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PRINCIPAL COMPONENT ANALYSIS

A typical phenomenon of datasets is *redundancy*. From a statistical perspective, one could say, that the measured variables in our data are typically not independent but correlated. The consequence is that knowing a small number of values derived from our measured variables might already describe the full dataset. Thus, the allegedly high-dimensional representation of many datasets is not their most compact form.¹ This redundancy is a common practical observation, and it motivates several questions. Vaguely speaking, one tries to find a mapping into a lower dimensional representation space which preserves (or selects) the relevant information. In this and following chapter, we will look into two methods which are examples for such mappings. Both belong to the domain of *dimensionality reduction methods*, which are essential tools in data science.

A difference in methodology to the previous chapters is that no simple solution criterion is usually known. While any good solution for a regression problem will provide a good approximation to the ground truth f , in dimensionality reduction there is often no single best answer. Two representations could capture or highlight different aspects of the data and might be useful for various applications. One could say that the condition “preserves information” or “reduces redundancy” leaves more space for different objective functions to minimize, which might also depend on the task at hand.

3.1 REASONS FOR REDUCING THE DIMENSION

The dimension d of a set of measurements can be too big by several means. For example, it can be *too big to understand*: A typical task for a given dataset is to answer a specific question or to gain new insights about inner workings. Here, a good visualization is a powerful tool to develop an idea or intuition on what is happening. The more dimensions our data has, the more challenging it is to visualize it.

¹ If you think of data compression you are not too far off, e.g. the term *redundancy* is also defined in information theory—which by the way provides a more rigorous investigation into terms we here use vaguely.

Send your solutions
to this chapter's tasks
until
December 1st.

While finding a suitable visualization is a topic on its own,² reducing the dimension can be a helpful start.

A computational reason for reducing d is scaling behavior. The runtime of many algorithms scales polynomially or even exponentially in the dimension of the input data. Furthermore, some methods do not perform well in high dimensions. We already saw for example that the k -nearest neighbors algorithm does only work for low dimensional data.

Therefore, dimensionality reduction as a preprocessing step can provide more expressive features for a learning algorithm. Another example would be non-linearly separable input whose low dimensional representation is linearly separable. Also, keep in mind that a low dimensional representation can be a regularization entailed by the reduction algorithm. The reason is that the algorithm usually enforces a particular model assumption.

In this sheet, we look at representations gained through a *linear* transformation.

LINEAR REPRESENTATIONS

Suppose we conducted an experiment and gained measurements in two variables, X_1 and X_2 . The plotted values might look as in [fig. 3.1](#). The data is two dimensional but visibly correlated: If X_1 is large so is X_2 (i.e., the covariance is positive). In this case, one might reduce the dimension to 1 and use a fitted line where each measurement is projected onto the line.

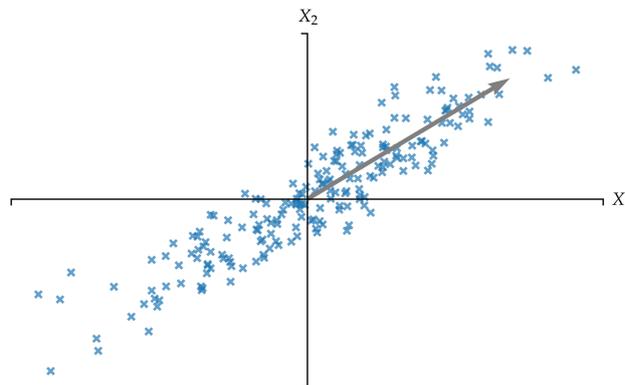


Figure 3.1: Plot of two measured variables in an experiment.

Then, the 1D values will be the points on this line, where we think of the line as a new axis. There is some freedom in this representation,

² The books of Edward R. Tufte might be useful for more information on great visualization from graphics design perspective.

namely in picking the center of this axis. Different centers will shift the 1D values.

We might be interested in two things in the calculation. The first could be the line itself corresponding to the mapping into a low dimensional representation, and the second would be the projections of our data onto this line, i.e., the coordinates w.r.t. the new axis.

In higher dimensions, it might not be sufficient to have only one axis (e.g., a plane in 3D). So generally we are interested in the set of orthogonal axes which can represent the most variation in the data.

3.2 DERIVATION OF PCA

In this chapter, we look into the classic method of *principal component analysis* (PCA). Despite its age [4, 7], it is the most popular method for linear dimensionality reduction.

Skip to [theorem 3.1](#).

