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

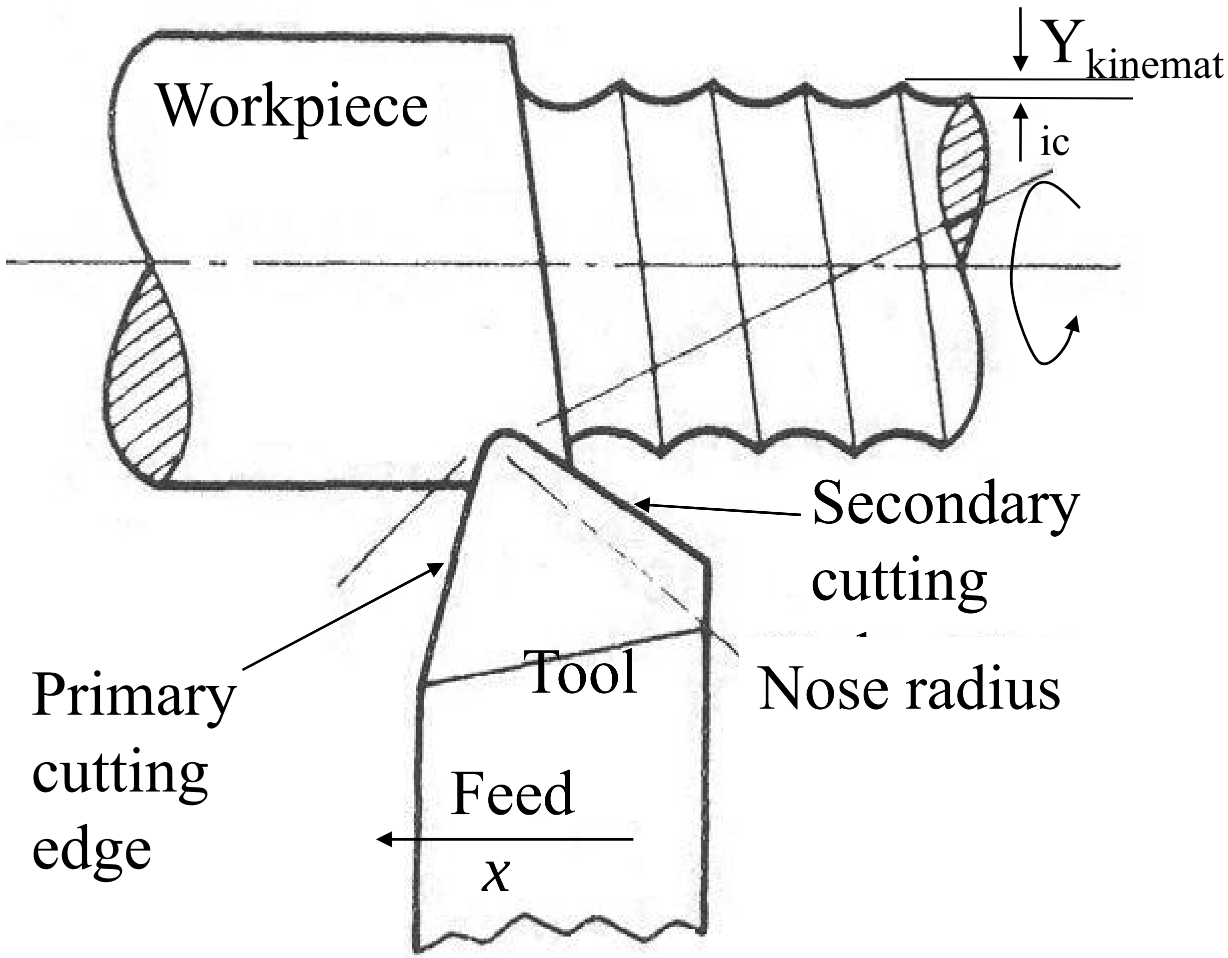
Engineering Models Vs Statistical Models

- 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?

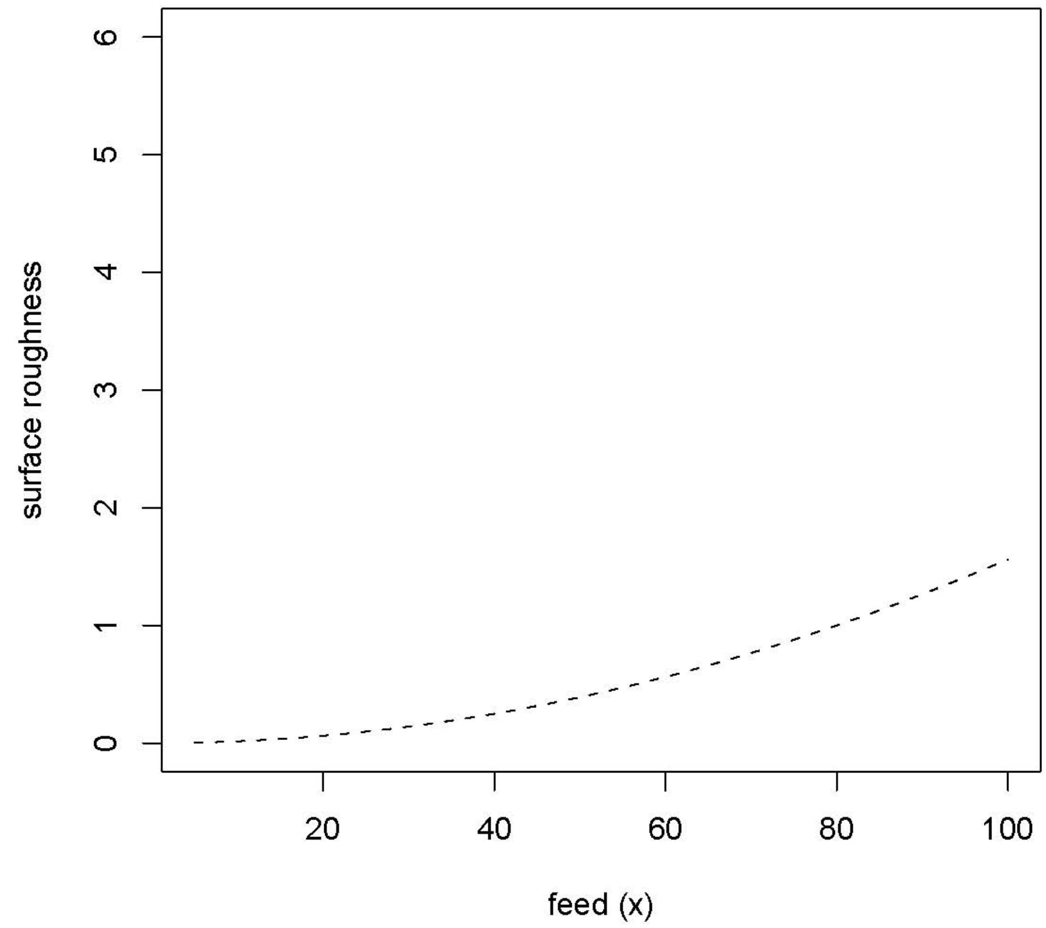
Engineering - Statistical Models

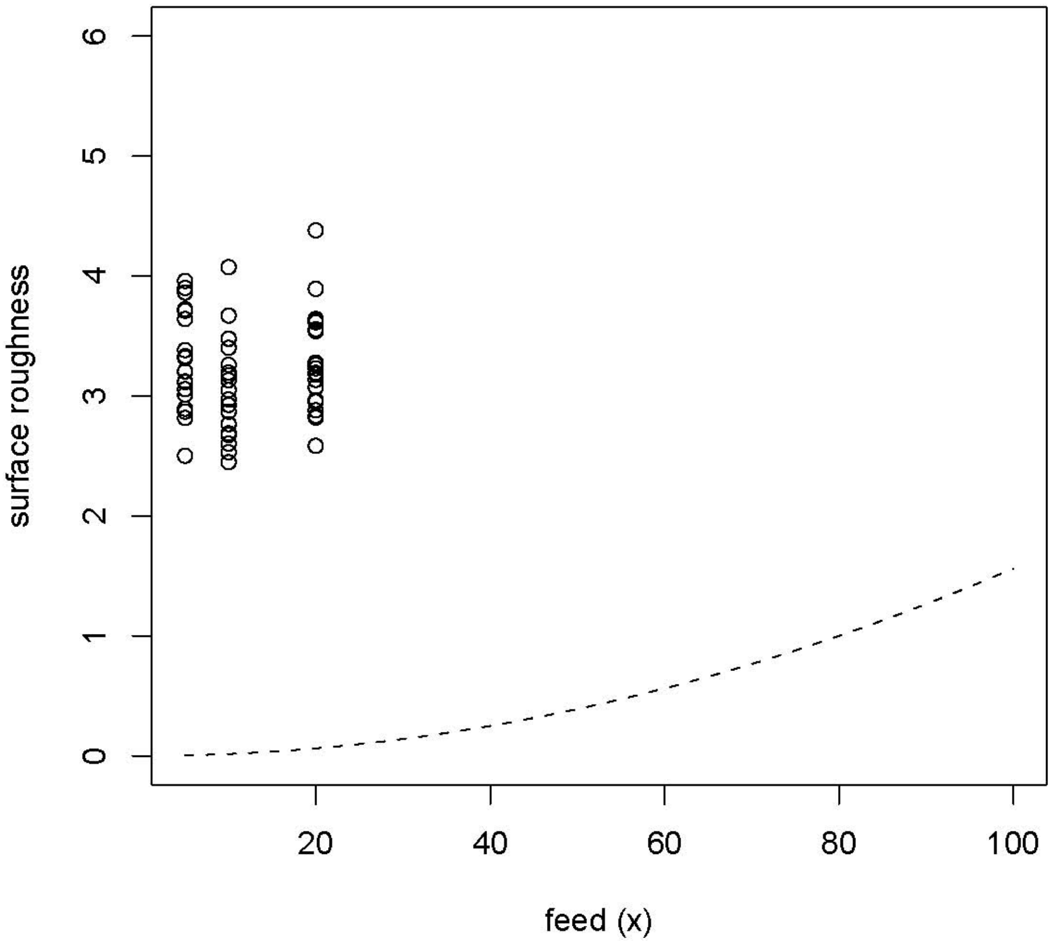
- Improve engineering models using data
  - More realistic predictions than engineering models
  - Less expensive than pure statistical models (fewer data)

