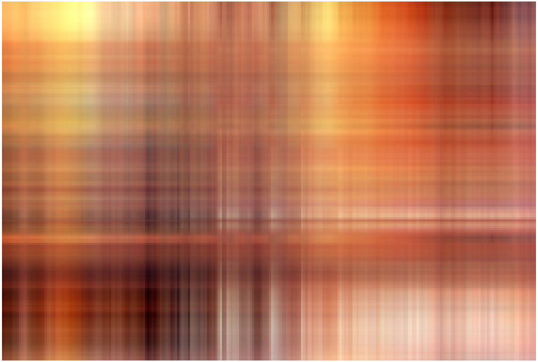
Principal component analysis

Ingo Blechschmidt

December 17th, 2014

Principal component analysis



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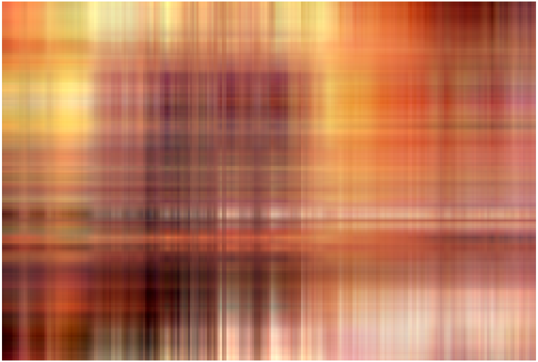

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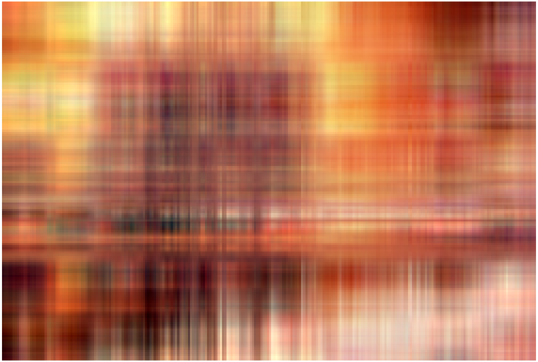

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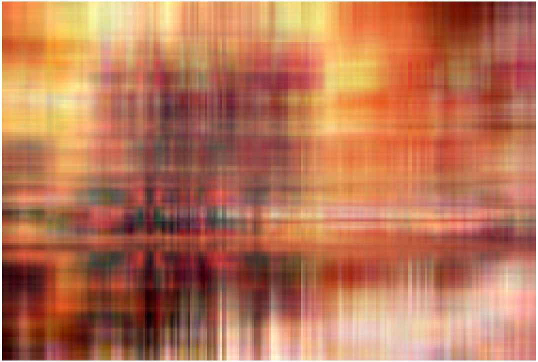

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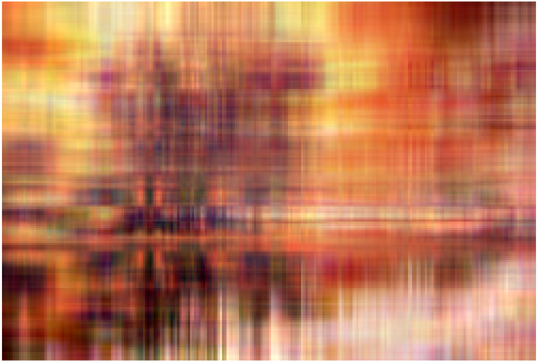

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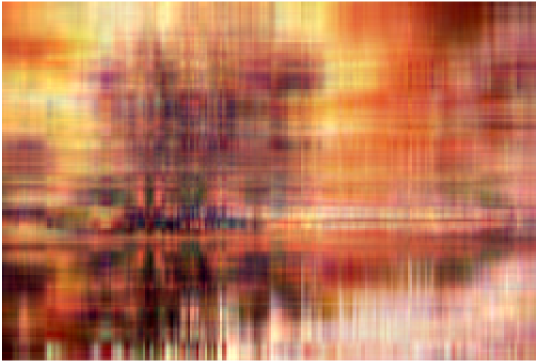

