COMP3223 Foundations of ML: Dimensionality reduction

by

Principal Components Analysis (PCA)

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$$\sum_{n=1}^{N} (r^n)^2 \quad = \quad \sum (y^n - f(\boldsymbol{x}^n; \boldsymbol{w}))^2$$

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- This is the $p > N$ problem

Revision: linear regression

- Linear model: $y = Xw$, X design matrix, $\widehat{w} = \left(X^{\mathsf{T}}X\right)^{-1} X^{\mathsf{T}}y$; also w_0 is the difference between averages of inputs and outputs:

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- **Centering**: $\widetilde{y}^n = y^n - \langle y \rangle$, $\widetilde{x}_i^n = x_i^n - \langle x_i \rangle$ and drop the column of ones from design matrix to form $\widetilde{X}$ with matrix elements $\left(\widetilde{X}\right)_{nj} = x_j^n - \langle x_j \rangle$.

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- $\frac{1}{N}\tilde{X}^{\mathsf{T}}\left(\tilde{y} - \tilde{X}\widehat{w}\right) = 0$ implies $\widehat{w} = \left(\frac{1}{N}\left(\tilde{X}^{\mathsf{T}}\tilde{X}\right)\right)^{-1}\left(\frac{1}{N}\tilde{X}^{\mathsf{T}}y\right)$, so

$$\widehat{w} = [\mathrm{cov}(X)^{-1}][\mathrm{cov}(X, y)].$$

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- Work with p-dim matrix not N-dim.

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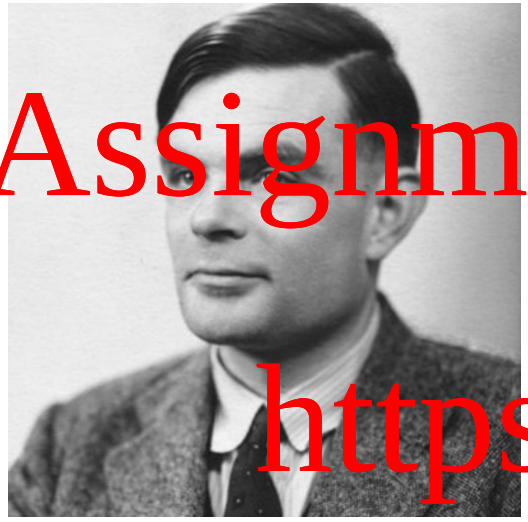

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Reconstruction for $r = 1, \ldots, 10$

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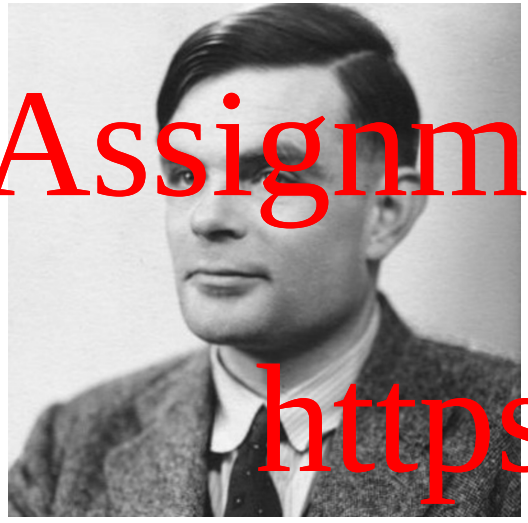

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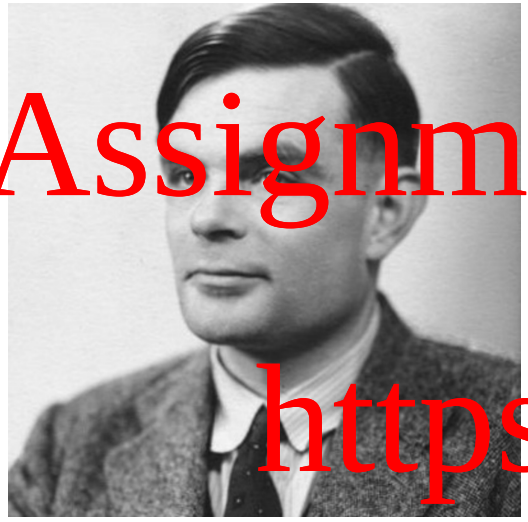

