Lecture 11

Vector Spaces and Singular Value Decomposition

Syllabus

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Purpose of the Lecture

View **m** and **d** as points in the space of model parameters and data

Develop the idea of transformations of coordinate axes

Show how transformations can be used to convert a weighted problem into an unweighted one

Introduce the Natural Solution and the Singular Value Decomposition

Part 1

the spaces of model parameters and data

what is a vector?

algebraic viewpoint a vector is a quantity that is manipulated (especially, multiplied) via a specific set of rules

geometric viewpoint a vector is a direction and length in space

what is a vector?

columna vector is a quantity that is manipulated (especially, multiplied) via a specific set of rules

> *geometric viewpoint* a vector is a direction and length in space in our case, a space of very high dimension



forward problem

$\mathbf{d} = \mathbf{G}\mathbf{m}$

maps an **m** onto a **d** maps a point in S(**m**) to a point in S(**d**)



inverse problem

$\mathbf{m} = \mathbf{G}^{-g}\mathbf{d}$

maps a **d** onto an **m** maps a point in S(**m**) to a point in S(**d**)



Part 2

Transformations of coordinate axes

coordinate axes are arbitrary

given *M*linearly-independent basis vectors $\mathbf{m}^{(i)}$

we can write any vector **m**^{*} as ...



... as a linear combination of these *basis vectors*



... as a linear combination of these *basis vectors*



 $\mathbf{m}_{i}^{*'} = \alpha_{i}$

might it be fair to say that the components of a vector are a column-vector ?



М $m_i^* = \sum_{i=1}^{\infty} v_j^{(i)} m_j^{*'} = \sum_{i=1}^{\infty} M_{ij} m_j^{*'}$ i=1 $\overline{i=1}$ matrix formed from basis vectors $M_{ij} = V_i^{(i)}$

transformation matrix **T**

$\mathbf{m}' = \mathbf{T}\mathbf{m}$ and $\mathbf{m} = \mathbf{T}^{-1}\mathbf{m}'$

transformation matrix **T**



different components

Q: does **T** preserve "length"? (in the sense that $\mathbf{m}^{T}\mathbf{m} = \mathbf{m}^{T}\mathbf{m}^{T}$)

 $L = \mathbf{m}^{\mathrm{T}}\mathbf{m} = \{\mathbf{T}^{-1}\mathbf{m}'\}^{\mathrm{T}}\{\mathbf{T}^{-1}\mathbf{m}'\} = \mathbf{m}'^{\mathrm{T}}\{\mathbf{T}^{-1}\mathbf{T}^{-1}\}\mathbf{m}'$

T so that $\{\mathbf{T}^{-1T}\mathbf{T}^{-1}\} = \mathbf{I}$

A: only when $\mathbf{T}^{\mathrm{T}} = \mathbf{T}^{-1}$

transformation of the model space axes

$d = Gm = GIm = [GT_m^{-1}] [T_mm] = G'm'$

d = Gmd = G'm'

same equation different coordinate system for **m**

transformation of the data space axes

$\mathbf{d'} = \mathbf{T}_{\mathrm{d}}\mathbf{d} = [\mathbf{T}_{\mathrm{d}}\mathbf{G}]\mathbf{m} = \mathbf{G''m}$

d = Gmd' = G''m

same equation different coordinate system for **d** transformation of both data space and model space axes

$d' = T_d d = [T_d G T_m^{-1}] [T_m m] = G'''m'$

Part 3

how transformations can be used to convert a weighted problem into an unweighted one

when are transformations useful?

remember this? minimize: $E + L = \mathbf{e}^{\mathrm{T}} \mathbf{W}_{e} \mathbf{e} + \mathbf{m}^{\mathrm{T}} \mathbf{W}_{m} \mathbf{m}$

when are transformations useful?

remember this? minimize: $E + L = \mathbf{e}^{\mathrm{T}} \mathbf{W}_{e} \mathbf{e} + \mathbf{m}^{\mathrm{T}} \mathbf{W}_{m} \mathbf{m}$ massage this into a pair of transformations

