Caltech

Transforming Data Across Environments Despite Structural Non-Identifiability

ACC 2019

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Overview

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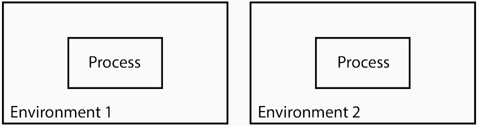
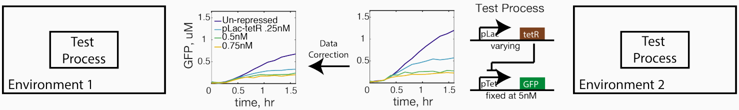
- Examples of problems:
  - batch variability reduction or data transformation
  - characterize subsystem behavior $\rightarrow$ predict system behavior

Transforming Process Behavior Across Environments



The Data Correction Problem



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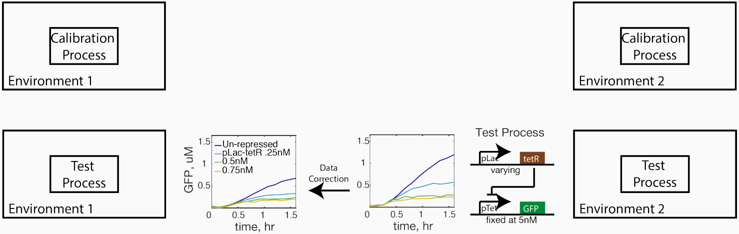

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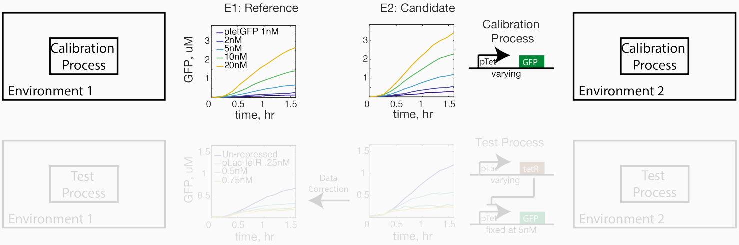
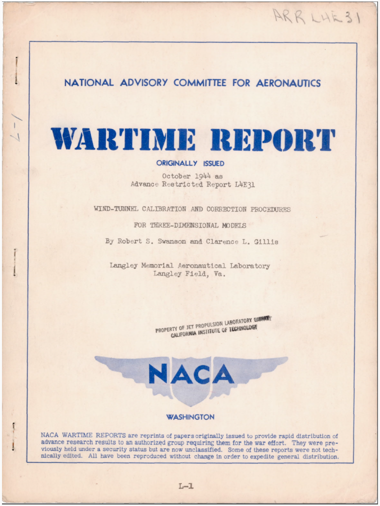


Solution: The Calibration-Correction Method



ARR L4E31

NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

WARTIME REPORT

ORIGINALLY ISSUED

October 1944 as
Advance Restricted Report L4E31

WIND-TUNNEL CALIBRATION AND CORRECTION PROCEDURES

FOR THREE-DIMENSIONAL MODELS

By Robert S. Swanson and Clarence L. Gillis

Langley Memorial Aeronautical Laboratory
Langley Field, Va.

NACA

WASHINGTON

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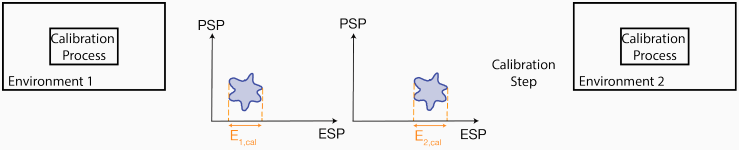
Solution: The Calibration-Correction Method

The usual practice of predicting the flying qualities of airplanes from wind-tunnel tests of relatively small-scale models makes it imperative that the model test results be corrected to free-air conditions. In addition, the large number of wind tunnels in use makes it desirable that a more or less standard calibration and correction procedure be adopted in order to make data from different tunnels as nearly comparable as possible. Not much com-

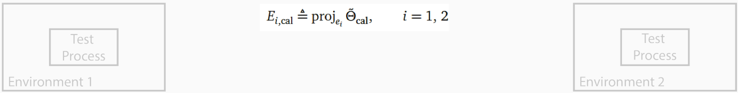
The Calibration-Correction Method: Calibration Step

