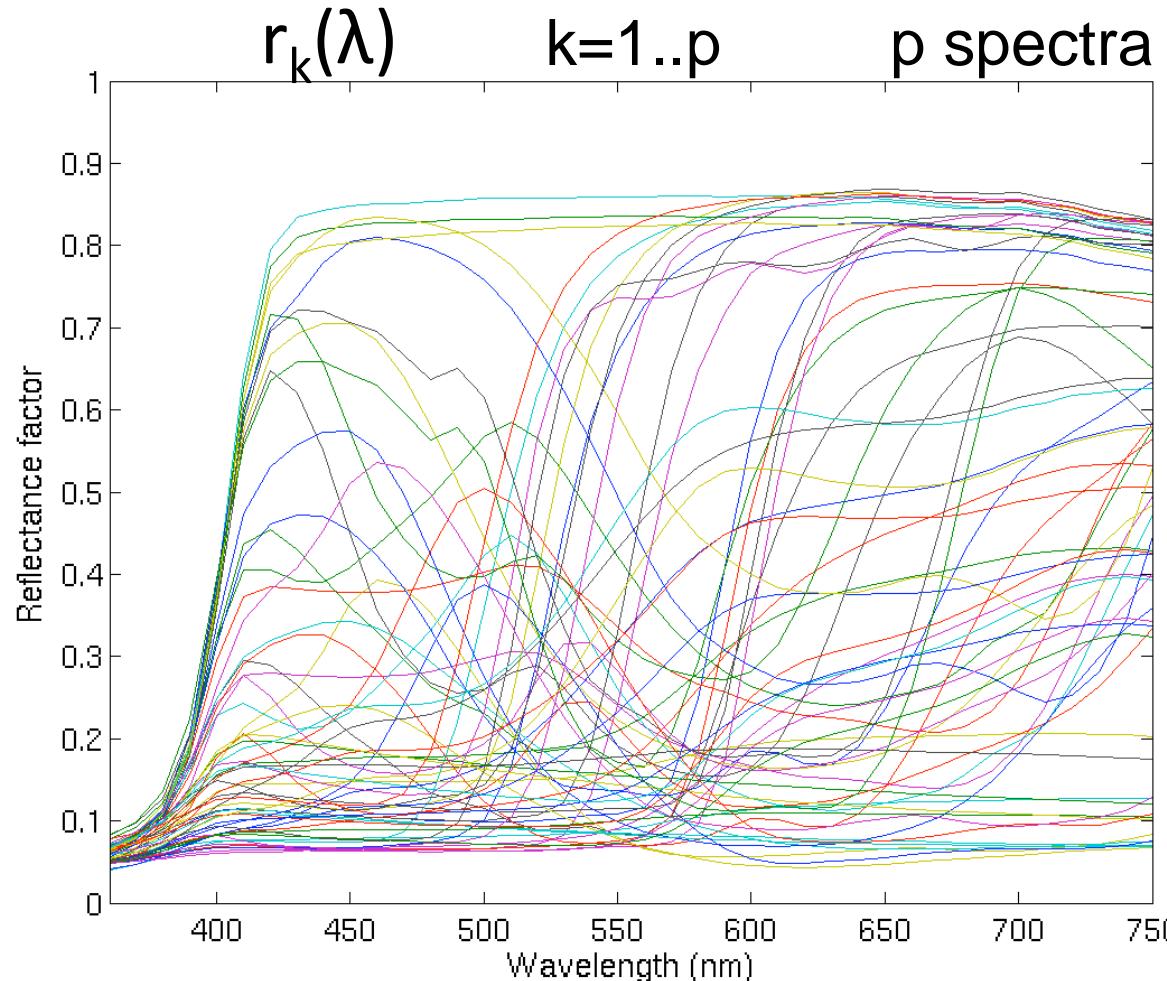
$$\mathbf{C}_y = (\mathbf{P}\mathbf{A}\mathbf{P}^T)/(n-1)$$

$$\mathbf{C}_y = \mathbf{D}/(n-1)$$

2. Dimensionality reduction: Principal Component Analysis

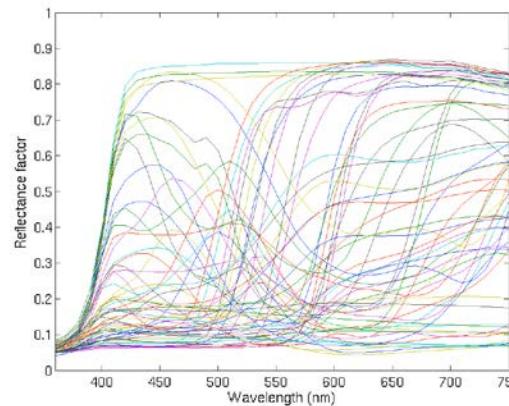
How to do with our set of spectra?

p spectral functions (radiances, illuminants or reflectances)



2. Dimensionality reduction: Principal Component Analysis

$r_k(\lambda)$



1) *correlation matrix*:

$$R_{ij}^k = r_k(\lambda_i)r_k(\lambda_j) ; \quad 1 \leq i, j \leq n$$

$$n = 61 \text{ for } 400 \leq \lambda \leq 700 \text{ nm}$$

$$\Delta\lambda = 5 \text{ nm}$$

$$R_T = \sum_{k=1}^p R^k \quad \text{p spectra}$$

R_T is a square matrix of $p \times p$ dimensions (i.e. 61×61)

2. Dimensionality reduction: Principal Component Analysis

R_T is a square matrix of pxp dimensions (i.e. 61x61)

SVD can be applied to this matrix to obtain the eigenvalues and eigenvectors. In Matlab, to obtain the PCA basis vectors you can use either [svd.m](#), [eig.m](#) or (in more recent versions), the specific function [pca.m](#).

[svd.m](#)

This function returns a vector of singular values

```
s = svd(X)  
[U,S,V] = svd(X)  
[U,S,V] = svd(X,0)  
[U,S,V] = svd(X,'econ')
```

[eig.m](#)

This function returns a column vector containing the eigenvalues of square matrix A

```
e = eig(A)  
[V,D] = eig(A)  
[V,D,W] = eig(A)  
e = eig(A,B)  
[V,D] = eig(A,B)  
[V,D,W] = eig(A,B)
```

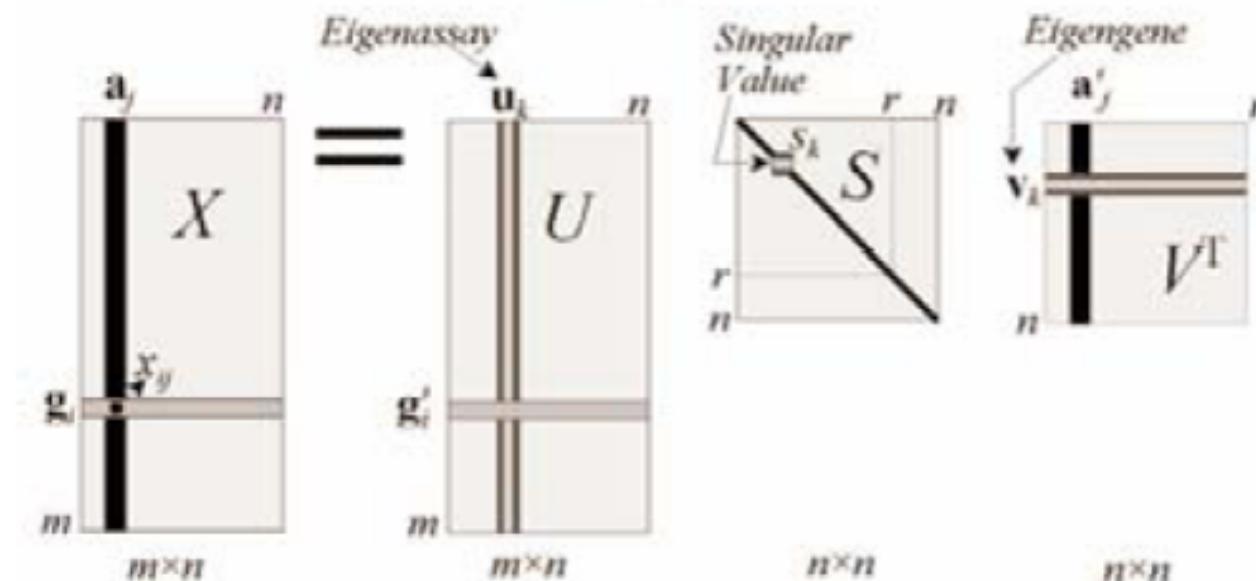
[pca.m](#)

This function returns the principal component coefficients, also known as loadings, for the n-by-p data matrix X.

```
coeff = pca(X)  
coeff = pca(X,Name,Value)
```

2. Dimensionality reduction: Principal Component Analysis

$$X = USV^T$$



Data X , one
row per data
point

US gives
coordinates
of rows of X
in the space
of principle
components

S is diagonal
 $S_k > S_{k+1}$,
 S_k^2 is kth
 largest
 eigenvalue

- Rows of V^T are unit length eigenvectors of $X^T X$.
- If cols of X have zero mean, then $X^T X = c \Sigma$ and eigenvects are the Principle Components

2. Dimensionality reduction: Principal Component Analysis

How many eigenvectors and eigenvalues?

Could we truncate this sum without loosing accuracy? *How many? Which ones?*

Remember **the eigenvectors are sorted by their corresponding eigenvalues** in descending order, establishing a **priority ranking** for the eigenvectors as a function of the degree of variance of the data that they are able to cover

- The magnitude of the eigenvalues corresponds to the variance of the data along the eigenvector directions

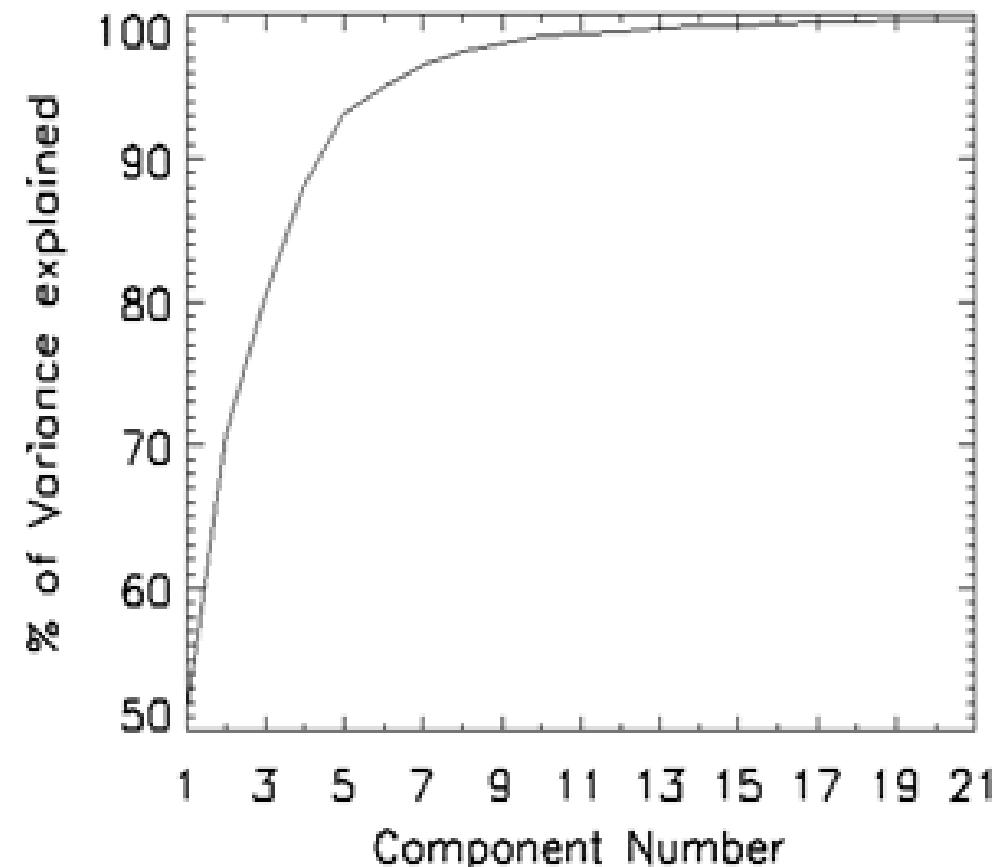
2. Dimensionality reduction: Principal Component Analysis

How many eigenvectors and eigenvalues?

- The magnitude of the eigenvalues corresponds to the variance of the data along the eigenvector directions
- To choose K (*see the elbow graph*), you can use the following criterion

$$VAF = \frac{\sum_{i=1}^K \lambda_i}{\sum_{i=1}^N \lambda_i}$$

VARIANCE ACCOUNTED FOR



Sometimes: Accumulated Energy

*related to the rank of the diagonalized covariance matrix

2. Dimensionality reduction: Principal Component Analysis

How many eigenvectors
and eigenvalues?

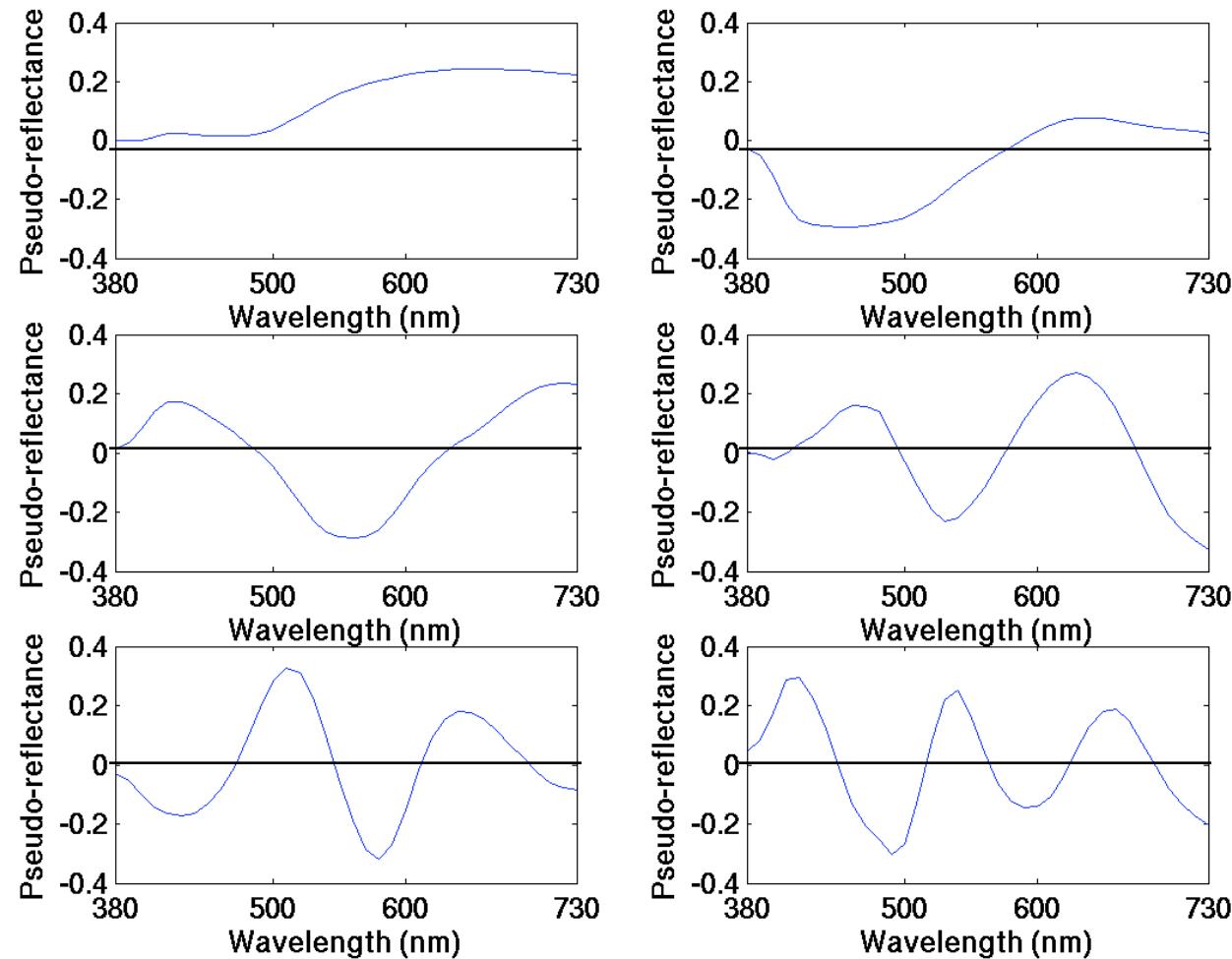
We perform PCA on three channel (R, G and B) data and the eigenvalues corresponding to the eigenvectors are 2, 1.5 and 0.5.

What will be the variance accounted for (VAF) if we consider the first two eigenvectors?

- a) 0.5
- b) 0.875
- c) 1.0
- d) 0.6875

2. Dimensionality reduction: Principal Component Analysis

First six
eigenvectors



What would happen if the first three eigenvectors are the spectral sensitivities of a camera R, G and B channels?

2. Dimensionality reduction: Principal Component Analysis

Reconstruction

1) exact:

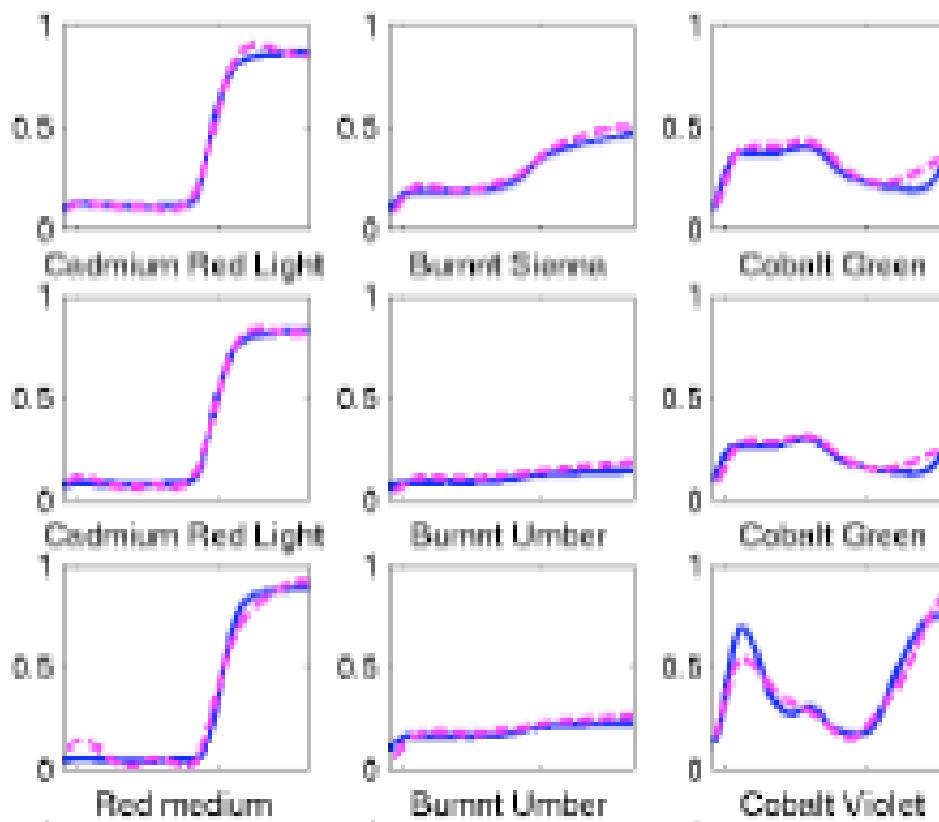
$$r(\lambda) = \sum_{k=1}^n \langle r(\lambda) | V_k(\lambda) \rangle V_k(\lambda)$$

2) approximated or recovered

or reconstructed or estimated:

$$r_R(\lambda) = \sum_{k=1}^m \langle r(\lambda) | V_k(\lambda) \rangle V_k(\lambda)$$

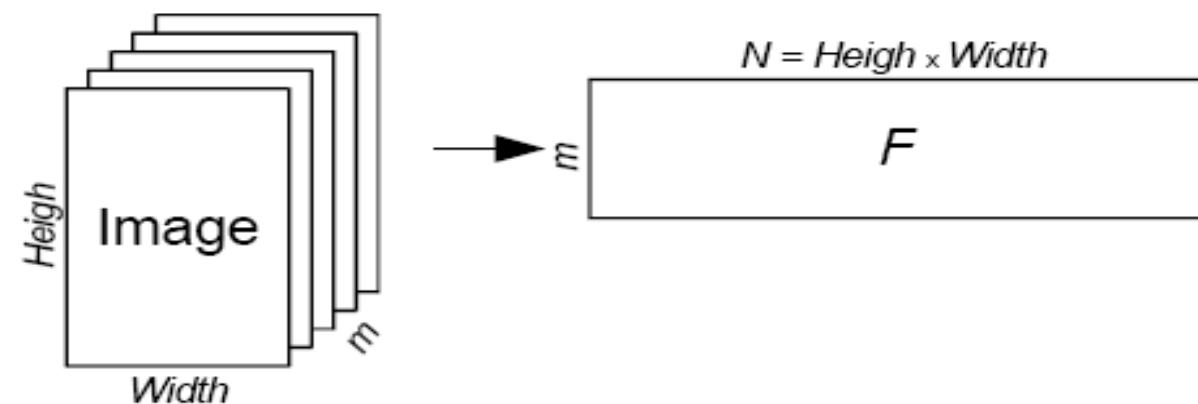
with $m < n$



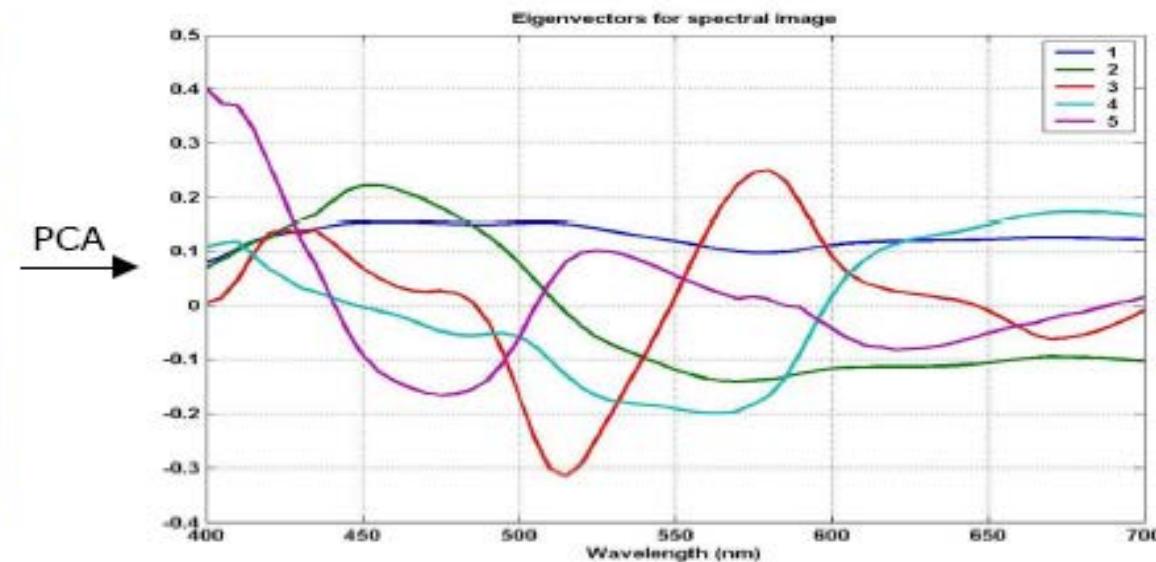
Which spectral metric to evaluate the similarity between $r_R(\lambda)$ and $r(\lambda)$?

2. Dimensionality reduction: Principal Component Analysis

PCA may be applied to spectral images



Spectral image as RGB-image

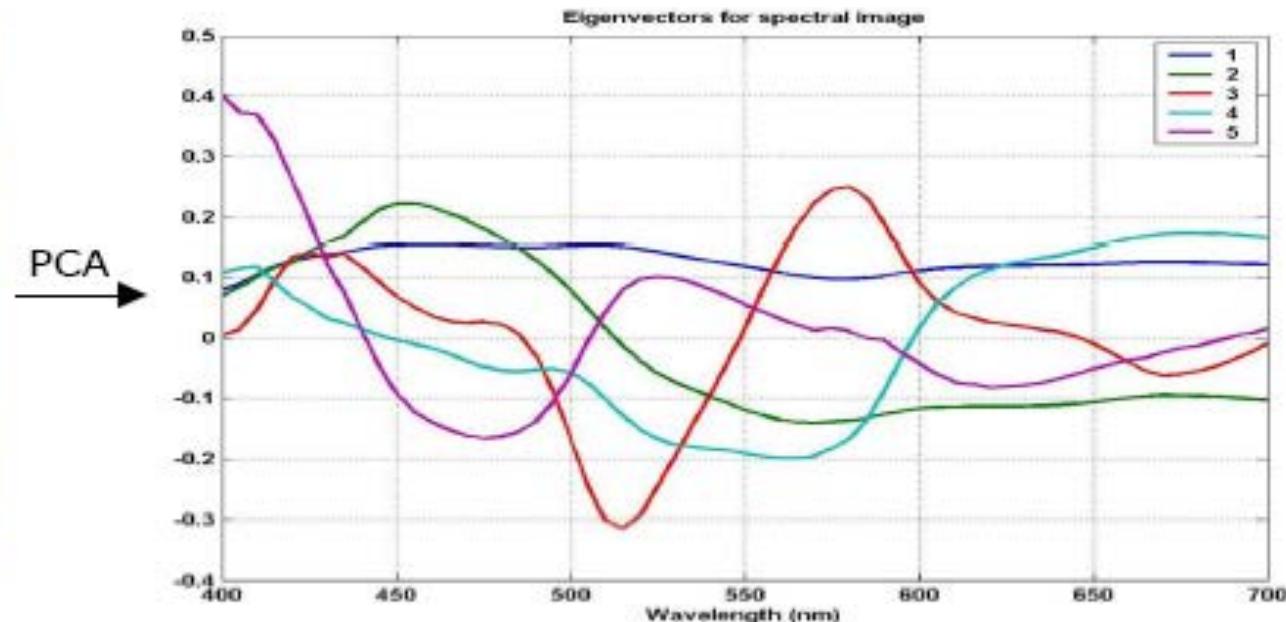


2. Dimensionality reduction: Principal Component Analysis

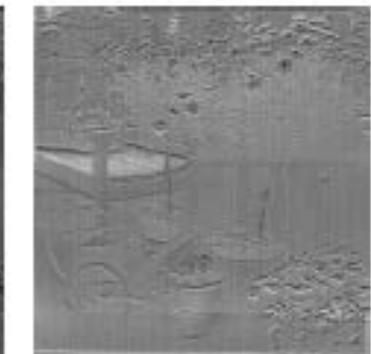
PCA may be applied to spectral images



Spectral image as RGB-image



Inner-product images between the spectral image and eigenvectors:



2. Dimensionality reduction: Principal Component Analysis

Cases studies if you want to know more....

