# General Introduction to $R^2$ in survival

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# Explained variation in linear regression - illustration 1

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# Explained variation in linear regression - illustration 2

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# Explained variation in linear regression - illustration 3

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Law of total variance

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Law of total variance

$$Var(Y) = E(Var(Y|X)) + Var(E(Y|X))$$

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In linear regression under the usual assumptions

$$\sigma^2_{Y} = \sigma^2_{Res} + \sigma^2_{Reg}$$

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In linear regression under the usual assumptions

$$\sigma^2_{Y} = \sigma^2_{Res} + \sigma^2_{Reg}$$

The population  $R^2$  is then defined as

$$R^2 = 1 - rac{\sigma^2_{Res}}{\sigma^2_{Y}}$$

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$$\begin{aligned} R^2 &= 1 - \frac{\sigma^2_{Res}}{\sigma^2_{Y}}\\ \sum (y_i - \bar{y})^2 &= \sum (y_i - \hat{y}_i)^2 + \sum (\hat{y}_i - \bar{y})^2 \end{aligned}$$

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$$SS_{tot} = SS_{res} + SS_{reg}$$

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$$R^{2} = 1 - \frac{\sigma^{2}_{Res}}{\sigma^{2}_{Y}}$$
$$\sum (y_{i} - \bar{y})^{2} = \sum (y_{i} - \hat{y}_{i})^{2} + \sum (\hat{y}_{i} - \bar{y})^{2}$$
$$SS_{tot} = SS_{res} + SS_{reg}$$
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$$\frac{SS_{tot}}{n - 1} = \frac{SS_{res}}{n - 1} + \frac{SS_{reg}}{n - 1}$$

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Most important: decomposition into explained and unexplained variation!!

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- If you lower the unexplained part, you increase the explained part by the same amount!

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- If you lower the unexplained part, you increase the explained part by the same amount!
- This ensures that we have a measure between 0 and 1

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J. R. Statist. Soc. A (1984), 147, Part 1, pp. 100-103

The Box-Wetz Criterion Versus R<sup>2</sup>

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By NORMAN R. DRAPER

University of Wisconsin, USA

### SUMMARY

The square of the multiple correlation coefficient in a regression fit,  $R^2$ , can be made small simply by increasing the number of repeat data points. It is argued here that  $R^2$ is misleading in such cases, and that the Box-Wetz (1973) criterion, and a simpler but essentially equivalent criterion, are not.

Keywords: MULTIPLE CORRELATION COEFFICIENT; PURE ERROR; REGRESSION WITH LARGE

### 1. INTRODUCTION

Figs 1(a) and (b) indicate two sets of data. In Fig. 1(a) there are five X locations r = 1, 2, ..., 5and one Y obscription at each location. In Fig. 1(b), there are then Y points at the five locations. Suppose we fit a straight line to each of these two sets and the underlying model is really a straight line. Because the additional data help to locate the true mean values at each location more precisely, the fit must be improved. However, the  $R^2$  statistic will be lower than before indicating, it would seem, a worre fit. Wenty  $R^2$ 



Fig. 1. Five data sites with (a) one run, (b) ten runs, per site.

### 2. ARGUMENT

The reason lies in the fact that it is impossible for a fitted model to explain pure error. Suppose we fit, by least squares, the model

$$Y = \eta + \epsilon = X\beta + Z\psi + \epsilon, \qquad (1)$$

where  $X\beta$  is the part to be tested in a "test for regression" and  $Z\psi$  represents effects such as the mean, block variables, time trends, and so on, that we wish to eliminate from the variation in

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### Box-Wetz Criterion Versus R<sup>2</sup>

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perhaps 3 $\theta$  or more for a regression worthy of further interpretation. With  $\theta$  = 5, a cautious value, this would imply that u should exceed 10 at minimum.

