

Lecture 09
Machine Learning 3:
classification (part 2)

2024-10-16

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1. Introduction

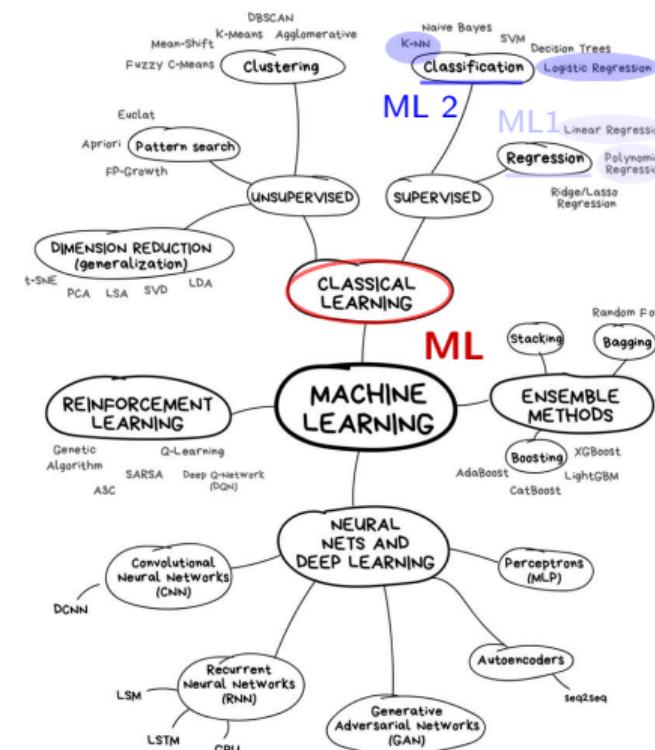
2. Principal Component Analysis (PCA)

3. Classification algorithms (perceptron + SVM)

4. Exercise

Introduction

Last week: classification part-1 (ML2)

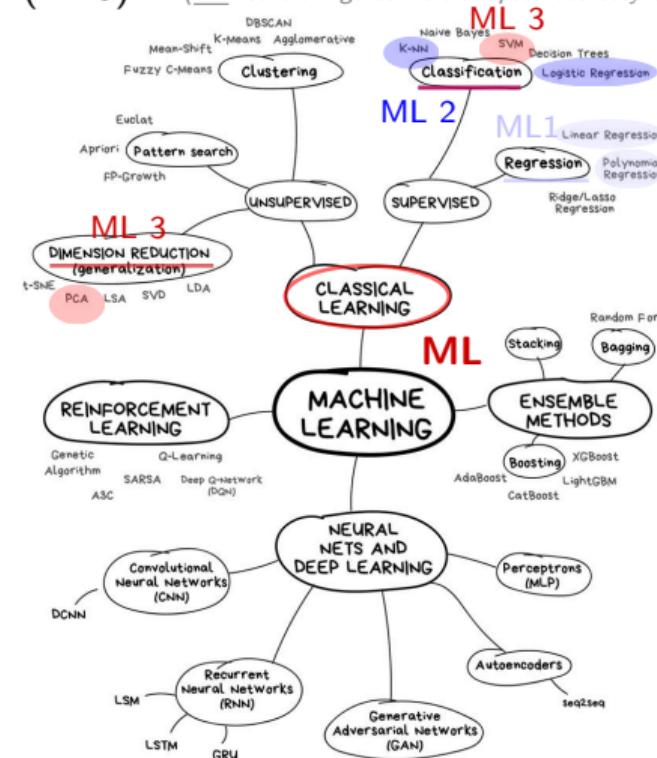


Introduction

Last week: **classification part-1 (ML2)**

This week: **classification part-2 (ML3)**

(NB: several figures were adapted courtesy of A. Ley & R. Hänsch from TU-Berlin)



Classification task

- Goal:

Learn the mapping between low level **features**, and
high level information (e.g. *semantic classes*)

- Steps:

1. features extraction (e.g. *handcrafted | learned*)
2. learning algorithm (e.g. *probability-based | not*)

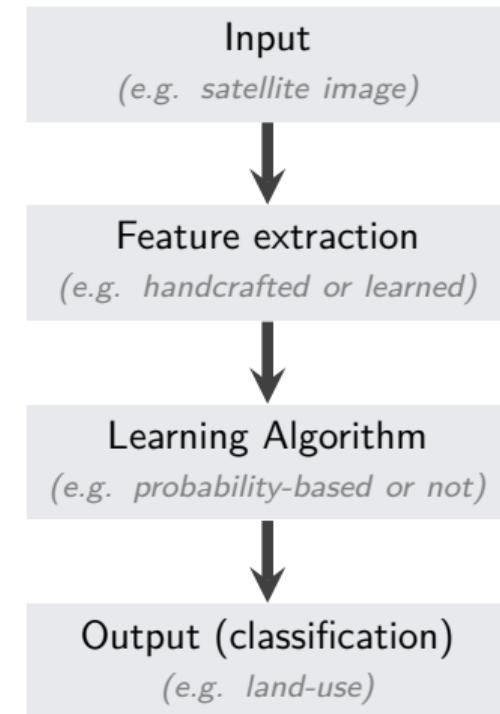
- Strategies:

⇒ **last week:**

handcrafted features + probability-based learning

⇒ **this week:**

learned features (PCA) + SVM learning



1. Introduction

2. Principal Component Analysis (PCA)

1. introduction
2. how it works
3. implementation steps

3. Classification algorithms (perceptron + SVM)

4. Exercise

2.1. introduction

Principal Component Analysis (PCA)

⇒ PCA is an **unsupervised learning** technique

→ in contrast to *supervised learning*, *unsupervised learning* algorithms operate on unlabeled data (we only have a set of k features X_1, X_2, \dots, X_k measured on n observations, without any associated target variable Y , thus we are not interested in any prediction task)

⇒ PCA is the most popular **dimensionality reduction algorithm**:

→ it is used to **reduce data dimensionality**, while preserving as much of the variance as possible
→ it is often used as data pre-processing technique before supervised techniques are applied (e.g. feature extraction to reduce computational load of the classifier)

⇒ Intuitive explanation: which angle captures the most information about the teapot?

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**1st principal component
= 1st “eigen vector”
(longest axis)**

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1st principal component
= 1st “eigen vector”
(longest axis)

2nd principal component
= 2nd “eigen vector”
(2nd longest axis \perp to 1st axis)

2.1. introduction

PCA toy example

We have several wine bottles in our cellar, 11 features (alcohol, acidity, etc.) describe its quality. Which features best define it, are there related features (i.e. covariant) which are redundant?



	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	5
1	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.8	5
2	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.8	5
3	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.8	6
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⇒ reduce data dimensions

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⇒ PCA does not select some features and discards others, instead it defines new features (using linear combinations of available features) which will best represent wine variability

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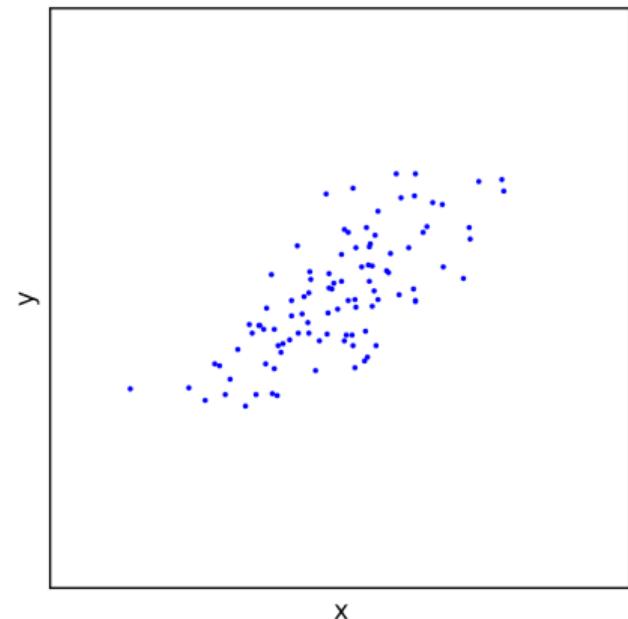
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How?

2.2. how it works

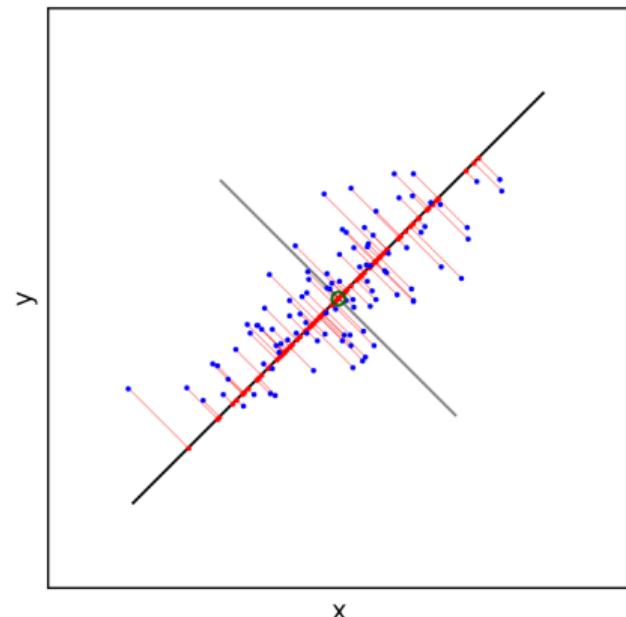
Consider 2 correlated features x and y :



2.2. how it works

Consider 2 correlated features x and y :

⇒ a new “feature” (red dots •) can be constructed by drawing a line through the cloud and projecting all points onto it

