Bayesian Estimation of Elastic Constants

University of California Santa Barbara

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Superalloys

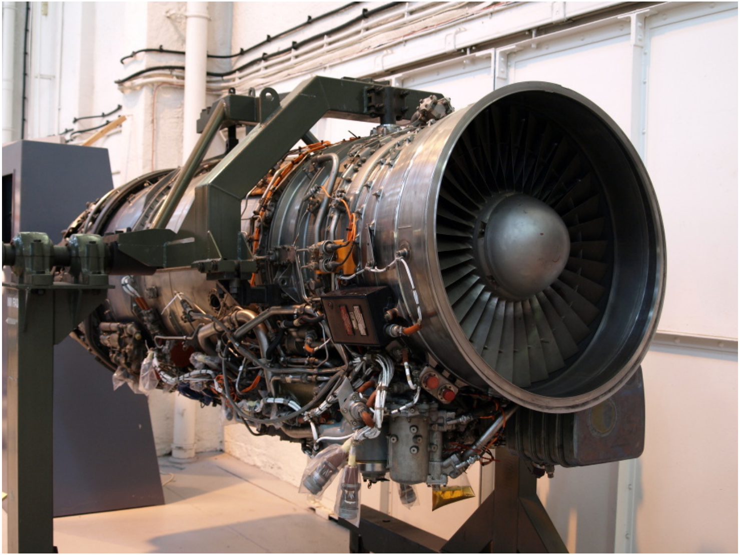
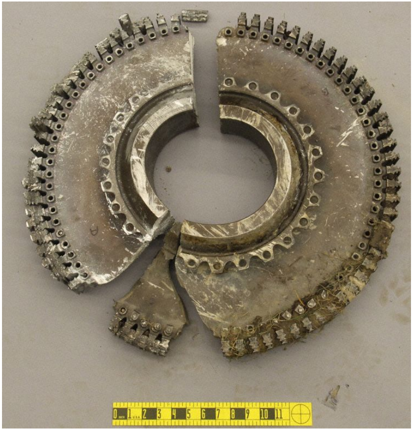


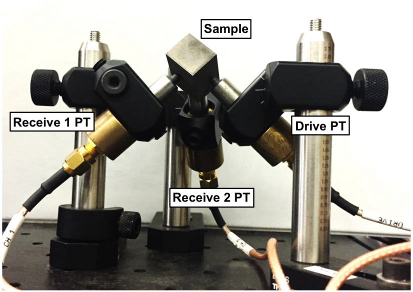
Image from https://commons.wikimedia.org/wiki/File:RB199_Cosford.JPG

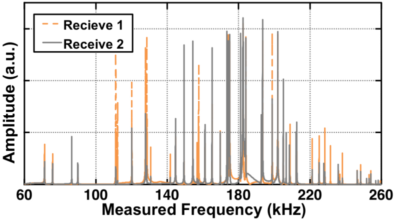
American B763, Chicago 2016



Pictures from `http://avherald.com/h?article=49ffa115`

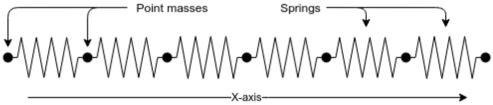
Experimental procedure





An example of mechanical resonance

- The simplest elastic materials obey Hooke's law: $F = -kd$
- If we hook a bunch of little point masses together with Hookean Springs,



- we can write out their equations of motion:

$$m\frac{\partial^2 d_i}{\partial t^2} = -k(d_i - d_{i-1}) + k(d_{i+1} - d_i)$$

- This is a second order linear ODE. The resonance modes are the square roots of the associated eigenvalue problem