García-Beltran et al. (1998)

PCA on reflectances from 5574 samples of acrylic paint on paper

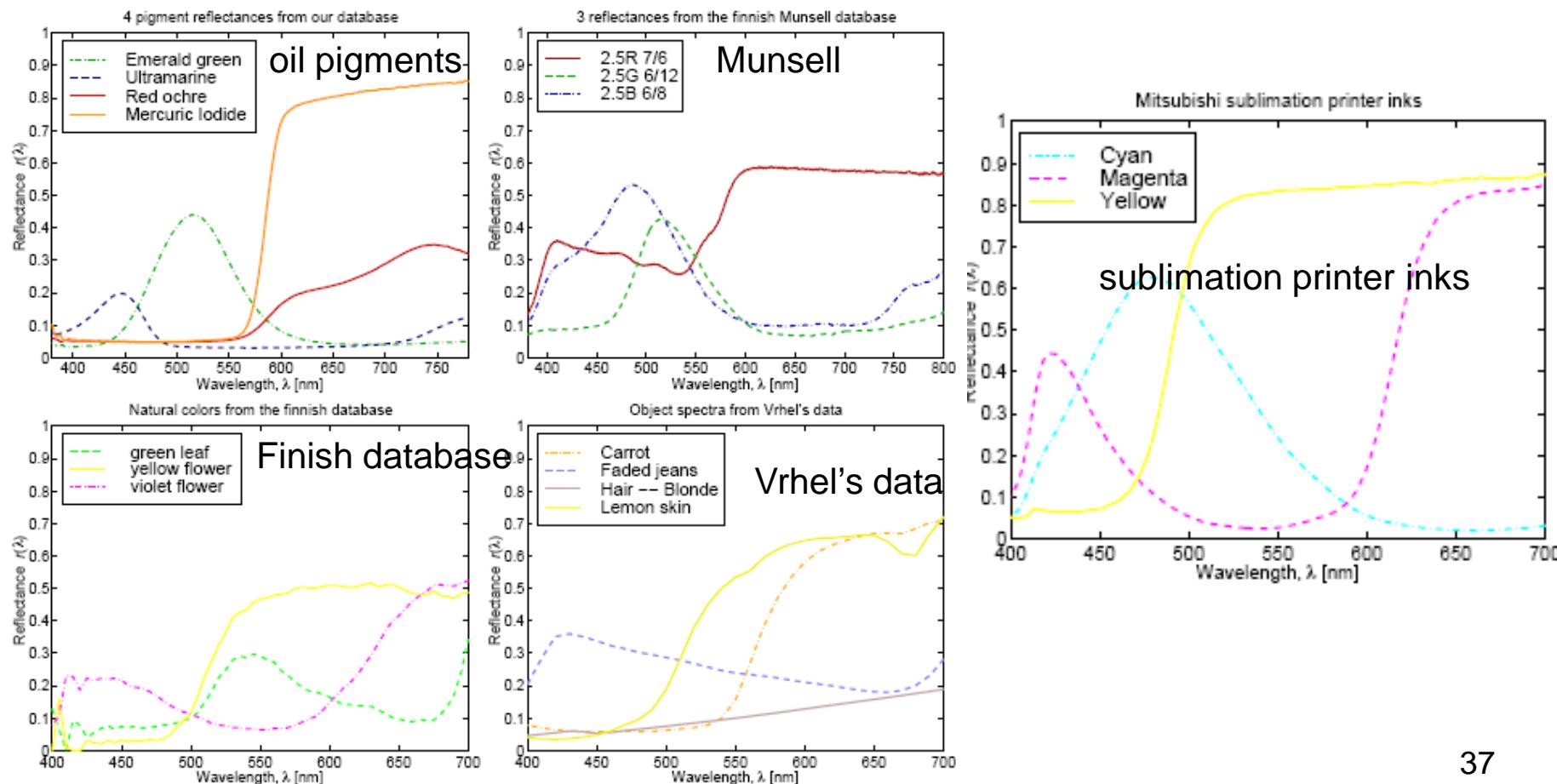
Romero et al. (1997)

PCA on natural and artificial illuminants: 99 measurements of daylight, or 48 daylight plus 7 CIE standard illuminants and 7 blackbody curves

2. Dimensionality reduction: Principal Component Analysis

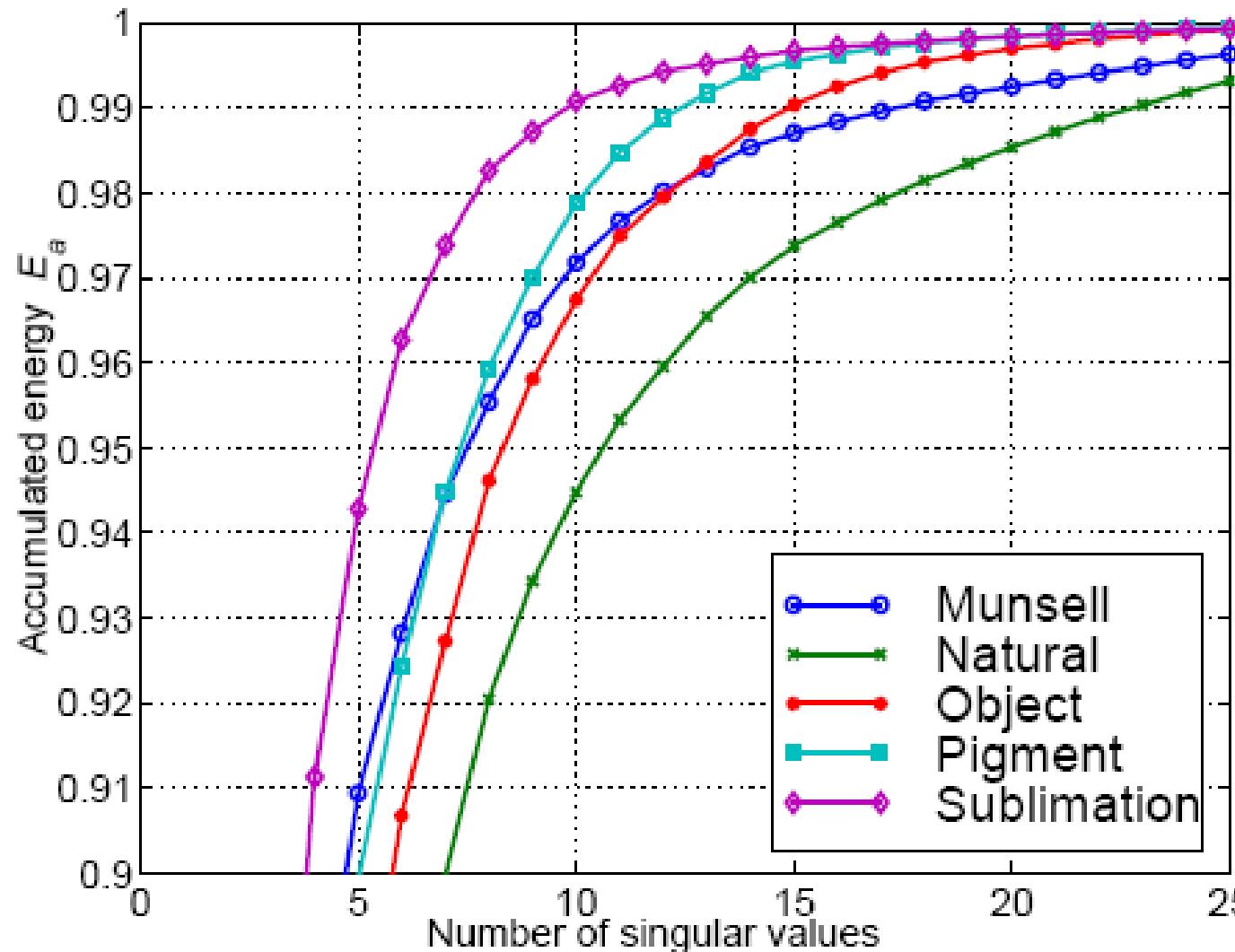
Cases studies if you want to know more....

Hardeberg (section 6.4). Reflectances from 5 different datasets and PCA using each individual group



2. Dimensionality reduction: Principal Component Analysis

how closely related are two different sets of eigenvectors?



*Remember
slide n. 29*

*From Hardeberg
(section 6.4).*

2. Dimensionality reduction: Principal Component Analysis

how closely related are two different sets of eigenvectors?

How many eigenvectors to reach a VAF threshold?

E_{req}	MUNSELL	NATURAL	OBJECT	PIGMENT	SUBLIM
0.90	5	8	6	6	4
0.99	18	23	15	13	10

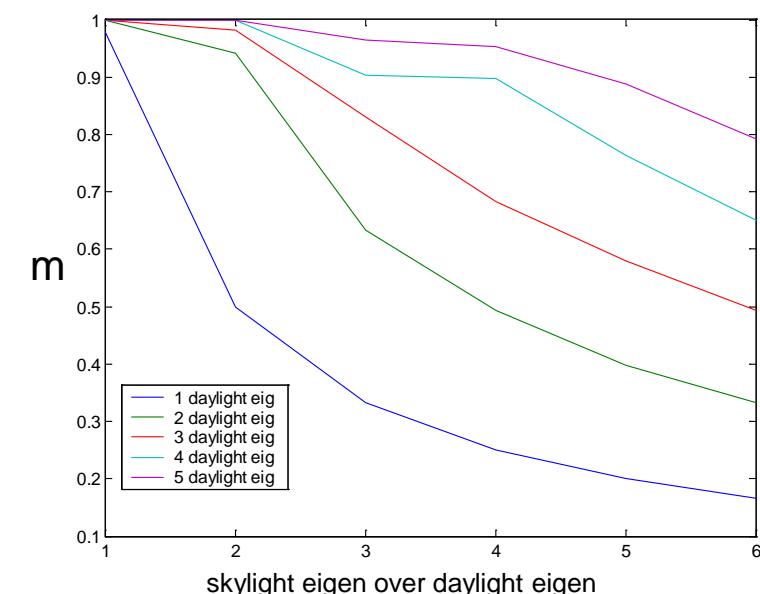
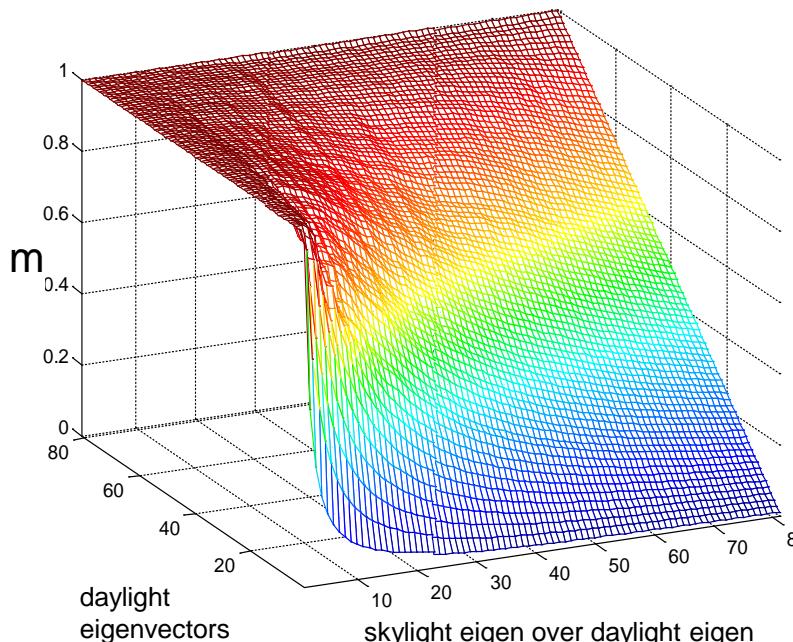
-Natural reflectances are more complex

- Important to adequately select the dataset best suited for our application if PCA is to be applied

*From Hardeberg
(section 6.4).*

2. Dimensionality reduction: Principal Component Analysis

how closely related are two different sets of eigenvectors?



$\mu \in (0,1)$ [S. Quan et.al. (2002) Journ. of Imag. Sc. and Tech. 46] describes the difference between two subspaces (in our case: skylight versus daylight subspaces).

$$\mu_A(S) = \frac{\text{Trace}\{O^T U U^T O\}}{\text{Trace}\{U U^T\}}$$

Finite-dimensional models $X = A B$

X ($m \times d$): m spectra sampled at d wavelengths

B ($n \times d$): n basis vectors

A ($m \times n$): matrix with weighting coefficients

How to compute basis vectors? **PCA, ICA, NNMF, NNICA** are some techniques... These techniques minimizes $\|X-AB\|^2$

A spectrum is modelled by projecting it onto the pseudoinverse of a set of basic vectors. The projection yields the weighting coefficients of the model. $w = x^T B^{-1}$

The PCA basic vectors are orthogonal so $B^{-1} = B^T$

For the other methods, the basis vectors are not orthogonal, so the pseudo-inverse of B , B^+ is used.

Finite-dimensional models $\mathbf{X} = \mathbf{A} \mathbf{B}$

$$\mathbf{w} = \mathbf{x}^T \mathbf{B}^{-1}$$

Except for PCA ($\mathbf{B}^{-1} = \mathbf{B}^T$) for the rest \mathbf{B}^+ is used.

- **PCA** finds basis vectors that are uncorrelated and orthogonal.
- **ICA** finds basis vectors that are uncorrelated and in addition are independent but not orthogonal.
- **Non-negative ICA (NNICA)** carries out ICA subject to the additional constraint of non-negativity in the resulting basis vectors.
- **Non-negative Matrix Factorization (NNMF)**: all entries in both A and B being nonnegative.

Finite-dimensional models $\mathbf{X} = \mathbf{A} \mathbf{B}$

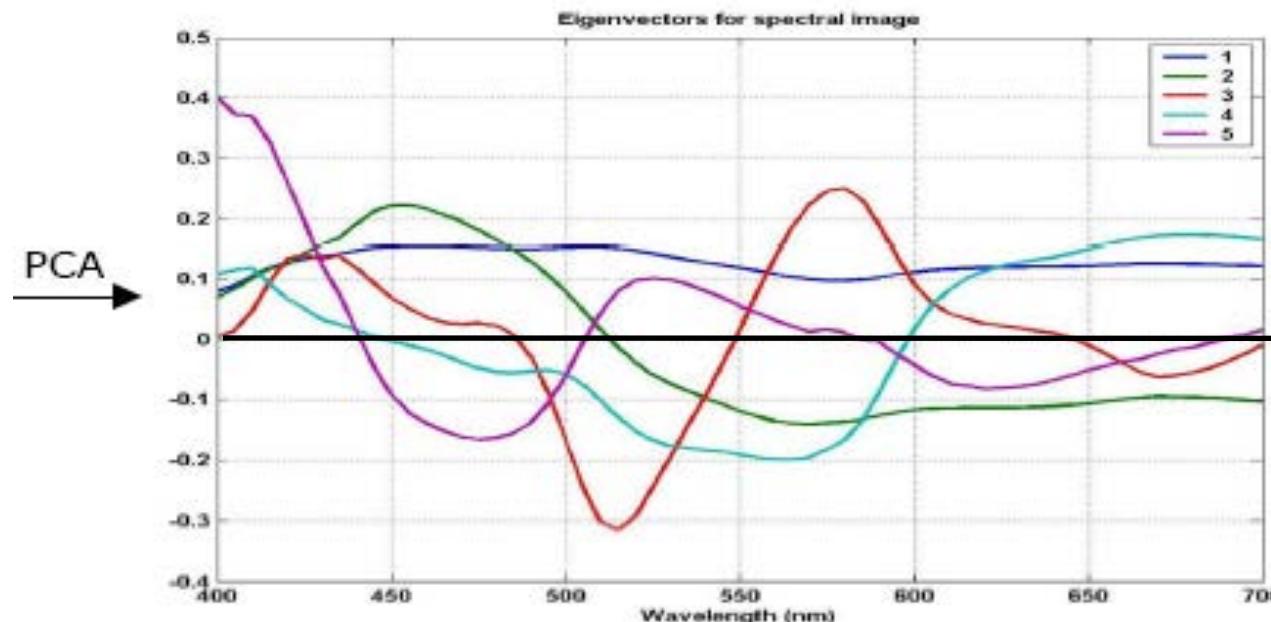
\mathbf{X} ($m \times d$): m spectra sampled at d wavelengths

\mathbf{B} ($n \times d$): n basis vectors

\mathbf{A} ($m \times n$): matrix with weighting coefficients

The output of an optical sensor can be described as the projection of the spectrum on the sensor's spectral sensitivity functions.

Is there a good basis for modelling spectra that also has the property that the pseudo-inverse of the basis might be used as physically realizable sensors?



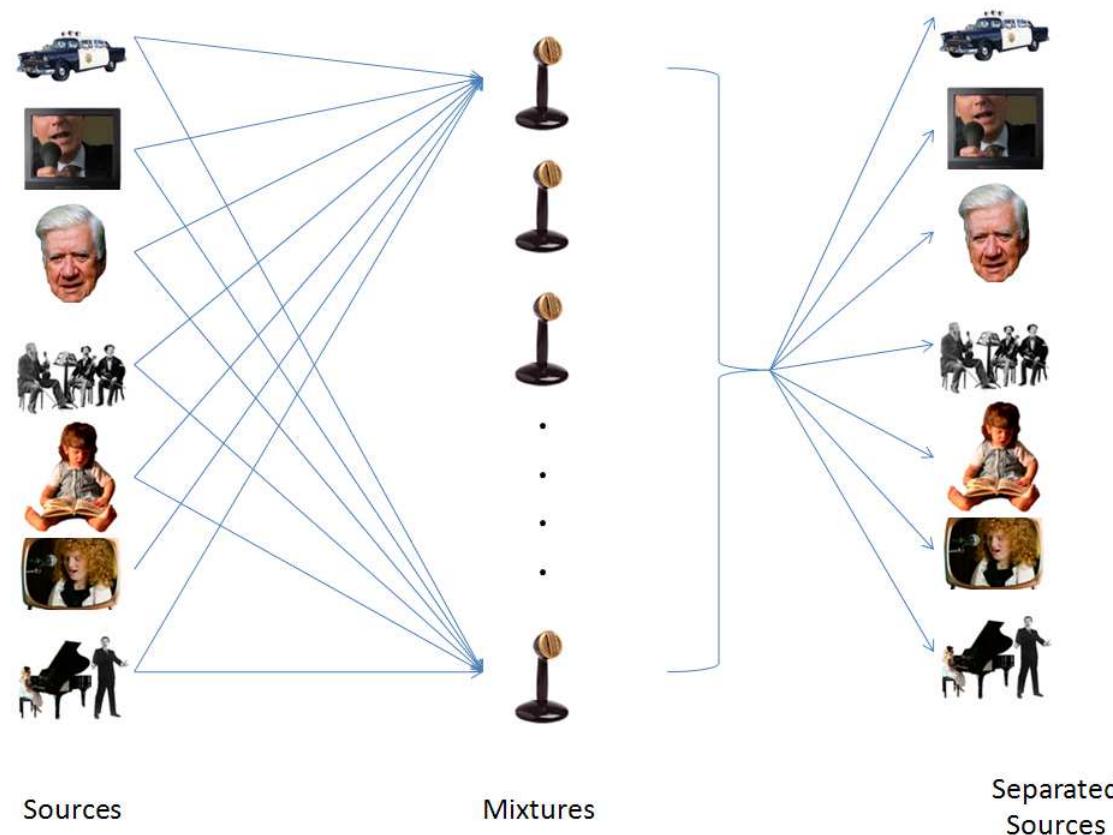
2. Dimensionality reduction

- Principal Component Analysis (PCA)
- **Independent Component Analysis (ICA)**
- Non-linear approaches of PCA and ICA (not in this course)
- Alternative methods for dimensionality reduction: NNMF
- Multidimensional scaling (not in this course)

2. Dimensionality reduction: Indep. Comp. Analysis (ICA)

- Example: 'cocktail-party'

- Example: Blind source separation
 - Original features $x_i(t)$ are microphones at a cocktail party
 - Each receives sounds from multiple people speaking
 - ICA outputs directions that correspond to individual speakers $y_k(t)$



2. Dimensionality reduction: **Indep. Comp. Analysis (ICA)**

- Also known as Blind Source Separation
- ICA seeks components that are independent in the statistical sense.
- Two variables x, y are *statistically independent* iff $P(x,y) = P(x)P(y)$.
- The idea: if the data vectors are linear combination of statistically independent data components, they should be separable in their components

2. Dimensionality reduction: **Indep. Comp. Analysis (ICA)**

Independent Component Analysis or ICA is a **blind-source separation method** which looks for components as **statistically independent as possible** in the data given as input to the algorithm.

Blind source: we do not have any a priori knowledge which we intend to use in the algorithm regarding the nature or features of the sources.

Statistical independence: there is not a correlation between the variables.

In math language: the joint probability distribution is the product of the two probability distributions corresponding to each variable.

2. Dimensionality reduction: Indep. Comp. Analysis (ICA)

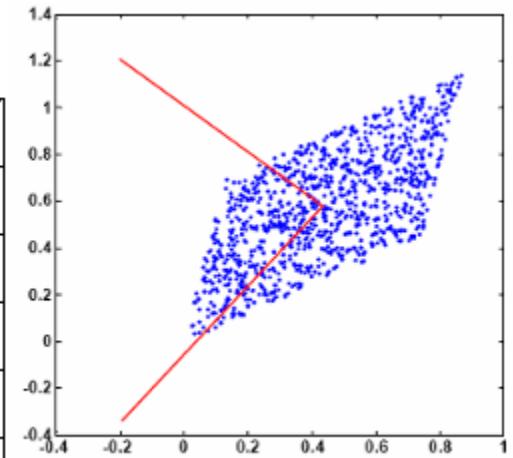
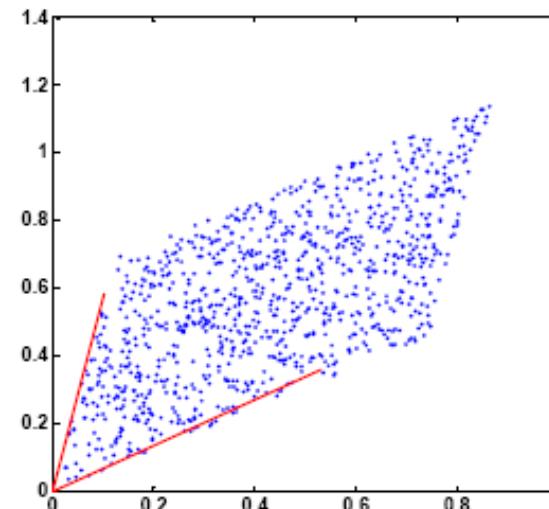
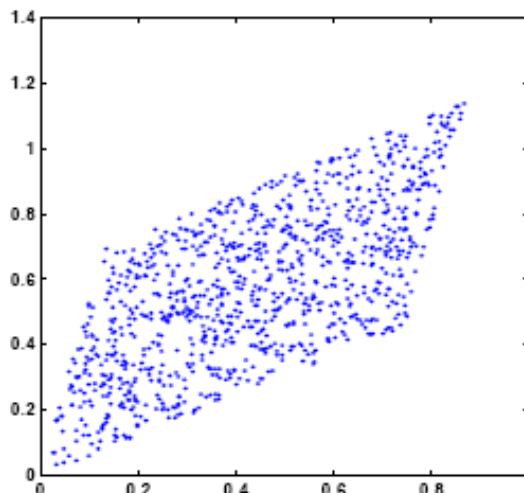
Independent Components Analysis

- PCA seeks directions $\langle Y_1 \dots Y_M \rangle$ in feature space X that minimize reconstruction error
 - In particular, choose projection that minimizes the squared error in reconstructing original data
- ICA seeks directions $\langle Y_1 \dots Y_M \rangle$ that are most *statistically independent*. I.e., that minimize $I(Y)$, the mutual information between the Y_j :

$$I(Y) = \left[\sum_{j=1}^J H(Y_j) \right] - H(Y)$$

Which maximizes their departure from Gaussianity!

2. Dimensionality reduction: Indep. Comp. Analysis (ICA)



- 2 directions appear on the data
- ICA extracts these directions (mixing matrix) to generate 2 independent sources

2. Dimensionality reduction: Indep. Comp. Analysis (ICA)

- Given m signals of length n, construct the data matrix

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_m \end{pmatrix}$$
.

INPUT to the algorithm

X is the data set (in our case, a matrix formed by columns which are spectral functions).

- We assume that X consists of m sources such that

$$\mathbf{X} = \mathbf{AS}$$

A= mixing matrix

S= ICs (Independent components)

Hyvärinen A., Karhunen J., Oja E. Independent Component Analysis. Wiley, 2001.

2. Dimensionality reduction: **Indep. Comp. Analysis (ICA)**

$$X = A S$$

It is quite common to work with the inverse of the A matrix (usually called the W matrix or filter matrix), which allows us to obtain the independent components of a given set of data X' different from the original data set X as:

$$W = A^{-1} \quad u = W X'$$

If our aim is to recover the dataset X' using ICA as a dimensionality reduction technique, then we would have to project the Independent Components u previously calculated onto the **basis functions** which form the mixing matrix, by:

$$X' = A u$$

2. Dimensionality reduction: **Indep. Comp. Analysis (ICA)**

How many basis functions for an appropriate dimensionality reduction?

The matrix A has in general as many basis functions as the original data (which in our case would be different wavelengths, and the A matrix would be square).

There is no defined criteria to rank them, but in many ICA algorithms they are ranked by norm.

But we can select a subset of them to recover the data and so the A matrix would not be square and the relation $AW=I$ (where I is the identity matrix) will not hold. We will have in this case to calculate W as the pseudoinverse matrix of A.

2. Dimensionality reduction: Indep. Comp. Analysis (ICA)

How to apply ICA to reduce dimensionality for spectral datasets?

1) We select the spectral dataset

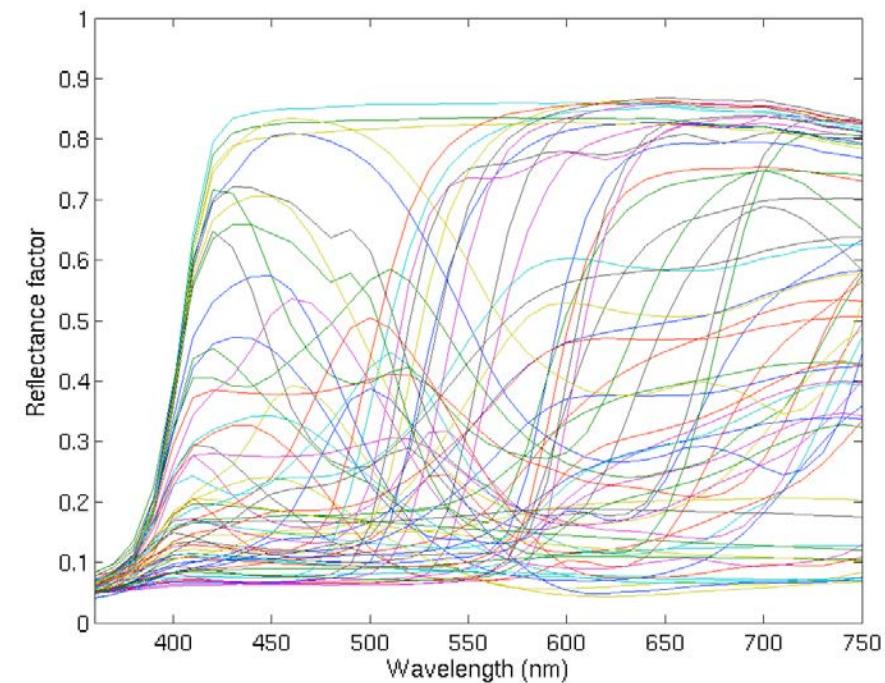
2) We choose the ICA algorithm

-Extended Infomax by Lee et

al. (1998)

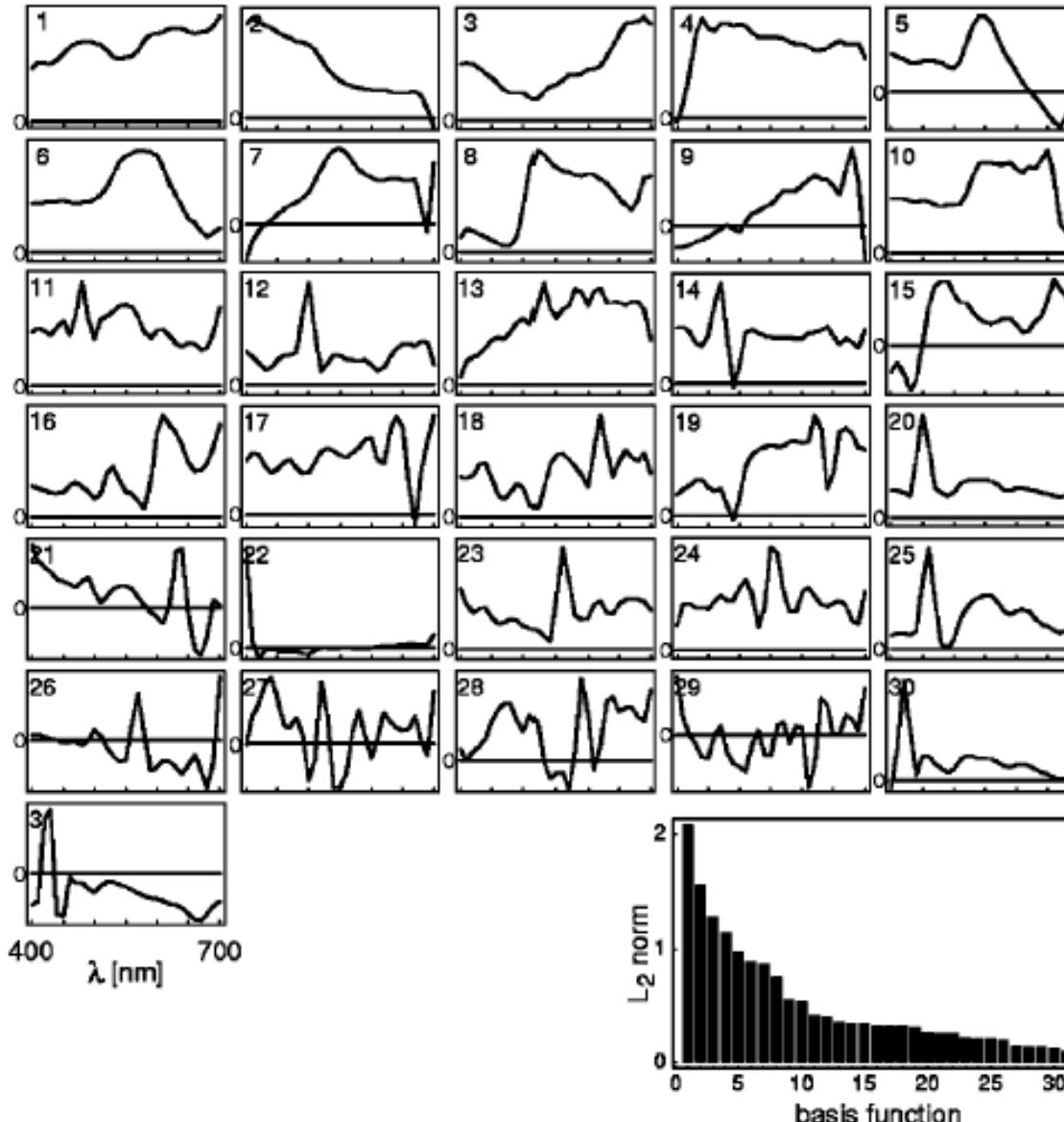
-FastICA by Oja, Hyvarinen et
al. (1999)

-JADE by Cardoso et al. (1999)



3) We obtain the IC and see the reconstructions (not recovering scale)

2. Dimensionality reduction: Indep. Comp. Analysis (ICA)



first 30 spectral IC
ranked according to
their L₂-norm

negative values!!!

