Overcoming model and observation error in data assimilation using manifold learning

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Joint work with John Harlim, Franz Hamilton, and Tim Sauer

Filtering Overview

- Consider the standard filtering problem,

$$x_i = f(x_{i-1}) + \omega_{i-1}$$
$$y_i = h(x_i) + \eta_i$$

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- Kalman-based Filtering:
  - Forecast: Local Linear (EKF) or Ensemble (EnKF)
  - Assimilate: Gaussian assumption + Bayesian posterior

Bias in Observation Models

- Consider the standard filtering problem,

$$x_i = f(x_{i-1}) + \omega_{i-1}$$
$$y_i = h(x_i) + \eta_i$$

- Model error: Specify variables, unknown dynamics
- Observation error: Specify dynamics, unknown mapping
- Both unknown: Underdetermined

Bias in Observation Models

- Consider the standard filtering problem,

$$x_i = f(x_{i-1}) + \omega_{i-1}$$
$$y_i = h(x_i) + \eta_i$$

- True observation function $h(x)$ is unknown
- Assume we have a guess $g(x)$ and

$$y_i = h(x_i) + \eta_i = g(x_i) + b_i + \eta_i$$

- Bias: $b_i \equiv h(x_i) - g(x_i)$

Bias in Observation Models

- Consider the standard filtering problem,

$$\begin{aligned} x_i &= f(x_{i-1}) + \omega_{i-1} \\ y_i &= h(x_i, \eta_i) \end{aligned}$$

- True observation function h is unknown
- Assume we have a guess g and

$$y_i = h(x_i, \eta_i) = g(x_i, \eta_i) + b_i$$

- Stochastic Bias: $b_i \equiv h(x_i, \eta_i) - g(x_i, \eta_i)$

Example 1: Lorenz-96

- 40-dimensions:

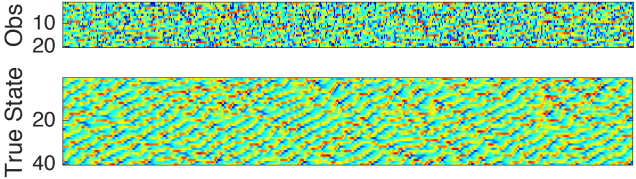
$$\dot{x}_j = x_{j-1}(x_{j+1} - x_{j-2}) - x_j + 8$$

- Observe 20 variables, 7 are 'cloudy'

$$h(x_k) = \begin{cases} x_k & \xi_i > 0.8 \\ \beta_k x_k - 8 & \text{else} \end{cases}$$

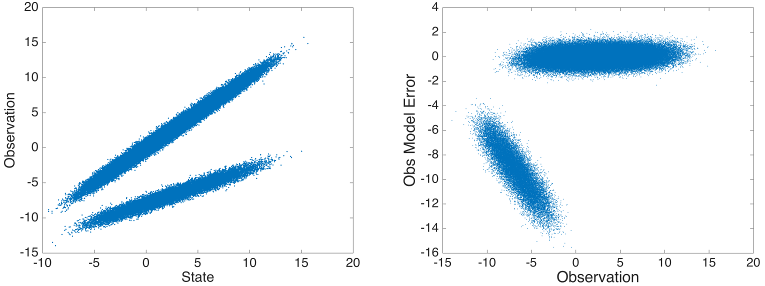
$$\beta_k \sim \mathcal{N}(0.5, 1/50).$$

$$\xi_i \sim \mathcal{U}(0, 1)$$



EXAMPLE 1: LORENZ-96

- The result is a bimodal distribution, “cloudy/clear”
- Obs Model Error = True Obs - g(True State)



CORRECTING THE BIAS

- Our goal is to find $p(b_i \mid y_i)$
- We can then correct our observation function

$$\hat{h}(x_i^f) \equiv g(x_i^f) + \hat{b}_i$$

- Where $\hat{b}_i = \mathbb{E}_{p(b_i \mid y_i)}[b_i]$
- Since $\hat{b}_i$ random:
  - Inflate the obs noise covariance
  - Use $\hat{R}_{b_i} = \mathbb{E}_{p(b_i \mid y_i)}[(b_i - \hat{b}_i)(b_i - \hat{b}_i)^\top]$

