Lecture 3: A first look at dimension reduction

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MSA220/MVE441 Statistical Learning for Big Data

28th March 2025

Dimension reduction and Predictive Modeling

One version of the curse of dimensionality

Samples tend to be further away from the origin

Let $\mathbf{x} \in [-1, 1]^p$ be a uniformly distributed random variable. For $0 \leq t \leq 1$ consider

$$q = \mathbb{P}(-t \leq x^{(1)} \leq t, \dots, -t \leq x^{(p)} \leq t) = \left(\frac{2t}{2}\right)^p$$

$$\Rightarrow \quad t = q^{1/p}$$

In a large enough sample about q percent of observations will be in $[-t, t]^p$.

In high dimensions, most data points are far away from the origin.

How should t be chosen so that about q percent of observations lie in $[-t, t]^p$?

p	$q = 1\%$	$q = 10\%$
2	$t \approx 0.01$	$t \approx 0.32$
3	$t \approx 0.22$	$t \approx 0.46$
10	$t \approx 0.63$	$t \approx 0.79$
100	$t \approx 0.95$	$t \approx 0.98$

Another version of the curse of dimensionality

Pairwise distances grow with dimension

If $\mathbf{x}, \mathbf{y} \in [0,1]^p$ uniformly distributed, then their pairwise distance $\|\mathbf{x} - \mathbf{y}\|_2$ grow with p.

The last column suggests that the mean pairwise distance grows as $O(\sqrt{p})$.

The standard deviations stay constant suggesting that observations have increasingly similar pairwise distances in high dimensions.

Mean and standard deviation of the pairwise distances of $n = 500$ simulated observations.

p	Mean	SD	Mean / $\sqrt{p}$
2	0.52	0.25	0.37
3	0.66	0.25	0.38
10	1.28	0.25	0.40
100	4.07	0.24	0.41
500	9.13	0.25	0.41
1000	12.91	0.24	0.41

High-dimensional predictive modeling

What does a predictive model do? The methods we have discussed so far try to capture some type of local, average behaviour - meaning, observations that are close borrow information from each other to come to a decision regarding the value of the outcome variable (numerical or class label). [.5em]

In high-dimensional settings, the notion of neighborhood breaks down.

In addition, many of the methods we have discussed will either be numerically unstable or ill-defined (i.e., can't estimate parameters) if the data dimension is to large.

What can be done about this dilemma?

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1. **Feature selection:** Deciding on a subset of the original features
   - We will talk a lot about feature selection later in class
   - Simplest strategy is some kind of pre-processing or *filtering*
   - Example: max variance features, features that are statistically associated with the label (t-test, ANOVA, correlation)

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2. **Feature transformation:** Combining existing features while reducing dimension (e.g. PCA)
    - The feature transformation might destroy/obscure relationships in the original data that it cannot capture
    - Since features are transformed, it is not guaranteed that uninformative features are actually filtered out

High-dimensional predictive modeling

When p is large

- kNN: notion of neighborhood breaks down

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High-dimensional predictive modeling

When p is large

- kNN: notion of neighborhood breaks down
- logistic regression: ill-defined/multicollinearity or numerically unstable model
- discriminant analysis: ill-defined/multicollinearity or numerically unstable model

Principal Component Analysis

Projection onto a subspace

Assume $\mathbf{x} \in \mathbb{R}^p$. Given **orthonormal vectors** $\mathbf{b}_1, \ldots, \mathbf{b}_m$, i.e.

$$\|\mathbf{b}_j\| = 1 \quad \text{and} \quad \mathbf{b}_j^\top \mathbf{b}_k = 0 \text{ for } j \neq k$$

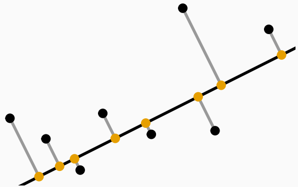
where $m < p$, the projection of $\mathbf{x}$ onto the m-dimensional linear subspace $V_m = \mathrm{span}(\mathbf{b}_1, \ldots, \mathbf{b}_m)$ is

$$\hat{\mathbf{x}} = \sum_{j=1}^{m} (\mathbf{x}^\top \mathbf{b}_j)\mathbf{b}_j = \underbrace{\left(\sum_{j=1}^{m} \mathbf{b}_j \mathbf{b}_j^\top\right)}_{\text{Projection matrix}} \mathbf{x}$$

The projection is **orthogonal**, i.e.

$$(\mathbf{x} - \hat{\mathbf{x}})^\top \mathbf{b}_j = 0$$

for all $\mathbf{b}_j$.