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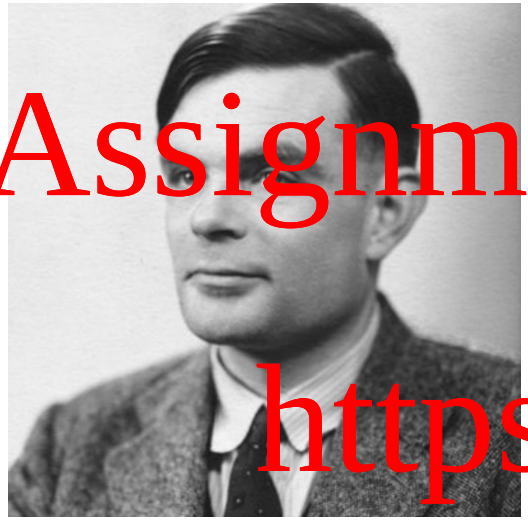

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- Variance of $\{z_1^n\}$ is λ_1.

PCA: principal components from variance decomposition

- Other eigenvectors w_k (from $Sw_k = \lambda_k w_k$) represent combinations that create $z_k^n = w_{k,1}x_1^n + w_{k,2}x_2^n + \cdots + w_{k,p}x_p^n$ decorrelated from z_1. $\text{cov}(z_i^n, z_j^n) = 0$ for $i \neq j$.

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Scale independence

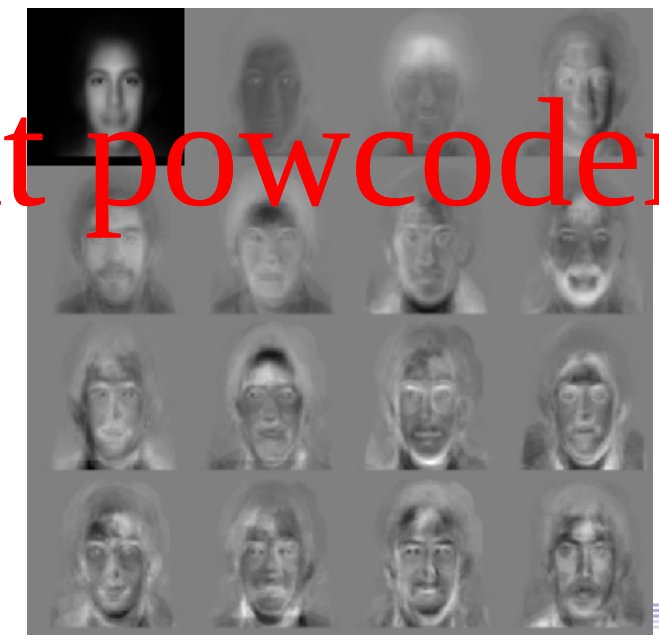
To make PCA independent of the *scale* of the data x^n, they might have to be first standardised such that all data entries x_k^n have equal range, eg by transforming them to unit variance.

Eigenfaces as features

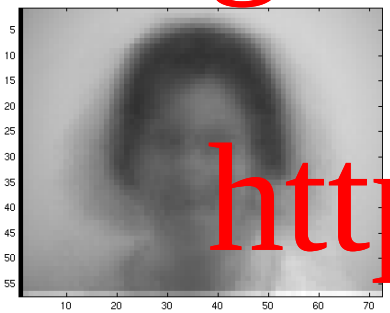
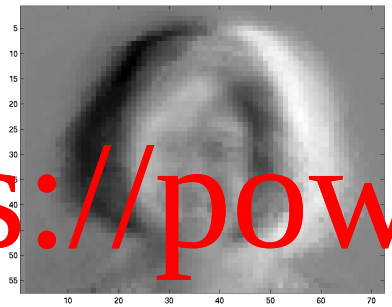
We will express arbitrary data vectors as linear combinations $v^n = \sum_{i=1}^{r} \alpha_i^n w_i$. of a set of eigenvectors $\{w_i\}$.

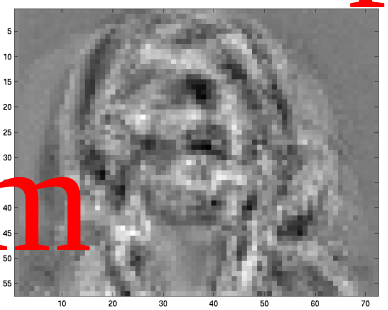
These are obtained from a certain data dependent matrix. Often most of the w_i are small (except for a small set of 'important' eigenvectors). In such a case we can represent a high dimensional data vector v^n effectively by a much smaller (and more robust) set of new 'coordinates' α_j^n

For a face recognition problem the vector v^n and the dominant **eigenfaces** may look like this:



Mean and eigenfaces



Mean face eigenface 1 eigenface 2 eigenface 30

Higher eigenfaces show only some random structure.

