Syllabus

Fri. 21.10.	(1)	0. Introduction
		A. Supervised Learning: Linear Models & Fundamentals
Fri. 27.10.	(2)	A.1 Linear Regression
Fri. 3.11.	(3)	A.2 Linear Classification
Fri. 10.11.	(4)	A.3 Regularization
Fri. 17.11.	(5)	A.4 High-dimensional Data
		B. Supervised Learning: Nonlinear Models
Fri. 24.11.	(6)	B.1 Nearest-Neighbor Models
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Fri. 8.12.	(8)	B.3 Decision Trees
Fri. 15.12.	(9)	B.4 Support Vector Machines
Fri. 12.1.	(10)	B.5 A First Look at Bayesian and Markov Networks
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Fri. 19.1.	(11)	C.1 Clustering
Fri. 26.1.	(12)	C.2 Dimensionality Reduction
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Outline

1. Principal Components Analysis
2. Probabilistic PCA & Factor Analysis
3. Non-linear Dimensionality Reduction
4. Supervised Dimensionality Reduction

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1. Principal Components Analysis
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4. Supervised Dimensionality Reduction

The Dimensionality Reduction Problem

Given

- a set $\mathcal{X}$ called **data space**, e.g., $\mathcal{X} := \mathbb{R}^m$,
- a set $X \subseteq \mathcal{X}$ called **data**,
- a function

$$D : \bigcup_{X \subseteq \mathcal{X}, K \in \mathbb{N}} (\mathbb{R}^K)^X \rightarrow \mathbb{R}_0^+$$

  called **distortion** where $D(P)$ measures how bad a low dimensional representation $P : X \rightarrow \mathbb{R}^K$ for a data set $X \subseteq \mathcal{X}$ is, and
- a number $K \in \mathbb{N}$ of latent dimensions,

find a low dimensional representation $P : X \rightarrow \mathbb{R}^K$ with K dimensions with minimal distortion $D(P)$.

Distortions for Dimensionality Reduction (1/2)

Let $d_{\mathcal{X}}$ be a distance on $\mathcal{X}$ and d_Z be a distance on the latent space $\mathbb{R}^K$, usually just the Euclidean distance

$$d_Z(v, w) := ||v - w||_2 = (\sum_{i=1}^{K}(v_i - w_i)^2)^{\frac{1}{2}}$$

Multidimensional scaling aims to find latent representations P that **reproduce the distance measure $d_{\mathcal{X}}$** as good as possible:

$$D(P) := \frac{2}{|X|(|X|-1)} \sum_{\substack{x,x' \in X \\ x \neq x'}} (d_{\mathcal{X}}(x, x') - d_Z(P(x), P(x')))^2$$

$$= \frac{2}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{i-1} (d_{\mathcal{X}}(x_i, x_j) - ||z_i - z_j||)^2, \quad z_i := P(x_i)$$

Distortions for Dimensionality Reduction (2/2)

Feature reconstruction methods aim to find latent representations P and reconstruction maps $r : \mathbb{R}^K \to \mathcal{X}$ from a given class of maps that **reconstruct features** as good as possible:

$$D(P, r) := \frac{1}{|X|} \sum_{x \in X} d_{\mathcal{X}}(x, r(P(x)))$$

$$= \frac{1}{n} \sum_{i=1}^{n} d_{\mathcal{X}}(x_i, r(z_i)), \quad z_i := P(x_i)$$

Singular Value Decomposition (SVD)

Theorem (Existence of SVD)

For every $A \in \mathbb{R}^{n \times m}$ there exist matrices

$$U \in \mathbb{R}^{n \times k}, V \in \mathbb{R}^{m \times k}, \Sigma := diag(\sigma_1, \ldots, \sigma_k) \in \mathbb{R}^{k \times k}, \qquad k := \min\{n, m\}$$

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_k = 0, \qquad r := \text{rank}(A)$$

$$U, V \text{ orthonormal, i.e., } U^T U = I, V^T V = I$$

with

$$A = U \Sigma V^T$$

σ_i are called **singular values of** *A.*

Note: $I := \text{diag}(1, \ldots, 1) \in \mathbb{R}^{k \times k}$ denotes the unit matrix.

Singular Value Decomposition (SVD; 2/2)

It holds:

a) σ_i^2 are eigenvalues and V_i eigenvectors of $A^T A$:

$$(A^T A) V_i = \sigma_i^2 V_i, \quad i = 1, \ldots, k, V = (V_1, \ldots, V_k)$$

b) σ_i^2 are eigenvalues and U_i eigenvectors of AA^T:

$$(AA^T) U_i = \sigma_i^2 U_i, \quad i = 1, \ldots, k, U = (U_1, \ldots, U_k)$$

proof:

$$\text{a) } (A^T A) V_i = V \Sigma^T U^T U \Sigma V^T V_i = V \Sigma^2 e_i = \sigma_i^2 V_i$$

$$\text{b) } (AA^T) U_i = U \Sigma^T V^T V \Sigma^T U^T U_i = U \Sigma^2 e_i = \sigma_i^2 U_i$$

Truncated SVD

Let $A \in \mathbb{R}^{n \times m}$ and $U \Sigma V^T = A$ its SVD. Then for $k' \leq \min\{n, m\}$ the decomposition

$$A \approx U' \Sigma' V'^T$$

with

$$U' := (U_{,1}, \ldots, U_{,k'}), V' := (V_{,1}, \ldots, V_{,k'}), \Sigma' := \text{diag}(\sigma_1, \ldots, \sigma_{k'})$$

is called **truncated SVD with rank k'**.

Low Rank Approximation

Let $A \in \mathbb{R}^{n \times m}$. For $k \leq \min\{n, m\}$, any pair of matrices

$$U \in \mathbb{R}^{n \times k}, V \in \mathbb{R}^{m \times k}$$

is called a **low rank approximation of A with rank k**.
The matrix

$$UV^T$$

is called the **reconstruction of A by U, V** and the quantity

$$||A - UV^T||_F = \sum_{i=1}^{n} \sum_{j=1}^{m} (A_{i,j} - U_i^T V_j)^2$$

the **L2 reconstruction error**.

