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# Headquarters U.S. Air Force

*Integrity - Service - Excellence*

## *Design of Experiments ( DOE ) for Validation of STORM Based on THUNDER*

**73rd MORSS, USMA 2005**
**WG 25 & 29**

**Mr. Tom Chwastyk**
**AFSAA/SAAT**

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STORM

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# Purpose

- THUNDER vs. STORM
- Goal of DOE here: V&V by comprehensive comparison
  - Why not VV&A?
- General and specific models of the V&V experiment
- DOE for adequate excitation to compare responses
  - Screening to reduce response model size
  - Adding design points to check for interactions
- Comparing THUNDER and STORM response
  - By Singular Value Decomposition
  - By Canonical Correlation
- Automating execution of runs and extraction of results
  - Work in progress – all feedback welcome
- Punch line: Massive quantitative validation experiment – uses computers and sophisticated techniques to exceed past human limits on data production and interpretation

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# THUNDER vs. STORM

- THUNDER: accepted standard
  - Not Government owned
  - Proprietary engine, SIMSCRIPT
    - CACI licenses – big $$$ / seat / year
  - Ground war:
    - "Pistons" define FLOT
    - Piston walls do not reorient as FLOT distorts
  - No study manager -- manual file configuration control
  - Minimal GUI
  - Minimal ISR

- STORM: AFSAA's next standard
  - Government owned
  - Open source, non-proprietary
    - Simulation engine in g++ ; maps, DB tools; even OS, all open
    - No per-seat license fees
  - Ground war:
    - Along arcs and within nodes
    - Shape of FLOT morphs naturally under network constraints
  - Study manager automates file configuration control
  - Extensive GUI – map tool, report tool, graph tool
  - Sat tool and other significant ISR developments

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# *V&V by Comparison (Not VV&A?)*

- **V&V**
  - **Verification: "Solve the Problem Right"**
    - **Identify and fix lurking code problems**
  - **Validation: "Solve the Right Problem"**
    - **Accepted referent is THUNDER but comparison is a hard problem**
  - **Comparison needed <u>over a set of scenarios of interest</u>**
    - **Are results "comparable to or better than" THUNDER? Just what does that mean?**
      - SME's "face validation" vs. statistical tools – both are needed
    - **Does DOE show effects of changes in STORM vs. THUNDER?**
- **Why V&V, not VV&A?**
  - **A ( Accreditation ) is PM's decision – balancing risk versus resources**
    - **Too little V&V: low resource expenditure but high risk**
    - **Too much V&V: little risk reduction for last expenditures**

# A General Model of an Experiment

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Excitation

What one offers up to Nature to excite a response

*Prior* = *before* running the experiment or getting the data

Prior "knowledge" or Belief

PURPOSE

Posterior "knowledge" or Belief

*Posterior* = *after* getting the data

Where and how one samples Nature's response

Response Sampling

# …Tailored to V&V and Comparison

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STORM uses next generation THUNDER campaign model

Excitation

Excitation is the set of scenarios, each with its experimental design and with levels for factors: <u>the INPUTS</u>

Prior knowledge or Belief

**PURPOSE**

Posterior knowledge or Belief

Response Sampling is MOMs + dofs extracted from simulation: <u>the OUTPUTS</u>

Response Sampling

**STORM improves on THUNDER – it's a good replacement**

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# V&V Scenario Set of Interest

- Consult with SMEs, see for what campaign models/scenarios THUNDER results (inputs and outputs) are already available and of interest
  - THUNDER has been much more expensive to run (small error ⇒ typically 60-100 reps) than STORM – hence, minimize additional THUNDER runs
- Choose among available THUNDER campaigns to agree on sufficiently complete V&V scenario set
- If necessary, add THUNDER or STORM work to achieve common and complete set of scenarios of significant interest for V&V

# Need to Reduce Input Dimensions

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| | | | |
|---|---|---|---|
| THUNDER | v6.9 | 99 | *.dat files |
| STORM | v1.3 | 115 | *.dat files (plus path.dat) |

- Typical .dat file has 10 to 1000+ parameters (inputs) – highly interrelated, often nonlinearly
- Too many parameters to screen individually
  - Use SME's to combine (cull?) inputs into fewer (10 to 100) factors $f_i \equiv_{def} [\, p_{i,j'} \,]$ parameter vectors
  - $p_{i,j}$ , $p_{i,k \neq j}$ need not be in same .dat file
  - Each parameter in a factor has two levels, A / B – goes A / B as its factor goes high / low – no "within-factor interactions"
- Factor screening takes place in STORM across entire V&V scenario set at once
- Whether the change in level of factor $f_i$ is significant depends both on the scenario set and on what MOM(s) or output dof(s) are of interest

