First Principle Model Simulation Study

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0.1 Quadratic Model

0.1.1 Intake Equation

$$E(t) = \beta_{\theta} + \beta_1 t + \beta_2 t^2$$

0.1.2 Time equation

$$t=min\big(\frac{-\beta_1\pm\left(\beta_1^2-4(\beta_\theta-E(t))\beta_2\right)^{1/2}}{2\beta2}$$

0.2 Thompson et al., 2017 First-Principles Dynamic Model

0.2.1 Oringinal Equation in paper

$$E(t) = \frac{E_{max}\theta\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}}-1\right)}{\theta\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}}+E_{max}r\right)}$$

0.2.2 Correct intake equation

• took the integral of the derivative/eating rate equation

$$\frac{dE}{dt} = (rE(t) = \theta) \left(1 - \frac{E(t)}{E_{max}} \right)$$

$$\int \frac{dE}{dt} = \int (rE(t) = \theta) \left(1 - \frac{E(t)}{E_{max}} \right)$$

$$\vdots$$

$$E(t) = \frac{E_{max}\theta \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}} - 1 \right)}{\theta \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}} + \frac{E_{max}r}{\theta} \right)}$$

$$= \frac{E_{max} \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}} + \frac{E_{max}r}{\theta} \right)}{e^{\frac{t(E_{max}r + \theta)}{E_{max}}} + \frac{E_{max}r}{\theta}}$$
(1)

 $\theta \neq 0$; integral constant $c \neq 1$; $\theta \neq +E_{max}r$

0.2.3 Correct time equation

$$E(t) = \frac{E_{max} \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}} - 1\right)}{e^{\frac{t(E_{max}r + \theta)}{E_{max}}} + \frac{E_{max}r}{\theta}}$$

$$E(t) \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}} + \frac{E_{max}r}{\theta}\right) = E_{max} \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}} - 1\right)$$

$$E(t) \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}}\right) + E(t) \left(\frac{E_{max}r}{\theta}\right) = E_{max} \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}}\right) - E_{max}$$

$$E(t) \left(\frac{E_{max}r}{\theta}\right) + E_{max} = E_{max} \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}}\right) - E(t) \left(e^{\frac{t(E_{max}r + \theta)}{E_{max}}}\right)$$

$$E_{max} \left(\frac{E(t)r}{\theta} + 1\right) = e^{\frac{t(E_{max}r + \theta)}{E_{max}}} \left(E_{max} - E(t)\right)$$

$$\frac{E_{max} \left(\frac{E(t)r}{\theta} + 1\right)}{E_{max} - E(t)} = e^{\frac{t(E_{max}r + \theta)}{E_{max}}}$$

$$ln \left(\frac{E_{max} \left(\frac{E(t)r}{\theta} + 1\right)}{E_{max} - E(t)}\right) = \frac{t(E_{max}r + \theta)}{E_{max}}$$

$$\frac{E_{max}}{E_{max}r + \theta} ln \left(\frac{E_{max} \left(\frac{E(t)r}{\theta} + 1\right)}{E_{max} - E(t)}\right) = t$$

0.3 Log likelihood

$$\begin{split} L(\hat{E(t)} + \epsilon, \sigma^2 | t, \theta, r, E_{max}) &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(E_i - E(t_i))^2}{2\sigma^2}} \\ &= \prod_{i=1}^n (2\pi\sigma^2)^{\frac{-1}{2}} \ e^{-\frac{1}{2\sigma^2}(E_i - E(t_i))^2} \\ &= (2\pi\sigma^2)^{\frac{-n}{2}} \ \prod_{i=1}^n e^{-\frac{1}{2\sigma^2}(E_i - E(t_i))^2} \end{split}$$

$$\ln\left(L(\hat{E}(t) + \epsilon, \sigma^{2} | t, \theta, r, E_{max})\right) = \ln\left((2\pi\sigma^{2})^{\frac{-n}{2}} \prod_{i=1}^{n} e^{-\frac{1}{2\sigma^{2}}(E_{i} - E(t_{i}))^{2}}\right)$$

$$= \ln\left((2\pi\sigma^{2})^{\frac{-n}{2}}\right) + \ln\left(\prod_{i=1}^{n} e^{-\frac{1}{2\sigma^{2}}(E_{i} - E(t_{i}))^{2}}\right)$$

$$= \ln\left((2\pi\sigma^{2})^{\frac{-n}{2}}\right) + \ln\left(e^{-\frac{1}{2\sigma^{2}}} \sum_{i}^{n} (E_{i} - E(t_{i}))^{2}\right)$$

