6.867 Machine Learning Fall 2017

Lecture 20. Principle Component Analysis

http://stellar.mit.edu/S/course/6/fa17/6.867/

Announcements

- Quiz 2
  - Thursday, November 30 7pm-9pm
  - Make up:
    - Tuesday, November 28, 4pm-6pm
  - Syllabus:
    - Till and including Lecture on November 16, 2017
  - Quiz Review:
    - Monday, November 27/Wednesday, November 29 TA OH
    - It will be posted online with solutions before Thanks Giving Break
    - It will cover concepts relevant for exam questions

Where Are We?

Date	Topic
9/7	Introduction, Overview, Basics
9/12	Regression: Risk Min., Max likelihood
9/14	Linear Regression: Shrinkage, Bias-Variance
9/19	Linear Regression: Bayesian
9/21	Classification: Discrim analysis; perceptron
9/26	Classification: Logistic reg
9/28	Classification: Support vector machines
10/3	Kernels
10/5	K-Nearest neighbors, VC-dimension
10/10	*Holiday*
10/12	Neural nets: basics, back-propagation
10/17	Neural nets: regularization, CNNs, auto-encoders
10/19	**Exam 1 7:30 - 9:30 PM**
10/24	Neural nets: recursive neural networks, LSTM
10/26	Neural nets: RNN sequence models, attention
10/31	Tree-models, Bagging, Random Forest
11/2	Bayesian networks: Learning and Inference
11/7	Mixture models: EM, K-means
11/9	Topic models
11/14	Deep generative models
11/16	Sampling method: Why, MCMC, Gibbs
11/21	Matrix data: principal component analysis
11/23	*Holiday*
11/28	Matrix data: recommendation systems
11/30	**Exam 2 7:30 - 9:30**
12/5	Matrix data: non-neg factor, PMI/Word2Vec
12/7	Reinforcement Learning – Part I
12/12	Reinforcement Learning – Part II

Regression

Classification

Non-linear methods

Supervised

Distribution Repr.