Estimate environment specific parameters



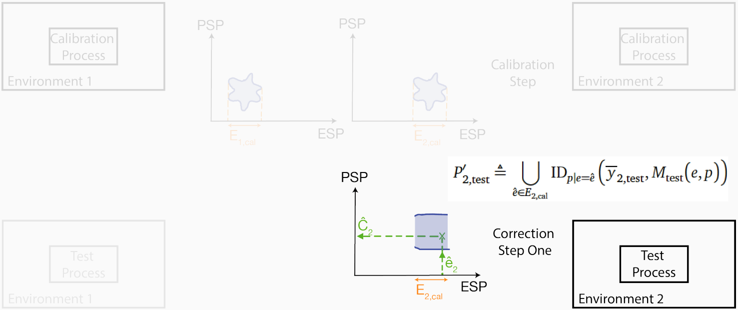
$$\tilde{\Theta}_{\text{cal}} \triangleq \left\{ (e_1, e_2, p) \,\middle|\, \overline{y}_{i,\text{cal}} = M_{\text{cal}}(e_i, p),\ i = 1, 2 \right\}$$

$$E_{i,\text{cal}} \triangleq \text{proj}_{e_i} \tilde{\Theta}_{\text{cal}}, \qquad i = 1, 2$$



The Calibration-Correction Method: Correction Step 1

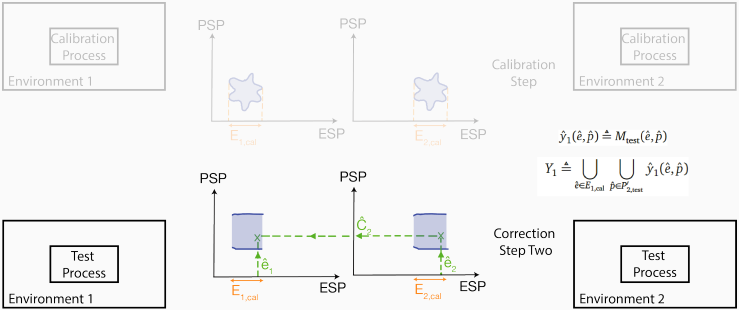
Estimate test process parameters in Extract 2



$$P'_{2,\text{test}} \triangleq \bigcup_{\hat{e} \in E_{2,\text{cal}}} \text{ID}_{p|e=\hat{e}}\left(\overline{y}_{2,\text{test}}, M_{\text{test}}(e,p)\right)$$

The Calibration-Correction Method: Correction Step 2

Predict test process behavior in Extract 1



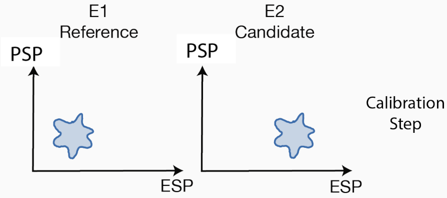
Parameter Consistency

Theorem

Consider the data correction problem in the model universe. Furthermore, consider the calibration-correction method, and the sets $\tilde{\Theta}_{\mathrm{cal}}$, $E_{1,\mathrm{cal}}$, $E_{2,\mathrm{cal}}$ *and* $C'_{2,\mathrm{test}}$. *Define* $\Theta_{i,\mathrm{test}} \triangleq \mathrm{ID}_\theta\left(\overline{y}_{i,\mathrm{test}}, \overline{M}_{\mathrm{test}}(\theta)\right)$ *for* $i = 1, 2$. *Then, the conditions,*

$$\tilde{\Theta}_{\mathrm{cal}} \neq \emptyset$$
$$E_{2,\mathrm{cal}} \subseteq \mathrm{proj}_e\, \Theta_{2,\mathrm{test}}$$
$$E_{1,\mathrm{cal}} \times C'_{2,\mathrm{test}} \subseteq \Theta_{1,\mathrm{test}},$$

are necessary and sufficient for the calibration-correction method to solve the data correction problem.



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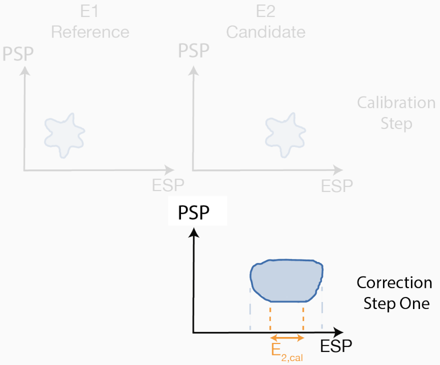