$$= \frac{-n}{2}\ln\left(2\pi\sigma^{2}\right) + -\frac{1}{2\sigma^{2}} \sum_{i}^{n} (E_{i} - E(t_{i}))^{2}$$
(2)

$$\sigma^2 = \frac{\sum_{i}^{n} (E_i - E(t_i))^2}{n}$$

$$\ln\left(L(\hat{E(t)} + \epsilon, \sigma^2 | t, \theta, r, E_{max})\right) = \frac{-n}{2} \ln\left(2\pi \left(\frac{\sum_{i=1}^{n} (E_i - E(t_i))^2}{n}\right)^2\right) + -\frac{1}{2\left(\frac{\sum_{i=1}^{n} (E_i - E(t_i))^2}{n}\right)^2} \sum_{i=1}^{n} (E_i - E(t_i))^2$$

1 Replication of Figure 1 from Thompson et al 2017

1.1 Compare by Sampling Rate

1.2 Paremeter Recovery by Sampling Rate

1.2.1 Parameter Recovery with Infrequent Bites (500 sims)

2 Simulations based on Fogel et al., 2017

2.1 Simulated Microbehaivor

Data were simulated from a multivariate normal distribution for the following microbehaviors:

- •: Number of Bites rounded to whole number
- •: Bite Size (g) restricted to be > 0
- •: Percent of Time Active (ie. eating) restricted be $\leq 100\%$
- •: Oral Exposure per Bite (sec)

2.1.1 Computed Microbehavior

The following microbehavior characteristics were calculated based on simulated data:

- \bullet : Total Oral Exposure (min); (Oral Exposure per Bite * Number of Bites)/60 restricted to be > 2 min to fit range reported in Fogel et. al., 2017
- •: Total Intake (g); Bite Size (g) * Number of Bites
- \bullet : Eating Rate (g/min); Total Intake (g)/Total Oral Exposure (min) restricted be >0 and <25 to approximate range depicted in Figure 1 in Fogel et al., 2017
- •: Meal Duration (min); Total Oral Exposure/(Percent of Time Active/100) restricted to be \leq 30 min as that was the longest duration the meal could go in the Fogel et al., 2017 paper

2.2 Correlations between Microstructure Behaviors

Table 1: Correlations between Microstructure Behaviors - Simulated

| | nBites | EatRate | TotalOE_min | ActiveMeal_pcent | BiteOE_sec |
|-----------------------------|----------------|-------------|-------------|------------------|---------------|
| nBites | NA | NA | NA | NA | NA |
| EatRate | 0.15** | NA | NA | NA | NA |
| $TotalOE_min$ | 0.54* | -0.05 | NA | NA | NA |
| $ActiveMeal_pcent$ | 0.11* | -0.02 | 0.33*** | NA | NA |
| $BiteOE_sec$ | -0.58**** | -0.25*** | 0.02 | 0.16** | NA |
| TotalIntake_g BiteSize_g | NA -0.42*** | NA 0.55* | NA -0.01 | NA 0.17** | NA 0.54*** |

2.2.2 Corrleations Simulated

Table 2: Correlations between Microstructure Behaviors - Simulated

| | nBites | EatRate | TotalOE_min | ActiveMeal_pcent | BiteOE_sec | TotalIntake_g |
|---------------------|--------|---------|-------------|------------------|------------|---------------|
| nBites | | | | | | |
| EatRate | 0.28* | | | | | |
| $TotalOE_min$ | 0.4* | -0.2* | | | | |
| $ActiveMeal_pcent$ | 0.17* | 0 | 0.38* | | | |
| $BiteOE_sec$ | -0.68* | -0.4* | 0.23* | 0.14* | | |
| TotalIntake_g | 0.47* | 0.67* | 0.5* | 0.22* | -0.14* | |
| BiteSize_g | -0.37* | 0.44* | 0.09* | 0.14* | 0.53* | 0.53* |