Note: $||A||_F$ is called Frobenius norm.
(Do not confuse this with the L2 norm $|| \cdot ||_2$ for matrices.)

Optimal Low Rank Approximation is Truncated SVD

Theorem (Low Rank Approximation; Eckart-Young theorem)

Let $A \in \mathbb{R}^{n \times m}$. For $k' \leq \min\{n, m\}$, the optimal low rank approximation of rank k' (i.e., with smallest reconstruction error)

$$(U^*, V^*) := \underset{U \in \mathbb{R}^{n \times k'}, V \in \mathbb{R}^{m \times k'}}{\arg\min} ||A - UV^T||_F^2$$

is the truncated SVD.

Note: As U, V do not have to be orthonormal, one can take $U := U'\Sigma'$, $V := V'$ for the SVD $A = U'\Sigma' V'^T$.

Principal Components Analysis (PCA)

Let $X := \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^m$ be a data set and $K \in \mathbb{N}$ the number of latent dimensions ($K \leq m$).

PCA finds

- K principal components $v_1, \ldots, v_K \in \mathbb{R}^m$ and
- latent weights $z_i \in \mathbb{R}^K$ for each data point $i \in \{1, \ldots, n\}$,

such that the linear combination of the principal components

$$x_i \approx \sum_{k=1}^{K} z_{i,k} v_k$$

reconstructs the original features x_i as good as possible:

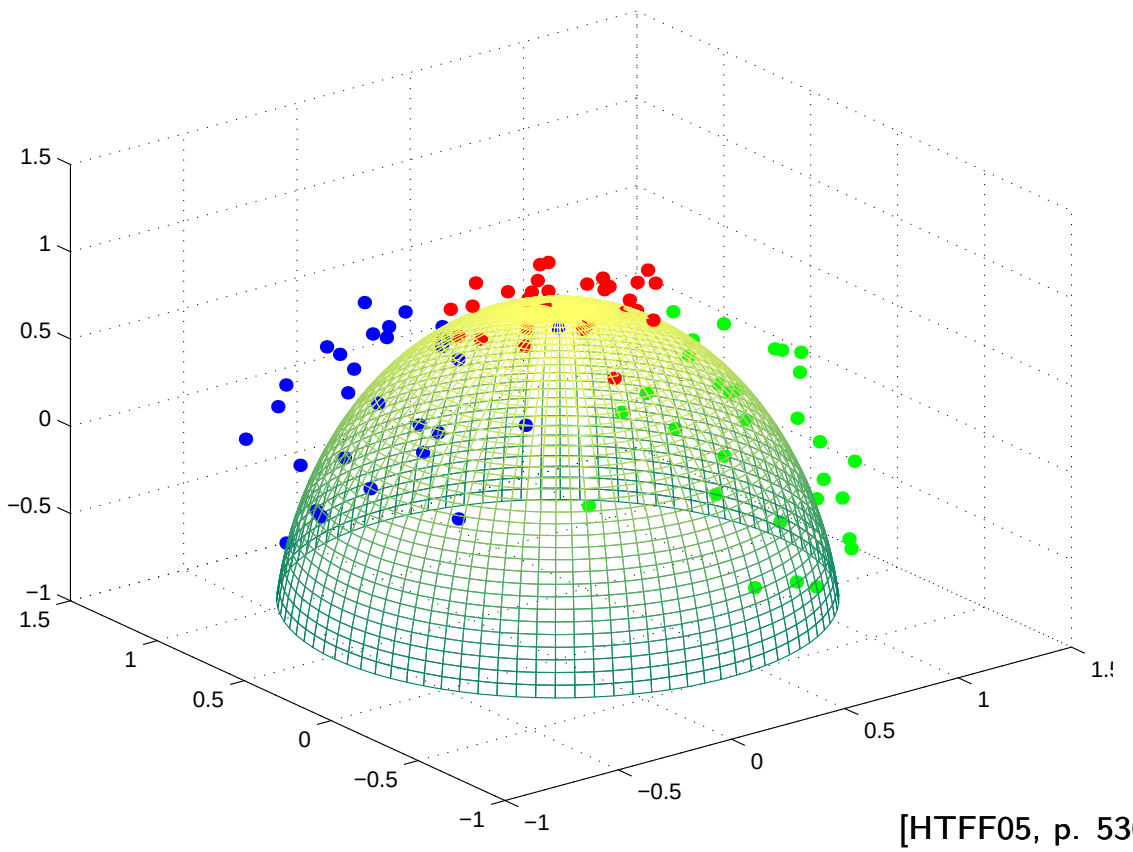
$$\underset{\substack{v_1, \ldots, v_K \\ z_1, \ldots, z_n}}{\arg\min} \sum_{i=1}^{n} ||x_i - \sum_{k=1}^{K} z_{i,k} v_k||^2$$