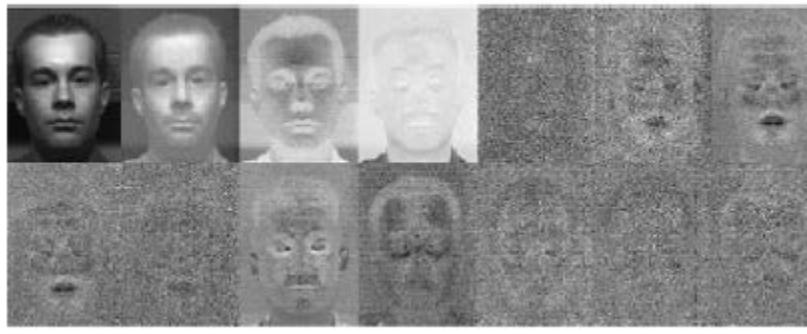
Usually, the mixing
functions (A) and
basis functions
($W = \text{pinv}(A)$) are not
ordered, so we can
order them by
vector norm
(Watchler et al.,
2001).

on

2. Dimensionality reduction

ICA versus PCA

PCA vs. ICA



PCA

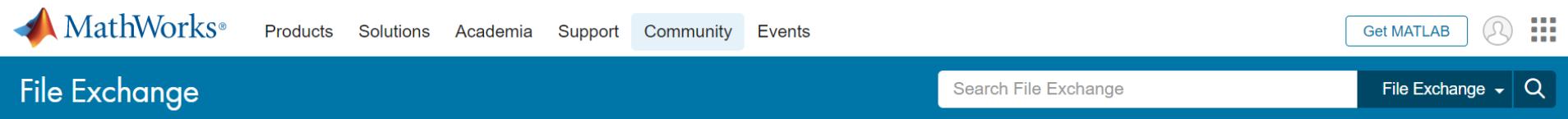
- PCA: first component is the mean; naturally ordered components by VAF
- PCA: Some components seem to be related to facial features

- ICA: There is no ordering rank emerging from the algorithm
- ICA: no apparent direct relation between particular features and the IC

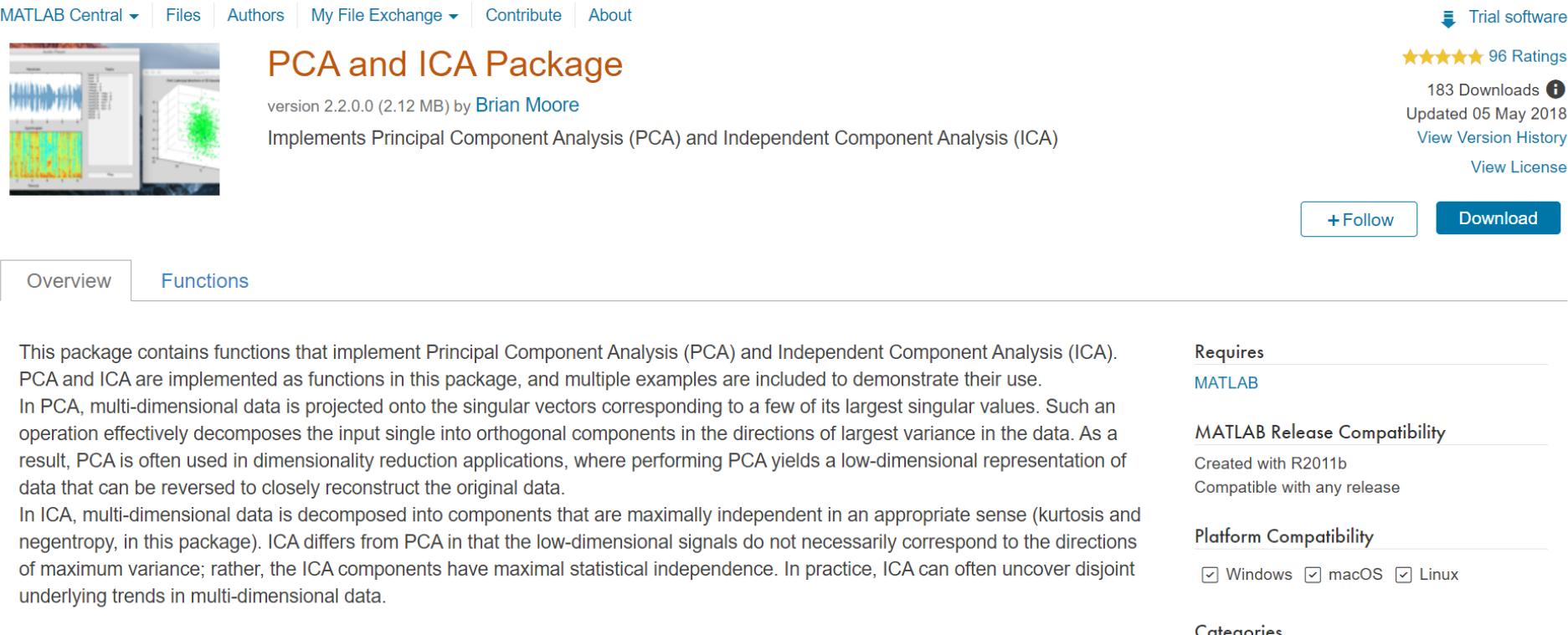


2. Dimensionality reduction

ICA & PCA in Matlab



The screenshot shows the MathWorks File Exchange interface. At the top, there are navigation links: Products, Solutions, Academia, Support, Community (which is highlighted in blue), and Events. To the right are buttons for "Get MATLAB", a user profile icon, and a search icon. Below the header, the page title is "File Exchange". A search bar says "Search File Exchange". Underneath, there's a breadcrumb menu: MATLAB Central ▾ / Files / Authors / My File Exchange ▾ / Contribute / About. On the left, there's a thumbnail image of the package interface showing various plots and data visualizations. The main title of the package is "PCA and ICA Package" in orange. Below it, it says "version 2.2.0.0 (2.12 MB) by Brian Moore". A brief description follows: "Implements Principal Component Analysis (PCA) and Independent Component Analysis (ICA)". To the right, there are ratings: "★★★★★ 96 Ratings", "183 Downloads", "Updated 05 May 2018", "View Version History", and "View License". At the bottom, there are two buttons: "+ Follow" and "Download".



This package contains functions that implement Principal Component Analysis (PCA) and Independent Component Analysis (ICA). PCA and ICA are implemented as functions in this package, and multiple examples are included to demonstrate their use. In PCA, multi-dimensional data is projected onto the singular vectors corresponding to a few of its largest singular values. Such an operation effectively decomposes the input single into orthogonal components in the directions of largest variance in the data. As a result, PCA is often used in dimensionality reduction applications, where performing PCA yields a low-dimensional representation of data that can be reversed to closely reconstruct the original data. In ICA, multi-dimensional data is decomposed into components that are maximally independent in an appropriate sense (kurtosis and negentropy, in this package). ICA differs from PCA in that the low-dimensional signals do not necessarily correspond to the directions of maximum variance; rather, the ICA components have maximal statistical independence. In practice, ICA can often uncover disjoint underlying trends in multi-dimensional data.

Requires
MATLAB

MATLAB Release Compatibility
Created with R2011b
Compatible with any release

Platform Compatibility
 Windows macOS Linux

Categories

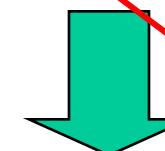
2. Dimensionality reduction

- Principal Component Analysis (PCA)
- Independent Component Analysis (ICA)
- **Non-linear approaches of PCA and ICA (not in this course)**
- Alternative methods for dimensionality reduction: NNMF
- Multidimensional scaling (not in this course)

2. Dimensionality reduction

Non-linear approaches of PCA and ICA (not in this course)

- Sometimes conventional linear PCA or ICA does not work because the assumption of linearity fails



- Strategy 1) introduce non-linearities in the mixing model

$$x_\lambda = a_{1\lambda}\phi_\lambda + a_{2\lambda}\phi_\lambda^2 + \dots$$

Polynomials or other non-linear functions...

- Strategy 2) move into another higher-dimensional space by a kernel transform and perform linear PCA there.

The Kernel trick

Non-linear approaches of PCA and ICA (not in this course)



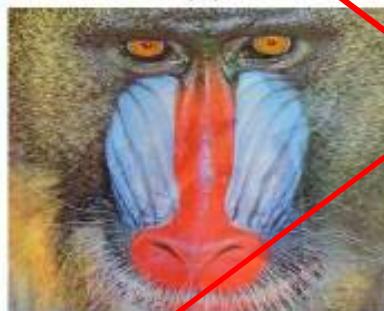
(a)



(b)



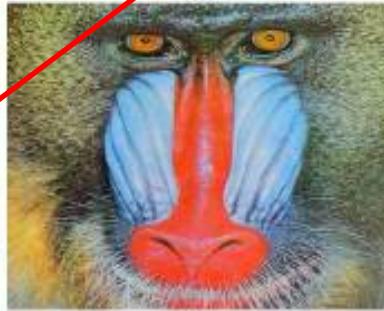
(c)



(d)



(e)



(f)

This technique may be used, for example, to separate reflections from images with relatively good results.



(a)



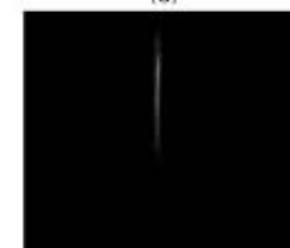
(b)



(c)



(d)



(e)



(f)

Fig 2: Image Separation of non-linear model. (a),(b): input images. (c),(d): ICA. (e),(f): KICA.

2. Dimensionality reduction

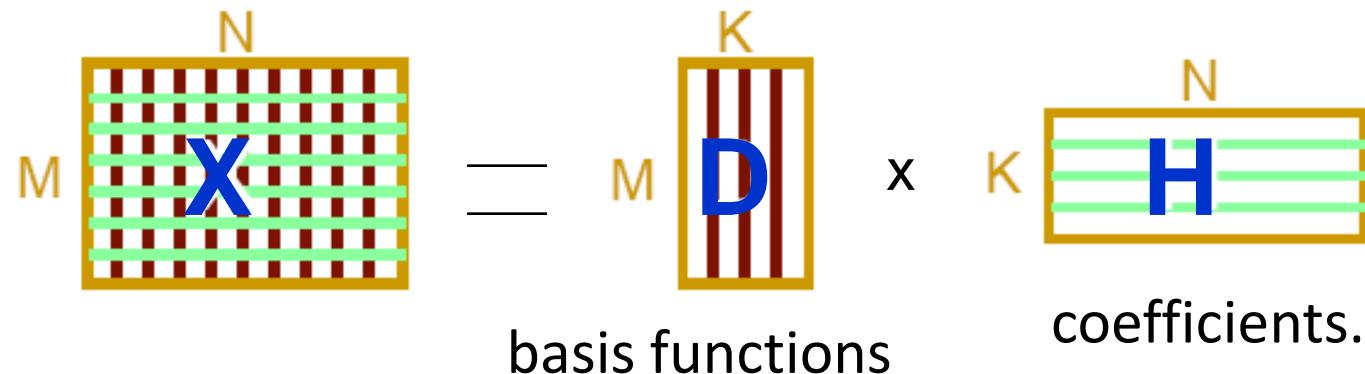
- Principal Component Analysis (PCA)
- Independent Component Analysis (ICA)
- Non-linear approaches of PCA and ICA (not in this course)
- **Alternative methods: NNMF**
- Multidimensional scaling (not in this course)

2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

Method for matrix decomposition into two all-positive matrices

- In matrix $X \approx DH$ s.t. $D, H \geq 0$



Dimension k must be known a priori, as it is fed into the algorithm.

Infinite number of possible solutions (algorithm selects the one minimizing distance between X and the matrix product DH).

2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

$$\mathbf{X} = \mathbf{D} \mathbf{H}$$

D basis functions
H coefficients

If we need to recover a given data set \mathbf{X}' , we would then calculate the inverse or pseudoinverse of matrix D, and then the coefficients would be the result of multiplying $\text{pinv}(\mathbf{D})$ by \mathbf{X}' . After that, the recovery would consist in multiplying D by the corresponding coefficient set.

2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

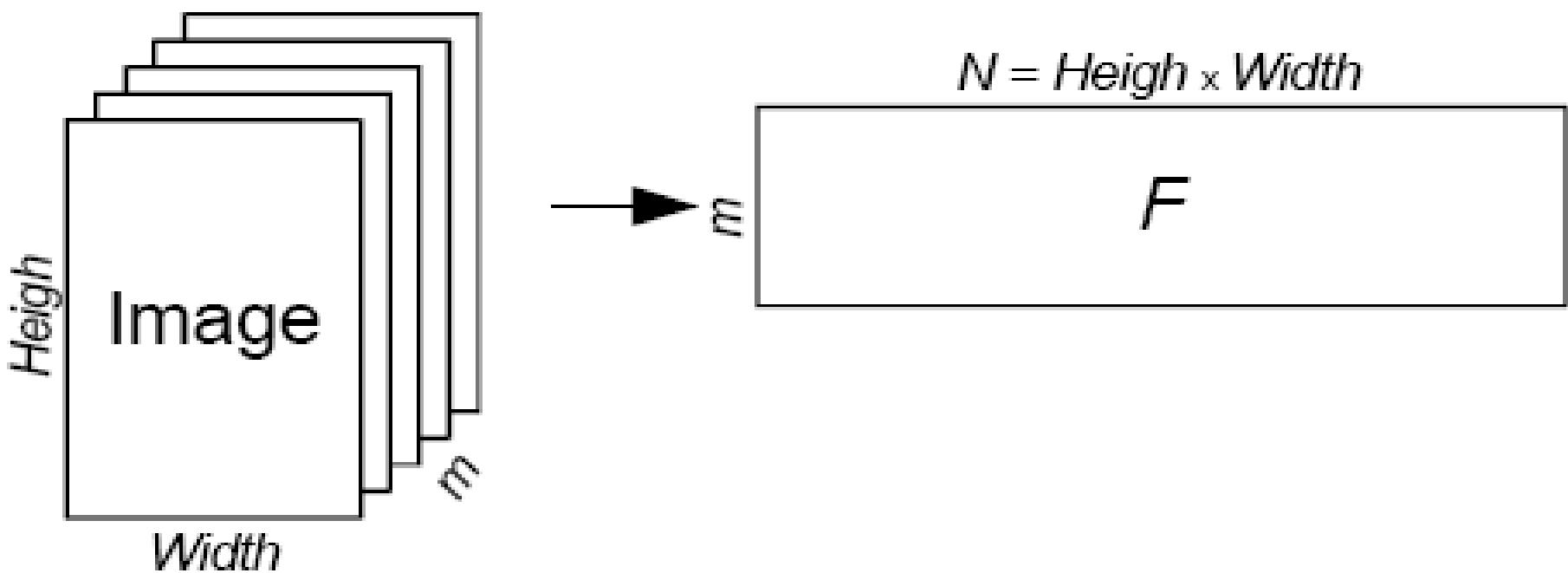
- Why Non-negative:
 - Many physical signals are non-negative by nature (pixel intensities, amplitude spectra, occurrence counts, etc.)
- Why NMF is not ICA
 - NMF does not learn anything about the relationships between parts: NMF assumes that the hidden variables are nonnegative, but makes no assumption about their statistical dependency.
- Basically an algorithmic minimization problem
 - Minimize divergence between X and DH

$$\min_{D,H \geq 0} D(X, DH)$$

2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

NNMF applied to multispectral data



2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

NNMF applied to multispectral data

$$N = \text{Height} \times \text{Width}$$

$$\begin{matrix} m \\ \rightarrow \end{matrix} \boxed{F} = \boxed{m \times r} W \times \boxed{n} H$$

2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

NNMF applied to multispectral data

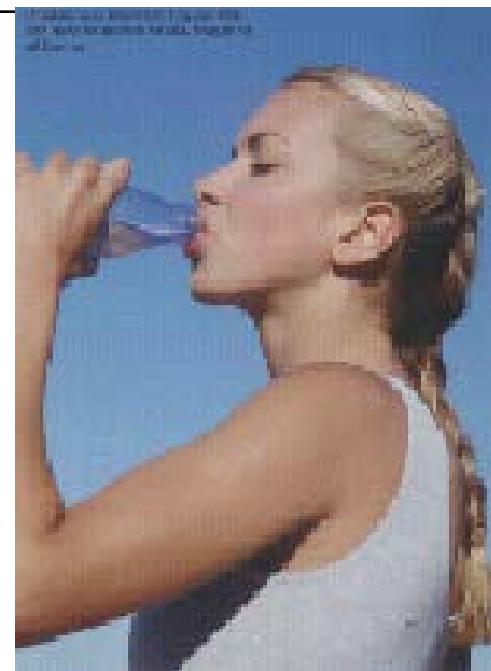
Number of components in reconstruction

1

5

all

From IFC, Joensuu



2. Dimensionality reduction: NNMF

Non-Negative Matrix Factorization (NNMF)

nnmf.m

[W,H] = nnmf(A,k)

[W,H] = nnmf(A,k,Name,Value)

[W,H,D] = nnmf(____)

[W,H] = nnmf(A,k) factors the n-by-m matrix A into nonnegative factors W (n-by-k) and H (k-by-m). The factorization is not exact; W^*H is a lower-rank approximation to A. The factors W and H minimize the root mean square residual D between A and W^*H .

2. Dimensionality reduction: PCA, ICA, NNMF....

Cases studies if you want to know more....

Weihua Xiong and Brian Funt (2005)

1781 reflectances and 102 illuminants (various sets)

PCA vs ICA vs NNMF number of basis functions required comparison

Ramanath et al., 2004, “Spectral Spaces and Color Spaces”, Color Research and Application

PCA vs ICA vs NNMF vs Nnets for three-dimensional representation of the Munsell data

2. Dimensionality reduction: PCA, ICA, NNMF....

Cases studies if you want to know more....

Weihua Xiong and Brian Funt (2005)

“Independent Component Analysis and Nonnegative Linear Model Analysis of Illuminant and Reflectance Spectra”

Principal Component Analysis (PCA), Independent Component Analysis (ICA), Non-Negative Matrix Factorization (NNMF) and Non-Negative Independent Component Analysis (NNICA) are all techniques that can be used to compute basis vectors for finite-dimensional models of spectra.

1781 reflectances and 102 illuminants (various sets)

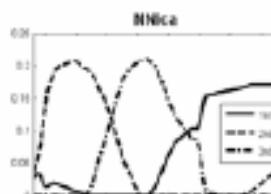
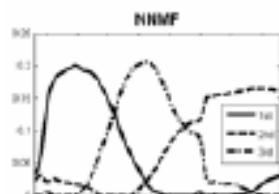
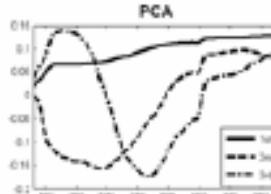
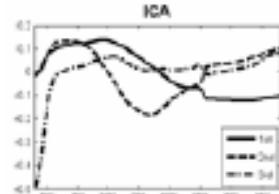
2. Dimensionality reduction: PCA, ICA, NNMF....

Cases studies if you want to know more....

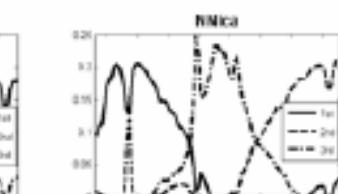
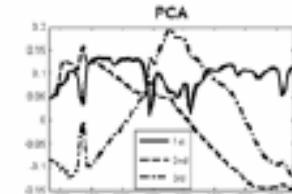
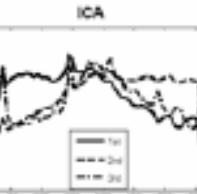
Weihua Xiong and Brian Funt (2005)

1781 reflectances and 102 illuminants (various sets)

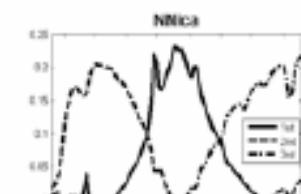
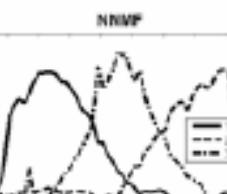
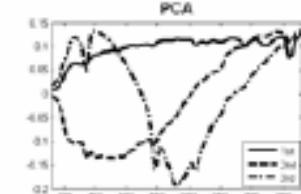
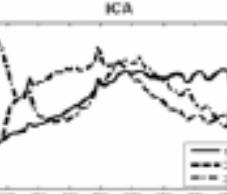
Surface Reflectance



Illumination



Colour Signal

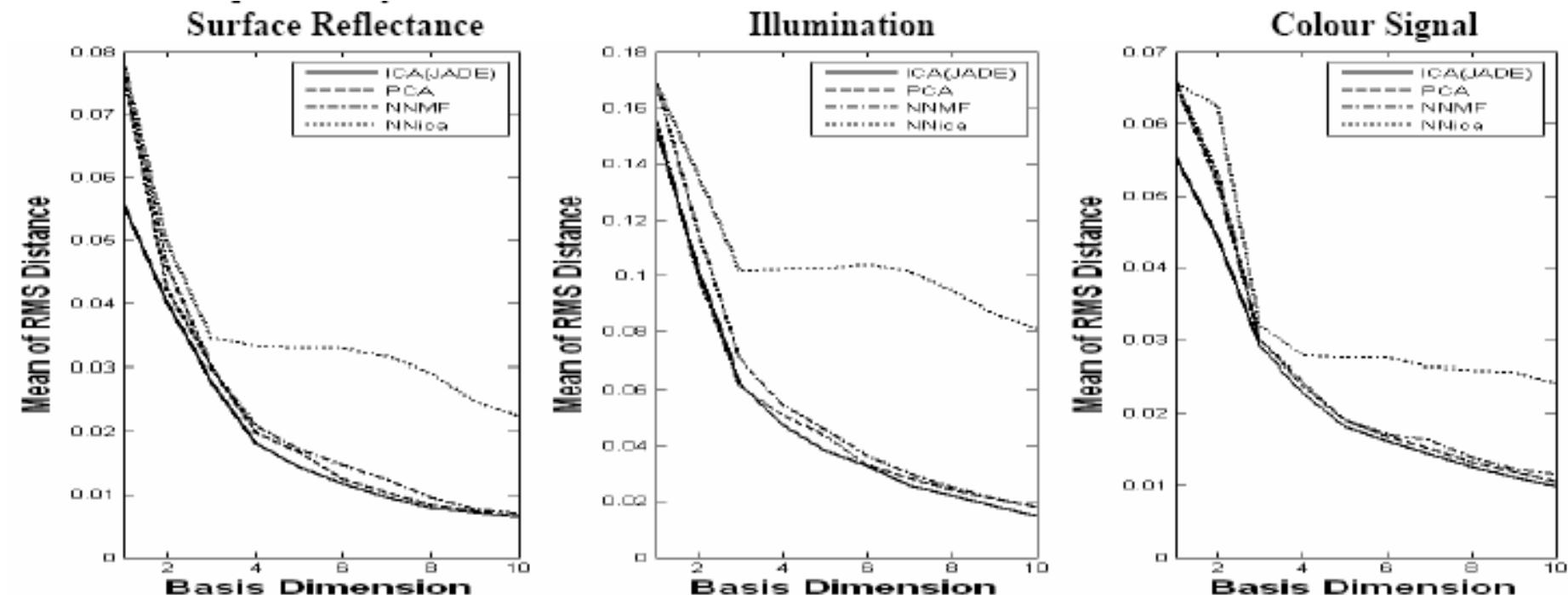


2. Dimensionality reduction: PCA, ICA, NNMF....

Cases studies if you want to know more....