2.3 Fast vs Slow Eaters Microstructure Characteristics

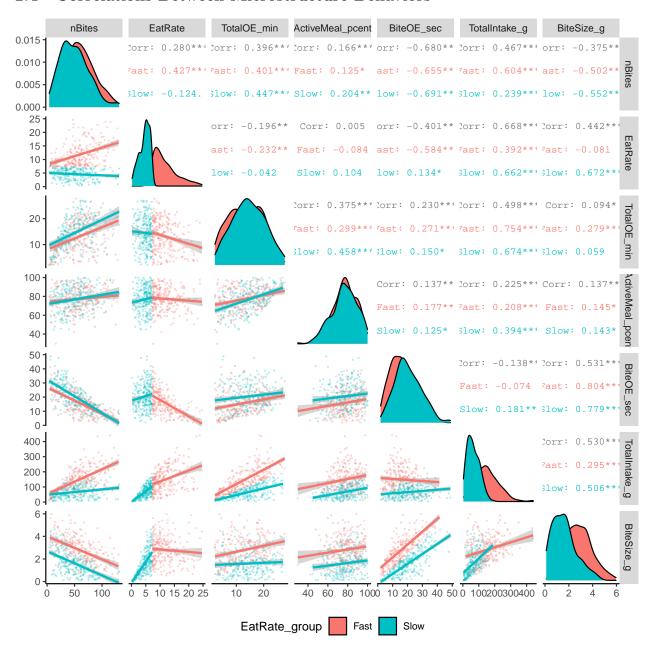
2.3.1 Means (SEM): Reported in Fogel et al., 2017 (Table 2)

| | Slow | Fast | t p |
|------------------------------|--------------|--------------------------|-------------------------|
| Bites(#) | 57.7 (2.5) | $\overline{68.4\ (2.5)}$ | $\overline{3.04}$ 0.003 |
| Bite Size (grams/bite) | 1.4(0.1) | 2.4(0.1) | 9.17 < 0.001 |
| Oral Exposure per Bite (sec) | 20.1(0.9) | 15.6 (0.5) | 4.11 < 0.001 |
| Active Mealtime (%) | 75.0(1.0) | $76.0\ (1.0)$ | 0.56 0.570 |
| Total Oral Exposure (min) | 15.1 (0.4) | 15.2(0.4) | 0.08 0.930 |
| Total Intake (kCal) | 175.3 (6.09) | 306.7(9.9) | 11.28 < 0.001 |

2.3.2 Means (SEM): From Simulated and Calculated Data

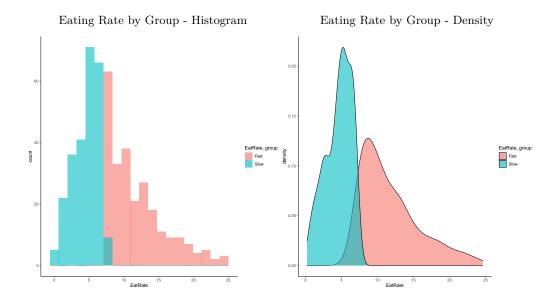
| | Slo | OW | F | ast | | |
|------------------------------|-------------|-------------|-------------|--------------|-------|---------|
| | Mean (SE) | Range | Mean (SE) | Range | t | p |
| Bites(#) | 50.28 (1.6) | 4 - 131 | 58.74 (1.7) | 5 - 130 | 15.53 | < 0.001 |
| Bite Size (grams/bite) | 1.6(0.1) | 0.1 - 4.6 | 2.8(0.1) | 0.5 - 6.0 | 12.56 | < 0.001 |
| Oral Exposure per Bite (sec) | 20.5(0.6) | 2.0 - 48.8 | 15.7(0.5) | 2.0 - 41.4 | -6.14 | < 0.001 |
| Active Mealtime (%) | 76.8(0.8) | 44.7 - 100 | 73.6(0.7) | 29.7 - 98.6 | 0.553 | 0.581 |
| Total Oral Exposure (min) | 14.5(0.4) | 2.2 - 27.0 | 13.1 (0.34 | 2.2 - 27.7 | -2.66 | 0.008 |
| Total Intake (grams) | 66.2(2.4) | 3.7 - 188.5 | 149.0 (4.8) | 16.3 - 441.3 | 15.53 | < 0.001 |