Mixtures, EM

Latent Variable Models

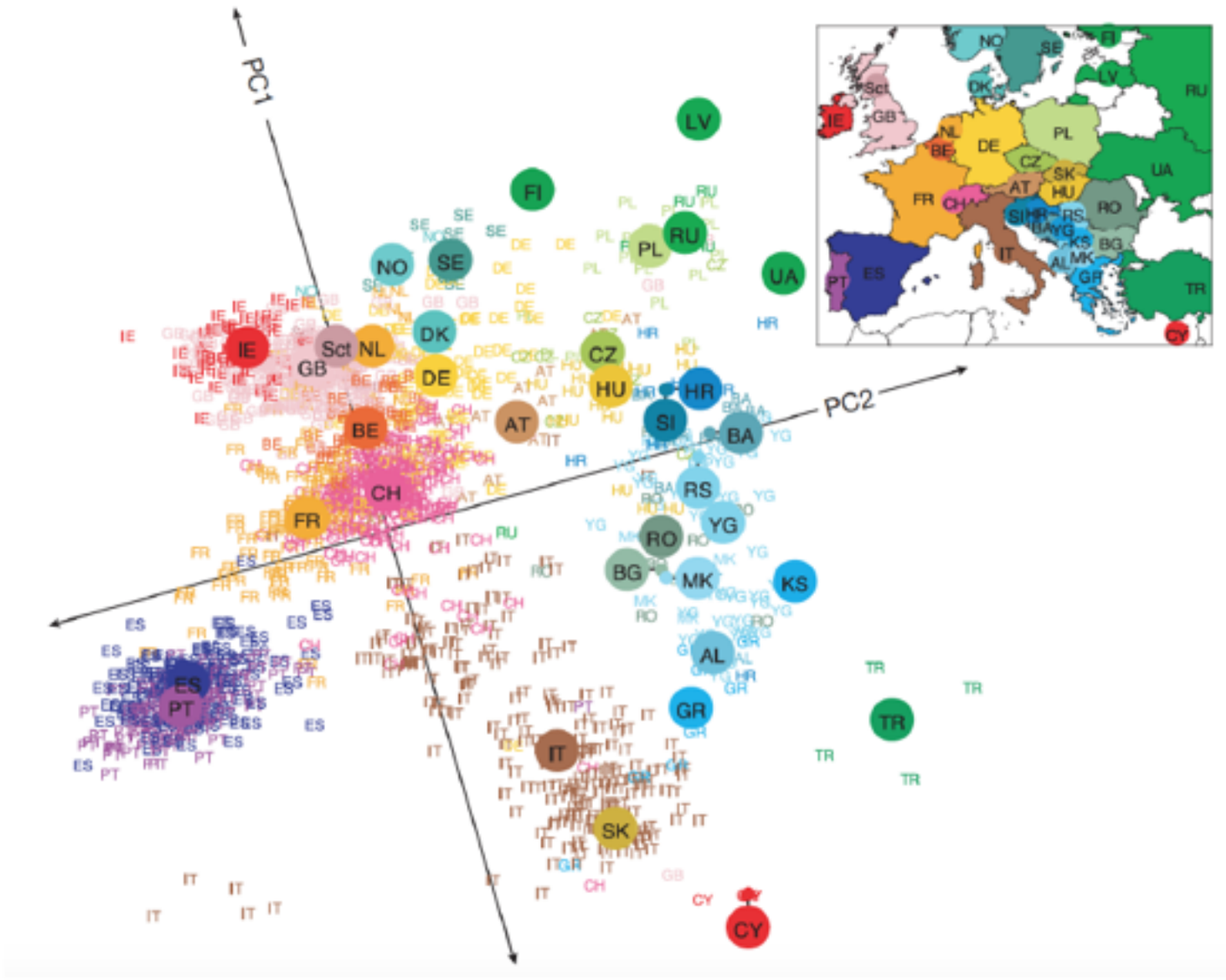
Sampling

Matrix data

Unsupervised

Re-inforcement learning

Example of Principle Component Analysis (PCA)



Genes Mirror Geography Within Europe, Novembre et al (2008)

Outline

- PCA (a la (*Kosambi-)Karhunen-Loeve* transformation)
    - Formulation
    - Applications
    - Implementation

- Probabilistic PCA
    - Maximum Likelihood
    - EM algorithm

- Non-linear PCA
    - Kernel PCA

What is PCA

- Answer 1: Maximizing variance
    - Project data into lower dimensional subspace
    - So that variance of projected data is maximized
- Answer 2: Minimizing error (or movement)
    - Project data into lower dimensional subspace
    - So that the square distance "movement" of data is minimized
- Both lead to the *same* algorithm

PCA via Maximizing Variance

- Setup
  - Data: $x_1, \ldots, x_N$ with $x_n \in \mathbb{R}^d$
  - Goal: project each x_n into $\mathbb{R}^m, \quad m \ll d$

- Example: linear projection with $m = 1$
  - Let $\mathbf{u}_1 \in \mathbb{R}^d$ such that $\mathbf{u}_1^T \mathbf{u}_1 = 1$
  - Projection: $x_n \to \mathbf{u}_1^T x_n, \quad n \in [N]$
  - Mean of projected data: $\mathbf{u}_1^T \bar{x}$ where $\bar{x} = \frac{1}{N}(\sum_n x_n)$
  - Variance of projected data:

$$\frac{1}{N} \sum_n \left(\mathbf{u}_1^T x_n - \mathbf{u}_1^T \bar{x} \right)^2$$

PCA via Maximizing Variance

- Re-writing variance

$$\frac{1}{N}\sum_n \left(\mathbf{u}_1^T x_n - \mathbf{u}_1^T \bar{x}\right)^2$$

$$= \frac{1}{N}\sum \left(\mathbf{u}_1^T (x_n - \bar{x})(x_n - \bar{x})^T \mathbf{u}_1\right)$$

$$= \mathbf{u}_1^T \left[\frac{1}{N}\sum_n (x_n - \bar{x})(x_n - \bar{x})^T\right] \mathbf{u}_1$$

$$= \mathbf{u}_1^T S \mathbf{u}_1, \quad S = \left[\frac{1}{N}\sum_n (x_n - \bar{x})(x_n - \bar{x})^T\right]$$

- Goal: find $\mathbf{u}_1 \in \mathbb{R}^d,\ \mathbf{u}_1^T \mathbf{u}_1 = 1$
  - so as to minimize $\mathbf{u}_1^T S \mathbf{u}_1$

PCA via Maximizing Variance

- Goal:

$$\begin{aligned} \text{minimize} \quad & \mathbf{u}_1^T S \mathbf{u}_1 \\ \text{such that} \quad & \mathbf{u}_1^T \mathbf{u}_1 = 1, \ \mathbf{u}_1 \in \mathbb{R}^d \end{aligned}$$

- Lagrangian:

$$L(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T S \mathbf{u}_1 - \lambda_1 (\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

$$\nabla_{\mathbf{u}_1} L(\mathbf{u}_1, \lambda_1) = 2S\mathbf{u}_1 - 2\lambda_1 \mathbf{u}_1$$

- Zero-gradient point satisfies

$$S\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$$

$$\mathbf{u}_1^T S \mathbf{u}_1 = \lambda_1 \mathbf{u}_1^T \mathbf{u}_1 = \lambda_1$$

PCA via Maximizing Variance

- That is, find $\mathbf{u}_1$
  - Eigenvector: $S\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$
  - With maximal eigenvalue: $\mathbf{u}_1^T S \mathbf{u}_1 = \lambda_1 \mathbf{u}_1^T \mathbf{u}_1 = \lambda_1$
  - Projection: $x_n \rightarrow \mathbf{u}_1^T x_n, \quad n \in [N]$

- PCA over $\mathbb{R}^m, \quad m < d$
  - Compute covariance matrix $S = \left[\frac{1}{N} \sum_n (x_n - \bar{x})(x_n - \bar{x})^T \right]$
  - Compute top m eigenvectors: $\mathbf{u}_1, \ldots, \mathbf{u}_m$
  - Projection: $x_n \rightarrow (\mathbf{u}_1^T x_n, , \ldots, \mathbf{u}_m^T x_n) \quad n \in [N]$