The goal is to find a linear transformation $P: \mathbb{R}^d \rightarrow \mathbb{R}^q$, with $q < d$, for a set of data points $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^d$ such that the new coordinates in \mathbb{R}^q describe the data (approximately).

More precisely we try to find a linear affine model $f: \mathbb{R}^q \rightarrow \mathbb{R}^d$ s.t.

$$f(\lambda_i) = \boldsymbol{\mu} + \mathbf{V}_q \lambda_i, \quad (3.1)$$

where $\mathbf{V}_q \in \mathbb{R}^{d \times q}$ is a matrix whose columns form an orthonormal basis, $\boldsymbol{\mu} \in \mathbb{R}^d$ is a location vector, and $\lambda_i = P(\mathbf{x}_i)$ are q dimensional coordinate vectors for the inputs $\mathbf{x}_i, i = 1, \dots, n$.

We fit the model using the least squares error

$$\sum_{i=1}^n \|\mathbf{x}_i - (\boldsymbol{\mu} + \mathbf{V}_q \lambda_i)\|^2$$

with respect to $\boldsymbol{\mu}, \mathbf{V}_q$ and λ_i .

To solve the system, first split up the optimization problem as

$$\min_{\boldsymbol{\mu}, \mathbf{V}_q, \{\lambda_i\}} \sum_{i=1}^n \|\mathbf{x}_i - (\boldsymbol{\mu} + \mathbf{V}_q \lambda_i)\|^2 = \min_{\mathbf{V}_q} \min_{\boldsymbol{\mu}, \{\lambda_i\}} \sum_{i=1}^n \|\mathbf{x}_i - (\boldsymbol{\mu} + \mathbf{V}_q \lambda_i)\|^2.$$

We solve the inner problem by using the first order necessary optimality condition

$$\begin{aligned} \sum_{i=1}^n (\boldsymbol{\mu} - \mathbf{x}_i + \mathbf{V}_q \lambda_i) &= 0, \\ \mathbf{V}_q^\top \mathbf{V}_q \lambda_i - \mathbf{V}_q^\top (\mathbf{x}_i - \boldsymbol{\mu}) &= 0 \quad \text{for } i = 1, \dots, n, \end{aligned}$$

which is also a sufficient optimality criterion in this case since the objective function is convex.

With $\mathbf{V}_q^\top \mathbf{V}_q = \mathbf{I}_q$ this is equivalent to

$$\begin{aligned} (\mathbf{I}_d - \mathbf{V}_q \mathbf{V}_q^\top) \boldsymbol{\mu} &= (\mathbf{I}_d - \mathbf{V}_q \mathbf{V}_q^\top) \bar{\mathbf{x}}, \\ \lambda_i &= \mathbf{V}_q^\top (\mathbf{x}_i - \boldsymbol{\mu}) \quad \text{for } i = 1, \dots, n. \end{aligned} \quad (3.2)$$

Here $\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$ denotes the mean.

The system in eq. (3.2) is under-determined (for $q < d$). The matrix $\mathbf{I}_d - \mathbf{V}_q \mathbf{V}_q^\top$ is the projection³ on the orthogonal complement \mathbf{V}_q^\perp . Since $\bar{\mathbf{x}}$ is a solution, all solutions to eq. (3.2) are of the form $\boldsymbol{\mu} = \bar{\mathbf{x}} + \text{span}(\mathbf{V}_q)$. So a solution to the inner minimization problem is

$$\boldsymbol{\mu} = \bar{\mathbf{x}} \quad \text{and} \quad \lambda_i = \mathbf{V}_q^\top (\mathbf{x}_i - \bar{\mathbf{x}}) \quad \text{for} \quad i = 1, \dots, n.$$

This leaves us with

$$\min_{\mathbf{V}_q} \sum_{i=1}^n \|(\mathbf{I}_d - \mathbf{V}_q \mathbf{V}_q^\top)(\mathbf{x}_i - \bar{\mathbf{x}})\|^2 \quad \text{subject to} \quad \mathbf{V}_q^\top \mathbf{V}_q = \mathbf{I}_q.$$

So we minimize the projection error onto the subspace⁴ spanned by the columns in \mathbf{V}_q . It is straightforward to calculate that the above minimization is equivalent to

$$\max_{\mathbf{V}_q} \sum_{i=1}^n \|\mathbf{V}_q^\top (\mathbf{x}_i - \bar{\mathbf{x}})\|^2 \quad \text{subject to} \quad \mathbf{V}_q^\top \mathbf{V}_q = \mathbf{I}_q. \quad (3.3)$$

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the matrix with rows $(\mathbf{x}_i - \bar{\mathbf{x}})^\top$, and denote the columns of \mathbf{V}_q by \mathbf{v}_i .