2.4 Correlations Between Microstructure Behaviors



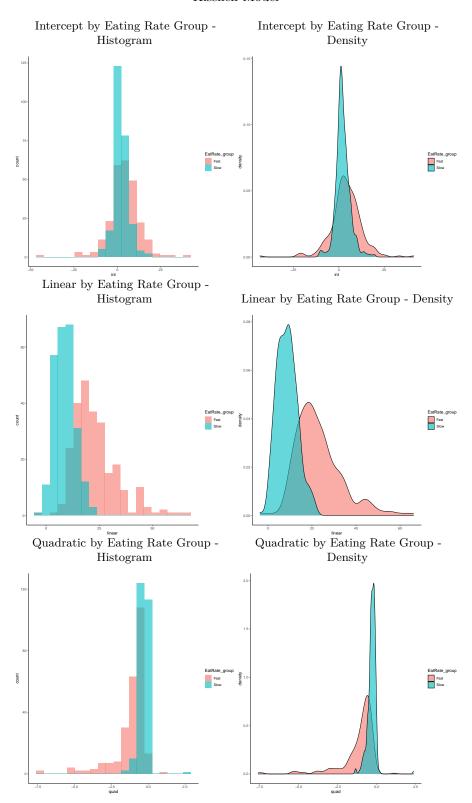
3 Parameter Distributions

3.1 Eating Rate Distribution



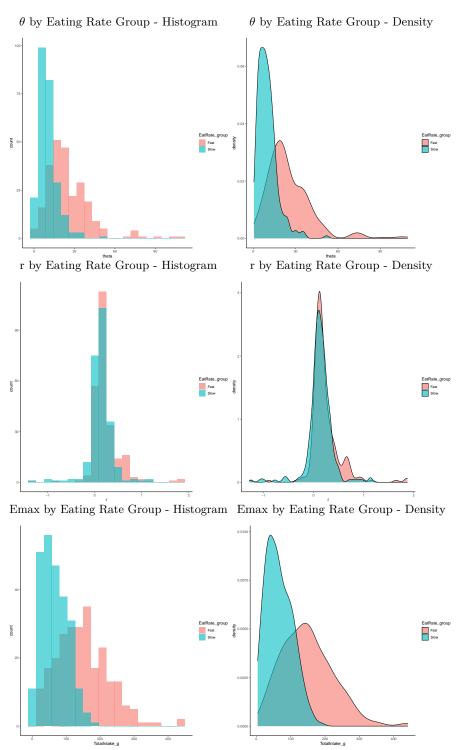
3.2 Kissileff's Quadratic Model

Kissileff Model

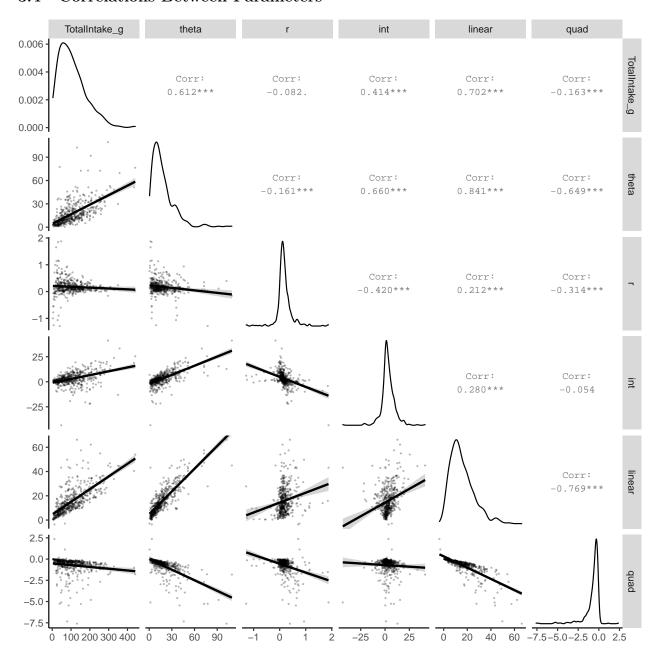


3.3 First Principles Model

First Principles Model



3.4 Correlations Between Parameters



4 Cumulative Intake Curves Accross Parameter Distributions

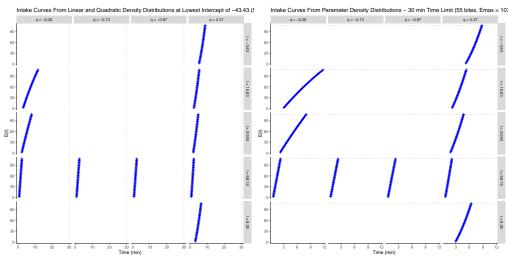
Set Emax and number of bites to the average of the distributions

4.1 Kissileff Quadratic Model

Kissileff Cumulative Intake Curves: Lowest Intercept (-43.43)