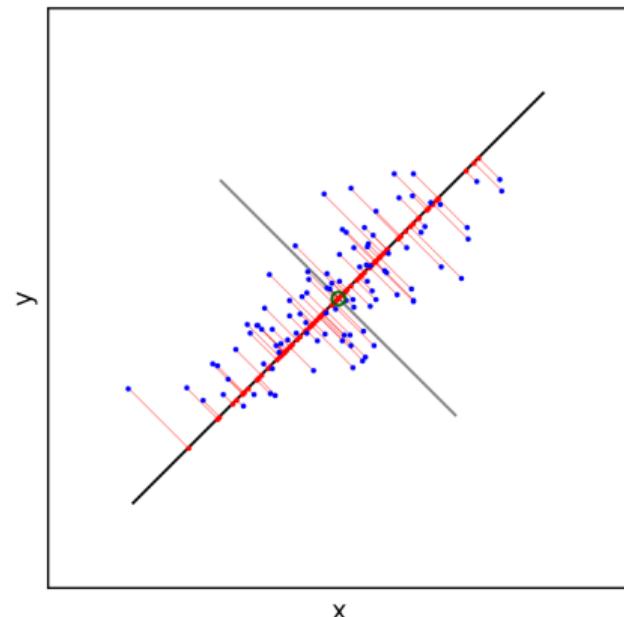


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⇒ linear combination $w_1x + w_2y$



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⇒ a new “feature” (**red dots** ●) can be constructed by drawing a line through the cloud and projecting all points onto it

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⇒ PCA will find the “best” line according to 2 criteria:

- maximum variance of the red dots (i.e., spread along black line)
- minimum distance to black line (i.e., length of red lines)

NB: run animation with PDF readers having built-in JavaScript engine

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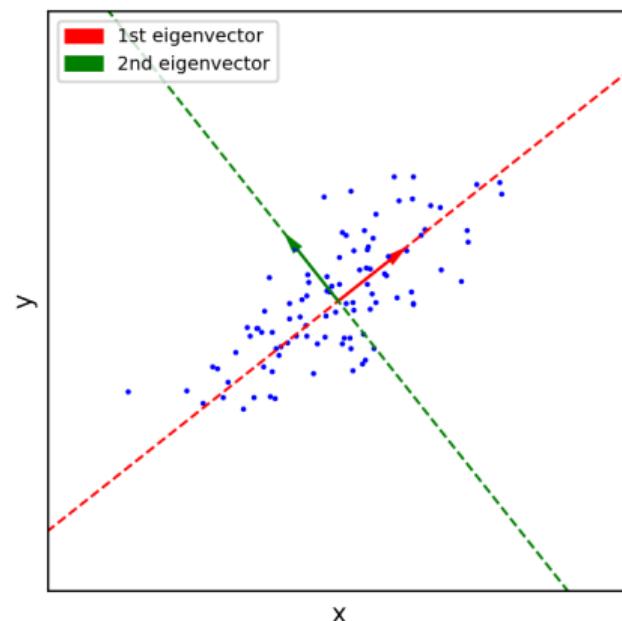
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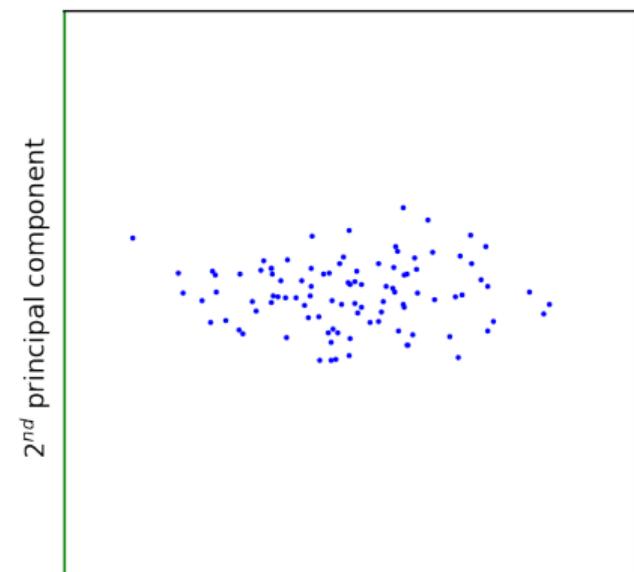
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⇒ we can project the data on the principal components, and thereby reduce dimensionality

NB: if only one eigenvector was kept, the transformed data would have only one dimension



1st principal component

2.3. implementation steps

Implementation steps

Math reminders

variance σ^2 = measure of the "spread" or "extent" of the data about some particular axis
= average of the squared differences from the mean
= square of standard deviation (σ)

$$\text{var}_x = \frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N}$$

$$\text{var}_y = \frac{\sum_{i=1}^N (y_i - \bar{y})^2}{N}$$

covariance = measure the level to which two variables vary together

$$\text{cov}_{x,y} = \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})}{N - 1}$$

$$\text{covariance matrix} = \begin{bmatrix} \text{var}_x & \text{cov}_{x,y} \\ \text{cov}_{y,x} & \text{var}_y \end{bmatrix}$$

2.3. implementation steps

Math reminders (continued)

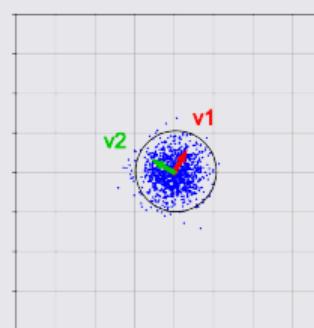
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Eigenvalue analysis of covariance matrix \Rightarrow find directions with maximal variance

- **eigenvectors** (\vec{v}_1, \vec{v}_2): represent the directions of the largest variance of the data
- **eigenvalues** (λ_1, λ_2): represent the magnitude of this variance in those directions

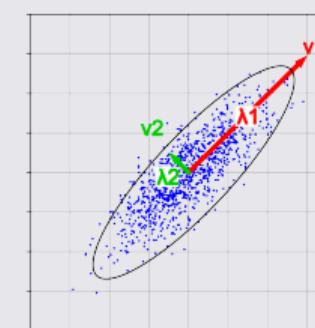
Determinant and trace of covariance matrix

- **determinant** $\det(\text{covmat}) = \lambda_1 \lambda_2$: measures the “spread” of the data captured by the covariance matrix
- **trace** $\text{trace}(\text{covmat}) = \lambda_1 + \lambda_2$: measures the “total variance” captured by the covariance matrix



$$\text{covmat} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

uncorrelated variables

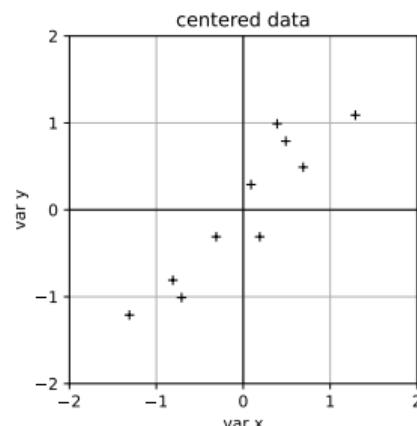


$$\text{covmat} = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}$$

highly correlated variables

2.3. implementation steps

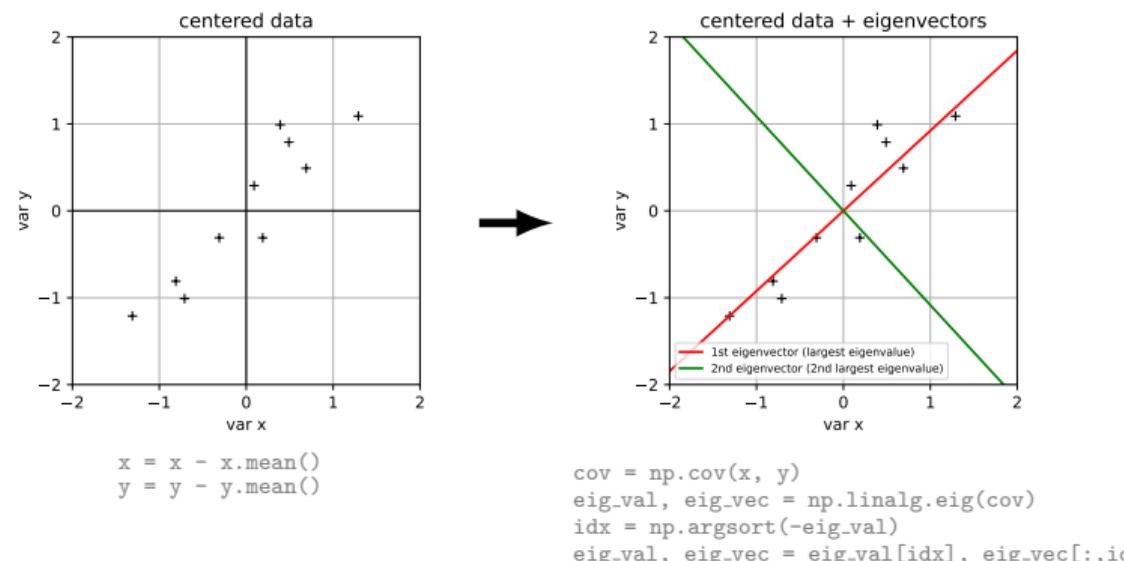
Implementation steps (example with 2 variables)



```
x = x - x.mean()  
y = y - y.mean()
```

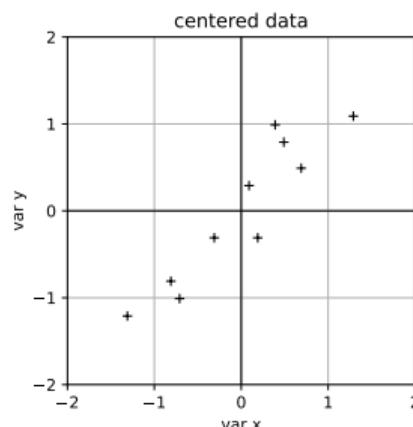
1. center points around origin (0,0)
2. compute covariance matrix → get eigenvalues & eigenvectors (= Principal Components) → sort by eigenvalue
 - ⇒ eigenvectors represent the directions of the largest variance of the data, eigenvalues represent the magnitude of this variance in those directions
 - ⇒ highest eigenvalue = direction with most variance (data dispersion) = 1st principal component
3. project the data onto the principal components (PCs)
 - ⇒ if only 1 eigenvector was kept, the 2 original features (var x, var y) could be reduced to 1 dimension