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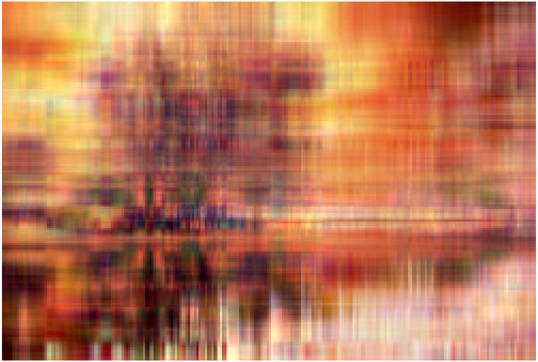

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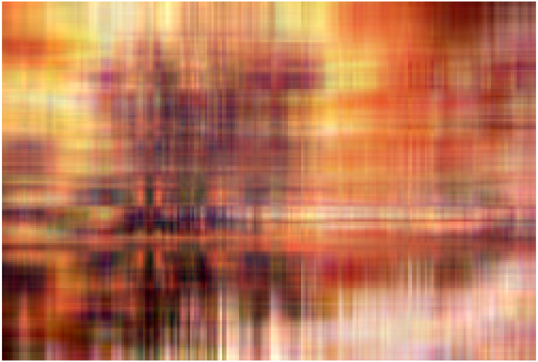

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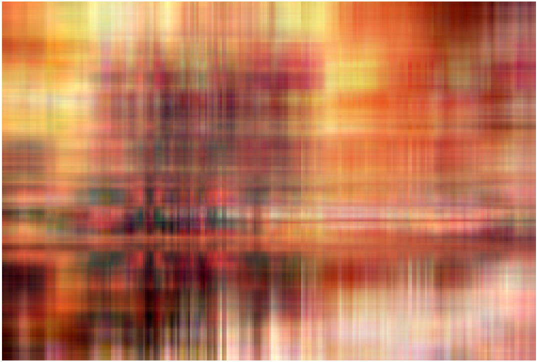

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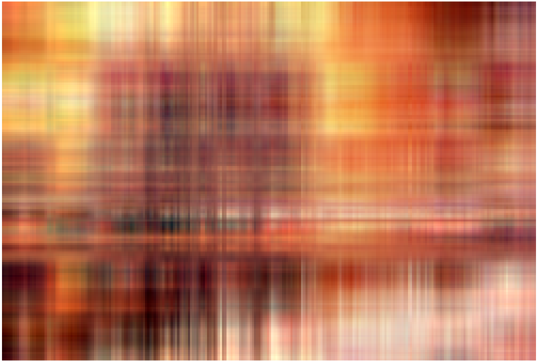

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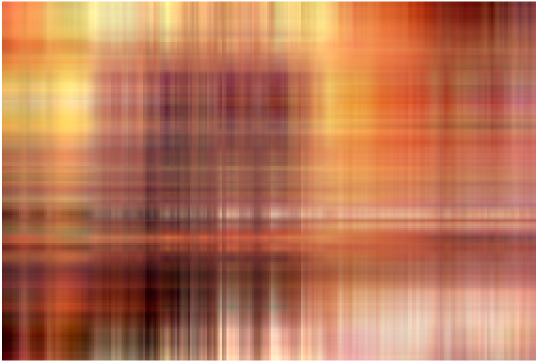

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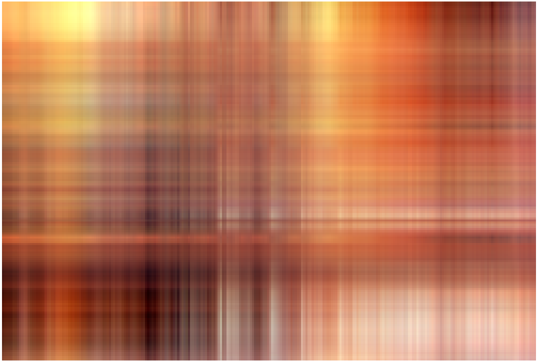

