

# NPL-SAMBA ITT projects

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# Outline

- 1 Data assimilation with engineering models
- 2 Spectral analysis associated with Gaussian Processes

# Quality engineering

- Functional requirement of a manufactured part
- Manufactured parts specified in terms of geometric shape, dimensions and tolerances in computer-aid design (CAD) drawings/files
- All designs usually refer to the ideal shape at 20 °C, the reference temperature for measurement
- Manufactured parts the output of a number of cutting, machining, drilling, polishing processes
- Each process likely to drift due to tool wear, environmental effects (especially temperature)
- Other sources of variation: tool, machine, operator

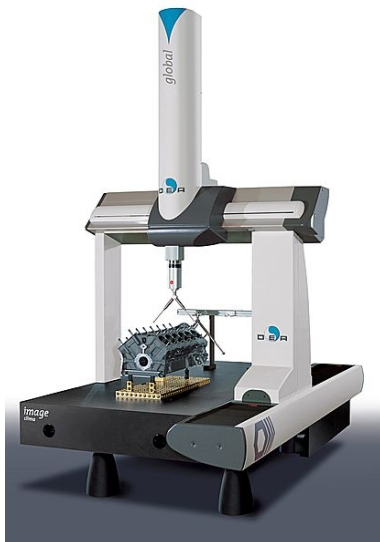
# Connecting rod from an internal combustion engine



# Traditional approach to inspection

- Assess a sample of objects from the production line to check dimensions and tolerances
- Plug gauges, ring gauges, hard gauges based on artefacts (yes/no test)
- Coordinate measuring machines (CMMs): gather  $x$ -,  $y$ - and  $z$ -coordinates of points  $\mathbf{x}_i$  on the workpiece.
- Apply algorithms to  $X = \{\mathbf{x}_i\}$  to check if the part (as presented by  $X$ ) conforms to specification
- Require workpiece to reach stable equilibrium at 20 °C
- Equilibrated workpiece: use a temperature measurement to scale back to 20 °C

# Coordinate measuring machine



# In-process measurement

Measure the workpiece , save time, money

- Workpiece ideal geometry at 20 °C specified, with tolerances
- Workpiece being manufactured: cutting, drilling, machining, cooling
- Measurements of the temperature at finite number of locations on the workpiece
- Measurements of the dimensions of a finite number of key features
- Using a FE model of artefact and the measurements, infer the workpiece shape at an equilibrated 20 °C

# Data assimilation

## Major tool in weather prediction

- **Forward model**: given the ideal geometry at 20 °C, known material properties, known boundary conditions, predict the geometric distortion due to thermal effects
- **Inverse problem**: incomplete, measured boundary conditions, approximate values of material properties
- Uncertainty quantification: how well can we infer the shape at 20 °C
- Degrees of freedom/surrogate models/machine learning: what measurement information is sufficient to make good inferences
- **Bing Ru Yang**, Bath, Louise Wright, Dale Partridge, NPL, project work



# Large engineering structures

- Aircraft wings, bridges
- Industry 4.0, digital twins



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# Fitting a model to data

- Standard data fitting model

$$\mathbf{y} = \mathbf{C}\mathbf{a} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \in \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$$

- $\mathbf{y}$  is an  $m \times n$  data vector,  $\mathbf{a}$  parameters of the model
- $\mathbf{C}$  is an  $m \times n$  observation matrix, e.g. basis functions evaluated at  $\mathbf{x}$
- $\boldsymbol{\epsilon}$  is an  $m \times n$  vector of independent random effects associated with the measuring system
- Least squares model fit

$$\hat{\mathbf{a}} = (\mathbf{C}^T \mathbf{C})^{-1} \mathbf{C}^T \mathbf{y} = \mathbf{R}_1^{-1} \mathbf{Q}_1^T \mathbf{y}, \quad \mathbf{C} = \mathbf{Q}_1 \mathbf{R}_1$$

$$\hat{\mathbf{y}} = \mathbf{C}\hat{\mathbf{a}} = \mathbf{C}(\mathbf{C}^T \mathbf{C})^{-1} \mathbf{C}^T \mathbf{y} = \mathbf{Q}_1 \mathbf{Q}_1^T \mathbf{y}$$