$\mathbf{m}^{\mathrm{T}}\mathbf{W}_{\mathrm{m}}\mathbf{m}$

$\mathbf{W}_{\mathrm{m}} = \mathbf{D}^{\mathrm{T}}\mathbf{D}$ or $\mathbf{W}_{\mathrm{m}} = \mathbf{W}_{\mathrm{m}}^{\frac{1}{2}} \mathbf{W}_{\mathrm{m}}^{\frac{1}{2}} = \mathbf{W}_{\mathrm{m}}^{\frac{1}{2}} \mathbf{W}_{\mathrm{m}}^{\frac{1}{2}}$

$\mathbf{m}^{\mathrm{T}}\mathbf{W}_{\mathrm{m}}\mathbf{m} = \mathbf{m}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\mathbf{D}\mathbf{m} = [\mathbf{D}\mathbf{m}]^{\mathrm{T}}[\mathbf{D}\mathbf{m}]$

when are transformations useful?

remember this? minimize: $E + L = \mathbf{e}^{\mathrm{T}} \mathbf{W}_{e} \mathbf{e} + \mathbf{m}^{\mathrm{T}} \mathbf{W}_{m} \mathbf{m}$

massage this into a pair of transformations

 $e^{T}W_{e}e$

 $W_e = W_e^{\frac{1}{2}} W_e^{\frac{1}{2}} = W_e^{\frac{1}{2}T} W_e^{\frac{1}{2}}$ OK since W_e symmetric

 $\mathbf{e}^{\mathrm{T}}\mathbf{W}_{\mathrm{e}}\mathbf{e} = \mathbf{e}^{\mathrm{T}}\mathbf{W}_{\mathrm{e}}^{\frac{1}{2}\mathrm{T}}\mathbf{W}_{\mathrm{e}}^{\frac{1}{2}}\mathbf{e} = [\mathbf{W}_{\mathrm{e}}^{\frac{1}{2}\mathrm{m}}]^{\mathrm{T}}[\mathbf{W}_{\mathrm{e}}^{\frac{1}{2}\mathrm{m}}]$

we have converted weighted least-squares minimize: $E + L = \mathbf{e}^{T} \mathbf{W}_{e} \mathbf{e} + \mathbf{m}^{T} \mathbf{W}_{m} \mathbf{m}$

into unweighted least-squares minimize: $E' + L' = e'^{T}e' + m'^{T}m'$

steps

- 1: Compute Transformations $\mathbf{T}_{m} = \mathbf{D} = \mathbf{W}_{m}^{\frac{1}{2}}$ and $\mathbf{T}_{e} = \mathbf{W}_{e}^{\frac{1}{2}}$
- 2: Transform data kernel and data to new coordinate system

$$\mathbf{G}''' = [\mathbf{T}_{e}\mathbf{G}\mathbf{T}_{m}^{-1}] \text{ and } \mathbf{d}' = \mathbf{T}_{e}\mathbf{d}$$

3: solve $\mathbf{G'''} \mathbf{m'} = \mathbf{d'}$ for $\mathbf{m'}$ using unweighted method

4: Transform **m'** back to original coordinate system $m=T_m^{-1}m'$

steps extra work 1: Compute Transformations $T_m = D = W_m^{\frac{1}{2}}$ and $T_e = W_e^{\frac{1}{2}}$

- 2: Transform data kernel and data to new coordinate system $G''' = [T_e G T_m^{-1}]$ and $d' = T_e d$
- 3: solve $\mathbf{G'''} \mathbf{m'} = \mathbf{d'}$ for $\mathbf{m'}$ using unweighted method
- 4: Transform **m'** back to original coordinate system $m=T_m^{-1}m'$

steps 1: Compute Transformations $T_m = D = W_m^{\frac{1}{2}}$ and $T_e = W_e^{\frac{1}{2}}$

2: Transform data kernel and data to new coordinate system

$$\mathbf{G}^{\prime\prime\prime} = [\mathbf{T}_{e}\mathbf{G}\mathbf{T}_{m}^{-1}] \text{ and } \mathbf{d}^{\prime} = \mathbf{T}_{e}\mathbf{d}$$

3: solve $\mathbf{G'''} \mathbf{m'} = \mathbf{d'}$ for $\mathbf{m'}$ using unweighted method

4: Transform **m'** back to original coordinate system $m=T_m^{-1}m'$

Part 4

The Natural Solution and the Singular Value Decomposition (SVD)



suppose that we could divide up the problem like this ...