2.3. implementation steps

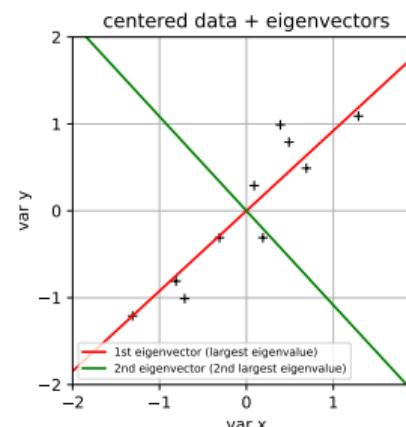
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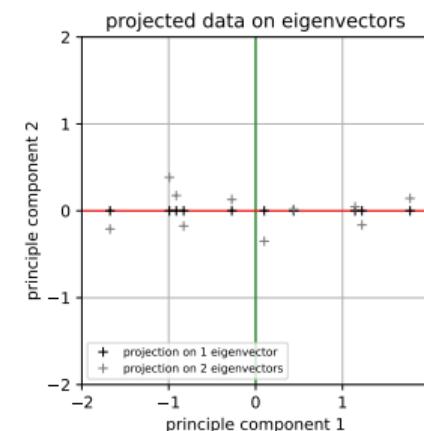
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Implementation steps (example with 2 variables)

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x = x - x.mean()
y = y - y.mean()
```



```
cov = np.cov(x, y)
eig_val, eig_vec = np.linalg.eig(cov)
idx = np.argsort(-eig_val)
eig_val, eig_vec = eig_val[idx], eig_vec[:,idx]
```