PCA via Minimizing Projection Error

- Another view of PCA
  - Project data into lower dimensional
  - So that the square distance "movement" of data is minimized

- Orthonormal basis of $\mathbb{R}^d$: $\mathbf{u}_1, \ldots, \mathbf{u}_d$
  - (affine) projection on $\mathbb{R}^m$, $m < d$:

$$x_n \to \tilde{x}_n = \sum_{i=1}^{m} z_{in}\mathbf{u}_i + \sum_{i=m+1}^{d} b_i \mathbf{u}_i$$

  - Goal: minimize

$$J = \frac{1}{N}\sum_n (x_n - \tilde{x}_n)^T (x_n - \tilde{x}_n)$$

PCA via Minimizing Projection Error

- Since $\mathbf{u}_1, \ldots, \mathbf{u}_d$ is orthonormal basis of $\mathbb{R}^d$

$$x_n = \sum_{i=1}^{d} \alpha_{in} \mathbf{u}_i, \quad \alpha_{in} = \mathbf{u}_i^T x_n$$

- Re-writing

$$J = \frac{1}{N} \Big(\sum_{i=1}^{m} \sum_{n} (\alpha_{in} - z_{in})^2 \Big) + \frac{1}{N} \Big(\sum_{i=m+1}^{d} \sum_{n} (\alpha_{in} - b_i)^2 \Big)$$

- To minimize J, we set

$$z_{in} = \alpha_{in}, \quad i \leq m$$

$$b_i = \frac{1}{N} \sum_{n} \alpha_{in} = \mathbf{u}_i^T \Big(\frac{1}{N} \sum_{n} x_n \Big) = \mathbf{u}_i^T \bar{x}, \quad m < i \leq d$$

PCA via Minimizing Projection Error

- In summary, given orthonormal basis of $\mathbb{R}^d$: $\mathbf{u}_1, \ldots, \mathbf{u}_d$

$$x_n = \sum_{i=1}^{d} \alpha_{in} \mathbf{u}_i, \quad \alpha_{in} = \mathbf{u}_i^T x_n$$

- The minimal projection error w.r.t. subspace formed by $\mathbf{u}_1, \ldots, \mathbf{u}_m$

$$J = \sum_{i=m+1}^{d} (\mathbf{u}_i^T \bar{x} - \mathbf{u}_i^T x_n)^2$$

$$= \sum_{i=m+1}^{d} \mathbf{u}_i^T S \mathbf{u}_i$$

- That is, to minimize J, we need to find $\mathbf{u}_1, \ldots, \mathbf{u}_d$
  - so that the last $(d - m)$ basis vector have minimal quadratic terms

PCA via Minimizing Projection Error

- In summary, given orthonormal basis of $\mathbb{R}^d$: $\mathbf{u}_1, \ldots, \mathbf{u}_d$

$$x_n = \sum_{i=1}^{d} \alpha_{in} \mathbf{u}_i, \quad \alpha_{in} = \mathbf{u}_i^T x_n$$

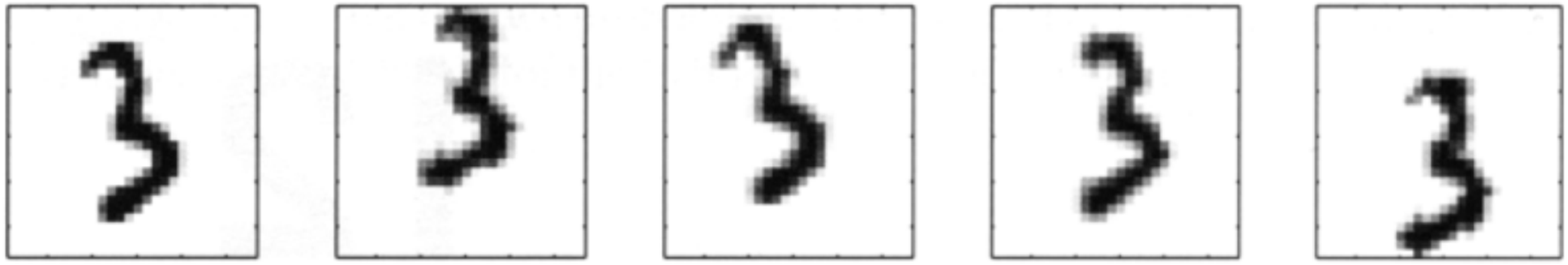
- The minimal projection error w.r.t. subspace formed by $\mathbf{u}_1, \ldots, \mathbf{u}_m$
  - minimizes $\sum_{i=m+1}^{d} \mathbf{u}_i^T S \mathbf{u}_i$

- These turn out to selecting $\mathbf{u}_1, \ldots, \mathbf{u}_d$
  - as eigenvectors of S
  - in decreasing order of eigenvalues!