Weihua Xiong and Brian Funt (2005)

1781 reflectances and 102 illuminants (various sets)

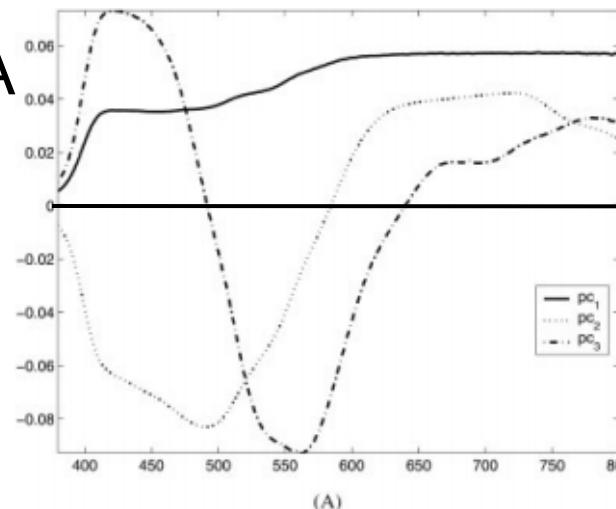


Cases study:

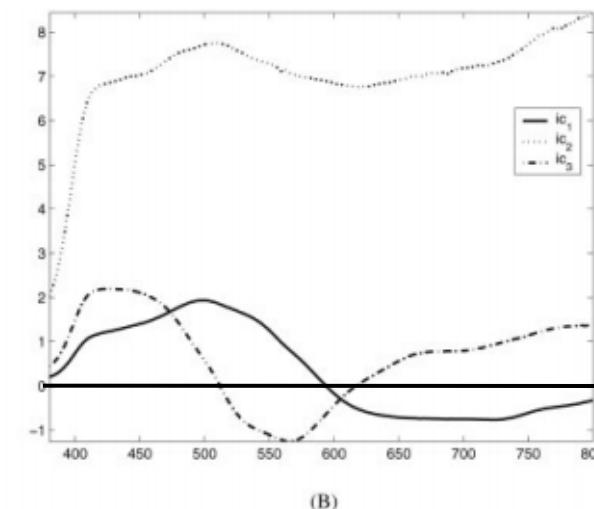
Ramanath et al., 2004

Munsell data

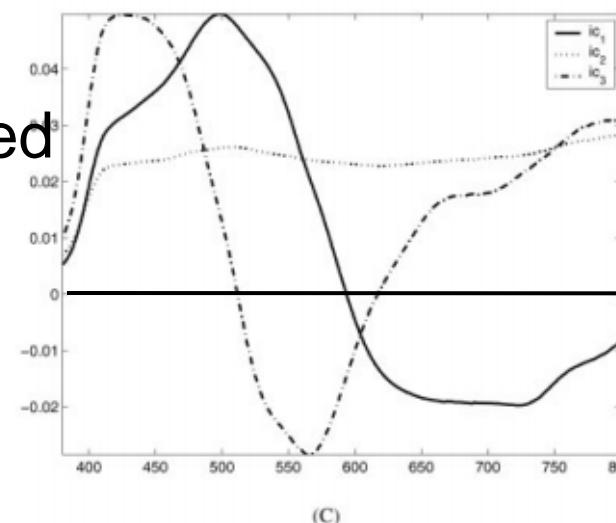
PCA



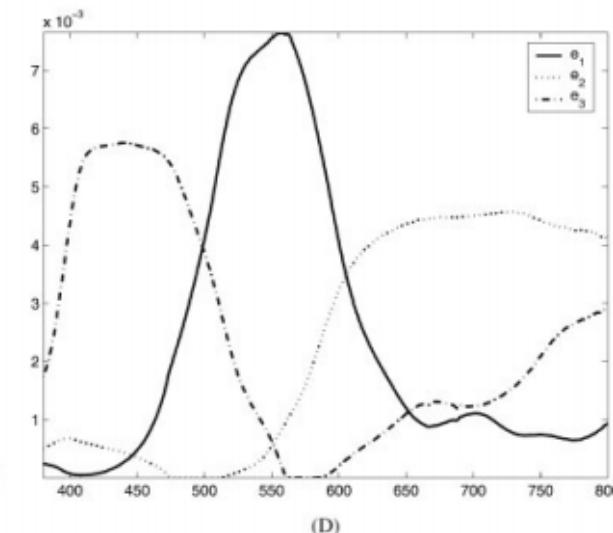
(A)



(B)

ICA
normalized

(C)



(D)

ICA

NNMF

FIG. 1. Basis functions for the Munsell spectral database when using the wavelength range of 380–800nm (A) Eigen functions corresponding to the top three eigenvalues using PCA, (B) using ICA, (C) ICA bases, normalized to unit vectors; note similarity to PCA bases, (D) using NMF. Note that the basis vectors span the same space if the sign is reversed. Also note that with ICA, the sequence of the bases is irrelevant.

Cases study: Ramanath et al., 2004 Munsell data

TABLE I. Error measures of the various reconstructions for the two wavelength ranges.

Method used		MSE	Max	Min	Variance	95th percentile
PCA	380–800 nm	0.3176	9.0823	0.0056	0.3098	1.0136
	430–660 nm	0.1071	2.3795	0.0005	0.0371	0.4324
ICA	380–800 nm	0.3581	9.2461	0.0113	0.3006	0.9324
	430–660 nm	0.9854	5.9959	0.0042	1.5119	3.5664
NMF	380–800 nm	0.3932	10.8585	0.0090	0.4442	1.1212
	430–660 nm	0.1257	2.5909	0.0002	0.0466	0.5568
CMFs	380–800 nm	25.8634	113.5626	0.4414	778.2233	86.5720
	430–660 nm	3.6709	16.6888	0.0507	15.1270	12.4693

Remember the question on chapter 4 about “How to present the data in a paper or in a report?”

2. Dimensionality reduction

- Principal Component Analysis (PCA)
- Independent Component Analysis (ICA)
- Non-linear approaches of PCA and ICA (not in this course)
- Alternative methods: NNMF
- **Multidimensional scaling (not in this course)**

2. Dimensionality reduction: Multidimensional scaling

- Generalization of PCA
 - PCA based on covariance-correlation matrices
 - Matrix algebra to find linear combinations between variables -> dimension reduction.
 - What's happen if relations are not linear?
 - What's happen if space is not euclidean?
- Non-parametric version of PCA
 - Correlation matrix can be considered as a similarity (dissimilarity) matrix:

$$d_{rs} = (c_{rr} + c_{ss} - 2c_{rs})^{1/2}$$

2. Dimensionality reduction: Multidimensional scaling

- Given an association (distance) matrix between units:
 - Tries to find a representation of the units in a given number of dimensions
 - Preserving the pattern/ordering in the association matrix
 - Thus, we could observe relations between variables

How it works:

- Provide association matrix (distances/similarity/dissimilarity)
- Provide number of dimensions
- Produce initial plot, perhaps using PCA
- Orders distances on plot, compares them with ordering of association matrix
- Computes STRESS
- Juggles points to reduce STRESS
- Go to 4, until STRESS is stabilized
- Output plot, STRESS
- Perhaps repeat with new starting conditions

2. Dimensionality reduction: Multidimensional scaling

- STRESS:

$$\sqrt{\frac{\sum_{i,j} (d_{ij} - \delta_{ij})^2}{\sum_{i,j} \delta_{ij}^2}}$$

- δ_{ij} associations between i and j
- d_{ij} associations between i and j predicted using distances on plot (by regression)
- The goal of MDS is to faithfully represent these (distances/dissimilarities/similarities) with the lowest possible dimensional space.

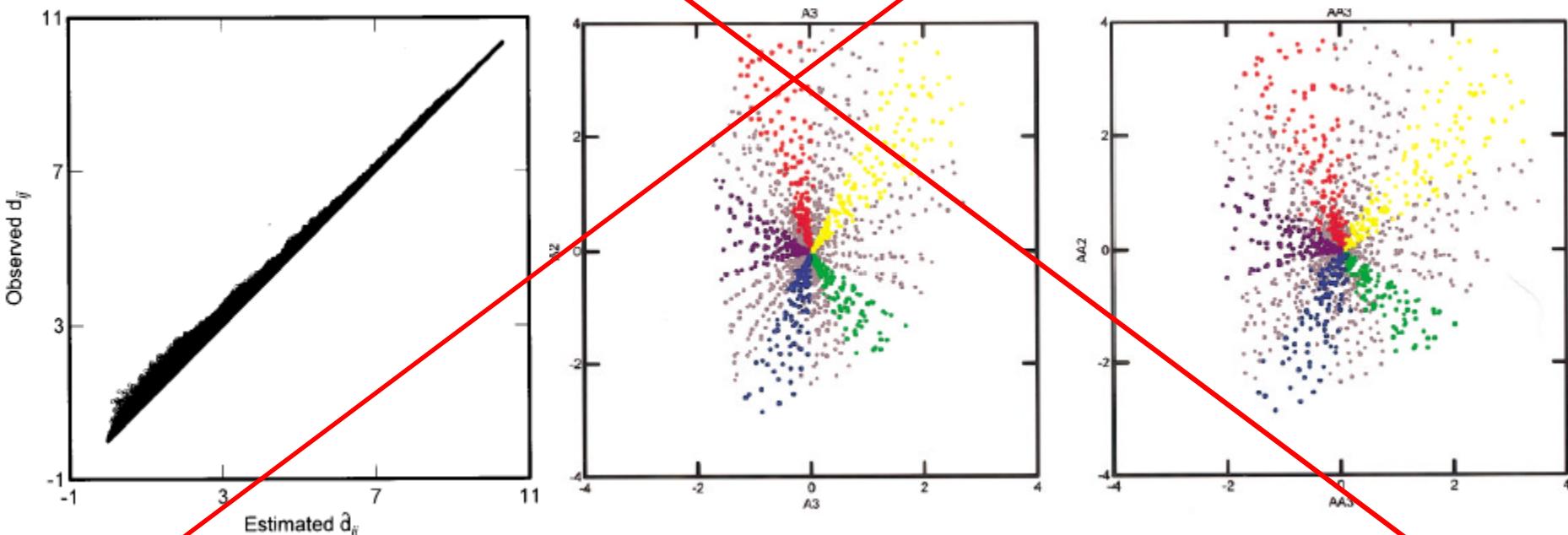
2. Dimensionality reduction: Multidimensional scaling

- How many dimensions?
 - STRESS <10% is “good representation”
 - Scree diagram
 - two (or three) dimensions for visual ease
- Metric or non-metric?
 - Metric has few advantages over PCA (unless many negative eigenvalues)
 - Non-metric does better with fewer dimensions

2. Dimensionality reduction: Multidimensional scaling

-MDS applied to spectral data (Romney and Indow, 2003)

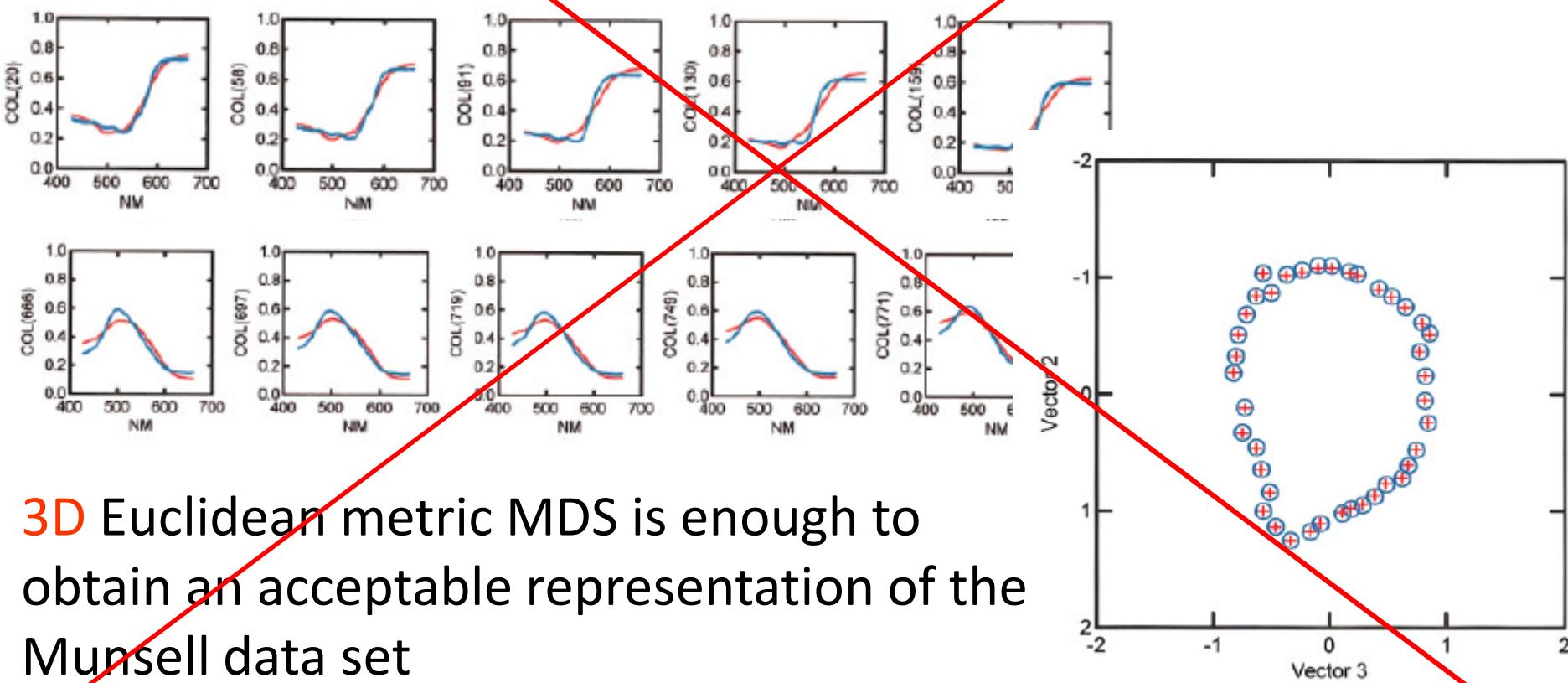
- Munsell chips, analyzed in terms of a 3-D MDS



- A specific color space suited to the Munsell spectra

2. Dimensionality reduction: Multidimensional scaling

- MDS applied to spectral data (Romney and Indow, 2003)
- After performing PCA, three coefficients seem to be enough (spectral range 430-660 nm)



3D Euclidean metric MDS is enough to obtain an acceptable representation of the Munsell data set

3. Algorithms for spectral estimation

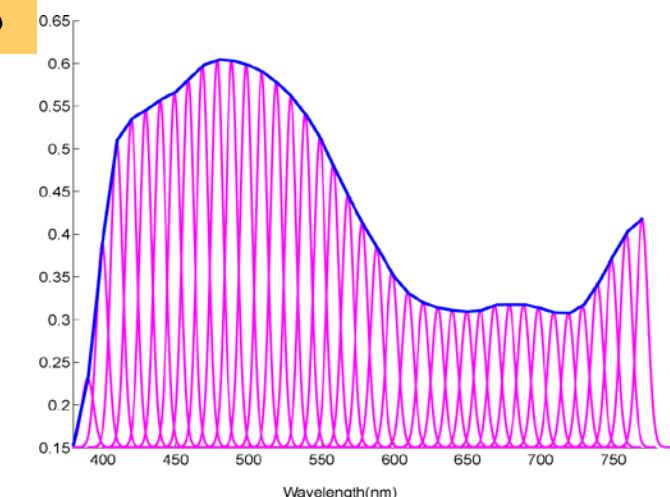
- Introduction
- Matrix notation
- Linear models
- Regression models
- Neural Network Model (not in this course)
- Others methods (not in this course)

3. What is spectral estimation?

Spectral Imaging Approaches

- Approach 1): to measure the spectral data accurately

⇒ A large amount of data



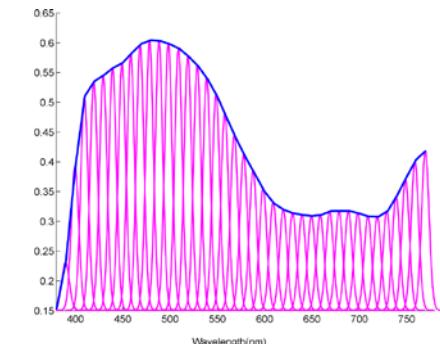
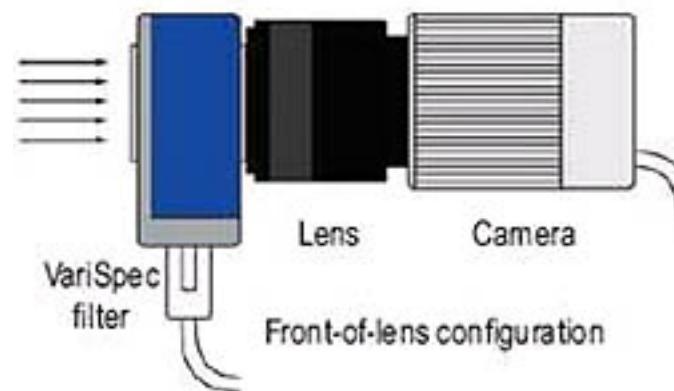
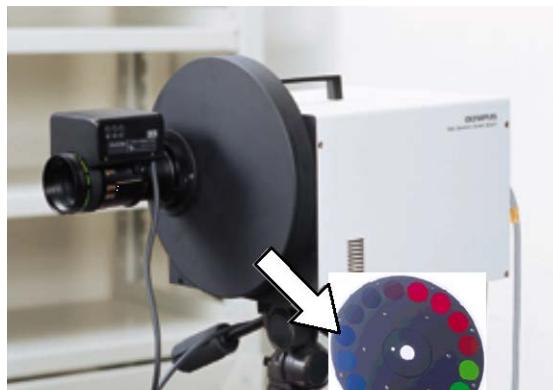
- Approach 2): to measure component images using a few optimally designed or optimal conventional color filters

⇒ Data is convenient for storing and transmission

⇒ Spectral image can be reconstructed computationally

3. What is spectral estimation?

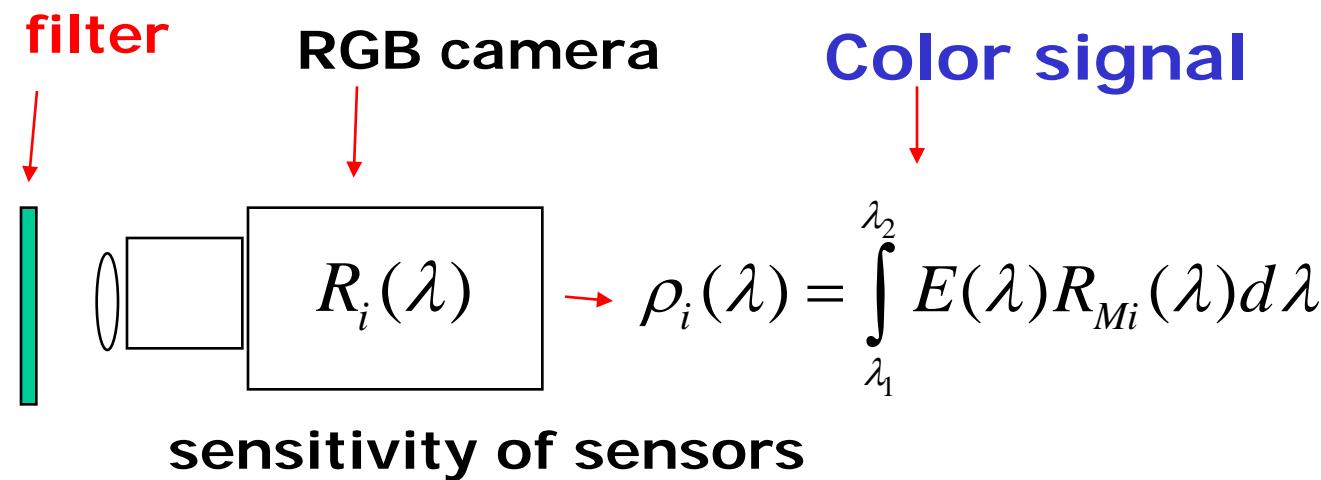
Approach 1) accurate measurements...



-Monochrome Camera + narrow band filter wheel or monochrome camera + LCTF (or similar spectral tuning device). Besides, algorithm relating camera responses to radiance (calibration target on the scene)

3. What is spectral estimation?

Approach 2) reduced set of images + estimation algorithm



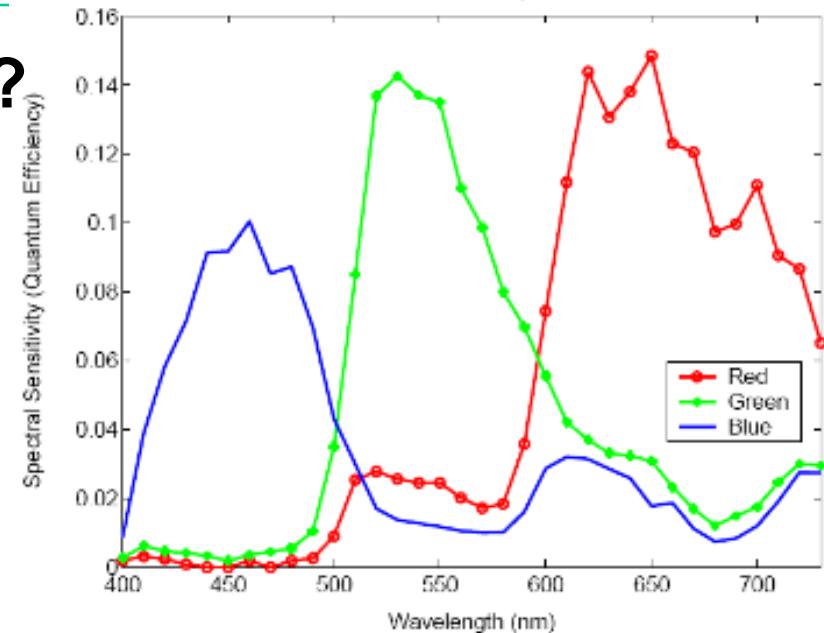
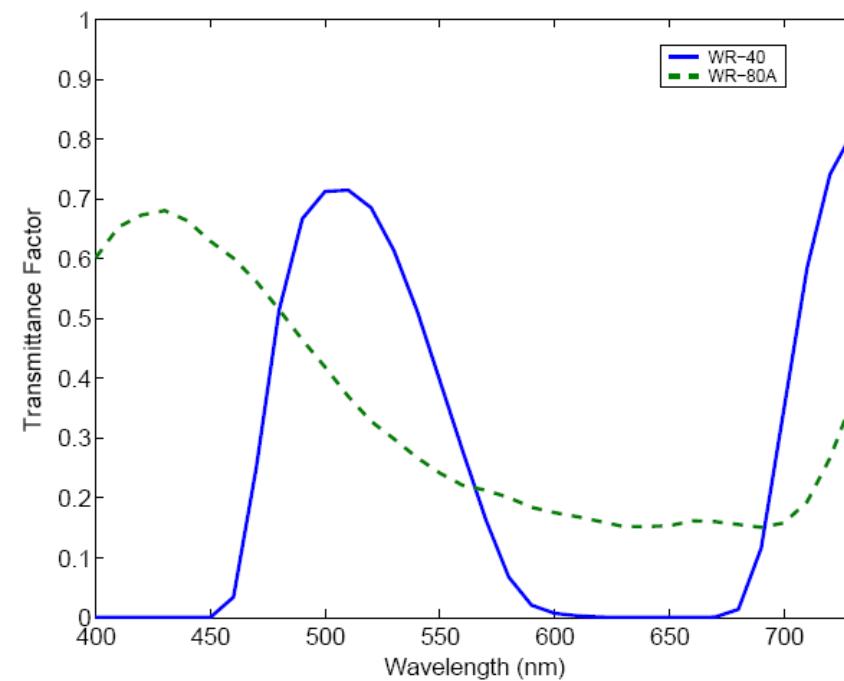
-Trichromatic Camera + small number of color filters.
Besides, algorithm relating camera responses to spectral functions (based on training: it is an undetermined problem)

Image from Nascimento et al. 2002

3. What is spectral estimation?

- Sensitivity of sensors:

Sensitivity of the sensors of the RGB camera: $R(\lambda)$



Spectral transmittance of the filters: $t(\lambda)$

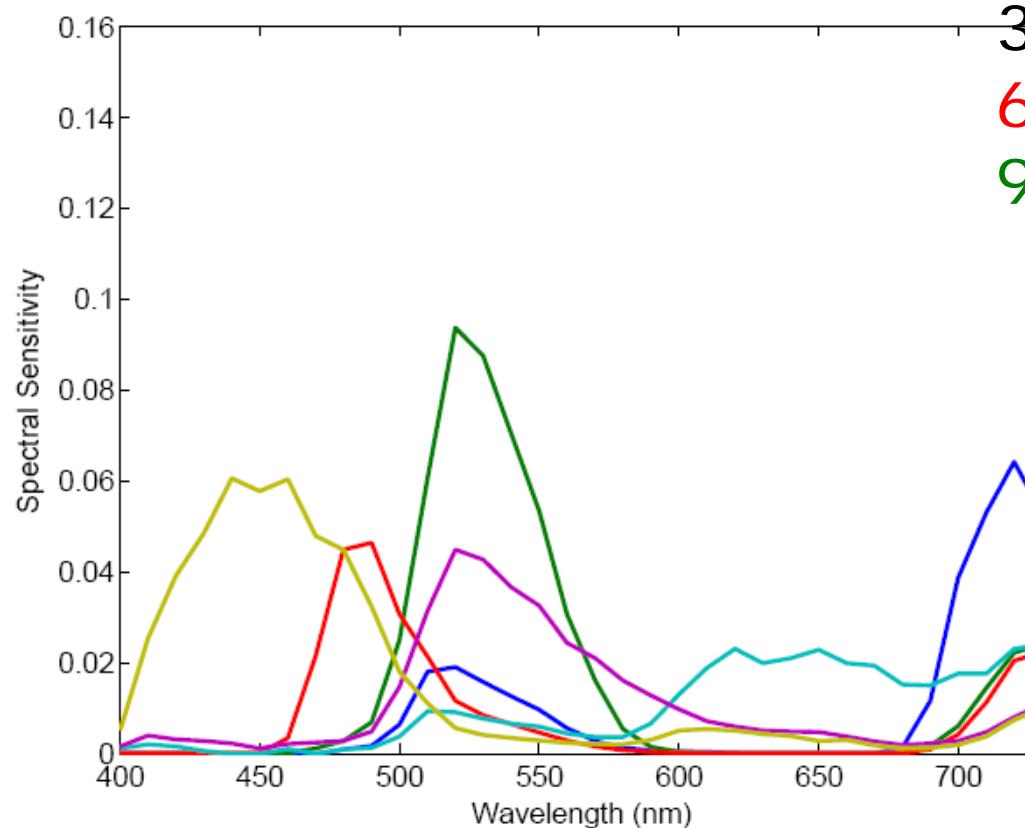


Kodak Wratten

3. What is spectral estimation?

- Spectral sensitivity of the sensors of the multispectral system: $R_M(\lambda) = t(\lambda)R(\lambda)$

Systems with:



3 sensors: RGB

6 sensors: RGB + 1 filter

9 sensors: RGB + 2 filters



3. Spectral estimation? Matrix notation

Fundamental equation for spectral estimation:

$$\rho = R^t E + \sigma$$

Color signals (Nx1)

Noise (kx1)

Transpose of matrix R of spectral sensitivities (Nxk)

Responses (kx1)

ρ : responses (kx1)
 R : transpose of matrix R of spectral sensitivities (Nxk)
 E : color signals (Nx1)
 σ : noise (kx1)

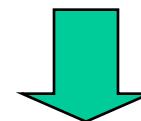
k: number of sensors
N: number of wavelength

3. Spectral estimation? Matrix notation

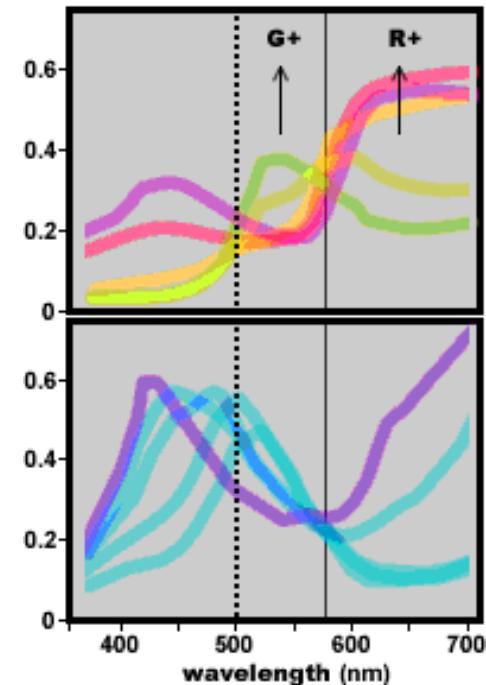
- **Problem:** more wavelengths than sensors ($N > k$)



Infinite solutions!!



- Algorithms of spectral estimation:



Based on a priori information of the spectra to be recovered

Some need a linear model to represent color signals: PCA, ICA, NMF, etc...

3. Algorithms or methods for spectral estimation

Main classification:

- **Direct methods (observational-model based methods)**
 - the spectral sensitivities of sensors and SPD of illuminant are known. $\rho = R^t E + \sigma$
- **Indirect methods (learning-based methods)**
 - depends on the quality of the learning set and on the regression method

Algorithms using dimensionality reduction of the spectral functions

1) Maloney-Wandell (1986):

$$\rho = R^t E$$

Training set of spectra to obtain the linear base V .

PCA, ICA, NMF

$$E = V \epsilon$$

$$\rho = \boxed{R^t V} \varepsilon = \boxed{\Lambda} \varepsilon$$

pseudoinverse of Λ : Λ^+

$$E_R = V \Lambda^+ \rho$$

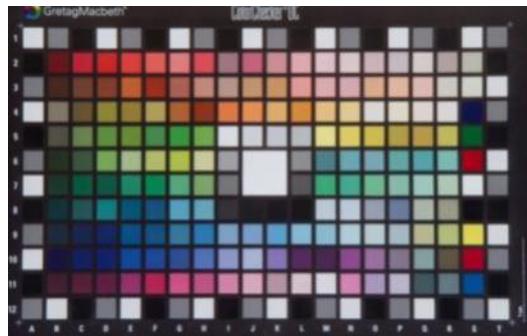
k: number of sensors
N: number of wavelength
n: number of basis vectors



- **Simple and fast**



- Knowledge about spectral sensitivities of the camera needed
- It is not robust against noise
 - Influence of “calibration errors” of the camera and of the spectral quality recovery



Linear Base (PCA,
ICA, NMF). Matrix
 V (columns)

Response
sensitivities Matrix
 R (columns)

$$\text{Matrix } \Lambda = R^t V$$

Estimated spectra

$$E_R = V \Lambda^+ \rho$$

2) Imai-Berns (1999):

Training spectrum set to obtain the linear base V .