```
XY = np.array([x, y]).T
XY_proj = np.dot(XY, eig_vec[:2].T)
```

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Implementation steps (back to our toy-example on wine quality)

⇒ do the same with the 11 features: search for the principal components in a 11-dimensional space

NB: the maximum number of components is restricted by the number of features

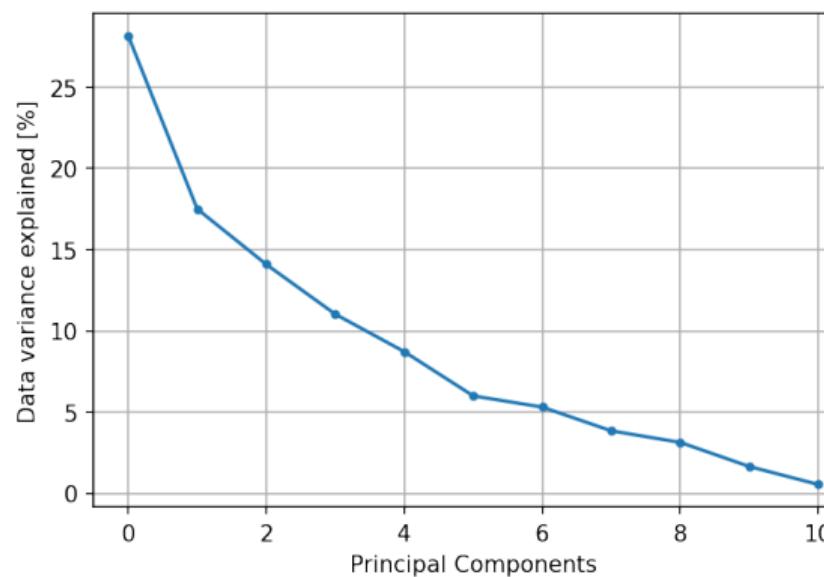
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Q1: How much data variance is explained by each principal component (eigenvector)?



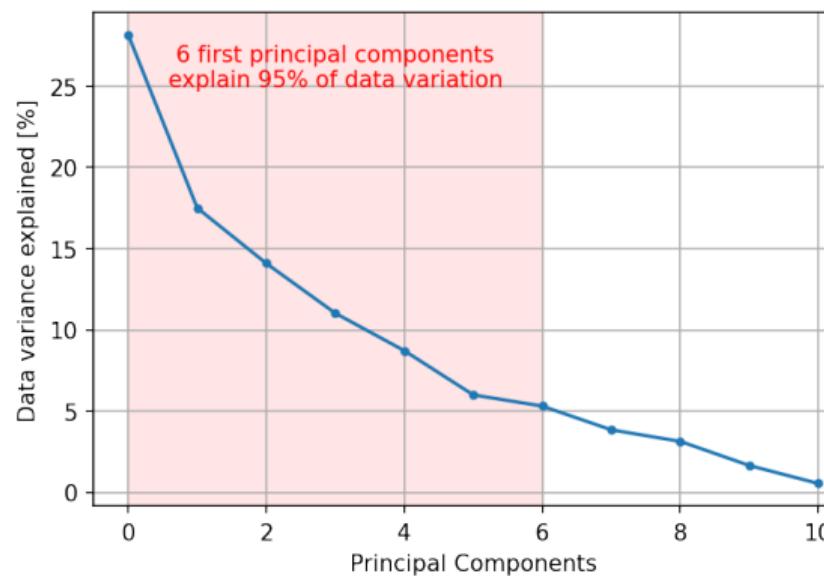
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Q1: How much data variance is explained by each principal component (eigenvector)?

Q2: How do the 11 eigenvectors (PCs) relate to the original feature space?

	0	1	2	3	4	5	6	7	8	9	10
0	0.489314	-0.238584	0.463632	0.146107	0.212247	-0.036158	0.023575	0.395353	-0.438520	0.242921	-0.113232
1	-0.110503	0.274930	-0.151791	0.272080	0.148052	0.513567	0.569487	0.233575	0.006711	-0.037554	-0.386181
2	-0.123302	-0.449963	0.236247	0.101283	-0.092614	0.428793	0.322415	-0.338871	0.057697	0.279786	0.471673
3	-0.229617	0.078960	-0.079418	-0.372793	0.666195	-0.043538	-0.034577	-0.174500	-0.003788	0.550872	-0.122181
4	-0.082614	0.218735	-0.058573	0.732144	0.246501	-0.159152	-0.222465	0.157077	0.267530	0.225962	0.350681
5	0.101479	0.411449	0.069593	0.049156	0.304339	-0.014000	0.136308	-0.391152	-0.522116	-0.381263	0.361645
6	-0.350227	-0.533735	0.105497	0.290663	0.370413	-0.116596	-0.093662	-0.170481	-0.025138	-0.447469	-0.327651
7	-0.177595	-0.078775	-0.377516	0.299845	-0.357009	-0.204781	0.019036	-0.239223	-0.561391	0.374604	-0.217626
8	-0.194021	0.129110	0.381450	-0.007523	-0.111339	-0.635405	0.592116	-0.020719	0.167746	0.058367	-0.037603
9	-0.249523	0.365925	0.621677	0.092872	-0.217671	0.248483	-0.370750	-0.239990	-0.010970	0.112320	-0.303015
10	0.639691	0.002389	-0.070910	0.184030	0.053065	-0.051421	0.068702	-0.567332	0.340711	0.069555	-0.314526

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6	-0.350227	-0.533735	0.105497	0.290663	0.370413	-0.116596	-0.093662	-0.170481	-0.025138	-0.447469	-0.327651	
7	-0.177595	-0.078775	-0.377516	0.299845	-0.357009	-0.204781	0.019036	-0.239223	-0.561391	0.374604	-0.217626	
8	-0.194021	0.129110	0.381450	-0.007523	-0.111339	-0.635405	0.592116	-0.020719	0.167746	0.058367	-0.037603	
9	-0.249523	0.365925	0.621677	0.092872	-0.217671	0.248483	-0.370750	-0.239990	-0.010970	0.112320	-0.303015	
10	0.639691	0.002389	-0.070910	0.184030	0.053065	-0.051421	0.068702	-0.567332	0.340711	0.069555	-0.314526	

$$PC\ 1 = 0.49 * feature0 + -0.24 * feature1 + 0.46 * feature2 + 0.15 * feature3 + 0.21 * feature4 + -0.04 * feature5 + 0.02 * feature6 + 0.40 * feature7 + -0.44 * feature8 + 0.24 * feature9 + -0.11 * feature10$$

2.3. implementation steps

Implementation steps (back to our toy-example on wine quality)

⇒ do the same with the 11 features: search for the principal components in a 11-dimensional space

NB: the maximum number of components is restricted by the number of features

Q1: How much data variance is explained by each principal component (eigenvector)?

