Statistical Adjustments to Engineering Models

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Model-based Quality Improvement

• Models are used for
  – Process control
  – Process optimization

• Two types of models
  – Statistical models
  – Engineering models
Statistical Models

- Statistical models
  - Developed based on data
  - Linear/nonlinear regression models
Engineering Models

• Engineering models
  – Developed based on engineering/physical laws
  – Analytical and finite element models
Engineering Models Vs Statistical Models

• Statistical models
  – Predictions are good closer to the data, but can be poor when made away from data

• Engineering models
  – Physically meaningful predictions, but often are not accurate because of the assumptions

• Can we integrate them to produce better models?
Engineering - Statistical Models

• Improve engineering models using data
  – More realistic predictions than engineering models
  – Less expensive than pure statistical models (fewer data)
Surface Roughness Prediction in Micro-Turning

- Workpiece
- Primary cutting edge
- Secondary cutting edge
- Tool
- Nose radius
- Feed
- \( Y_{\text{kinemat}} \)
- \( \text{ic} \)
Engineering model:  \[ Y_{\text{kinematic}} = \frac{x^2}{8r} \]
Statistical model: \( Y = \beta_0 + \beta_1 x + \beta_2 x^2 \)
Existing methods

• Mechanistic model calibration
  – Estimate unknown parameters (calibration parameters) from data
  – Box, Hunter, Hunter (1978), Kapoor et al. (1998)
  – Not a general method

• Bayesian calibration
  – Kennedy and O’Hagan (2001)
Bayesian Methodology

• Take engineering model as the prior mean
• Get data from the physical experiment
• Obtain posterior distribution
• Engineering-Statistical model is the posterior mean
Engineering model → Prior distribution → Posterior distribution → Eng.-Stat. Model
Methodology-continued

- Output: $Y$
- Factors: $\boldsymbol{x} = (x_1, \ldots, x_p)'$
- Random error: $\epsilon \sim \mathcal{N}(0, \sigma^2)$

$$Y = \mu(\boldsymbol{x}) + \epsilon$$

- Objective: Find $\mu(\boldsymbol{x})$
- Engineering model: $f(\boldsymbol{x}; \eta)$
- Calibration parameters: $\eta = (\eta_1, \ldots, \eta_q)'$
- Data: $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$
Sequential Model Building

**Flowchart Diagram:**

1. **Engineering Model**
   - If Positive relation:
     - Yes: **Constant adjustment**
     - No: **Check & Correct**

2. **Is MI large?**
   - No: **Engineering Model**
   - Yes: **Functional Adjustment Model**

3. **Is MI large?**
   - No: **Engineering Model**
   - Yes: **Constant Adjustment Model**
Methodology-continued

• Check the usefulness of engineering model using graphical analysis
• If it is useful

\[ MI = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu}_i^E)^2 \]

• If MI is small, then stop. Engineering model is good.
Constant adjustment model

\[ \mu(x) - f(x) = \beta_0 + \beta_1 (f(x) - \bar{f}) \]

\[ MI = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu}_i^C)^2 \]

- If MI is small, then stop. CAM is good.
Functional adjustment model

\[ \mu(x) - \mu^C(x) = \delta(x; \alpha) \]
\[ \delta(x; \alpha) = \sum_{i=0}^{m} \alpha_i u_i(x) \]

• Add terms until MI is small enough.
Constant adjustment model

\[ Y - f(x) = \beta_0 + \beta_1 (f(x) - \bar{f}) + \epsilon \]

\[ \epsilon \sim \mathcal{N}(0, \sigma^2), \quad \beta_0 \sim \mathcal{N}(0, \tau_0^2), \quad \beta_1 \sim \mathcal{N}(0, \tau_1^2) \]

\[ y - f = F\beta + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I) \]

\[ \beta \sim \mathcal{N}(0, \Sigma) \]
Posterior distribution

- posterior distribution is

$$\beta|y \sim \mathcal{N}\left((F'F + \sigma^2 \Sigma^{-1})^{-1} F'(y - f), \sigma^2(F'F + \sigma^2 \Sigma^{-1})^{-1}\right)$$

- constant adjustment predictor is

$$\hat{\mu}^C(x) = f(x) + \hat{\beta}_0 + \hat{\beta}_1(f(x) - \bar{f})$$

- Prediction interval

$$\hat{\mu}^C(x) \pm z_{\alpha/2}\sigma\left\{1 + \frac{1}{n + \sigma^2/\tau_0^2} + \frac{(f(x) - \bar{f})^2}{S + \sigma^2/\tau_1^2}\right\}^{1/2}$$
Simplification