- PCA, NMF or ICA

Training to obtain matrix G: relation between responses of the sensors and linear coefficients for m spectra taken from the '*training set*'.

G estimation by pseudoinverse

Color signal recovery from response of sensors.

k: number of sensors

N: number of wavelength

n: number of basis vectors

m: training set number

$$E = V \varepsilon$$

$$\varepsilon_{ts} = G \rho_{ts}$$

$n \times m \quad n \times k \quad k \times m$

$$G = \varepsilon_{ts} \rho_{ts}^+$$

$$E_R = V G \rho$$

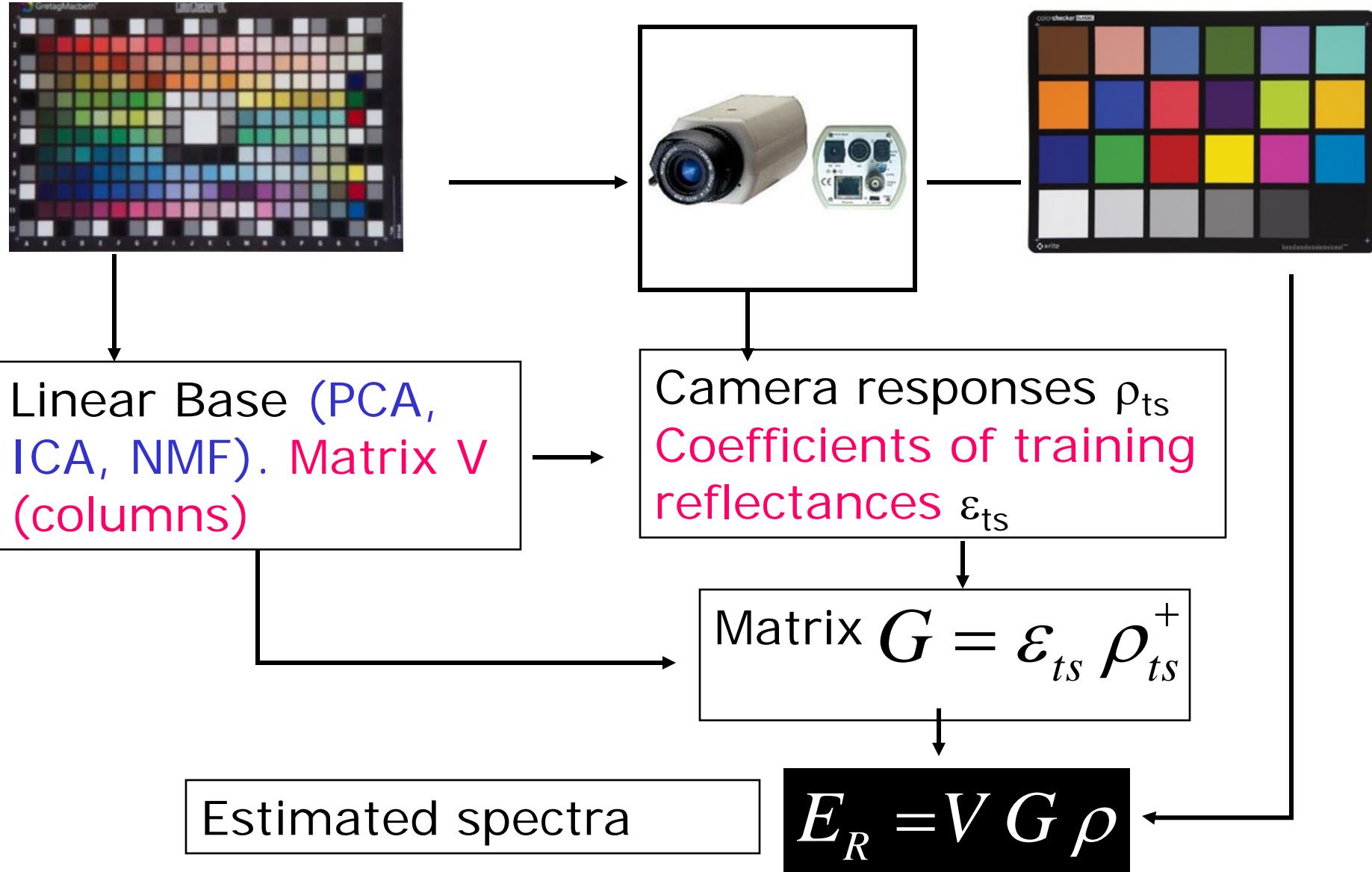
$N \times 1 \quad N \times n \quad n \times k \quad k \times 1$



- Quite simple and fast
- Takes noise into account



- Knowledge about spectral sensitivities of the camera needed (**only in case of simulations**)
- Needs two training sets (one for V and one for G)
- Influence of “calibration errors” of the camera and of the spectral recovery quality (**only in case of simulations**)



k: number of sensors
N: number of wavelength
n: number of basis vectors

Common conclusions for the Maloney-Wandell and Imai-Berns algorithms :

Optimal number of vectors (n)? Normally $n=k$ (number of sensors).

Maximum accuracy reached when $n=k$

Both algorithms allow $n>k$ but this implies:

- pseudoinverting rather than inverting ($n=k$)
- if $n=k$ solution is univocal
- pseudoinverting means to apply Moore-Penrose to a problem with more unknowns than equations.
- ambiguity in the solution
- noise affects more when dealing with big matrixes.

What happens if $n \leq k$ and n is not large enough to accurately recover spectra?

3) Shi-Healey (2002):

$$\rho = R^t E + \sigma$$

Smart method allowing $n > k$ without reducing quality of spectral recoveries

$$n > k$$

n (number of vectors)

k (number of sensors)

Subspace of spectra E (generated by changing the n parameters ε in the linear basis) compatible with the same sensors' responses

$$E = V_1 \varepsilon_1 + V_2 \varepsilon_2$$

$1, \dots, n-k$

$n-k+1, \dots, n$

$$E = V \varepsilon$$

$$\rho = R^t (V_1 \varepsilon_1 + V_2 \varepsilon_2)$$

Only one spectrum is the right one.

To select one criterion to select the appropriate spectrum.

Shi-Healey propose to select the one closer to one of the training set

3) Shi-Healey (2002):

Training: linear base V

$n > k$

$$E = V_1 \varepsilon_1 + V_2 \varepsilon_2$$

$1, \dots, n-k \quad n-k+1, \dots, n$

$$E = V \varepsilon$$

PCA, ICA, NMF

$$\rho = R^t (V_1 \varepsilon_1 + V_2 \varepsilon_2)$$

E vectors with different ε can generate the same ρ
 Aim: to associate a single recovered E_R with a ρ

From sensors' responses and m training spectra:

$$\left. \begin{array}{l} \rho_{k \times 1} \\ E_{ts} \\ N \times m \end{array} \right\} \Rightarrow \varepsilon_1^* \Rightarrow E^*$$

$(n-k) \times m$

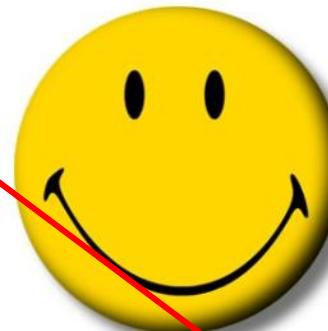
$$\varepsilon_1^* = \left(V_1 - V_2 (R^t V_2)^{-1} R^t V_1 \right)^+ \left(E_{ts} - V_2 (R^t V_2)^{-1} \rho^* \right)$$

$$\text{N} \times \text{m} \quad E^* = V_1 \varepsilon_1^* + V_2 (R^t V_2)^{-1} (\rho - R^t V_1 \varepsilon_1^*)$$

E_R is chosen from the set of E^* which minimizes

$$\| E_i^* - E_{ts_i} \|$$

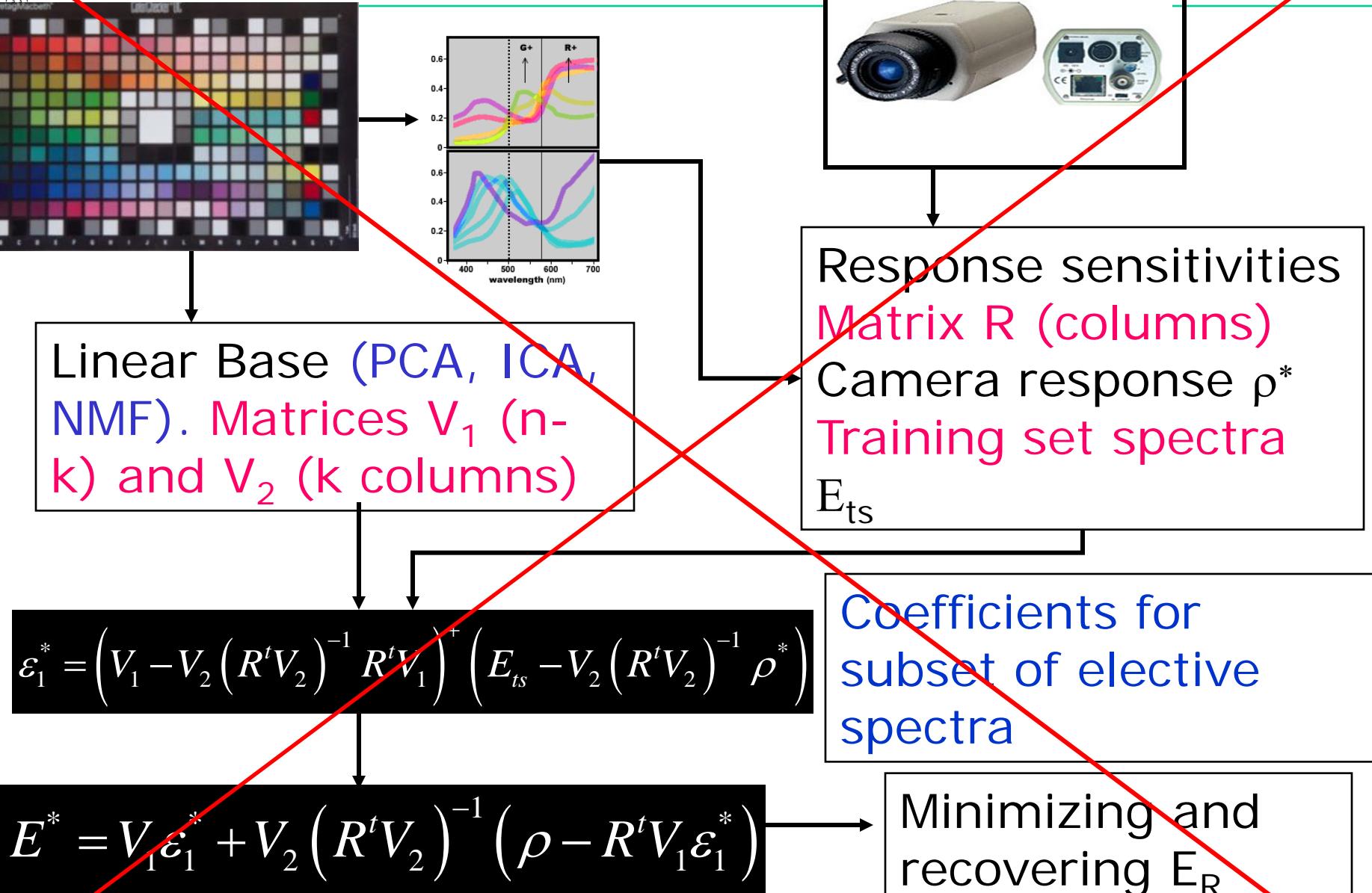
Disadvantage: for every given sensor response ρ we have to calculate m estimated spectra for E^* and choose the minimum of m distances. If m is large, the algorithm is extremely slow.



- It allows $n > k$
- Takes noise into account



- Knowledge about spectral sensitivities of the camera needed
 - Needs info about the spectra and camera responses of the training set
 - Influence of “calibration errors” of the camera
- Rather slow for big training sets



Algorithms without dimensionality reduction of the spectral functions

4) Wiener (Haneishi et al., 2000):

Training spectrum set E_{ts}

$$\rho = R^t E + \sigma$$

Camera sensitivities and noise estimation of the capture system

$$W = E_{ts} E_{ts}^t R \left(R^t E_{ts} E_{ts}^t R + \sigma_{ts} \sigma_{ts}^t \right)^{-1}$$

Estimated spectra

$$E_R = W \rho$$



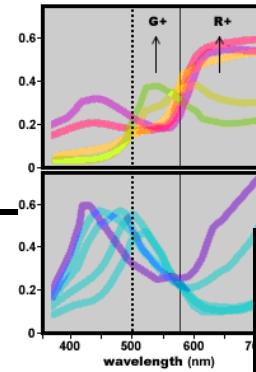
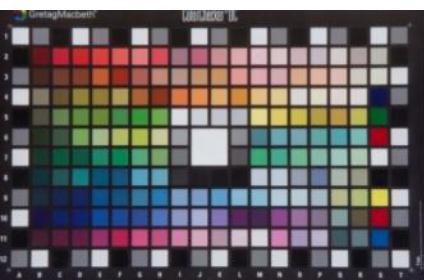
Real camera responses to the spectral functions which are to be estimated



- **Simple and fast**
- **Takes noise into account**



- Knowledge about spectral sensitivities of the camera needed
- Influence of “calibration errors” of the camera
- Noise estimation procedure needed as a previous step (Shimano 2005 for an experimental method to do so)



Camera
sensitivities R
Noise variance σ

$$W = E_{ts} E_{ts}^t R \left(R^t E_{ts} E_{ts}^t R + \sigma_{ts} \sigma_{ts}^t \right)^{-1}$$

Estimated spectra

$$E_R = W \rho$$

5) Pseudo-Inverse (PI) or Linear regression (Day, 2003):

-*Training of the system*: establishing the relation between m training spectra and their responses.

- W estimation by pseudoinverse

-Spectral recovery from real sensor responses. Noise taken into account.

-Non-linear versions lately developed, but no significative improvement found which compensates for the increased complexity

k: number of sensors

N: number of wavelength

m: training set number

$$E_{ts} = W_L \rho_{ts}$$

Nxm Nxk kxm

$$W_L = E_{ts} \rho_{ts}^+$$

$$E_R = W_L \rho$$

5b) Non linear regression (Shimano 2007, López-Álvarez 2007)

$$W_L = E_{ts} \rho_{ts}^+$$

$$W_{NL} = E_{ts}$$

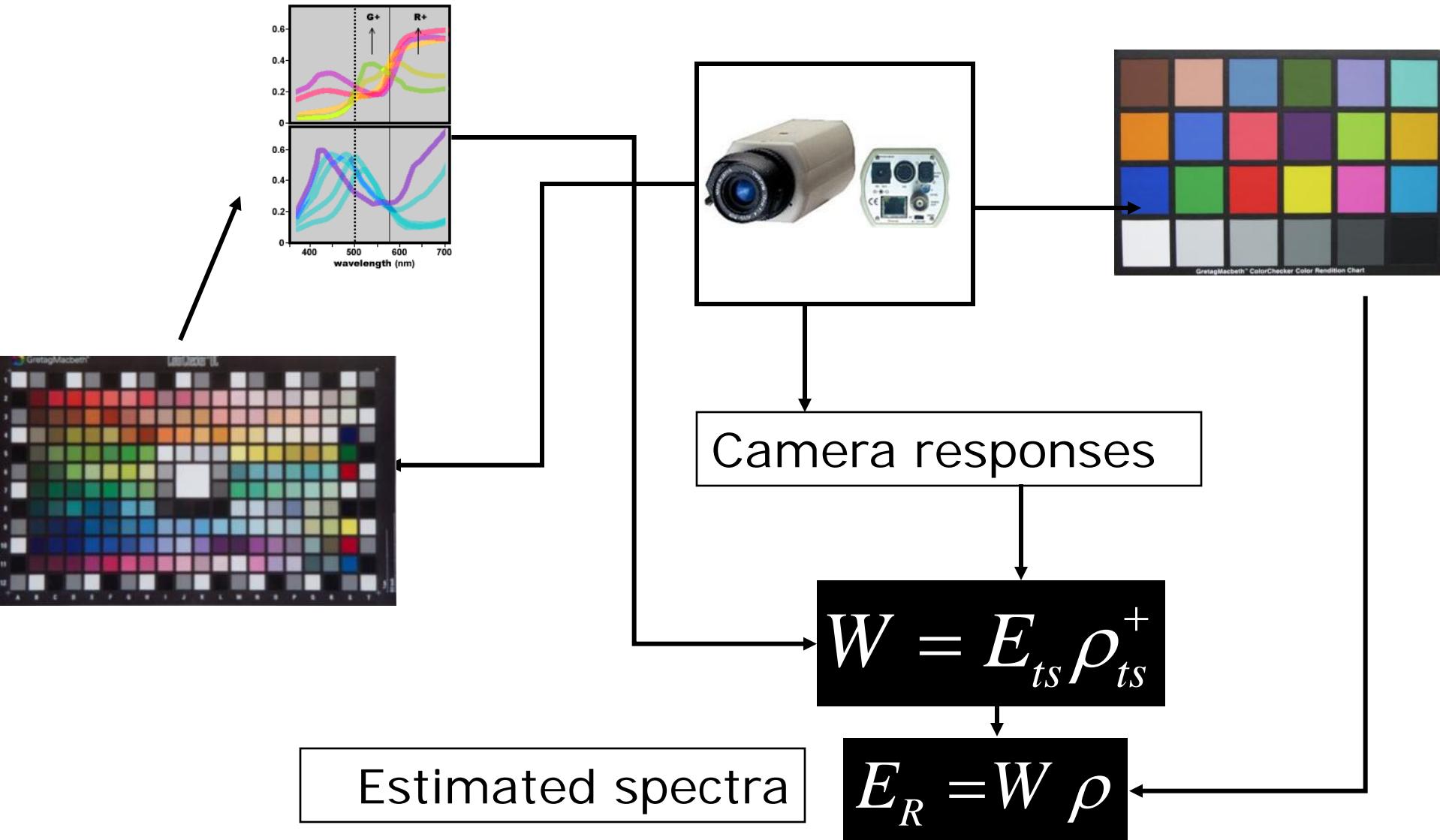
$$\begin{bmatrix} 1 \\ \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_1\rho_2 \\ \rho_1\rho_3 \\ \rho_2\rho_3 \\ \rho_1^2 \\ \rho_2^2 \\ \rho_3^2 \end{bmatrix}^+$$



- Simple and fast
- Takes noise into account
- No knowledge about the spectral sensitivities needed



- When applied computationally, not robust against noise
- In some occasions, the real camera responses to the training spectra are needed (**in case of simulations**)



6) Matrix-R method (Zhao et al., 2005): PROPOSED AS A SEMINAR

Theoretical basis: Wyzszecki hypothesis + matrix R theory

Any spectral distribution:
decomposed into **fundamental spectrum** + metameric black
(zero tristimulus values)

Method for obtaining the
fundamental stimulus
and metameric blacks
from a given spectrum

Weight matrix A Orthogonal projector P

$$A_{ij} = E_{i\lambda} CMF_{\lambda j}$$

$$P = A(A^t A)^{-1} A^t$$

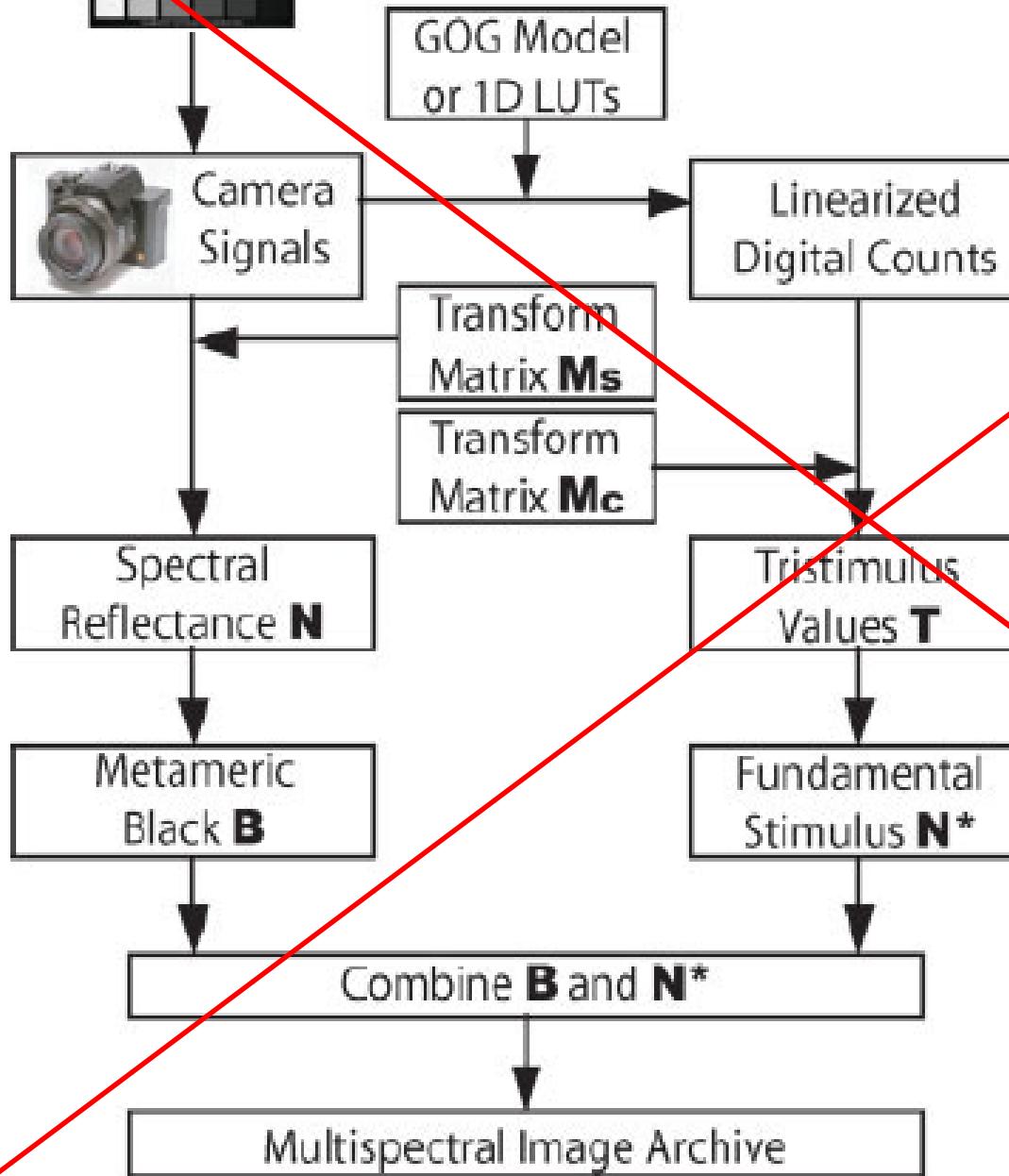
For a given
spectrum N:

Fundamental

Metameric black

$$N^* = PN = A(A^t A)^{-1} T$$

$$B = (I - P)N = N - N^*$$

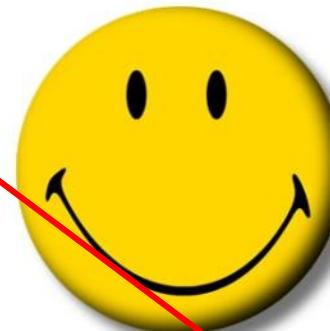


$$M_s = E_{ts} \rho_{ts}^+$$

Transformation matrix **Mc**: derived from LSE minimization using CIEDE2000 color difference formula

GOG model:
gamma correction with offset

$$D_{Li} = (\alpha_{Li} D_i + \beta_{Li})^{\gamma_i}$$



- Original approach
- Takes noise into account
- No knowledge about the spectral sensitivities needed



- More complex than previous estimation algorithms
- The real camera responses to the training spectra are needed



	Maloney Wandell	Imai- Berns	Shi-Healey	Wiener	Regression (linear or non-linear)	Matrix R method
Linear base	yes	yes	yes	No	No	No
Training set of spectra	yes (for linear base)	yes (for linear base and the matrix inversion)	yes (for linear base and exhaustive comparison)	yes (for the matrix inversio n)	yes (for the matrix inversion)	yes (for calculation of fundamental and m. blacks)
Knowled ge of spectral sensitivi ties	yes	No	yes	yes	No	No
Computation time	fast	fast	slow	fast	fast	Relatively fast

Other algorithms for spectral estimation/recovery:

- **POCS (Projection Onto Convex Sets)**

H. Stark, *Vector Space Projections*, (John Wiley&Sons, 1998).

- **Neural Networks**

M. D. Buhmann, *Radial Basis Functions: Theory and Implementations*, (Cambridge University Press, 2003).

A. Mansouri, F. S. Marzani ; P. Gouton, “Neural networks in two cascade algorithms for spectral reflectance reconstruction” IEEE International Conference on Image Processing 2005

- **Kernel**

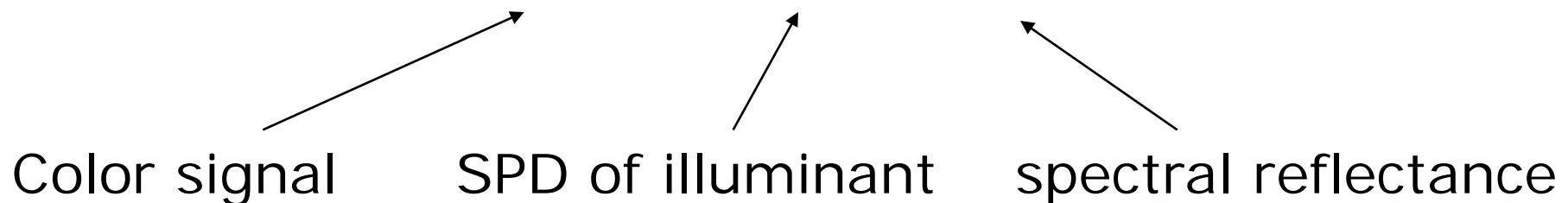
V. Heikkinen, R. Lenz, T. Jetsu, J. Parkkinen, M. Hauta-Kasari, T. Jääskeläinen. “Evaluation and unification of some methods for estimating reflectance spectra from RGB images”, J. Opt. Soc. Am. A **25**, 2444-2458 (2008).

- etc...

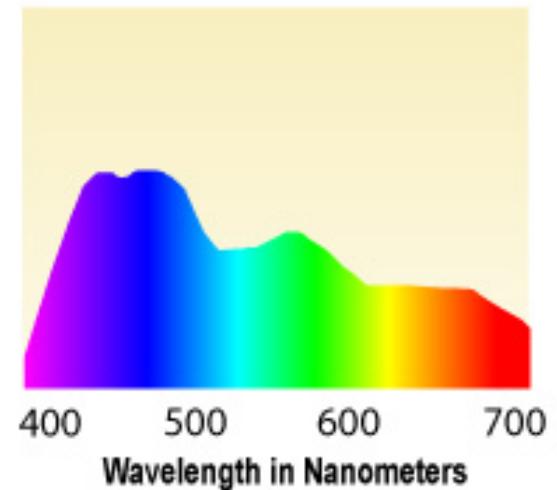
Reflectances from Color Signals?