Applications of PCA

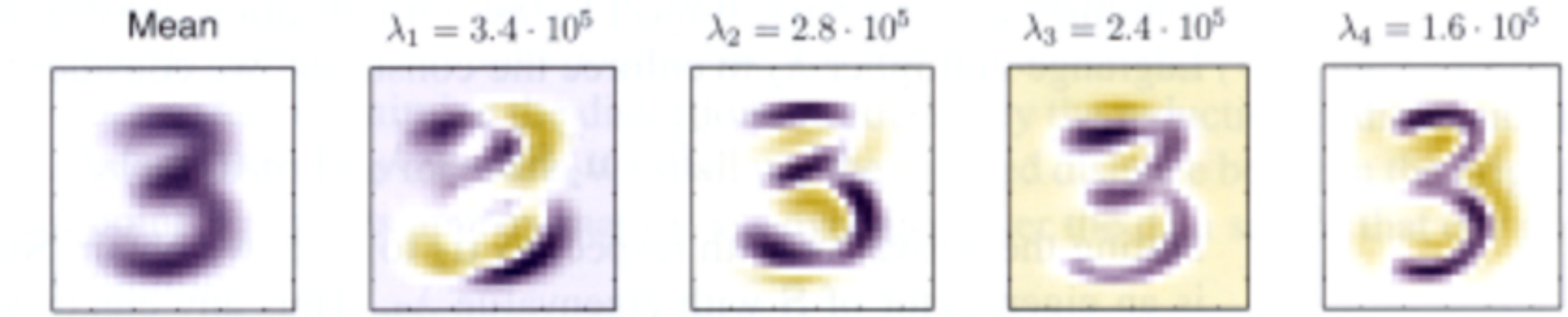
- Visualization, data compression, data pre-processing, …

- A Data Compression Example (Bishop, Chapter 12):



A synthetic data set obtained by taking one of the off-line digit images and creating multiple copies in each of which the digit has undergone a random displacement and rotation within some larger image field. The resulting images each have $100 \times 100 = 10,000$ pixels.