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# Input Sensitivity Screening

- Initial screening in STORM of two-level factors
  - Resolution V (preferred) or IV (if necessary) fractional factorial (FF) – possibly even res. III for initial stab?
    - If resolution IV necessary, follow up with resolution V (res. IV significant factors only, plus all 2-factor interactions) to screen for significant interactions
  - 256 reps ( resolution IV ) $\Rightarrow$ up to 128 factors
    - Comparable to # of reps in STORM V&V reports for previous releases ( 19 + cases x 10 repeated reps / case )
    - Likely fewer factors ($\leq$64, $\leq$32) if long reps ($t_{sim}$>>10 days)
  - ***<u>However</u>***, 256 reps ( resolution V ) $\Rightarrow$ <u>only 12 to 17</u> factors ( + all 2-level interactions )
- In any case –
  - NOT One-Factor-At-a-Time as before!
  - NO replicated design points (reps)!

# Matrix Model Equations

$$\mathbf{Y} = \mathbf{XB} + \mathbf{E}$$

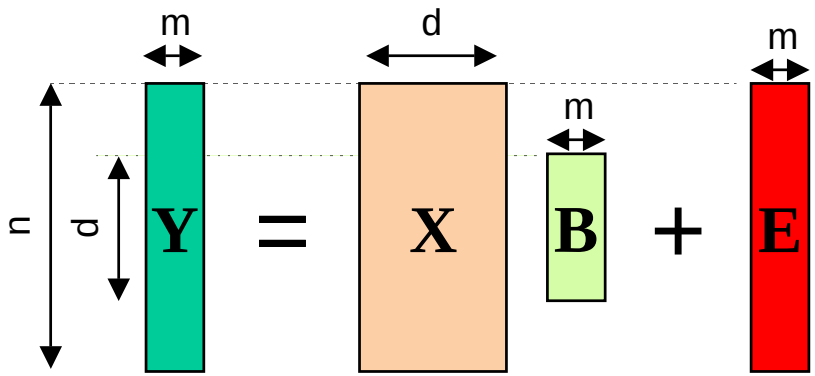
$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{B}} + \hat{\mathbf{E}}(\mathbf{s})$$

$$\hat{\mathbf{E}}'_i = \left[ f_1(s_i) \ \cdots \ f_j(s_i) \ \cdots \ f_m(s_i) \right]'$$

$\hat{\mathbf{B}}$ is by least squares, minimizes

$$rss = \Sigma_i \Sigma_j (y_{ij} - \hat{y}_{ij})^2$$

# Not Your Usual Few Responses




m = # of response variables

d = # of design variables ( factors )

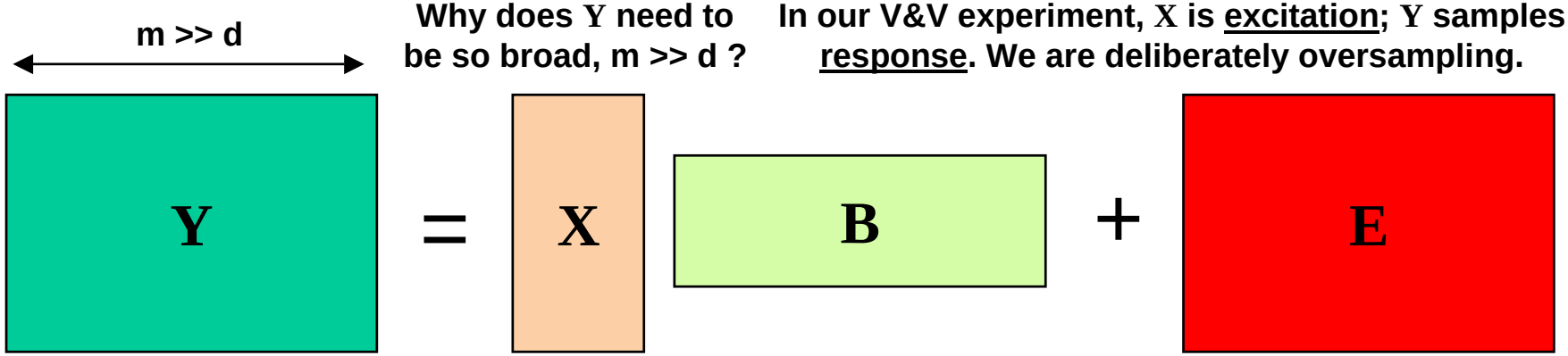
n = # of runs

n > d (always)

m << d (usually)