Surface Roughness Prediction in Micro-Turning



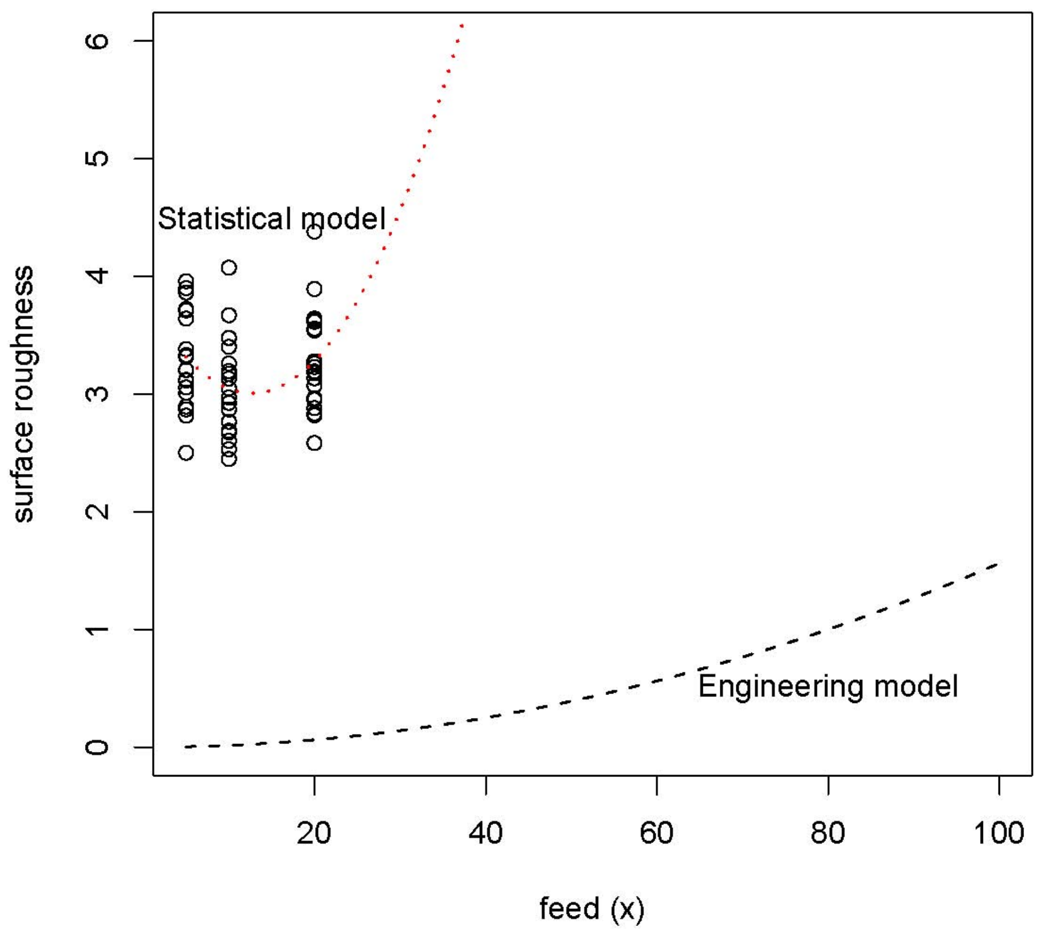
Engineering model: $Y_{kinematic} = \frac{x^2}{8r}$

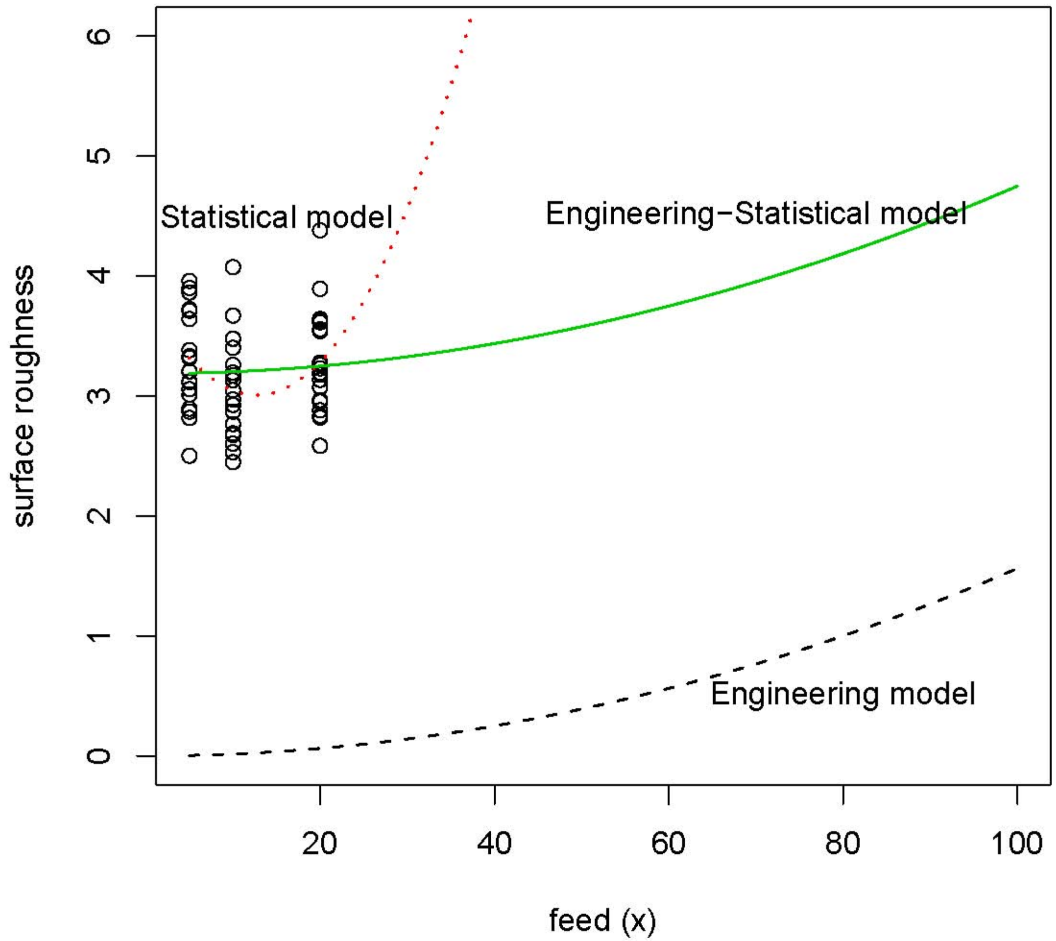




surface roughness
feed (x)
0
1
2
3
4
5
6
20
40
60
80
100

Statistical model: $Y = \beta_0 + \beta_1 x + \beta_2 x^2$





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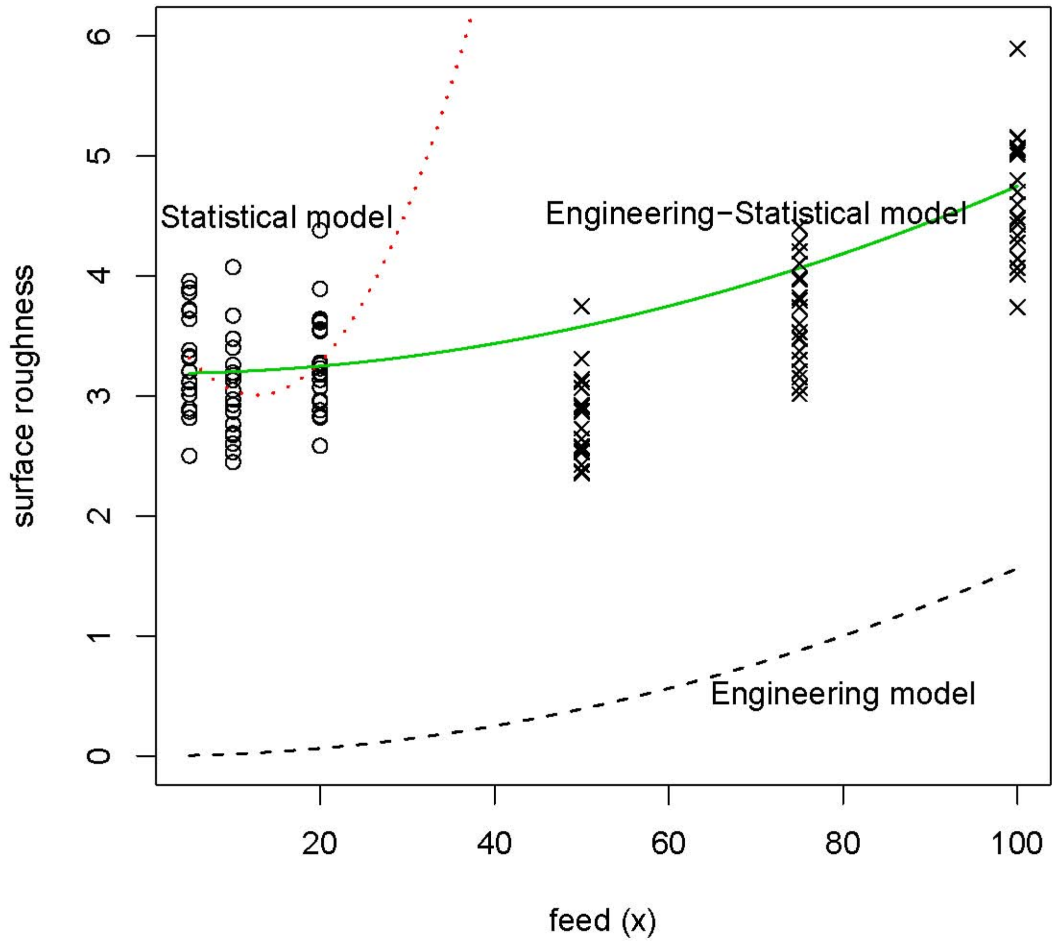


