Advanced Data Analysis and Machine Learning

Lecture: Dimensionality Reduction

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Outline

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Data dimensionality

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- Various direct or indirect measurements as sources of information produce information on the measurement target.
- The data can be used to characterise the measurement target and model its behaviour.
- However, adding different kinds of measurements does not guarantee better characterisation or model because of the varying representativeness of a measurement, or noise.
- Data dimensionality increases with the number of measurement channels, and processing the data requires more computational effort.
- More samples are needed to estimate the parameters of a model characterising the measurement target or process.
- However, the measurements generating the optimal or good enough characterisation for a specific purpose can be selected.

Dimensionality reduction

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- Data dimensionality can be reduced intelligently.
- Various linear and nonlinear methods exist for the purpose.
- Several methods are based on the idea that the data lies on or near a low-dimensional manifold (residing in the high-dimensional space).
- In addition to these methods, data preprocessing can be used to efficiently remove data characteristics problematic for efficient reduction of dimensions.
- Dimensionality reduction is a useful tool in data analysis and machine learning since it mitigates undesired properties of high number of dimensions.

Problem of dimensionality reduction

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- The purpose of dimensionality reduction is to find a manifold to characterise a specific set of data optimally or well enough, and represent the data by using the manifold.
- Problem definition [2]:
  - Let us have a $n \times D$ matrix $\boldsymbol{X}$ consisting of n vectors of data x_i with dimensionality D. The dataset has intrinsic dimensionality d where $d < D$, and often $d \ll D$.
  - A dimensionality reduction technique transforms dataset $\boldsymbol{X}$ into a new dataset $\boldsymbol{Y}$ with dimensionality d, while retaining the geometry of the data as much as possible.
  - Dimensionality reduction is an ill-posed problem because generally the geometry of the manifold embedded in the high-dimensional space and the intrinsic dimensionality d of the dataset $\boldsymbol{X}$ are unknown $\Rightarrow$ it is necessary to make assumptions of the data to solve the problem.

Purpose of reducing dimensions

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- The purpose of dimensionality reduction is to transform high-dimensional data into a representation of reduced dimensionality.
- In an ideal situation, the new representation corresponds to the intrinsic dimensionality of the data.
- The intrinsic dimensionality of data is the minimum number of parameters needed to account for the observed properties of the data [1].
- Where from do we get the number of intrinsic dimensions?

Dimensionality reduction methods

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- Dimensionality reduction approaches can be diveded into the following categories [2]:
  - Linear methods
    such as principal component analysis (PCA)
  - Global nonlinear methods
    such as multidimensional scaling (MDS)
  - Local nonlinear methods
    such as locally linear embedding (LLE)
  - Variants of local nonlinear methods
    such as conformal eigenmaps
  - Global linear-model alignment methods
    such as locally linear coordination (LLC)

Dimensionality reduction concepts

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- Convex methods optimise an objective function that does not contain any local optima, that is, the solution space is convex. A common form for the objective function is $\phi(\boldsymbol{Y}) = \frac{\boldsymbol{Y}^\intercal \boldsymbol{A} \boldsymbol{Y}}{\boldsymbol{Y}^\intercal \boldsymbol{B} \boldsymbol{Y}}$ (generalized Rayleigh quotient to get either exact or approximate eigenvalues).
- Non-convex methods optimise objective functions that do contain local optima.
- Full spectral methods perform an eigendecomposition of a full matrix capturing the covariances between dimensions, or the pairwise similarities between datapoints.
- Sparse spectral methods solve a sparse eigenproblem, and they commonly aim to retain the local structure in the data.

Method taxonomy

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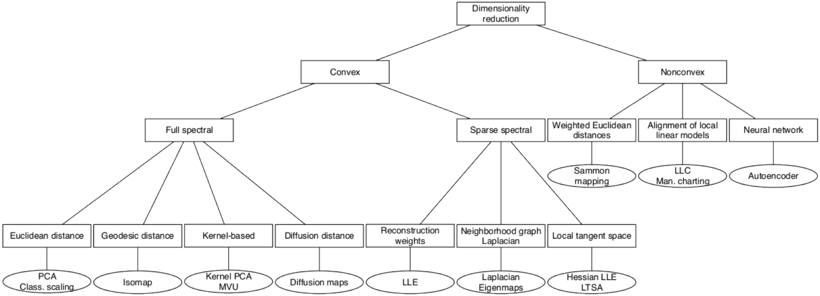

Dimensionality reduction (DR) method taxonomy [3].

