# ON THE APPLICATION OF DURBIN-WATSON STATISTICS TO TIME-SERIES-BASED REGRESSION MODELS

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A fundamental tenet in (linear) regression analysis is that errors associated with a model must be random and independent from observation to observation in an experiment, with expectation (or mean value) zero. Various aspects of residual behavior are routinely discussed in modern texts on probability and statistics. The distribution of

$$e_k = y_k - \hat{y}_k;\ k = 1, \ldots, n$$

should show a random scatter when plotted against

$$x_k,\ y_k,\ \text{or}\ \hat{y}_k$$

as abscissa.

If the statistical experiment involves observations in a time sequence, and the error at time instant $t_k$ is influenced by the error at the immediately previous time instant $t_{k-1}$, the resulting "influential carryover"[1,2] violates the error-independence criterion. The errors may be negatively or positively correlated.

The technique introduced by Durbin and Watson[3] more than fifty years ago is a popular and straightforward test for the existence of autocorrelation in time-series analysis (*e.g.,* in forecasting). Only a small number of textbooks on probability and statistics intended for engineering and natural sciences treats this subject matter, however.

The purpose of this article is to demonstrate the application of the Durbin-Watson (DW) technique to regression analysis concerning chemical engineering processes where the "regressor"[4] sequence occurs as a time series. Regression problems of this kind appear routinely in reaction kinetics/chemical reaction engineering, applied transport phenomena, process control, and engineering economics and plant design, thus touching all major domains of the undergraduate curriculum.

The DW technique is illustrated by two examples. The first is related to decisions concerning the order of a chemical reaction. The second illustrates its usefulness in determining if a regression model is statistically admissible, and as such, is of major interest to chemical (and other) engineers.

## BRIEF THEORY

Given the general first-order autoregressive process[5]

$$Y_k = \beta_0 + \sum_{i=1}^{p-1} \beta_k x_{k,i} + e_k \qquad k = 1, \ldots, n \tag{1}$$

where the errors are assumed to obey the first-order autocorrelation

$$e_k = \rho e_{k-1} + u_k \tag{2}$$

with $|\rho| < 1$, and independent random $u_k$ belonging to the normal distribution with zero mean and variance $\rho^2$. The regressor set $\{x_n\}$ contains observations obtained at consecutive time instants $t_1, t_2, \ldots, t_n$. In the case of correlated errors, the variance of each error term is given by

$$\sigma^2(e_k) = \frac{\sigma^2}{1 - \rho^2} \tag{3}$$

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and the covariance of adjacent errors is

$$\sigma^2(e_k;e_{k-1}) = \rho\sigma^2(e_k) \tag{4}$$

To test the null hypothesis $H_0 : \rho = 0$ against an appropriate alternative hypothesis $H_1$, the Durbin-Watson statistic

$$D = \frac{\sum_{k=2}^{n}(e_k - e_{k-1})^2}{\sum_{k=1}^{n} e_k^2} = \frac{SSED}{SSE} \tag{5}$$

is computed and compared to upper ($d_U$) and lower ($d_L$) limits of D, as a function of observation size, in critical tables.[3,5,6] The decision scheme is given in Table 1.

The D-statistic is related to the Lag 1 autocorrelation[5,7] coefficient of residuals defined as[5]

$$r_1 = \frac{\sum_{k=2}^{n} e_k e_{k-1}}{\sum_{k=1}^{n} e_k^2} \tag{6}$$

by the simple relationship

$$D = 2(1 - r_1) \tag{7}$$

which is particularly useful for $n < 15$ since critical tables do not extend outside the $15 \leq n \leq 100$ range. If the inequality $|r_1| > 2/\sqrt{n}$ stands, the independence of errors is in serious doubt. The size of observations in the first example is sufficiently large to use critical tables, whereas tables cannot be used in the second example.

### TABLE 1

**Decision Schemes in the DW Statistical Test**

*Note: Rejection of $H_0$ is a stastistically stronger result than failure to reject it.*

| *Test Hypotheses* | *Criterion* | *Decision* |
|---|---|---|
| $H_0 : \rho = 0;\ H_1 : \rho > 0$ | $D < d_L$ | Reject $H_0$ in favor of $H_1$ |
| | $D > d_U$ | Fail to reject $H_0$ |
| $H_0 : \rho = 0;\ H_1 : \rho < 0$ | $(4\text{-}D) < d_L$ | Reject $H_0$ in favor of $H_1$ |
| | $(4 - D) > d_U$ | Fail to reject $H_0$ |
| | $d_L \leq D \leq d_U$ | Inconclusive |
| | $d_L \leq (4 - D) \leq d_U$ | Inconclusive |

## EXAMPLE 1

### *Kinetics of the Bromination of Metaxylene*

The rate equation written in terms of bromine concentration

$$\frac{dc}{dt} = -kc^m \tag{8}$$

has the rate constant $k \approx 0.1\ (dm^3/mol)^{1/2}\ min^{-1}$ and apparent order $m = 1.5$ at 17 °C.[8] As can be seen from Table 2 (next page), the errors do not appear to be correlated, since the DW-statistic D is larger than $d_U$ values at levels of significance $\alpha$.