- least squares estimate

$$\tilde{\beta}_0 = \bar{y} - \bar{f} \quad \text{and} \quad \tilde{\beta}_1 = \sum_{i=1}^{n} (y_i - f_i)(f_i - \bar{f})/S$$

$$S = \sum_{i=1}^{n} (f_i - \bar{f})^2$$

$$\hat{\beta}_0 = \frac{\tau_0^2}{\tau_0^2 + \sigma^2/n} \tilde{\beta}_0 \quad \text{and} \quad \hat{\beta}_1 = \frac{\tau_1^2}{\tau_1^2 + \sigma^2/S} \tilde{\beta}_1$$
Empirical Bayes estimation

- Estimate hyperparameters by maximizing

\[
l = -\frac{1}{2} \log \det (F \Sigma F' + \sigma^2 I) - \frac{1}{2} (y - f)'(F \Sigma F' + \sigma^2 I)^{-1} (y - f)
\]

\[
\hat{\tau}_0^2 = \left( \tilde{\beta}_0^2 - \sigma^2 / n \right)_+ \quad \text{and} \quad \hat{\tau}_1^2 = \left( \tilde{\beta}_1^2 - \sigma^2 / S \right)_+
\]

\[
\hat{\beta}_0 = \left( 1 - \frac{1}{z_0^2} \right)_+ \tilde{\beta}_0 \quad \text{and} \quad \hat{\beta}_1 = \left( 1 - \frac{1}{z_1^2} \right)_+ \tilde{\beta}_1,
\]

\[
z_0 = \frac{|\tilde{\beta}_0|}{\sigma / \sqrt{n}} \quad \text{and} \quad z_1 = \frac{|\tilde{\beta}_1|}{\sigma / \sqrt{S}}.
\]
Approximate frequentist procedure

- Fit the simple linear regression

\[ y_i - f_i = \beta_0 + \beta_1 (f_i - \bar{f}) + \epsilon_i \]

and force \( \beta_j \) to be 0 if \( |z_j| < \sqrt{2} \).
Surface roughness example

- Engineering model: \( f_i = \frac{x_i^2}{6400} \)

- There is a positive relation
Example-continued

• From replicates \[ \hat{\sigma}^2 = s^2 = .183 \]

\[
MI = \frac{1}{120} \sum_{i=1}^{120} (y_i - f_i)^2 = 9.12.
\]

• Engineering model is not good for prediction

\[
MI > \frac{r - 1}{r} s^2 + \frac{\sigma^2}{n} \chi^2_{q, \alpha}.
\]
Constant adjustment model

$$\hat{\mu}^C(x) - f(x) = 2.98 - .11(f(x) - .4857)$$

$$MI = \frac{1}{120} \sum_{i=1}^{120} (y_i - \hat{\mu}^C_i)^2 = .255$$
Functional adjustment model

\[ Y - \mu^C(x) = \delta(x; \alpha) + \epsilon \]

\[ \delta(x; \alpha) = \alpha_0 + \sum_{i=1}^{m} \alpha_i u_i(x) \]

\[ \alpha \sim N(0, \gamma^2 R) \]
Two-stage estimation

- Use the estimate of $\mu^C(x)$ from the constant adjustment model.

\[
\hat{\mu}^F(x) = \hat{\mu}^C(x) + \sum_{i=0}^{m} \hat{\alpha}_i u_i(x)
\]

\[
\hat{\alpha} = (U'U + \frac{\sigma^2}{\gamma^2}R^{-1})^{-1}U'(y - \hat{\mu}^C)
\]

\[
l = -\frac{1}{2} \log \det(\gamma^2 URU' + \sigma^2 I) - \frac{1}{2}(y - \hat{\mu}^C)'(\gamma^2 URU' + \sigma^2 I)(y - \hat{\mu}^C)
\]
Approximate frequentist procedure

- Fit a multiple linear regression
- Do a variable selection
Surface roughness example

\[
\hat{\mu}^F(x) - \hat{\mu}^C(x) = 0.015(x - 43.33) - 0.593(\log(1 + x) - 3.35)
\]

\[
MI = \frac{1}{120} \sum_{i=1}^{120} (y_i - \hat{\mu}^F_i)^2 = 0.215
\]
Calibration parameters