Correcting the bias

- Need to find $p(b_i \mid y_i)$
- From the forecast step we have a prior $p(b_i)$
  - Forecast $x_i^f \Rightarrow$ Bias estimate: $y_i - g(x_i^f)$
  - Prior $p(b_i) = \mathcal{N}(y_i - g(x_i^f), P_i^y)$
- Use Bayes' $p(b_i \mid y_i) = p(b_i)p(y_i \mid b_i)$
- Need the likelihood $p(y_i \mid b_i)$
- Use kernel estimation of conditional distributions

Learning the Conditional Distribution

- Given training data (y_i, b_i) our goal is to learn $p(y_i \mid b_i)$
- For a kernel $K(\alpha, \beta) = e^{-\frac{||\alpha - \beta||^2}{\delta^2}}$ we define Hilbert spaces

$$\mathcal{H}_y = \left\{ \sum_{i=1}^{N} a_i K(y_i, \cdot) \ : \ \vec{a} \in \mathbb{R}^N \right\}$$

$$\mathcal{H}_b = \left\{ \sum_{i=1}^{N} a_i K(b_i, \cdot) \ : \ \vec{a} \in \mathbb{R}^N \right\}$$

- Eigenvectors ϕ_ℓ of $K_{ij} = K(y_i, y_j)$ are a basis for $\mathcal{H}_y$.
- Similarly φ_k are a basis for $\mathcal{H}_b$.

Learning the conditional distribution

- We assume that $p(y \mid b)$ can be approximated in $\mathcal{H}_y \otimes \mathcal{H}_b$
- Let $C^{yb}_{ij} = \langle \phi_i, \varphi_j \rangle$ and $C^{bb}_{ij} = \langle \varphi_i, \varphi_j \rangle$ then define

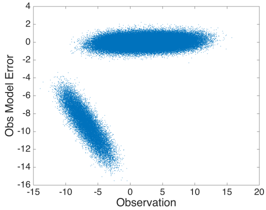
$$C^{y|b} = C^{yb} \left(C^{bb} + \lambda I \right)^{-1}$$

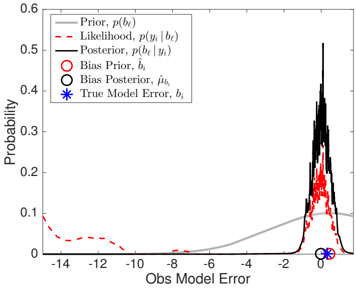
- We can then define a consistent estimator of $p(y \mid b)$ by

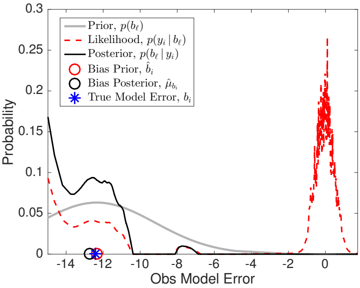
$$\hat{p}(y \mid b) = \sum_{i,j=1}^{N} C^{y|b}_{i,j} \phi_i(y) \varphi_j(b) \hat{q}(y)$$

Correcting the bias

- Below plots have $y_i \approx -4$
- Left is clear, right is cloudy
- Notice bimodal likelihood



