

Using Bayesian Methods to Improve a Calibration Program

Calibration of a Pressure Transducer

Using Dynamic Linear Modelling

by

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1 What is pressure?

Pressure is a measure of the impact of molecules of a gas or liquid bombarding the containing walls of the vessel for which they are confined. Its magnitude is the force of impacts per unit area, i.e.

$$p = \frac{F}{A}.$$

The SI unit for measuring pressure is the pascal, abbreviated Pa, which represents one newton per square meter (N/m^2). In relation to the world we live, a pascal is a very small quantity. Atmospheric pressure is roughly 100,000 Pa. Other common units of pressure are the bar, millibar, pound-force per square in, torr.

Various instruments are used to measure pressure, eg. barometers, manome-

ters, transducers, dead weight gauges, and several others. In this study the statistical calibration of pressure transducers is considered.

2 Pressure Transducers

One instrument among the many that the NIST Pressure Measurements Division calibrates is the pressure transducer gauge. The pressure transducer is an instrument that converts pressure in a manifold to an electrical signal. How it operates can be easily understood by comparing it to a simple electrical condenser, ie. two parallel plates separated by a distance d with a voltage applied to one plate and the other grounded. The electrical field, \vec{E} ,

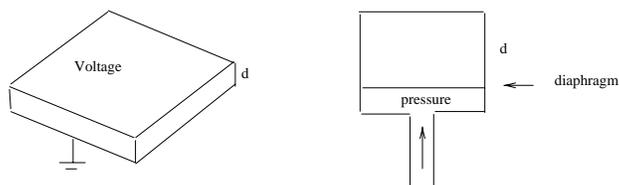


Figure 1: Illustration of condenser and transducer

created between the plates has components $E_x = 0$ and $E_y = V/d$ where V is the magnitude of the applied voltage. Thus, the capacitance and other electrical constants associated with the condenser all depend on the separation distance, d of the plates. Similarly, the upper part of the transducer acts

like a condenser and as pressure enters the gauge it deforms the diaphragm thus changing the electric field. From principals of physics one can derived a pressure reading from the deformation of the electric field.

Because of degradation of the mechanical parts, the transducer has to be periodically recalibrated to correct for inaccuracies that occur over time. A more accurate and stable comparison pressure gauge is used to determine how far off the readings of the inaccurate instrument are from the truth.

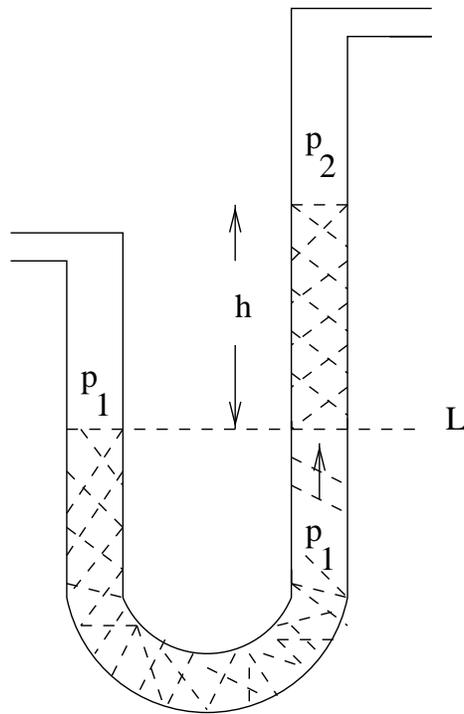


Figure 2: Illustration of Manometer

One such gauge used by NIST to calibrate a transducer is the manometer. The manometer is essentially a liquid filled *U – tube* where the vertical separation of the liquid’s surfaces gives a measure of the difference between the pressures at the ends. The liquid is usually mercury, water or oil, whose densities, ρ , are well known. The constant h denotes the height of the column of liquid above the p_1 equilibrium level. The pressures p_1 and p_2 at the ends of the manometer are related by

$$\begin{aligned} p_1 &= p_2 + \text{pressure caused by the column of liquid above } p_1 \text{ equilibrium level} \\ &= p_2 + g\rho h \end{aligned} \tag{1}$$

where g denotes the graviational constant. Because of its simplicity and because the constants on the right hand side of Eq. (1) can be very accurately determined, NIST uses a manometer to calibrant pressure gauges over a certain range. For high pressures the manometer would not be a reasonable instrument since the column of liquid would have to reach an unmanageable height. In this study transducers are considered in the pressure range of .01 torr to 1 torr. A torr is approximately 133 pascals. So these are low vaccum pressures.