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⇒ how about using PCA on images?
→ Sentinel-2 exercise: a crop of 900 pixels (4-bands 15×15 pixels) can be reduced
fairly accurately to 32 points! (i.e., projection in a 32-dimensional space, first 32 pcs)

1. Introduction
2. Principal Component Analysis (PCA)
3. Classification algorithms (perceptron + SVM)
 1. Perceptron
 2. Support Vector Machine (SVM)
4. Exercise

Once features have been extracted, we can feed to the classifier! (recall last week lecture)

⇒ the classification algorithm needs to learn the decision boundary (*i.e. surface separating the different classes*) in an N -dimensional **feature space**:

- probabilistic approaches:

- **Logistic Regression** ⇒ *last week*
 - **Softmax Regression** ⇒ *last week*
 - **Naive Bayes**

- non-probabilistic approaches:

- **k-Nearest Neighbors (kNN)** ⇒ *last week*
 - **Perceptron** ⇒ *today!*
 - algorithm finding a hyperplane to separate classes, adjusting weights based on misclassified points
 - **Support Vector Machines (SVM)** ⇒ *today!*
 - algorithm finding the optimal hyperplane that maximizes the margin between classes
 - **Random Forest** ⇒ *next lectures*
 - **Convolutional Neural Networks (CNNs)** ⇒ *next lectures*

Choosing a classifier

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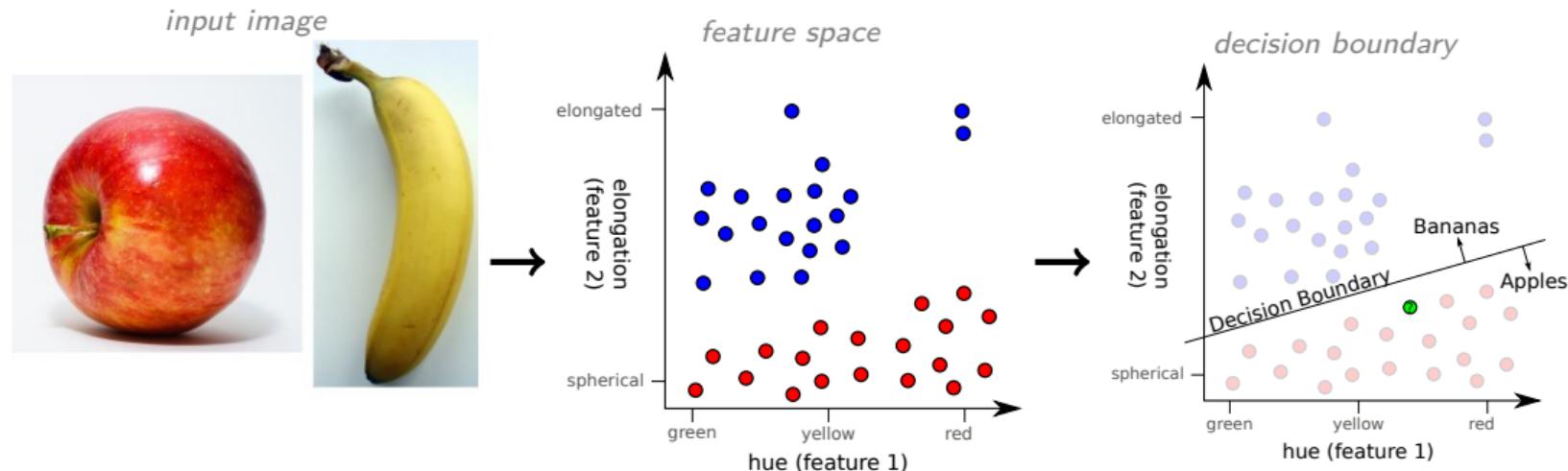
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3.1. Perceptron

Recall our toy example from last week: classify fruit images into either bananas or apples



⇒ how is the decision boundary learned?

3.1. Perceptron

Perceptron classifier

⇒ algorithm which classifies data based on linear decision boundary

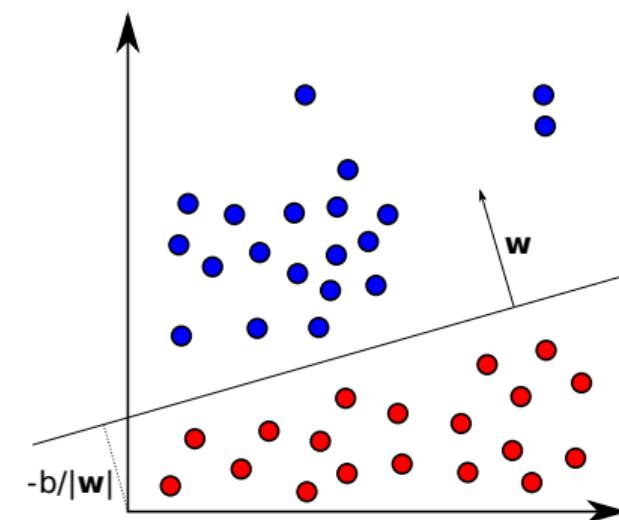
NB: the original perceptron algorithm is a binary classifier (similar to logistic regression but non-probabilistic)

NB: in an N -dimensional feature space, the decision boundary is a hyperplane

⇒ perceptron:

$$\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + \mathbf{b})$$

- $\hat{y} \in \{-1, 1\}$: predicted class → banana or apple
- $\mathbf{x} \in \mathbb{R}^2$: feature vector → hue, elongation
- $\mathbf{w} \in \mathbb{R}^2$: weight vector → needs to be learned
- $\mathbf{b} \in \mathbb{R}$: bias → needs to be learned
- sign: sign function returning the sign of a real number



3.1. Perceptron

Perceptron classifier

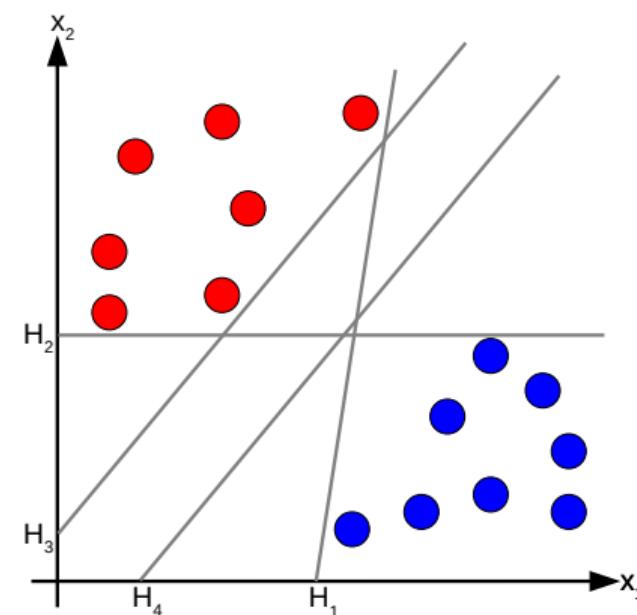
⇒ perceptron: $\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + \mathbf{b})$

⇒ problem: multiple “good” boundaries can be found

⇒ need to find the *optimal hyperplane*

= boundary with maximal margins

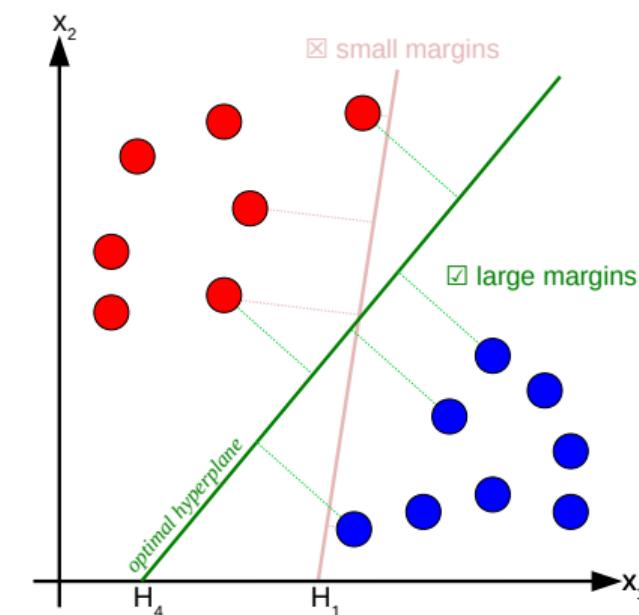
= perceptron of maximal stability to new inputs



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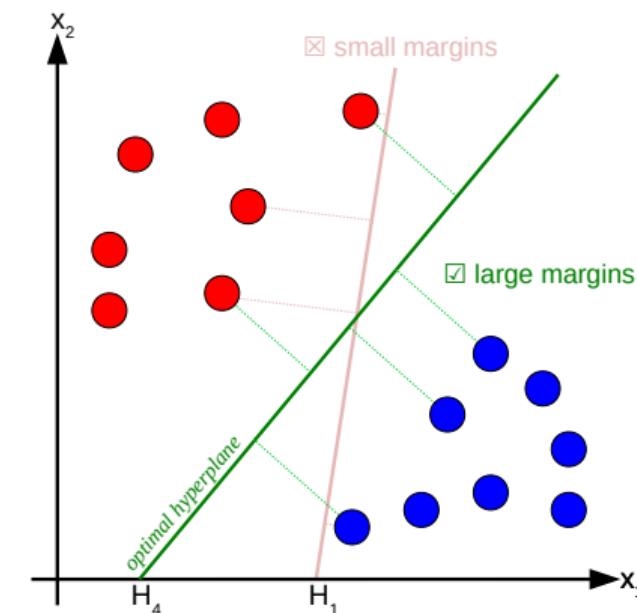
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Perceptron classifier

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- ⇒ problem: multiple “good” boundaries can be found
- ⇒ need to find the *optimal hyperplane*
= boundary with **maximal margins**
= perceptron of maximal stability to new inputs