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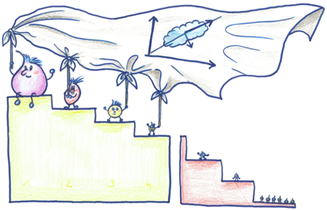
Outline

1. Theory
   - Singular value decomposition
   - Pseudoinverses
   - Low-rank approximation



2. Applications
   - Image compression
   - Proper orthogonal decomposition
   - Principal component analysis
   - Eigenfaces
   - Digit recognition

Singular value decomposition

Let $A \in \mathbb{R}^{n\times m}$. Then there exist

- numbers $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m \geq 0$,
- an orthonormal basis $\mathbf{v}_1, \ldots, \mathbf{v}_m$ of $\mathbb{R}^m$, and
- an orthonormal basis $\mathbf{w}_1, \ldots, \mathbf{w}_n$ of $\mathbb{R}^n$,

such that

$$A\mathbf{v}_i = \sigma_i \mathbf{w}_i, \quad i = 1, \ldots, m.$$

In matrix language:

$$\begin{aligned} A &= W\Sigma V^t, \\ \text{where} \quad V &= (\mathbf{v}_1|\ldots|\mathbf{v}_m) \in \mathbb{R}^{m\times m} \text{ orthogonal}, \\ W &= (\mathbf{w}_1|\ldots|\mathbf{w}_n) \in \mathbb{R}^{n\times n} \text{ orthogonal}, \\ \Sigma &= \operatorname{diag}(\sigma_1, \ldots, \sigma_m) \in \mathbb{R}^{n\times m}. \end{aligned}$$

- The singular value decomposition (SVD) exists for any real matrix, even rectangular ones.

- The singular values σ_i are unique.

- The basis vectors are not unique.

- If A is orthogonally diagonalizable with eigenvalues λ_i (for instance, if A is symmetric), then $\sigma_i = |\lambda_i|$.

- $\|A\|_{\text{Frobenius}} = \sqrt{\sum_{ij} A_{ij}^2} = \sqrt{\text{tr}(A^t A)} = \sqrt{\sum_i \sigma_i^2}$.

- There exists a generalization to complex matrices. In this case, the matrix A can be decomposed as $W \Sigma V^\star$, where $V^\star$ is the complex conjugate of V^t and W and V are unitary matrices.

- The singular value decomposition can also be formulated in a basis-free manner as a result about linear maps between finite-dimensional Hilbert spaces.

Existence proof (sketch):

1. Consider the eigenvalue decomposition of the symmetric and positive-semidefinite matrix $A^t A$: We have an orthonormal basis $\mathbf{v}_i$ of eigenvectors corresponding to eigenvalues λ_i.

2. Set $\sigma_i := \sqrt{\lambda_i}$.

3. Set $\mathbf{w}_i := \frac{1}{\sigma_i} A\mathbf{v}_i$ (for those i with $\lambda_i \neq 0$).

4. Then $A\mathbf{v}_i = \sigma_i \mathbf{w}_i$ holds trivially.

5. The $\mathbf{w}_i$ are orthonormal: $(\mathbf{w}_i, \mathbf{w}_j) = \frac{1}{\sigma_i \sigma_j}(A^t A\mathbf{v}_i, \mathbf{v}_j) = \frac{\lambda_i \delta_{ij}}{\sigma_i \sigma_j}$.

6. If necessary, extend the $\mathbf{w}_i$ to an orthonormal basis.

This proof gives rise to an algorithm for calculating the SVD, but unless $A^t A$ is small, it has undesirable numerical properties. (But note that one can also use AA^t!) Since the 1960ies, there exists a stable iterative algorithm by Golub and van Loan.