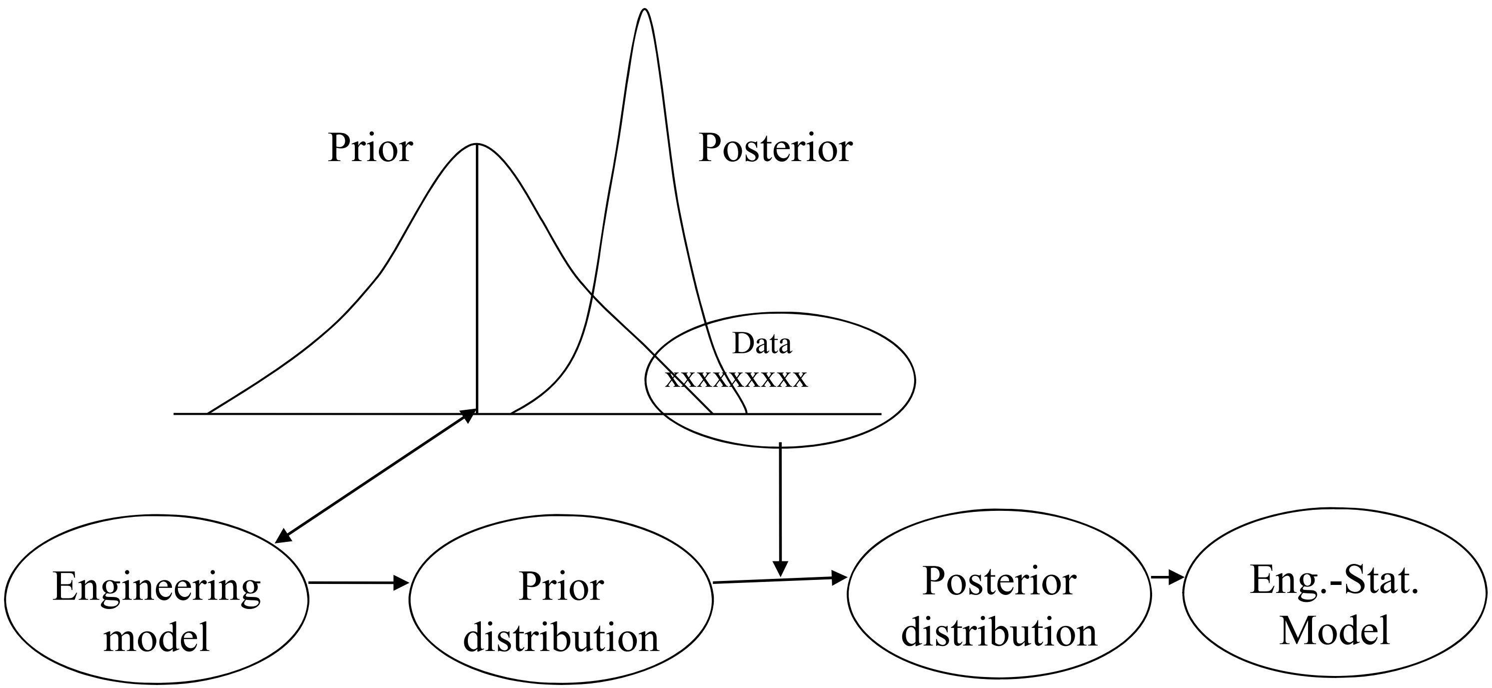
surface roughness
feed (x)
0
1
2
3
4
5
6
20
40
60
80
100
Statistical model
Engineering−Statistical model
Engineering model

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)
  - Reese et al. (2004), Higdon et al. (2004), Bayarri et al. (2007), Qian and Wu (2008).

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


Prior
Posterior
Data
xxxxxxxxx
Engineering model
Prior distribution
Posterior distribution
Eng.-Stat. Model

Methodology-continued

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

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

- Objective: Find $\mu(\boldsymbol{x})$

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

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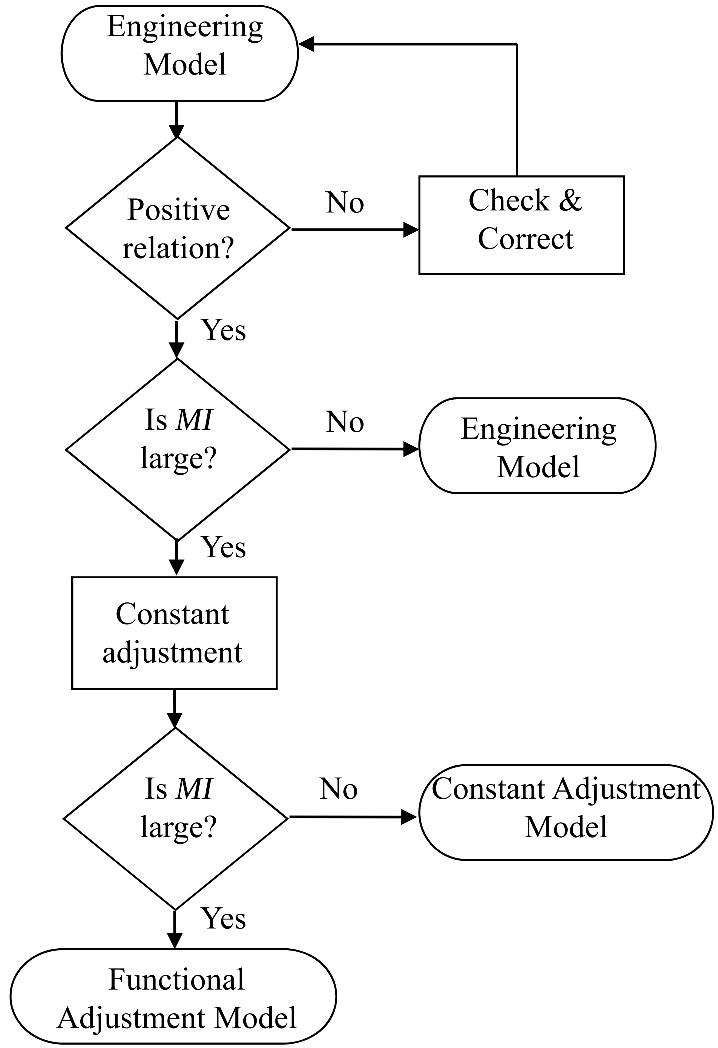
Sequential Model Building



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

$$\mu(\boldsymbol{x}) - f(\boldsymbol{x}) = \beta_0 + \beta_1 (f(\boldsymbol{x}) - \bar{f})$$

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

- If MI is small, then stop. CAM is good.

Functional adjustment model

$$\mu(\boldsymbol{x}) - \mu^{C}(\boldsymbol{x}) = \delta(\boldsymbol{x};\boldsymbol{\alpha})$$

$$\delta(\boldsymbol{x};\boldsymbol{\alpha}) = \sum_{i=0}^{m} \alpha_i u_i(\boldsymbol{x})$$

- Add terms until MI is small enough.

Constant adjustment model

$$Y - f(\boldsymbol{x}) = \beta_0 + \beta_1 (f(\boldsymbol{x}) - \bar{f}) + \epsilon$$

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

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

$$\boldsymbol{\beta} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma})$$

Posterior distribution

- posterior distribution is

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

- constant adjustment predictor is

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

- Prediction interval

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

Simplification

- least squares estimate

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

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

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

Empirical Bayes estimation

- Estimate hyperparameters by maximizing

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

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

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

$$z_0 = \frac{|\tilde{\beta}_0|}{\sigma/\sqrt{n}} \ \text{ and } \ z_1 = \frac{|\tilde{\beta}_1|}{\sigma/\sqrt{S}}.$$

Approximate frequentist procedure

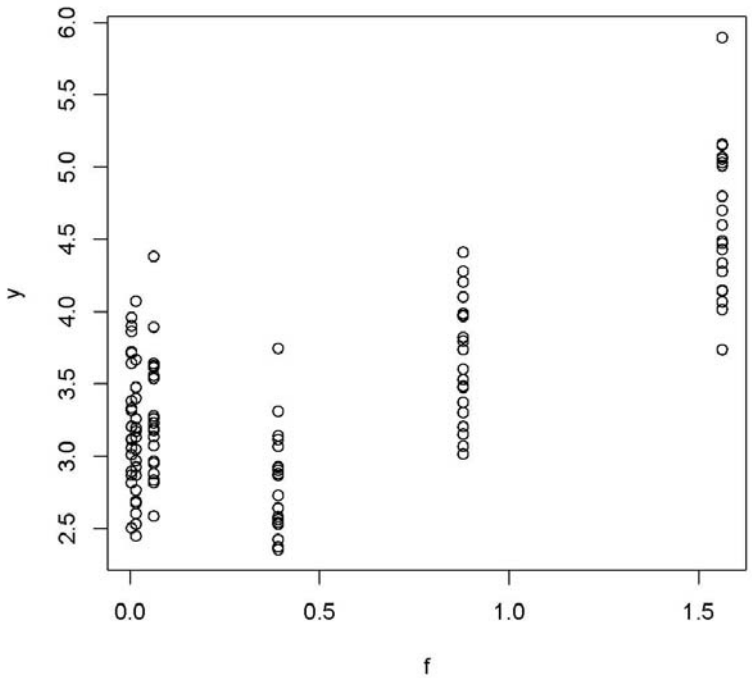
- Fit the simple linear regression

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

$$\text{and force } \beta_j \text{ to be 0 if } |z_j| < \sqrt{2}.$$

Surface roughness example

- Engineering model: $f_i = x_i^2/6400$



- There is a positive relation

Example-continued

- From replicates $\hat{\sigma}^2 = s^2 = .183$

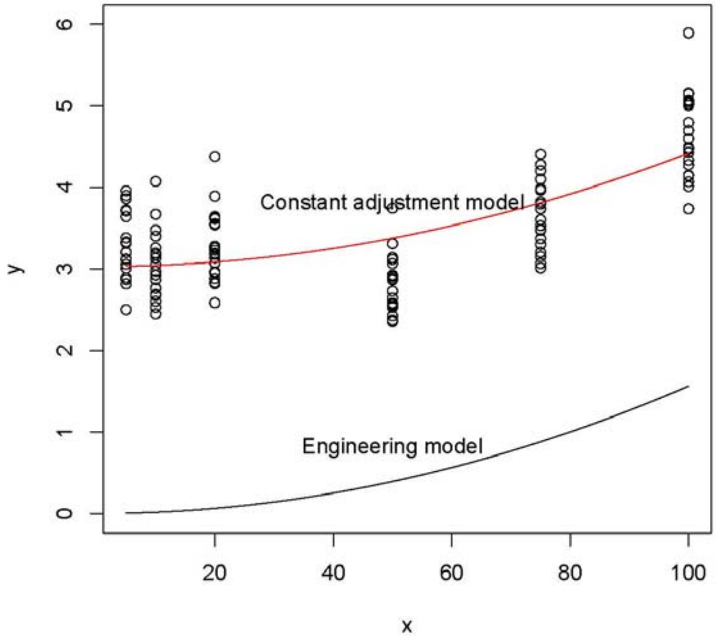
$$MI = \frac{1}{120}\sum_{i=1}^{120}(y_i - f_i)^2 = 9.12.$$

- 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

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



$$MI = \frac{1}{120}\sum_{i=1}^{120}(y_i - \hat{\mu}_i^C)^2 = .255$$

Functional adjustment model

$$Y - \mu^C(\boldsymbol{x}) = \delta(\boldsymbol{x}; \boldsymbol{\alpha}) + \epsilon$$

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

$$\boldsymbol{\alpha} \sim \mathcal{N}(\mathbf{0}, \gamma^2 \boldsymbol{R})$$

Two-stage estimation

- Use the estimate of $\mu^C(\boldsymbol{x})$ from the constant adjustment model
- $$\hat{\mu}^F(\boldsymbol{x}) = \hat{\mu}^C(\boldsymbol{x}) + \sum_{i=0}^{m} \hat{\alpha}_i u_i(\boldsymbol{x})$$