From (11) we see that, if  $w_m$  is fixed, and if  $(\max x_p^* - \min x_p^*)/\epsilon$  remains more or less constant as N is increased, a behaviour we would anticipate, then u increases as N<sup>2</sup>. (A partillel argument shows that the observed F for regression given  $b_0$  increases as  $N - w_m$ .) Thus, as N increases, the practical usefulness of the regression as measure by  $v_1$  (and F) will improve. This behaviour seems more sensible than that of  $R^3$ , in the circumstances discussed. Note also that if  $a^2$  remains fixed and p is reduced, u increases. The practical implication is that models with un-needed terms will be rated lower than the model which has the non-significant terms removed, a result which accords with commonsense.

Darlington (1982) provided partial motivation for the analysis above; his review contains statements which imply that a regression based on a large data-soti-s not useful when  $\mathbb{R}^3$  is small; "ovin if the F for regression given  $h_0$  is large. As explained above, it appears that the reverse is true.

### ACKNOWLEDGEMENTS

Partial support was provided by the United States Army under Contract No. DAAG29-80-C-0041 and by the University of Wisconsin Graduate School through the Wisconsin Alumni Research Foundation. Helpful comments from G. E. P. Box and W. J. Raynor are greatly appreciated.

### REFERENCES

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J. R. Statist. Soc. A (1985) 148, Part 4, p. 357

### Corrections

The Box-Wetz Criterion Versus R<sup>2</sup>

### By NORMAN R. DRAPER

### (J. R. Statist. Soc. A, 147, 1984, 100-103.)

Professor J. S. Cramer has kindly pointed out an error in this note. It lies immediately after equation (10) where my assumption that  $\gamma_m$  can be kept fixed while the  $n_l$  increase is untrue, and so subscuent remarks about  $R^2$  are now wrong.

The correct conclusion from (10) is that, approximately,  $R^2 < \sigma_0^2/(\sigma_0^2 + \sigma^3)$ , the right hand side being the limit of  $R^2$  as N increases, if the model is correct. For a useful regression, we would ward  $\sigma_0/\sigma$  beink measures the ratio of the spread of the  $\eta$ 's to the spread of the errors to be large, and we see that  $R^2$  provides good information on this since, for large N,  $\sigma_0/\sigma \approx R(1-R^2)^{6}$ .

The behaviour of u and F is sensitive to N, however. From equation (11), if we assume the range of the  $j_{1}$  to he "about  $B_{n_{1}}$  and with  $v \approx n$ , we find  $u \approx N^{*0}(a_{n_{1}})\partial u_{m_{2}}$ . Furthermore  $F \approx (N - u_{m_{1}} - 1)(a_{n_{1}}^{2}\partial^{2})u_{m_{2}}$ . Thus, even if  $a_{n_{2}}/a$  is the simulation of the regression. Rather than compare F with the usual percentage point, we may perhaps with to recalibrate the test, and this is wind Box and Berreen (1973).

Overall then, it appears that  $R^2$  is a useful indicator for large data sets whereas F can be misleading if used in the ordinary way; thus Darlington (1982) is right.

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The behaviour of u and F is sensitive to N, however. From equation (11), if we assume the range of the  $\hat{\gamma}_1$  to be "about  $\delta \sigma_0$ ," and with  $z \circ \infty$ , we find  $u \approx N^{-0}(\sigma_0/\phi) m_0^{-1}$ . Furthermore  $F \approx (N - u_m - 1)(\sigma_0^2/\sigma^2) v_m$ . Thus, even if  $\sigma_0/\sigma$  is small, observed values of u and F can be large for large  $\Lambda$ , and may give a miledading intersion of the expression. Rather than compare F with the usual percentage point, we may perhaps with to recalibrate the test, and this is wind Box and West (1973) investigated for moderate sample size.

Overall then, it appears that  $R^2$  is a useful indicator for large data sets whereas F can be misleading if used in the ordinary way; thus Darlington (1982) is right.

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# Misunderstanding - R2 is NOT a measure of fit





# Misunderstanding - R2 is NOT a measure of fit



# Explained variation in survival analysis

Many measures proposed under different names

- explained variation
- explained randomness
- prognostic value
- correlation
- concordance
- ...