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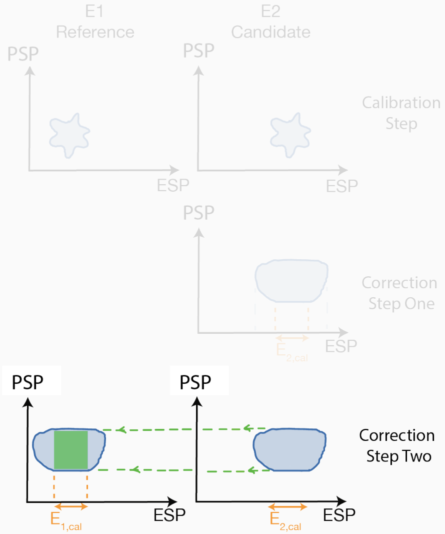
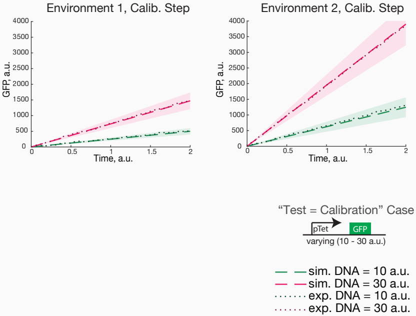


Consider the Test = Calibration Process Case



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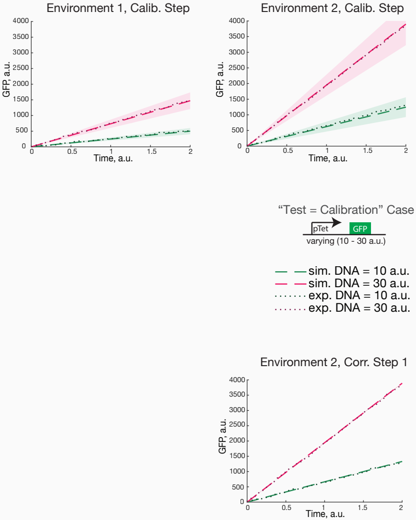
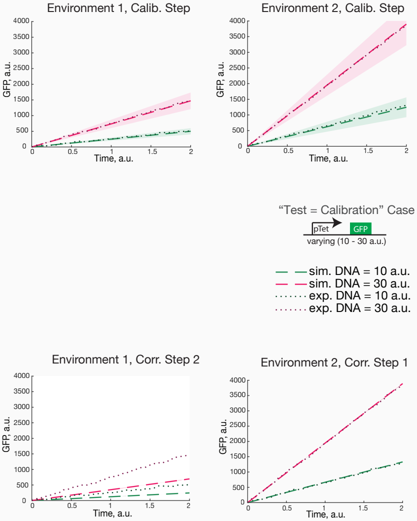
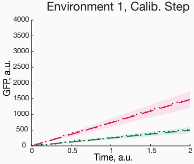
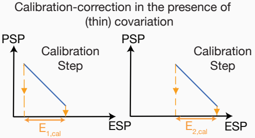


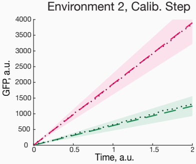
Correcting the Calibration Data Fails

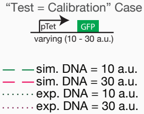


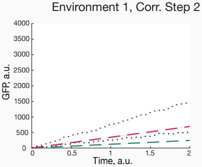
Parameter Covariation Could be a Problem

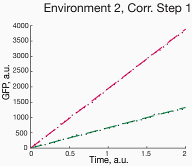












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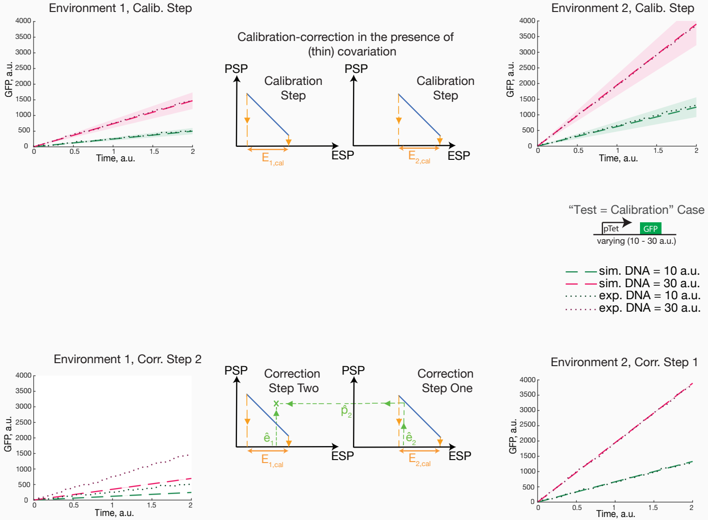