Rayleigh Quotient

Let $\mathbf{A} \in \mathbb{R}^{k\times k}$ be a symmetric matrix. For $\mathbf{0} \neq \mathbf{x} \in \mathbb{R}^k$ define

$$J(\mathbf{x}) = \frac{\mathbf{x}^\top \mathbf{A}\mathbf{x}}{\mathbf{x}^\top \mathbf{x}}$$

$J(\mathbf{x})$ is called the **Rayleigh Quotient** for $\mathbf{A}$.

Maximizing the Rayleigh Quotient

The maximization problem

$$\max_{\mathbf{x}} J(\mathbf{x}) \quad \text{subject to} \quad \mathbf{x}^\top \mathbf{x} = 1$$

is solved by a **unit eigenvector** $\mathbf{x}$ of $\mathbf{A}$ corresponding to the **largest eigenvalue** λ of $\mathbf{A}$.

Note: $-\mathbf{x}$ is also a solution.

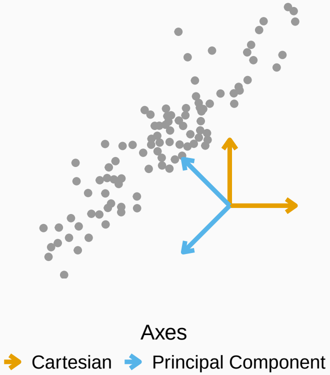
Principal Component Analysis (PCA) (I)

Goal: Given continuous data, find an orthogonal coordinate system such that the variance of the data is maximal along each direction.

Given data points $\mathbf{x}_1, \dots, \mathbf{x}_n$ and a unit vector $\mathbf{r}$, the **variance of the data along $\mathbf{r}$** is

$$S(\mathbf{r}) = \sum_{l=1}^{n} (\mathbf{r}^\top(\mathbf{x}_l - \overline{\mathbf{x}}))^2 = (n-1)\mathbf{r}^\top \widehat{\boldsymbol{\Sigma}}\mathbf{r}$$

where $\widehat{\boldsymbol{\Sigma}}$ is the empirical covariance matrix.



Principal Component Analysis (PCA) (II)

Direction with maximal variance: Find $\mathbf{r}$ such that

$$\max_{\mathbf{r}} S(\mathbf{r}) \quad \text{subject to} \quad \|\mathbf{r}\|^2 = \mathbf{r}^\top \mathbf{r} = 1$$

- This is the same problem as maximizing the **Rayleigh Quotient** for the matrix $\widehat{\boldsymbol{\Sigma}}$.
- The **solution** is the eigenvector $\mathbf{r}_1$ of $\widehat{\boldsymbol{\Sigma}}$ corresponding to the largest eigenvalue λ_1.

How do we find the other directions?

Project data on orthogonal complement of $\mathbf{r}_1$, i.e.

$$\hat{\mathbf{x}}_l = \left(\mathbf{I}_p - \mathbf{r}_1\mathbf{r}_1^\top\right)\mathbf{x}_l$$

and repeat the procedure above.

Intermezzo: Pre-processing

Data is often pre-processed before it is used in computational methods.

Given a data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, let

- $\mathbf{m}_r \in \mathbb{R}^n$ be the vector of row-means,
- $\mathbf{m}_c \in \mathbb{R}^p$ be the vector of column-means, and
- $\mathbf{s} \in \mathbb{R}^p$ be the vector of per-column standard deviations.