New engineering model

- $R(x)$ is calculated using a combination of analytical formulas and finite element simulations

$$f(x; \eta) = Y_{\text{kinematic}} + Y_{\text{plastic}} = \frac{x^2}{8r} + \eta_0 + \eta_1 \log(R(x))$$
Statistical adjustments

- First use least squares estimate

\[ \tilde{\eta} = \arg \min_{\eta \in [\eta_L, \eta_U]} \sum_{i=1}^{n} [y_i - f_i(\eta)]^2 \]

\[ f(x; \tilde{\eta}) = \frac{x^2}{8r} - 24.83 + 4.49 \log R(x) \]

- MI= .209 (new engineering model is good)
Constant adjustment model

\[ Y - f(x; \eta) = \beta_0 + \beta_1(f(x; \eta) - f(\eta)) + \epsilon \]

\[ A(\eta) = \frac{1}{\sigma^2} \sum_{i=1}^{n} [y_i - f_i(\eta)]^2 + \log(1 + (z_0^2(\eta) - 1)_+) \]

\[ + \log(1 + (z_1^2(\eta) - 1)_+) - (z_0^2(\eta) - 1)_+ - (z_1^2(\eta) - 1)_+ \]

\[ \hat{\beta}_0 = \left(1 - \frac{1}{z_0^2(\hat{\eta})}\right)_+ \hat{\beta}_0(\hat{\eta}) \] and \[ \hat{\beta}_1 = \left(1 - \frac{1}{z_1^2(\hat{\eta})}\right)_+ \hat{\beta}_1(\hat{\eta}) \]
Approximate frequentist procedure

• Fit a nonlinear regression

\[ y_i = f_i(\eta) - \beta_0 - \beta_1(f_i(\eta) - \bar{f}(\eta)) + \epsilon_i \]

and force \( \beta_j \) to be 0 if \( |z_j| < \sqrt{2} \).
A Spot Welding Example

• Higdon et al. (2004) and Bayarri et al. (2007)
  – Three factors: Load, Current, and Gage
  – One calibration parameter
\( \hat{\mu}^F(x) - \hat{\mu}^C(x) = .12x_1 - .21(x_2 - .03) + .65x_3 + .44x_1x_2 + .40(x_2x_3 - .33) \)
Eng. Model (Black-dashed) : 0.69
Joseph&Melkote (Red-solid): 0.23
Bayarri et al. (Blue-dotted) : 0.20
Example: LAMM

Laser assisted mechanical micromachining (LAMM) integrates *thermal softening* with *mechanical micro cutting*.
Objective

Find optimum processing conditions that minimize cutting/thrust forces and thermal damage.
Thermal Model

- Mapped dense mesh (25 μm x 12.5 μm x 20μm)
- An 8 noded 3-D thermal element (Solid70) is used
- Gaussian distribution of heat flux applied to a 5x5 element matrix which sweeps the mesh on the front face
Geometric Model

\[
\gamma_{chip} = 2V \frac{\gamma_{chip}}{\sqrt{2 \sin(\pi / 4 + \theta_{PD}) PD}} \\
\gamma_{work} = 2V \frac{\gamma_{work}}{\sqrt{2 \sin(\pi / 4 + \theta_{PD}) PD + \frac{\sin(\psi + \theta / 2)}{PC}}}
\]

\[
\gamma_{chip} = \frac{\sqrt{2 \sin \theta_{PD}}}{\sin(\pi / 4 + \theta_{PD})} + \frac{\cos(\alpha_{avg} + \theta_{PD})}{\cos(\alpha_{avg} - \phi) \sin(\phi + \theta_{PD})}
\]

\[
\gamma_{work} = \frac{\sqrt{2 \sin \theta_{PD}}}{\sin(\pi / 4 + \theta_{PD})} + \frac{\sin(\theta_{PD} + \theta / 2)}{\sin(\psi + \theta / 2)} + \frac{\sin \theta / 2}{\sin(\theta_{PB} + \theta / 2) \sin(\theta_{PB} + \theta_{PD})}
\]

\[
\gamma_{eff} = \frac{v_{chip} \gamma_{chip} + v_{work} \gamma_{work}}{v_{chip} + v_{work}}
\]