**Why does Y need to be so broad, m >> d ?**

**In our V&V experiment, X is <u>excitation</u>; Y samples <u>response</u>. We are deliberately oversampling.**




**We oversample by several times the dimensionality of our excitation in a "shotgun approach", hoping we catch most of the significant dimensions of model response.**

# Why Fit Is Always Too Good

$$\mathbf{Y} = \mathbf{X}\,\mathbf{B} + \mathbf{E}$$

$$\hat{\mathbf{Y}} = \mathbf{X}\,\hat{\mathbf{B}} + \hat{\mathbf{E}}$$

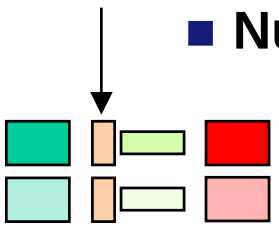
$$\mathbf{X}'\,\mathbf{E} \neq 0 = \mathbf{X}'\,\hat{\mathbf{E}}$$

# Elements of Matrix Model

- Starts as typical multivariate response model
  - Response matrix $\mathbf{Y}$ (n×m)
  - Design matrix $\mathbf{X}$ (n×d)
  - Effects matrix $\mathbf{B}$ (d×m)
  - "Out-of-model" matrix $\mathbf{E}$ (n×m)
  - Estimates "hatted": $\hat{\mathbf{E}}$ , $\hat{\mathbf{B}}$
- Beyond typical model:
  - *Compute* $\mathbf{Y}$ from $\mathbf{X}$ in permuted order $pco^{(1)}$, $pco^{(2)}$, $pco^{(3)}$, but *record* $\mathbf{Y}$ in design order (picture of $\mathbf{Y}$, $pco_i$ , $pco^{(i)}$ later)
  - Record random seed and permuted computational order [ $s_i$ $pco_i$ ] for row $i$ (nx2)

# Design Matrix X - Words

- **ROWS in the design matrix X**
  - Give particular combination of factor levels for each design point
  - Cover all scenarios of interest
  - Contain a non-zero entry in only one of the columns indicating scenarios
- **COLUMNS in the design matrix X**
  - Signify design (input) factors
  - Signify scenarios for estimating mean
    - Decompose sum of squares due to scenario means
    - Number of means is included in d, # of design variables



# Design Matrix - Picture

**X**

| scenario # 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 factor level |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 1 | 3 | 5 | 7 | 2 | 8 |
| 1 | 0 | 0 | 0 | 2 | 4 | 6 | 7 | 2 | 8 |
| 1 | 0 | 0 | 0 | 2 | 4 | 5 | 7 | 2 | 8 |
| 1 | 0 | 0 | 0 | 1 | 3 | 6 | 7 | 2 | 8 |
| 0 | 1 | 0 | 0 | 1 | 3 | 5 | 8 | 7 | 1 |
| 0 | 1 | 0 | 0 | 2 | 4 | 6 | 8 | 7 | 1 |
| 0 | 1 | 0 | 0 | 2 | 4 | 5 | 8 | 7 | 1 |
| 0 | 1 | 0 | 0 | 1 | 3 | 6 | 8 | 7 | 1 |
| 0 | 0 | 1 | 0 | 1 | 3 | 6 | 8 | 7 | 8 |
| 0 | 0 | 1 | 0 | 1 | 3 | 5 | 8 | 2 | 1 |
| 0 | 0 | 1 | 0 | 1 | 3 | 6 | 7 | 7 | 8 |
| 0 | 0 | 1 | 0 | 1 | 4 | 5 | 7 | 2 | 1 |
| 0 | 0 | 1 | 0 | 1 | 4 | 6 | 8 | 7 | 8 |
| 0 | 0 | 1 | 0 | 1 | 4 | 5 | 7 | 2 | 1 |
| 0 | 0 | 0 | 1 | 1 | 4 | 6 | 8 | 2 | 8 |
| 0 | 0 | 0 | 1 | 2 | 3 | 6 | 7 | 2 | 8 |
| 0 | 0 | 0 | 1 | 1 | 3 | 6 | 8 | 2 | 1 |
| 0 | 0 | 0 | 1 | 2 | 3 | 5 | 7 | 7 | 1 |
| 0 | 0 | 0 | 1 | 1 | 3 | 5 | 7 | 7 | 8 |
| 0 | 0 | 0 | 1 | 2 | 4 | 5 | 8 | 7 | 8 |