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Kent and O'Quigley's

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(This is really just an approximation to Kent & O'Quigley, but ok)

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$$R^{2} = rac{D^{2}/\sqrt{(8/\pi)}}{D^{2}/\sqrt{(8/\pi)} + \sigma_{\epsilon}^{2}}$$

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$$R^2 = rac{\operatorname{Var}(eta' Z)}{\operatorname{Var}(eta' Z) + rac{\pi^2}{6}}$$

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$$R^2 = rac{D^2/\sqrt{(8/\pi)}}{D^2/\sqrt{(8/\pi)} + \sigma_{\epsilon}^2}$$

The others are said to perform poorly.

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The recommended measures have the following properties (among others)

- They assume that the model holds everywhere
- They do not allow for covariates or effects to change in time
- They cannot be used with repeated events
### The authors' recommendation is based on one criterium

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The authors' recommendation is based on one criterium

### **Bias under censoring**

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The authors' recommendation is based on one criterium

#### **Bias under censoring**

(Sounds reasonable)

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 generate covariates (decide on number - often 1, distribution often uniform, range).

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- generate survival times, conditional on covariates under some model, often exponential.

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Stare (SLO)

if comparing measures - choose the one with the smallest (or no) bias.

#### 7 is wrong, so 8 may be wrong!

- generate covariates (decide on number often 1, distribution often uniform, range).
- generate survival times, conditional on covariates under some model, often exponential.
- fit a model, calculate a measure (or more) on this uncensored data.
- generate censoring times, given a required proportion of censoring. Censoring distribution often **uniform**.
- Solution censor survival times, fit the model, calculate the measure again.
- see if the value of the measure on censored data is close to the value on uncensored (on average).
- if not conclude bias.
- if comparing measures choose the one with the smallest (or no) bias.

#### I'd better say: 7 doesn't make much sense!

Stare (SLO)

#### Usual reporting of simulation results in papers

#### Table 42 : Effect of censoring

		censoring	
paper		0%	50%
1996	some measure	0.276	0.187
2011	some measure	0.139	41.8 % increase

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### What is going on?



No censoring

time

We estimate a measure on such data.

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### What is going on?



Uniform censoring (50 %)

Why do we think that we should get the same value on such data?



### What is going on?



Type I censoring

One can study bias up to  $\tau$ , nothing else!

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$$\int_0^\infty S(t)dt$$

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$$\int_0^\infty S(t)dt \qquad \qquad \int_0^{\tau} S(t)dt$$

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$$\int_0^\infty S(t) dt \qquad \neq \qquad \int_0^{\tau} S(t) dt$$

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$$\int_0^\infty S(t)dt \qquad \neq \qquad \int_0^{\tau} S(t)dt$$

#### Estimator A

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If we have a model for S(t) and ASSUME that it holds everywhere, we can correct B.

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If we have a model for S(t) and ASSUME that it holds everywhere, we can correct B.

Some measures inherently assume that the model holds everywhere, so they SEEM better than the others.

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$$\rho^2 = 1 - e^{-E(LR)},\tag{1}$$

where E(LR) is

$$E(LR) = 2 \int_{D(x)} \int_0^\infty \log \frac{f_M(t|x)}{f_0(t)} dF_M(t|x) dG(x)$$
(2)

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where E(LR) is

$$E(LR) = 2 \int_{D(x)} \int_0^\infty \log \frac{f_M(t|x)}{f_0(t)} dF_M(t|x) dG(x)$$
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If there is a time  $\tau$  beyond which all the observations are censored, we CANNOT estimate (2).

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For parametric models, we replace the densities with values of  $S(\tau|x)$ , for the Cox model we drop them from the likelihood.

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Neither helps (of course)!

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So, again, why do we think we should estimate (2) with observations limited to  $\tau$ ?

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For the Cox model we used the following estimator:

$$\hat{E}(LR) = \frac{2}{k}\sum_{i=1}^{k}(\hat{LR})_i.$$

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So k (number of events), **NOT** n (number of cases)!