If we assume for the sake of argument, however, that the decomposition is first order ($m = 1$), the test results depend on the selected level of significance. Since $R^2$, $R_{adj}^2$, and the residual distributions (not shown) are not appreciably different, the model carrying $m = 1.5$ is a better fit.

This conclusion is also supported by the 95% confidence intervals for the true regression parameter $b_0$ : (-0.6494; 0.3079) when $m = 1.5$ and (-3.6478; -2.01306) when $m = 1$; in the second case, the correct value of zero does not even fall into the interval

What happens if the decomposition is assumed to be of zero order? With $m = 0$ in Eq. (8), the bromine concentration would be a linear function of time. The $c = \beta_0 + \beta_1 t$ + error model would have the sample regression parameters $b_0 = 0.25849$ and $b_1 = -0.004119$, with $R^2 = 0.857$ and $s_e^2 = 0.00724$ (including the $t = 63.00$; $c = 0.0482$ observation pair, lost by the rate-averaging process discussed in Ref. 8). Since SSE = 0.03558 and SSED = 0.02419, however, the DW statistic $D \approx 0.7$ is less than the $d_L$ values shown in Table 2, indicating a positive correlation between errors. The residual distribution also being parabolic (*i.e.,* definitely non-random), the postulation of zero-order kinetics would be statistically most questionable, apart from its physical improbability.

## EXAMPLE 2

### *Effect of Temperature/Humidity Index on the Level of Pollution*

The level of pollution as a function of the temperature/humidity index, recorded on ten consecutive days at a certain location[9] are shown in Table 3. The problem assignment in Ref. 9 is to determine if the data are suitable for a linear regression analysis.

Table 4 illustrates that increasing the degree of the polynomial is not particularly effective, inasmuch as the adjusted $R^2$ values indicate that even at best, only about 65% of the variations in the pollution index are explained by variations in the temperature/humidity index. The error variances are also very similar.

The residual distribution in all three cases is reasonably random, and the numerical values of the Lag 1 autocorrelation coefficient magnitude are well below the numerical value of $2/\sqrt{10} = 0.632$. The errors appear to be unrelated.

It is instructive to note that the power relationship $Y = \beta_0 x_1^{\beta}$ would not yield a better fit with a nonlinear $R^2 = 0.690$ (linearization yields $\ln(b_0) = -5.77981$ and $b_1 = 1.52312$; the residual distribution is quasi-random).

## FURTHER COMMENTS ON THE DURBIN-WATSON TECHNIQUE

If the DW-statistic falls into the inconclusiveness zone, "remedial measures" for autocorrelation may be applied: addition of independent variables, transformation of variables, the Cochrane-Orcutt procedure, and the Hildreth-Lu procedure. The discussion of these techniques is beyond the scope of this paper and may be

**TABLE 3**

**Pollution as Function of Temperature/Humidity Index**

*x - temperature/humidity index; Y - coded pollution level*

| *Day k* | *1* | *2* | *3* | *4* | *5* | *6* | *7* | *8* | *9* | *10* |
|---|---|---|---|---|---|---|---|---|---|---|
| x $^0$F | 77 | 95 | 30 | 45 | 85 | 50 | 65 | 60 | 63 | 82 |
| Y | 1.5 | 4.0 | 0.5 | 1.4 | 2.0 | 0.8 | 2.5 | 2.0 | 1.7 | 2.8 |

**TABLE 2**

**Application of DWT to the Kinetics of Metaxylene Bromination.**

*Experimental data are taken from Ref. 8, Table 3.1.1.*

| *k* | *1* | *2* | *3* | *4* | *5* | *6* | *7* | *8* | *9* | *10* | *11* | *12* | *13* | *14* | *15* | *16* | *17* | *18* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $t_k$ | 0 | 2.25 | 4.50 | 6.33 | 8.00 | 10.25 | 12.00 | 13.50 | 15.60 | 17.85 | 19.60 | 27.00 | 30.00 | 38.00 | 41.00 | 45.00 | 47.00 | 57.00 |
| $x_k$ | 0.3150 | 0.2812 | 0.2555 | 0.2353 | 0.2153 | 0.1980 | 0.1852 | 0.1713 | 0.1566 | 0.1465 | 0.1295 | 0.1107 | 0.0942 | 0.0799 | 0.0736 | 0.0692 | 0.0615 | 0.0518 |
| $y_k$ | 16.44 | 13.56 | 11.48 | 11.68 | 9.11 | 8.00 | 7.73 | 7.71 | 5.87 | 4.06 | 3.64 | 3.23 | 2.79 | 2.10 | 1.55 | 1.35 | 1.25 | 1.18 |