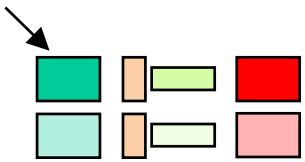
constant factor level within scenario says significance of factor is not tested within scenario

1's account for scenario means, ssq

Notional design only, not $2^{k-p}$

# Response Matrix Y - Words

- **ROWS in the response matrix Y**
  - **Correspond to design matrix rows**
- **COLUMNS in the response matrix Y signify**
  - **Scalar or vector MOMs / dofs**
  - **Consistent responses for each row and scenario**
    - **Squadrons or other entity types handled differently by planning files on different design points should <u>not</u> re-use the same response columns <u>unless</u>**
      - **the difference in response due to difference in planning file parameters is the effect being sought and**
      - **the difference in planning file parameters is reflected in one or more factors**



# Response Matrix - Picture

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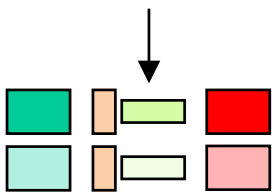
| pco $^{(i)}$ | pco $_i$ | scenario # | i = row # in X | Scalar MOM 1 | Scalar MOM 2 | Scalar MOM 3 | Vector dof 1 day 1 | Vector dof 1 day 2 | Vector dof 1 day 3 | … | Vector dof 1 day n-1 | Vector dof 1 day n | Scalar MOM 4 | Vector dof 2 day 1 | Vector dof 2 day 2 | Vector dof 2 day 3 | … | Vector dof 2 day n-1 | Vector dof 2 day n | Scalar MOM 5 | Vector dof 3 day 1 | Vector dof 3 day 2 | … | Vector dof 3 day n-1 | Vector dof 3 day n | Vector dof 4 day 1 | … etc. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 14 | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | |
| 11 | 3 | 1 | 2 | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | 5 | 1 | 3 | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | 9 | 1 | 4 | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | 11 | 2 | 5 | | | | | | | | | | | | | | | | | | | | | | | | |
| 10 | 12 | 2 | 6 | | | | | | | | | | | | | | | | | | | | | | | | |
| 12 | 4 | 2 | 7 | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | 8 | 2 | 8 | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | 13 | 3 | 9 | | | | | | | | | | | | | | | | | | | | | | | | |
| 14 | 6 | 3 | 10 | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | 2 | 3 | 11 | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | 7 | 3 | 12 | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | 1 | 3 | 13 | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 | 10 | 4 | 14 | | | | | | | | | | | | | | | | | | | | | | | | |
| … | … | … | … | | | | | | | | | | | | | | | | | | | | | | | | |

Y

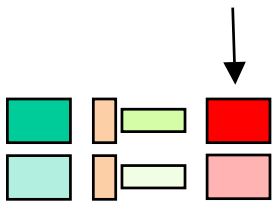
# Effects Matrix B, B hat

- ROWS in the effects matrix B
  - Correspond to design variables
  - For SME-aggregated factors, coefficient shows effect of change in level
  - For scenario indicator variables, coefficient shows scenario mean for each response
- COLUMNS in the effects matrix B
  - Correspond to response MOMs, dofs



# Out-of-Model Matrix E, E hat

- Part of E is assumed due to stochastic effects
  - Neither random seed value $s_i$ nor its effect $f_j(s_i)$ on each response $y_{ij}$ is known to the fitting process
  - $s_i$ and $f_j(\bullet)$ — hence $f_j(s_i)$ — are termed <u>exo</u>genous (excluded from model)
- Effects of exogenous variables, *including stochastic effects*, alias to an unknown extent onto <u>endo</u>genous (included in model) effects $b_j$



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# Interactions, Response Surface

- Once factors and 2-factor interactions are identified as significant at resolution V, high-low level only …
- Add intermediate levels as appropriate to gain Response Surface Model (RSM)
  - Central composite design if appropriate
- Retain only <u>statistically</u> significant factors (and interactions) for comparing STORM to THUNDER
  - Not normal statistical practice to "cherry pick" interactions without physical model justification
  - Empirically justifiable because RSM is <u>descriptive</u> only, not first principles
  - We are a long way off from this