$$= \sum_{i=1}^{n} ||x_i - Vz_i||^2, \quad V := (v_1, \ldots, v_K)^T$$

PCA Algorithm

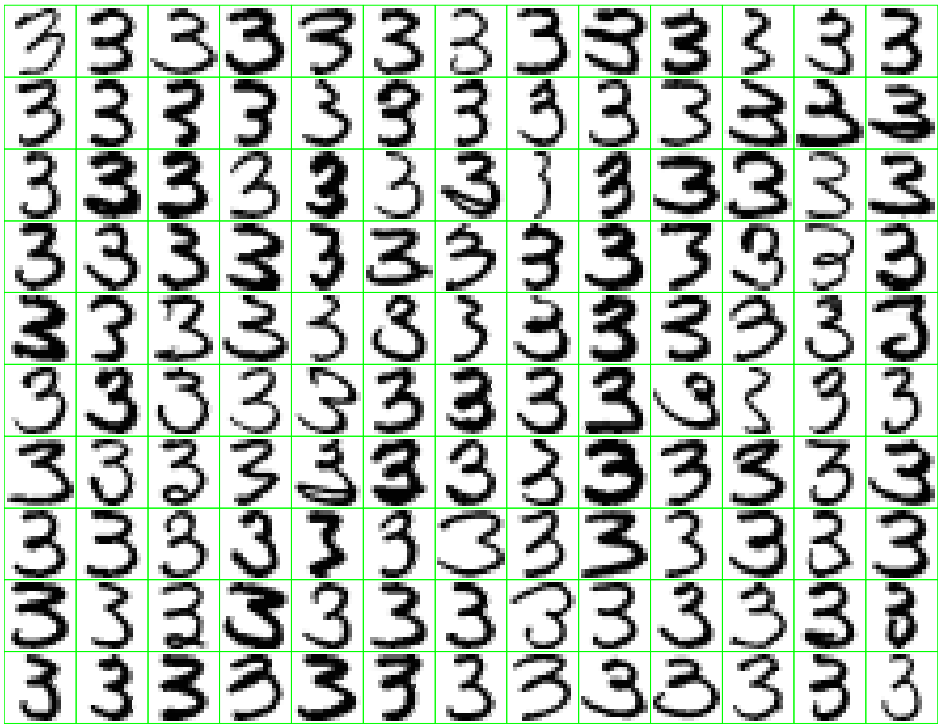
procedure DIMRED-PCA($\mathcal{D} := \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^M, K \in \mathbb{N}$)
  $X := (x_1, x_2, \ldots, x_N)^T$
  $(U, \Sigma, V) := \text{svd}(X)$
  $Z := U_{.,1:K} \cdot \Sigma_{1:K,1:K}$
  return $\mathcal{D}^{\text{dimred}} := \{Z_{1,.}, \ldots, Z_{N,.}\}$

Principal Components Analysis (Example 1)



[HTFF05, p. 536]

Principal Components Analysis (Example 2)



[HTFF05, p. 538]

Outline

Probabilistic Model

Probabilistic PCA provides a probabilistic interpretation of PCA.

It models for each data point

- a multivariate normal distributed latent factor z,
- that influences the observed variables linearly:

$$p(z) := \mathcal{N}(z; 0, I)$$
$$p(x \mid z; \mu, \sigma^2, W) := \mathcal{N}(x; \mu + Wz, \sigma^2 I)$$

Probabilistic PCA Loglikelihood

$$\begin{aligned}
&\ell(X, Z; \mu, \sigma^2, W) \\
&\quad = \sum_{i=1}^{n} \ln p(x_i \mid z_i; \mu, \sigma^2, W) + \ln p(z_i) \\
&\quad = \sum_{i} \ln \mathcal{N}(x_i; \mu + Wz_i, \sigma^2 I) + \ln \mathcal{N}(z_i; 0, I) \\
&\quad \propto \sum_{i} -\frac{1}{2} \log \sigma^2 - \frac{1}{2\sigma^2}(x_i - \mu - Wz_i)^T (x_i - \mu - Wz_i) - \frac{1}{2} z_i^T z_i \\
&\quad \propto -\sum_{i} \log \sigma^2 + \frac{1}{\sigma^2}(\mu^T \mu + z_i^T W^T W z_i - 2x_i^T \mu - 2x_i^T W z_i + 2\mu^T W z_i) \\
&\qquad\qquad + z_i^T z_i
\end{aligned}$$

remember: $\mathcal{N}(x; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^m |\Sigma|^{\frac{1}{2}}}} e^{-\frac{1}{2}(x-\mu)\Sigma^{-1}(x-\mu)}$.

PCA vs Probabilistic PCA

$$\ell(X, Z; \mu, \sigma^2, W)$$
$$\propto \sum_i -\frac{1}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(x_i - \mu - Wz_i)^T(x_i - \mu - Wz_i) - \frac{1}{2}z_i^T z_i$$

- as PCA: Decompose with minimal L2 loss

$$x_i \approx \mu + \sum_{k=1}^{K} z_{i,k} v_k$$
$$\text{with } v_k := W_{\cdot,k}$$

- different from PCA: L2 regularized row features z.
  - cannot be solved by SVD. Use EM as learning algorithm!
- additionally also regularization of column features W possible (through a prior on W).

EM / Block Coordinate Descent: Outline

$$\ell(X, Z; \mu, \sigma^2, W)$$
$$\propto -\sum_i \log\sigma^2 + \frac{1}{\sigma^2}(\mu^T\mu + z_i^T W^T W z_i - 2x_i^T\mu - 2x_i^T W z_i + 2\mu^T W z_i) + z_i^T z_i$$

1. **expectation step**: $\forall i$

$$\frac{\partial \ell}{\partial z_i} \stackrel{!}{=} 0 \qquad \rightsquigarrow z_i = \ldots \qquad (0)$$

2. **minimization step**:

$$\frac{\partial \ell}{\partial \mu} \stackrel{!}{=} 0 \qquad \rightsquigarrow \mu = \ldots \qquad (1)$$
$$\frac{\partial \ell}{\partial \sigma^2} \stackrel{!}{=} 0 \qquad \rightsquigarrow \sigma^2 = \ldots \qquad (2)$$
$$\frac{\partial \ell}{\partial W} \stackrel{!}{=} 0 \qquad \rightsquigarrow W = \ldots \qquad (3)$$

EM / Block Coordinate Descent

$$\ell(X, Z; \mu, \sigma^2, W)$$
$$\propto -\sum_i \log \sigma^2 + \frac{1}{\sigma^2}(\mu^T\mu + z_i^T W^T W z_i - 2x_i^T\mu - 2x_i^T W z_i + 2\mu^T W z_i) + z_i^T z_i$$

$$\frac{\partial \ell}{\partial z_i} = -\frac{1}{\sigma^2}(2z_i^T W^T W - 2x_i^T W + 2\mu^T W) - 2z_i^T \stackrel{!}{=} 0$$
$$(W^T W + \sigma^2 I)\, z_i = W^T(x_i - \mu)$$
$$z_i = (W^T W + \sigma^2 I)^{-1} W^T (x_i - \mu) \qquad (0)$$

$$\frac{\partial \ell}{\partial \mu} = -\frac{1}{\sigma^2}\sum_i 2\mu^T - 2x_i^T + 2z_i^T W^T \stackrel{!}{=} 0$$
$$\mu = \frac{1}{n}\sum_i x_i - W z_i \qquad (1)$$

Note: As $\mathbb{E}(z_i) = 0$, μ often is fixed to $\mu := \frac{1}{n}\sum_i x_i$.