The pseudoinverse of a matrix

Let $A \in \mathbb{R}^{n\times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the solutions to the optimization problem

$$\|A\mathbf{x} - \mathbf{b}\|_2 \longrightarrow \min$$

under $\mathbf{x} \in \mathbb{R}^m$ are given by

$$\mathbf{x} = A^+\mathbf{b} + V \begin{pmatrix} 0 \\ \star \end{pmatrix},$$

where $A = W\Sigma V^t$ is the SVD and

$$A^+ = W\Sigma^+ V^t,$$
$$\Sigma^+ = \operatorname{diag}(\sigma_1^{-1}, \dots, \sigma_m^{-1}).$$

- In the formula for Σ^+, set $0^{-1} := 0$.
- If A happens to be invertible, then $A^+ = A^{-1}$.
- The pseudoinverse can be used for polynomial approximation: Let data points $(x_i, y_i) \in \mathbb{R}^2$, $1 \leq i \leq N$, be given. Want to find a polynomial $p(z) = \sum_{k=0}^{n} \alpha_i z^i$, $n \ll N$, such that

$$\sum_{i=1}^{N} |p(x_i) - y_i|^2 \longrightarrow \min.$$

In matrix language, this problem is written

$$\|A\mathbf{u} - \mathbf{y}\|_2 \longrightarrow \min$$

where $\mathbf{u} = (\alpha_0, \ldots, \alpha_N)^T \in \mathbb{R}^{n+1}$ and

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^n \end{pmatrix} \in \mathbb{R}^{N \times (n+1)}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \in \mathbb{R}^N.$$

Low-rank approximation

Let $A = W\Sigma V^t \in \mathbb{R}^{n\times m}$ and $1 \leq r \leq n, m.$ Then a solution to the optimization problem

$$\|A - M\|_{\text{Frobenius}} \longrightarrow \min$$

under all matrices M with $\operatorname{rank} M \leq r$ is given by

$$\begin{aligned} M &= W\Sigma_r V^t, \\ \text{where} \quad \Sigma_r &= \operatorname{diag}(\sigma_1, \ldots, \sigma_r, 0, \ldots, 0). \end{aligned}$$

The approximation error is

$$\|A - W\Sigma_r V^t\|_{\mathrm{F}} = \sqrt{\sigma_{r+1}^2 + \cdots + \sigma_m^2}.$$

- This is the Eckart–Young(–Mirsky) theorem.
- Beware of false and incomplete proofs in the literature!

Image compression

- Think of images as matrices.
- Substitute a matrix $W\Sigma V^t$ by $W\Sigma_r V^t$ with r small.
- To reconstruct $W\Sigma_r V^t$, only need to know
  - the r singular values $\sigma_1, \dots, \sigma_r$, $\quad r$
  - the first r columns of W, and $\quad \text{height} \cdot r$
  - the top r rows of V^t. $\quad \text{width} \cdot r$
- Total amount:
  $r \cdot (1 + \text{height} + \text{weight}) \ll \text{height} \cdot \text{width}$

- See http://speicherleck.de/iblech/stuff/pca-images.pdf for sample compressions and http://pizzaseminar.speicherleck.de/skript4/08-principal-component-analysi svd-image.py for the Python code producing theses images.

- Image compression by singular value decomposition is mostly of academic interest only.

- This might be for the following reasons: other compression algorithms have more efficient implementations; other algorithms taylor to the specific properties of human vision; the basis vectors of other approaches (for instance, DCT) are similar to the most important singular basis vectors of a sufficiently large corpus of images.

- See http://dsp.stackexchange.com/questions/7859/relationship-between-dct-and-pca.