For plane strain conditions,

\[
\varepsilon = \gamma_{eff} / \sqrt{3}
\]

\[
\varepsilon = \gamma_{eff} / \sqrt{3}
\]
Shear Flow Strength

\[ \sigma(\varepsilon, \dot{\varepsilon}, T, HRC) = \left( A + B \varepsilon^n + C \ln(\varepsilon + \varepsilon_0) + D \right) \left( 1 + E \ln\left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_n} \right) \right) \left( 1 - (T^*)^m \right) \]

\[ S = \sigma / \sqrt{3} \]

Yan et al., 2007

Distance from the center of the tool face along tool edge at 100 μm from the center of the laser beam (μm)

10W laser power, 10 mm/min speed, 100 μm laser-tool distance and 110 μm spot size
Forces

- Cutting and thrust forces,

\[
F_c = \{(h - p) \cot \phi + h + r_n \sin \theta - (k - 1) \delta\} \sum_{i=1}^{n} S(i)w(i)
\]

\[
F_t = \{(h - p) \cot \phi - h + r_n \sin \theta + (k - 1) \delta \cot \psi\} \sum_{i=1}^{n} S(i)w(i)
\]
Equilibrium Forces/Deflection

1. Initialize $h = h_{initial}$
2. Calculate Force, $F(t, h)$ from force model
3. Determine $k_{equil}$

$h_{new} = h - \varepsilon$

- Calculate new thrust force $F_{new}$ based on new depth of cut, $h_{new}$

$\left| \frac{F_{new}}{h_{initial} - h_{new}} \right| - k_{equil} \leq 0.1$

- $h = h_{new}$

- Calculate equilibrium depth of cut, $h$
- Calculate the equilibrium force, $F_e$ and $F_t$
Force model

Thermal Model

Temperature Distribution, $T$

Geometric Model

Material Model

$\sigma = f(\varepsilon, \dot{\varepsilon}, T, HRC)$

Stress Distribution, $S$

Force Model

Elastic Deflection

Forces, $F_c$ and $F_t$

Actual Depth of Cut, $h$
Force prediction

- Positive relation, but predictions are smaller than actual
Force prediction-continued

- Better than cutting force, but slightly smaller than actual
Engineering-Statistical Force Models

Plot of measured vs. predicted cutting and thrust forces

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Optimization Problem

- For a given depth of cut \( (t) \), find the optimum levels of set depth of cut, laser power, laser speed, and distance from tool to minimize cutting/thrust forces while making sure there is no heat affected zone.

\[
\begin{align*}
\min_{x_1, x_2, x_3, x_4} & \quad \hat{y}_c^2 + \hat{y}_t^2 \\
\text{subject to} & \quad \text{doc} = t \\
& \quad T_2 \leq A_{c_1}
\end{align*}
\]
Nonlinear programming

\[
\min \left\{ 1.54x_1^{0.89} \exp(0.0014x_2 - 0.009x_3e^{-0.0034x_4}) \right\}^2 + \left\{ 1.03x_1^{0.8} \exp(0.0014x_2 - 0.043x_3e^{-0.0034x_4}) \right\}^2
\]

\[
x_1 - 0.57x_1^{0.8} \exp(0.0014x_2 - 0.196x_3e^{-0.0034x_4}) = t
\]

\[
25 + 196.4x_3 \exp(-0.0021x_1x_3 - 0.00045x_2x_3) \leq 800
\]

\[
10 \leq x_1 \leq 25, \ 10 \leq x_2 \leq 50, \ 0 \leq x_3 \leq 10, \ 100 \leq x_4 \leq 200
\]
Optimization Results

- For example, for depth of cut = 10 μm

- Set depth of cut ($x_1$) = 12.30 μm

- Cutting speed ($x_2$) = 10 mm/min

- Laser power ($x_3$) = 4.5 W

- Laser location from the tool edge ($x_4$) = 100 μm
Validation

Before machining

After machining

Hardness measurement

Epoxy 400X 75 μm

Distance (mm)

Before machining

After machining

Height (μm)

Distance (mm)

Before machining

After machining 10 μm

硬度 (HRC)

10 μm groove depth

25 μm groove depth

Distance from the edge of groove (μm)
Conclusions

• Engineering models can be improved by using data
• Engineering-Statistical models perform better than engineering models and statistical models
• Need relatively less amount of data
• They use the physics of the process
Process Optimization

Factors & Levels

Experiment

Statistical model

Engineering knowledge

Engineering model

Engineering-Statistical model

Optimize

Optimize
Conclusions-continued

• Simple procedure
  – Fit two linear/nonlinear regressions
  – Do variable selection

• Easy-to-implement
  – No additional programming is required