EM / Block Coordinate Descent: Summary

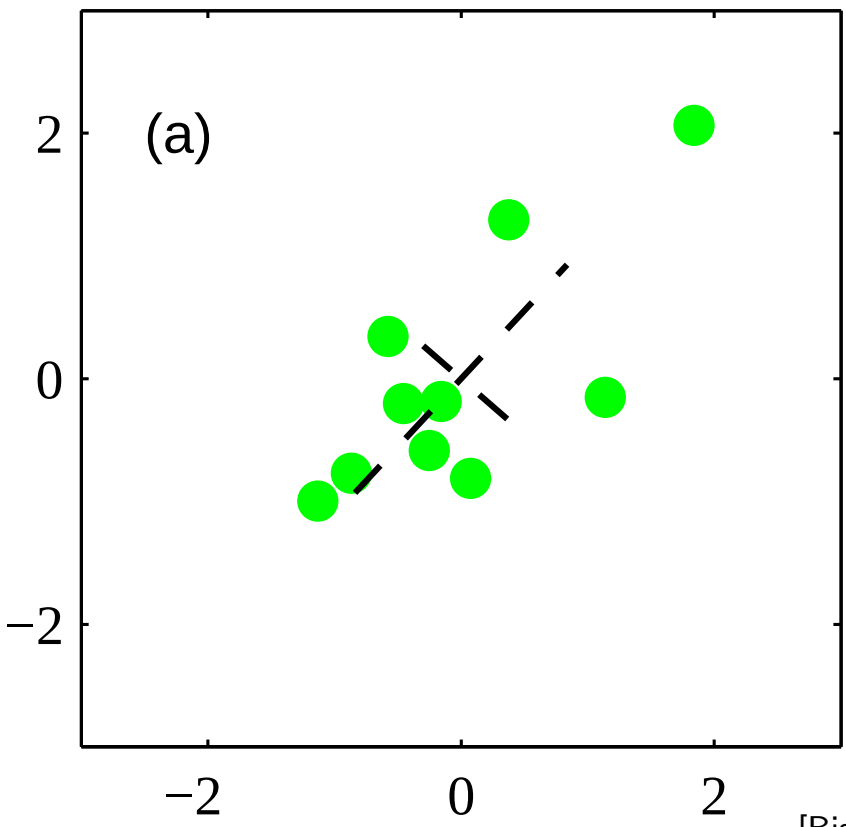
alternate until convergence:

1. **expectation step**: $\forall i$
$$z_i = (W^T W + \sigma^2 I)^{-1} W^T (x_i - \mu) \qquad (0)$$
2. **minimization step**:
$$\mu = \frac{1}{n}\sum_i x_i - W z_i \qquad (1)$$
$$\sigma^2 = \frac{1}{n}\sum_i (x_i - \mu - W z_i)^T (x_i - \mu - W z_i) \qquad (2)$$
$$W = \sum_i (x_i - \mu) z_i^T \Big(\sum_i z_i z_i^T\Big)^{-1} \qquad (3)$$

Probabilistic PCA Algorithm (EM)

procedure DIMRED-PPCA($\mathcal{D} := \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^M, K \in \mathbb{N}, \epsilon \in \mathbb{R}^+$)
  allocate $z_1, \ldots, z_N := 0 \in \mathbb{R}^K, \mu := 0 \in \mathbb{R}^M, W := 0 \in \mathbb{R}^{N \times K}, \sigma^2 := 1 \in \mathbb{R}$
  repeat
    $\sigma^2_{\text{old}} := \sigma^2, z^{\text{old}} := z$
    for $n := 1, \ldots, N$ **do**
      $z_n := (W^T W + \sigma^2 I)^{-1} W^T (x_n - \mu)$
    $\mu_{\text{old}} := \mu$
    $\mu := \frac{1}{n} \sum_i x_i - W z_i$
    $\sigma^2 := \frac{1}{n} \sum_i (x_i - \mu_{\text{old}} - W z_i)^T (x_i - \mu_{\text{old}} - W z_i)$
    $W := \sum_i (x_i - \mu_{\text{old}}) z_i^T (\sum_i z_i z_i^T)^{-1}$
  until $\frac{1}{N} \sum_{n=1}^N ||z_n - z_n^{\text{old}}|| < \epsilon$
  return $\mathcal{D}^{\text{dimred}} := \{z_1, \ldots, z_N\}$

EM / Block Coordinate Descent: Example



[Bis06, p. 581]

Regularization of Column Features W

$$p(W) := \prod_{j=1}^{m} \mathcal{N}(w_j; 0, \tau_j^2 I), \quad W = (w_1, \ldots, w_m)$$

$$\rightsquigarrow \ell = \ldots + \sum_{j=1}^{m} -K \log \tau_j^2 - \frac{1}{2\tau_j^2} w_j^T w_j$$