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

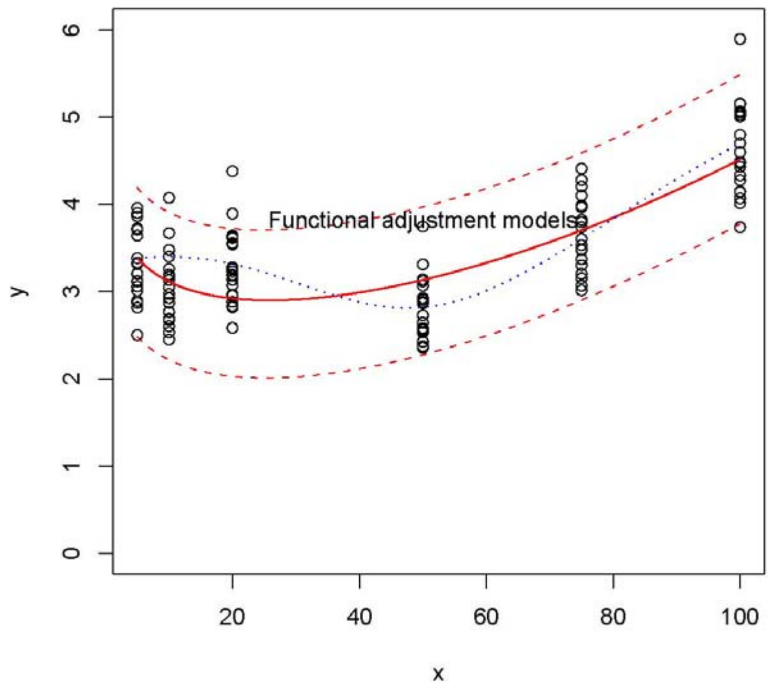
$$l = -\frac{1}{2}\log det(\gamma^2 \boldsymbol{U}\boldsymbol{R}\boldsymbol{U}' + \sigma^2 \boldsymbol{I}) - \frac{1}{2}(\boldsymbol{y} - \hat{\boldsymbol{\mu}}^C)'(\gamma^2 \boldsymbol{U}\boldsymbol{R}\boldsymbol{U}' + \sigma^2 \boldsymbol{I})(\boldsymbol{y} - \hat{\boldsymbol{\mu}}^C)$$

Approximate frequentist procedure

- Fit a multiple linear regression
- Do a variable selection

Surface roughness example

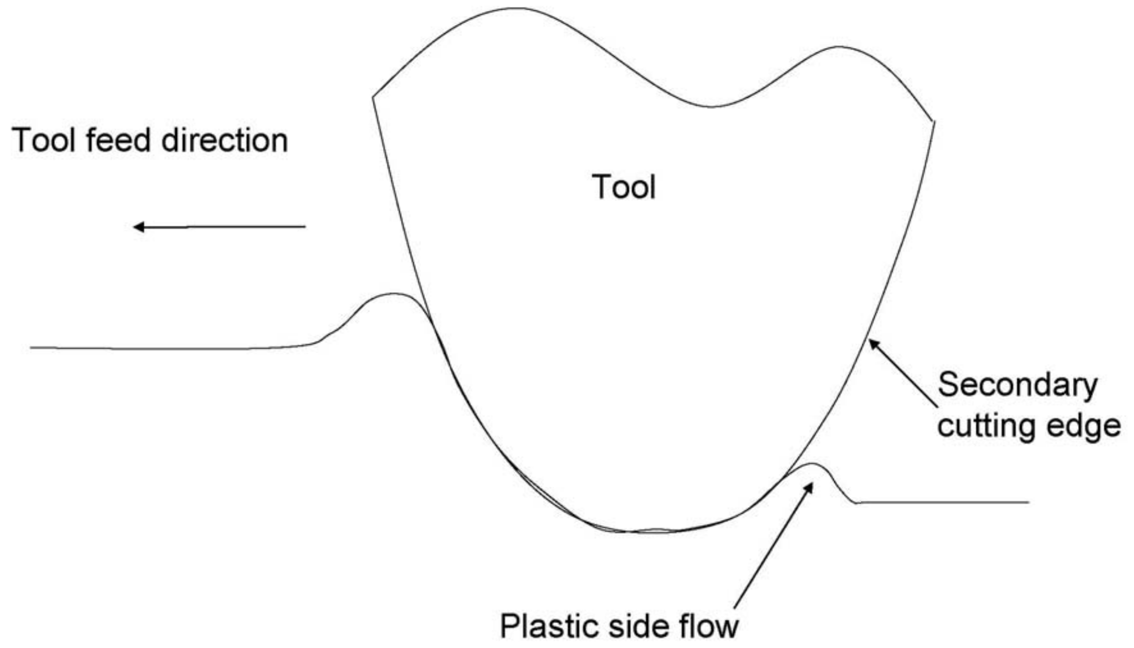
$$\hat{\mu}^F(x) - \hat{\mu}^C(x) = .015(x - 43.33) - .593(\log(1+x) - 3.35)$$



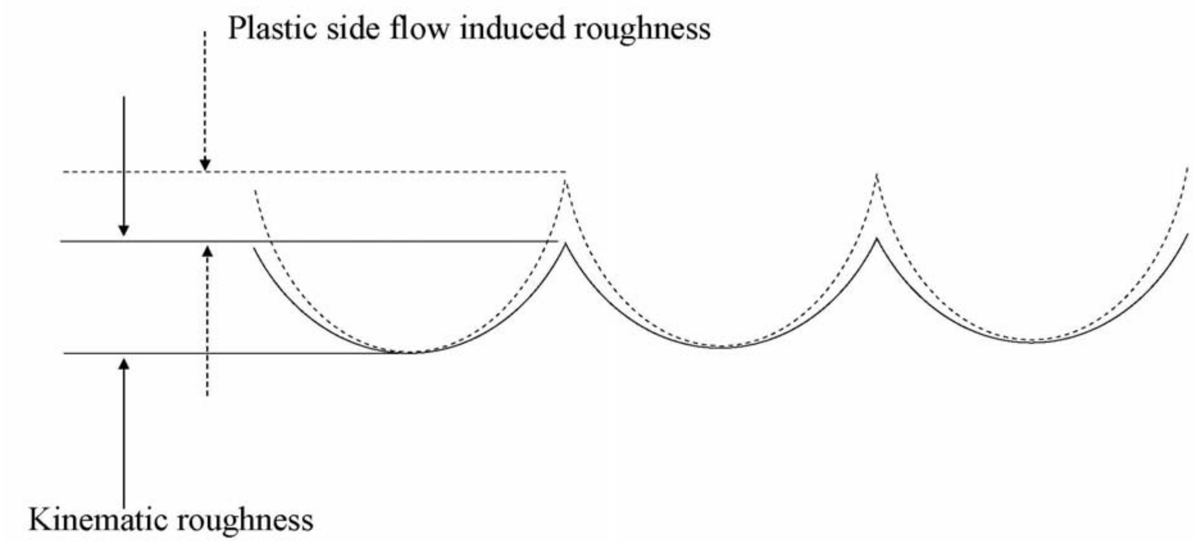
$$MI = \frac{1}{120}\sum_{i=1}^{120}(y_i - \hat{\mu}_i^F)^2 = .215$$

Calibration parameters

- Liu and Melkote (2006)



New engineering model



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

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

Statistical adjustments

- First use least squares estimate

$$\tilde{\boldsymbol{\eta}} = \arg \min_{\boldsymbol{\eta} \in [\boldsymbol{\eta}_L, \boldsymbol{\eta}_U]} \sum_{i=1}^{n} [y_i - f_i(\boldsymbol{\eta})]^2$$

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

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

Constant adjustment model

$$Y - f(\boldsymbol{x};\boldsymbol{\eta}) = \beta_0 + \beta_1(f(\boldsymbol{x};\boldsymbol{\eta}) - f(\boldsymbol{\eta})) + \epsilon$$

$$\begin{aligned} A(\boldsymbol{\eta}) &= \frac{1}{\sigma^2}\sum_{i=1}^{n}[y_i - f_i(\boldsymbol{\eta})]^2 + \log(1 + (z_0^2(\boldsymbol{\eta}) - 1)_+) \\ &+ \log(1 + (z_1^2(\boldsymbol{\eta}) - 1)_+) - (z_0^2(\boldsymbol{\eta}) - 1)_+ - (z_1^2(\boldsymbol{\eta}) - 1)_+ \end{aligned}$$

$$\hat{\beta}_0 = \left(1 - \frac{1}{z_0^2(\hat{\boldsymbol{\eta}})}\right)_+ \tilde{\beta}_0(\hat{\boldsymbol{\eta}}) \text{ and } \hat{\beta}_1 = \left(1 - \frac{1}{z_1^2(\hat{\boldsymbol{\eta}})}\right)_+ \tilde{\beta}_1(\hat{\boldsymbol{\eta}})$$