Proper orthogonal decomposition

Given data points $\mathbf{x}_i \in \mathbb{R}^N$, want to find a low-dimensional linear subspace which **approximately contains** the $\mathbf{x}_i$.

Minimize

$$J(U) := \sum_i \|\mathbf{x}_i - P_U(\mathbf{x}_i)\|^2$$

under all r-dimensional subspaces $U \subseteq \mathbb{R}^N$, $r \ll N$, where $P_U : \mathbb{R}^N \to \mathbb{R}^N$ is the orthogonal projection onto U.

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More concrete formulation: Minimize

$$J(\mathbf{u}_1, \dots, \mathbf{u}_r) := \sum_i \left\| \mathbf{x}_i - \sum_{j=1}^{r} \langle \mathbf{x}_i, \mathbf{u}_j \rangle \mathbf{u}_j \right\|^2,$$

where $\mathbf{u}_1, \dots, \mathbf{u}_r \in \mathbb{R}^N$, $\langle \mathbf{u}_j, \mathbf{u}_k \rangle = \delta_{jk}$.

- In the first formulation, the optimization domain is the *Grassmannian* of r-dimensional subspaces in $\mathbb{R}^N$. It is a compact topological space (in fact a manifold of dimension $r \cdot (N - r)$). Since $J(U)$ depends continuously on U, the optimization problem is guaranteed to have a solution.

- The solution is in general not unique, not even locally. For instance, consider the four data points $(\pm 1, \pm 1)$ in $\mathbb{R}^2$. Then any line U through the origin solves the optimization problem, with functional value $J(U) = 4$.

- In the more concrete formulation, we look for an orthonormal basis of a suitable subspace. In this case, the optimization domain is a compact subset of $\mathbb{R}^{N \times r}$.

- Since a given subspace possesses infinitely many orthonormal bases (at least for $r \geq 2$), solutions to this refined problem are never unique, not even locally.

- Note that this is a non-convex optimization problem. Therefore common numerical techniques do not apply.

Collect the data points $\mathbf{x}_i$ as columns of a matrix

$$X = (\mathbf{x}_1 | \cdots | \mathbf{x}_\ell) \in \mathbb{R}^{N \times \ell}$$

and consider its singular value decomposition

$$X = W \Sigma V^t.$$

Then a solution to the minimization problem is given by the first r columns of W, with approximation error

$$J = \sum_i \|\mathbf{x}_i\|^2 - \sum_{j=1}^{r} \sigma_j^2.$$

- Proper orthogonal decomposition (POD) cannot be used to find low-dimensional *submanifolds* which approximately contain given data points. But check out *kernel principal component analysis*.

- Also, POD does not work well with *affine* subspaces. But in this case, the fix is easy: Simply shift the data points so that their mean is zero.

- POD is a general method for *dimension reduction* and can be used as a kind of "preconditioner" for many other algorithms: Simply substitute the given points $\mathbf{x}_i$ by their projections $P_U(\mathbf{x}_i)$.

Principal component analysis

Given observations $x_i^{(k)}$ of random variables $X^{(k)}$, want to find **linearly uncorrelated** principal components.

Write $X = (\mathbf{x}_1 | \cdots | \mathbf{x}_\ell) \in \mathbb{R}^{N \times \ell}$. Calculate $X = W \Sigma V^t$. Then the principal components are the variables

$$Y^{(j)} = \sum_k W_{kj} X^{(k)}.$$

Most of the variance is captured by $Y^{(1)}$; second to most is captured by $Y^{(2)}$; and so on.

- For instance, in a study about circles, the variables *radius*, *diameter*, and *circumference* are linearly correlated.

- Principal component analysis (PCA) would automatically pick one of these attributes as a principal component.

- We have to normalize the data to have zero empirical mean first. Then XX^t is the empirical covariance matrix.