Clearly, for any solution \mathbf{V}_q we would obtain new solutions by composing with an orthogonal transformation. To encode further semantics we look for a solution \mathbf{V}_q such that the matrices \mathbf{V}_k containing the first $k \leq q$ columns are a solution to the corresponding smaller problems

$$\max_{\mathbf{V}_k} \sum_{i=1}^n \|\mathbf{V}_k^\top (\mathbf{x}_i - \bar{\mathbf{x}})\|^2 \quad \text{subject to} \quad \mathbf{V}_k^\top \mathbf{V}_k = \mathbf{I}_k.$$

In this way, the columns are ordered w.r.t. their contribution to the error reduction.

Using Lagrange multipliers and induction over q , one can show that such an optimal solution must fulfill

$$(\mathbf{X}^\top \mathbf{X}) \mathbf{v}_k = \lambda_k \mathbf{v}_k \quad \text{for} \quad k = 1, \dots, q,$$

for some $\lambda_k \in \mathbb{R}$, $k = 1, \dots, q$. So the columns \mathbf{v}_i of \mathbf{V}_q must be eigenvectors of $\mathbf{X}^\top \mathbf{X}$.

Now consider the *singular value decomposition* (SVD) of \mathbf{X} :

$$\mathbf{X} = \mathbf{U} \mathbf{D} \mathbf{W}^\top \quad \text{with} \quad \mathbf{D} = \text{diag}(\sigma_1, \dots, \sigma_d),$$

(such that $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_d \geq 0$).

One can see that the columns of \mathbf{W} are eigenvectors of $\mathbf{X}^\top \mathbf{X}$ with eigenvalues $\sigma_1^2, \dots, \sigma_d^2$.

³ This is exactly the term in Gram-Schmidt.

⁴ This can be also seen as the reconstruction error from going to the low dimensional representation and back, as in the original introduction of PCA [7].

Since the columns of \mathbf{W} and of \mathbf{V}_q form an orthonormal basis, we can find a family of orthogonal maps⁵ $F_{\mathbf{V}_q}$ such that the image of all basis vectors from \mathbf{W} includes the basis vectors of \mathbf{V}_q , and all eigenspaces map into themselves. We denote with $\hat{\mathbf{W}} := F_{\mathbf{V}_q}(\mathbf{W})$ the matrix whose columns are mapped column-wise, and we obtain the SVD

$$\mathbf{X} = \hat{\mathbf{U}}\mathbf{D}\hat{\mathbf{W}}^\top,$$

for an orthogonal matrix $\hat{\mathbf{U}}$ which can be derived from \mathbf{D} and $\hat{\mathbf{W}}$.

So $\mathbf{V}_q^\top \hat{\mathbf{W}} \in \mathbb{R}^{q \times d}$ is a permutation matrix. For any vector \mathbf{z} follows

$$\|\mathbf{V}_q^\top \hat{\mathbf{W}}\mathbf{z}\|^2 = \sum_{k \in \Gamma} z_k^2 \quad (3.4)$$

for certain indices $\Gamma \subseteq \{1, \dots, d\}$. We obtain

$$\begin{aligned} \sum_{i=1}^n \|\mathbf{V}_q^\top (\mathbf{x}_i - \bar{\mathbf{x}})\|^2 &= \sum_{i=1}^n \|\mathbf{V}_q^\top \hat{\mathbf{W}}\mathbf{D}^\top \hat{\mathbf{U}}^\top \mathbf{e}_i\|^2 \\ &= \sum_{i=1}^n \sum_{k \in \Gamma} (\sigma_k \hat{\mathbf{U}}_{i,k})^2 && \text{(use eq. (3.4))} \\ &= \sum_{k \in \Gamma} \sigma_k^2. && \text{(columns of } \hat{\mathbf{U}} \text{ have norm 1)} \end{aligned}$$

Therefore, we can solve the problem from eq. (3.3) by letting the columns of \mathbf{V}_q be orthogonalized unit eigenvectors belonging to the q largest eigenvalues.

Let us summarize this in the following Theorem.