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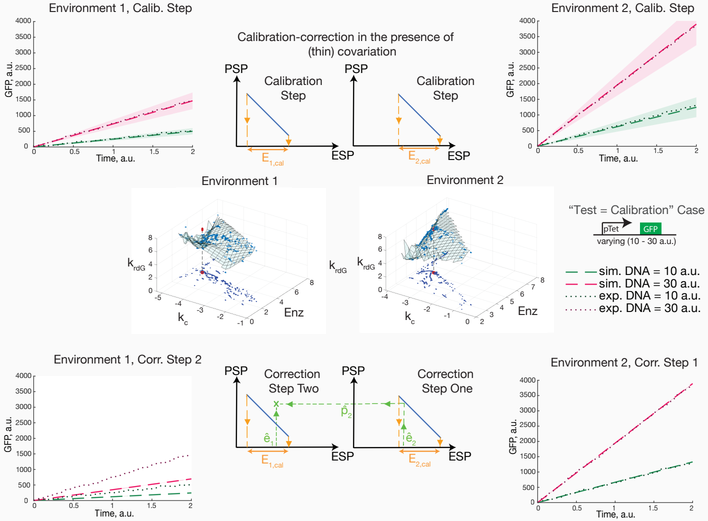
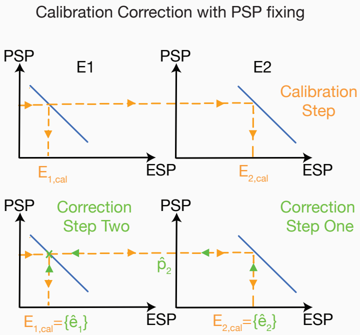


PSP Fixing Helps



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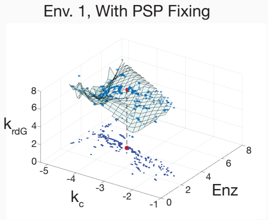
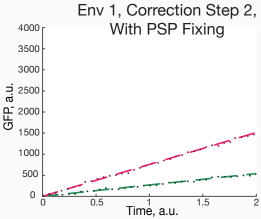
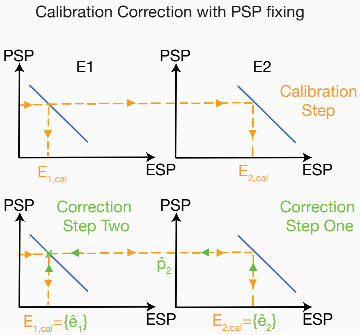






Formally...

Proposition

Consider the 'Test = Calib' case of the DCP. Assume the conditions

$$\begin{aligned} &\tilde{\Theta}_{\text{cal}} \neq \emptyset, \\ &C'_{2,\text{cal}} \subseteq \operatorname{proj}_c \Theta_{1,\text{cal}}, \\ &E_{i,\text{cal}} \subseteq \operatorname{proj}_e \Theta_{i,\text{cal}}, \qquad i = 1, 2, \end{aligned}$$

hold, but the set

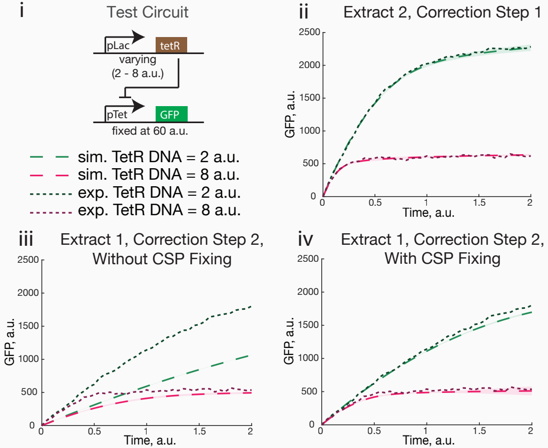
$$\Theta'_{1,\text{cal}} \triangleq \Theta_{1,\text{cal}} \cap \left(E_{1,\text{cal}} \times \operatorname{proj}_c \Theta_{2,\text{cal}}\right)$$

has covariation with respect to the (e, c) partition. Then, the calibration-correction method fails to solve this problem.