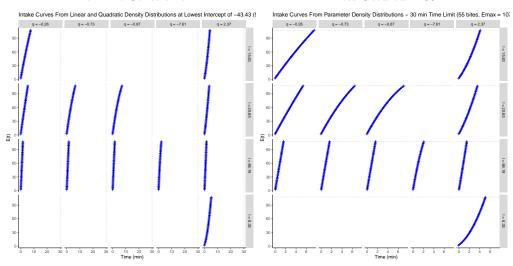
All Bites Occured in 30 min



Kissileff Cumulative Intake Curves: Mean Intercept (3.13)

No Time Constraint

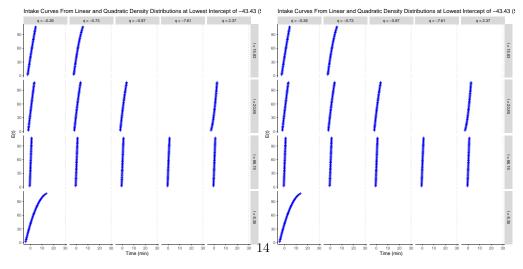
All Bites Occured in 30 min



Kissileff Cumulative Intake Curves: Highest Intercept (41.2)

No Time Constraint

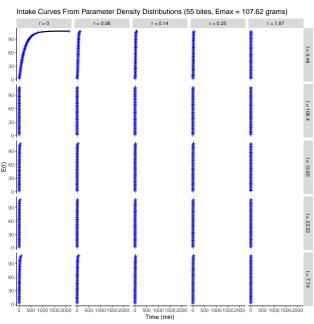
All Bites Occured in 30 min



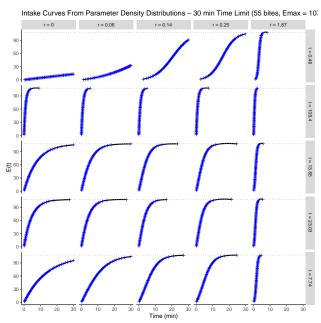
4.2 First Principles Model

First Prinicples Model Cumulative Intake Curves

No Time Constraints



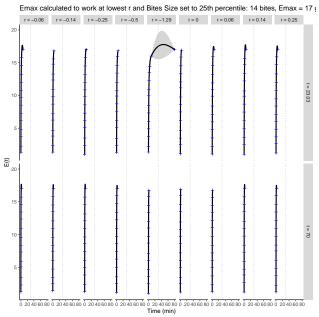
All Bites Occured in 30 min



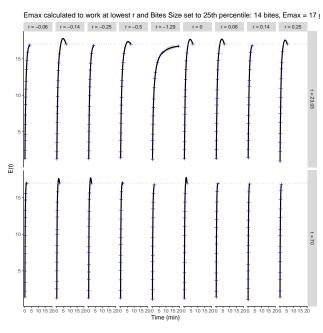
4.2.1 Zoom in on r - negative and small values

First Prinicples Model Cumulative Intake Curves

No Time Constraints



All Bites Occured in 30 min



5 Parameter Recovery

5.1 Recovery Tables from 100 Random Samples

5.1.1 First Principles Model

Table 3: Recovery of r within 95 percent confidence bounds

| | Measurement noise | No noise | Process noise |
|-------|-------------------|----------|---------------|
| FALSE | 32 | 27 | 30 |
| TRUE | 68 | 73 | 70 |

Table 4: Recovery of theta within 95 percent confidence bounds

| | Measurement noise | No noise | Process noise |
|-------|-------------------|----------|---------------|
| FALSE | 3 | 0 | 1 |
| TRUE | 97 | 100 | 99 |

5.1.2 Kissileff's Quadratic Model

Table 5: Recovery of intercept within 95 percent confidence bounds

| | Measurement noise | No noise | Process noise |
|-------|-------------------|----------|---------------|
| FALSE | 10 | 8 | 8 |
| TRUE | 90 | 92 | 92 |

Table 6: Recovery of linear coefficient within 95 percent confidence bounds

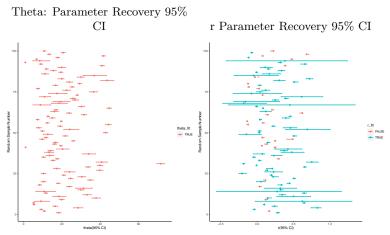
| | Measurement noise | No noise | Process noise |
|-------|-------------------|----------|---------------|
| FALSE | 15 | 15 | 14 |
| TRUE | 85 | 85 | 86 |