Theorem 3.1. *Let $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ be a set of vectors from \mathbb{R}^d , and let $q \in \mathbb{N}$ with $q \leq d$. The minimization problem*

$$\min_{\substack{\boldsymbol{\mu} \in \mathbb{R}^d, \lambda_i \in \mathbb{R}^q, \\ \mathbf{V}_q \in \mathbb{R}^{d \times q}}} \sum_{i=1}^n \|\mathbf{x}_i - (\boldsymbol{\mu} + \mathbf{V}_q \lambda_i)\|^2 \quad \text{subject to} \quad \mathbf{V}_q^\top \mathbf{V}_q = \mathbf{I}_q$$

is solved for $\boldsymbol{\mu} = \bar{\mathbf{x}}$, $\lambda_i = \mathbf{V}_q^\top (\mathbf{x}_i - \bar{\mathbf{x}})$, and \mathbf{V}_q contains column-wise q orthogonalized unit eigenvectors of $\mathbf{X}^\top \mathbf{X}$ for the q largest eigenvalues.

Remark. The solution is not unique. The orthonormal basis of each eigenspace is only unique up to an orthogonal transformation (composition of reflections).

3.2.1 Numerical Computation

We have seen two basic problems we could solve to get a PCA:

1. Compute eigenvectors of $\mathbf{X}^\top \mathbf{X}$.

⁵ Complete the basis \mathbf{V}_q , then the linear map that maps the corresponding basis vectors on to each other does the job.

Effectively, we now pick a SVD matching our orthonormal basis vectors from \mathbf{V}_q . The SVD is not unique in \mathbf{W} and \mathbf{U} .

2. Compute a singular value decomposition of \mathbf{X} .

Of course, both are related and several solvers exist for each. An optimal choice might depend on the size of n , p , and d , and if speed is more important than accuracy.

Let us implement the PCA and test it on a toy example we understand. The accompanying material includes a JUPYTER notebook which should be used as a template for your solution. The material also includes the datasets and some PYTHON code you may use. Please check the README file for further details.

Also check if the routine returns eigenvectors as columns or rows!

Task 3.1. Implement a PCA routine whose inputs are $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ and q . Use a NUMPY/SCIPY routine to compute either eigenvectors directly or use a SVD. In the case of eigenvectors, make sure your routine does actually return an orthonormal basis (consult the documentation of your solver).

The toy example is a 2D dataset which is embedded into 4D by rotating and translating it, also noise was added. We would like to recover the 2D representation. Each point in the dataset is labeled among five categories. We also check the results we get for non-linear data.

Task 3.2. Test your PCA implementation on the provided toy dataset.

- Plot a slice of the 4D toy data. Compute the PCA representation for $q = 2$ and plot it as described in the notebook. To check your result: The plot should reveal a perfectly round and familiar shape.
- Map the 2D representation onto a distorted ellipse in 3D, the code for the transformation is provided. Do a PCA of this 3D data for $q = 2$ and plot the result. Repeat this for a few ellipses and describe in words how the PCA does pick the coordinate system \mathbf{V}_q .

3.3 STATISTICAL PERSPECTIVE

The method we described is known by several names. The name PCA is especially popular in statistics [4]. We quickly sketch the statistics approach to get another perspective of the method.

Suppose we have a vector-valued random variable $\hat{\mathbf{X}} \in \mathbb{R}^d$. The covariance matrix is a real $d \times d$ matrix and it is defined as

$$\text{Cov}[\hat{\mathbf{X}}]_{ij} := \mathbb{E}[(\hat{\mathbf{X}}_i - \mathbb{E}[\hat{\mathbf{X}}_i])(\hat{\mathbf{X}}_j - \mathbb{E}[\hat{\mathbf{X}}_j])].$$

To simplify notation we assume that $\hat{\mathbf{X}}$ has zero mean, so

$$\text{Cov}[\hat{\mathbf{X}}] = \mathbb{E}[\hat{\mathbf{X}}^\top \hat{\mathbf{X}}].$$

Let $\mathbf{v}_1 \in \mathbb{R}^d$ be a vector with unit-norm. We consider the real random variable Y_1 defined by $Y_1 := \mathbf{v}_1^\top \hat{\mathbf{X}}$. We now wish to maximize its variance

$$\text{Var}[Y_1] := \mathbb{E}[(Y_1 - \mathbb{E}[Y_1])^2] = \mathbb{E}[Y_1^2]$$

w.r.t. to the direction \mathbf{v}_1 . This is motivated by the idea, that since the variance is a measure of how much a random variable varies, we want to find the direction along which our data varies the most. This direction is defined to be a the *first principal component*.