Approximate frequentist procedure

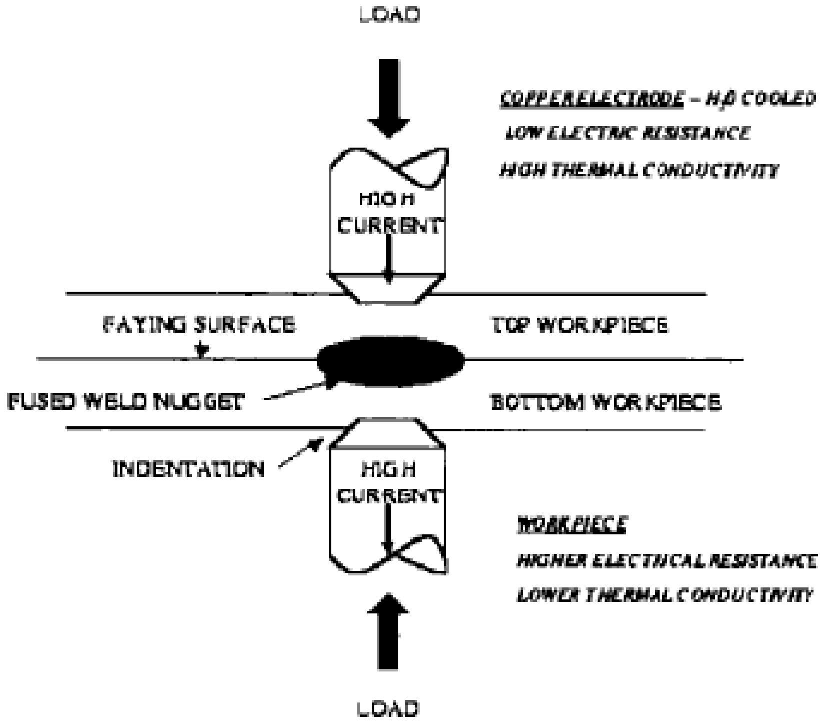
- Fit a nonlinear regression

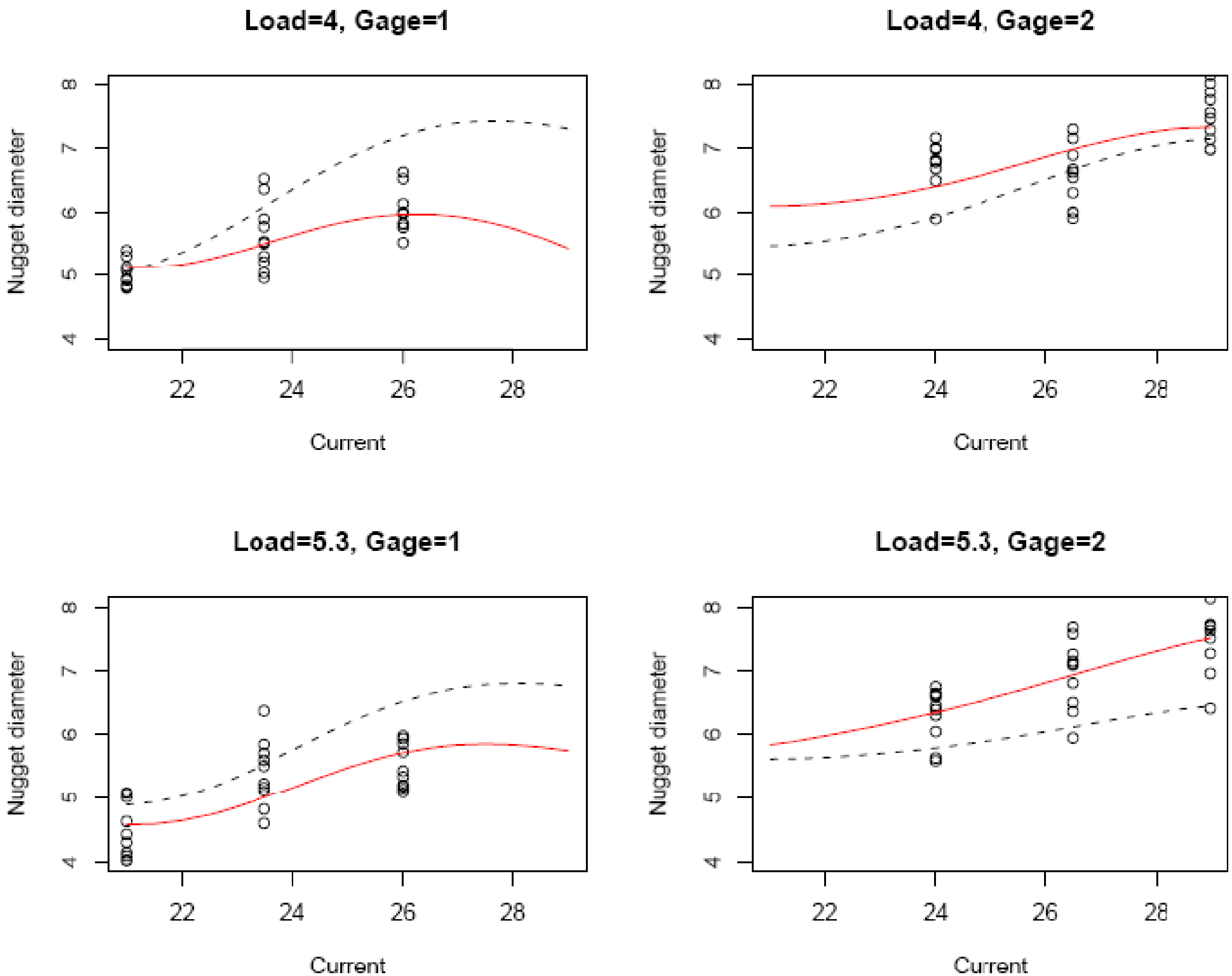
$$y_i = f_i(\boldsymbol{\eta}) - \beta_0 - \beta_1(f_i(\boldsymbol{\eta}) - \bar{f}(\boldsymbol{\eta})) + \epsilon_i$$

and force β_j to be 0 if $|z_j| < \sqrt{2}$.

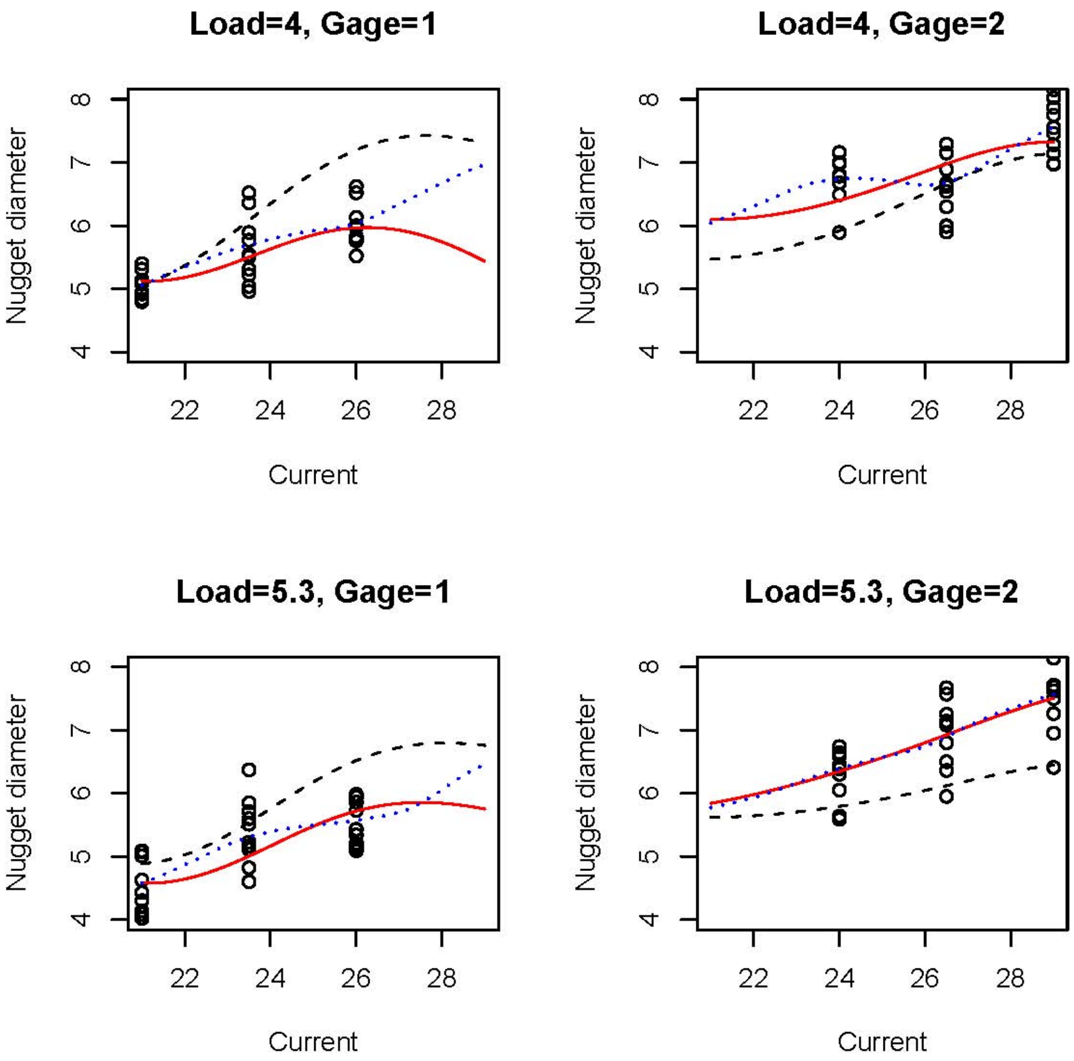
A Spot Welding Example

- Higdon et al. (2004) and Bayarri et al. (2007)
  - Three factors: Load, Current, and Gage
  - One calibration parameter





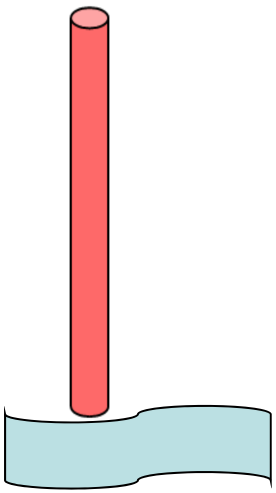
$$\hat{\mu}^F(\boldsymbol{x}) - \hat{\mu}^C(\boldsymbol{x}) = .12x_1 - .21(x_2 - .03) + .65x_3 + .44x_1x_2 + .40(x_2x_3 - .33)$$



Eng. Model (Black-dashed) : 0.69
Joseph&Melkote (Red-solid): 0.23
Bayarri et al. (Blue-dotted) : 0.20

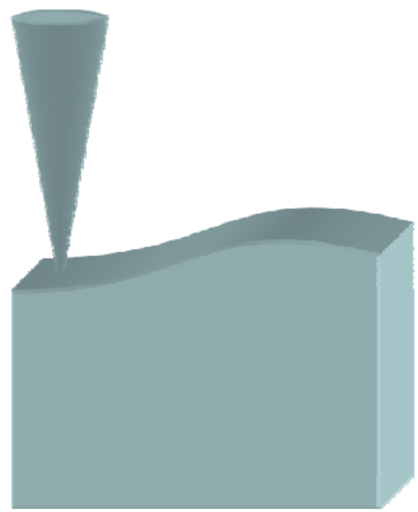
Example: LAMM

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



Laser heating

+



Mechanical micromachining

= LAMM

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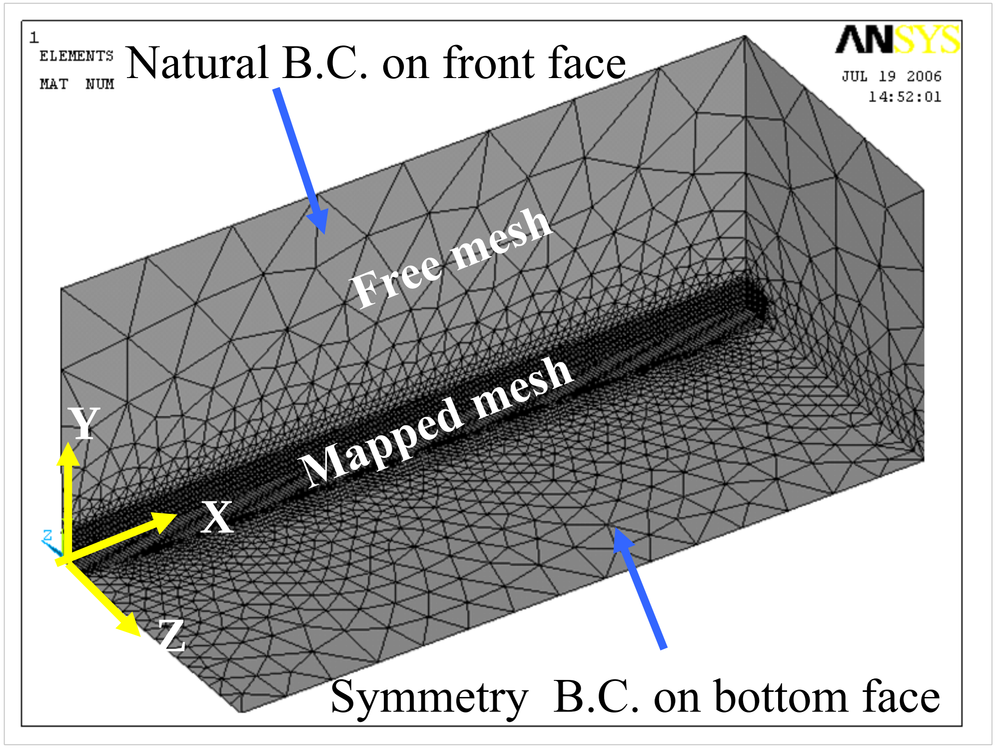
Objective