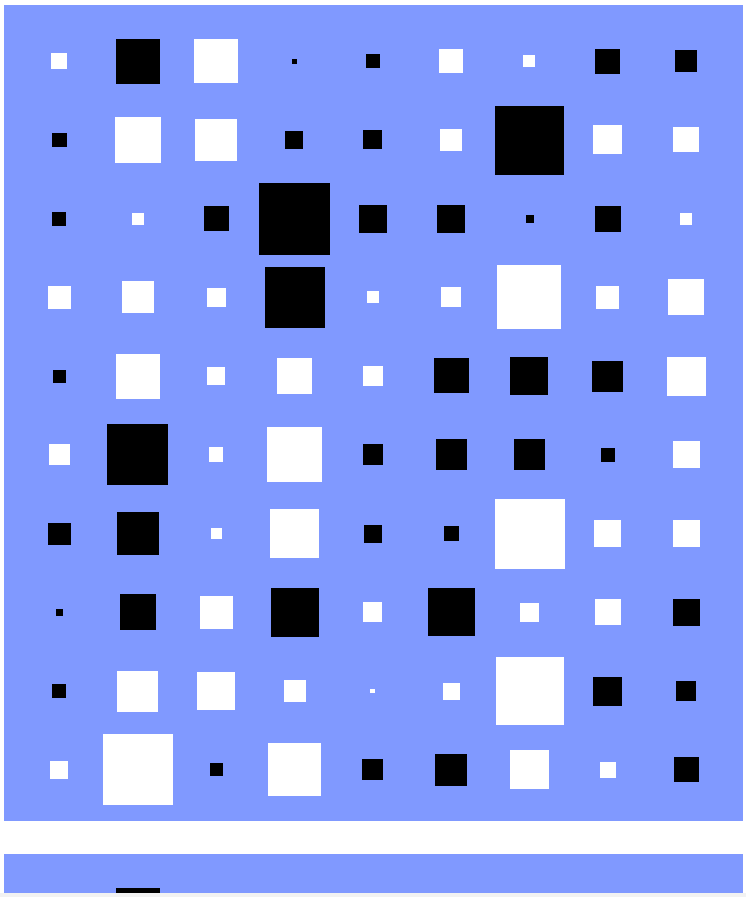
$$\frac{\partial \ell}{\partial W} = \ldots - W \operatorname{diag}(\frac{1}{\tau_1^2}, \ldots, \frac{1}{\tau_m^2})$$

$$W = \sum_i (x_i - \mu) z_i^T (\sum_i z_i z_i^T + \sigma^2 \operatorname{diag}(\frac{1}{\tau_1^2}, \ldots, \frac{1}{\tau_m^2}))^{-1} \qquad (3')$$

$$\frac{\partial \ell}{\partial \tau_j} = -K \frac{1}{\tau_j^2} + \frac{1}{(\tau_j^2)^2} w_j^T w_j \stackrel{!}{=} 0$$

$$\tau_j = \frac{1}{K} w_j^T w_j \qquad (4)$$

Bayesian PCA: Example



[Bis06, p. 584]

Factor Analysis

$$p(z) := \mathcal{N}(z; 0, I)$$
$$p(x \mid z; \mu, \Sigma, W) := \mathcal{N}(x; \mu + Wz, \Sigma), \quad \Sigma \text{ diagonal}$$

$$\ell(X, Z; \mu, \Sigma, W)$$
$$\propto \sum_i -\frac{1}{2}\log|\Sigma| - \frac{1}{2}(x_i - \mu - Wz_i)^T\Sigma^{-1}(x_i - \mu - Wz_i) - \frac{1}{2}z_i^T z_i$$

EM:

$$z_i = (W^T\Sigma^{-1}W + I)^{-1}W^T\Sigma^{-1}(x_i - \mu) \qquad (0')$$
$$\mu = \frac{1}{n}\sum_i x_i - Wz_i \qquad (1)$$
$$\Sigma_{j,j} = \frac{1}{n}\sum_i ((x_i - \mu_i - Wz_i)_j)^2 \qquad (2')$$

Note: See appendix for derivation of EM formulas.

Outline

Linear Dimensionality Reduction

Dimensionality reduction accomplishes two tasks:

1. compute lower dimensional representations for **given data points** x_i
   - for PCA:

$$u_i = \Sigma^{-1} V^T x_i, \quad U := (u_1, \ldots, u_n)^T$$

2. compute lower dimensional representations for **new data points** x (often called "fold in")
   - for PCA:

$$u := \arg\min_u ||x - V\Sigma u||^2 = \Sigma^{-1} V^T x$$

PCA is called a **linear dimensionality reduction technique** because the latent representations u depend linearly on the observed representations x.

Kernel Trick

Represent (conceptionally) non-linearity by linearity in a higher dimensional embedding

$$\phi : \mathbb{R}^m \to \mathbb{R}^{\tilde{m}}$$

but compute in lower dimensionality for methods that depend on x only through a scalar product

$$\tilde{x}^T \tilde{\theta} = \phi(x)^T \phi(\theta) = k(x, \theta), \quad x, \theta \in \mathbb{R}^m$$

if k can be computed without explicitly computing ϕ.

Kernel Trick / Example

Example:

$$\phi : \mathbb{R} \to \mathbb{R}^{1001},$$
$$x \mapsto \left(\left(\begin{pmatrix} 1000 \\ i \end{pmatrix}^{\frac{1}{2}} x^i \right)_{i=0,\ldots,1000} \right. = \begin{pmatrix} 1 \\ 31.62\, x \\ 706.75\, x^2 \\ \vdots \\ 31.62\, x^{999} \\ x^{1000} \end{pmatrix}$$

$$\tilde{x}^T \tilde{\theta} = \phi(x)^T \phi(\theta) = \sum_{i=0}^{1000} \begin{pmatrix} 1000 \\ i \end{pmatrix} x^i \theta^i = (1 + x\theta)^{1000} =: k(x, \theta)$$

Naive computation:

- 2002 binomial coefficients, 3003 multiplications, 1000 additions.

Kernel computation:

- 1 multiplication, 1 addition, 1 exponentiation.