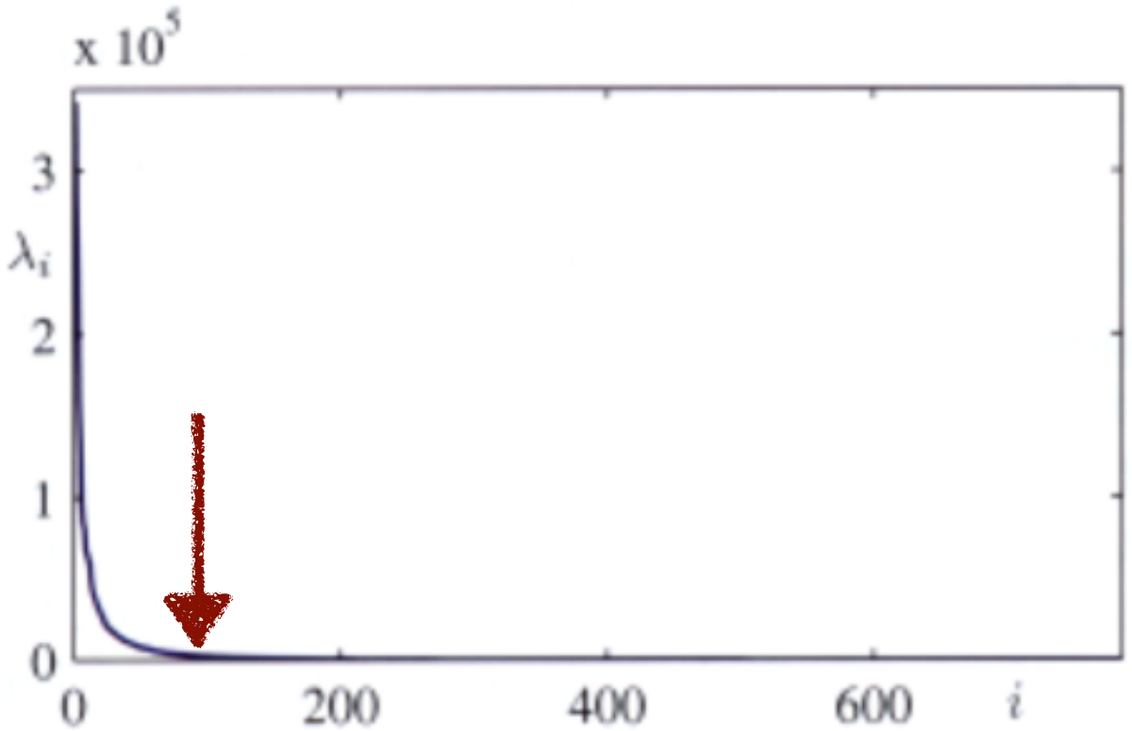
Applications of PCA



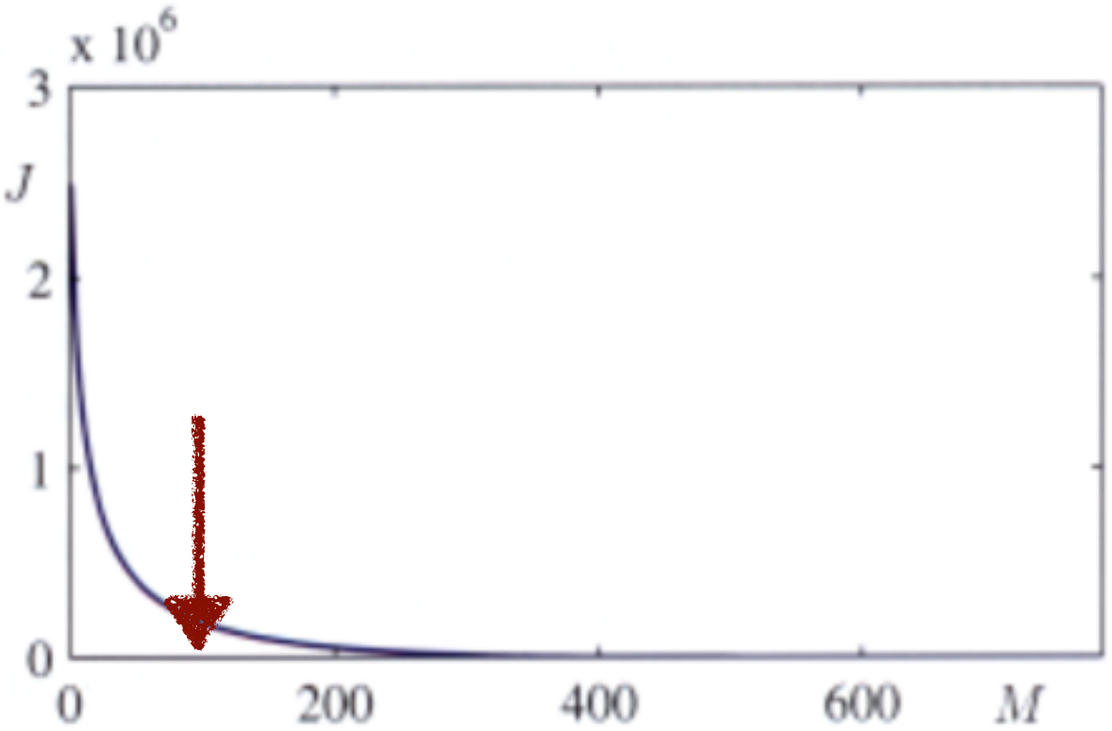
The mean vector $\overline{\mathbf{x}}$ along with the first four PCA eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_4$ for the off-line digits data set, together with the corresponding eigenvalues.

Applications of PCA

compressed fraction = 100/10000 = 1%



eigenvalues of correlation matrix



projection error vs projection dim

Applications of PCA

- Principle Component Regression (PCR)
- Recall setting of Regression
    - Given observed features $\mathbf{x} \in \mathbb{R}^d$ predict target $\mathbf{y} \in \mathbb{R}$
    - Training data $(x_n, y_n),\ 1 \leq n \leq N$

- PCR (at high level)
    - Perform PCA for data matrix of features

$$X^T X \in \mathbb{R}^{d \times d},\ X = \left[x_n^T\right]$$

    - Using Ordinary Least Squares, learn model on "projected" features
    - "lift" model back to original space

Applications of PCA

- Principle Component Regression (PCR)
  - Spectral decomposition of data matrix $X^T X = V \Lambda V^T$
  - Projected data $W_m = XV_m$
    $= [X\mathbf{v}_1, \ldots, X\mathbf{v}_m]$
  - PCR model estimate
    $$\hat{\beta}_m = (W_m^T W_m)^{-1} W_m^T \mathbf{y}$$
  - Final model estimate
    $$\hat{\beta} = V_m \hat{\beta}_m$$

- Benefits of PCR
  - Variance reduction, Addressing Multi-collinearity, Dimensionality Reduction, Induced Regularization, Efficiency.

PCA: Implementation

- PCA: usually N < d
  - Compute d x d correlation matrix: N x d x d
  - Computing *top* m eigenvectors: md^2
- A useful implementation trick
  - Compute N x d matrix: $X = \begin{bmatrix} (x_1 - \bar{x})^T \\ \dots \\ (x_N - \bar{x})^T \end{bmatrix}$
  - Then $S = \frac{1}{N} X^T X$
  - Therefore

$$\frac{1}{N} X^T X \mathbf{u}_i = \lambda_i \mathbf{u}_i$$

PCA: Implementation

- Continuing:

$$\frac{1}{N}X^T X\mathbf{u}_i = \lambda_i \mathbf{u}_i \;\Rightarrow\; \frac{1}{N}XX^T(X\mathbf{u}_i) = \lambda_i(X\mathbf{u}_i)$$