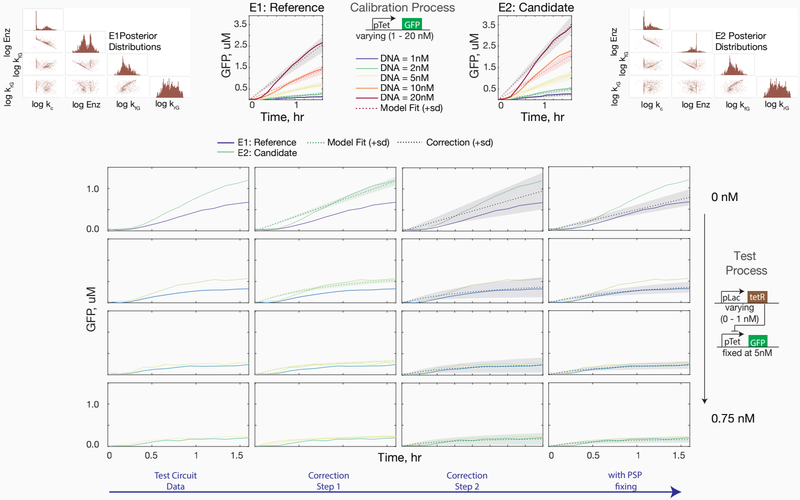
Proposition

Consider the sets $\Theta_{i,\text{cal}} \triangleq \text{ID}_\theta\left(\overline{y}_{i,\text{cal}}, M_{\text{cal}}(\theta)\right)$ for $i = 1, 2$, and the partition $\theta = (e, c)$. Assume that the $\Theta_{i,\text{cal}}$ have thin covariation in their c coordinates with respect to their e coordinates. Then, the calibration-correction method with CSP fixing is able to solve the DCP for the 'Test = Calib' case.

PSP Fixing Helps for New Test Data Too



PSP Fixing Helps with Experimental Data



Acknowledgements

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Research supported by:

The Data Correction Problem

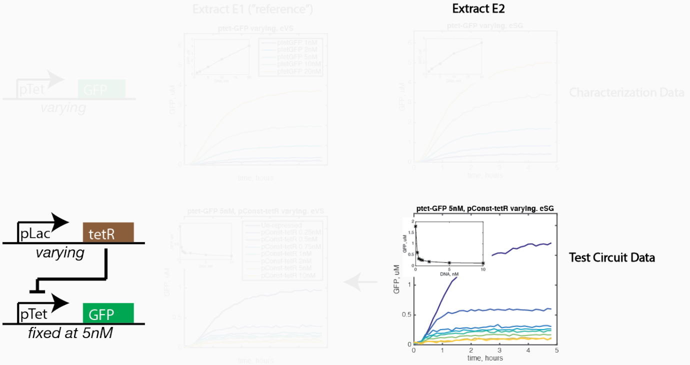


Figure 1: Given: Experimental data ($\bar{y}_{2,t}$) for a circuit in an extract, E2. The subscript t stands for test circuit.

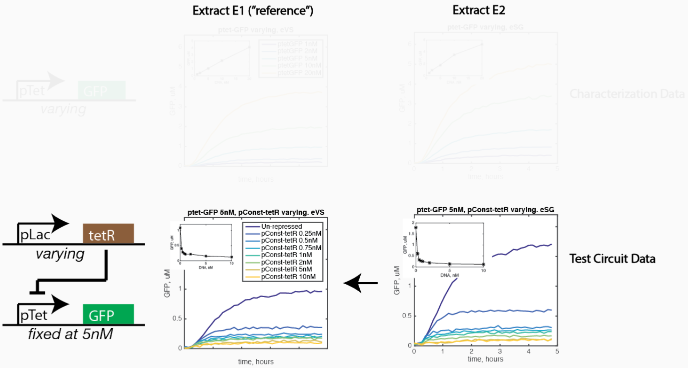


Figure 2: Goal: Transform it into a the behavior ($\bar{y}_{1,t}$) of that experiment in a different extract, E1, which we call the 'reference' extract.

The Data Correction Problem

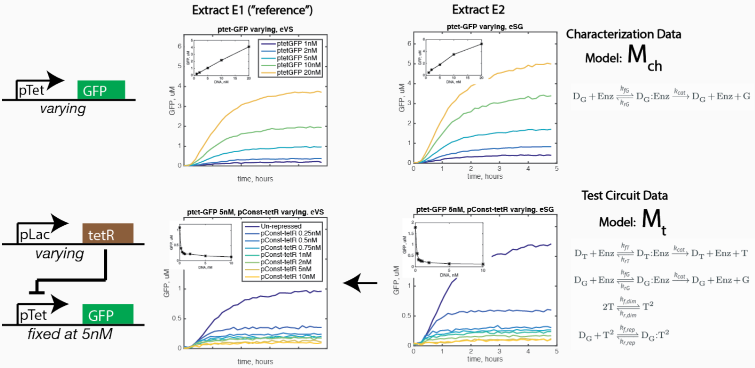


Figure 3: Available tools: Choice of a set of characterzation experiments $(\bar{y}_{1,ch}, \bar{y}_{2,ch})$ and corresponding models for both the characterization (M_{ch}) and test (M_t) circuits.