- Recovery of spectral reflectance from color signals:

$$E(\lambda) = S(\lambda)r(\lambda)$$

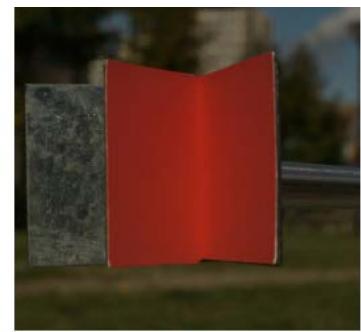
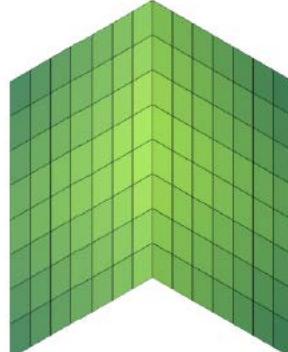
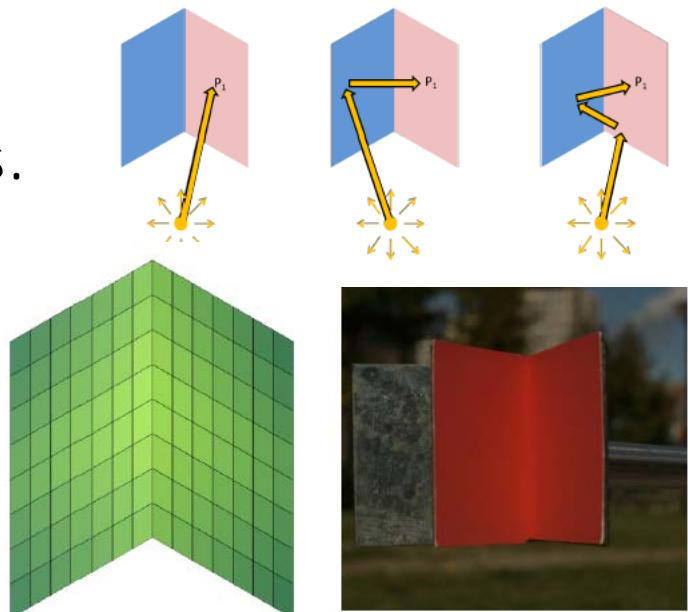


An estimation or measurement of the SPD of the illumination is needed



- Some estimation algorithms

- grey world hypothesis
- including a white in the scene:
planar or spherical
- specular reflections
- retinex algorithm
- others: i.e. using self-interreflections in concave objects.



(a) Two Munsell sheets with an angle of 45°

Spectral estimation algorithms or methods

Cases studies if you want to know more....

Nieves et al.(2007)

Spectral recovery of artificial illuminants

López-Alvarez et al.(2007)

Spectral recovery of natural illuminants

Zhao et al., 2004

Spectral recovery of reflectances

Valero et al., 2007

Spectral recovery of reflectances from natural scenes

Cases studies if you want to know more....

1) Recovering artificial illuminants (Nieves et al., 2007):

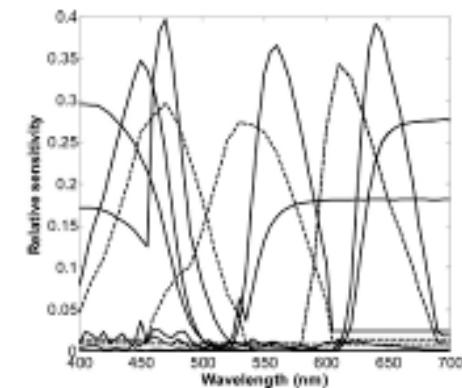


RGB camera plus 0, 1, 2 or 3 color filters?
How accurate?
Which filters?
How many?

Cases studies if you want to know more....

1) Recovering artificial illuminants (Nieves et al., 2007):

- Different methods for obtaining the linear base (PCA, ICA, NNMF with different rank factorizations).
- Comparison with linear regression method (no need for linear base)
- Recovery of artificial illuminants (some cases of “spiky” SPDs), computational and experimental approaches.



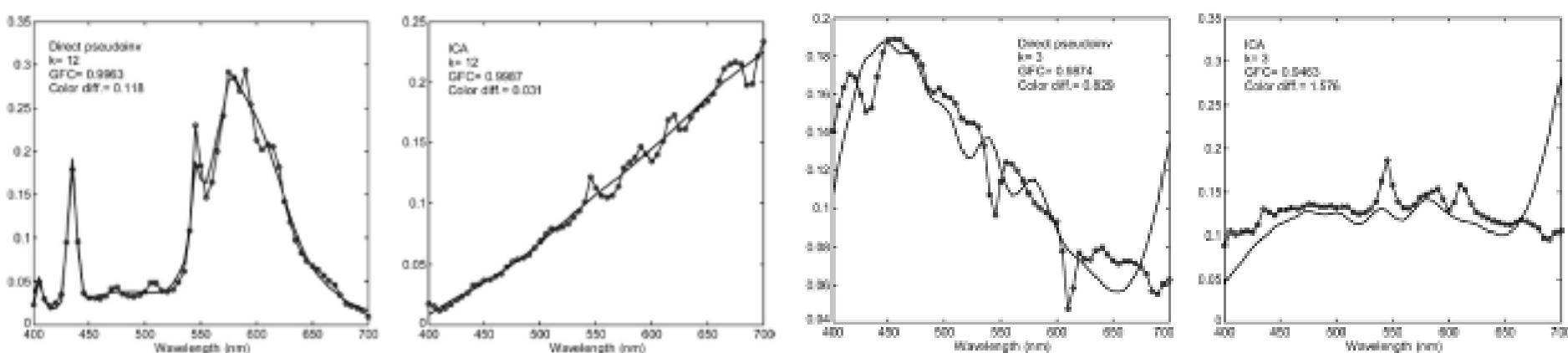
Simulations (test spectra):

Table 2. Mean and Sample Standard Deviation of GFC and ΔE^*ab Values Obtained for the Test Spectra

Without noise

Measure	Algorithm	Number of Sensors					
		$k = 3$		$k = 6$		$k = 9$	
Mean	SD	Mean	SD	Mean	SD	Mean	SD
GFC	NMF Euclidean	0.95062	0.06239	0.97873	0.02209	0.97961	0.02272
	NMF divergence	0.95065	0.06240	0.97949	0.02280	0.97949	0.02280
	ICA	0.95062	0.06240	0.97870	0.02207	0.97981	0.02238
	Direct pseudoinv	0.95065	0.06240	0.97873	0.02205	0.97984	0.02236
	PCA	0.89926	0.07683	0.94410	0.04599	0.98543	0.01167
ΔE^*ab	NMF Euclidean	1.9421	1.7096	0.7395	0.7485	0.4043	0.4300
	NMF divergence	1.9479	1.7170	0.3926	0.3946	0.3926	0.3946
	ICA	1.9464	1.7161	0.7438	0.7472	0.3625	0.3400
	Direct pseudoinv	1.9467	1.7169	0.7451	0.7473	0.3621	0.3406
	PCA	3.0078	1.5298	1.8320	1.3003	0.4600	0.2593

^aOnly the maximum rank of factorization ($u = 29$ in the case of NMF algorithms) is shown for each number



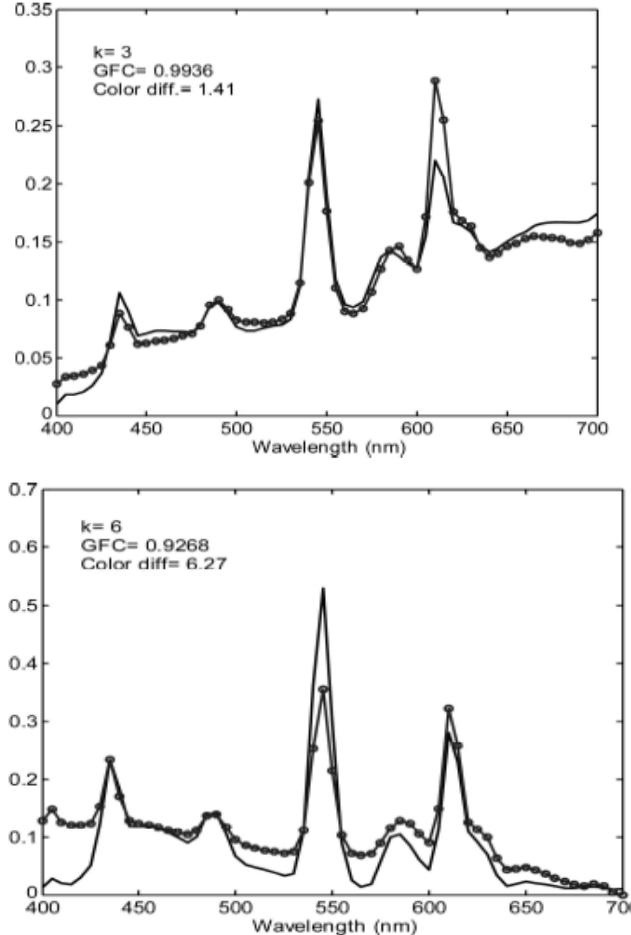
Experimental results:

Table 4. Average Spectral and Colorimetric Quality Classification of Test Illuminants Using the Direct Pseudoinverse Method with Different Numbers of Sensors^a

		Simulated Digital Counts		Experimental Results	
		GFC	ΔE^*ab	GFC	ΔE^*ab
$k = 3$	Mean	0.9474	2.33	0.9128	1.67
	SD	0.0811	2.08	0.0637	0.68
$k = 6$	Mean	0.9816	2.20	0.7978	4.33
	SD	0.0153	0.98	0.0492	0.99
$k = 9$	Mean	0.9715	2.36	0.7975	9.26
	SD	0.0312	0.83	0.0052	0.14
$k = 12$	Mean	0.9741	2.37		
	SD	0.0284	0.89		

^aThe results are for computational and experimental results.

- Recovery is acceptable only for low number of sensors
- If a reduced training set of illuminants is used, we can obtain good classification results without the need of an a priori classification of the training set
- Useful for illuminant estimation in a scene captured by an RGB camera

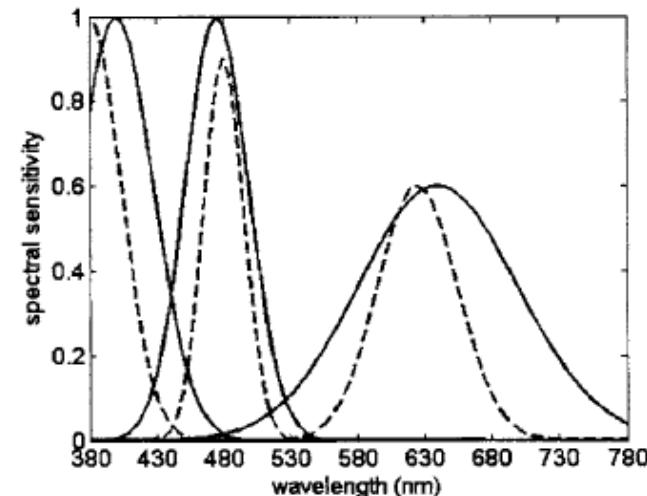


Cases studies if you want to know more....

2) Recovering natural illuminants (López-Álvarez et al., 2007):

Theoretical work (with simulations):

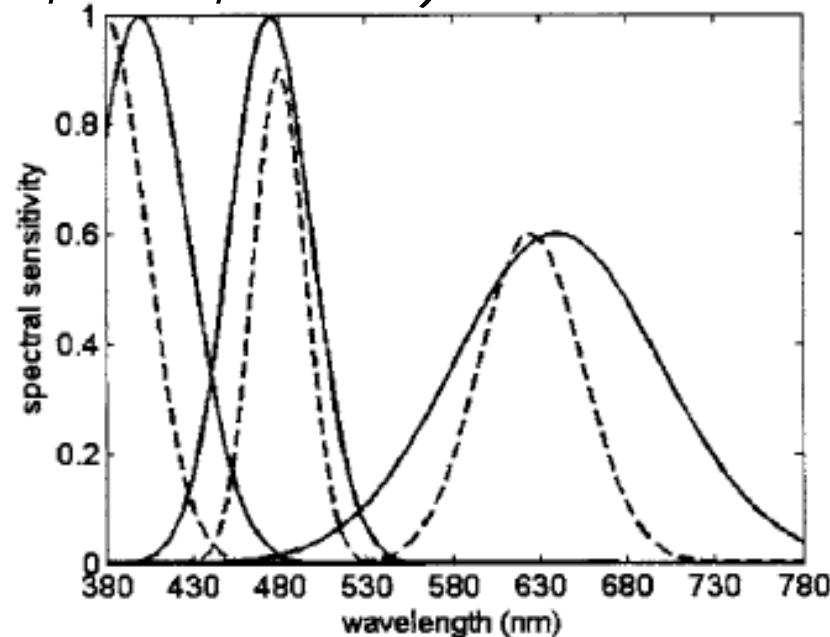
- Can we estimate the spectra of natural daylight from the response of few Gaussian sensors?
- How accurate? Which metric to evaluate it?
- How many sensors? Optimization search!
- The more the better?
- Which FWHM?
- How many spectra for the training set?
- What is the influence of noise?
- Which estimation algorithm is the best?
- Which dimensionality reduction algorithm?



One application:
The Design of a Low-Cost Radiometric System for Photovoltaic Solar Cells, IEEE Journal of Photovoltaics 2016

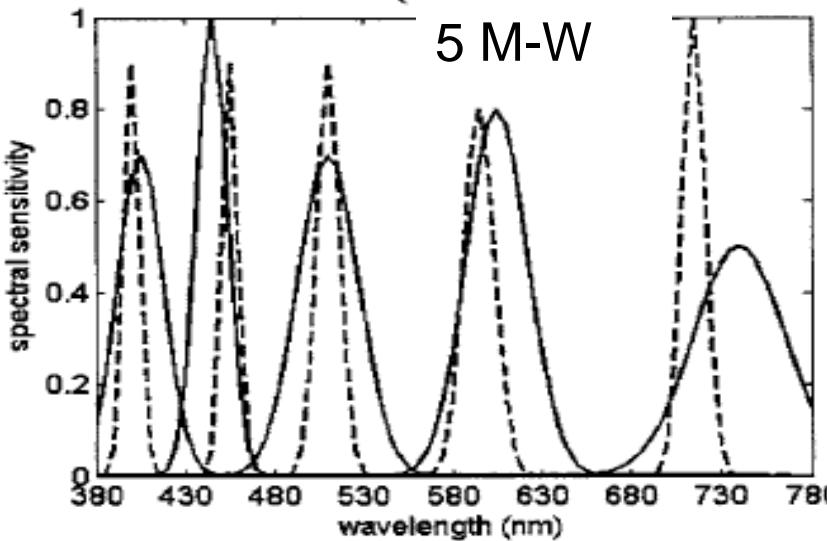
2) Recovering natural illuminants (López-Álvarez et al., 2007):

- Selection of algorithms, sensors (3 to 5) and linear basis for daylight recovery from camera responses (search for optimal sensors by simulated annealing)
- Different additive noise levels (SNR of 40 dB, 30 dB and 26 dB, which corresponds to 1%, 3%, 5% random, normally distributed noise)
- Different training set sizes (20, 156, 1567)
- Different recovery methods (M-W, I-B, S-H, LR)
- Different dimensionality reduction methods (PCA, ICA, NMF)



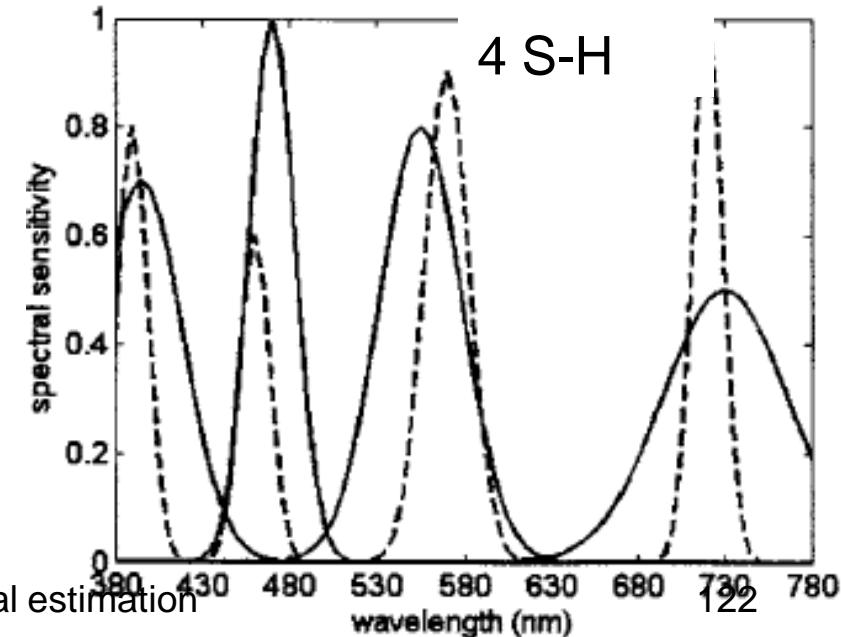
Cases studies if you want to know more....

Spectral profile of optimum sensors

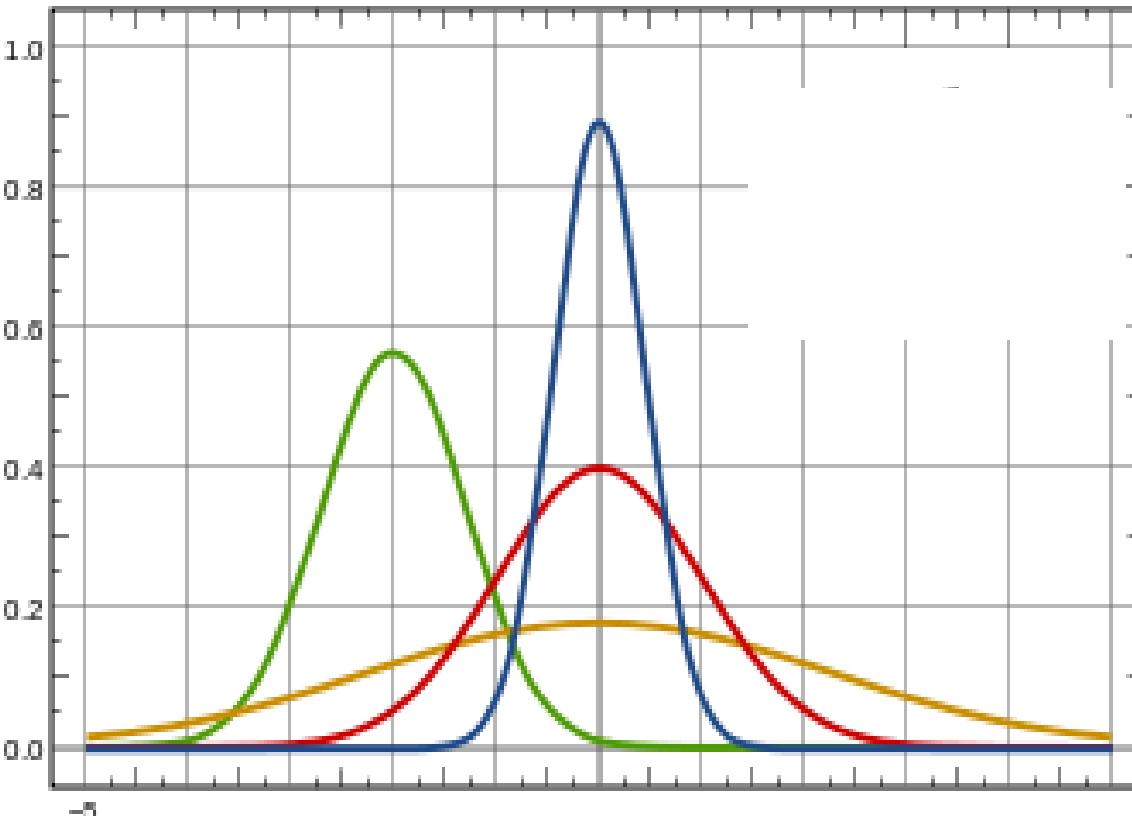


- Influence of noise level: it sharpens the sensors and (for M-W method) shifts peak wavelengths to the left
- No significant influence of the training set size

- Much sharper sensors for the S-H method.
- The peak wavelengths tend to be similar to the positions of the absorption bands of typical daylight SPDs.



Cases studies if you want to know more....



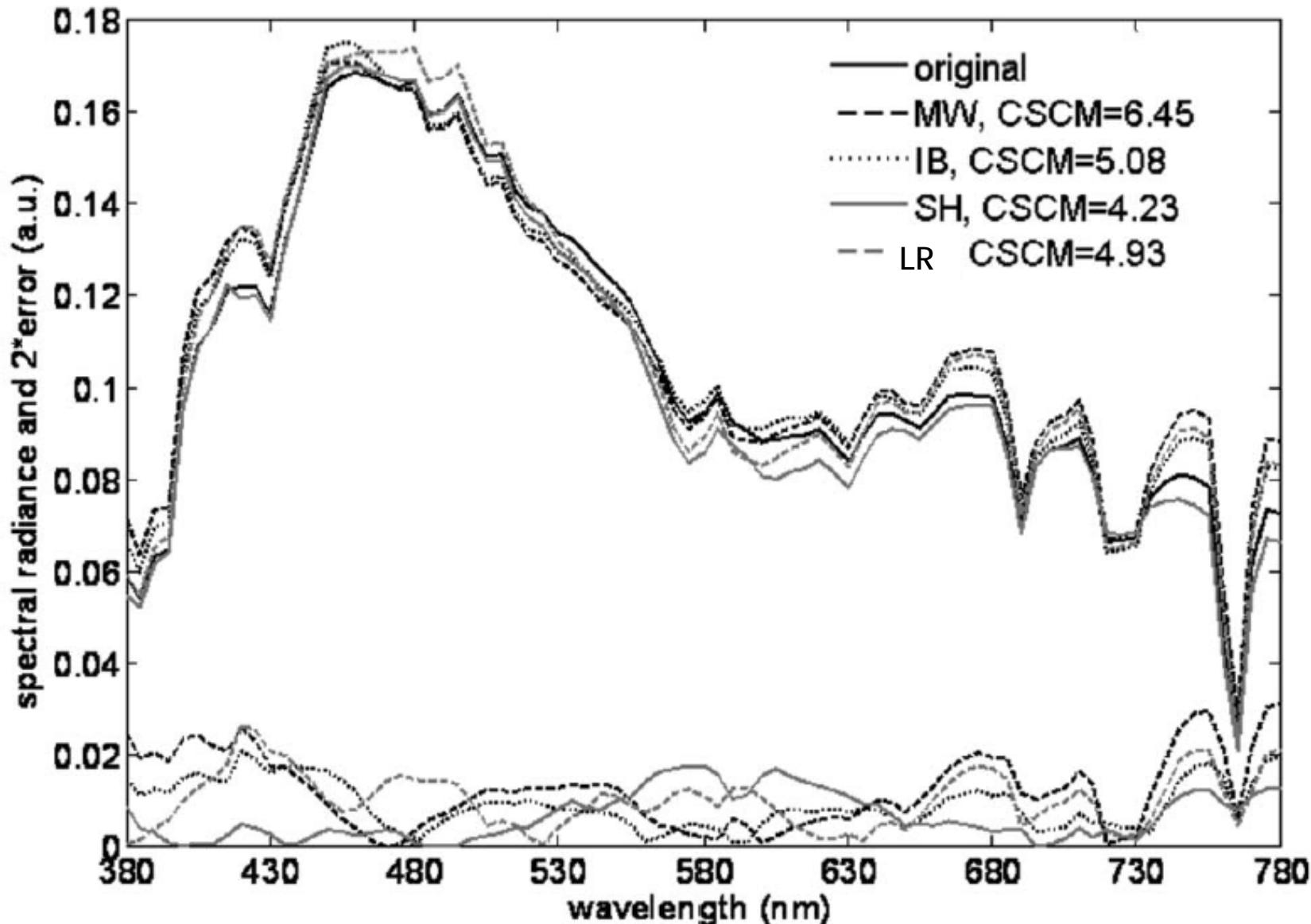
$$n_c = \frac{N!}{n!(N-n)!}$$

N=available filters
n=selected filters

Simulated annealing

$$CSCM = Ln(1 + 1000(1 - GFC)) + \Delta E_{ab}^* + IRE(\%)$$

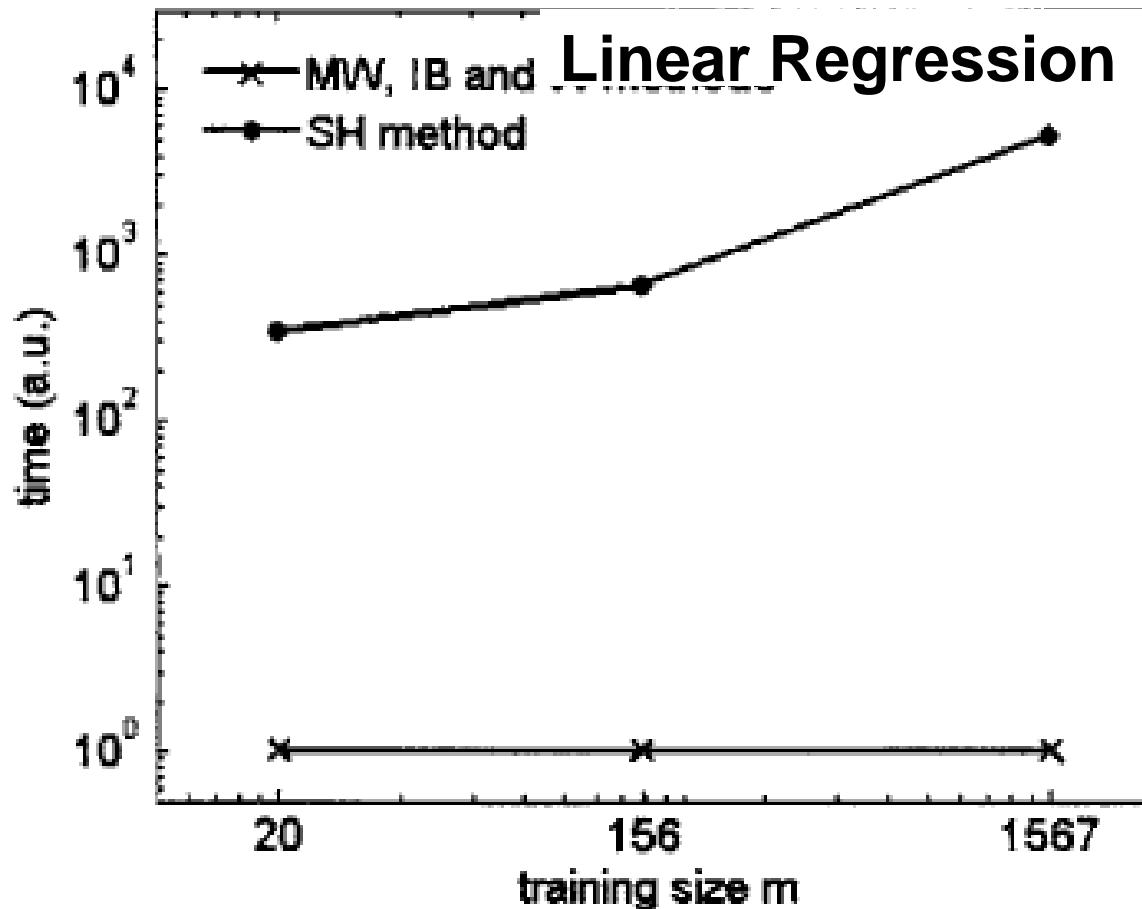
Accuracy of the spectral recovery



Cases studies if you want to know more....

And the winner is....

- Balancing speed and performance, best is maybe **Linear Regression**



Cases studies if you want to know more....

3) Recovering reflectances (Zhao et al, 2004):

- Can we estimate spectral reflectances from an RGB camera + color filters?
- How accurate?
- How many sensors? Which filters?
- Which estimation algorithm is the best?
- Which dimensionality reduction algorithm?
- How many spectra for the training set?
- Which is the best training set?



Cases studies if you want to know more....

3) Recovering reflectances (Zhao et al, 2004):

- Three recovery algorithms compared for reflectance recovery: LR, matrix-R, and CCR (canonical correlation regression, based on cross-product terms of the camera responses).
 - Six-channel camera (two color filters used)
 - Training with ColorChecker DC, six more color targets used as test



- Transformation of RGB to tristimulus offered as comparison

Cases studies if you want to know more....