Table 7: Recovery of quadratic coefficient within 95 percent confidence bounds

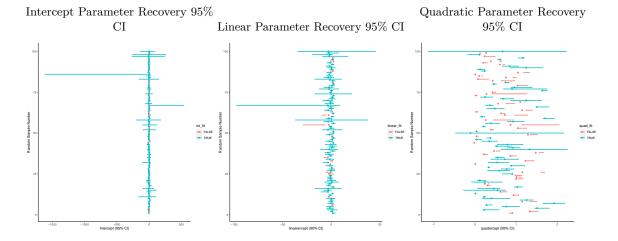
| | Measurement noise | No noise | Process noise |
|-------|-------------------|----------|---------------|
| FALSE | 47 | 45 | 37 |
| TRUE | 53 | 55 | 63 |

5.2 100 Random Multivariate Samples: No Noise

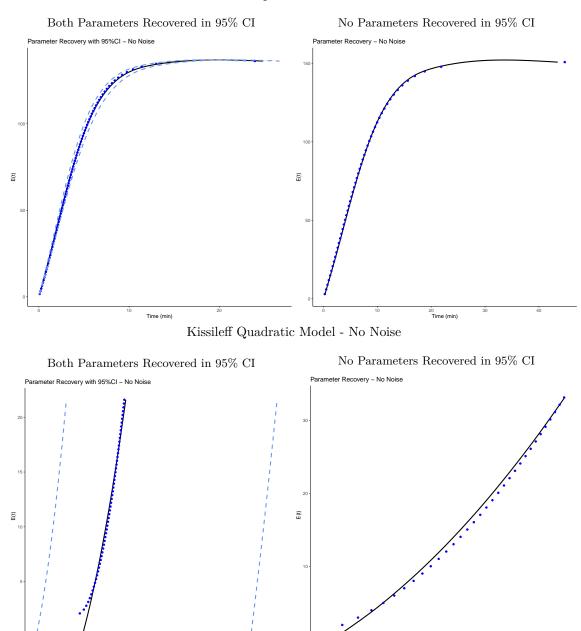
First Principles Model: No Noise



Kissileff Quadratic Model: No Noise



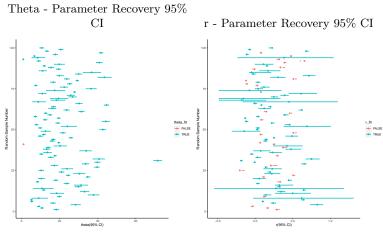
First Principles Model - No Noise



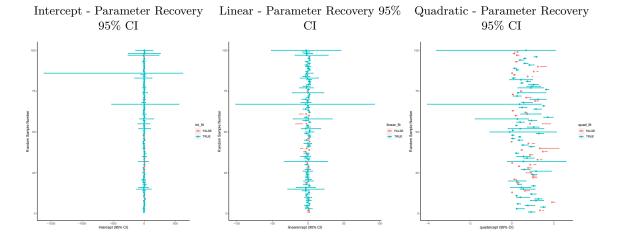
Time (min)

7 Time (min)

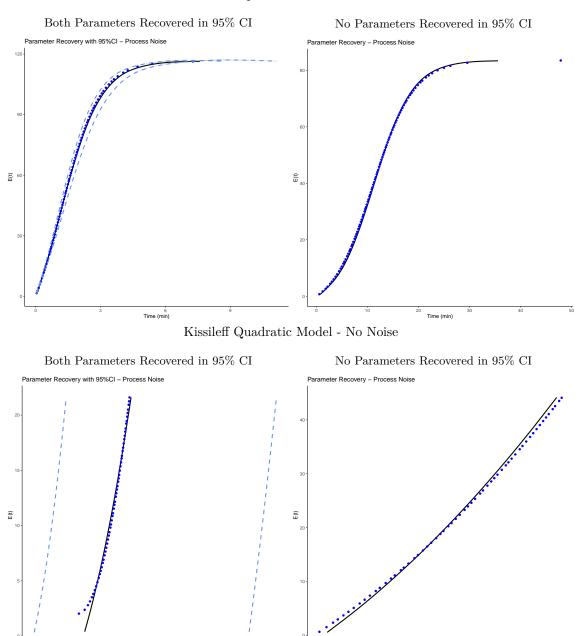
First Principles Model - Process Noise



Kissileff Quadratic Model - Process Noise



First Principles Model - Process Noise



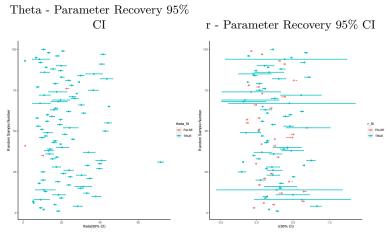
100 Time (min)