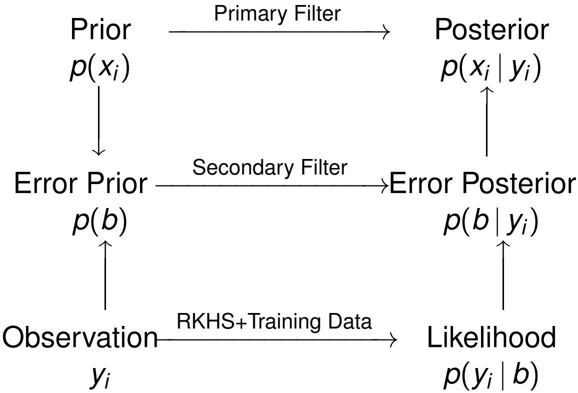




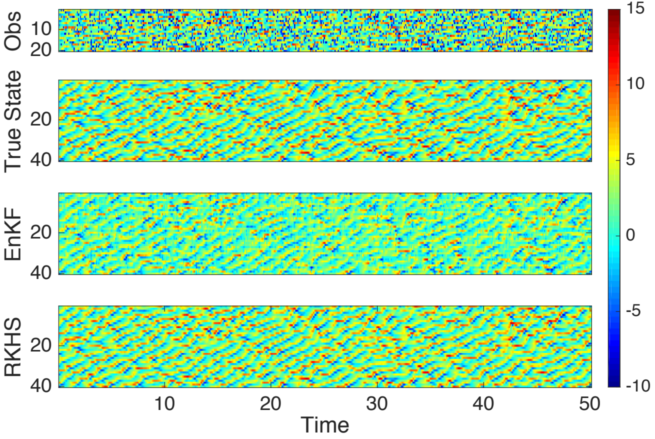
OVERVIEW

- **Learning Phase:** Given training data set (x_i, y_i)
  - Compute the biases $b_i = y_i - g(x_i)$
  - Learn the conditional distribution $p(y \mid b)$
- **Filtering:** Forecast $x_i^f \Rightarrow$ Bias estimate: $y_i - g(x_i^f)$
  - Prior $p(b) = \mathcal{N}(y_i - g(x_i^f), P_i^y)$
  - Likelihood $p(y_i \mid b)$ from learning phase
  - Apply Bayes: $p(b \mid y_i) = p(b)p(y_i \mid b)$
- Estimate bias $\hat{b}_i$ and correct the observation

Overview

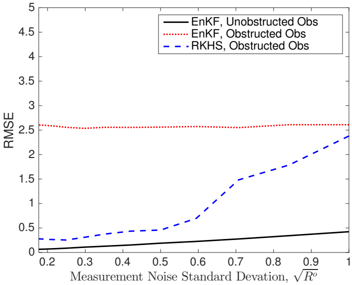

Prior
$p(x_i)$
Primary Filter
Posterior
$p(x_i \mid y_i)$
Error Prior
$p(b)$
Secondary Filter
Error Posterior
$p(b \mid y_i)$
Observation
y_i
RKHS+Training Data
Likelihood
$p(y_i \mid b)$

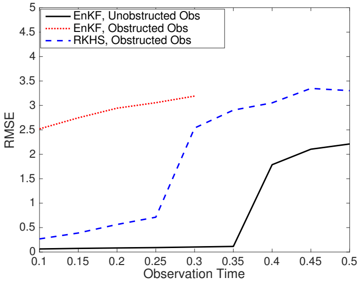
Lorenz-96 Results



Lorenz-96 Results

- Works well with small measurement noise
- Observations need to be precise, but not accurate





Bias in Observation Models

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$$x_i = f(x_{i-1}) + \omega_{i-1}$$
$$y_i = h(x_i) + \eta_i$$

- True observation function $h(x)$ is unknown
- Guess $g(x)$ and bias: $b_i \equiv h(x_i) - g(x_i)$

- Previously: Given training data, $\{(x_i, y_i)\}$
- Now: Only have observations, $\{y_i\}$.
- Idea: Iteratively estimate the bias

Iterative Bias Estimation

- Get the filter running with the bad obs g (inflate R)

$$\hat{b}_k^{(0)} = y_k - g\left(x_k^{(0)}\right)$$

- Takens' embedding to identify similar states:

$$z_k = [y_k, y_{k-1}, \ldots, y_{k-d}]$$

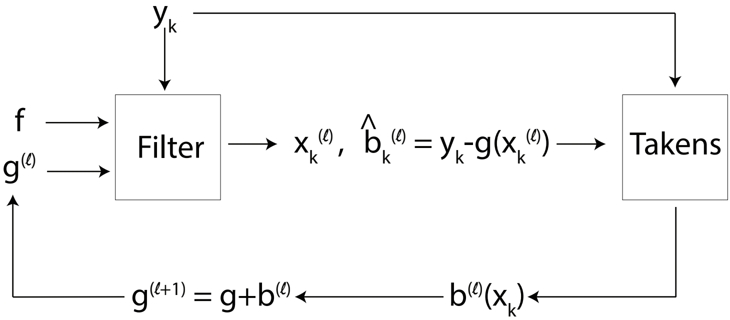
- Smooth the bias with local linear interpolation:

$$b^{(0)}(x_k) = \sum_i e^{-\frac{||z_k - z_i||^2}{\epsilon^2}} \hat{b}_i^{(0)}$$