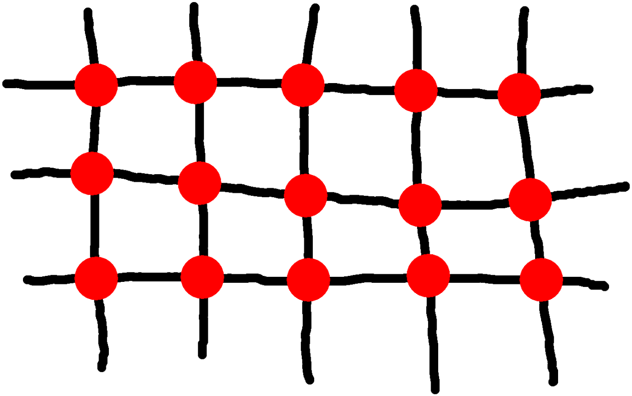
$$-m\omega^2\mathbf{d} = \begin{bmatrix} -k & k & 0 & \\ k & -2k & k & \\ 0 & k & -2k & \\ & & & \ldots \end{bmatrix}\mathbf{d}, -m\omega^2\mathbf{d} = \mathbf{K}\mathbf{d} \qquad (1)$$

Slightly fancier mechanics

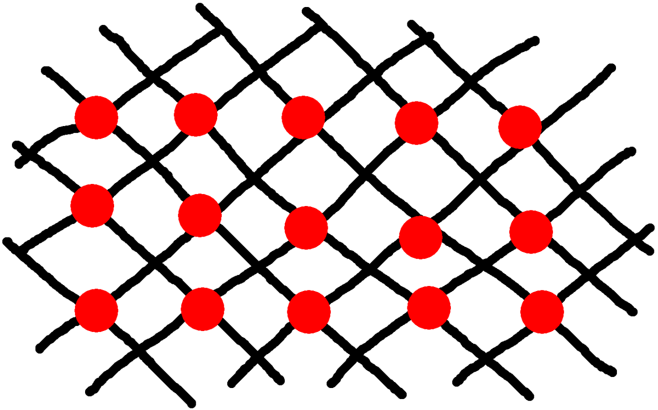
- The inverse problem attached to this is a classic method of estimating elastic constants (see references slide at end).
- The mechanics in an actual turbine blade are similar to the example, but are parameterized with a 6x6 matrix of elastic coefficients determined by the symmetry of the crystal (instead of just one).

$$\underbrace{\begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix}}_{\text{Cubic crystal symmetry (Cu, Au, Al)}} \quad \underbrace{\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & (c_{11} - c_{12})/2 \end{bmatrix}}_{\text{Hexagonal crystal symmetry (Co, Mg, Ti)}}$$

Crystal lattice



Crystal lattice 2



Simple model

```
data {
  int<lower = 1> N;
  real<lower = 0.0> y[N - 1];
  real m;
}
parameters {
  real<lower = 0.0> k;
  real<lower = 0.0> sigma;
}
```

```
transformed parameters {
  vector[N - 1] eigs;
  {
    matrix[N, N] K = f(k);
    eigs = eigenvalues_sym(K)[2:N];
  }
}
model {
  k ~ normal(1.0, 1.0);
  sigma ~ normal(0.0, 1.0);
  y ~ normal(sqrt(eigs), sigma);
}
```