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So *k* (number of events), **NOT** *n* (number of cases)! We imputed values for censored observations after  $t_{max}$ .
# Example continued - estimation of information gain measure

For the Cox model we used the following estimator:

$$\hat{E}(LR) = \frac{2}{k}\sum_{i=1}^{k}(\hat{LR})_i.$$

So *k* (number of events), **NOT** *n* (number of cases)! We imputed values for censored observations after  $t_{max}$ .

For parametric models the story is different.

### Some results on Information gain measure

Table 43 : Cox model

% censored	$\rho_i^2$	se	$\rho^2$	se
90	0.43	0.12	0.44	0.04
80	0.43	0.08	0.44	0.04
70	0.44	0.05	0.44	0.04
60	0.43	0.05	0.43	0.04
50	0.45	0.04	0.45	0.04
40	0.43	0.04	0.43	0.04
30	0.43	0.04	0.43	0.04
20	0.44	0.04	0.44	0.04
10	0.44	0.04	0.44	0.04

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• We need to distinguish between censoring BEFORE  $t_{max}$  and after  $t_{max}$  where  $t_{max}$  is the last observed event time.

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- Our estimates should be unbiased (or at least consistent) until t<sub>max</sub>.
- When we censor with a uniform distribution, we will always have a maximum observable event time τ, everything beyond that is censored. And, BTW, using exponential will not solve the problem.

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- If some measure pretends to be (or looks) unbiased on the whole support of *T*, then we should be suspicious.
- All measures (?) can be made to look unbiased on the whole support of T.

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 Consistency (unbiasedness) up to τ. Most (all?) measures can be adjusted to meet this criterium.

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- Expected value. And add variance of the estimator as a bonus.



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- Scale? Approaching 1?

- Consistency (unbiasedness) up to τ. Most (all?) measures can be adjusted to meet this criterium.
- Expected value. And add variance of the estimator as a bonus.
- Scale? Approaching 1?
- Time dependent covariates and effects.

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Once we satisfy these criteria, not many measures will be left ...

#### ... but at least one will

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#### A Measure of Explained Variation for Event History Data

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# Explained risk ranking

Rank of event under model

$$r^{(M)}(t)$$

Stare (SLO)

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Rank of event under model $r^{(M)}(t)$ Rank of event under perfect knowledge $r^{(P)}(t)$ 

 $r^{(M)}(t)$ 

 $r^{(P)}(t) r^{(0)}(t)$ 

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 $r^{(M)}(t)$ 

 $r^{(P)}(t)$  $r^{(0)}(t)$ 

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Difference  $r^{(0)}(t) - r^{(P)}(t)$  needs to be explained

 $r^{(M)}(t)$ 

 $r^{(P)}(t)$ 

 $r^{(0)}(t)$ 

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Difference  $r^{(0)}(t) - r^{(P)}(t)$  needs to be explained Difference  $r^{(0)}(t) - r^{(M)}(t)$  *is* explained

 $r^{(M)}(t)$ 

 $r^{(P)}(t)$ 

 $r^{(0)}(t)$ 

P

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Difference  $r^{(0)}(t) - r^{(P)}(t)$  needs to be explained Difference  $r^{(0)}(t) - r^{(M)}(t)$  *is* explained

$$R_E \simeq \frac{\sum_t (r^{(0)}(t) - r^{(M)}(t))}{\sum_t (r^{(0)}(t) - r^{(P)}(t))}$$

$${m R}_{E} = rac{\sum_{i} \, \int_{0}^{ au} \left\{ \, \left( r_{i}^{(0)}(t) - r_{i}^{(M)}(t) 
ight) \, / \hat{G}_{it} 
ight\} \, dN_{i}(t)}{\sum_{i} \, \int_{0}^{ au} \left\{ \, \left( r_{i}^{(0)}(t) - r_{i}^{(P)}(t) 
ight) \, / \hat{G}_{it} 
ight\} \, dN_{i}(t)}$$