The Data Correction Problem (DCP)

- Have
  - Data for test circuit in E2, the candidate extract, $\overline{y}_{2,t}$
  - Ability to choose characterization experiments, and collect data $\overline{y}_{1,ch}$,$\overline{y}_{2,ch}$
  - Ability to choose models, M_{ch} and M_t
- Find a method that gives $\hat{y}_{1,t}$, such that $\hat{y}_{1,t} = \overline{y}_{1,t}$

Some Notation

- *Extracts* vs *Circuits*
- Model parameter vector (θ) coordinates partitioned into Extract Specific Parameters (e) and Circuit Specific Parameters (c), so that $\theta = (e, c)$

ESPs vs CSPs

$$\mathrm{D_G} + \mathrm{P} \underset{k_{rG}}{\overset{k_{fG}}{\rightleftharpoons}} \mathrm{D_G{:}P} \xrightarrow{k_c} \mathrm{D_G} + \mathrm{P} + \mathrm{G}$$

$$\mathrm{D} + \mathrm{pol} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{D{:}pol} \xrightarrow{k_c} \mathrm{D} + \mathrm{protein} + \mathrm{pol}$$

$$\mathrm{D_T} + \mathrm{P} \underset{k_{rT}}{\overset{k_{fT}}{\rightleftharpoons}} \mathrm{D_T{:}P} \xrightarrow{k_c} \mathrm{D_T} + \mathrm{P} + \mathrm{T}$$

$$\mathrm{D_G} + \mathrm{P} \underset{k_{rG}}{\overset{k_{fG}}{\rightleftharpoons}} \mathrm{D_G{:}P} \xrightarrow{k_c} \mathrm{D_G} + \mathrm{P} + \mathrm{G}$$

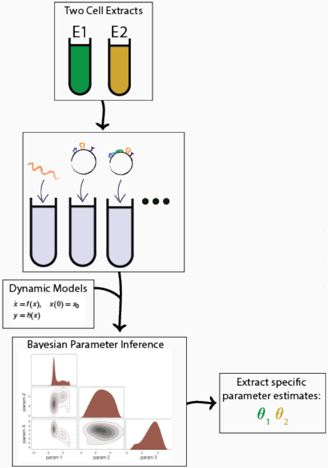
$$2\mathrm{T} \underset{k_{r,dim}}{\overset{k_{f,dim}}{\rightleftharpoons}} \mathrm{T}^2$$

$$\mathrm{D_G} + \mathrm{T}^2 \underset{k_{r,rep}}{\overset{k_{f,rep}}{\rightleftharpoons}} \mathrm{D_G{:}T^2}$$

- Environment specific parameters, e: $[\mathrm{P}]_{\mathrm{total}}$, k_c
- Process specific parameters, c: everything else

Proposed Solution

The Calibration-Correction Method - Calibration Step



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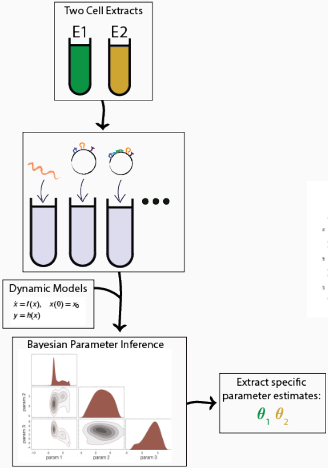

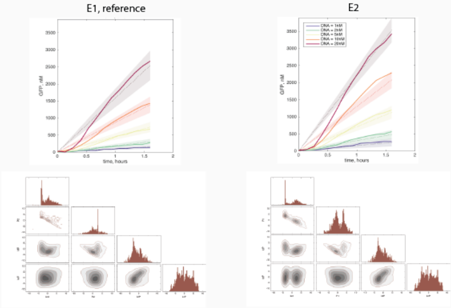

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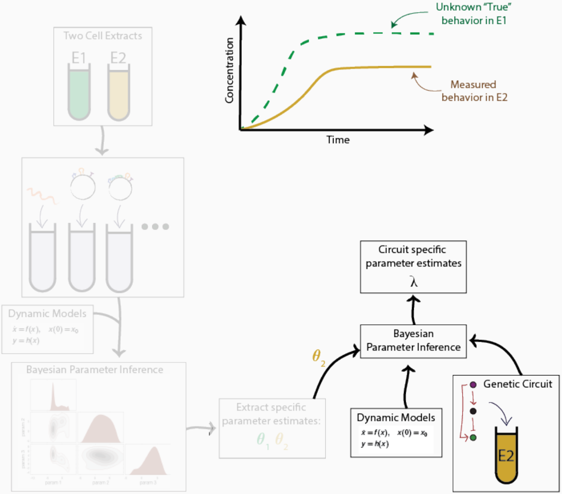
  - find $\hat{e}_{i,ch}$ such that $\bar{y}_{i,ch} = M_{ch}(\hat{e}_{i,ch}, c_{i,ch})$ for some $c_{i,ch}$.
  - All such points:

$$E_{i,ch} \triangleq \text{proj}_e \, \text{ID}_\theta(\overline{y}_{i,ch}, M_{ch}) \qquad \forall i \in \{1, 2\}. \tag{1}$$

The Calibration-Correction Method - Correction Step1



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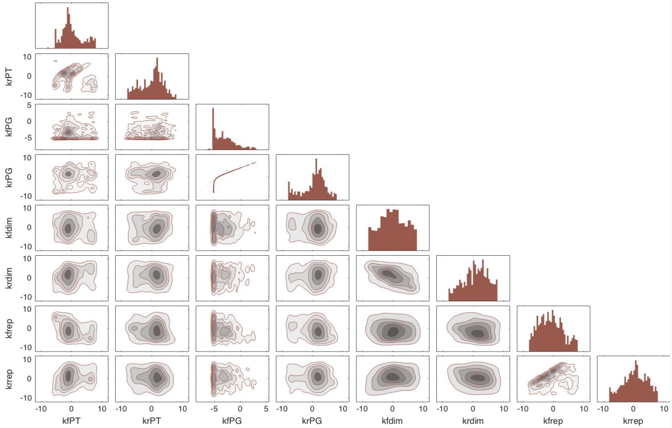

The Calibration-Correction Method - Correction Step 1

- **Correction Step One**: Test data, Extract 2. ($\overline{y}_{2,t}$) + extract parameters fixed at $\hat{e}_{2,ch} \rightarrow$ identify test parameters $\hat{c}_{2,t}$

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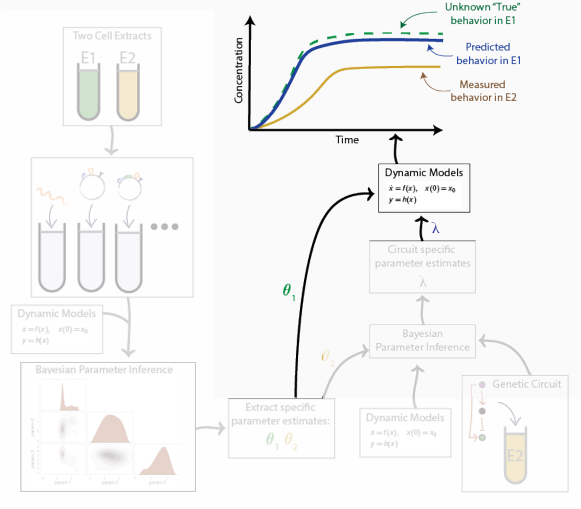
  - All such points:

$$C'_{c,t} \triangleq \bigcup_{\hat{e} \in E_{2,ch}} \mathrm{ID}_{c|e=\hat{e}}\left(\overline{y}_{2,t}, M_t\left(e, c\right)\right)$$

The Calibration-Correction Method - Correction Step 2



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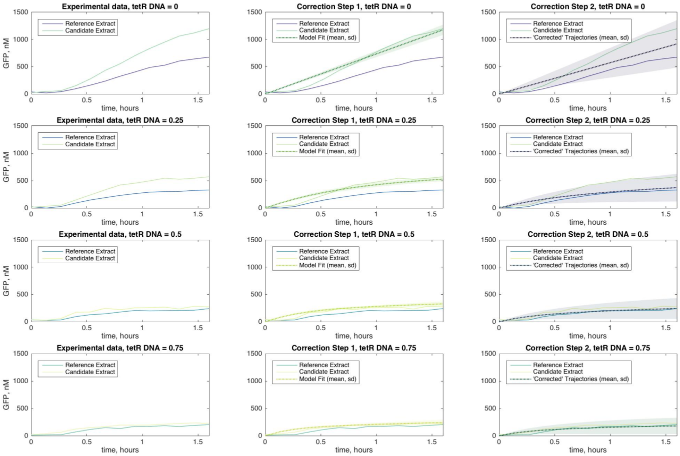