Time (min)

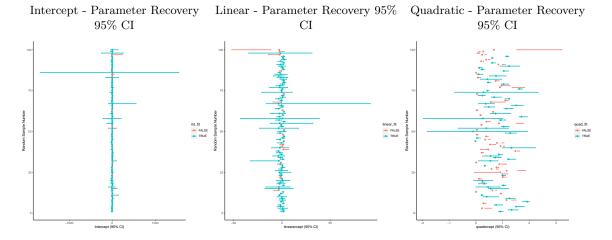
5.3 100 Random Multivariate Samples - Process Noise and Measurement Error

Measurement error: uses average bite size and jittered bite timing

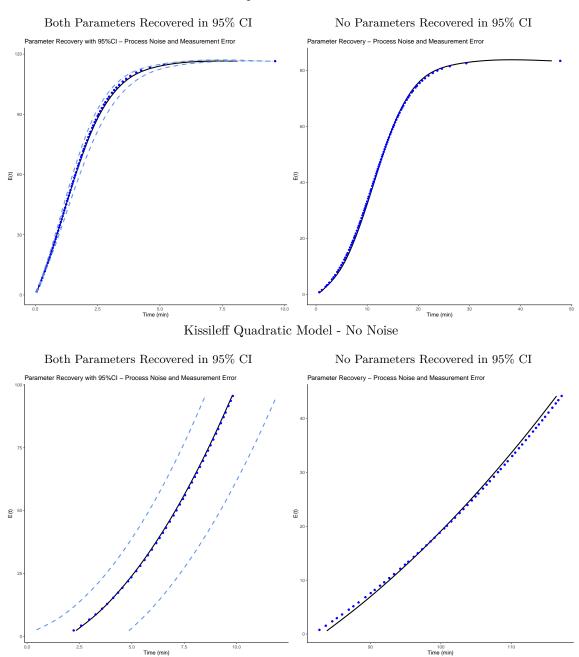
First Principles Model - Process Noise and Measurement Noise



Kissileff Quadratic Model - Process Noise



First Principles Model - Process Noise

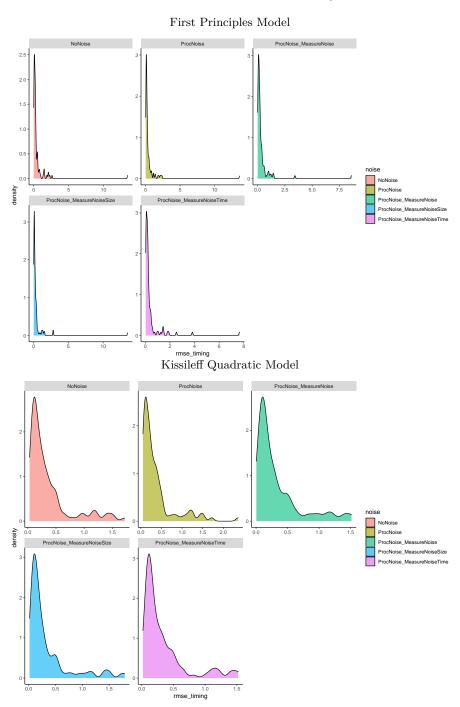


Time (min)

6 Root Mean Square Error

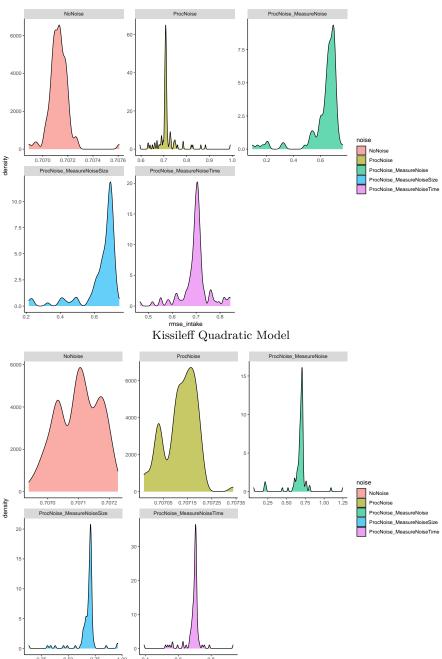
6.1 Distributions

RMSE Distribution for Bite Timing



RMSE Distribution for Intake

First Principles Model



6.2 number of NA's (estimated from recovered parameters)