- Update the observation function:

$$g^{(1)} = g + b^{(0)}$$

Iterative Bias Estimation



Example 2: Lorenz-63

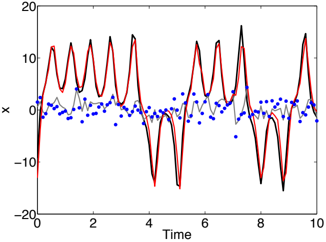
- 3-dimensional chaotic ODE
- True Obs:

$$h(\vec{x}) = h\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) = \begin{bmatrix} \sin(x_1) \\ x_2 - 6 \\ \cos(x_3) \end{bmatrix}$$

- Guess:

$$g(\vec{x}) = g\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

EXAMPLE 2: LORENZ-63



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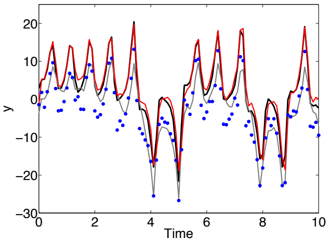
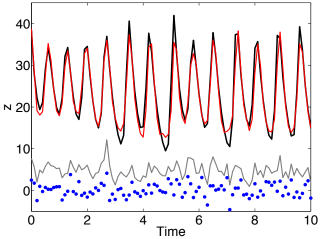
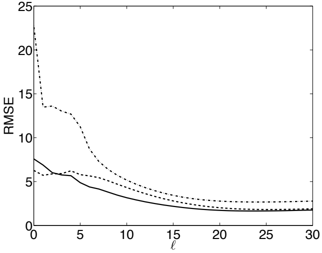


(b)



(c)

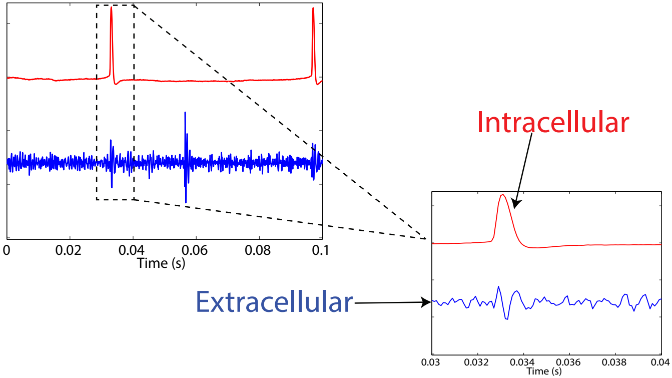


(d)

Putting the Two Methods Together

- Step 1: Iterative Estimation
  - Using historical observations, offline
- Step 2: Conditional Estimation
  - Use data from step 1 to train RKHS, online

Example 3: Intracellular from Extracellular



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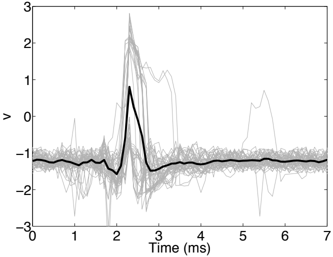

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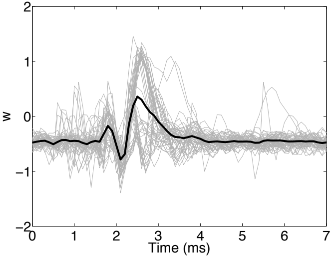
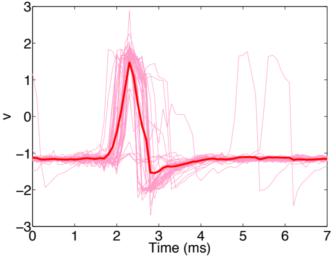