Then (with $\mathbf{1}_n = (1, \dots, 1)^\top \in \mathbb{R}^n$)

- the matrix $\mathbf{X} - \mathbf{m}_r \mathbf{1}_p^\top$ has row means zero (**row-centred**),
- the matrix $\mathbf{X} - \mathbf{1}_n \mathbf{m}_r^\top$ has column means zero (**column-centred**), and
- the matrix $\mathbf{X}\,\mathrm{diag}(1/\mathbf{s})$ has column standard deviations one (**standardised columns**)

Principal Component Analysis (PCA) (III)

Computational Procedure:

1. **Centre** (and possibly **standardise**) the columns of the data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$
2. Calculate the **empirical covariance matrix** $\widehat{\mathbf{\Sigma}} = \frac{1}{n-1}\mathbf{X}^\top \mathbf{X}$
3. Determine the **eigenvalues** λ_j and corresponding orthonormal **eigenvectors** $\mathbf{r}_j$ of $\widehat{\mathbf{\Sigma}}$ for $j = 1, \dots, p$ and order them such that
$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$$
4. The vectors $\mathbf{r}_j$ give the direction of the **principal components (PC)** $\mathbf{r}_j^\top \mathbf{x}$ and the eigenvalues λ_j are the **variances along the PC directions**

Note: Set $\mathbf{R} = (\mathbf{r}_1, \dots, \mathbf{r}_p)$ and $\mathbf{D} = \mathrm{diag}(\lambda_1, \dots, \lambda_p)$ then

$$\widehat{\mathbf{\Sigma}} = \mathbf{R}\mathbf{D}\mathbf{R}^\top \quad \text{and} \quad \mathbf{R}^\top\mathbf{R} = \mathbf{R}\mathbf{R}^\top = \mathbf{I}_p$$

PCA and Dimension Reduction

Recall: For a matrix $\mathbf{A} \in \mathbb{R}^{k \times k}$ with eigenvalues $\lambda_1, \ldots, \lambda_k$ it holds that

$$\operatorname{tr}(\mathbf{A}) = \sum_{j=1}^{k} \lambda_j$$

For the empirical covariance matrix $\widehat{\boldsymbol{\Sigma}}$ and the variance of the j-th feature $\mathrm{Var}[x_j]$

$$\operatorname{tr}(\widehat{\boldsymbol{\Sigma}}) = \sum_{j=1}^{p} \mathrm{Var}[x_j] = \sum_{j=1}^{p} \lambda_j$$

is called the **total variation**.

Using only the first $m < p$ principal components leads to

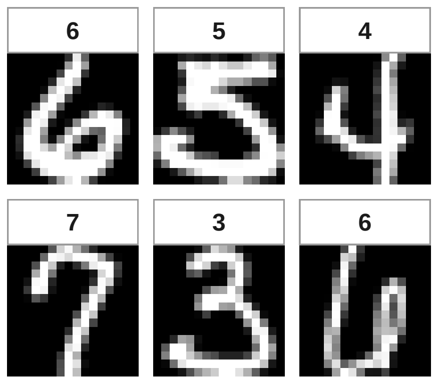
$$\frac{\lambda_1 + \cdots + \lambda_m}{\lambda_1 + \cdots + \lambda_p} \cdot 100\% \quad \text{of } \textbf{explained variance}$$

PCA and Dimension Reduction: Example (I)

Variant of the MNIST handwritten digits dataset

($n = 7291$, 16×16 greyscale images, i.e. $p = 256$)

Digit	Frequency
0	0.16
1	0.14
2	0.10
3	0.09
4	0.09
5	0.08
6	0.09
7	0.09
8	0.07
9	0.09



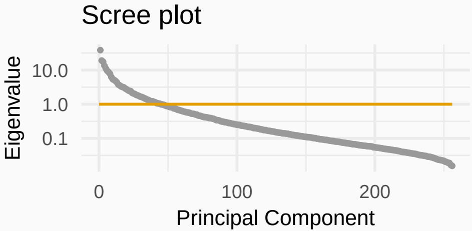
PCA and Dimension Reduction: Example (II)

For standardized variables

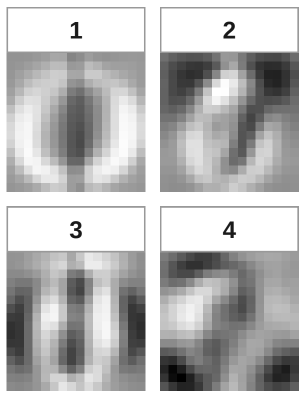
$$\operatorname{tr}(\widehat{\boldsymbol{\Sigma}}) = p$$