- Note that, in the given sample, the $Y^{(j)}$ are indeed uncorrelated:

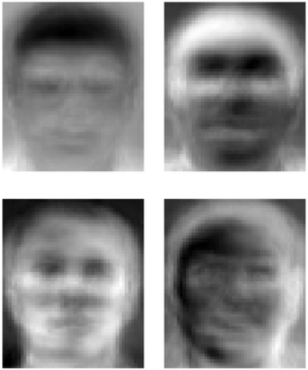
$$\begin{aligned} E(Y^{(j)}XX^tY^{(k)}) &= (W\mathbf{e}_j)^tXX^t(W\mathbf{e}_k) \\ &= \mathbf{e}_j^tW^tW\Sigma V^tV\Sigma^tW^tW\mathbf{e}_k \\ &= \mathbf{e}_j^t\Sigma\Sigma^t\mathbf{e}_k. \end{aligned}$$

- Beware that PCA cannot resolve nonlinear correlation.

- Also note that PCA is sensitive to outliers and is not scaling-independent.

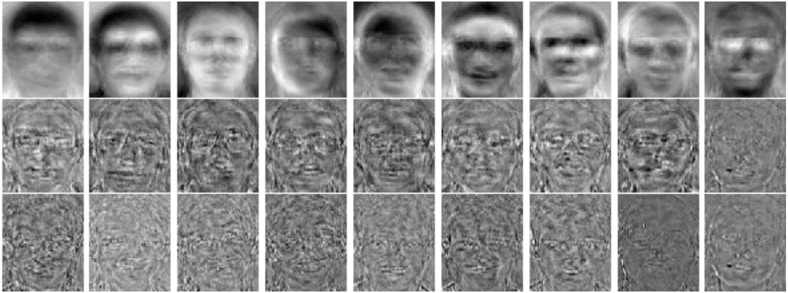
Eigenfaces

- Record sample faces $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^{\text{width}\cdot\text{height}}$.
- Calculate a POD basis of **eigenfaces**.
- Recognize faces by looking at the coefficients of the most important eigenfaces.



Eigenfaces resemble faces.

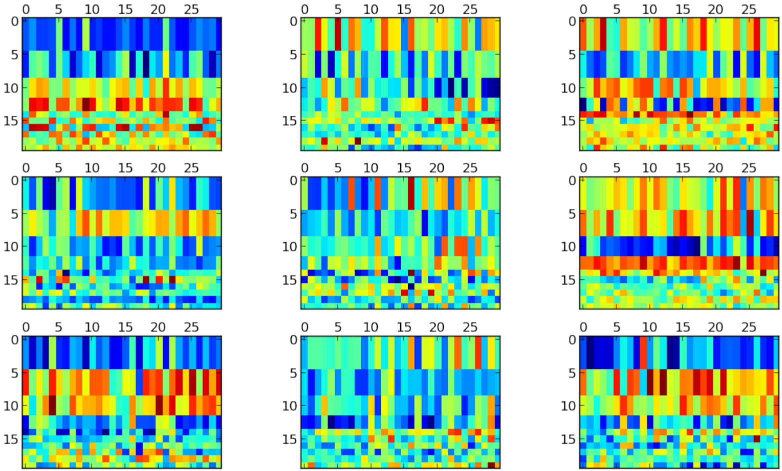
More eigenfaces



- A naive approach is very sensitive to lighting, scale and translation.
- But extensions are possible, for instance considering the eyes, the nose, and the mouth separately; this leads to eigeneyes, eigennoses, and eigenmouths.
- Image credit:
  http://upload.wikimedia.org/wikipedia/commons/6/67/Eigenfaces.png
  http://www.cenparmi.concordia.ca/~jdong/eigenface.gif
- Live demo:
  http://cognitrn.psych.indiana.edu/nsfgrant/FaceMachine/faceMachine.html
- Examples:
  http://www.cs.princeton.edu/~cdecoro/eigenfaces/

Digit recognition

Apply POD for dimension reduction, then use some similarity measure or clustering technique. Results:



- These images were produced by a Python program. The actual numerical code is very short (a few lines). Of course, the MNIST data set was used.