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$$R_{E} = \frac{\int_{0}^{\tau} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(M)}(t) \right) \right\} dN_{i}(t)}{\int_{0}^{\tau} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(P)}(t) \right) \right\} dN_{i}(t)}$$

 $\begin{array}{ll} \mbox{continuous variable} \\ \mbox{$\sharp$ at risk$} & 10 \\ \mbox{rank}_{null} & 5.5 \\ \mbox{rank}_{perfect} & 1 \\ \mbox{rank}_{model}(t_5) & 3 \end{array}$ 



$$R_{E} = \frac{\int_{0}^{\tau} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(M)}(t) \right) / \hat{G}_{it} \right\} dN_{i}(t)}{\int_{0}^{\tau} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(P)}(t) \right) / \hat{G}_{it} \right\} dN_{i}(t)}$$

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 $\begin{array}{ll} \mbox{continuous variable} \\ \mbox{$\sharp$ at risk$} & 5 \\ \mbox{rank}_{null} & 3 \\ \mbox{rank}_{perfect} & 1 \\ \mbox{rank}_{model}(t_{10}) 3 \end{array}$ 



 $R_E$ 

Variance of  $R_E$  - in short...

•

$$\begin{aligned} \operatorname{Var}(R_{E}) &= \\ & \frac{1}{n^{2}Q_{2}(\tau)^{2}} \int_{0}^{\tau} \sum_{i} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(M)}(t) \right)^{2} / \hat{G}_{it}^{2} \right\} \hat{\lambda}_{i}(t|\mathscr{F}_{t-}) dt \\ & - \frac{2Q_{1}(\tau)}{n^{2}Q_{2}(\tau)^{3}} \int_{0}^{t} \sum_{i} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(M)}(t) \right) \right. \\ & \times \left( r_{i}^{(0)}(t) - r_{i}^{(P)}(t) \right) / \hat{G}_{it}^{2} \right\} \hat{\lambda}_{i}(t|\mathscr{F}_{t-}) dt \\ & + \frac{Q_{1}(\tau)^{2}}{n^{2}Q_{2}(\tau)^{4}} \int_{0}^{\tau} \sum_{i} \left\{ \left( r_{i}^{(0)}(t) - r_{i}^{(P)}(t) \right)^{2} / \hat{G}_{it}^{2} \right\} \hat{\lambda}_{i}(t|\mathscr{F}_{t-}) dt \end{aligned}$$

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#### Population value

$$\mathcal{R}_{E} = 2 \frac{E\left\{\int_{0}^{\tau} S(t) H_{t}(u) \alpha(t | \mathscr{F}_{t-}, u) dt\right\}}{E\left\{\int_{0}^{\tau} S(t) \alpha(t | \mathscr{F}_{t-}, u) dt\right\}} - 1,$$

Special cases, uncensored Cox survival, univariate X

$$\mathcal{R}_{E} = 1 - \frac{4}{\beta} \int_{0}^{1} \log\left(\frac{2e^{\beta x}}{1 + e^{\beta x}}\right) dx \qquad X \sim U(0, 1)$$
$$\mathcal{R}_{E} = \frac{1}{2} \left(\frac{e^{\beta} - 1}{e^{\beta} + 1}\right) \qquad X \sim Ber(0.5)$$

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# Some simulations

 ⊢⊣ variance of the R<sub>E</sub> estimates
 ⊢⊣ average of variance estimates

```
sample size: 20 \rightarrow 1000
\beta = 1
no censoring
100 simulation runs
```



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# Some simulations



#### **Properties**



the null model IS always the same



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- the null model IS always the same
- 2  $R_E$  CAN be used with time dependent covariates or effects

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- the null model IS always the same
- R<sub>E</sub> CAN be used with time dependent covariates or effects
- explained variation interpretation?