Typical selection rule: Components with

$$\lambda_j \geq \frac{1}{p}\operatorname{tr}(\widehat{\boldsymbol{\Sigma}}) \quad (= 1)$$



Visualisations of the first four principal components

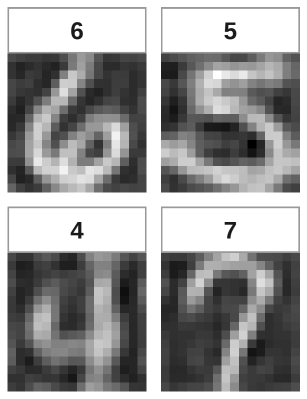


PCA and Dimension Reduction: Example (III)

Using the selection rule leads to 44 components. Using the projection

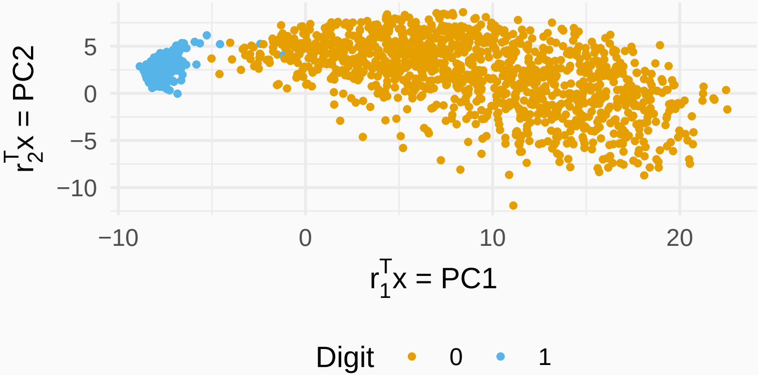
$$\hat{\mathbf{x}} = \left(\sum_{j=1}^{44} \mathbf{r}_j \mathbf{r}_j^\top \right) \mathbf{x}$$

creates a **reconstruction** of $\mathbf{x}$.



PCA and Dimension Reduction: Example (IV)

Projecting the digits onto the first two principal component directions gives a very clear distinction of digits 0 and 1.



Importance of standardisation (I)

The overall issue: **Subjectivity vs Objectivity**

(Co-)variance is scale dependent: If we have a sample (size n) of variables x and y, then their empirical covariance is

$$s_{xy} = \frac{1}{n-1} \sum_{l=1}^{n} (x_l - \overline{x})(y_l - \overline{y})$$

If x is scaled by a factor c, i.e. $z = c \cdot x$, then

$$\begin{aligned} s_{zy} &= \frac{1}{n-1} \sum_{l=1}^{n} (z_l - \overline{z})(y_l - \overline{y}) \\ &= \frac{1}{n-1} \sum_{l=1}^{n} (c \cdot x_l - c \cdot \overline{x})(y_l - \overline{y}) = c \cdot s_{xy} \end{aligned}$$

Importance of standardisation (II)

(Co-)variance is scale dependent: $s_{zy} = c \cdot s_{xy}$ where $z = c \cdot x$

- By scaling variables we can therefore make them as large/influential or small/insignificant as we want, which is a very **subjective** process
- By standardising variables we can get of rid of **scaling** and reach an **objective** point-of-view
- **Do we get rid of information?**
  - The **typical range** of a variable is compressed
  - The overall shape of the data is preserved
  - Outliers will still be outliers