An illustration of the coupling used in the calibration is shown in the figure below. The gauges are connected by a manifold, which is connected to

a pressure generator. At the start of the calibration, pressure at a certain level is released into the manifold. This pressure produces pressures at both the manometer and the transducer and they are recorded as a pair (x_1, y_1) . Then, this starting pressure is ramped up to create two new pressures at the two instruments, (x_2, y_2) and so on until say n comparison values are produced (x_n, y_n) . At each pressure setting the pressure induced at the manometer can be accurately determined. Based on these data a calibration curve is found between the x 's and y 's.

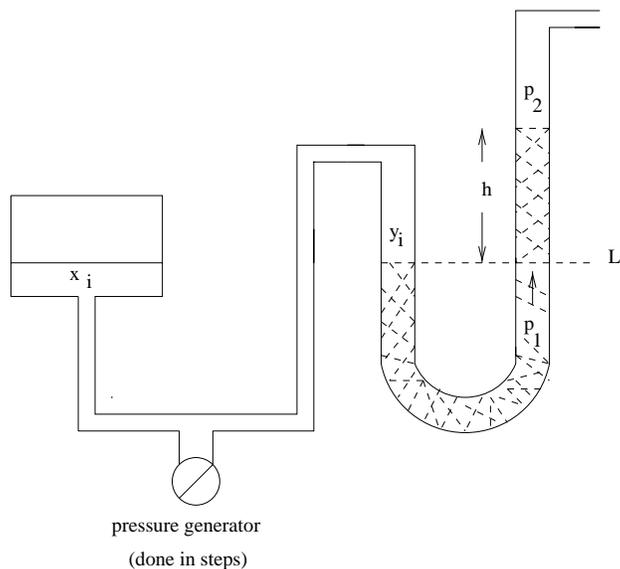


Figure 3: Illustration of Calibration Set-Up

For example, consider transducer XX007 that was sent to NIST for cal-

ibration with comparison data given below Obviously, the residuals suggest

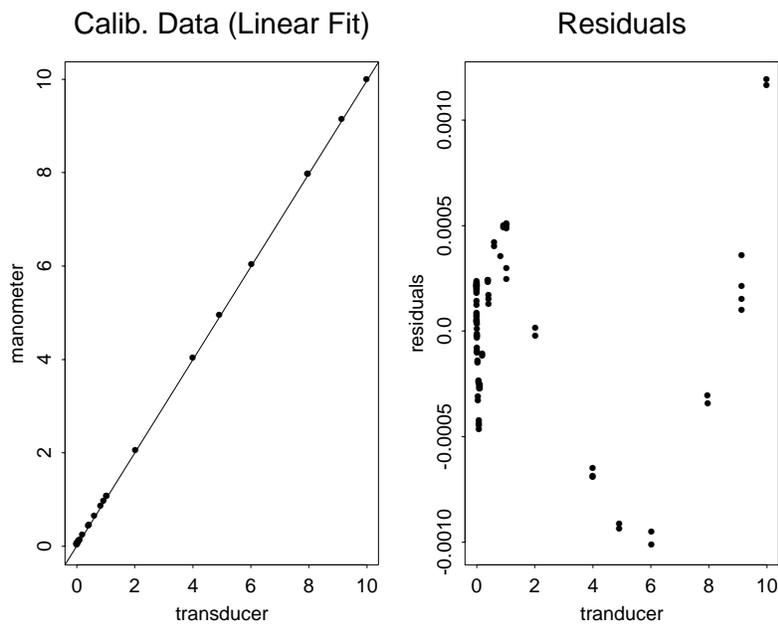


Figure 4: Calibration data for Transducer XX007

that a polynomial fit would be a better calibration curve than a straight line, for example one might try a fifth degree polynomial, ie.