$t_k$ : observation time (min)
$x_k$ : mean bromine concentration (mol/dm$^3$)
$y_k$ : mean rate of reaction - $10^3\ \Delta c/\Delta t$ (mol/dm$^3$ min)

| | $Y=\beta_0 + \beta_1 x^{1.5} + \text{error}$ | $Y = \beta_0 + \beta_1 x + \text{error}$ |
|---|---|---|
| $b_0$ | -0.170746 | -2.830640 |
| $b_1$ | 94.494843 | 57.830640 |
| $R^2$ | 0.987 | 0.977 |
| $R_{adj}^2$ | 0.986 | 0.976 |
| $s_c^2$ | 0.3054 | 0.5305 |
| SSED | 8.54756 | 9.86520 |
| SSE | 4.88721 | 8.48330 |
| D | 1.749 | 1.162 |
| Decision on errors | Not correlated at<br>$\alpha$=0.01; 0.025; 0.05 | $\alpha$ = 0.01: Not correlated<br>$\alpha$=0.025: No conclusions<br>$\alpha$=0.05: Borderline positive correlation |

*Critical values of the DW statistic at n = 19*[3,5,6]

| *α* | *$d_L$* | *$d_U$* |
|---|---|---|
| *0.05* | *1.16* | *1.39* |
| *0.025* | *1.03* | *1.26* |
| *0.01* | *0.90* | *1.12* |

found elsewhere.[10]

The DW technique may not indicate autocorrelated errors associated with a second-order autoregressive pattern

$$e_k = \rho_1 e_{k-1} + \rho_2 e_{k-2} + u_k \qquad (9)$$

and hence it is not robust against incorrect model specifications.

Alternative tests of autocorrelation include the Theil-Nagar procedure[10,11] and the Olmstead-Tukey, Mann-Kendall, Hotelling-Pabst, and von Neumann tests summarized briefly by Powell.[6] To the author's knowledge, the Durbin-Watson technique is more widely used.

## CONCLUSIONS

Owing to the relative ease of its use, the inclusion of the Durbin-Watson technique in a probability and statistics course is well advised for the undergraduate chemical engineering curriculum. It is somewhat surprising that the technique is treated only by a small number of engineering textbooks, notably the ones cited in this paper. Routine teaching of the technique would further emphasize for students the importance of error structure analysis and help counteract their often-demonstrated inclination to assign inflated significance to the $R^2$ parameter.

## ACKNOWLEDGMENT

Useful discussions with Dr. Tom Duever of the Department of Chemical Engineering are hereby gratefully acknowledged.

## NOMENCLATURE

| | |
|---|---|
| $b_i$ | sample regression parameters, *i.e.*, least-squares estimators of true regression parameters $\beta_i$, i = 1,...,p |
| c | concentration |
| D | Durbin-Watson statistic (Eq. 5) |
| $d_L$, $d_U$ | lower and upper level bounds, respectively, in critical tables of the Durbin-Watson statistic |
| e | error (or residual), defined as the difference between the observed and regressed value of the dependent variable |
| k | rate constant (Eq. 8) |
| m | reaction order (Eq. 8) |
| n | length of the time series and size of the observation set |
| p | size of the regression polynomial (simple linear: 2; quadratic: 3, etc.) |
| $R^2$ | coefficient of determination; $R_{adj}^2$ its adjusted value, defined as 1 - [SSE/(n-p)]/[SST/(n-1)] |
| $r_1$ | Lag 1 autocorrelation coefficient (Eq. 6) |
| $s_e^2$ | sample error variance, defined as SSE/(n-p) |
| t | time; $t_k$ the k-th instant in the time series |
| u | random variable (Eq. 2) |
| x | independent variable (regressor) |
| Y | dependent variable; $\hat{Y}$ regressed dependent variable |

### *Greek Symbols*

| | |
|---|---|
| $\alpha$ | level of significance in hypothesis testing |
| $\beta_i$ | true population regression parameters, k = 1,...,p |
| $\sigma^2$ | true (population) variance |
| $\rho$ | true (population) correlation coefficient |

### *Special Symbols*

| | |
|---|---|
| SSE | sum of the squared errors (Eq. 5) |
| SSED | sum of the squared error differences (Eq. 5) |
| SST | total sum of squares in regression theory |

**TABLE 4**

**Application of DWT to the Pollution Problem of Example 2.**

*Data are taken from Ref. 9*

| | *Simple linear model* | *Quadratic model* | *Cubic model* |
|---|---|---|---|
| $b_0$ | -0.80347 | 0.36495 | -6.62620 |
| $b_1$ | 0.041771 | 0.001023 | 0.395176 |
| $b_2$ | - | $3.2274 \times 10^{-4}$ | $-6.470 \times 10^{-3}$ |
| $b_3$ | - | - | $3.644 \times 10^{-5}$ |
| $R^2$ | 0.684 | 0.700 | 0.766 |
| $R_{adj}^2$ | 0.644 | 0.614 | 0.649 |
| $s_c^2$ | 0.364 | 0.395 | 0.359 |
| SSED | 6.4739 | 6.0833 | 3.7614 |
| SSE | 2.9144 | 2.7654 | 2.1568 |
| D | 2.221 | 2.200 | 1.744 |
| $\|r_1\|$ | 0.110 | 0.100 | 0.128 |

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