- That is:

$$\frac{1}{N}XX^T\mathbf{v}_i = \lambda_i \mathbf{v}_i$$

- And again

$$\frac{1}{N}X^T X(X^T\mathbf{v}_i) = \lambda_i(X^T\mathbf{v}_i)$$

- In summary, PCA with N < d:
  - Compute eigenvectors $\mathbf{v}_i,\ i \leq N$ of $Q = \frac{1}{N}XX^T$ in $O(N^3)$
  - Obtain eigenvectors $\mathbf{u}_i,\ i \leq N$ of S as

$$\mathbf{u}_i \propto X^T\mathbf{v}_i$$

PCA: Implementation

- In summary:
  - Let N x d data matrix: $X = \begin{bmatrix} (x_1 - \bar{x})^T \\ \dots \\ (x_N - \bar{x})^T \end{bmatrix}$
  - Compute eigenvectors $\mathbf{v}_i,\ i \leq N$ of $Q = \frac{1}{N} X X^T$
  - The m dimensional projection of N points is given by N x m matrix:

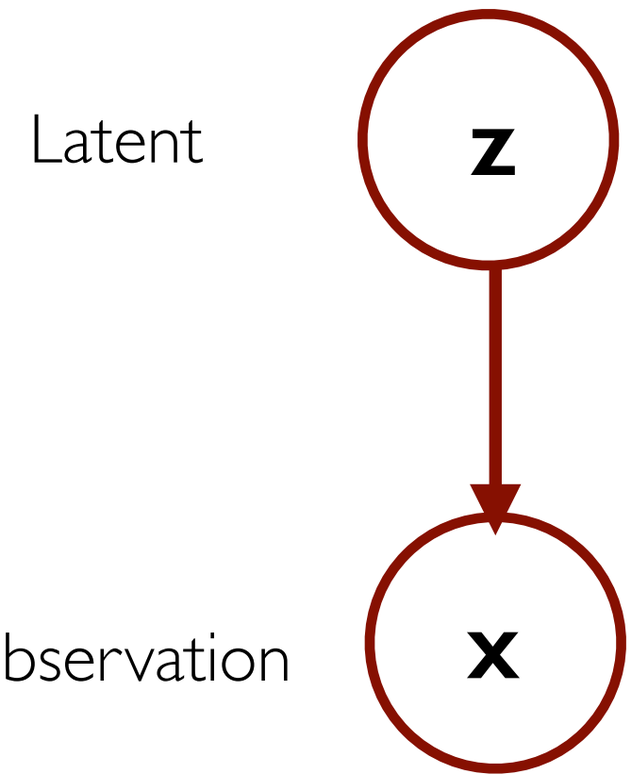
$$\left[c_1 \mathbf{v_1} \cdots c_m \mathbf{v_m} \right]$$

- Because

$$\begin{aligned} X \mathbf{u}_i &\propto X X^T \mathbf{v}_i \\ &\propto Q \mathbf{v}_i \\ &\propto \lambda_i \mathbf{v}_i \end{aligned}$$

Probabilistic PCA

- Probabilistic latent variable model:



$$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \in \mathbb{R}^m$$

$$\mathbf{x}|\mathbf{z} \sim \mathcal{N}(\mathbf{W}\mathbf{z} + \mu, \sigma^2\mathbf{I}) \in \mathbb{R}^d$$

$$\mathbf{W} \in \mathbb{R}^{d \times m}$$

- Equivalently:

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \mu + \varepsilon, \quad \varepsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I}) \in \mathbb{R}^d$$

Probabilistic PCA

- Probabilistic latent variable model:

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \mu + \varepsilon, \quad \varepsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I}) \in \mathbb{R}^d$$

- Hence

$$\mathbf{x} \sim \mathcal{N}(\mu_\mathbf{x}, \Sigma_\mathbf{x}) \in \mathbb{R}^d$$

$$\begin{aligned}\mu_\mathbf{x} &= \mathbb{E}[\mathbf{x}] \\ &= \mathbf{W}\mathbb{E}[\mathbf{z}] + \mu \\ &= \mu\end{aligned}$$

$$\begin{aligned}\mathbf{\Sigma_x} &= \mathbb{E}[\mathbf{x}\mathbf{x}^T] - \mu\mu^T \\ &= \mathbf{W}\mathbb{E}[\mathbf{z}\mathbf{z}^T]\mathbf{W} + \mathbb{E}[\varepsilon\varepsilon^T] \\ &= \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I} \\ &\equiv \mathbf{C} \in \mathbb{R}^{d\times d}\end{aligned}$$

Probabilistic PCA

- Probabilistic latent variable model:

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \mu + \varepsilon, \quad \varepsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I}) \in \mathbb{R}^d$$

- Conversely

$$\mathbf{z}|\mathbf{x} \sim \mathcal{N}(\mu_{\mathbf{z}|\mathbf{x}}, \mathbf{\Sigma}_{\mathbf{z}|\mathbf{x}})$$

$$\mu_{\mathbf{z}|\mathbf{x}} = \mathbf{M}^{-1}\mathbf{W}^T(\mathbf{x} - \mu) \qquad \Sigma_{\mathbf{z}|\mathbf{x}} = \sigma^2\mathbf{M}^{-1}$$

where $\mathbf{M} = \mathbf{W}^T\mathbf{W} + \sigma^2\mathbf{I} \in \mathbb{R}^{m \times m}$