The idea is iteratively continued by searching normed directions $\mathbf{v}_2, \mathbf{v}_3, \dots$, perpendicular to all previous ones, while maximizing the variance subject to

$$\text{Var}[\mathbf{v}_1^\top \hat{\mathbf{X}}] \geq \text{Var}[\mathbf{v}_2^\top \hat{\mathbf{X}}] \geq \dots$$

It turns out that a solution is given by picking eigenvectors of $\mathbb{E}[\hat{\mathbf{X}}^\top \hat{\mathbf{X}}]$ belonging to the largest eigenvalues. Moreover, the eigenvalues λ_i are equal to the variances of the random variables Y_i .

The dots to our derivation can be connected by switching to approximations of the expected values using observed values (samples) for $\hat{\mathbf{X}}$, which we shall denote by $\mathbf{x}_1, \dots, \mathbf{x}_n$. Following this idea we notice that the singular values from above fulfill $\sigma_i^2 \approx \lambda_i = \text{Var}[Y_i]$.

A common approach on how to decide how large q should be chosen, is to look at the variances σ_i^2 . One usually picks q as the smallest number such that σ_i^2 is below a given threshold, or such that the *percentage of captured variance*⁶

$$\frac{\sum_{i=1}^q \text{Var}[\mathbf{v}_i^\top \hat{\mathbf{X}}]}{\text{Var}[\hat{\mathbf{X}}]} = \frac{\sum_{i=1}^q \lambda_i}{\sum_{i=1}^d \lambda_i} \approx \frac{\sum_{i=1}^q \sigma_i^2}{\sum_{i=1}^d \sigma_i^2} \quad (3.5)$$

is above a given threshold.

We revisit the Iris dataset to check how PCA can be utilized there.

Task 3.3. Use PCA for the Iris dataset:

- Compute all (four) singular values of \mathbf{X} using a suitable function from NUMPY. Compute the captured variance percentage from eq. (3.5) when using only the first principal component, and for the first two principal components.
- Compute the PCA transformation onto the first two principal components of the Iris dataset. Plot the transformed data in a 2D scatter plot such that the three labels are distinguishable. Do the same for 1D and use the provided function to plot it. What do you observe?
- Using the insights from the visualization in b) build classifiers for the whole Iris dataset which use a 4D, 2D, or 1D PCA respectively as the first step, and two linear SVMs as a second and third step to classify a data-point as one of the three labels. You can copy your SVM code from sheet 2, but we recommend using SCIKIT-LEARN.

Do not forget to square the singular values.

With a better understanding of PCA we now turn our attention to the analysis of a larger dataset.

⁶ Also known as percentage of explained variance.



Figure 3.2: Ten pedestrian images and ten garbage (non-pedestrian) images from the dataset.

3.4 PEDESTRIAN CLASSIFICATION

Detecting people in video footage is a topic interesting for many entities. One important application would be in the self-driving car industry. The task can be split broadly into several connected steps:

- How to gather the image material.
- Find region proposals in an image which could be interesting.
- Decide if a given region shows a pedestrian.

We dive deeper into the last problem. The second step is known as a *segmentation problem* in computer vision, it is also tackled as an unsupervised learning problem.

Our dataset consists of labeled pictures of size 100x50 pixel, it is derived from the TUD dataset [8]. Half of the pictures show a pedestrian, the other half does not. A separation into training and test data is provided. We begin by preparing the data.

Task 3.4. *Prepare the data.*

- Load the test and training images into NUMPY arrays. The template contains a routine which will help you. Normalize the pixel values to $[0, 1]$.*
- Write a routine `plot_im` to plot an image using MATPLOTLIB's `imshow` (to get consistent contrast, provide constant values for its arguments `vmin` and `vmax`). Create a plot with ten randomly chosen training images showing a pedestrian and ten randomly chosen training images not showing a pedestrian. You can use the `subplot` method⁷ from MATPLOTLIB.*

Our training data consists of $n = 2000$ points, with dimension $d = 15000$ (the pixels of an image for three colors). Compared to what we

⁷ You should implement an optional argument `ax` for `plot_im`, so you can use it for the subplot, see `plt.gca()`.

saw so far, one could say that the dimension is quite large. Arguably, visualization of a single data-point, i.e., image, is straight-forward, but our goal is to classify the images using the color values of the pixels. Trying to find an algorithm by just looking at the numbers is hard.⁸

Unsurprisingly, our next step is to compute a PCA to reduce d to a much smaller number. Note that the coordinate axes calculated by the PCA can be interpreted as images and we represent the data in terms of coefficients for the corresponding eigenvectors, which are called *eigenpedestrians*.