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

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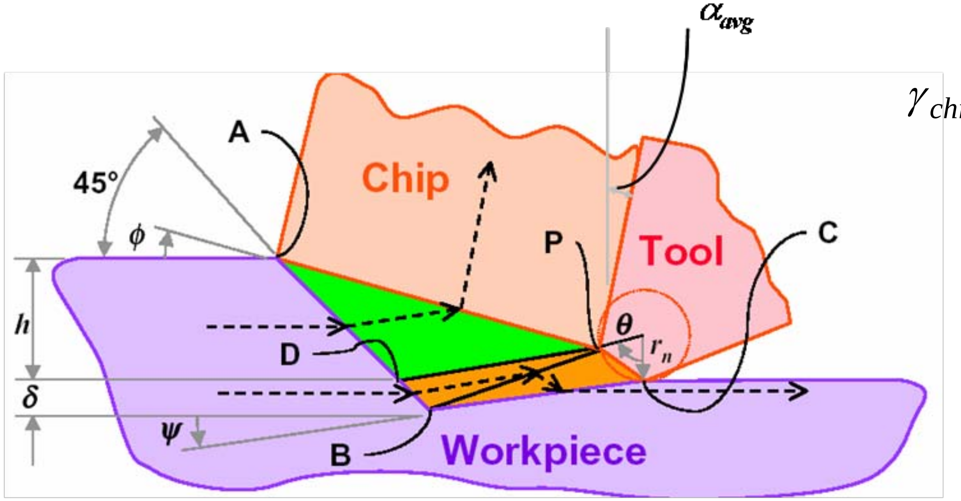
Geometric Model



(Manjunathiah et. al, 2000)

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

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

$$\dot{\gamma}_{chip} = 2V\frac{\gamma_{chip}}{\sqrt{2}\sin(\pi/4+\theta_{PD})\overline{PD}}$$

$$\dot{\gamma}_{work} = 2V\frac{\gamma_{work}}{\sqrt{2}\sin(\pi/4+\theta_{PD})\overline{PD} + \frac{\sin(\psi+\theta/2)}{\sin\psi}\overline{PC}}$$

$$\gamma_{eff} = \frac{v_{chip}\gamma_{chip} + v_{work}\gamma_{work}}{v_{chip}+v_{work}}$$

$$\dot{\gamma}_{eff} = \frac{v_{chip}\dot{\gamma}_{chip} + v_{work}\dot{\gamma}_{work}}{v_{chip}+v_{work}}$$

For plane strain conditions,

$$\varepsilon = \gamma_{eff}/\sqrt{3}$$

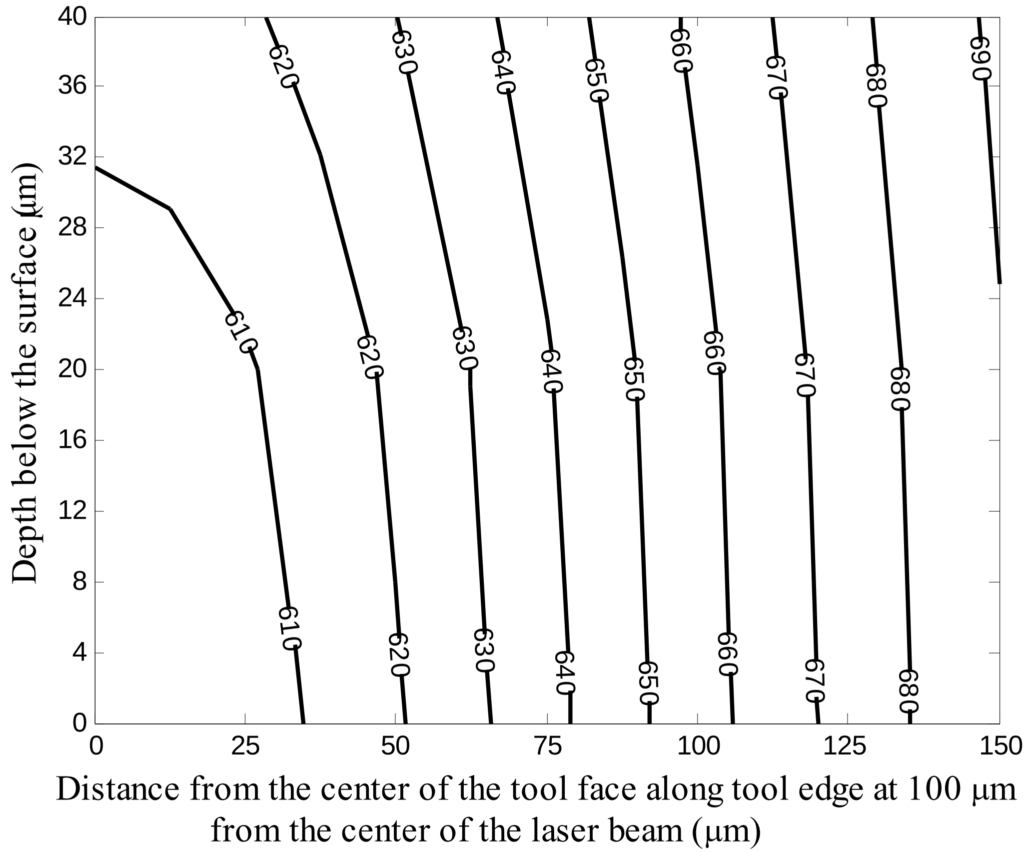
$$\dot{\varepsilon} = \dot{\gamma}_{eff}/\sqrt{3}$$

Shear Flow Strength

$$\sigma(\varepsilon,\dot{\varepsilon},T,HRC)=\left(A+B\varepsilon^{n}+C\,ln(\varepsilon+\varepsilon_0)+D\right)\left(1+E\,ln\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)\right)\left(1-\left(T^{*}\right)^{m}\right)$$

Yan et al., 2007

$$S=\sigma/\sqrt{3}$$



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

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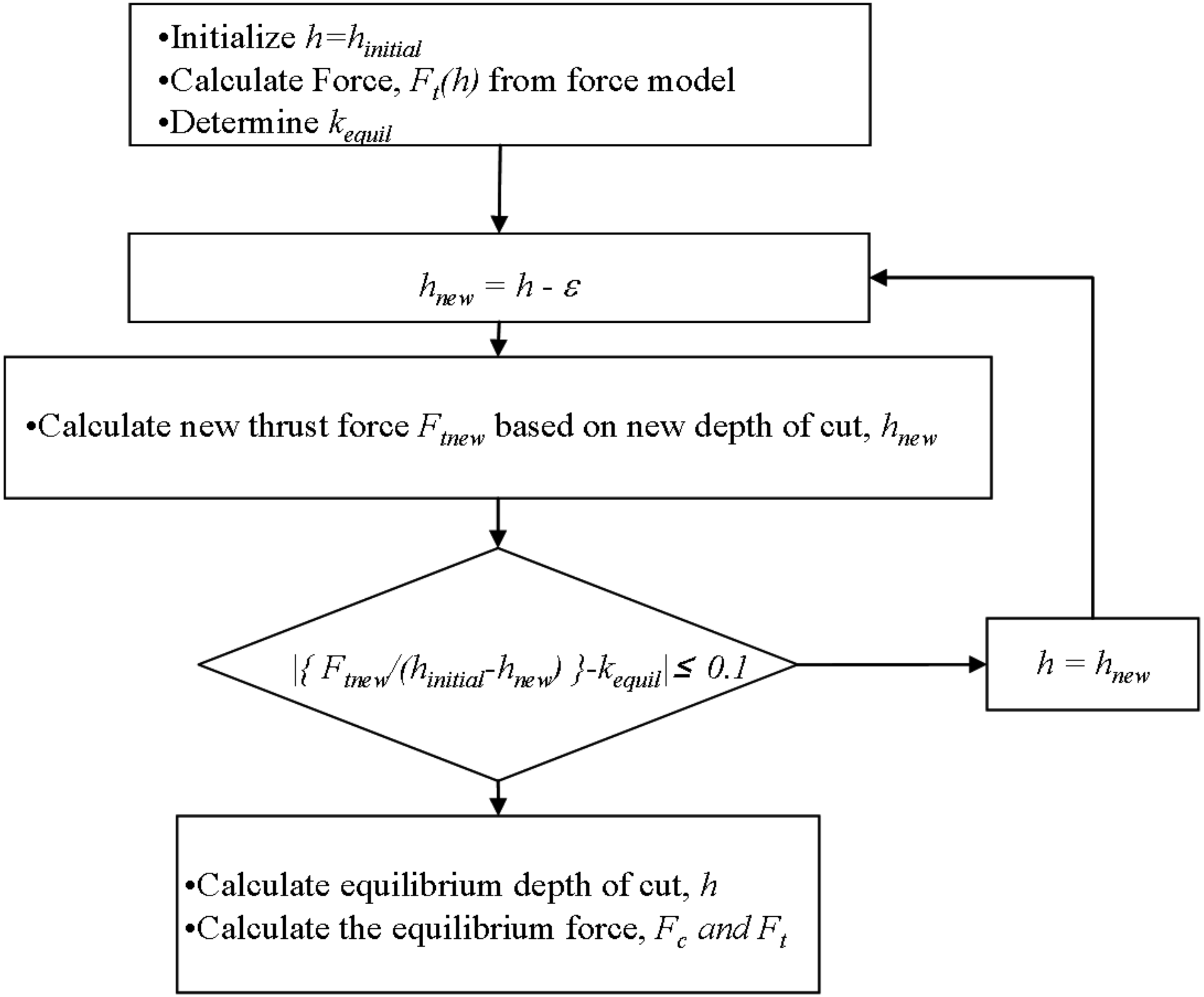
Forces