- ⇒ the **Support Vector Machine** (SVM) algorithm will find the *optimal hyperplane* and learn the best *weights w* and *bias b* to classify the data



3.2. Support Vector Machine (SVM)

Support Vector Machine (SVM)

⇒ perceptron: $\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + \mathbf{b})$

⇒ definitions:

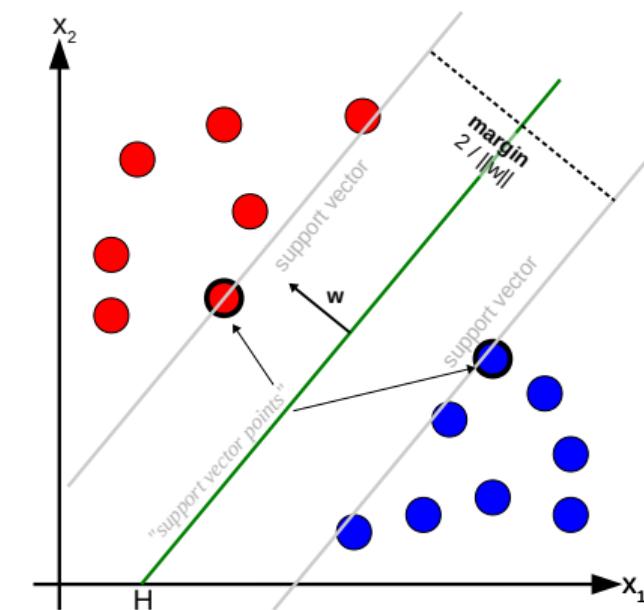
- **support vector points** = points closest to the hyperplane
(only these points are contributing to the result, other points are not)
- **margin** = distance between hyperplane & support vector points
 $= \frac{2}{\|\mathbf{w}\|}$

⇒ maximize margin:

$$\max_{\mathbf{w}} \frac{2}{\|\mathbf{w}\|}, \text{ subject to } \begin{cases} \mathbf{w}^T \mathbf{x}_i + b \geq 1 & \text{if } y_i = +1 \\ \mathbf{w}^T \mathbf{x}_i + b \leq -1 & \text{if } y_i = -1 \end{cases}$$

which is equivalent to:

$$\min_{\mathbf{w}} \|\mathbf{w}\|^2, \text{ subject to } y_i(\mathbf{w}^T \mathbf{x}_i - b) \geq 1$$



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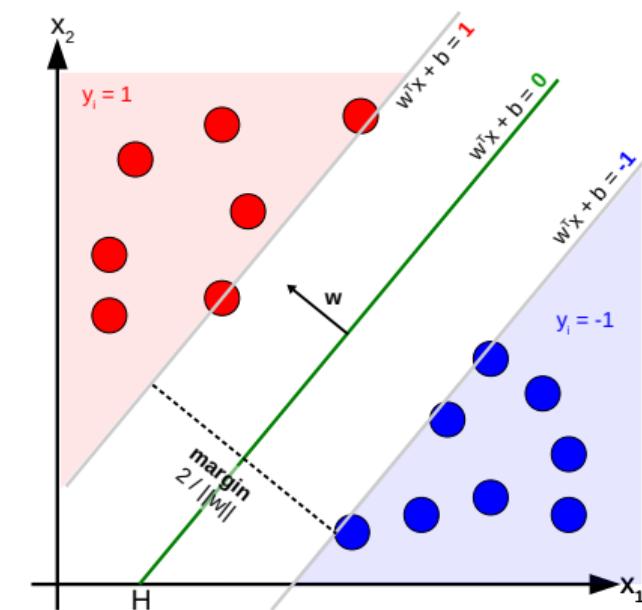
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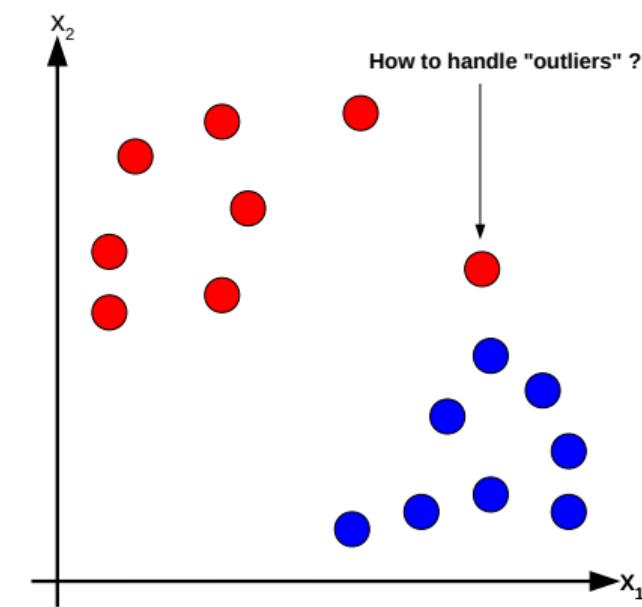
⇒ How can outliers be handled?

- ⇒ is a hard-margin with 100% accuracy good?
- ⇒ no, allow small errors (soft-margin) to favour overall better model
- ⇒ tolerate margin violation & favour large margin boundaries
- ⇒ optimization becomes:

$$\min_{w, \xi} \|w\|^2 + C \sum_i^N \xi_i \text{, subject to } y_i(w^T x_i - b) \geq 1 - \xi_i$$

where:

C	regularization parameter - small $C \Rightarrow$ constraints easily ignored, large margin - large $C \Rightarrow$ towards hard-margin SVM
ξ_i	slack variable for each data point



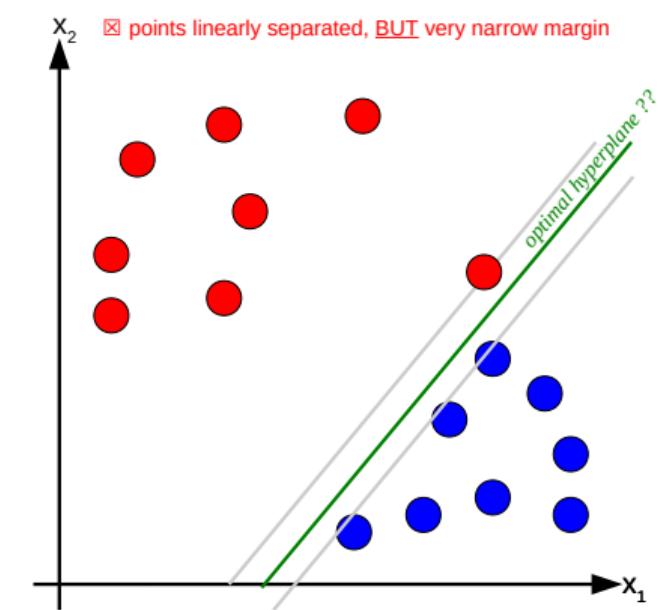
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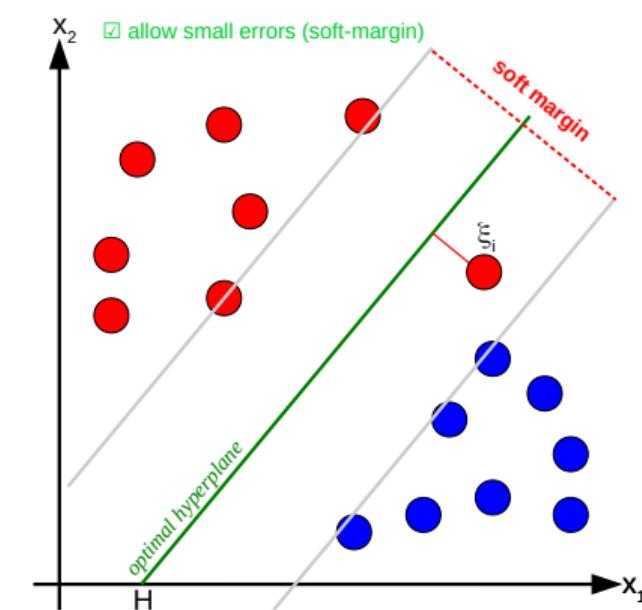
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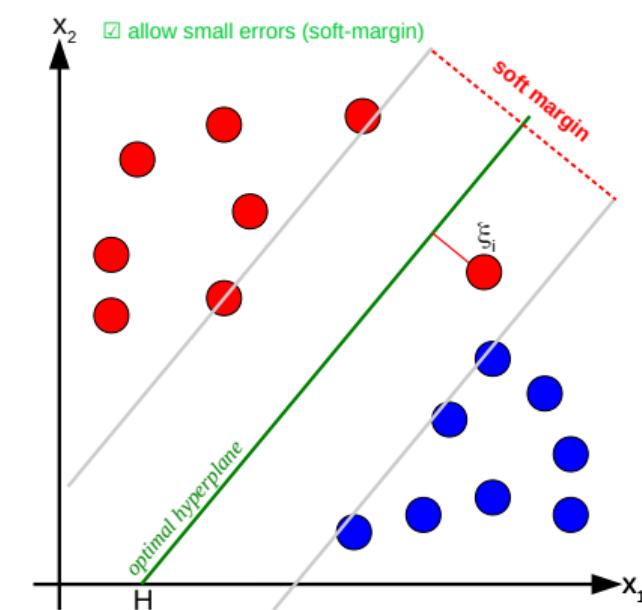
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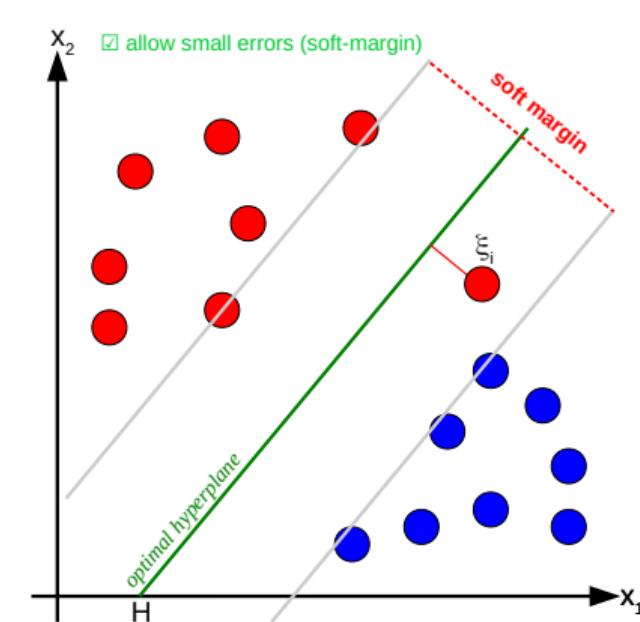
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3.2. Support Vector Machine (SVM)

Side note: reformulating optimization in terms of **regularization** and **loss function** (anticipating DL lectures)

Learning an SVM has been formulated as a constrained optimization problem over w and ξ :

$$\min_{w, \xi_i} \|w\|^2 + C \sum_i^N \xi_i \quad \text{subject to: } y_i(w^T x_i - b) \geq 1 - \xi_i$$

The constraint $y_i(w^T x_i - b) \geq 1 - \xi_i$ can be written more concisely as: $y_i f(x_i) \geq 1 - \xi_i$

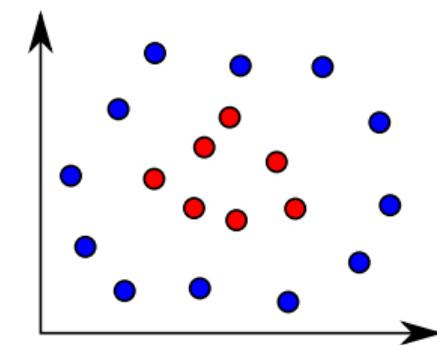
Together with $\xi_i > 0$, it is equivalent to: $\xi_i = \max(0, 1 - y_i f(x_i))$

Hence the learning problem is equivalent to the unconstrained optimization problem over w :

$$\min_w \underbrace{\|w\|^2}_{\text{regularization}} + C \sum_i^N \underbrace{\max(0, 1 - y_i f(x_i))}_{\text{loss function (Hinge loss)}}$$

Support Vector Machine (SVM)

- What if the features x_i are not linearly separable?

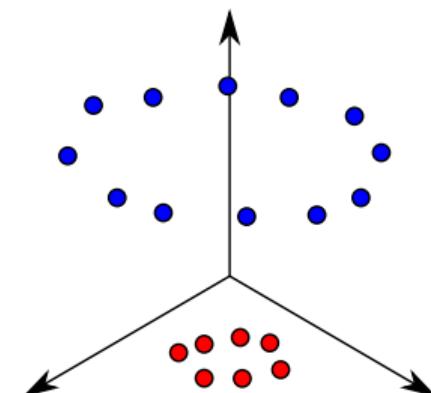


Support Vector Machine (SVM)

- **What if the features x_i are not linearly separable?**