$$manometer = const + a_1 * transducer + a_2 * transducer^2 + \dots + a_5 * transducer^5 + error$$

The residuals of this fit look better. The following curve was eventually used as the calibration curve for the full range of pressure values

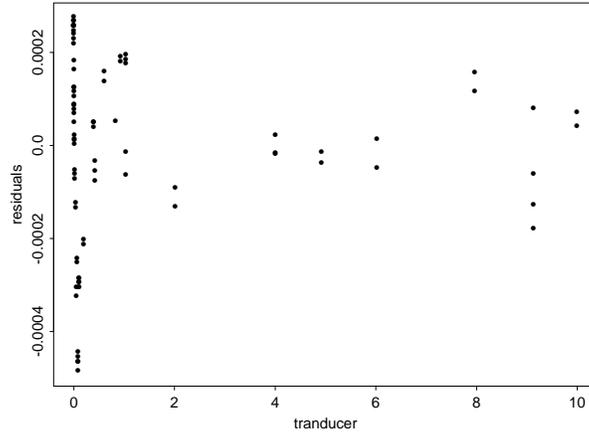


Figure 5: Residuals for a 5th Degree Polynomial Fit

3 Prior Calibrations

The transducer discussed in the previous section was recalibrated 5 times over the last ten years, 1990, 1992, 1994, 1996 and 1999. Each time the calibration was done at NIST's Pressure Measurements Division calibration laboratory. The data for each calibration is filed and given by

$$(x_i(t), y_i(t)) = \text{calibration data } t = 1990, 1992, 1994, 1996, 1999$$

$$x_i(t) = \text{ith transducer reading at time period } t$$

$$y_i(t) = \text{ith manometer reading at time period } t$$

An analysis of the data led to models of following form for calibration

curves

$$y = a_0 + a_1x + \dots + a_jx^j + b_1\text{Log}_{10}(x) + b_2(\text{Log}_{10}(x))^2$$

Note that inverse calibration is used, i.e. the primary standard is taken as the y-value. This was done because the variability between the primary standard and the transducer is very small, for each calibration period.

4 Bayesian Calibration

Calibration is a prediction problem. On one hand, one has a very well made, precise instrument (call it the standard) and on the other hand, one has a not so precise instrument (call it the test). Both instruments measure the same quantity and one wants to correct the inaccuracy in the test instrument based on a comparison with the standard. So, the prediction problem is: for each new observation on the test instrument, find a correction for it based on the comparison data $(transducer_i, primary\ standard_i), i = 1, \dots, n$. In terms of the model above one wants to find a predicted value for the correction y based on seeing a value x from the test.

Since calibration is a prediction problem, the predictive density plays a major role in bayesian calibration. For a random sample $y_i, i = 1, \dots, n$ from

a density $p(y | \theta)$, the predictive density of observing another independent value y from $p(y | \theta)$ is given by

$$p(y | y_1, \dots, y_n) = \int_{\Theta} p(\theta | y_1, \dots, y_n) p(y | \theta) d\theta$$

where $p(\theta | y_1, \dots, y_n)$ is the posterior density of $p(\theta)$, the prior density. In the calibration problem one seeks the predictive density, $p(y | x, data)$. This requires a prior and a posterior density.

Because the instrument has been calibrated several times before, these data sets provide excellent prior information. Below an algorithm is given that ties these prior data sets together in such a way that at time t a posterior density can be determined and thus a predictive density for the calibration. Now at NIST, the data used to calibrate a gauge is just the present calibration data. It does not use prior calibration data. Bayesian calibration provides a means to use these prior sets of data, and thus producing a better and more efficient method of calibration.