Table 8: Number of random draws with an NAs in estimation of bite timing

| | NoNoise | ${\bf ProcNoise}$ | ${\bf ProcNoise_MeasureNoise}$ | ${\bf ProcNoise_MeasureNoiseSize}$ | ${\bf ProcNoise_MeasureNoiseTime}$ |
|---|---------|-------------------|---------------------------------|-------------------------------------|-------------------------------------|
| N | 325 | 330 | 345 | 365 | 335 |
| Y | 175 | 170 | 155 | 135 | 165 |

Table 9: Averge number of bites with NA timepoints (limited to the those with NAs)

| | x |
|-------------------------------------|----------|
| NoNoise | 1.971429 |
| ProcNoise | 2.147059 |
| ProcNoise_MeasureNoise | 1.967742 |
| ${\bf ProcNoise_MeasureNoiseSize}$ | 2.296296 |
| ${\bf ProcNoise_MeasureNoiseTime}$ | 1.969697 |

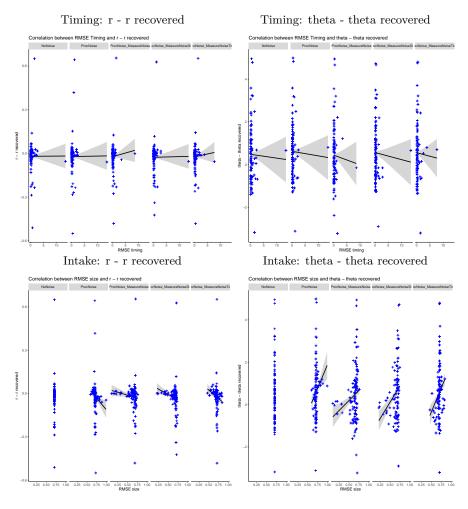
Table 10: Range in the number of bites with NA timepoints (limited to the those with NAs)

| | X |
|-------------------------------------|------|
| NoNoise | 1, 5 |
| ProcNoise | 1, 6 |
| ProcNoise_MeasureNoise | 1, 5 |
| ${\bf ProcNoise_MeasureNoiseSize}$ | 1, 6 |
| ${\bf ProcNoise_MeasureNoiseTime}$ | 1, 6 |

6.3 Correlation between Parameter Recovery Difference and RMSE

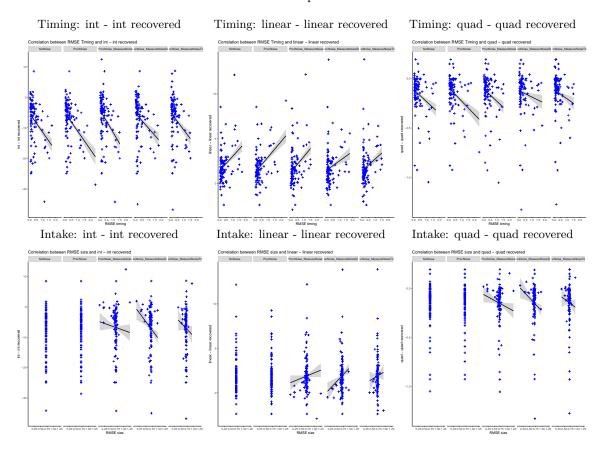
6.3.1 First Prinicples Model

 RMSE correlation with parameter - recovered



6.3.2 Kissileff Quadratic Model

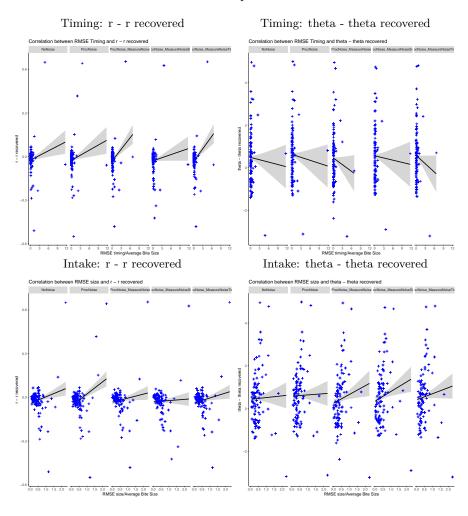
 RMSE correlation with parameter - recovered



${\bf 6.4}$ Correlation between Parameter Recovery Difference and RMSE/Avg Bite Size

6.4.1 First Prinicples Model

 RMSE correlation with parameter - recovered



6.4.2 Kissileff Quadratic Model

 RMSE correlation with parameter - recovered