# Effective number of degrees of freedom in a model

- If  $\hat{\mathbf{y}} = H\mathbf{y}$ , the sum of the eigenvalues of  $H$  is a measure of the number of degrees of freedom associated with the model.
- Least squares model fit

$$\hat{\mathbf{y}} = C(C^T C)^{-1} C^T = Q_1 Q_1^T \mathbf{y}$$

- $Q_1 Q_1^T$  is a projection with  $n$  eigenvalues equal to 1, all others 0.

# Correlated systematic effects

- Extension of the standard model:

$$\mathbf{y} = \mathbf{C}\mathbf{a} + \mathbf{e} + \epsilon, \quad \mathbf{e} \in \mathcal{N}(\mathbf{0}, V_0), \quad \epsilon \in \mathcal{N}(\mathbf{0}, \sigma^2 I)$$

# Gauss Markov regression

- Combined variance matrix, Choleski decomposition

$$V = V_0 + \sigma^2 I = LL^T, \quad \tilde{\mathbf{y}} = L^{-1}\mathbf{y}, \quad \tilde{C} = L^{-1}C$$

$$\tilde{\mathbf{y}} = \tilde{C}\mathbf{a} + \tilde{\epsilon}, \quad \tilde{\epsilon} \in N(\mathbf{0}, I)$$

- Effective degrees of freedom: transformed problem

$$\hat{\tilde{\mathbf{y}}} = \tilde{Q}_1 \tilde{Q}_1^T \tilde{\mathbf{y}}$$

- Effective degrees of freedom: original problem

$$\hat{\mathbf{y}} = L\hat{\tilde{\mathbf{y}}} = L\tilde{Q}_1 \tilde{Q}_1^T L^{-1}\mathbf{y}$$

# Explicit effects model

- Same extended model

$$\mathbf{y} = \mathbf{C}\mathbf{a} + \mathbf{e} + \boldsymbol{\epsilon}, \quad \mathbf{e} \in \mathcal{N}(\mathbf{0}, V_0), \quad \boldsymbol{\epsilon} \in \mathcal{N}(\mathbf{0}, \sigma^2 I)$$

- Introduce parameters to describe the systematic effects,

$$\mathbf{e} = L_0 \mathbf{d}, \quad V_0 = L_0 L_0^T$$

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{C} & L_0 \\ & I \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{d} \end{bmatrix} + \begin{bmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{\delta} \end{bmatrix} \quad \boldsymbol{\epsilon} \in \mathcal{N}(\mathbf{0}, \sigma^2 I), \quad \boldsymbol{\delta} \in \mathcal{N}(\mathbf{0}, I)$$

# Augmented system

$\tilde{\mathbf{y}} = \tilde{\mathbf{C}}\tilde{\mathbf{a}} + \tilde{\boldsymbol{\epsilon}}$ , where

$$\tilde{\mathbf{y}} = \begin{bmatrix} \mathbf{y}/\sigma \\ \mathbf{0} \end{bmatrix}, \quad \tilde{\mathbf{C}} = \begin{bmatrix} \mathbf{C}/\sigma & \mathbf{L}_0/\sigma \\ & \mathbf{I} \end{bmatrix}$$

and

$$\tilde{\mathbf{a}} = \begin{bmatrix} \mathbf{a} \\ \mathbf{d} \end{bmatrix}, \quad \tilde{\boldsymbol{\epsilon}} = \begin{bmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{\delta} \end{bmatrix} \quad \tilde{\boldsymbol{\epsilon}} \in \mathbf{N}(\mathbf{0}, \mathbf{I})$$