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# Dimension Reduction (1): RSM

- Add face and center points for significant factors to get central composite design if feasible
- Possibly use intermediate points for near-orthonormal Latin Square
- Get response surface model (RSM) – polynomial or spline
  - Stop on Mallow's $C_p$ or other measure of complexity vs. goodness of fit
- <u>Retains coordinates of original model space</u>

# Weight Questions (1)

- **Question 1: What is the proper weight or scale per MOM / dof(s) in the penalty function for lack of fit?**
  - **That is, how much should lack of fit in one column (or set of columns) of Y count relative to lack of fit in another column (or set of columns)?**
- **Question 2: Same as Question 1 but for one scenario (set of rows) versus another**

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# Weight Answers (Partial) (2)

- Depends on user goal and on STORM / THUNDER comparison approach
  - Data for SVD, canonical correlation should have zero scenario mean
  - Appears no natural scale for Singular Value Decomposition (SVD); use unit column variance for consistency with canonical correlation
  - Scale set to unit column variance by definition of canonical correlation, but meaning and appropriateness to user goal are not clear
  - Beware augury / mysticism / wise chin-scratching

# Equations in Passing

- Final dry run for this brief commented that there were way too many equations, too few graphics
- Graphics proved far more time consuming to produce than initially expected
- Equations were retained more as art objects and speaking totems than as detailed communication tools
- Equations past the basic “Matrix Model Equations” will not be on the midterm or the final

# Dim. Red. (2): SVD (1)

- **Singular Value Decomposition (SVD) on responses Y adjusted to zero-scenario-mean, scaled to unit Y column norm, and transposed*:**

* not a good idea, but not fatal

$$\underset{(n\times m)}{\mathbf{Y}_{zsm}} = \mathbf{Y}(\mathbf{I}_n - \underbrace{\mathbf{X}_{sm}(\mathbf{X}_{sm}'\mathbf{X}_{sm})^{-1}\mathbf{X}_{sm}'}_{\mathbf{X}_{sm}\,=\,\text{only columns for scenario means}})$$

$$\underset{(m\times n)}{\mathbf{A}} = \left(\hat{\mathbf{Y}}_{zsm}\right)', \left(\hat{y}_{zsm}\right)_{ij} = \left(y_{zsm}\right)_{ij} \Big/ \sqrt{\sum_{i'=1}^{n}\left(y_{zsm}\right)_{i'j}^{2}}$$

$$\mathbf{A} = \mathbf{ODV}' \begin{cases} \mathbf{O}'\mathbf{O} = \mathbf{I}_n, (m > n) \Rightarrow \mathbf{OO}' \neq \mathbf{I}_m \\ \mathbf{D}\ \text{diagonal, p.s.d.}, (i < j) \Rightarrow (d_{ii} \geq d_{jj}) \\ \mathbf{VV}' = \mathbf{V}'\mathbf{V} = \mathbf{I}_n \end{cases}$$

# … SVD (2)

- **Continuing,**

$$\mathbf{A}'\mathbf{A} = \mathbf{Z} = \mathbf{V}\mathbf{D}'\mathbf{O}'\mathbf{O}\mathbf{D}\mathbf{V}'$$

$$= \mathbf{V}\mathbf{D}^2\mathbf{V}'$$

$$\mathbf{Z}\mathbf{V} = \mathbf{V}\mathbf{D}^2\mathbf{V}'\mathbf{V} = \mathbf{V}\mathbf{D}^2$$

$$\mathbf{Z}\mathbf{V} = \mathbf{V}\boldsymbol{\Lambda} \quad \text{(symmetric eigenproblem)}$$

$$d_{ii} = \sqrt{\lambda_i} \quad (\text{sorted } \lambda_1 \geq \lambda_2 \geq \ldots \lambda_n \geq 0)$$

$$\mathbf{O}_i = \mathbf{A}\mathbf{V}_i d_{ii}^{-1} \quad \text{canonical column } i \text{ of } \mathbf{A} \text{ for } d_{ii} > 0$$

- **Why is this significant?**

# … SVD (3)

- **This is significant *because*…**

$$\mathbf{A} = \mathbf{ODV}' = \sum d_{ii}\mathbf{OV}' \text{ (exactly!) and}$$

$$\sum_j \sum_k (\mathbf{O}_i \mathbf{V}_i')^2_{jk} = \sum_j \sum_k (o_{ji} v_{ik})^2 = \sum_j o_{ji}^2 \sum_k v_{ik}^2 = 1,$$