Consider the calibration problem where an instrument has been previously calibrated at times $t = t_1, t_2, \dots, t_{m-1}$ and a calibration is sought at time $t = t_m$. At each time period t the data are modeled as

$$y_i(t) = \theta_1(t) + \theta_2(t)f_1(x_i(t)) + \dots, \theta_p(t)f_p(x_i(t)) + \phi\epsilon_i(t) \quad i = 1, \dots, n(t).$$

for some known functions $f_i(x)$ and $\phi = 1/\sigma$ denotes the precision. The model can be written more succinctly in vector form:

$$Y(t) = X(t)\theta(t) + \phi\epsilon(t)$$

where $Y(t) = (y_1(t), \dots, y_n(t))^t$, $X(t) = (f_i(x_j))$, $1 \leq i \leq n(t)$, $1 \leq j \leq p$ an $n(t) \times p$ matrix, $\epsilon(t) = (\epsilon_1(t), \dots, \epsilon_n(t))^t$ and $\theta(t) = (\theta_1(t), \dots, \theta_n(t))^t$. The error vector, $\epsilon(t)$ has a multivariate normal distribution with mean zero and variance-covariance matrix the identity matrix.

Consider the inverse calibration model where the test is the independent variable. So, $y_i(t)$ represents the standard and $x_i(t)$ represents the test. Then the calibration problem is identical to the regression problem. The dynamic linear model is

$$Y(t) = X(t)\theta(t) + \phi\epsilon(t) \tag{2}$$

$$\theta(t) = \theta(t-1) + \phi\omega(t) \tag{3}$$

where $\omega(t)$ has a multivariate normal distribution with mean zero and variance-covariance matrix $V(t)$. It is assumed that $\omega(t)$ is independent of $\theta(t-1)$ and $\epsilon(t)$. This is the standard dynamic linear model with parameters (θ, ϕ) , see Pole, West and Harrison (1994).

At each time period, $t = t_i$ the priors are chosen recursively, start with

a vague Normal Gamma prior on $(\theta(t_0), \phi)$. The vector $(\theta(t_0), \phi)$ is said to have a normal gamma prior with parameters $\mu(t_0), \lambda(t_0), \alpha(t_0), \beta(t_0)$ if its density is given by

$$p(\theta(t_0), \phi) = N_p(\theta(t_0) \mid \mu(t_0), \phi\lambda(t_0))Ga(\phi \mid \alpha(t_0), \beta(t_0))$$

where $N_p(z \mid \mu, \lambda)$ denotes the p dimensional multivariate normal density with mean μ and precision matrix λ and $Ga(\phi \mid \alpha, \beta) = e^{-\phi\beta} x^{\alpha-1} \Gamma(\alpha) / \beta^\alpha$ is the gamma density.

By a vague prior one means a prior density that is flat, i.e. it looks in some sense like a uniform prior. For a normal random variable, this can be done by making the precision very small. For a gamma random variable, this can be done by making β very small and making α reasonably large. Indeed, for β small one can approximate the gamma density by $x^{\alpha-1} \Gamma(\alpha) / \beta^\alpha$. Using the fact that $\log(\Gamma(\alpha)) = (\alpha - .5)\log(\alpha) - \alpha + \textit{smaller order terms}$, one has $\log Ga(\phi \mid \alpha, \beta) = (\alpha - .5)\log(\alpha) - \alpha + (\alpha - 1)\log(x) - \alpha\log(\beta)$. So, for α big this term will be dominated by the constant $\alpha\log(\alpha)$ for reasonably sized x . Caution if α is taken too large, computing $\gamma(\alpha)$ can slow ones computations.

The dynamic linear modeling algorithm goes as follow:

- Start with a Vague Normal Gamma Prior on $(\theta(t_0), \phi)$ with parameters

$\mu(t_0), \lambda(t_0), \alpha(t_0), \beta(t_0)$

e.g. $\theta_p(t_0) = 0, \lambda(t_0) = 10^{-6}I, \alpha(t_0) = 10^4, \beta(t_0) = 10^{-6}$.

- Use the state equation $\theta(t_1) = \theta(t_0) + \phi\omega(t_1)$ to compute a derived prior for $(\theta(t_1), \phi)$.