$$L = \mathbf{m}^{\mathrm{T}}\mathbf{m} = [\mathbf{m}_{\mathrm{p}} + \mathbf{m}_{0}]^{\mathrm{T}}[\mathbf{m}_{\mathrm{p}} + \mathbf{m}_{0}] = \mathbf{m}_{\mathrm{p}}^{\mathrm{T}}\mathbf{m}_{\mathrm{p}} + \mathbf{m}_{0}^{\mathrm{T}}\mathbf{m}_{0}$$
$$E = [\mathbf{d}_{\mathrm{p}} + \mathbf{d}_{0} - \mathbf{G}\mathbf{m}_{\mathrm{p}}]^{\mathrm{T}}[\mathbf{d}_{\mathrm{p}} + \mathbf{d}_{0} - \mathbf{G}\mathbf{m}_{\mathrm{p}}] = [\mathbf{d}_{\mathrm{p}} - \mathbf{G}\mathbf{m}_{\mathrm{p}}]^{\mathrm{T}}[\mathbf{d}_{\mathrm{p}} - \mathbf{G}\mathbf{m}_{\mathrm{p}}] + \mathbf{d}_{0}^{\mathrm{T}}\mathbf{d}_{0}$$



$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

$$\begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{d}_{p} - \mathbf{G}\mathbf{m}_{p} \end{bmatrix}^{T} + \mathbf{d}_{0}^{T} \mathbf{d}_{0}$$

natural solution

determine \mathbf{m}_{p} by solving \mathbf{d}_{p} - $\mathbf{G}\mathbf{m}_{p}$ =0

set $\mathbf{m}_0 = \mathbf{0}$





Singular Value Decomposition (SVD)

 $\mathbf{G} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathrm{T}}$

$N \times N$ matrix of eigenvectors $\mathbf{U} = \begin{bmatrix} \mathbf{u}^{(1)} & \mathbf{u}^{(2)} & \mathbf{u}^{(3)} & \cdots & \mathbf{u}^{N} \end{bmatrix}$

$M \times M \text{ matrix of eigenvectors}$ $\mathbf{V} = \begin{bmatrix} \mathbf{v}^{(1)} & \mathbf{v}^{(2)} & \mathbf{v}^{(3)} & \dots & \mathbf{v}^M \end{bmatrix}$ $\Lambda \text{ is an } N \times M \text{ diagonal matrix}$

singular value decomposition

 $\mathbf{G} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathrm{T}}$

$\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{I}$ and $\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}$



suppose only $p \lambda$'s are non-zero

$\boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_{\mathrm{p}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}$

suppose only $p \lambda$'s are non-zero



$\mathbf{U}_{p}^{T}\mathbf{U}_{p}=\mathbf{I} \text{ and } \mathbf{V}_{p}^{T}\mathbf{V}_{p}=\mathbf{I}$ since vectors mutually pependicular and of unit length

$\mathbf{U}_{p}\mathbf{U}_{p}^{T} \neq \mathbf{I}$ and $\mathbf{V}_{p}\mathbf{V}_{p}^{T} \neq \mathbf{I}$ since vectors do not span entire space

The part of **m** that lies in V_0 cannot effect **d**

$\mathbf{d} = \mathbf{G}\mathbf{m} = \mathbf{U}_{\mathrm{p}}\mathbf{\Lambda}_{\mathrm{p}}\mathbf{V}_{\mathrm{p}}^{\mathrm{T}}\mathbf{m}$

since $\mathbf{V}_{\mathbf{p}}^{\mathsf{T}}\mathbf{V}_{\mathbf{0}}=\mathbf{0}$

so \mathbf{V}_0 is the model null space

The part of **d** that lies in \mathbf{U}_0 cannot be affected by **m**

 $\mathbf{d} = \mathbf{G}\mathbf{m} = \mathbf{U}_{\mathrm{p}}\mathbf{\Lambda}_{\mathrm{p}}\mathbf{V}_{\mathrm{p}}^{\mathrm{T}}\mathbf{m}$

since $\Lambda_p V_p^T m$ is multiplied by U_p and $U_0^T U_p^T = 0$

so \mathbf{U}_0 is the data null space

The Natural Solution

$\mathbf{m}^{\text{est}} = \mathbf{V}_{\text{p}} \mathbf{\Lambda}_{\text{p}}^{-1} \mathbf{U}_{\text{p}}^{\text{T}} \mathbf{d}$