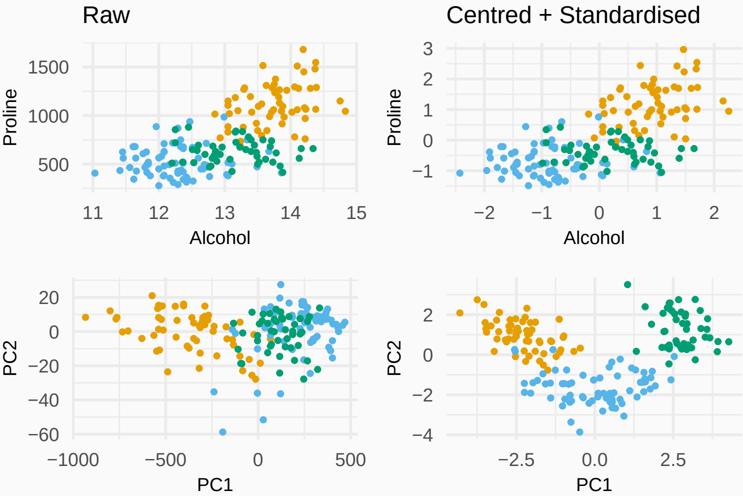
UCI Wine Data Set

UCI Wine Data Set[1]

- Results of a chemical analysis on multiple samples from three different origins of wine
- $n = 178$ samples (59 origin 1, 71 origin 2, 48 origin 3)
- $p = 13$ features
  - e.g. alcohol in %, ash, colour intensity, magnesium, …

[1] *https://archive.ics.uci.edu/ml/datasets/Wine*

Importance of standardisation (III)



Singular Value Decomposition

Singular Value Decomposition (SVD)

The **singular value decomposition (SVD)** of a matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, $n \geq p$, is

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$$

where $\mathbf{U} \in \mathbb{R}^{n \times p}$ and $\mathbf{V} \in \mathbb{R}^{p \times p}$ with

$$\mathbf{U}^\top\mathbf{U} = \mathbf{I}_p \quad \text{and} \quad \mathbf{V}^\top\mathbf{V} = \mathbf{V}\mathbf{V}^\top = \mathbf{I}_p$$

and $\mathbf{D} \in \mathbb{R}^{p \times p}$ is diagonal. Usually

$$d_{11} \geq d_{22} \geq \cdots \geq d_{pp}$$

Note: Due to the **orthogonality conditions** on $\mathbf{U}$ and $\mathbf{V}$

$$\mathbf{X}\mathbf{X}^\top\mathbf{U} = \mathbf{U}\mathbf{D}^2$$

$$\mathbf{X}^\top\mathbf{X}\mathbf{V} = \mathbf{V}\mathbf{D}^2$$

SVD and PCA

In PCA the empirical covariance matrix $\widehat{\boldsymbol{\Sigma}}$ is in focus, whereas SVD focuses on the data matrix $\mathbf{X}$ directly.

Connection: For centred variables

$$\widehat{\boldsymbol{\Sigma}} = \frac{\mathbf{X}^\top \mathbf{X}}{n-1} = \frac{\mathbf{V}\mathbf{D}\mathbf{U}^\top \mathbf{U}\mathbf{D}\mathbf{V}^\top}{n-1} = \mathbf{V}\left(\frac{\mathbf{D}^2}{n-1}\right)\mathbf{V}^\top$$

The PC directions are in $\mathbf{V}$ and the eigenvalues of $\widehat{\boldsymbol{\Sigma}}$ are $d_{jj}^2/(n-1)$.

Note: This is how PCA is typically calculated. SVD is a **more general tool** and is used in many other contexts as well.

SVD and best rank-q-approximation / dimension reduction

Write $\mathbf{u}_j$ and $\mathbf{v}_j$ for the columns of $\mathbf{U}$ and $\mathbf{V}$, respectively. Then

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top = \sum_{j=1}^{p} d_{jj} \underbrace{\mathbf{u}_j \mathbf{v}_j^\top}_{\text{rank-1-matrix}}$$

Best rank-q-approximation: For $q < p$

$$\mathbf{X}_{q} = \sum_{j=1}^{q} d_{jj} \mathbf{u}_j \mathbf{v}_j^\top$$

with **approximation error**

$$\left\| \mathbf{X} - \mathbf{X}_q \right\|_F^2 = \left\| \sum_{j=q+1}^{p} d_{jj} \mathbf{u}_j \mathbf{v}_j^\top \right\|_F^2 = \sum_{j=q+1}^{p} d_j^2$$

Cautionary Remarks

- PCA with leading eigenvectors may not preserve the signal in your data about the outcome Y - alternatives like PLS (partial least squares), CCA (canonical correlation analysis), etc.
- Pre-processing (centring and standardisation) is important if data is collected on different scales...
- but.... Is the relative scale of features a nuisance or informative?
- What about binary or categorical data?
  - Binary - may be misleading - careful about centering as well
  - Categorical/Ordinal - use one-shot encoding
  - Generalized PCA (MSE loss replaced with Deviance for the distribution family) or MCA (multiple correspondence analysis) - looking for co-occurences of factor levels.
  - Lot's of packages - even for mixed type data.