(b)



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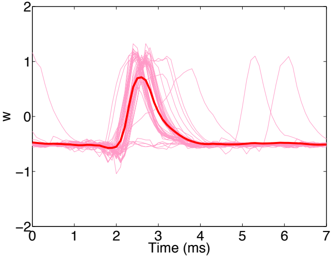


(d)

EXAMPLE 4: MULTI-CLOUD "SATELLITE-LIKE" OBS

- Consider a 7-dim'l model for a column of atmosphere
  - Baroclinic anomaly potential temperatures, θ_1 and θ_2
  - Boundary layer anomaly potential temperature, θ_{eb}
  - Vertically averaged water vapor content, q
  - Cloud fractions: congestus f_c, deep f_d, and stratiform f_s
- Extrapolate anomaly potential temperature at height z

$$T(z) = \theta_1 \sin(\frac{z\pi}{Z_T}) + 2\theta_2 \sin(\frac{2z\pi}{Z_T}), \quad z \in [0, 16]$$

Khouider, B., J. Biello, and A. J. Majda, 2010: A stochastic multicloud model for tropical convection.

Example 4: Multi-cloud "Satellite-like" obs

- Extrapolate anomaly potential temperature at height z

$$T(z) = \theta_1 \sin(\frac{z\pi}{Z_T}) + 2\theta_2 \sin(\frac{2z\pi}{Z_T}), \quad z \in [0, 16]$$

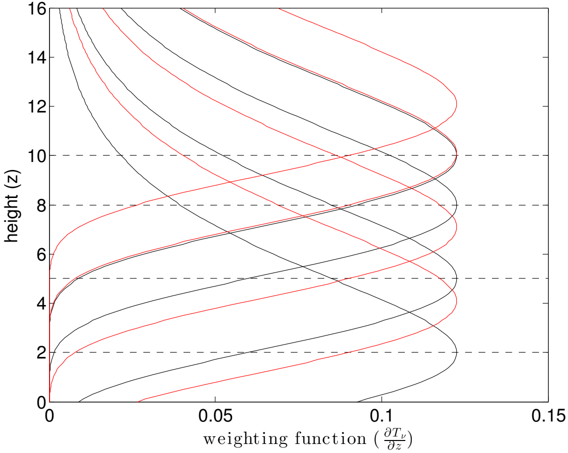
- Brightness temperature-like quantity at wavenumber-ν

$$\begin{aligned} h_\nu(x, f) = (1 - f_d - f_s)\Big[(1 - f_c)\big(\theta_{eb} T_\nu(0) + \int_0^{z_c} T(z)\frac{\partial T_\nu}{\partial z}(z)\,dz\big) \\ + f_c T(z_c) T_\nu(z_c) + \int_{z_c}^{z_d} T(z)\frac{\partial T_\nu}{\partial z}(z)\,dz\Big] \\ + (f_d + f_s) T(z_d) T_\nu(z_d) + \int_{z_d}^{\infty} T(z)\frac{\partial T_\nu}{\partial z}(z)\,dz, \end{aligned} \tag{1}$$

- Setting $f = 0$ is the clear sky model

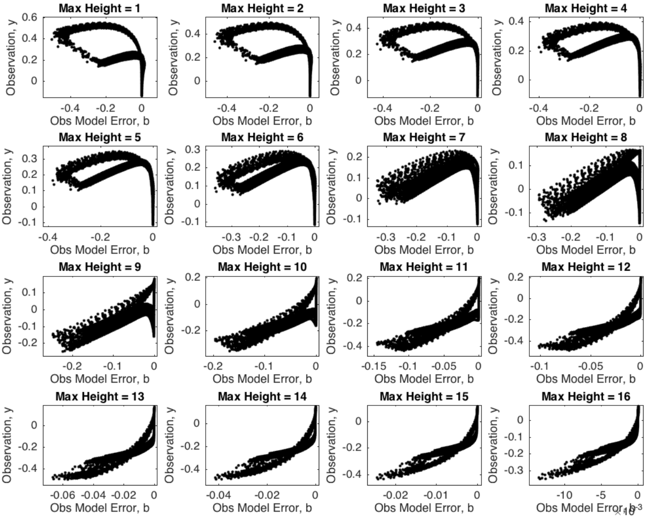
EXAMPLE 4: MULTI-CLOUD "SATELLITE-LIKE" OBS