Task 3.5. *Take a look at the eigenpedestrians. From now on use the PCA implementation of SCIKIT-LEARN.*

- a) *Compute the PCA with $q = 200$ for the full training set (i.e., with pedestrian and non-pedestrian samples combined).*
- b) *Plot the first 20 eigenpedestrians, as well as eigenpedestrians 50 to 60 and eigenpedestrians 100 to 110. What do you observe? Provide a guess on what these eigenpedestrians might encode.*

We now use our PCA representation to train a linear SVM.

Task 3.6. *Train a linear SVM (use `LinearSVC` from `SCIKIT-LEARN`) using the PCA representation of the full training dataset for values of q between 10 and 200 in steps of 5. For each q compute and store the prediction accuracy (use the `score` method) on the training and test dataset. Plot the scores for q . Which q seems the best choice? Compare the situation to [task 3.3 c](#)) w.r.t. q .*

The prediction results are not bad, but for self-driving cars probably not acceptable.

3.4.1 Histogram of Oriented Gradients

To improve the prediction quality, we use a handcrafted feature map as an additional step before applying PCA. In particular, we will use the so-called *Histogram of Oriented Gradients* (HOG), which became quite popular after the well-received experiments by Dalal and Triggs [2] were published. Before we explain what HOG is we take a quick excursion into computer vision.

A very common tool in computer vision are image gradients. Starting from the difference quotient

$$\lim_{\varepsilon \rightarrow 0} \frac{f(x + \varepsilon) - f(x)}{\varepsilon}$$

we can define a gradient for images by using a discrete approximation. Let $\mathbf{I} \in \mathbb{R}^{h \times w}$ be a matrix representing one color channel of an image. The entries of the matrix represent pixel values for this color.

⁸ This is the problem fundamental to the field of computer vision.

We can compute the partial derivatives in y - and x -direction by using a centered difference quotient, for example

$$\frac{\mathbf{I}_{y+1,x} - \mathbf{I}_{y-1,x}}{2} \text{ and } \frac{\mathbf{I}_{y,x+1} - \mathbf{I}_{y,x-1}}{2}. \quad (3.6)$$

One might argue that the scaling factor of 2 is not canonical since the two units color value and pixel distance have no natural choice for their ratio's unit. Indeed, it is common to pick the factor to normalize the result into a suitable range. Furthermore, since for many algorithms not the scale but the relative size of the derivatives is important, the scaling factor can be considered to be flexible. A popular choice is 1, which is what we will use.⁹

Often, one can represent the derivative calculation by a *convolution*—whose continuous counterpart might be known from integration theory. Given a *filter* matrix $\mathbf{K} \in \mathbb{R}^{p \times q}$ we define the convolution $\mathbf{I} * \mathbf{K}$ of \mathbf{K} and \mathbf{I} point-wise by

We use zero-based indexing

$$(\mathbf{I} * \mathbf{K})_{y,x} := \sum_{\substack{0 \leq i < p \\ 0 \leq j < q}} \mathbf{K}_{i,j} \mathbf{I}_{y+k_y-i, x+k_x-j}$$

with *shifts*¹⁰ k_x and k_y . The result is a new color channel whose entries were computed using weighted sums of the surroundings of each pixel of \mathbf{I} . Another example for a popular filter is Gaussian smoothing, here the entries of \mathbf{K} are computed using a Gaussian kernel.

The new color channel is either smaller, or one has to specify how the missing pixel values outside of the border of \mathbf{I} are extrapolated. In our case we are extending \mathbf{I} by the constant value 0. The y - and x -derivatives can be computed using `scipy.ndimage.convolve` with the filters $[-1, 0, 1]^\top$ and $[1, 0, -1]$, which correspond to eq. (3.6) with scaling factor 1.

In HOG, the gradient norm and direction is computed for each pixel and each color channel. For a RGB image this would give three sets of gradient norms and directions. To reduce the sets of gradient norms and directions to one set, we pick for every pixel a maximum over all channels w.r.t. to the gradient norms. This means, for every pixel we consider all color channels and pick a channel such that the gradient norm of this channel at this pixel is maximal among all gradient norms for this pixel.