Kernel PCA

$$\phi : \mathbb{R}^m \to \mathbb{R}^{\tilde{m}}, \quad \tilde{m} \gg m$$

$$\tilde{X} := \begin{pmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_n) \end{pmatrix}$$

$$\tilde{X} \approx U \Sigma \tilde{V}^T$$

We can compute the columns of U as eigenvectors of $\tilde{X}\tilde{X}^T \in \mathbb{R}^{n \times n}$ without having to compute $\tilde{V} \in \mathbb{R}^{\tilde{m} \times k}$ (which is large!):

$$\tilde{X}\tilde{X}^T U_i = \sigma_i^2 U_i$$

Kernel PCA / Removing the Mean

Issue 1: The $\tilde{x}_i := \phi(x_i)$ may not have zero mean and thus distort PCA.

$$\begin{aligned}
\tilde{x}'_i :=& \tilde{x}_i - \frac{1}{n}\sum_{i=1}^{n}\tilde{x}_i \\
=& \tilde{X}^T(I - \frac{1}{n}\mathbb{1}) \\
\tilde{X}' :=& (\tilde{x}'_1, \ldots, \tilde{x}'_n)^T = (I - \frac{1}{n}\mathbb{1})\tilde{X}^T \\
K' :=& \tilde{X}'\tilde{X}'^T = (I - \frac{1}{n}\mathbb{1})\tilde{X}^T\tilde{X}(I - \frac{1}{n}\mathbb{1}) \\
=& HKH, \quad H := (I - \frac{1}{n}\mathbb{1}) \text{ centering matrix}
\end{aligned}$$

Thus, the kernel matrix K' with means removed can be computed from the kernel matrix K without having to access coordinates.

Note: $\mathbb{1} := (1)_{i=1,\ldots,n,j=1,\ldots,n}$ vector of ones,
$I := (\delta(i=j))_{i=1,\ldots,n,j=1,\ldots,n}$ unity matrix.

Kernel PCA / Fold In

Issue 2: How to compute projections u of new points x (as $\tilde{V}$ is not computed)?

$$u := \arg\min_u ||x - \tilde{V}\Sigma u||^2 = \Sigma^{-1}\tilde{V}^T x$$

With

$$\begin{aligned}
\tilde{V} &= \tilde{X}^T U \Sigma^{-1} \\
u &= \Sigma^{-1}\tilde{V}^T x = \Sigma^{-1}\Sigma^{-1}U^T\tilde{X}x = \Sigma^{-2}U^T(k(x_i, x))_{i=1,\ldots,n}
\end{aligned}$$

u can be computed with access to kernel values only (and to U, Σ).

Kernel PCA / Summary

Given:

- data set $X := \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^m$,
- kernel function $k : \mathbb{R}^m \times \mathbb{R}^m \rightarrow R$.

task 1: Learn latent representations U of data set X:

$$K := (k(x_i, x_j))_{i=1,\ldots,n, j=1,\ldots,n} \tag{0}$$

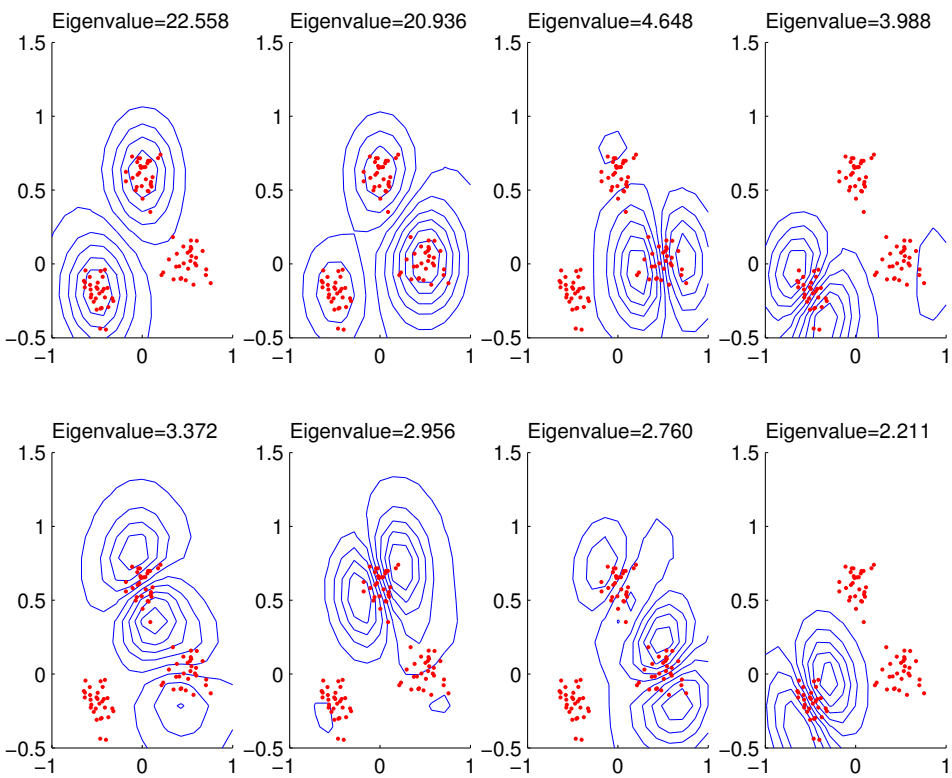
$$K' := HKH, \quad H := (I - \frac{1}{n}\mathbb{1}) \tag{1}$$

$$(U, \Sigma) := \text{eigen decomposition } K'U = U\Sigma \tag{2}$$

task 2: Learn latent representation u of new point x:

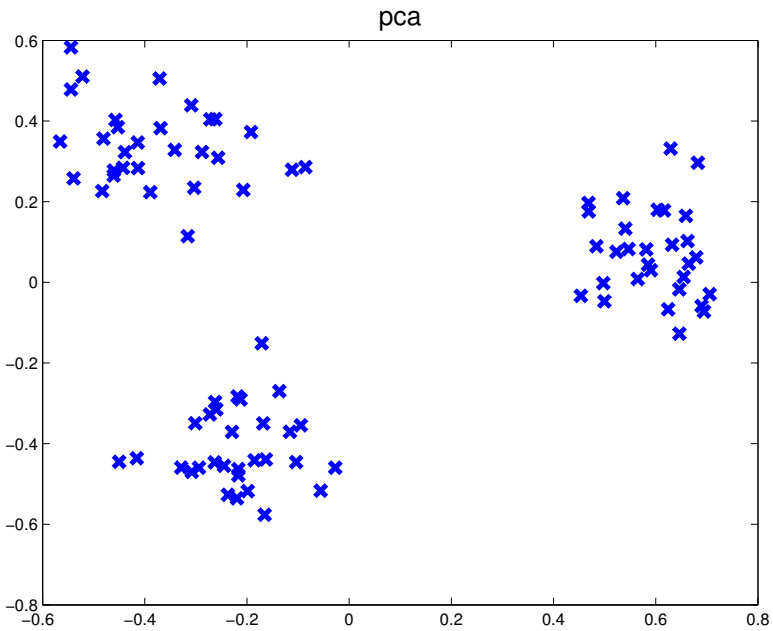
$$u := \Sigma^{-2} U^T (k(x_i, x))_{i=1,\ldots,n} \tag{3}$$