- Eigenvalues

$$\hat{\tilde{\mathbf{y}}} = \mathbf{P}\tilde{\mathbf{y}} = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} \mathbf{y}/\sigma \\ \mathbf{0} \end{bmatrix}$$

$$\hat{\mathbf{y}} = P_{11}\mathbf{y}$$

- $n \leq \sum_j \lambda_j(P_{11}), \sum_j \lambda_j(P_{22}) \leq m$



# Gaussian Processes

- Same extended model

$$\mathbf{y} = \mathbf{C}\mathbf{a} + \mathbf{e} + \epsilon, \quad \mathbf{e} \in \mathcal{N}(\mathbf{0}, V_0), \quad \epsilon \in \mathcal{N}(\mathbf{0}, \sigma^2 I)$$

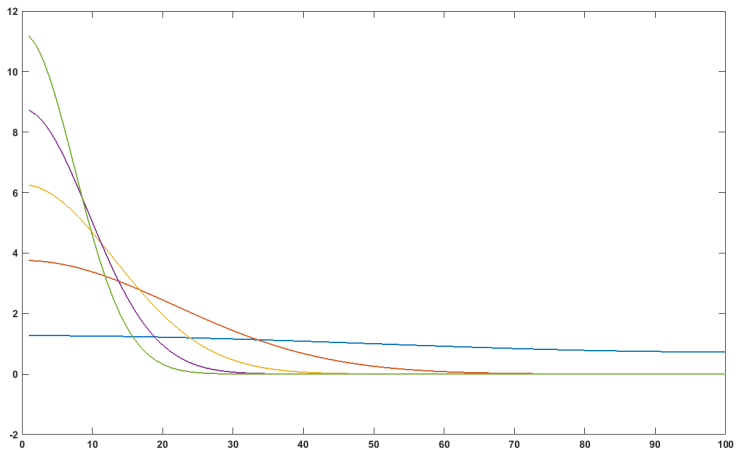
- $C_{ij} = b_j(t_i)$ ,  $\text{cov}(\mathbf{e}, \mathbf{e}') = k(t, t')$ , e.g.

$$k(t, t') = \sigma_E^2 \exp \{ -(t - t')^2 / \tau^2 \}$$

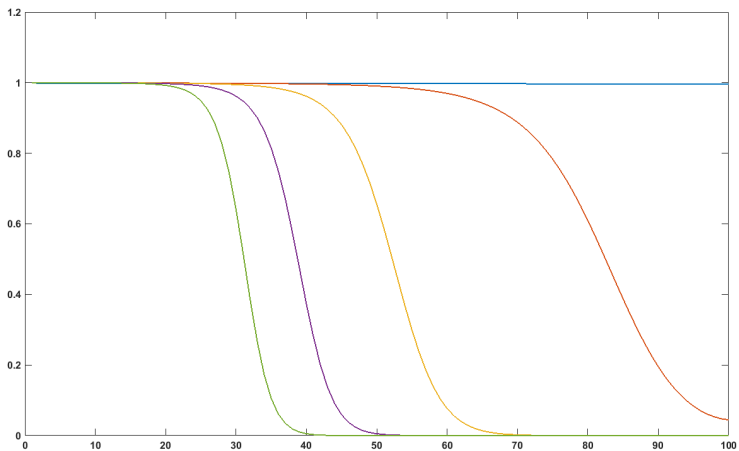
- Equally spaced  $t_i$

$$V = \sigma_E^2 \begin{bmatrix} 1 & v & v^4 & v^9 & v^{16} & \dots \\ v & 1 & v & v^4 & v^9 & \dots \\ v^4 & v & 1 & v & v^4 & \dots \\ & & & \ddots & & \end{bmatrix}$$