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- If $q < p$, dimensional reduction. Instead of basis vectors $e_k = (0, \cdots, 0, \underbrace{1}_{k}, 0, \ldots, 0)^T$, $k = 1, \ldots, p$, use v_i, $i = 1, \ldots, q$. The co-ordinates are α_i^n

Exercise

- Minimising with respect to $\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_{(1)}$ and $\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_{(2)}$,

$$\left\| \begin{pmatrix} x_1^{(n)} \\ x_2^{(n)} \end{pmatrix} - \begin{pmatrix} v_{1;1} & v_{2;1} \\ v_{1;2} & v_{2;2} \end{pmatrix} \begin{pmatrix} \alpha_1^{(n)} \\ \alpha_2^{(n)} \end{pmatrix} \right\|^2$$

(in $v_{j;i}$, j the label for the vector, i the row index),

$$\begin{pmatrix} \alpha_1^{(n)} \\ \alpha_2^{(n)} \end{pmatrix} = \begin{pmatrix} v_{1;1} & v_{2;1} \\ v_{1;2} & v_{2;2} \end{pmatrix}^{-1} \begin{pmatrix} x_1^{(n)} \\ x_2^{(n)} \end{pmatrix}.$$

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- Extend to q-dimensional representation of $x^n \in \mathbb{R}^p$,

$$\begin{pmatrix} \alpha_1^{(n)} \\ \vdots \\ \alpha_q^{(n)} \end{pmatrix} = \underbrace{\begin{pmatrix} v_{1;1} & v_{2;1} & \cdots & v_{q;1} \\ \vdots & \vdots & \ddots & \vdots \\ v_{1;p} & v_{2;p} & \cdots & v_{q;p} \end{pmatrix}^T}_{\text{columns of matrix } V_q \text{ are orthogonal vectors}} \begin{pmatrix} x_1^{(n)} \\ \vdots \\ x_p^{(n)} \end{pmatrix}.$$

PCA: Low rank projection

- q-dimensional representation of $x^n \in \mathbb{R}^p$, with orthonormal vectors as columns of V_q:

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- $\|X - V_q V_q^T X\|^2$ is the minimum residual.

Compare PCA pre-processed regression with regularisation

- Regularisation using the 2-norm of $\boldsymbol{w}$ involves minimising the loss function $\ell(\boldsymbol{w})$

$$
\begin{aligned}
\widehat{\boldsymbol{w}}_{\text{ridge}} &= \operatorname{argmin}_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|^2 + \lambda\|\boldsymbol{w}\|^2 \\
\implies \widehat{\boldsymbol{w}}_{\text{ridge}} &= (\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X} + \lambda\mathbb{I})^{-1}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{y} \\
&= \boldsymbol{V}(\boldsymbol{S}^2 + \lambda\mathbb{I})^{-1}\boldsymbol{S}\boldsymbol{U}^{\mathsf{T}}\boldsymbol{y} \\
&= \sum_{k=1}^{\min(p,N)} (\boldsymbol{u}_k^{\mathsf{T}}\boldsymbol{y})\,\frac{\sigma_k}{\sigma_k^2 + \lambda}\boldsymbol{v}_k
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- **Sparse PCA**: $A_{p\times q} := (\alpha_1, \ldots, \alpha_q)$, $B_{p\times q} := (\beta_1, \ldots, \beta_q)$, $A^T A = \mathbb{I}_q$, so that $AA^T = P_q$ a q-dim projector:

$$\begin{aligned} \widehat{\beta} &= \text{argmin}_{A,B} \sum_{i=1}^{N} \|x_i - AB^T x_i\|^2 + \lambda_2 \|\beta\|^2 + \lambda_1 \|\beta\|_1 \\ v_i &= \widehat{\beta}_i / \|\widehat{\beta}\| \end{aligned}$$

v_i sparse PCA components

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  - **Lasso**: $\widehat{w}_{\text{lasso}} = \text{argmin}_w \|y - Xw\|^2$ s.t. $\lambda \sum_i |w_i| \leq 1$.
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- Implement PCA via neural network with linear activation function. If non-linear, we arrive at an **autoencoder**, trained via backprop.