- Weighting functions define RTM at different wavenumbers



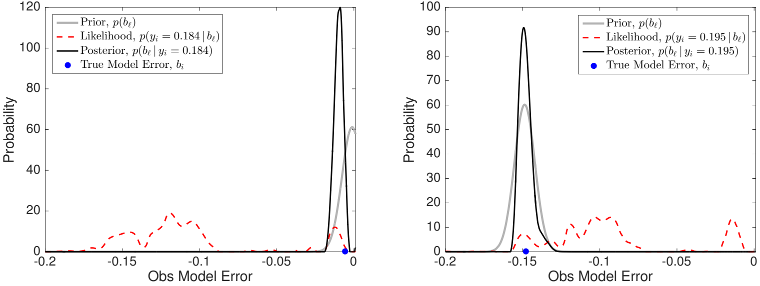
Example 4: Multi-cloud "Satellite-like" obs

- Biases at the 16 observed wavenumbers

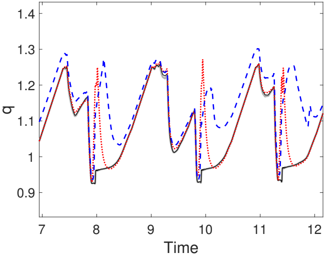


Example 4: Multi-cloud "Satellite-like" obs

- Multimodal likelihood functions



Example 4: "Satellite-like" obs (Iterative)



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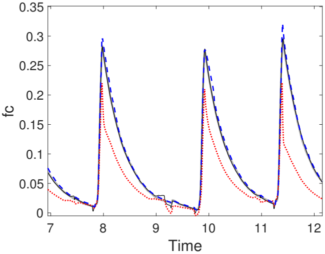

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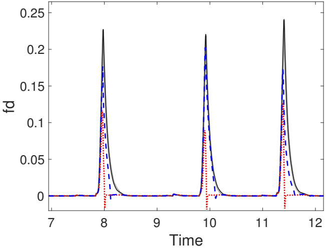
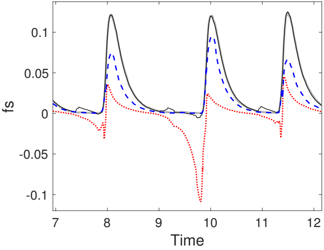
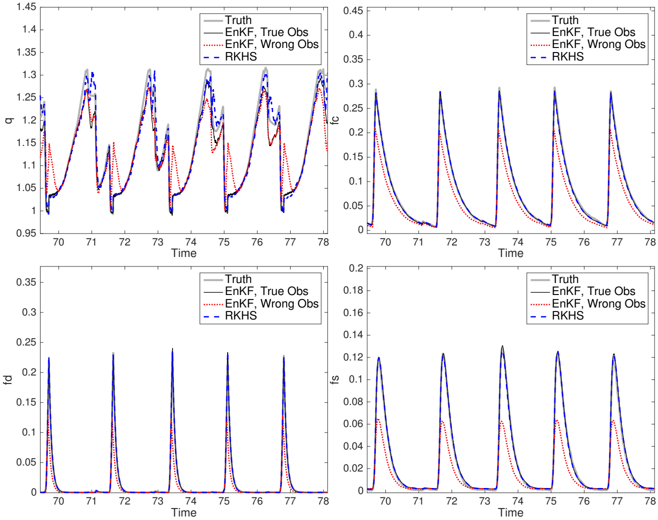




Example 4: "Satellite-like" obs (RKHS)



References

http://math.gmu.edu/~berry/

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- F. Hamilton, T. Berry, T. Sauer, Correcting Observation Model Error in Data Assimilation (preprint).
- F. Hamilton, T. Berry, T. Sauer, Tracking intracellular dynamics through extracellular measurements. PloS One (2018).