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- **Correction Step Two**: Predict $\hat{y}_{1,t} = M_t(\hat{e}_{1,ch}, \hat{c}_{2,t})$
  - All such trajectories:

$$Y_1 \triangleq \bigcup_{\hat{e} \in E_{1,ch}} \bigcup_{\hat{c} \in C'_{2,t}} \widetilde{y}_1(\hat{e}, \hat{c}), \tag{2}$$

where,

$$\widetilde{y}_1(\hat{e}, \hat{c}) = M_t(\hat{e}, \hat{c}). \tag{3}$$

Failure Conditions for this Method

- A parameter identification step is attempted when no parameter exists such that the model fits the data
- Correction step two is able to produce a trajectory not equal to the true trajectory

Results

Characterization Experiments Must be at Least as Informative as the Data to be Corrected

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Define,

$$E_{1,t} \triangleq \mathrm{proj}_e \, \mathrm{ID}_\theta(\overline{y}_{1,t}, \overline{M}_t),$$
$$E_{2,t} \triangleq \mathrm{proj}_e \, \mathrm{ID}_\theta(\overline{y}_{2,t}, \overline{M}_t).$$

Characterization Experiments Must be at Least as Informative as the Data to be Corrected

Define,

$$E_{1,t} \triangleq \text{proj}_e \, \text{ID}_\theta(\overline{y}_{1,t}, \overline{M}_t),$$
$$E_{2,t} \triangleq \text{proj}_e \, \text{ID}_\theta(\overline{y}_{2,t}, \overline{M}_t).$$

The first two conditions are,

$$E_{1,ch} \subseteq E_{1,t}$$
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Proof Ideas: If $E_{2,ch} \subseteq E_{2,t}$ does not hold, parameter estimation of the $C_{2,t}$ fails in first correction step. If $E_{1,ch} \subseteq E_{1,t}$ does not hold, then the prediction of a correct trajectory $\hat{y}_{1,t}$ is impossible for any c.

Process Specific Parameter Estimates for the Test Process Must Agree in Both Environments

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Recall that,

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Proof Idea: In the second correction step, the prediction $\hat{y}_{1,t}$ is generated by plugging in an arbitrary point from $C'_{2,t}$ into what would have been $C'_{1,t}$.

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Proof idea: In the second correction step, we pick arbitrary points from the sets $E_{1,ch}$ and $C'_{2,t}$ as a proxy for a point in $\Theta_{1,t}$.

Supplement

Definition (Parameter Identification)

Let the set $\mathscr{M}_Y$ be the set of all pairs $(\overline{y}, M(\theta, u, x_0))$ for which there exists a parameter $\hat{\theta} \in \Omega$ such that $\overline{y} = M(\hat{\theta}, u, x_0)$. Also, let $\mathscr{P}(\Omega)$ be the power set of Ω. We define the *parameter identification of* θ as an operator $\text{ID}_\theta : \mathscr{M}_Y \to \mathscr{P}(\Omega)$, with $\text{ID}_\theta(\overline{y}, M) = \{\hat{\theta} \in \Omega \mid \overline{y} = M(\hat{\theta}, u, x_0)\}$

Parameter Identifiability

Definition

$M(\theta_A)$ and $M(\theta_B)$ *output-indistinguishable* if,

$$\begin{aligned} &\theta_A,\ \theta_B \in \Omega, \\ y(t,\theta_A,u,x_0) &= y(t,\theta_B,u,x_0) \quad \forall t \geq 0,\ \forall u \in \mathscr{U},\ \forall x_0 \in \chi. \end{aligned} \tag{4}$$

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Definition

$M(\theta)$ SGI if all its parameters θ_i are SGI.

Proof: Necessity of $E_{2,ch} \subseteq E_{2,t}$

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- This implies $\nexists \tilde{c}$ s.t. $M_t(\tilde{e}, \tilde{c}) = \overline{y}_{2,t}$.
- $\implies$ parameter ID fails at correction step one (first failure condition).

Proof: Necessity of $E_{1,ch} \times C'_{2,t} \subseteq \Theta_{1,t}$

- Split into three sub conditions

$$
\begin{aligned}
E_{1,ch} \subseteq E_{1,t} &\triangleq \operatorname{proj}_e \mathrm{ID}_\theta(\overline{y}_{1,t}, \overline{M}_t), \\
C'_{2,t} &\subseteq C'_{1,t}, \\
E_{1,ch} \times C'_{2,t} &\subseteq \Theta_{1,t},
\end{aligned}
$$

Sufficiency is straightforward

The argument is a simple exercise in checking that the parameters that get picked are in sets such that the correct trajectories get generated.