- Cutting and thrust forces,

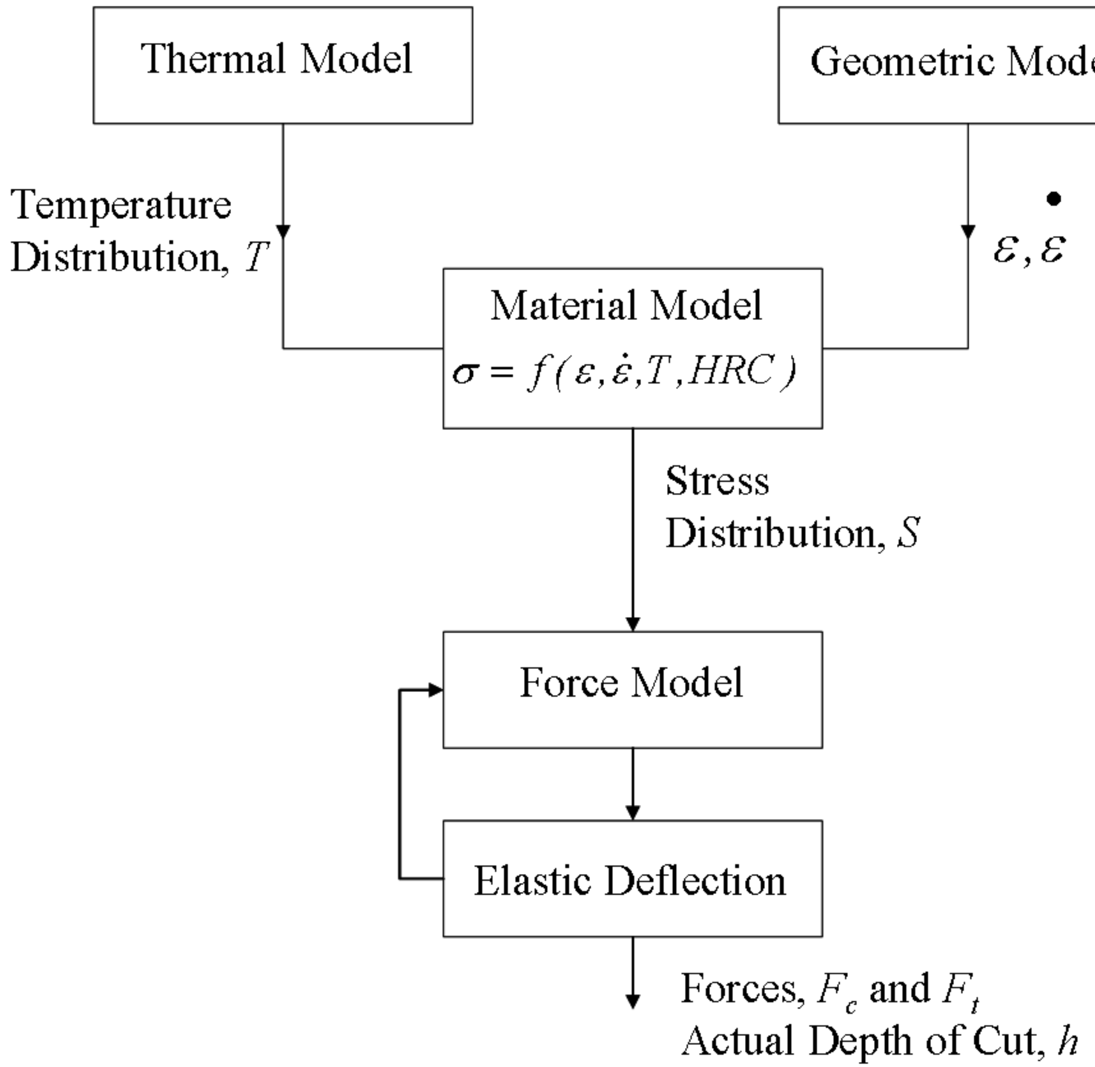
$$F_c = \{(h-p)\cot\phi + h + r_n \sin\theta - (k-1)\delta\}\sum_{i=1}^{n}\bar{S}(i)w(i)$$

$$F_t = \{(h-p)\cot\phi - h + r_n \sin\theta + (k-1)\delta\cot\psi\}\sum_{i=1}^{n}\bar{S}(i)w(i)$$

Equilibrium Forces/Deflection

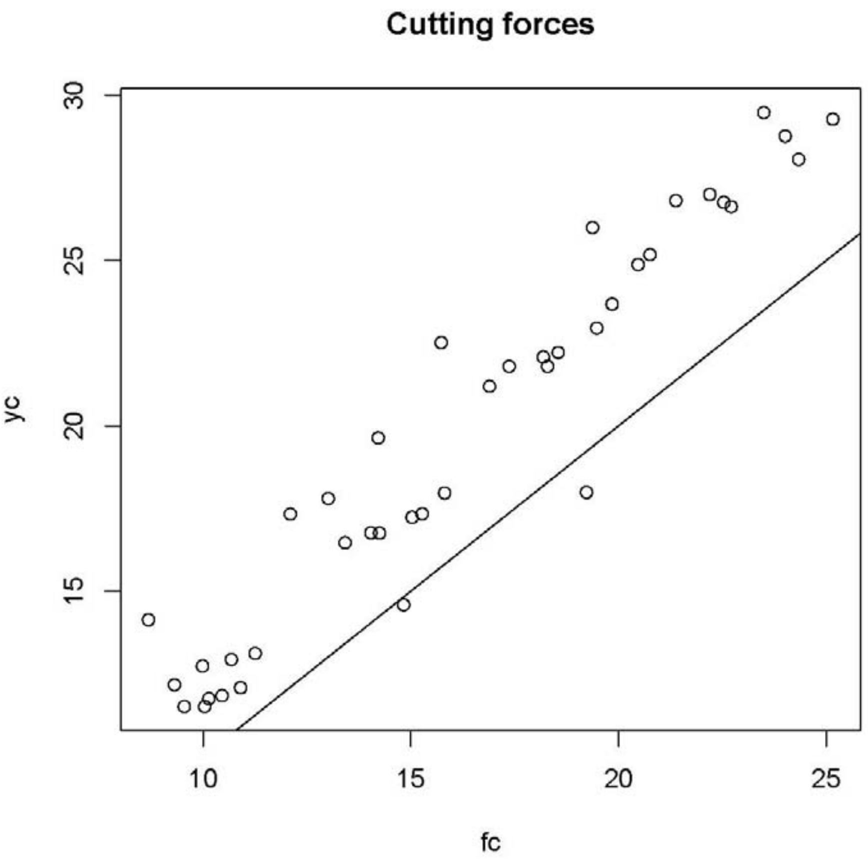


Force model



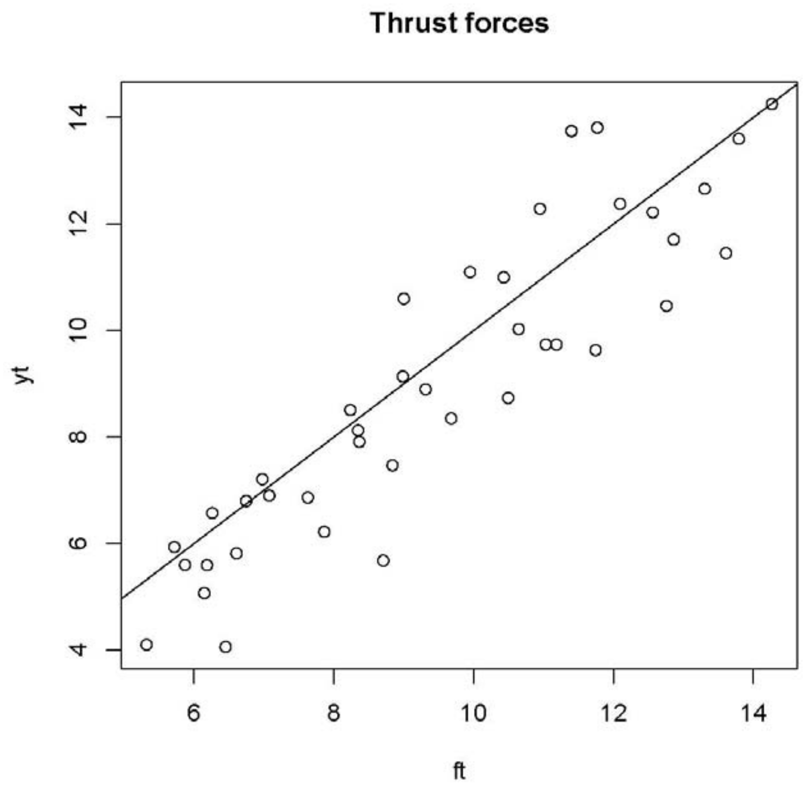
Thermal Model
Geometric Model
Temperature Distribution, T
$\dot{\varepsilon}, \varepsilon$
Material Model
$\sigma = f(\varepsilon, \dot{\varepsilon}, T, HRC)$
Stress Distribution, S
Force Model
Elastic Deflection
Forces, F_c and F_t
Actual Depth of Cut, h

Force prediction



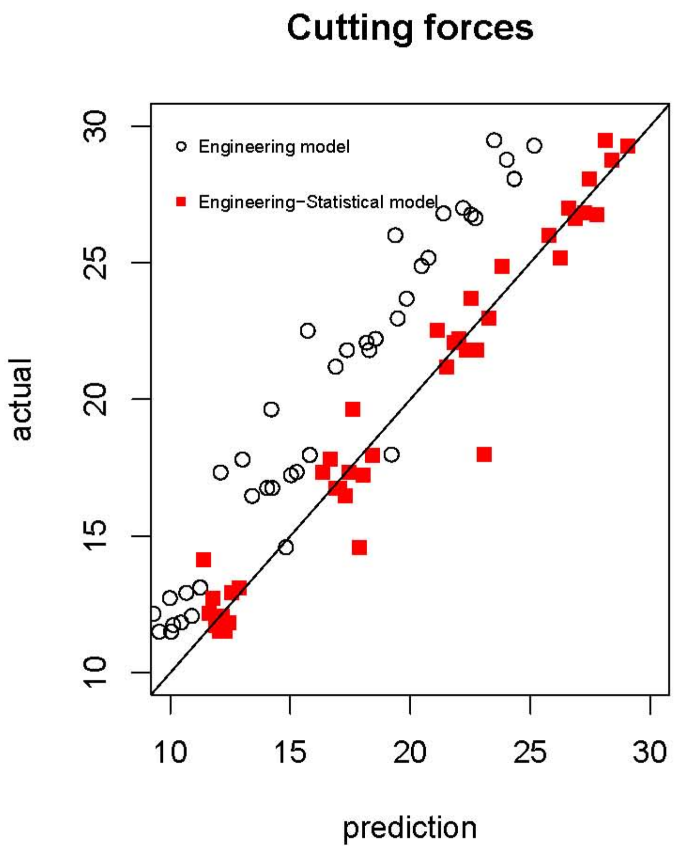
- Positive relation, but predictions are smaller than actual