**so all scale information is in the "singular values" $d_{ii}$ in the sense that $d_{ii}^2$ shows how many unit rows of $\mathbf{A}$ are expressed by $d_{ii}\mathbf{V}'_i$.**

- **This means that the completeness $R^2(k,m)$ of expressing all $m$ unit rows of the response matrix $\mathbf{A}$ using only $k$ coefficients is**

$$R^2_{k,m} = \left(\sum_{i=1}^{k} d_{ii}^2\right) \Big/ \left(\sum_{i'=1}^{m} d_{i'i'}^2\right)$$

- **More on SVD follows after discussion on Canonical Correlation**

# DR (3): Canonical Correlation (1)

- Two response sets, say $\mathbf{T}=\hat{\mathbf{Y}}'_T$ for THUNDER and $\mathbf{S}=\hat{\mathbf{Y}}'_S$ for STORM
- $m$ ROWS of $\mathbf{T}$, $\mathbf{S}$
  - Zero scenario mean, unit variance as for SVD
  - Same row $\Leftrightarrow$ same MOM or dof for $\mathbf{T}$ as for $\mathbf{S}$
- $n$ COLUMNS of $\mathbf{T}$, $\mathbf{S}$ are in same order as design matrix rows, although design points were computed in permuted sequence(s)

# … CanCorr (2)

- **Canonical correlation (CanCorr) gives $m \times 2$ coefficients [ $\mathbf{lca}_k$ $\mathbf{lcb}_k$ ] for successive $n \times 2$ linear composites [ $\mathbf{u}_k$ $\mathbf{w}_k$ ], such that for $\mathbf{u}_k' = \mathbf{lca}_k'\mathbf{T}$, $\mathbf{w}_k' = \mathbf{lcb}_k'\mathbf{S}$, $k = 1, 2, \ldots, \min(m,n)$**
  - **$\mathbf{u}_k$ and $\mathbf{w}_k$ have maximal correlation $\rho^*_k$ between any two linear composites of $\mathbf{T}$, $\mathbf{S}$ <u>not</u> spanned by $[\mathbf{u}_1\ \mathbf{u}_2\ \ldots\ \mathbf{u}_{k-1}]'$, $[\mathbf{w}_1\ \mathbf{w}_2\ \ldots\ \mathbf{w}_{k-1}]'$**
  - **$\mathrm{Var}(\mathbf{u}_k) = \mathrm{Var}(\mathbf{u}_k) = 1$**
  - **$\rho^*_1 \geq \rho^*_2 \geq \rho^*_3 \geq \ldots \rho^*_{\min(m,n)} \geq 0$**
  - **For $j > k$, $\mathbf{u}_j$ and $\mathbf{w}_k$ are uncorrelated, i.e.,**

$$\mathbf{u}_j'(\mathbf{I} - \mathbf{1}(\mathbf{1}'\mathbf{1})^{-1}\mathbf{1}')\,\mathbf{w}_k = 0$$

# … CanCorr (3)

- **How does this work? From the zero scenario means, unit row norms, and definition of variance we get**

$$\underset{(2m\times 1)}{\mathbf{0}} = \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \end{bmatrix} \underset{(n\times 1)}{\mathbf{1}}$$

$$\underset{(2m\times 2m)}{\boldsymbol{\Sigma}} = \frac{1}{n - n_{zsm}} \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \end{bmatrix}'$$

$$= \begin{pmatrix} \boldsymbol{\Sigma}_{\mathbf{TT}} & \boldsymbol{\Sigma}_{\mathbf{TS}} \\ \boldsymbol{\Sigma}_{\mathbf{ST}} & \boldsymbol{\Sigma}_{\mathbf{SS}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}$$

# … CanCorr (4)

- **Then it can be shown in about 3 textbook pages that**

$$\begin{bmatrix} \mathbf{u}_k \\ \mathbf{w}_k \end{bmatrix} = \begin{bmatrix} \underbrace{\mathbf{e}_k{}'\boldsymbol{\Sigma}_{11}^{-1/2}}_{\mathbf{lca}_k}\mathbf{T} \\ \underbrace{\mathbf{f}_k{}'\boldsymbol{\Sigma}_{22}^{-1/2}}_{\mathbf{lcb}_k}\mathbf{S} \end{bmatrix}, \text{ where}$$

$\mathrm{Corr}(\mathbf{u}_k, \mathbf{w}_k) = \rho_k^*$ is the $k^{\text{th}}$ largest eigenvalue of

$\boxed{\boldsymbol{\Sigma}_{11}^{-1/2}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1/2}}$, with eigenvector $\mathbf{e}_k$, and also of

$\boxed{\boldsymbol{\Sigma}_{22}^{-1/2}\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1/2}}$, with eigenvector $\mathbf{f}_k$.