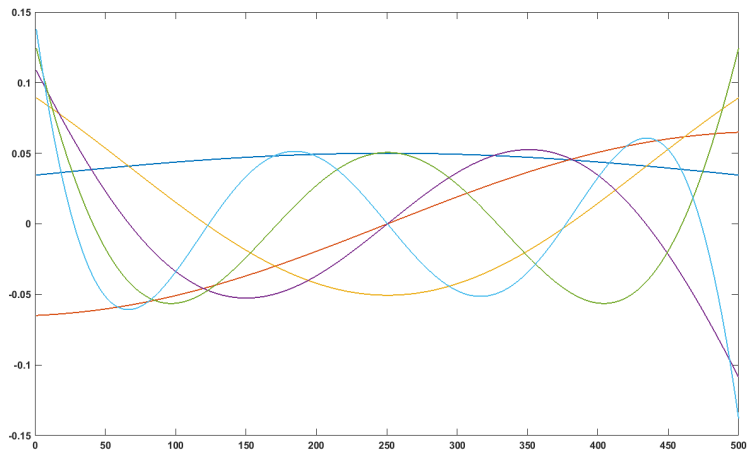
# Eigenvalues of $V$ for different $\tau$



# Eigenvalues of $P_{11}$ for different $\tau$



# Eigenvectors of $V$



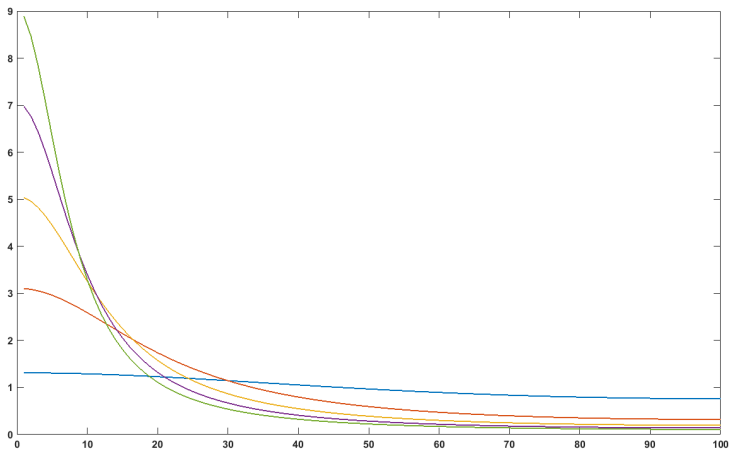
# Eigenvectors as Chebyshev polynomials

0.0838	-0.0002	0.0549	0.0009	0.0400	0.0018
0.0001	0.0724	-0.0004	-0.0485	-0.0013	-0.0366
-0.0077	0.0001	0.0697	0.0007	0.0461	0.0017
-0.0000	-0.0078	0.0001	-0.0687	-0.0009	-0.0449
0.0003	-0.0000	-0.0079	-0.0001	0.0681	0.0011
0.0000	0.0004	-0.0000	0.0080	0.0002	-0.0677
-0.0000	0.0000	0.0004	0.0000	-0.0081	-0.0002
-0.0000	-0.0000	0.0000	-0.0005	-0.0000	0.0081
0.0000	-0.0000	-0.0000	-0.0000	0.0005	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0005

# Chebyshev polynomials as eigenvectors

11.1174	0.0445	-8.8230	0.0275	-0.6102	0.0337
-0.0000	12.8329	0.1027	-9.1725	0.0586	-0.9364
1.1822	0.0047	12.3875	0.1628	-9.1967	0.0874
-0.0000	-1.4056	-0.0112	-12.5111	-0.2227	9.1655
0.0785	0.0003	1.4235	0.0180	12.6002	0.2820
-0.0000	-0.0869	-0.0007	-1.4731	-0.0250	-12.6561
0.0034	0.0000	0.0874	0.0011	1.5080	0.0320
0.0000	-0.0036	-0.0000	-0.0900	-0.0015	-1.5330
0.0001	0.0000	0.0036	0.0000	0.0920	0.0019
0.0000	-0.0001	-0.0000	-0.0037	-0.0001	-0.0935

Eigenvalues of  $V$ ,  $k(t, t') \propto \exp\{-|t - t'|/\tau\}$



# Eigenvectors of $V$ , $k(t, t') \propto \exp\{-|t - t'|/\tau\}$