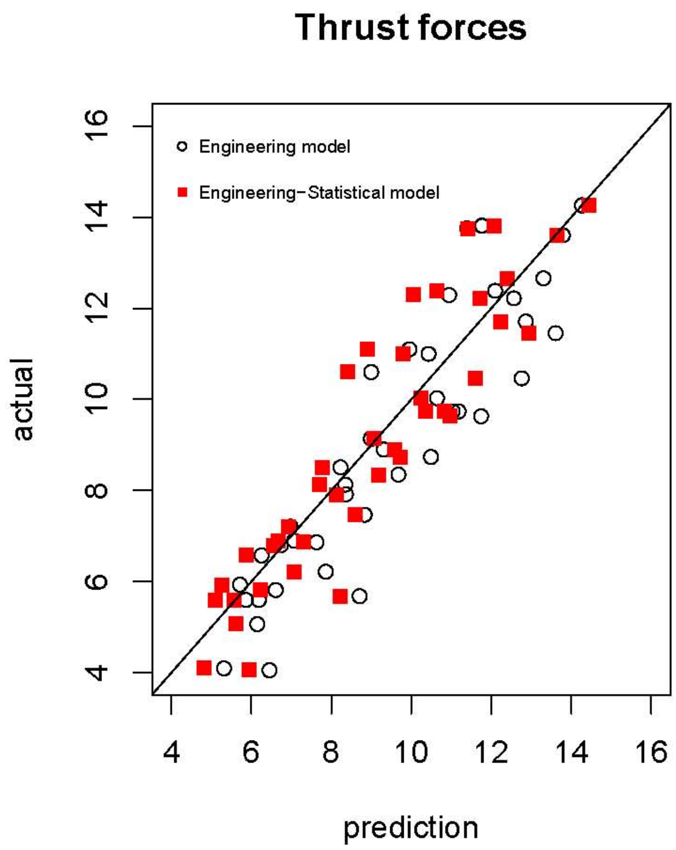
Force prediction-continued



- Better than cutting force, but slightly smaller than actual

Engineering-Statistical Force Models





Plot of measured vs. predicted cutting and thrust forces

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.

$$\min_{x_1, x_2, x_3, x_4} \hat{y}_c^2 + \hat{y}_t^2$$

$$\text{subject to} \quad doc = t$$

$$T_2 \leq A_{c_1}$$

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Nonlinear programming

$$\min \left\{1.54 x_1^{0.89} \exp(0.0014 x_2 - 0.009 x_3 e^{-0.0034 x_4})\right\}^2 + \left\{1.03 x_1^{0.8} \exp(0.0014 x_2 - 0.043 x_3 e^{-0.0034 x_4})\right\}^2$$

$$x_1 - 0.57 x_1^{0.8} \exp(0.0014 x_2 - 0.196 x_3 e^{-0.0034 x_4}) = t$$

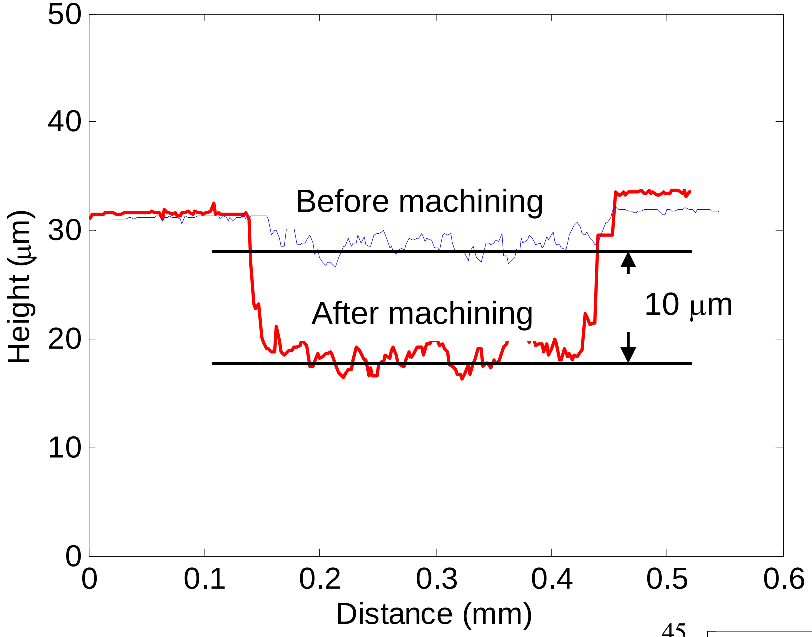
$$25 + 196.4 x_3 \exp(-0.0021 x_1 x_3 - 0.00045 x_2 x_3) \le 800$$

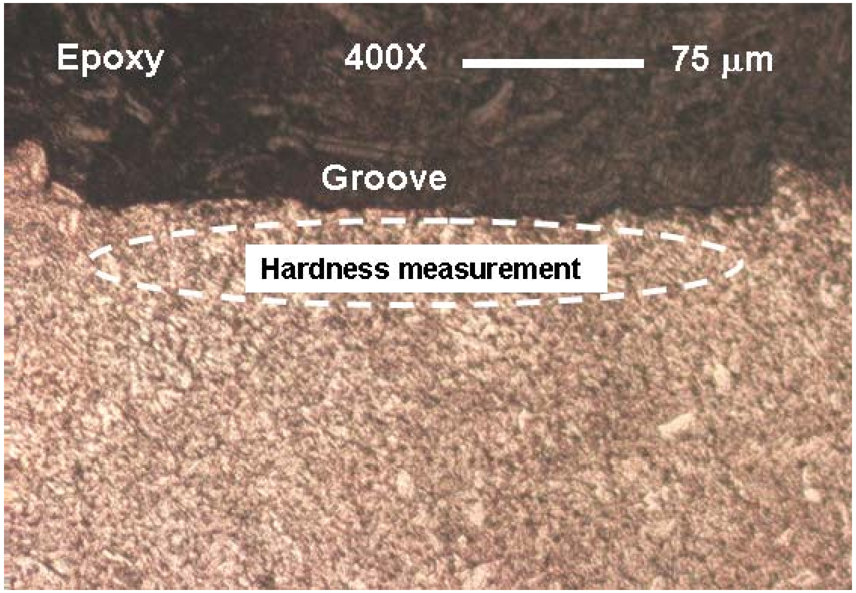
$$10 \le x_1 \le 25,\ 10 \le x_2 \le 50,\ 0 \le x_3 \le 10,\ 100 \le x_4 \le 200$$

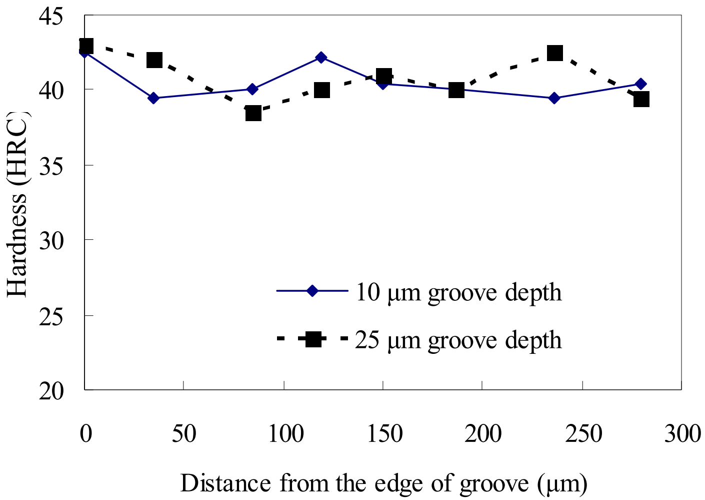
Optimization Results

- 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







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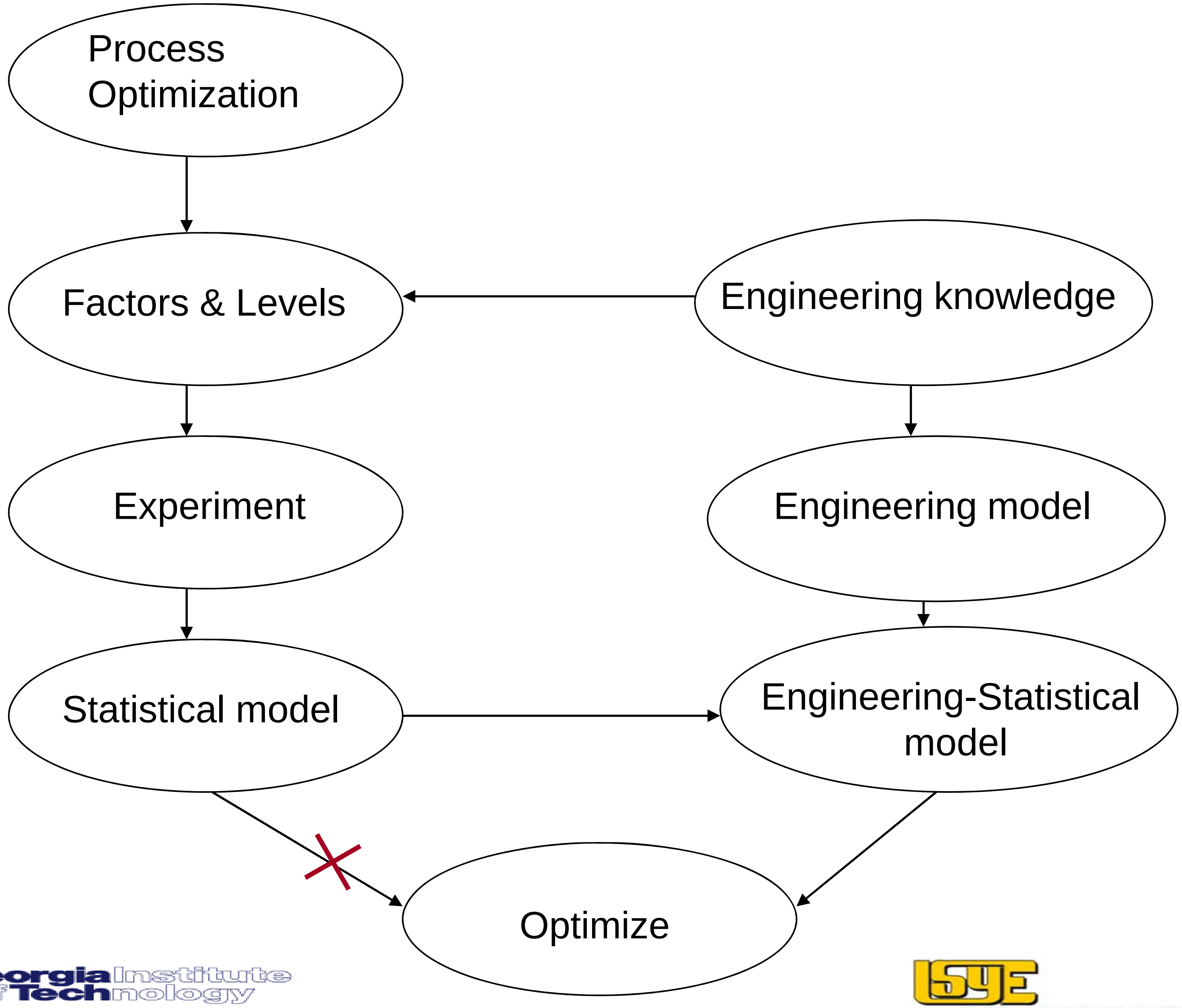
Conclusions

- 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
Engineering knowledge
Experiment
Engineering model
Statistical model
Engineering-Statistical
model
Optimize

Conclusions-continued

- Simple procedure
  - Fit two linear/nonlinear regressions
  - Do variable selection
- Easy-to-implement
  - No additional programming is required