Probabilistic PCA

- Maximum Likelihood Estimator
  - data: $x_1, \ldots, x_N$
  - (model) parameters: $\mu, \mathbf{W}, \sigma^2$
  - log-likelihood: recall $\mathbf{C} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I} \in \mathbb{R}^{d\times d}$

$$
\begin{aligned}
-\log \mathbb{P}\left(x_1, \ldots, x_N | \mu, \mathbf{W}, \sigma^2\right) &\propto \frac{1}{2}\sum_{n=1}^{N}(x_n-\mu)^T\mathbf{C}^{-1}(x_n-\mu) \\
&\quad + \frac{N}{2}\log|\mathbf{C}| \\
&\equiv F(\mu, \mathbf{C})
\end{aligned}
$$

- Goal: find $\mu, \mathbf{C}$ that minimizes $F(\mu, \mathbf{C})$

Probabilistic PCA

- Setting partial derivative with respect to μ to 0 leads to

$$\mu = \bar{x} = \frac{1}{N}\sum_{n} x_n$$

- Therefore, we wish to find $\mathbf{C}$ to minimize $F(\bar{x}, \mathbf{C})$

$$F(\bar{x}, \mathbf{C}) = \frac{N}{2}\Big(\log|C| + \mathrm{Tr}\big(\mathbf{C}^{-1}\mathbf{S}\big)\Big)$$

- Recall

$$S = \frac{1}{N}X^T X \quad \text{where} \quad X = \begin{bmatrix} (x_1 - \bar{x})^T \\ \dots \\ (x_N - \bar{x})^T \end{bmatrix}$$

$$\mathbf{C} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I} \in \mathbb{R}^{d\times d}$$

Probabilistic PCA

- Minimizing choice of $\mathbf{C}$ or equivalently $\mathbf{W}, \sigma^2$ are such that

$$\mathbf{W}_{\mathrm{ML}} = \mathbf{U}_{\mathrm{ML}} \left(\mathbf{L}_{\mathrm{ML}} - \sigma^2 \mathbf{I} \right)^{\frac{1}{2}} \mathbf{R}$$

  - $\mathbf{U}_{\mathrm{ML}}$ is d x m matrix with top m eigenvectors of $\mathbf{S}$ as columns
  - $\mathbf{L}_{\mathrm{ML}}$ is m x m diagonal matrix with corresponding eigenvalues
  - $\mathbf{R}$ being any m x m orthonormal matrix

- Notice that as $\sigma \to 0$ and $\mathbf{R} = \mathbf{I}$

$$\mathbf{W}_{\mathrm{ML}} \to \mathbf{U}_{\mathrm{ML}} \mathbf{L}_{\mathrm{ML}}^{\frac{1}{2}}$$

Probabilistic PCA

- The corresponding mean latent variable for a given data $\mathbf{x}$

$$\begin{aligned}\mathbb{E}[\mathbf{z}|\mathbf{x}] &= \mathbf{M}^{-1}\mathbf{W}^T(\mathbf{x}-\mu) \\ &= \left(\mathbf{W}_{\mathrm{ML}}^T\mathbf{W}_{\mathrm{ML}}\right)^{-1}\mathbf{W}_{\mathrm{ML}}^T\left(\mathbf{x}-\bar{\mathbf{x}}\right)\end{aligned}$$

- That is, projection of $\mathbf{x}-\bar{\mathbf{x}}$ on space spanned by columns of $\mathbf{W}_{\mathrm{ML}}$
- And, as $\sigma \to 0$, the columns of $\mathbf{W}_{\mathrm{ML}}$ are top e.v. of $\mathbf{S}$
- That is, we recover the PCA algorithm:
    - Identify top m eigenvectors of $\mathbf{S}$
    - Project data points on space spanned by these m eigenvectors

Probabilistic PCA: via EM

- Starting point of EM is maximum likelihood:

$$\text{maximize } \mathbb{E}_{\mathbf{z}}\Big[\log \mathbb{P}\big(x_1,\ldots,x_n;z_1,\ldots,z_n|\mathbf{W},\mu,\sigma^2\big)\Big]$$
$$\text{over } \mu,\mathbf{W},\sigma^2$$

  - The log likelihood can be written as

$$-\mathbb{E}_{\mathbf{z}}\Big[\log \mathbb{P}\big(x_1,\ldots,x_n;z_1,\ldots,z_n\big)\Big] = -\sum_{n=1}^{N}\mathbb{E}_{\mathbf{z}}\Big[\log \mathbb{P}(x_n|z_n)+\log \mathbb{P}(z_n)\Big]$$
$$\propto \sum_{n=1}^{N}\frac{d}{2}\log(2\pi\sigma^2)+\frac{1}{2}\mathrm{Tr}\big(\mathbb{E}_{\mathbf{z}}\big[z_n z_n^T\big]\big)+\frac{1}{2\sigma^2}\|x_n-\mu\|^2$$
$$-\frac{1}{\sigma^2}\mathbb{E}_{\mathbf{z}}\big[z_n^T\big]\mathbf{W}^T(x_n-\mu)+\frac{1}{2\sigma^2}\mathrm{Tr}\big(\mathbb{E}_{\mathbf{z}}\big[z_n z_n^T\big]\mathbf{W}^T\mathbf{W}\big)$$