Principal component analysis

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- Constructs a representation of the data by finding a linear basis of reduced dimensionality in which the variance is maximal.
- PCA seeks for a linear mapping $\boldsymbol{M}$ which maximises trace$(\boldsymbol{M}^\mathsf{T}\boldsymbol{\Sigma}\boldsymbol{M})$ where $\Sigma_{ij} = \mathrm{cov}(x_i, x_j) = \mathrm{E}\left[(x_i - \mu_i)(x_j - \mu_j)\right]$.
- The principal components (PCs) are the eigenvectors of the covariance matrix $\boldsymbol{\Sigma}$. They are found by solving $\boldsymbol{\Sigma}\boldsymbol{M} = \lambda\boldsymbol{M}$, and the new representation $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{M}$.
- To reduce the number of dimensions, only the the first l eigenvectors (in the decreasing order of variance) are selected while minimising the total reconstruction error $\|\boldsymbol{X} - \boldsymbol{X}_L\|_2$.
- The main disadvantage of PCA is that the size of the covariance matrix is proportional to the data dimensionality, but alternative ways to determine the eigenvectors exist.

Multidimensional scaling

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- Nonlinear DR method with various modifications.
- Produces a new representation by minimising a loss function taking into account the pairwise distances between the datapoints in both the low and high-dimensional spaces.
- The loss function can be defined a various ways: for example, the raw stress function $\phi(\boldsymbol{Y}) = \sum_{ij}(\|x_i - x_j\|^2 - \|y_i - y_j\|^2)$ where x is a high-dimensional datapoint, y is a low-dimensional datapoint, and $\|\cdot\|$ is the Euclidean distance ($y_i = x_i\boldsymbol{M}$ and $\|m_j\|^2 = 1\ \forall j$).
- The loss function can be minimised, for example, by performing the eigendecomposition of a pairwise dissimilarity matrix, or with the conjugate gradient method.
- Selection of the number of dimensions affects the difficulty of interpreting the results.

Locally linear embedding

- Local and nonlinear DR method.
- Constructs a low-dimensional representation of the original datapoints with the aim to preserve only the local properties of the manifold around each datapoint.
- The method describes each datapoint x_i as a linear combination W_i of its k nearest neighbours x_{i_j} by fitting a hyperplane (assumes the manifold to be locally linear) through the datapoint and its neighbours.
- LLE tries to retain the datapoint reconstruction weights in the low-dimensional representation as good as possible by minimising the cost function $\phi(\boldsymbol{Y}) = \sum_i \|y_i - \sum_{j=1}^k w_{ij} y_{i_j}\|^2$ (subject to $\|y^{(k)}\|^2 = 1 \; \forall k$).
- The points in the low-dimensional representation y_i minimising the cost function can be computed by finding the eigenvectors corresponding to the smallest d nonzero eigenvalues of the inproduct of $(\boldsymbol{I} - \boldsymbol{W})$.

Conformal eigenmaps

- Local nonlinear techniques for dimensionality reduction do not employ information on the geometry of the manifold that is contained in discarded eigenvectors (with small eigenvalues).
- A conformal transformation preserves the angles between neighbouring datapoints in dimensionality reduction.
- Conformal eigenmaps starts with a local nonlinear method for dimensionality reduction to reduce the high-dimensional data to a dataset of dimensionality d_t where $d < d_t < D$.
- Based on the previous representation and guided by a conformality measure, conformal eigenmaps constructs a d-dimensional representation that preserves the angles between the neighbouring datapoints as well as possible.

Locally linear coordination

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- LLC computes a number of locally linear models and aligns the models globally.
- The method has two steps:
  1. Compute a mixture of local linear models (factor analysers) on the data by using the expectation maximisation (EM) algorithm. The mixture of models represents joint variations (correlations) in the high-dimensional data, and the idea is to seek for latent unobserved variables (factors) explaining the variations.
  2. Align the models by finding a linear transformation based on the data models that minimizes the LLE cost function (by solving a generalised eigenproblem).

Number of intrinsic dimensions

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- The intrinsic dimensionality of data is the minimum number of parameters needed to account for the observed properties of the data [1].
- The intrinsic number of dimensions can be estimated by local or global estimators.
- Local estimators:
  - Rely on the idea that the number of datapoints within radius r from a data point increases proportional to r^d where d is the intrinsic dimensionality (around that datapoint).
  - Average over local dimensionality estimates.
- Global estimators:
  - Treat the data as a whole.
  - For examples, make use of eigenvalues, r-coverings (how many hyperspheres are needed to cover the whole dataset) or spanning trees.

Summary

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- The purpose of dimensionality reduction is to find a manifold to characterise a specific set of data optimally or well enough, and represent the data by using the manifold.
- Various linear and nonlinear methods exist for the purpose, and the intrinsic dimensionality of a dataset can be estimated by using either a local or global estimator.
- Dimensionality reduction is a useful tool in data analysis and especially in machine learning since it mitigates undesired properties of high number of dimensions.

References

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