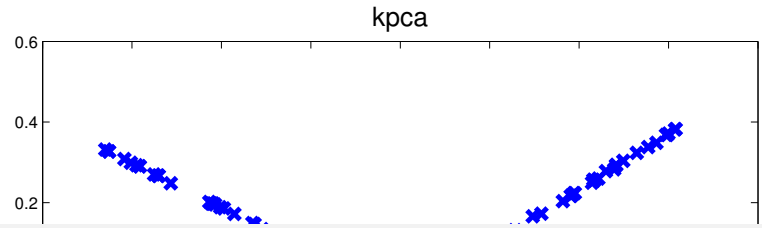
Kernel PCA: Example 1



[Mur12, p. 493]

Kernel PCA: Example 2





[Mur12, p. 495]

Outline

Dimensionality Reduction as Pre-Processing

Given a prediction task and
a data set $\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_n, y_n)\} \subseteq \mathbb{R}^m \times \mathcal{Y}$.

1. compute latent features $z_i \in \mathbb{R}^K$ for the objects of a data set by means of dimensionality reduction of the predictors x_i.
   - e.g., using PCA on $\{x_1, \ldots, x_n\} \subseteq \mathbb{R}^m$
2. learn a prediction model

$$\hat{y} : \mathbb{R}^K \to \mathcal{Y}$$

   on the latent features based on

$$\mathcal{D}'^{\text{train}} := \{(z_1, y_1), \ldots, (z_n, y_n)\}$$

3. treat the number K of latent dimensions as hyperparameter.
   - e.g., find using grid search.

Dimensionality Reduction as Pre-Processing

Advantages:

- simple procedure
- generic procedure
  - works with any dimensionality reduction method and any prediction method as component methods.
- usually fast

Disadvantages:

- dimensionality reduction is **unsupervised**, i.e., not informed about the target that should be predicted later on.
  - leads to the very same latent features regardless of the prediction task.
  - likely not the best task-specific features are extracted.

Supervised PCA

$$p(z) := \mathcal{N}(z; 0, 1)$$
$$p(x \mid z; \mu_x, \sigma_x^2, W_x) := \mathcal{N}(x; \mu_x + W_x z, \sigma_x^2 I)$$
$$p(y \mid z; \mu_y, \sigma_y^2, W_y) := \mathcal{N}(y; \mu_y + W_y z, \sigma_y^2 I)$$

- like two PCAs, coupled by shared latent features z:
  - one for the predictors x.
  - one for the targets y.
- latent features act as **information bottleneck**.
- also known as **Latent Factor Regression** or **Bayesian Factor Regression**.

Supervised PCA: Discriminative Likelihood

A simple likelihood would put the same weight on

- reconstructing the predictors and
- reconstructing the targets.

A weight $\alpha \in \mathbb{R}_0^+$ for the reconstruction error of the predictors should be introduced (**discriminative likelihood**):

$$L_\alpha(\Theta; x, y, z) := \prod_{i=1}^{n} p(y_i \mid z_i; \Theta) p(x_i \mid z_i; \Theta)^\alpha p(z_i; \Theta)$$

α can be treated as hyperparameter and found by grid search.

Supervised PCA: EM

- The M-steps for μ_x, σ_x^2, W_x and μ_y, σ_y^2, W_y are exactly as before.
- the coupled E-step is:

$$z_i = \left(\frac{1}{\sigma_y^2} W_y^T W_y + \alpha \frac{1}{\sigma_x^2} W_x^T W_x\right)^{-1} \left(\frac{1}{\sigma_y^2} W_y^T (y_i - \mu_y) + \alpha \frac{1}{\sigma_x^2} W_x^T (x_i - \mu_x)\right)$$

Conclusion (1234/4)

- Dimensionality reduction aims to find a **lower dimensional representation of data** that **preserves the information** as much as possible. — "Preserving information" means
  - to preserve **pairwise distances between objects** (**multidimensional scaling**).
  - to be able to reconstruct the original object features (**feature reconstruction**).
- The **truncated Singular Value Decomposition (SVD)** provides the best **low rank factorization** of a matrix in two factor matrices.
  - SVD is usually computed by an algebraic factorization method (such as QR decomposition).
- **Principal components analysis (PCA)** finds latent object features and latent variable features that provide the **best linear reconstruction** (in L2 error).
  - PCA is a truncated SVD of the data matrix.
- **Probabilistic PCA** (PPCA) provides a probabilistic interpretation of

Readings

- Principal Components Analysis (PCA)
  - [HTFF05], ch. 14.5.1, [Bis06], ch. 12.1, [Mur12], ch. 12.2.
- Probabilistic PCA
  - [Bis06], ch. 12.2, [Mur12], ch. 12.2.4.
- Factor Analysis
  - [HTFF05], ch. 14.7.1, [Bis06], ch. 12.2.4.
- Kernel PCA
  - [HTFF05], ch. 14.5.4, [Bis06], ch. 12.3, [Mur12], ch. 14.4.4.