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# … CanCorr (5)

- **First approach will be to look at initial canonical variables (cv's) as long as $\rho_k$ are well separated**
  - **If $\rho_k$ are closely spaced, eigenvectors and hence cv's are determined only up to rotations**
- **Second approach will be to look at residuals once projections on all cv's from 1 to k are removed, for k's such that**
  - **k is not in the middle of a closely spaced block of $\rho_k$**
  - **k is not so far beyond 1 that any patterns apparent in residuals are as likely to be artifacts of numerical methods as of remaining THUNDER vs. STORM relationships**
- **<u>We have not done this before; any advice would be welcome.</u>**

# SVD versus CanCorr: SVD (4)

- $\mathbf{A'A} = \mathbf{Z}$ of the SVD development can now be seen as $\Sigma_{22}$ of CanCorr.
- We also have $\Sigma_{12}$, the covariation of T with S. We can estimate what we would expect for T based on S using the first k singular vectors of S as

$$\hat{\mathbf{T}}(\mathbf{S},k) = \mathbf{\Sigma}_{12}\left(\mathbf{\Sigma}_{22}\right)^{-1|k} = \mathbf{\Sigma}_{12}\mathbf{O}\begin{pmatrix} d_{11}^{-1} & 0 & \cdots & & & & \\ 0 & \ddots & & & & & \\ \vdots & & d_{kk}^{-1} & & & & \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & & 0 \end{pmatrix}\mathbf{O}'$$

# SVD versus CanCorr: SVD (5)

- Similar remarks and approaches as for CanCorr apply to SVD
  - Singular vectors are less well defined as eigenvalues become closely spaced
  - We may look at the fits (estimated values) first if most of the significance falls into a few numerically stable patterns
  - We will look at residuals as well, particularly at breaks in a block-type pattern of decrease in singular values / eigenvalues

# SVD versus CanCorr: SVD (6)

- **The big, big difference between SVD and CanCorr is**
  - **SVD aims to compactly express the variation of a *single* data set**
  - **Covariation with the other data set is dealt with almost as an afterthought.**
- **CanCorr aims to compactly express the covariation of *both* data sets, without favor for one or the other.**

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# Automating Runs and Results (1)

- Again, a work in progress – all feedback welcome
- Number of parameters, factors, runs makes manual DOE setup and execution unattractive for all but small problems
  - Manual "baby steps" on small problems for debugging
- Concept is to factor problem into DOE files giving
  - Design matrix, source citation, permuted computational order
  - Factors and associated parameters, with .DAT file levels for parameters as .DOE factor goes between its levels

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# Automating Runs and Results (2)

- Automate run process
  - Substituting parameter .DAT levels into .DOE files
  - Write result to temporary .DAT files
  - Execute runs in permuted order
- Automate DOE post process
  - Extract results
  - Transfer to statistical software
  - Use stat tools for evaluation and comparison between THUNDER, STORM results on nominally equivalent models

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# Punch Line: Quantitative V&V?

- This is a massive quantitative validation experiment
  - Uses computers to exceed past human limits on data production
  - Uses computers and sophisticated math to surpass unaided human limits on data interpretation
  - Unexpected differences between THUNDER and STORM will constitute new knowledge
  - Finding only differences explainable as due to known deliberate changes would be a disappointment

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# Nothing to Lose But Uncertainty

- The author's involvement stems from > 20 years trying to compare test data with modeling results
  - 16 years shock testing nuclear powered ships and their components
  - 9 years with robotic test equipment testing composite material systems
    - Assumed material response theory (dissipated energy density) said could account for 60K data points via 125 coefficients and constraints
    - Ability to so compactly model test data gave massive support to underlying theory
- It is long past time for a similar quantitative approach to V&V – and comparing THUNDER and STORM should be a milestone in that effort.

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# Questions?