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- explained variation interpretation?
- Scale? Is the difference between 0.5 and 0.45 the same as between 0.7 and 0.65?
- 🗿 approaching 1? 💽
- O dependency on censoring?
- CAN be used with any model

 $\ddot{-}$  between 0 and 1

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- ö between 0 and 1
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- between 0 and 1
- imple interpretation
- $\ddot{-}$  computationally simple
- $\ddot{-}$  partial  $R_E$  can be easily computed

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- $\ddot{-}$  computationally simple
- partial R<sub>E</sub> can be easily computed
- only ranks are important –
- $\ddot{-}$  For single episodes with time-constant effects and covariates

$$R_E = 2(c - 1/2)$$

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#### Freireich data - remission times of leukaemia patients

42 patients, 12 events covariate: treatment (binary: 21/21)

 $R_E = 0.374$ 

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312 patients, 125 events covariates: age, log bilirubin, log albumin, presence of edema, log blood clotting time

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$$R_E = 0.580$$

#### Stablein data

95 patients, 78 events covariate: rx (binary: 48/47)

$$R_E = 0.127$$

#### Stablein data - improving the fit



R<sub>E</sub>

#### Measure in time - Stablein data

95 patients, 78 events covariate: rx binary: 48/47

$$R_E = 0.127$$



 $R_E$ 

# Measure in time - asymmetric Z



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#### Measure in time - asymmetric Z



 $R_E$ 

# Instead of conclusions



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#### Instead of conclusions



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- Can we do better than  $R_E$ ?
- Hopefully. (ask me in a year)

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# Explained variation interpretation

What is variation?



What is variation?

Any measure of the extent to which a distribution is not degenerate (Nagelkerke).

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What is variation?

Any measure of the extent to which a distribution is not degenerate (Nagelkerke).

$$\left(r_{i}^{(0)}(t)-r_{i}^{(P)}(t)\right)=\left(r_{i}^{(0)}(t)-r_{i}^{(M)}(t)\right)+\left(r_{i}^{(M)}(t)-r_{i}^{(P)}(t)\right).$$

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$$\begin{split} R_E := & \frac{\sum\limits_{i=1}^{n} [r_{null}(t_i) - r_{model}(t_i)]}{\sum\limits_{i=1}^{n} [r_{null}(t_i) - 1]} &= & \frac{\sum\limits_{i=1}^{n} r_{null}(t_i)}{\sum\limits_{i=1}^{n} [r_{null}(t_i) - 1]} - & \frac{\sum\limits_{i=1}^{n} r_{model}(t_i)}{\sum\limits_{i=1}^{n} [r_{null}(t_i) - 1]} \\ &= & a + b \sum\limits_{i=1}^{n} r_{model}(t_i) \end{split}$$

 $R_E$  is simply a linear function of the sum of predicted conditional ranks of failures!

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#### Example - Cox model

#### Binary covariate

$$E(R_E) = 2p(1-p) \frac{e^{\beta x_1} - e^{\beta x_2}}{e^{\beta x_1} + e^{\beta x_2}} \stackrel{\beta \to \infty}{\to} 2p(1-p)$$

$$\beta = 5.03$$
  $R_E = 0.493, \ E(R_E) = 0.493$ 

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# Example - Cox model

Uniform covariate			
	$\hat{eta}$	$R_E$	
	0.8	0.141	
	1.9	0.284	
	3.0	0.435	
	3.9	0.502	
	5.0	0.575	
	6.9	0.667	
	10.1	0.762	
	13.8	0.810	
	18.8	0.863	
	25.1	0.890	

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## The effect of censoring before the last observed failure





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# The effect of censoring before the last observed failure





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#### Conclusion

 $R_E$  does not depend on censoring before the last observed failure

# The effect of censoring at a given time

eta = 1sample size 250 100 runs  $Z \sim \mathcal{N}(0, 1)$  $Z \sim Unif[0, 1]$  $Z \sim asymmetric$ 



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# The effect of censoring at a given time

eta = 1sample size 250 100 runs  $Z \sim \mathcal{N}(0, 1)$  $Z \sim Unif[0, 1]$  $Z \sim asymmetric$ 



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#### Conclusion

The effect of censoring at a given time depends on the covariate distribution. Possible solution: imputation.