4) Computational simulations of reflectance recovery for natural scenes (Valero et al, 2007):

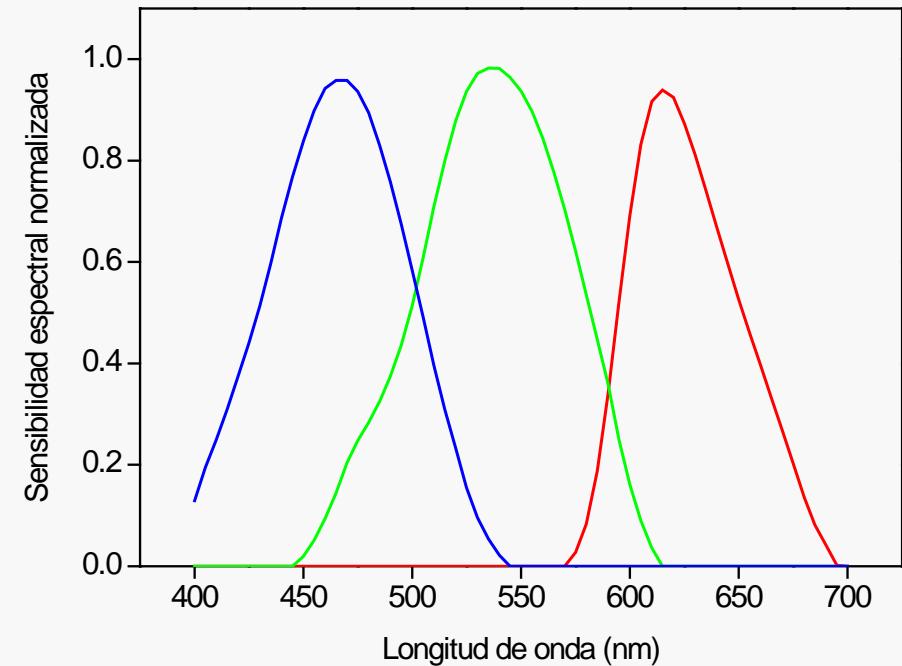
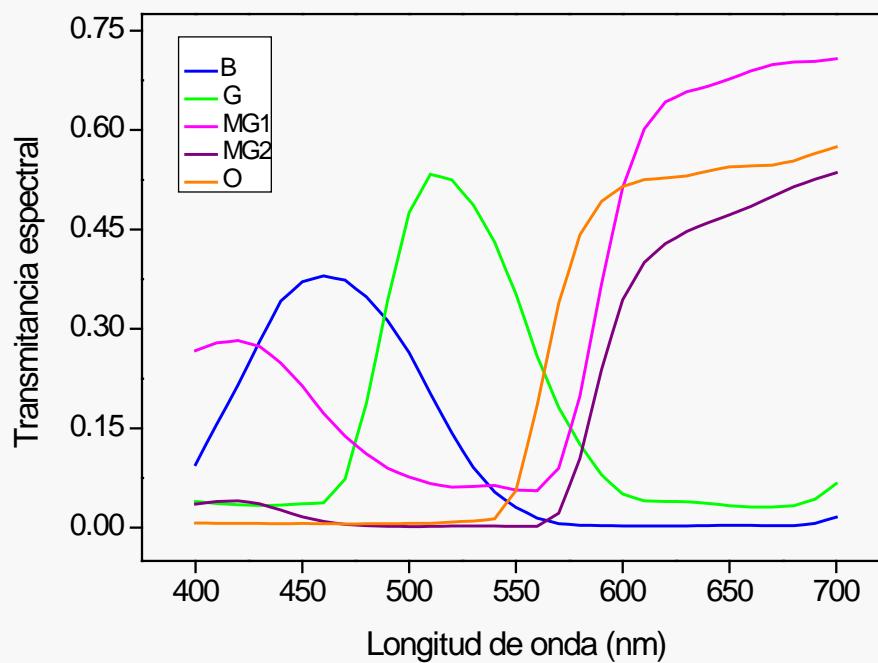
- Can we estimate spectral reflectances of natural images?
- RGB + color filters? How many filters? How accurate?
- How many sensors? Which filters?
- Which estimation algorithm is the best?
- Which dimensionality reduction algorithm?
- How many spectra for the training set?
- Which is the best training set?



4) Computational simulations of reflectance recovery for natural scenes (Valero et al, 2007):

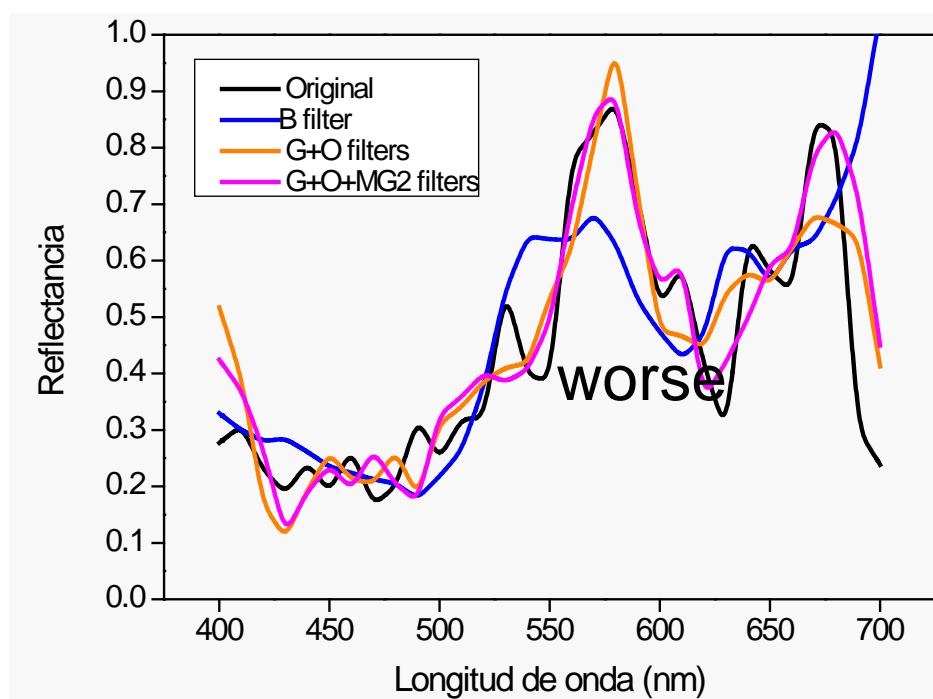
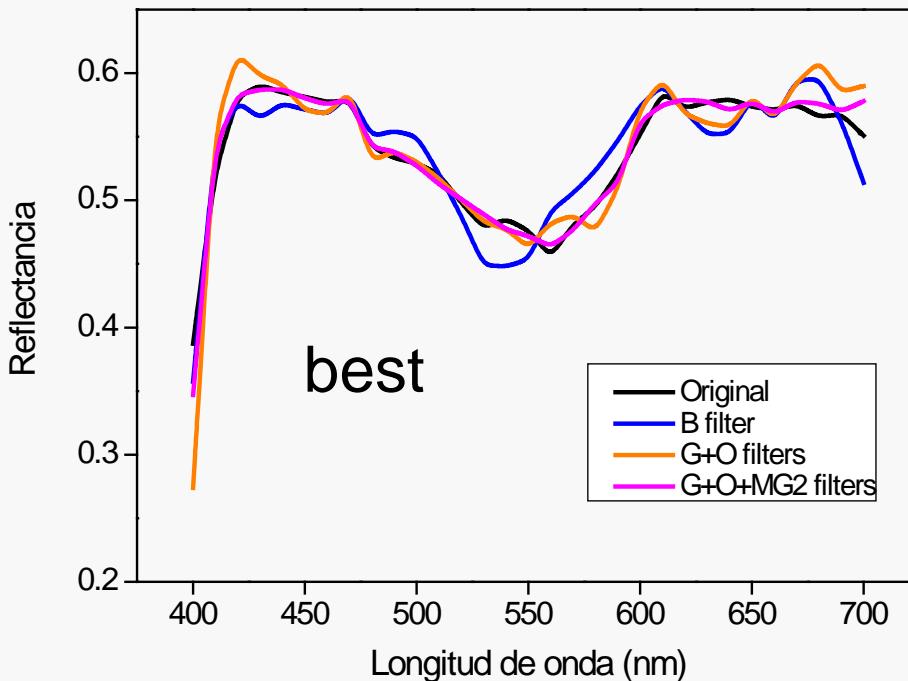


- LR method (no noise added in the simulated camera responses). Ground-truth data: rural and urban scenes captured by a monochrome camera + LCTF
- The best combinations of one, two or three color filters are studied.



- 30 scenes, 151x151 pixel fragments: training set of 684030 reflectances
- Test set: 3 sets of different scenes or different fragments of the training scenes

		Color filters							
Index	Test set	3 sensors	MG 1	MG 2	B	G	O	G+O	G+O+MG2
GFC (%)	1	99.07 (1.65)	99.45 (1.09)	99.49 (1.07)	99.63 (0.70)	99.35 (1.17)	99.59 (0.69)	99.75 (0.42)	99.90 (0.10)
	2	96.45 (8.18)	98.00 (4.62)	98.13 (4.28)	98.63 (2.96)	97.64 (5.44)	98.39 (3.17)	98.99 (2.58)	99.31 (1.79)
	3	96.26 (6.30)	97.18 (3.87)	97.30 (3.75)	98.02 (3.32)	96.86 (4.21)	97.64 (3.40)	98.68 (2.40)	98.96 (1.97)
RMSE (%)	1	7.24 (5.27)	5.49 (4.15)	5.20 (4.12)	4.51 (3.45)	6.03 (4.27)	4.88 (3.28)	3.75 (2.77)	2.47 (1.32)
	2	5.54 (6.11)	3.59 (3.65)	3.47 (3.57)	3.17 (3.34)	3.96 (3.96)	3.41 (3.38)	2.68 (2.88)	2.02 (2.04)
	3	2.23 (1.40)	2.25 (1.25)	2.18 (1.23)	1.63 (1.13)	2.46 (1.35)	1.99 (1.13)	1.40 (0.92)	1.25 (0.80)
ΔE^*_{ab}	1	1.03 (0.66)	0.53 (0.42)	0.54 (0.45)	0.50 (0.27)	0.42 (0.39)	0.57 (0.44)	0.24 (0.16)	0.18 (0.14)
	2	1.15 (0.94)	0.67 (0.84)	0.73 (0.82)	0.61 (0.55)	0.53 (0.79)	0.73 (0.85)	0.25 (0.33)	0.22 (0.32)
	3	1.83 (1.25)	1.07 (0.74)	1.18 (0.82)	0.60 (0.55)	0.83 (0.63)	1.26 (0.96)	0.31 (0.33)	0.27 (0.31)



- Satisfactory recovery with two color filters successively added in front of the lens
- When rural scenes alone are used as training, urban scenes are recovered worse, and so with urban scenes as training, although the rural matrix is more robust

1. How are the spectral curves we are dealing with?

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3. Algorithms for spectral estimation

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- Others methods

4. Selection of samples

5. Selection of filters (or LEDs)

6. Influence of noise

4. Selection of samples

Most of spectral estimation algorithms depends on training sets in different ways.

Theoretically: the training set should be representative of the target set of spectra.
Training set depending on the application.

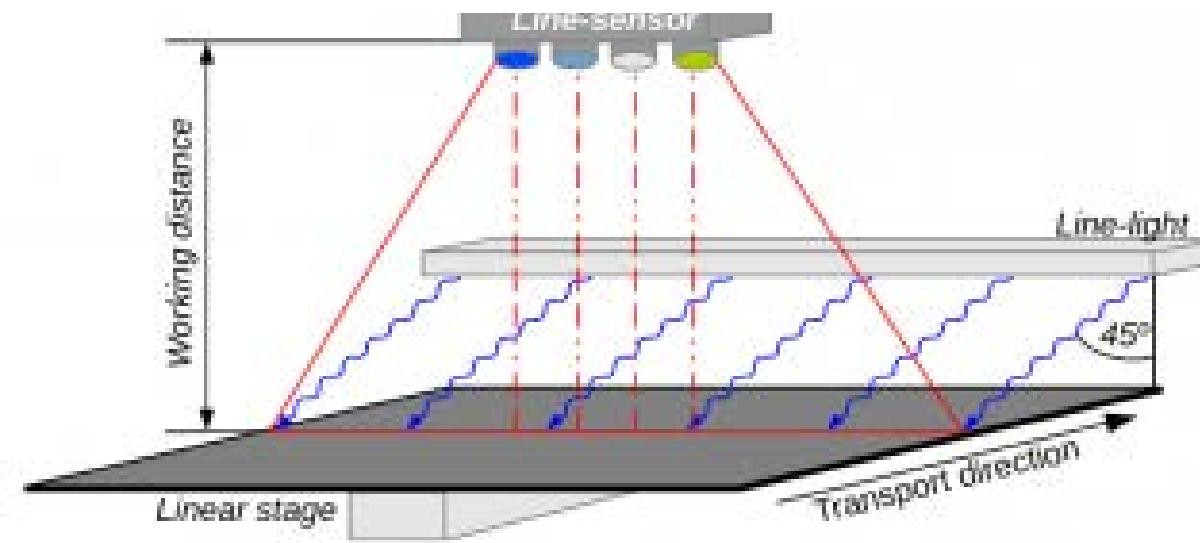
Training set and test set?

1. Training set different from test set.
2. Training and test are subsets of a unique set.



4. Selection of samples

TruePixa from Chromasens?



(a)



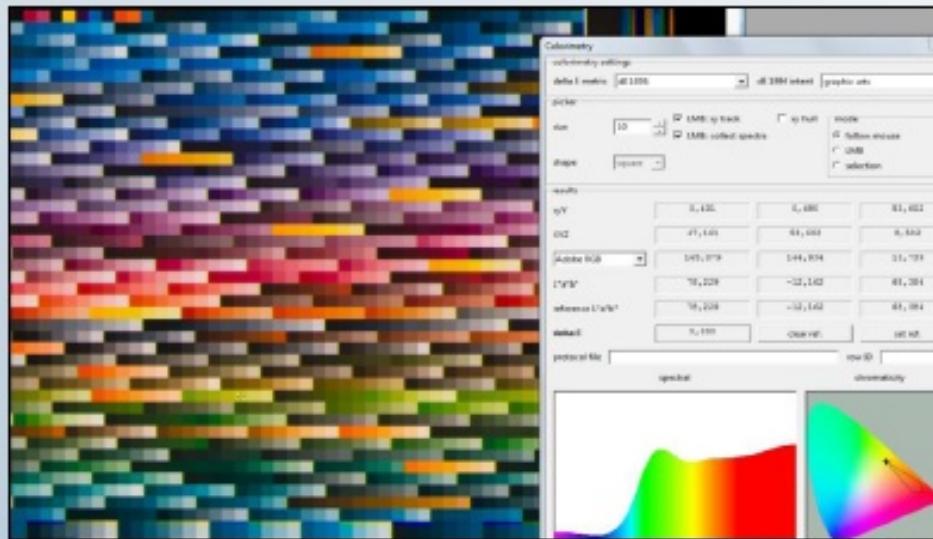
(b)

4. Selection of samples

TruePixa from Chromasens? The same instrument for different applications? Same training set? Different?

Sample applications for line-scanning based MSI using truePIXIA

- Print inspection / print control / print color measurement*



from Timo Eckhard's slides (2016)

4. Selection of samples

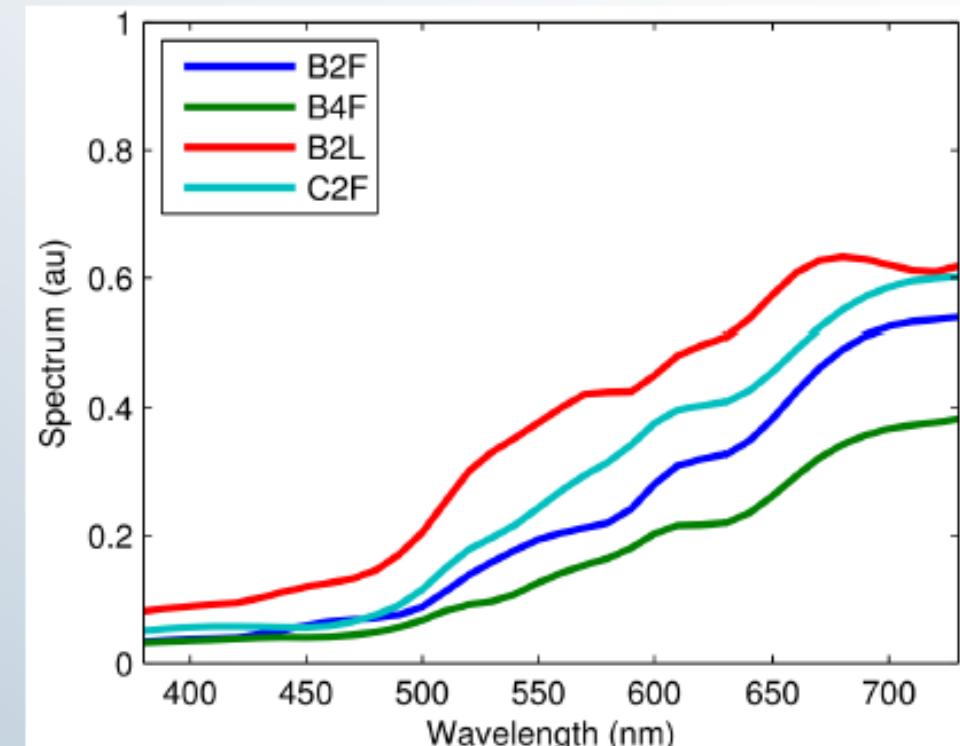
TruePixa from Chromasens? The same instrument
for different applications? Same training set?
Different?

Image classification: tobacco leafs



Segmented images

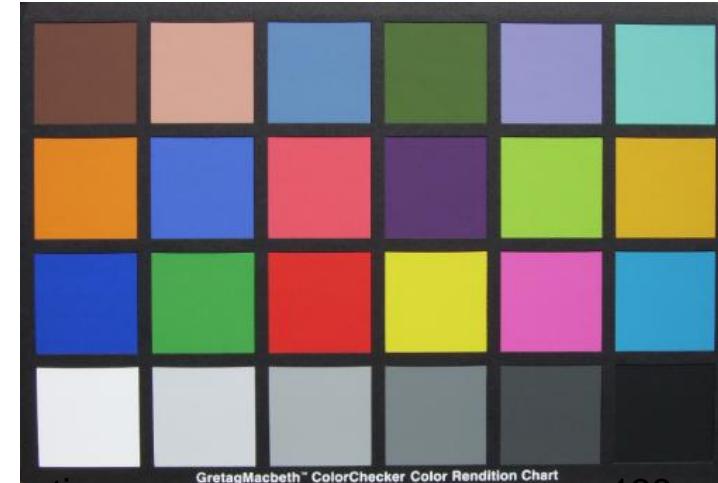
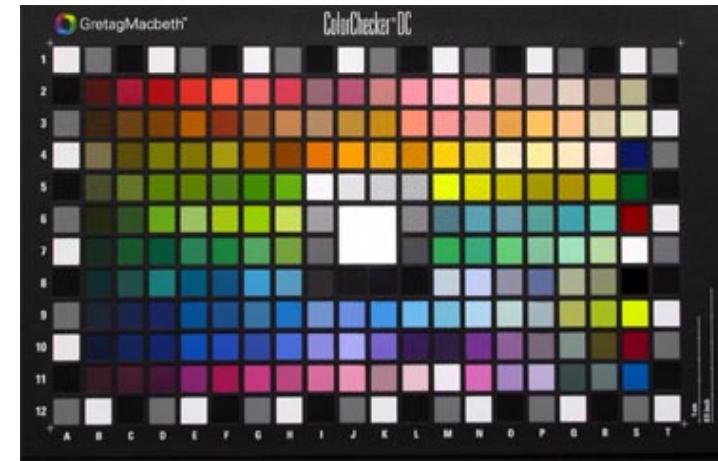
from Timo Eckhard's slides (2016)



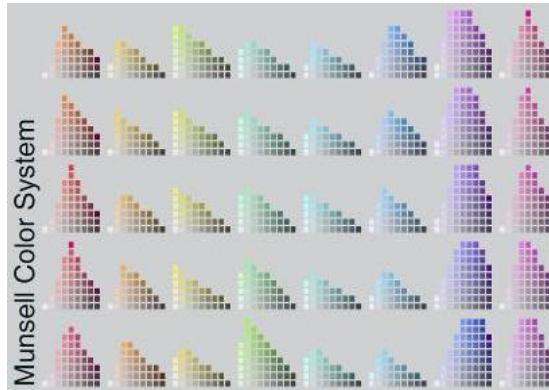
Spectral reflectances

4. Selection of samples

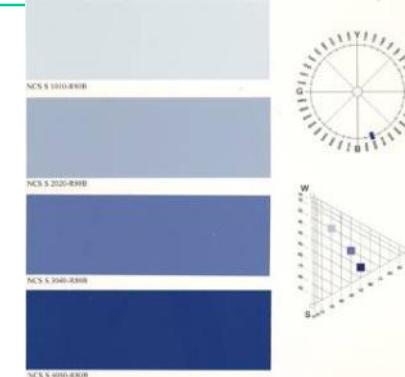
- The **training data** must be as **similar** to the data we intend to recover as possible.
- If the data are not representative of a very particular kind of surface or radiance curve, then a standard set is a good option
- Very often used: Gretag-Macbeth ColorChecker (DC or reduced 24 patches versions)



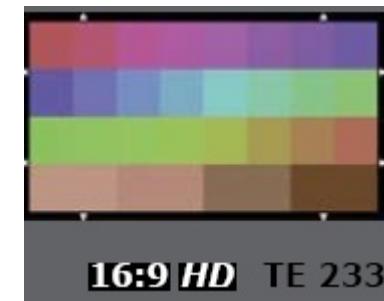
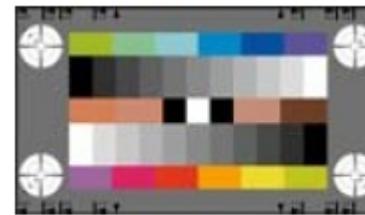
Munsell



NCS



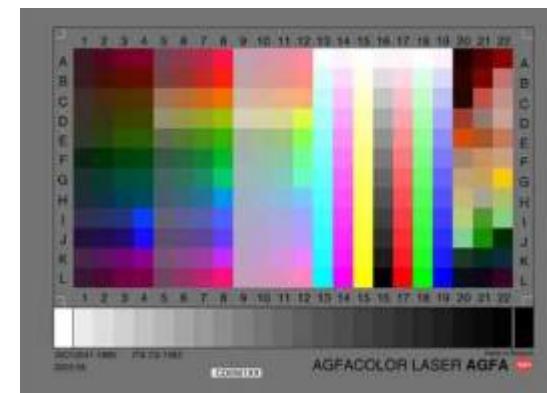
Esser



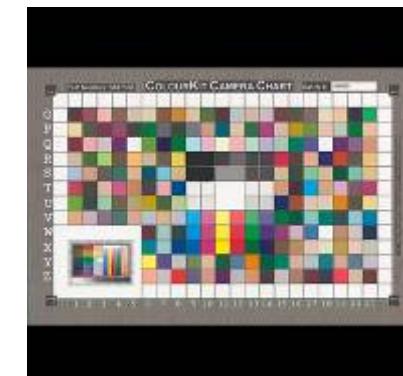
Kodak



AGFA



FFEI



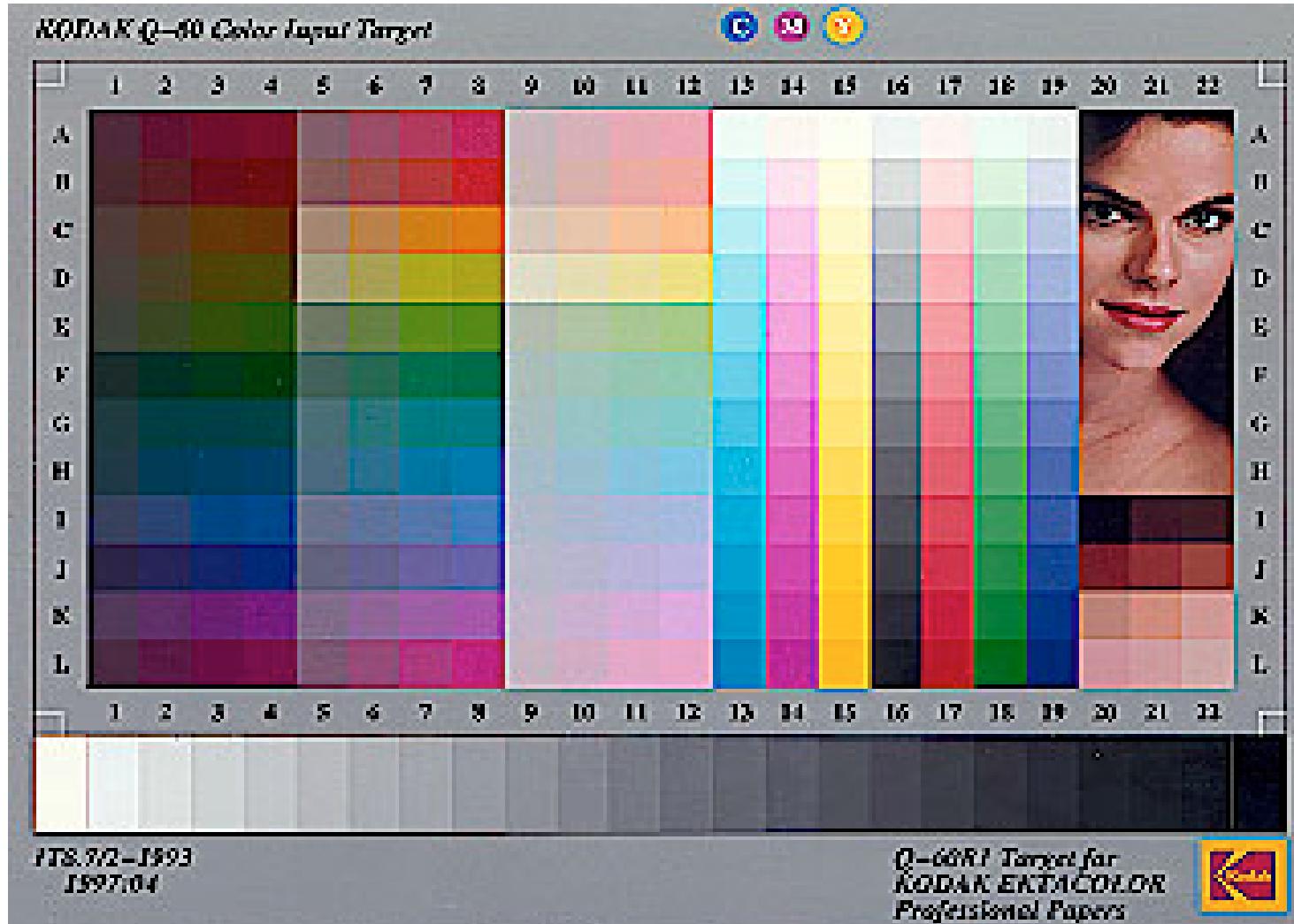
Selection criteria

- There are many possibilities available. So what to do before tackling training data selection?