⇒ compute new features $x_i \mapsto \phi(x)$

$\phi(x)$ is a **feature map**, mapping x to $\phi(x)$ where data is separable



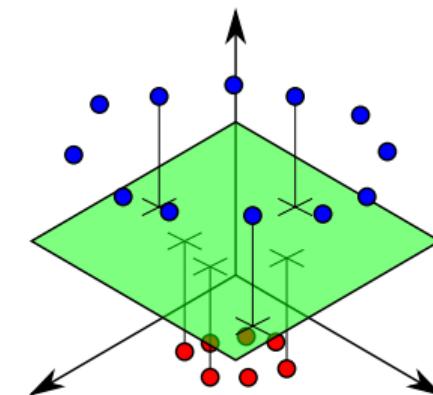
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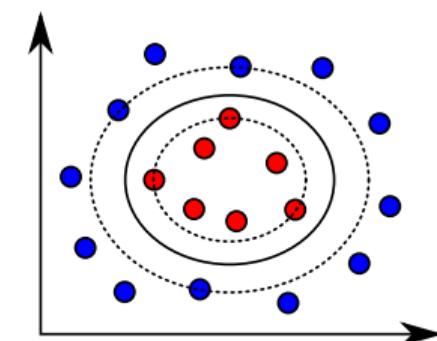
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⇒ data not linearly-separable in original feature space become separable



Kernel trick

The Representer Theorem states that the solution \mathbf{w} can be written as a linear combination of the training data:

$$\mathbf{w} = \sum_{j=1}^N \alpha_j y_j \mathbf{x}$$

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Using the feature map $\phi(\mathbf{x})$, it can be reformulated as:

$$\begin{aligned} f(\mathbf{x}) &= \sum_i^N \alpha_i y_i (\phi(\mathbf{x}_i)^T \phi(\mathbf{x})) + b \\ &= \sum_i^N \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b \end{aligned}$$

where $k(\mathbf{x}_i, \mathbf{x})$ is known as a **Kernel**

3.2. Support Vector Machine (SVM)

Kernel trick

- Classifier can be learnt and applied without explicitly computing $\phi(x)$
- All that is required is the kernel $k(x, x')$
- Multiple kernels exist:
 - linear kernels: $k(x, x') = x^T x'$
 \rightarrow very fast and easy to train, but very simple
 - polynomial kernels: $k(x, x') = (1 + x^T x')^d$
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Kernel trick

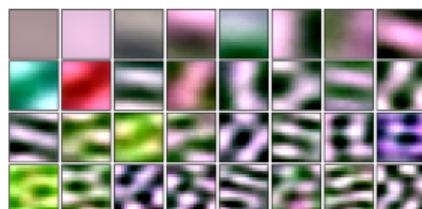
- Classifier can be learnt and applied without explicitly computing $\phi(x)$
- All that is required is the kernel $k(x, x')$
- Multiple kernels exist:
 - linear kernels: $k(x, x') = x^T x'$
 \rightarrow very fast and easy to train, but very simple
 - polynomial kernels: $k(x, x') = (1 + x^T x')^d$
 \rightarrow contains all polynomial terms up to degree d
 - gaussian kernels: $k(x, x') = \exp(-||x - x'||^2 / 2\sigma^2)$ (RBF kernel)
 \rightarrow kernel very powerful and most often used

1. Introduction
2. Principal Component Analysis (PCA)
3. Classification algorithms (perceptron + SVM)
4. Exercise

EXERCISE:

classify land-use in satellite images (Sentinel-2) using PCA and SVM

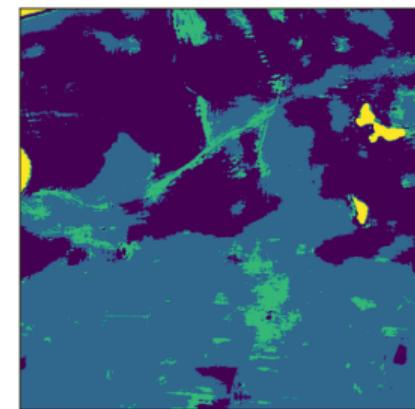
PCA dimensionality reduction



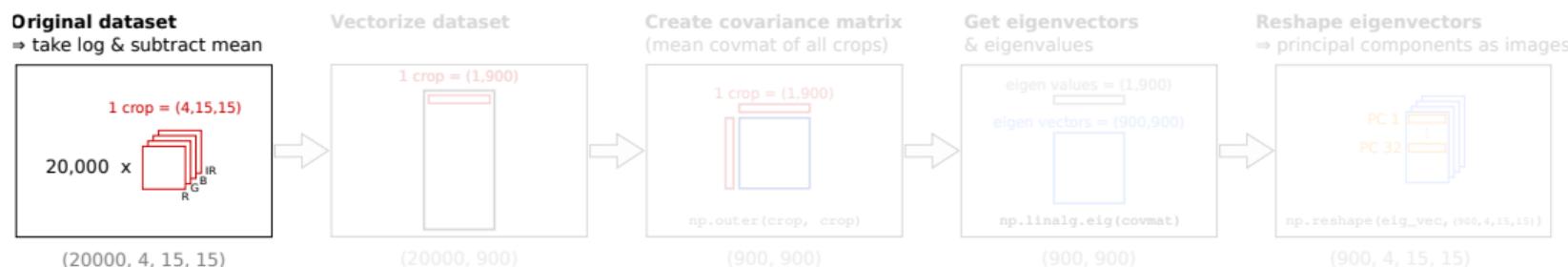
train SVM & apply



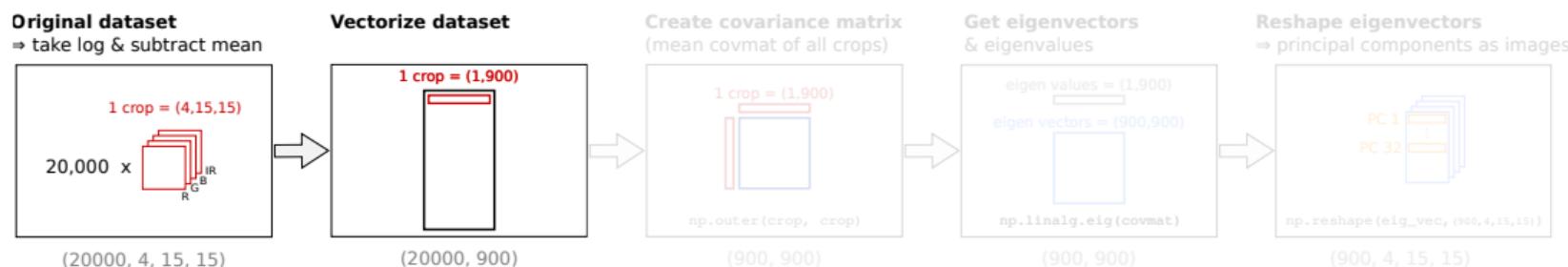
land-use classification



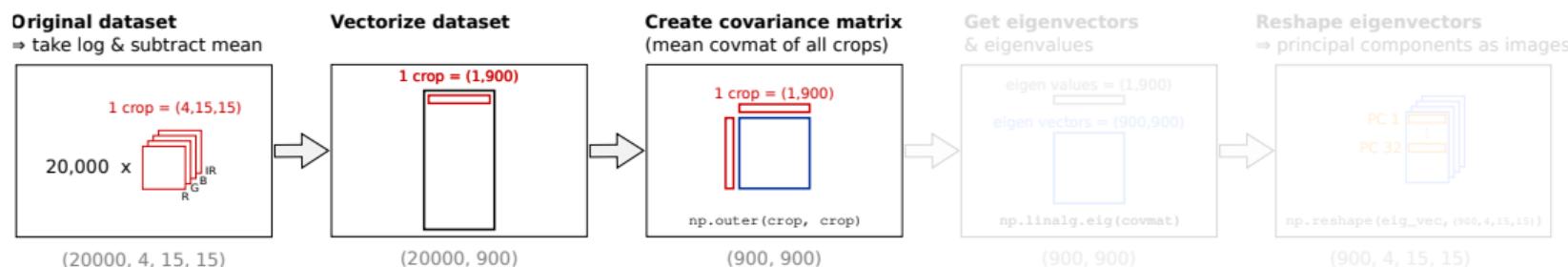
Part 1: apply PCA on satellite image crops



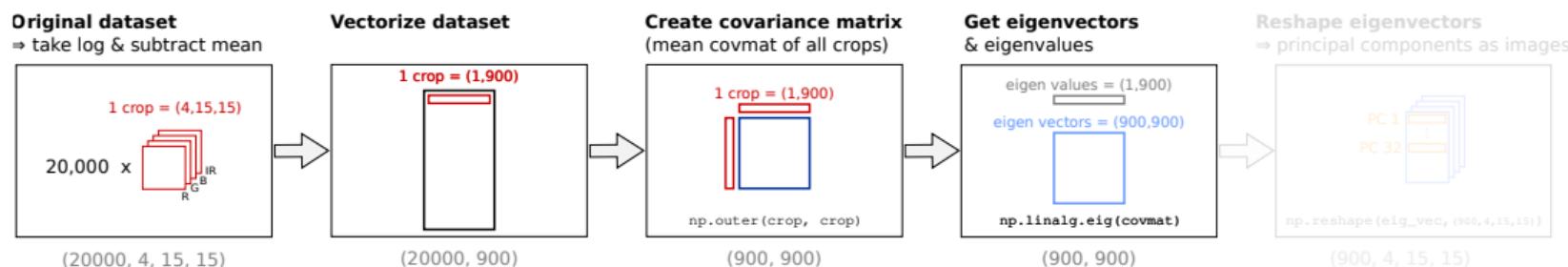
Part 1: apply PCA on satellite image crops



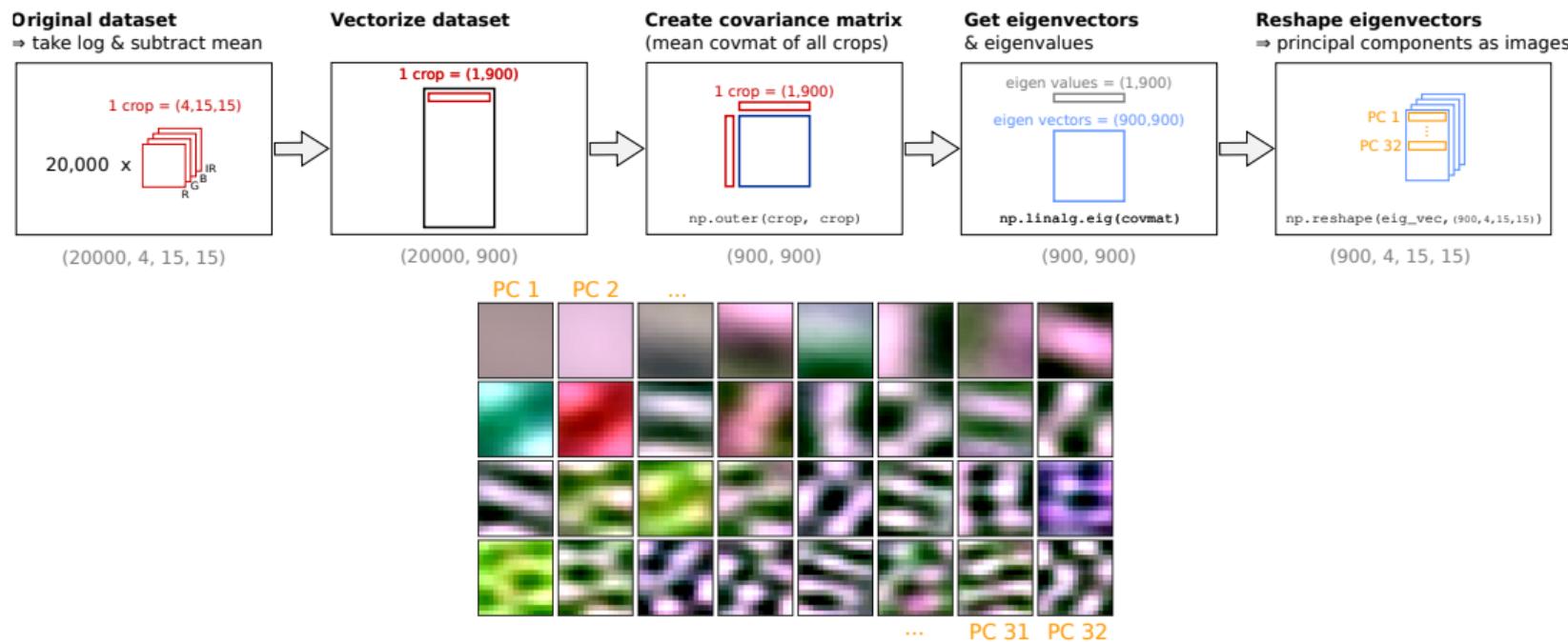
Part 1: apply PCA on satellite image crops



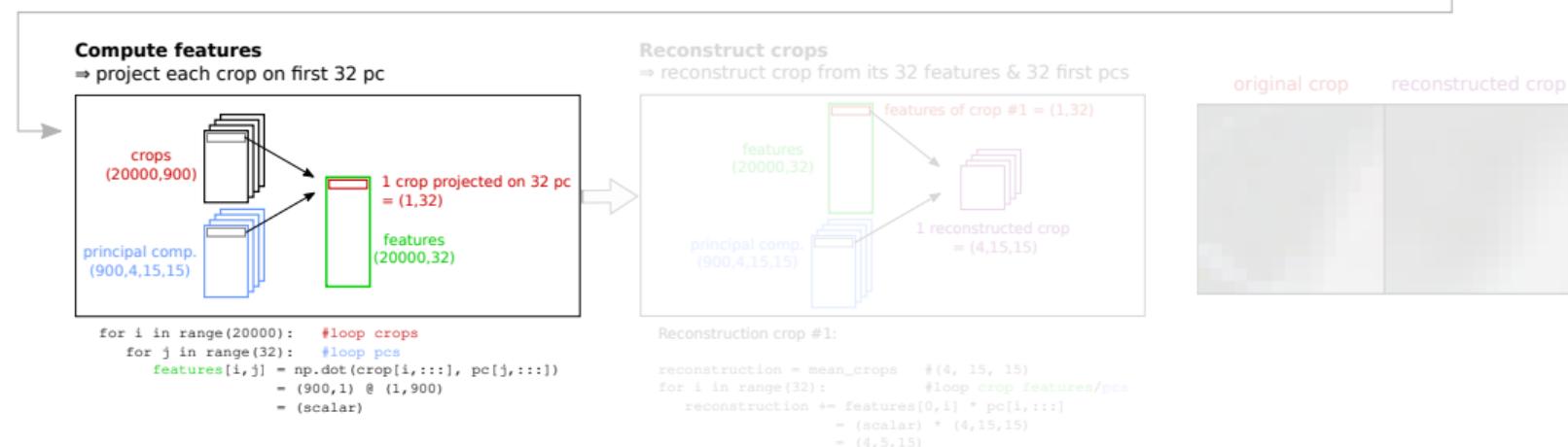
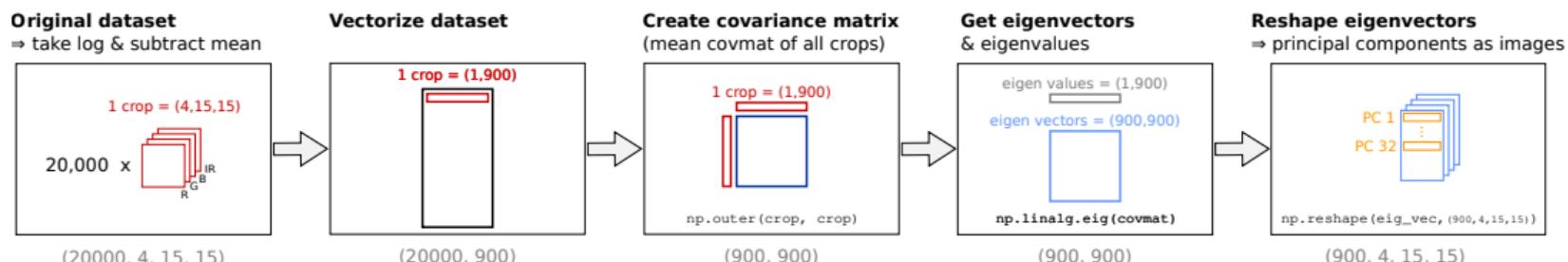
Part 1: apply PCA on satellite image crops



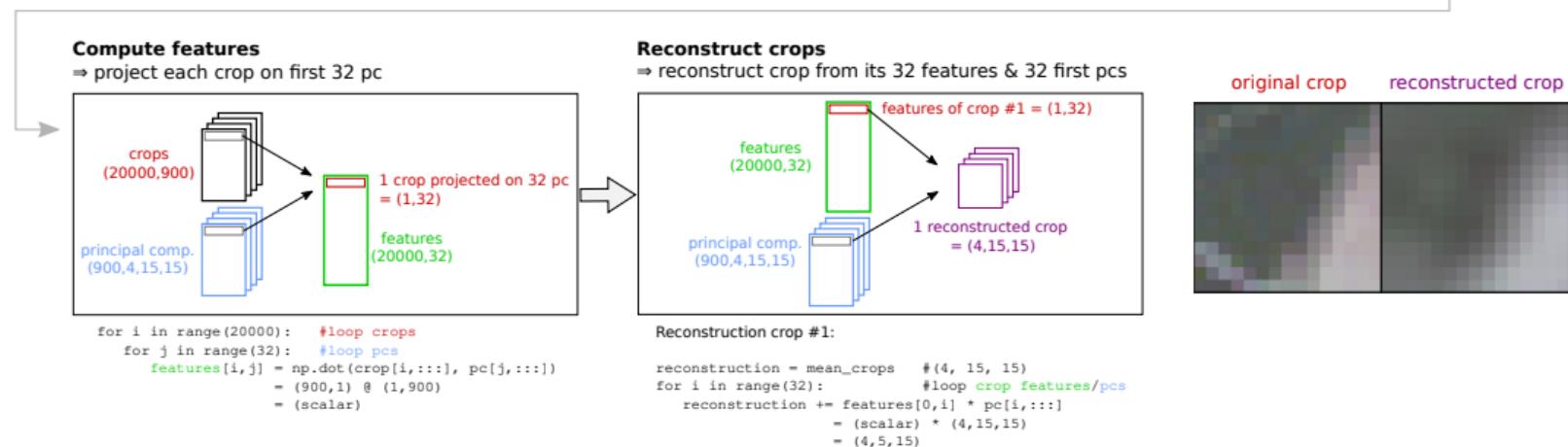
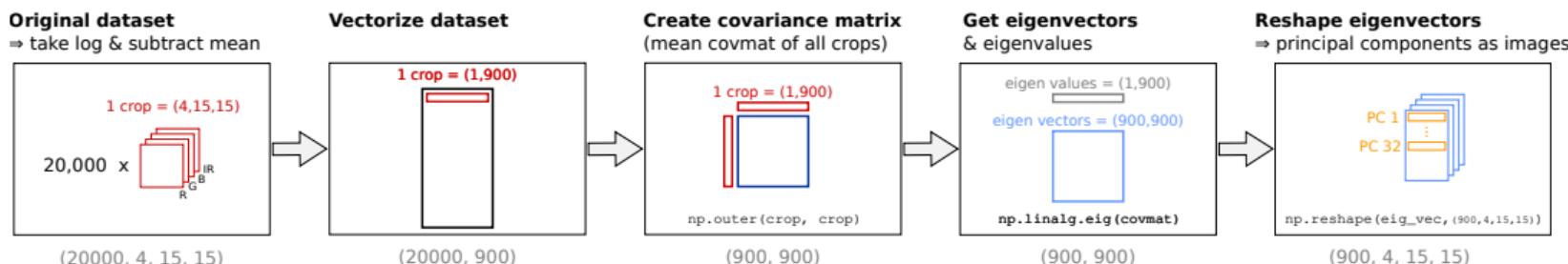
Part 1: apply PCA on satellite image crops



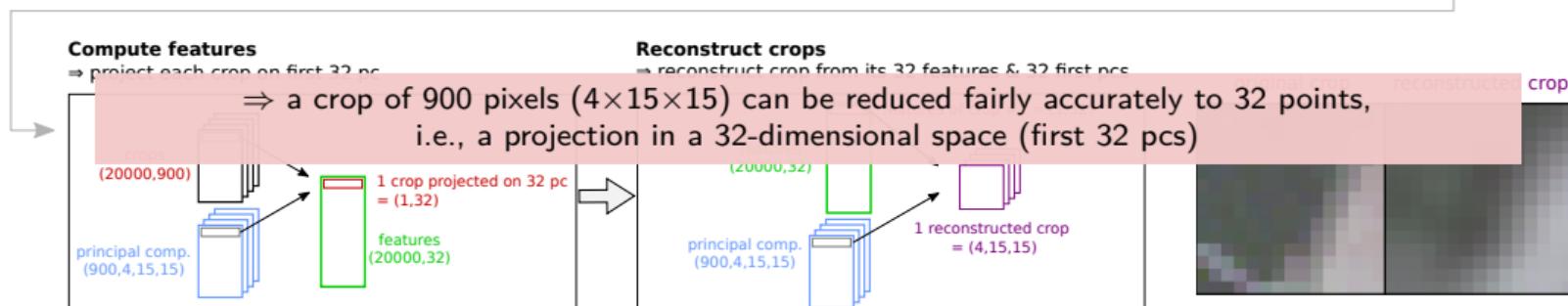
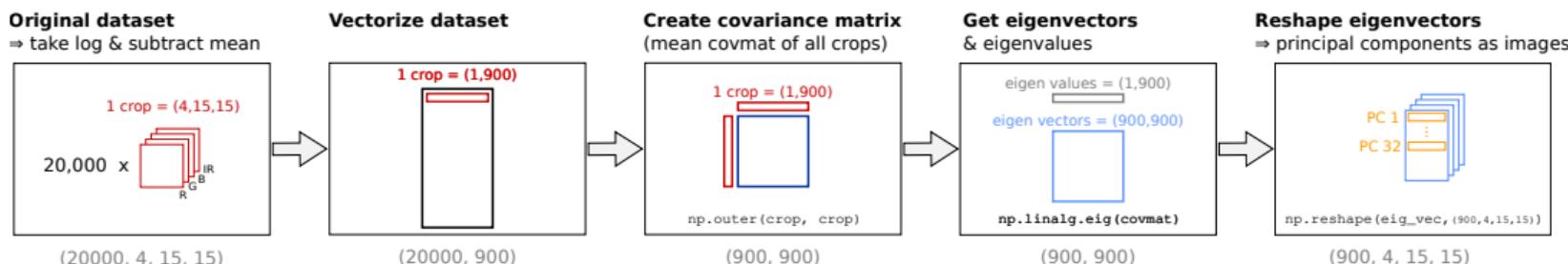
Part 1: apply PCA on satellite image crops



Part 1: apply PCA on satellite image crops



Part 1: apply PCA on satellite image crops



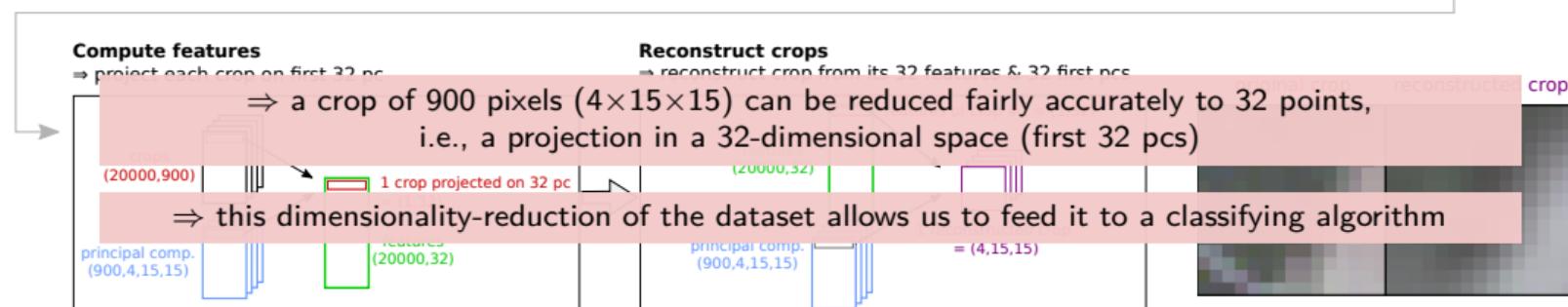
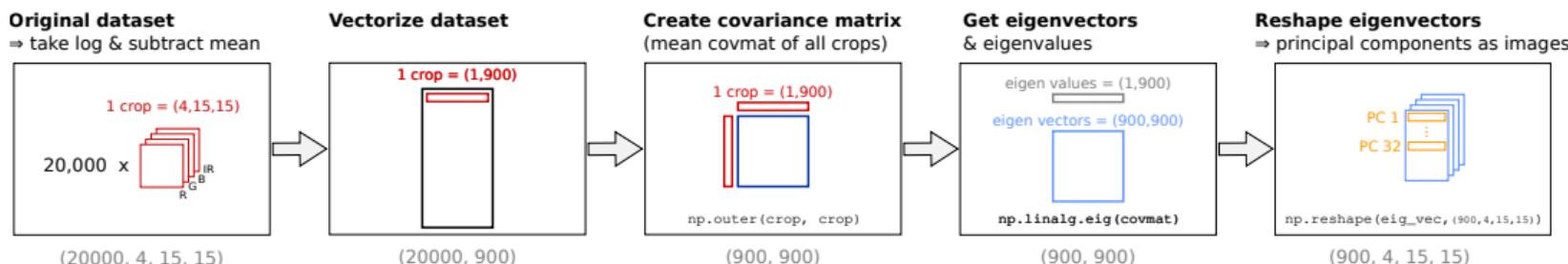
```