Probabilistic PCA

- EM suggests iterative way to solve this:
    - E-step: assume parameters fixed
        - evaluate conditional distribution of $\mathbf{Z}$ given the parameters
    - M-step: maximize overall log-likelihood over choice of parameters
        - using the conditional distribution of $\mathbf{Z}$ evaluated in E-step
    - Iterate the above E and M steps

- Let's see these in our context next

Probabilistic PCA

- E-step

$$\mathbb{E}[z_n] = \mathbf{M}^{-1}\mathbf{W}^T(x_n - \bar{x})$$

$$\mathbb{E}[z_n z_n^T] = \mathrm{Cov}[z_n] + \mathbb{E}[z_n]\mathbb{E}[z_n]^T$$

$$= \sigma^2\mathbf{M}^{-1} + \mathbf{M}^{-1}\mathbf{W}^T(x_n - \bar{x})(x_n - \bar{x})^T\mathbf{W}\mathbf{M}^{-1}$$

- M-step

$$\mathbf{W}_{\mathrm{new}} = \left[\sum_{n=1}^{N}(x_n - \bar{x})\mathbb{E}[z_n]^T\right]\left[\sum_{n=1}^{N}\mathbb{E}[z_n z_n^T]\right]^{-1}$$

$$\sigma^2_{\mathrm{new}} = \frac{1}{Nd}\sum_{n=1}^{N}\left\{\|x_n - \bar{x}\|^2 - 2\mathbb{E}[z_n]^T\mathbf{W}_{\mathrm{new}}^T(x_n - \bar{x})\right.$$

$$\left. + \mathrm{Tr}\left(\mathbb{E}[z_n z_n^T]\mathbf{W}_{\mathrm{new}}^T\mathbf{W}_{\mathrm{new}}\right)\right\}$$

Probabilistic PCA

- Assuming normalized data ($\bar{x} = \mathbf{0}$), PCA is utilizes matrix

$$S = \frac{1}{N} \sum_n x_n x_n^T$$

- Consider non-linear transformation: $\mathbf{x} \rightarrow \phi(\mathbf{x})$

$$S' = \frac{1}{N} \sum_n \phi(x_n)\phi(x_n)^T$$

- And let top m eigenvectors of S' be

$$S'\mathbf{v}_i = \lambda_i \mathbf{v}_i, \ i \in [m]$$

Probabilistic PCA

- That is

$$\frac{1}{N}\sum_n \phi(x_n)\left(\phi(x_n)^T \mathbf{v}_i\right) = \lambda_i \mathbf{v}_i$$

- Equivalently

$$\mathbf{v}_i = \sum_n a_{in}\phi(x_n)$$

- Using this back into definition of eigenvector, we obtain

$$\frac{1}{N}\sum_n \phi(x_n)\phi(x_n)^T \sum_{p=1}^{N} a_{ip}\phi(x_p) = \lambda_i \sum_{p=1}^{N} a_{ip}\phi(x_p)$$

Probabilistic PCA

- Define kernel

$$k(x, x') = \phi(x)^T \phi(x')$$

- Multiplying both sides with $\phi(x_\ell)$

$$\frac{1}{N} \sum_n \phi(x_\ell)^T \phi(x_n) \sum_{p=1}^{N} a_{ip} \phi(x_n)^T \phi(x_p) = \lambda_i \sum_{p=1}^{N} a_{ip} \phi(x_\ell)^T \phi(x_p)$$

- That is

$$\frac{1}{N} \sum_n K(x_\ell, x_n) \sum_{p=1}^{N} a_{ip} K(x_n, x_p) = \lambda_i \sum_{p=1}^{N} a_{ip} K(x_\ell, x_p)$$

- Equivalently

$$\mathbf{K}^2 \mathbf{a}_i = \lambda_i N \mathbf{K} \mathbf{a}_i \quad \Rightarrow \quad \mathbf{K} \mathbf{a}_i = \lambda_i N \mathbf{a}_i$$

Probabilistic PCA

- Projection:

$$
\begin{aligned}
y_i(x) &= \phi(x)^T \mathbf{v}_i \\
&= \sum_n a_{in} \phi(x)^T \phi(x_n) \\
&= \sum_n a_{in} K(x, x_n)
\end{aligned}
$$

- This suggests a way to find projection of a new data point *without* re-computing PCA!

Beyond PCA

- Independent component analysis
    - When distribution over latent variables factorizes

- Auto-encoder
    - Using neural networks for modeling latent variable model
    - We've seen already seen this in class

- Matrix latent variable model
    - We shall discuss this in the next lecture