Then, each (y, x) -position is assigned (*binned*) to a square cell of size $|c| \in \mathbb{N}$. The cells span over $|c|$ pixels in both directions and form a regular grid. Similarly, the orientations are binned into $\#b \in \mathbb{N}$ equally sized intervals which partition either the full circle $\alpha := 2\pi$ or only the half circle $\alpha := \pi$, in which case one calls the orientations *unsigned*. The intervals are

$$\left[\left(\frac{\alpha}{\#b} \right) i, \left(\frac{\alpha}{\#b} \right) (i + 1) \right), \quad \text{for } i = 0, \dots, \#b - 1.$$

⁹ An argument for this factor is, that in the case of integer division the precision loss from rounding down is avoided at the cost of a higher number range.

¹⁰ In SciPy these are chosen to center the filter by default.

In other words, the gradient norms are accumulated into a histogram¹¹ $H(c_y, c_x, b_i)$ where we collect

- the y - and x -positions into cells, indexed by (c_y, c_x) , and
- the orientations into the former intervals for each cell, indexed by b_i .

More precisely, for a gradient norm $\|\nabla_{y,x}\|$ and direction $\phi \in [-\pi, \pi]$ at position (y, x) we consider the interval whose center is below or equal to

$$\hat{\phi} := \phi \pmod{\alpha},$$

and the interval whose center is above $\hat{\phi}$ (wrapping around), as well as preceding and succeeding cells in y - and x -direction in the same fashion, i.e., with respect to their center¹² (out of bound cells are ignored). The gradient norms $H(c_y, c_x, b_i)$ for those neighbors are then updated by adding a fraction of the gradient norm at position (y, x) . The fraction for each $H(c_y, c_x, b_i)$ is defined by the coefficients of a convex combination whose terms can be found in [algorithm 3.3](#).

The last step is to combine the cells into blocks, which are then normalized and clipped. If $|B| \in \mathbb{N}$ is the block size, then a block consists of $|B|$ consecutive cells in y -direction and $|B|$ consecutive cells in x -direction. The blocks do overlap, but only full blocks are considered. Consequently, $|B|$ has to be chosen less than or equal to the minimum number of cells in y - and x -direction respectively. The HOG feature vector consists of the entries of all blocks (in any order).

Task 3.7. (Optional bonus task) Test the HOG features for the dataset.

- Implement [algorithm 3.3](#) either yourself in Python, or build a Python binding to the provided C++ implementation.
- Repeat the experiment from [task 3.6](#) for values of q between 10 and 200 in steps of 5 but use the HOG features as input for the PCA instead.

Be aware that [task 3.7](#) is expected to be challenging. If you want to implement [algorithm 3.3](#) in Python you should try to avoid stating the loops over all pixels as Python loops. Instead, a suitable NUMPY routine should be used. This means the algorithm as stated here should not be implemented in a straightforward way with NUMPY. A way to use NUMPY more efficiently is to compute all inner variables ($f_x, c_{x,prec}, \dots$) as matrices containing the results for all pixels. Then, each update of the histogram can be done cell-wise, here `scipy.ndimage.sum` could be handy. To test your implementation values for intermediate steps of the algorithm are available (for a single layer), see the notebook for details.

¹¹ The histogram was introduced by Karl Pearson, the inventor of PCA [7].

¹² The NUMPY routines `np.digitize` and `np.arange` can be useful for these steps.

Algorithm 3.3 Computation of HOG-features.

Input: An image $\mathbf{I} \in \mathbb{R}^{h \times w \times 3}$, a number of bins $\#b$ (default: 9), a cell size $|c|$ (default: 8), a block size $|B|$ (default: 2), whether to use unsigned directions (default: yes), and a clip value C (default: 0.2).

Output: A feature vector.

$$\alpha \leftarrow \begin{cases} \pi & \text{if use unsigned directions,} \\ 2\pi & \text{else.} \end{cases}$$

$$|b| \leftarrow \alpha / \#b$$

Initialize $H(c_y, c_x, b_i)$ to zero for all cell indices c_y, c_x and all bin indices b_i .

for all pixel positions y, x **do**

$dy^{(i)}, dx^{(i)} \leftarrow$ derivatives at y, x using zero boundary conditions on channel i , for $i = 1, 2, 3$.