for i in range(20000):      #loop crops
    for j in range(32):      #loop pcs
        features[i,j] = np.dot(crop[i,:,:], pc[j,:,:])
        = (900,1) @ (1,900)
        = (scalar)
    
```

```

reconstruction = mean_crops    #(4, 15, 15)
for i in range(32):            #loop crop features/pcs
    reconstruction += features[0,i] * pc[i,:,:]
    = (scalar) * (4,15,15)
    = (4,5,15)
    
```

Part 1: apply PCA on satellite image crops



```

for i in range(20000):    #loop crops
    for j in range(32):    #loop pcs
        features[i,j] = np.dot(crop[i,:,:], pc[j,:,:])
        = (900,1) @ (1,900)
        = (scalar)
    
```

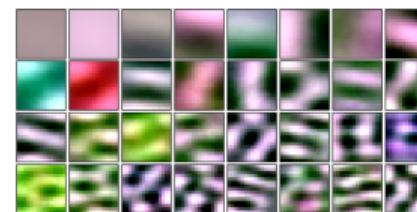
```

Reconstruction crop #1:

reconstruction = mean_crops    #(4, 15, 15)
for i in range(32):            #loop crop features/pcs
    reconstruction += features[0,i] * pc[i,:,:]
    = (scalar) * (4,15,15)
    = (4,5,15)
    
```

Part 2: train SVM on principal components and apply to classify full image

PCA dimensionality reduction



land-use classification