Simple model posterior

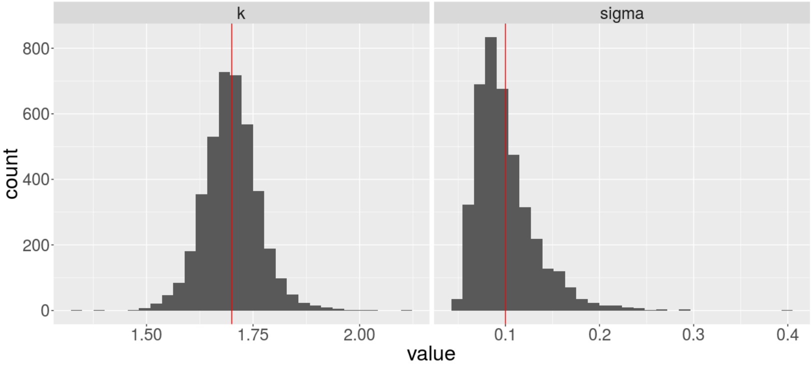
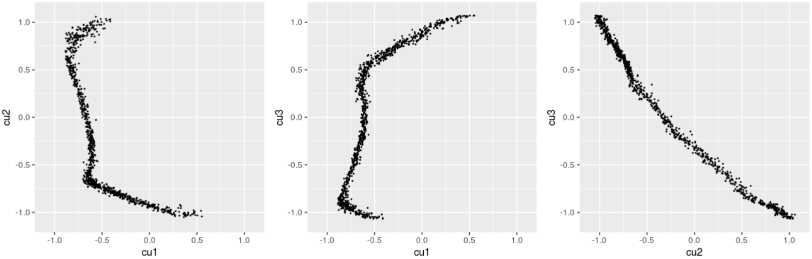


Table of results [Goodlet et al., 2018]

Specimen name	$\mathbf{c_{11}}$ (GPa) mean ± sd	$\mathbf{c_{44}}$ (GPa) mean ± sd	**A** (unitless) mean ± sd
CMSX-4-A	249.0 ± 2.3	129.2 ± 0.29	2.811 ± 0.011
CMSX-4-B	248.3 ± 2.0	129.6 ± 0.28	2.817 ± 0.0097
Co-Ternary-A	257.3 ± 0.79	149.9 ± 0.13	3.219 ± 0.0045
Co-Ternary-B	256.7 ± 0.58	150.0 ± 0.10	3.217 ± 0.0035
Co-2Ta-A	258.8 ± 1.8	147.7 ± 0.26	3.134 ± 0.0085
Co-2Ta-B	259.3 ± 1.6	147.9 ± 0.23	3.141 ± 0.0077
Co-6Ti-A	248.1 ± 1.4	145.4 ± 0.24	3.188 ± 0.0086
Co-6Ti-B	250.7 ± 1.8	145.2 ± 0.23	3.211 ± 0.0086
CoNi-A1	256.7 ± 0.36	142.1 ± 0.08	2.868 ± 0.0029
CoNi-A2	256.4 ± 0.41	141.9 ± 0.09	2.873 ± 0.0032
CoNi-A+1	256.7 ± 0.86	142.2 ± 0.11	2.880 ± 0.0036
CoNi-A+2	255.9 ± 0.66	142.0 ± 0.09	2.880 ± 0.0030
CoNi-B1	257.1 ± 1.3	141.6 ± 0.21	2.864 ± 0.0068
CoNi-B2	257.5 ± 1.0	141.7 ± 0.17	2.868 ± 0.0057
CoNi-C1	256.0 ± 0.67	140.3 ± 0.13	2.828 ± 0.0044
CoNi-C2	256.1 ± 0.75	140.6 ± 0.14	2.825 ± 0.0048
CoNi-D1	256.2 ± 0.60	141.2 ± 0.09	2.853 ± 0.0029
CoNi-D2	257.8 ± 0.78	141.3 ± 0.12	2.849 ± 0.0036

Not all those who wander are lost



Folks that worked on this project that aren't here

Brent Goodlet

Leah Mills

Tresa Pollock

Linda Petzold

If you haven't had enough already

- `https://github.com/bbbales2/stancon_2018` $\leftarrow$ rus.html has more details
- [Bales et al., 2018]
- [Goodlet et al., 2018]

An incomplete list of people smarter than me

- [Bernard et al., 2015] $\leftarrow$ This one is also Bayesian!
- [Migliori and Maynard, 2005]
- [Sarrao et al., 1994]
- [Maynard, 1992]
- [Visscher et al., 1991] $\leftarrow$ I quite like this one
- [Ohno, 1976]
- [Demarest, 1971]
- [Holland, 1968]
- [Bower, 2009] $\leftarrow$ This is a general reference on mechanics

References I

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