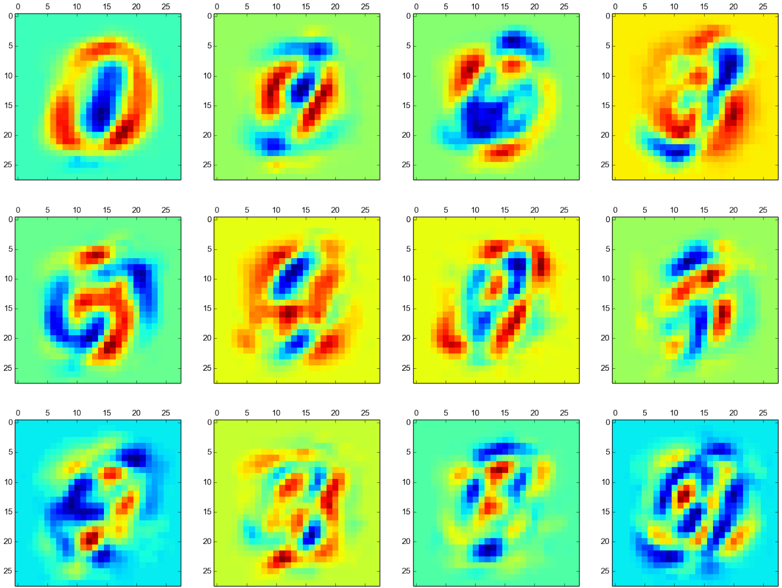
  `http://pizzaseminar.speicherleck.de/skript4/08-principal-component-analysis/digit-recognition.py`

- The nine images show the values of the first ten POD coefficients of the first 30 samples of the digits 1 to 9. Each column corresponds to a different sample. The first four POD coefficients are drawn using more vertical space, so that visual weight aligns with importance.

- One can clearly see that the POD coefficients differ for the different digits.

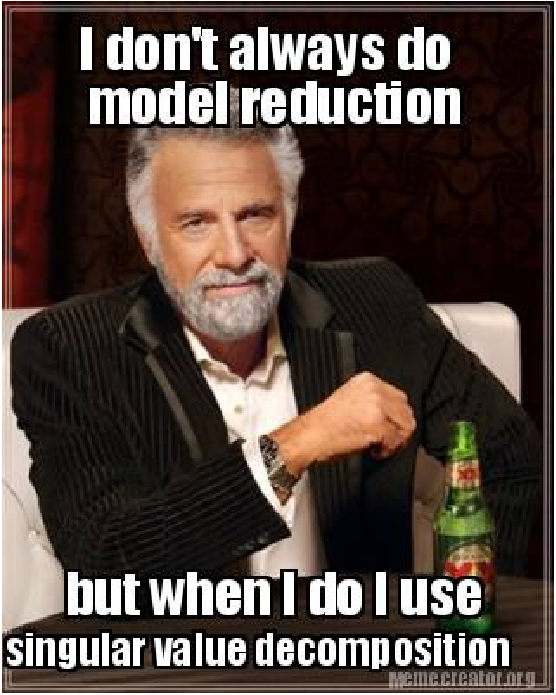
- Also, one can see that the difference is not so great for similar digits like 5 and 8 or 7 and 9.

Eigendigits



- These images show the first 12 POD basis vectors. The first basis vector is a kind of “prototypical digit”. The other basis vectors give subsequent “higher-order terms”.

- Because I didn’t implement a similarity measure or clustering technique, I couldn’t calculate the percentage of correctly classified digits. However, presumably the success rate would not be too high: Like the eigenfaces approach, this naive implementation is sensitive to the specific position of the digits in the bounding box. Refined techniques are discussed in the literature.


I don't always do model reduction
but when I do I use
singular value decomposition
memecreator.org