Further Readings

- (Non-negative) Matrix Factorization
  - [HTFF05], ch. 14.6
- Independent Component Analysis, Exploratory Projection Pursuit
  - [HTFF05], ch. 14.7 [Bis06], ch. 12.4 [Mur12], ch. 12.6.
- Nonlinear Dimensionality Reduction
  - [HTFF05], ch. 14.9, [Bis06], ch. 12.4

Factor Analysis: Loglikelihood

$$
\begin{aligned}
&\ell(X, Z; \mu, \Sigma, W) \\
&\quad = \sum_{i=1}^{n} \ln p(x \mid z; \mu, \Sigma, W) + \ln p(z) \\
&\quad = \sum_{i} \ln \mathcal{N}(x; \mu + Wz, \Sigma) + \ln \mathcal{N}(z; 0, I) \\
&\quad \propto \sum_{i} -\frac{1}{2} \log |\Sigma| - \frac{1}{2}(x_i - \mu - Wz_i)^T \Sigma^{-1} (x_i - \mu - Wz_i) - \frac{1}{2} z_i^T z_i \\
&\quad \propto -\sum_{i} \log |\Sigma| + (x_i^T \Sigma^{-1} x_i + \mu^T \Sigma^{-1} \mu + z_i^T W^T \Sigma^{-1} W z_i - 2 x_i^T \Sigma^{-1} \mu \\
&\qquad\qquad - 2 x_i^T \Sigma^{-1} W z_i + 2 \mu^T \Sigma^{-1} W z_i) + z_i^T z_i
\end{aligned}
$$

remember: $\mathcal{N}(x; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^m |\Sigma|}^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu)\Sigma^{-1}(x-\mu)}$.

Factor Analysis: EM / Block Coordinate Descent

$$
\begin{aligned}
&\ell(X, Z; \mu, \Sigma, W) \\
&\quad \propto -\sum_{i} \log |\Sigma| + (x_i^T \Sigma^{-1} x_i + \mu^T \Sigma^{-1} \mu + z_i^T W^T \Sigma^{-1} W z_i - 2 x_i^T \Sigma^{-1} \mu \\
&\qquad\qquad - 2 x_i^T \Sigma^{-1} W z_i + 2 \mu^T \Sigma^{-1} W z_i) + z_i^T z_i
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \ell}{\partial z_i} &= -(2 z_i^T W^T \Sigma^{-1} W - 2 x_i^T W \Sigma^{-1} + 2 \mu^T \Sigma^{-1} W) - 2 z_i^T \\
(W^T \Sigma^{-1} W + I)\, z_i &= W^T \Sigma^{-1} (x_i - \mu) \\
z_i &= (W^T \Sigma^{-1} W + I)^{-1} W^T \Sigma^{-1} (x_i - \mu)
\end{aligned}
$$

$$
\frac{\partial \ell}{\partial \mu} = -\sum_{i} 2 \mu^T \Sigma^{-1} - 2 x_i^T \Sigma^{-1} + 2 z_i^T W^T \Sigma^{-1} \stackrel{!}{=} 0
$$

Note: As $\mathbb{E}(z_i) = 0$, μ often is fixed to $\mu := \frac{1}{n} \sum_i x_i$.

$$
\mu = \frac{1}{n} \sum_{i} x_i - W z_i \qquad (1')
$$

References

Christopher M. Bishop.
Pattern recognition and machine learning, volume 1.
springer New York, 2006.

Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin.
The elements of statistical learning: data mining, inference and prediction, volume 27.
Springer, 2005.

Kevin P. Murphy.
Machine learning: a probabilistic perspective.
The MIT Press, 2012.

Matrix Trace

The function

$$\mathrm{tr} : \bigcup_{n \in \mathbb{N}} \mathbb{R}^{n \times n} \to \mathbb{R}$$

$$A \mapsto \mathrm{tr}(A) := \sum_{i=1}^{n} a_{i,i}$$

is called **matrix trace**. It holds:

a) invariance under permutations of factors:

$$\mathrm{tr}(AB) = \mathrm{tr}(BA)$$

b) invariance under basis change:

$$\mathrm{tr}(B^{-1}AB) = \mathrm{tr}(A)$$

proof:

$$\text{a)} \quad \mathrm{tr}(AB) = \sum_i \sum_j A_{i,j} B_{j,i} = \sum_i \sum_j B_{i,j} A_{j,i} = \mathrm{tr}(BA)$$

$$\text{b)} \quad \mathrm{tr}(B^{-1}AB) = \mathrm{tr}(BB^{-1}A) = \mathrm{tr}(A)$$

Frobenius Norm

The function $||\cdot||_F : \bigcup_{n,m\in\mathbb{N}} \mathbb{R}^{n\times m} \rightarrow \mathbb{R}_0^+$

$$A \mapsto ||A||_F := (\sum_{i=1}^{n}\sum_{j=1}^{m} a_{i,j}^2)^{\frac{1}{2}}$$

is called **Frobenius norm**. It holds:

a) trace representation:

$$||A||_F = (\mathrm{tr}(A^T A))^{\frac{1}{2}}$$

b) invariance under orthonormal transformations:

$$\mathrm{tr}(UAV^T) = \mathrm{tr}(A), \quad U, V \text{ orthonormal}$$

proof:

$$\text{a) } \mathrm{tr}(A^T A) = \sum_i \sum_j A_{j,i} A_{j,i} = ||A||_2^2$$

$$\text{b) } ||UAV||_F^2 = \mathrm{tr}(VA^T U^T UAV^T) = \mathrm{tr}(VA^T AV^T)$$
$$= \mathrm{tr}(A^T AV^T V) = \mathrm{tr}(A^T A) = ||A||_F^2$$

Frobenius Norm (2/2)

c) representation as sum of squared singular values:

$$||A||_F = \sum_{i=1}^{\min\{m,n\}} \sigma_i^2$$

proof:

c) let $A = U\Sigma V^T$ the SVD of A

$$||A||_F = ||U\Sigma V^T||_F = ||\Sigma||_F = \mathrm{tr}(\Sigma^T\Sigma) = \sum_{i=1}^{\min\{m,n\}} \sigma_i^2$$