- 1) Getting as much info as possible about the target spectral functions**
- 2) Collect all the reference charts in the lab**
- 3) Develop and run a selection-optimization algorithm to get as few and most representative examples from the charts or objects...**
- 4) Select our own "customized" reference data set for training**

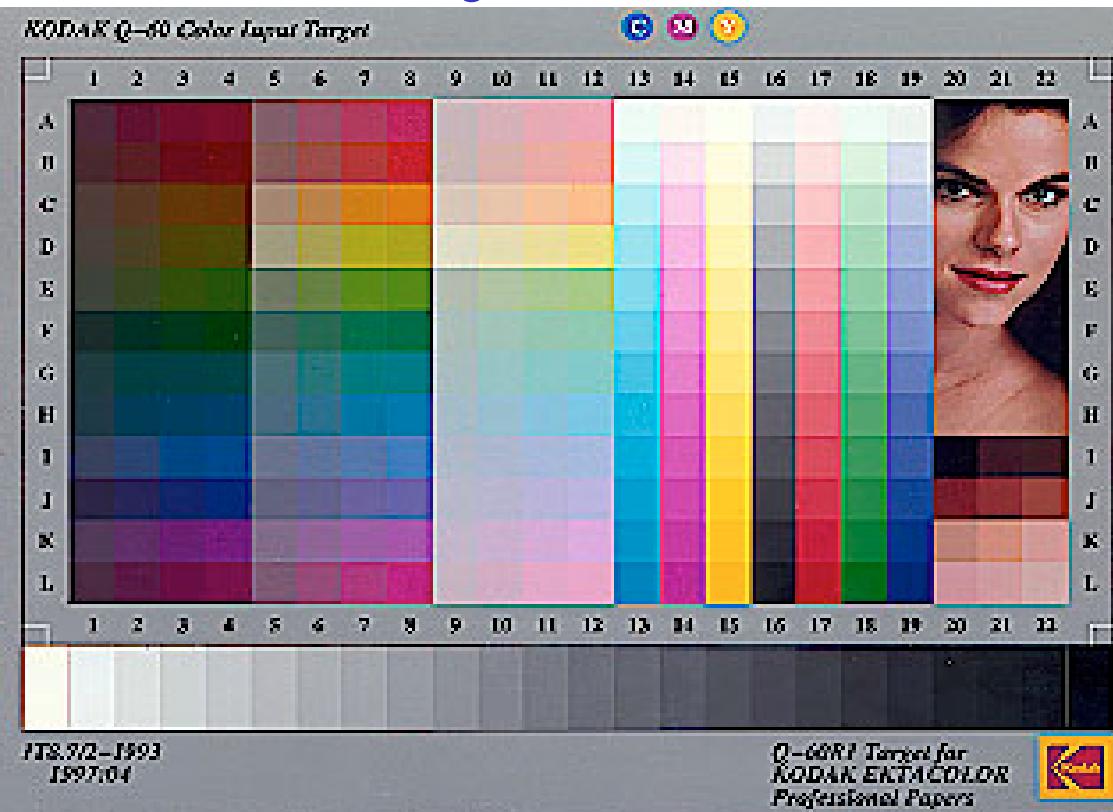
How to select the most significant patches?

The more the better?



How to select the most significant patches?

- As Mohammadi et al. (2004, 2005) have shown, performance does not depend on number of colors or gamut, but on spectral properties of samples, and it stabilizes beyond a certain number of samples.



- A saturated sample predicts quite well the mixtures of white with itself, and so more samples with different chroma values would not be necessary.

How to select the most significant patches?

Selection processes:

1. Random selection

2. Iterative process

1. Find a spectrum which is as different as possible from the other target spectra.
2. Select the second spectrum as the one which minimizes the condition number of a matrix with the first two spectra
3. Repeat the procedure.

Hardeberg (1999) showed that this iterative process is better than a heuristically selection.

3. Other methods?

Training approaches for training

from Eckhard et al.
Applied Optics, 2014

global vs local

1. **global training:** estimation is computed using the same transformation for all test samples.
2. **local training:** the transformation used is different for each specific sample, and therefore is adaptive to the sample features.

bottom-up vs top-down

1. **bottom-up:** starts with an empty set and successively adds samples to the set
2. **top-down:** start with a full set and reject samples consecutively until the final training set is obtained

general purpose vs application dependent selection

1. **general purpose:** the selection is not optimized for a specific application but rather to a specific objective, such as to select most distinct colors from a set of available samples
2. **application dependent:** perform the sample selection based on the objective to enhance a specific type of estimation application.

What is k-fold cross validation?

k-fold cross validation: widely used in statistics to validate a model.

Randomly partitions the given sample into k subsamples of equal size.

- $k-1$ subsamples merged together as training set
- the other as test set.

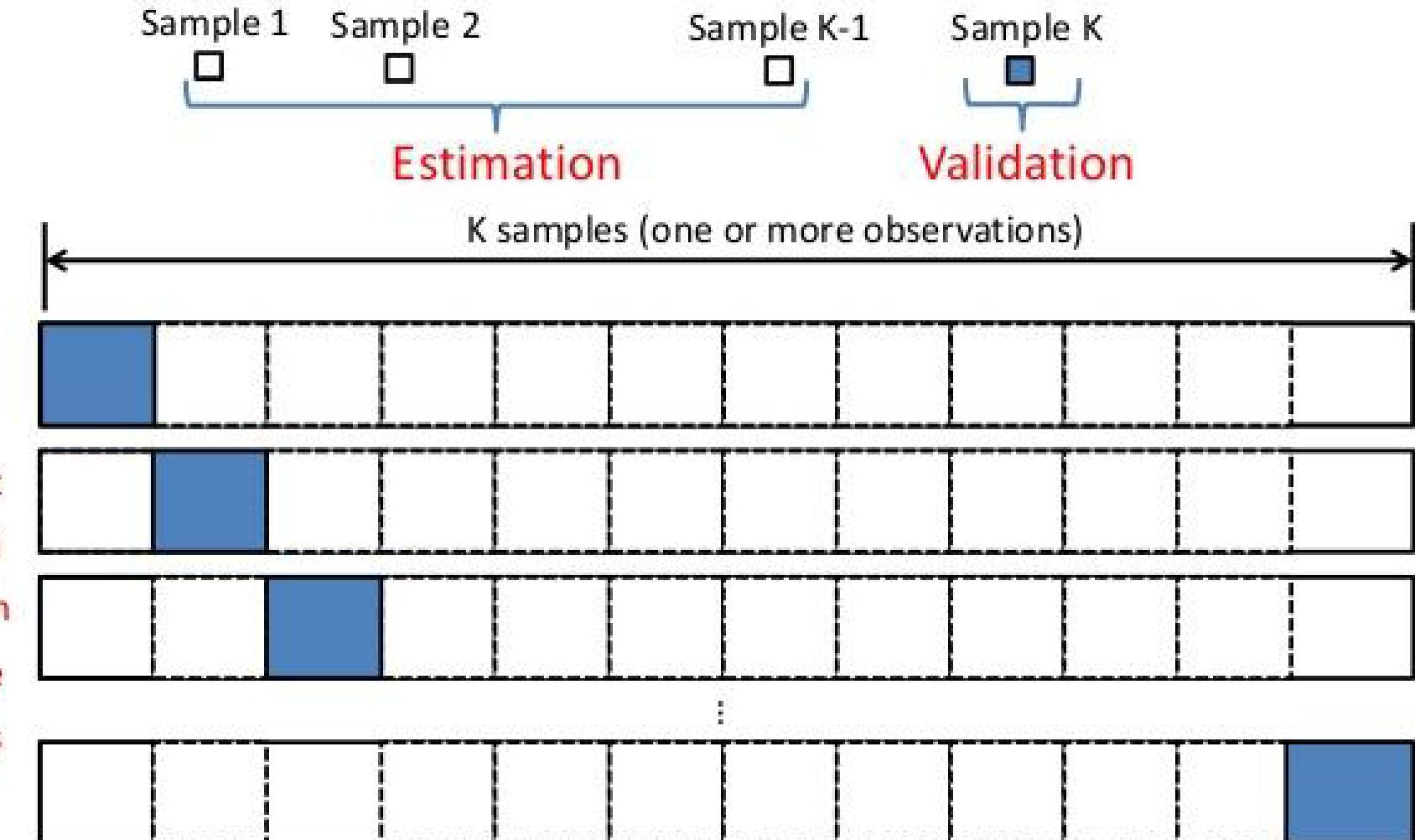
Repeated k times.

Normally $k=10$

Cross-validation is unbiased.

What is k-fold cross validation?

- K-fold cross-validation:



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Camera + color filters

Which filters will give the best spectral accuracy?



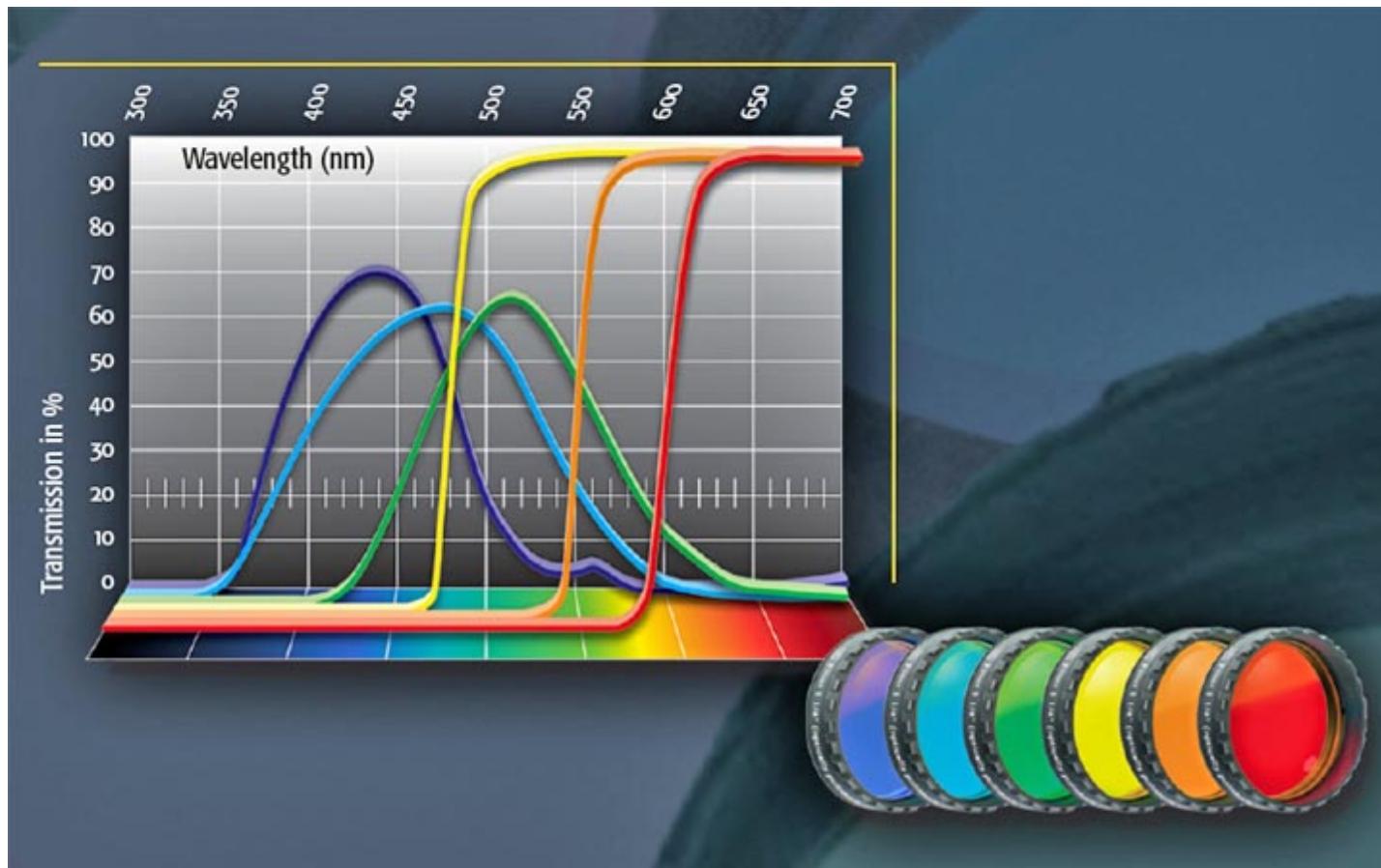
1st approach: to choose from an optimized set of commercially available color filters (for example, interference filters, Kodak Wratten gelatin filters, ...)

2nd approach: to design optimal color filters computationally

- adaptive to various applications
- rewritable filter based imaging system needed

1st approach: to choose from an optimized set of commercially available color filters

Advantage: not having to build the filters once the optimization process is ended



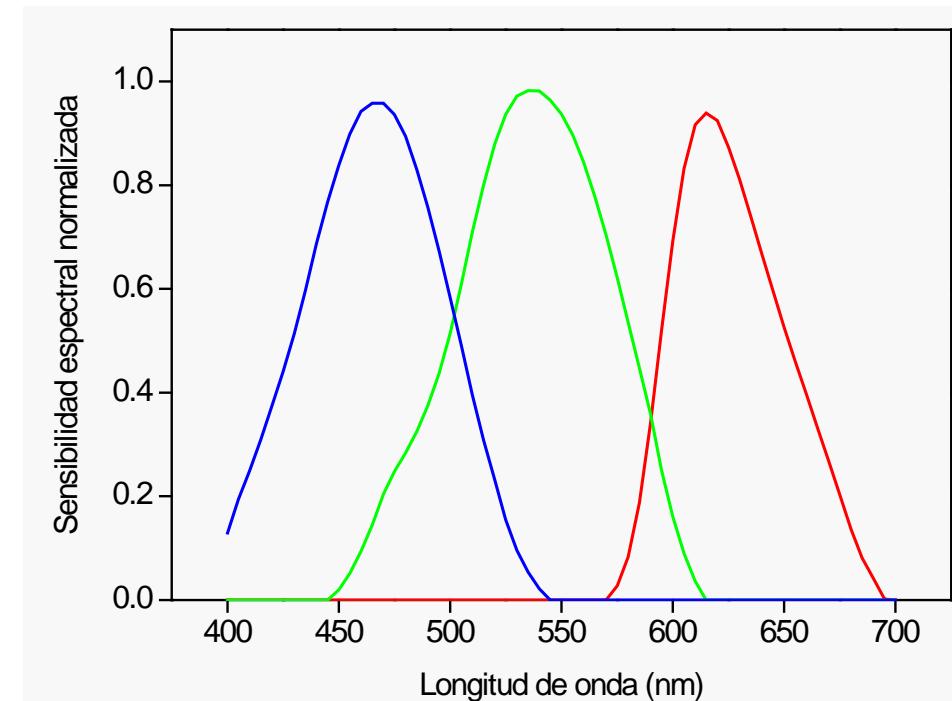
But how to select the optimal filters (or LEDs)?

Selection method	Considered information	Comput. complex.	Optimization criterion	Scheme
Equi-spacing (6.5.1.1)	None	Immediate	None	Heuristic
Exhaustive search (6.5.1.2)	<i>a posteriori</i>	Very high	Any	Combinatorial
Progressive optimal (6.5.1.3)	Filter, camera, illuminant, reflectances	Very low	Correlation to optimal filters	Each filter chosen individually. Clearly sub-optimal
Max orthogonality (6.5.1.4)	Filter, camera, illuminant	Low	Filter/channel orthogonality	Sub-optimal. Constructive (each filter chosen considering already chosen filters)
Orthog. in charac. reflectance space (6.5.1.5)	Filter, camera, illuminant, reflectances	Low	“Camera response” orthogonality	Sub-optimal. Constructive

1) Not searching, but using evenly spaced central peak wavelengths

- This is not guaranteed to be the optimal choice!
- Maybe good option for a first trial

Related with the Shannon-Whitakker theorem

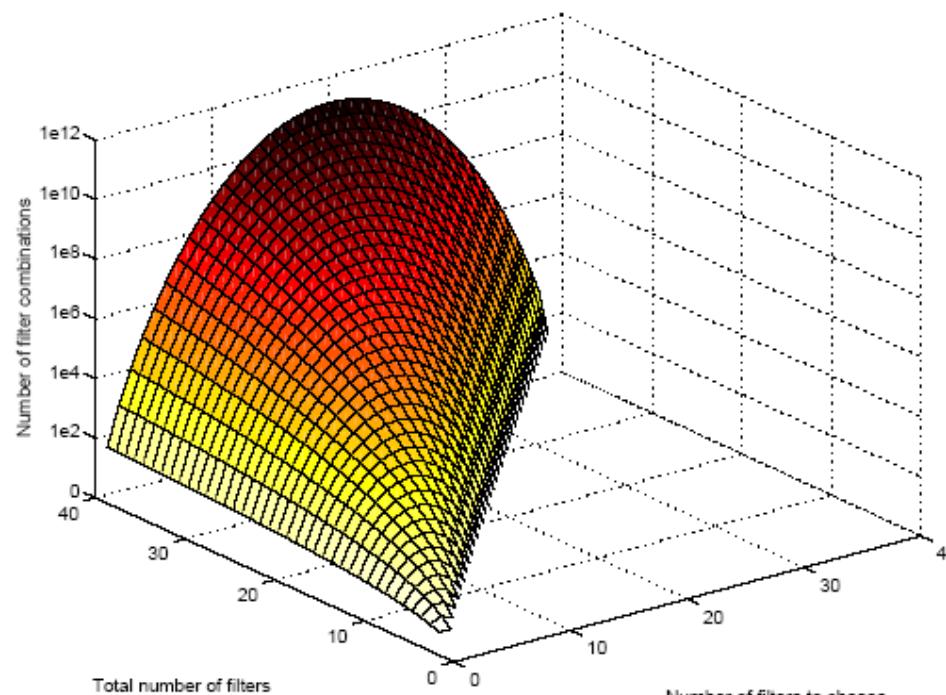


2) Trial and error (exhaustive search, binary search, brute-force search)

- Often prohibitively expensive in computation time

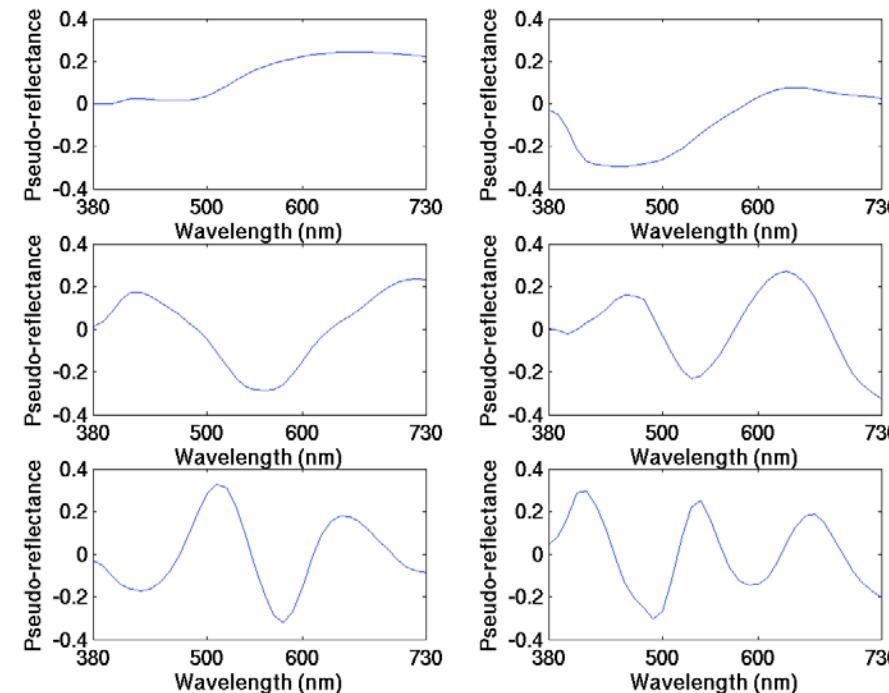
$$n_c = \frac{N!}{n!(N-n)!}$$

N=available filters
n=selected filters



3) Progressive optimal filters - POF (Mahy et al., 1994)

- First, PCA is performed on the training reflectance set
- Secondly, a set of progressive optimal filters is built (the k th POF is a linear combination of the first k basis vectors with positivity constraint)
- Thirdly, select from the commercially available set the filters most closely resembling the POFs



4) Maximizing filter orthogonality

- a) To start, choose the filter transmitting the maximum energy (having the highest norm)
- b) Then, choose the filter which has the maximum orthogonal component to the first

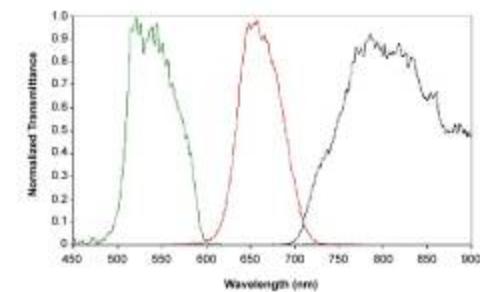
$$b_2 = \max \left\| y_k - (b_1(b_1^t y_k)) \right\|$$

- c) Go on iteratively choosing the filter most orthogonal to the subspace spanned by the rest of the chosen filters (orthogonal base)



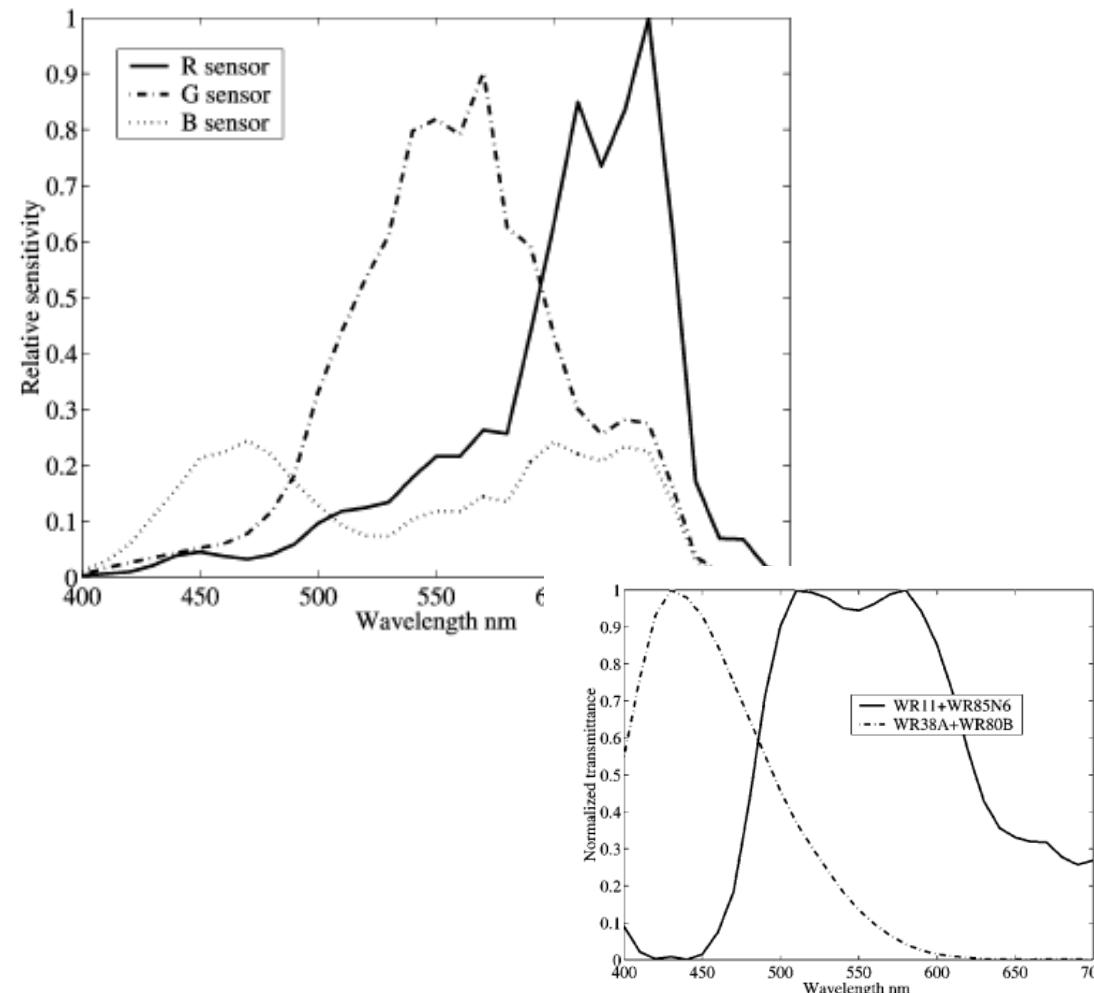
5) Maximizing filter orthogonality in characteristic reflectance space

- a) Perform PCA on the reflectance set and calculate the available sensors responses to the first r eigenvectors ($g_{k,j}$).
- b) Choose as first filter the one having the highest projection norm
- c) Go on iteratively choosing the filter most orthogonal to the subspace spanned by the projections of the rest of the chosen filters (orthogonal base)



6) Other methods

Computational filter design: subspace matching method (Du-Yong and Allebach, 2006)



- The very basics: one tries to find the set of filters (with smoothness and positivity constraints) which make the camera sensors subspace best match the subspace spanned by the reflectance training set

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Influence of noise in the recovery of spectral functions

- We have previously seen that there are some algorithms including noise in the camera model (I-B, S-H, W, LR) or using real camera responses (matrix-R). Adding noise to the systems always leads to a worse recovery performance.

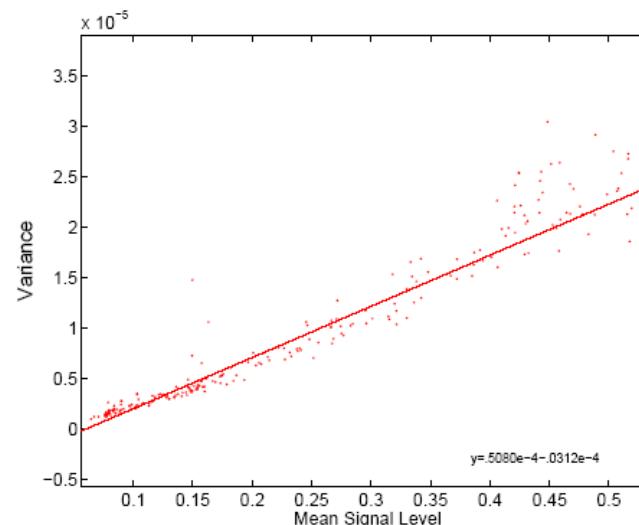


- But noise can be included in the camera model, usually as additive signals different for each channel.

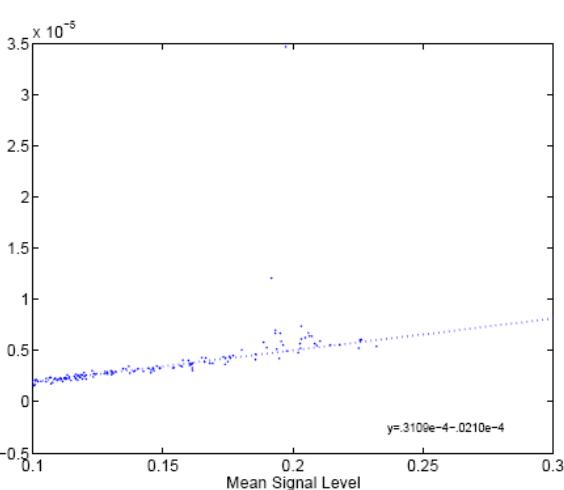
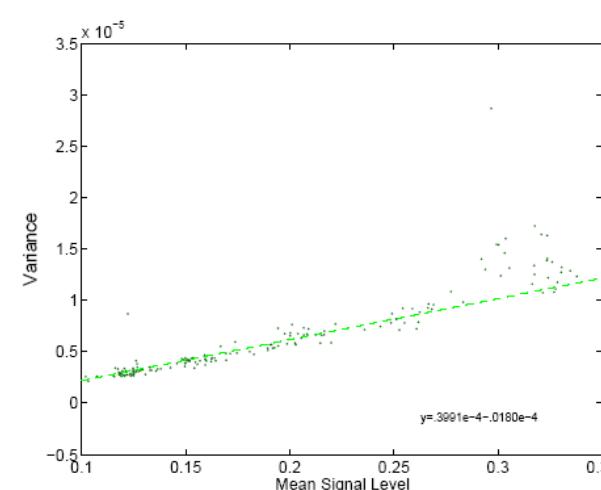
- In general, using simulated noiseless digital counts results in recovery matrices not robust to noise.

$$\rho = \alpha R^t E + \sigma$$

- One can perform a **complete noise characterization** of the camera (as seen in Chapter 3), or else **take some pictures of a training set target under similar conditions** of illumination to those which will be used in the simulations, and study the variance in the camera signals (Day, 2003).



a. Red



c. Blue

- Afterwards, one can simulate noiseless DC and introduce additive gaussian noise of the appropriate variance

To simulate additive noise in the device

How? Which kind of noise? Which amount of noise?

Valero et al. (2014):

- Modeled noise: shot noise and flicker noise, which depend on the magnitude of the camera response
- Quantization noise (assuming 10 bits per channel): rescaling and rounding camera responses to the nearest integer in the range [0–1024]
- Thermal and dark-current not considered.
- Level: 30 dB
- 100 different noise values for each noise-free camera response
- Noise values normally distributed with a standard deviation σ_i

$$\rho = \rho_{free} + \sigma$$

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