It will be normal gamma with parameters

$$\mu_d(t_1) = \mu(t_0), \quad \lambda_d(t_1)\lambda(t_0) + V(t_1)$$

$$\alpha_d(t_1) = \alpha(t_0) \quad \beta_d(t_1) = \beta(t_0)$$

- Compute the posterior density of $(\theta(t_1), \phi)$ given the data $y(t_1), X(t_1)$.

It will be normal gamma with parameters

$$\mu_{pos}(t_1) = (\lambda_d(t_1) + X(t_1)^t X(t_1))^{-1}((\lambda_d(t_1)\mu(t_0) + X^t(t_1)Y(t_1)))$$

$$\lambda_{pos}(t_1) = \lambda_d(t_1) + X(t_1)^t X(t_1)$$

$$\alpha_{pos}(t_1) = \alpha_d(t_0) + \frac{1}{2}n(t_1)$$

$$\beta_{pos}(t_1) = \beta_d(t_1) + \frac{1}{2}(Y(t_1) - X(t_1)\theta(t_1))^t Y(t_1) + \frac{1}{2}(\mu_d(t_1) - \mu_{pos}(t_1)\lambda_d(t_1))\mu_d(t_1)$$

Compute the marginal density $\theta(t_1)$. It will be Student T with known parameters. Use its mean to estimate $\theta(t_1)$. This can be used to check fit

with the data, $\hat{y}(t_1) = X(t_1)E[\theta(t_1) | Data]$. Compute the predictive density of $y_{fut}(t_1)$ it will be Student T with known parameters.

At time t_2 , use the posterior of $(\theta(t_1), \phi)$ as the prior for for the next iteration at time $t = t_2$

Repeat.

The following equations curves were supplied as calibration curves for the transducer at times t1=1990,t2=1992, t3=1994,t4=1996,t5=1999.

$$y(90) = 5.1400207E - 4 + .99706543 * x(90) - 7.59022E - 5 * x(90)^2 + 1.0655982E - 5 * x(90)^3 \\ + .0012814899 * \log_{10}(x(90)) + 4.096750E - 4 * (\log_{10}(x(90)))^2$$

$$y(92) = .416733E - 4 + .995612 * x(92) - .712361E - 4 * x(92)^2 + .963455E - 5 * x(92)^3 \\ + .103228E - 2 * \log_{10}(x(92)) + .383161E - 3 * (\log_{10}(x(92)))^2$$

$$y(94) = -7.38460E - 4 + 9.96765E - 1 * x(94) - 6.00106E - 4 * x(94)^2 + 8.31965E - 5 * x(94)^3 \\ - 3.39525E - 6 * r^4 + 8.28179E - 5 * \log_{10}(x(94)) + 1.44930E - 4 * (\log_{10}(x(94)))^2$$

$$y(96) = 0.995150 * x(96) - 4.46523E - 4 * x(96)^2 + 6.59320E - 5 * x(96)^3 \\ - 2.71946E - 6 * x(96)^4 + 1.14660E - 3 * \log_{10}(x(96)) + 5.14573E - 4 * (\log_{10}(x(96)))^2$$

$$y(99) = 5.79384E - 4 + 0.994388 * x(99) + 9.36232E - 5 * x(99)^2 + 1.57063E - 3 * \log_{10}(x(99))$$

$$+ 5.80231E - 4 * (\log_{10}(x(99)))^2$$

These models were used in the dynamic linear model algorithm above. Below is a comparison of NIST's previous calibration results and the Bayesian calibration results based on the dynamic linear model algorithm. The comparison is based on the fitted models $\hat{y}(t) = X(t)\theta(t)$ and $\hat{y}(t) = X(t)E[\theta(t) | Data]$, ie. their R^2 parameters are compared.

NIST	$R^2(1990) = 0.225292$	$R^2(1992) = .0000889048$	$R^2(1994) = 1.61953$	$R^2(1996)$
Bayesian	$R^2(1990) = 1.71688E - 06$	$R^2(1992) = .0000874232$	$R^2(1994) = 1.28331$	$R^2(1996)$

Other comparisons are in the works. For example a comparison of predicted values. Here one row is removed from each data set and a comparison is made to determine which method is better in predicting the value of the deleted row.