Connections to Discriminant Analysis

Discriminant Analysis and the Inverse Covariance Matrix

From PCA or SVD we get $\widehat{\boldsymbol{\Sigma}} = \mathbf{V}\mathbf{D}\mathbf{V}^\top$ where $\mathbf{V}^\top\mathbf{V} = \mathbf{V}\mathbf{V}^\top = \mathbf{I}_p$ and $d_{11} \geq \cdots \geq d_{pp} \geq 0$. Then

$$\widehat{\boldsymbol{\Sigma}}^{-1} = \mathbf{V}\mathbf{D}^{-1}\mathbf{V}^\top = \mathbf{V}\mathbf{D}^{-1/2}\mathbf{D}^{-1/2}\mathbf{V}^\top = \left(\widehat{\boldsymbol{\Sigma}}^{-1/2}\right)^\top \widehat{\boldsymbol{\Sigma}}^{-1/2}$$

where $(\mathbf{D}^{-1/2})_{jj} := 1/\sqrt{d_{jj}}$ and $\widehat{\boldsymbol{\Sigma}}^{-1/2} := \mathbf{D}^{-1/2}\mathbf{V}^\top$.

In LDA the term involving the inverse covariance matrix is then

$$\begin{aligned}(\mathbf{x} - \widehat{\boldsymbol{\mu}})^\top\widehat{\boldsymbol{\Sigma}}^{-1}(\mathbf{x} - \widehat{\boldsymbol{\mu}}) &= (\mathbf{x} - \widehat{\boldsymbol{\mu}})^\top \left(\widehat{\boldsymbol{\Sigma}}^{-1/2}\right)^\top \widehat{\boldsymbol{\Sigma}}^{-1/2}(\mathbf{x} - \widehat{\boldsymbol{\mu}}) \\ &= \left(\mathbf{V}^\top(\mathbf{x} - \widehat{\boldsymbol{\mu}})\right)^\top \mathbf{D}^{-1} \left(\mathbf{V}^\top(\mathbf{x} - \widehat{\boldsymbol{\mu}})\right) \\ &= \sum_{j=1} \frac{1}{d_{jj}}(\tilde{x}_j - \tilde{\mu}_j)^2\end{aligned}$$

Inverse of the eigenvalues can lead to **numerical instability**.

Regularised Discriminant Analysis (RDA)

The empirical covariance matrix used by LDA can be **stabilized**:

$$\widehat{\mathbf{\Sigma}}_\lambda := \widehat{\mathbf{\Sigma}} + \lambda \mathbf{I}_p = \mathbf{V}(\mathbf{D} + \lambda \mathbf{I}_p)\mathbf{V}^\top$$

where $\lambda > 0$ is a tuning parameter.

- Using $\widehat{\mathbf{\Sigma}}_\lambda$ in LDA is called **regularised discriminant analysis (RDA)**.
- Instead of $1/d_{jj}$ the scaling factors are now $1/(d_{jj} + \lambda)$.
- For small d_{jj} this can lead to **numerical stability**, whereas large d_{jj} are not much affected.
- For increasingly large λ the d_{jj} will have diminishing impact and RDA starts to become **nearest centroids**.
- RDA can be used with QDA as well by considering:

$$\widehat{\mathbf{\Sigma}}_{i,\lambda} := \underbrace{\widehat{\mathbf{\Sigma}}_i}_{\text{QDA}} + \lambda \underbrace{\widehat{\mathbf{\Sigma}}}_{\text{LDA}}$$

Take-home message

- Principal component analysis gives a convenient decomposition of the variance of the data
- Pre-processing (centring and standardisation) is important if data is collected on different scales
- Singular value decomposition is a universal workhorse for in numerical methods