$$i_{\max} \leftarrow \arg \max_{i=1,2,3} \sqrt{(dy^{(i)})^2 + (dx^{(i)})^2}$$

$$\|\nabla_{y,x}\| \leftarrow \sqrt{(dy^{(i_{\max})})^2 + (dx^{(i_{\max})})^2}, dx \leftarrow dx^{(i_{\max})}, dy \leftarrow dy^{(i_{\max})}.$$

$$\hat{\phi} \leftarrow \text{atan2}(dy, dx) \bmod \alpha$$

$b_{\text{prec}} \leftarrow$ index of orientation interval preceding the orientation $\hat{\phi}$ w.r.t. the interval's center (can be -1)

$c_{x,\text{prec}} \leftarrow$ index of horizontally preceding cell w.r.t. its center (can be -1)

$c_{y,\text{prec}} \leftarrow$ index of vertically preceding cell w.r.t. its center (can be -1)

$$f_b \leftarrow \frac{\hat{\phi} - [b_{\text{prec}}|i| + \frac{1}{2}|i|]}{|i|}$$

$$f_x \leftarrow \frac{x - [(c_{x,\text{prec}} + 1)|c| - \frac{1}{2}|c| - 0.5]}{|c|}$$

$$f_y \leftarrow \frac{y - [(c_{y,\text{prec}} + 1)|c| - \frac{1}{2}|c| - 0.5]}{|c|}$$

$$b_{\text{succ}} \leftarrow b_{\text{prec}} + 1 \bmod \#b, b_{\text{prec}} \leftarrow b_{\text{prec}} \bmod \#b$$

$$c_{x,\text{succ}} \leftarrow c_{x,\text{prec}} + 1, c_{y,\text{succ}} \leftarrow c_{y,\text{prec}} + 1$$

(The cells with indices -1 and $\lfloor h/|c| \rfloor$ or $\lfloor w/|c| \rfloor$ can be stored in H but must not be considered for the blocks)

$$H(c_{y,\text{prec}}, c_{x,\text{prec}}, b_{\text{prec}}) \leftarrow \text{add } \|\nabla_{y,x}\| (1 - f_x) (1 - f_y) (1 - f_b)$$

$$H(c_{y,\text{prec}}, c_{x,\text{prec}}, b_{\text{succ}}) \leftarrow \text{add } \|\nabla_{y,x}\| (1 - f_x) (1 - f_y) f_b$$

$$H(c_{y,\text{succ}}, c_{x,\text{prec}}, b_{\text{prec}}) \leftarrow \text{add } \|\nabla_{y,x}\| (1 - f_x) f_y (1 - f_b)$$

$$H(c_{y,\text{succ}}, c_{x,\text{prec}}, b_{\text{succ}}) \leftarrow \text{add } \|\nabla_{y,x}\| (1 - f_x) f_y f_b$$

$$H(c_{y,\text{prec}}, c_{x,\text{succ}}, b_{\text{prec}}) \leftarrow \text{add } \|\nabla_{y,x}\| f_x (1 - f_y) (1 - f_b)$$

$$H(c_{y,\text{prec}}, c_{x,\text{succ}}, b_{\text{succ}}) \leftarrow \text{add } \|\nabla_{y,x}\| f_x (1 - f_y) f_b$$

$$H(c_{y,\text{succ}}, c_{x,\text{succ}}, b_{\text{prec}}) \leftarrow \text{add } \|\nabla_{y,x}\| f_x f_y (1 - f_b)$$

$$H(c_{y,\text{succ}}, c_{x,\text{succ}}, b_{\text{succ}}) \leftarrow \text{add } \|\nabla_{y,x}\| f_x f_y f_b$$

end for

for all blocks **do**

Normalize the block w.r.t. the Euclidean (vector) norm.

Clip the block entries to be below C , normalize again.

Add the block entries to the feature vector.

end for

Building a C++ binding is a quite technical task and therefore challenging as well. Some experience in programming Python and C, C++, or Fortran could be very helpful. A skeleton of the binding with learning resources is provided in the README of the accompanying material.

3.5 OUTLOOK

At the time, the HOG features managed to increase the prediction rate notably. They are one of many examples where sophisticated hand-crafted features were developed to solve a problem. A lot of work can go into such feature maps and they might be problem specific. In recent years, the deep learning community has provided powerful tools to tackle computer image vision problems. One advantage is, that (convolutional) neural networks can learn feature maps on their own, but the training is not well understood and can be painful. Manually created feature a still a valuable tool in the machine learning workflow.

For further details about pedestrian classification in particular we refer to the reviews [1, 3].

Finally, more information on PCA can be found in the book by Jolliffe [5]. For dimensionality reduction in general see [6], which also covers PCA.

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