The part of \mathbf{m}^{est} in \mathbf{V}_0 has zero length

 $\mathbf{V}_0^{\mathrm{T}}\mathbf{m}^{\mathrm{est}} = \mathbf{V}_0^{\mathrm{T}}\mathbf{V}_{\mathrm{p}}\mathbf{\Lambda}_{\mathrm{p}}^{-1}\mathbf{U}_{\mathrm{p}}^{\mathrm{T}}\mathbf{d} = \mathbf{0}$

The error has no component in \mathbf{U}_{p}

 $\mathbf{U}_{p}^{T}\mathbf{e} = \mathbf{U}_{p}^{T}[\mathbf{d} - \mathbf{G}\mathbf{m}^{est}] = \mathbf{U}_{p}^{T}[\mathbf{d} - \mathbf{U}_{p}\boldsymbol{\Lambda}_{p}\mathbf{V}_{p}^{T}\mathbf{V}_{p}\boldsymbol{\Lambda}_{p}^{-1}\mathbf{U}_{p}^{T}\mathbf{d}]$ $= \mathbf{U}_{p}^{T}[\mathbf{d} - \mathbf{U}_{p}\mathbf{U}_{p}^{T}\mathbf{d}] = \mathbf{U}_{p}^{T}\mathbf{d} - \mathbf{U}_{p}^{T}\mathbf{d} = \mathbf{0}$

computing the SVD

[U, L, V] = svd(G); lambda = diag(L);

determining p use plot of λ_i vs. *i*

however

case of a clear division between $\lambda_i > 0$ and $\lambda_i = 0$ rare



Natural Solution

and the model parameters are estimated as

mest = Vp*((Up'*dobs)./lambdap);



resolution and covariance

$$\mathbf{R} = \mathbf{G}^{-g}\mathbf{G} = \{\mathbf{V}_{p}\boldsymbol{\Lambda}_{p}^{-1}\mathbf{U}_{p}^{T}\}\{\mathbf{U}_{p}\boldsymbol{\Lambda}_{p}\mathbf{V}_{p}^{T}\} = \mathbf{V}_{p}\mathbf{V}_{p}^{T}$$
$$\mathbf{N} = \mathbf{G}\mathbf{G}^{-g} = \{\mathbf{U}_{p}\boldsymbol{\Lambda}_{p}\mathbf{V}_{p}^{T}\}\{\mathbf{V}_{p}\boldsymbol{\Lambda}_{p}^{-1}\mathbf{U}_{p}^{T}\} = \mathbf{U}_{p}\mathbf{U}_{p}^{T}$$

$$= \sigma_d^2 \{ \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \} \{ \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \}^T = \sigma_d^2 \mathbf{V}_p \mathbf{\Lambda}_p^{-2} \mathbf{V}_p^T$$

resolution and covariance

$$\mathbf{R} = \mathbf{G}^{-g}\mathbf{G} = \{\mathbf{V}_{p}\boldsymbol{\Lambda}_{p}^{-1}\mathbf{U}_{p}^{T}\}\{\mathbf{U}_{p}\boldsymbol{\Lambda}_{p}\mathbf{V}_{p}^{T}\} = \mathbf{V}_{p}\mathbf{V}_{p}^{T}$$

$$\mathbf{N} = \mathbf{G}\mathbf{G}^{-g} = \big\{\mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T\big\}\!\big\{\mathbf{V}_p\mathbf{\Lambda}_p^{-1}\mathbf{U}_p^T\big\} = \mathbf{U}_p\mathbf{U}_p^T$$

 $[\operatorname{cov} \mathbf{m}^{\operatorname{est}}] = \mathbf{G}^{-g}[\operatorname{cov} \mathbf{d}]\mathbf{G}^{-gT} =$

$$= \sigma_d^2 \{ \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \} \{ \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \}^T = \sigma_d^2 \mathbf{V}_p \mathbf{\Lambda}_p^{-2} \mathbf{V}_p^T$$

large covariance if any λ_p are small

Is the Natural Solution the best solution?

Why restrict a priori information to the null space

when the data are known to be in error?

A solution that has slightly worse error but fits the a priori information better might be preferred ...