

Data assimilation with and without a model

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Parameter estimation and UQ
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Tyrus Berry, Postdoc, GMU



Franz Hamilton, Postdoc, NC State



OUTLINE OF TALK

1. EnKF and applications

- ▶ Parameters
- ▶ Network edge detection

2. Problem: Don't know noise covariances

- ▶ Adaptive filtering

3. Problem: Model error

- ▶ Multimodel DA

4. Problem: Model unknown

- ▶ Kalman-Takens filter

DATA ASSIMILATION

$$x_k = f(x_{k-1}) + \eta_k \quad \eta_k \in N(0, Q)$$

$$y_k = h(x_k) + \nu_k \quad \nu_k \in N(0, R)$$

Main Problem. Given the model above plus observations y_k ,

- ▶ **Filtering:** Estimate the current state $p(x_k | y_1, \dots, y_k)$
- ▶ **Forecasting:** Estimate a future state $p(x_{k+\ell} | y_1, \dots, y_k)$
- ▶ **Smoothing:** Estimate a past state $p(x_{k-\ell} | y_1, \dots, y_k)$
- ▶ **Parameter estimation**

We'll apply the ensemble Kalman filter (EnKF) to attempt to achieve these goals.

DATA ASSIMILATION

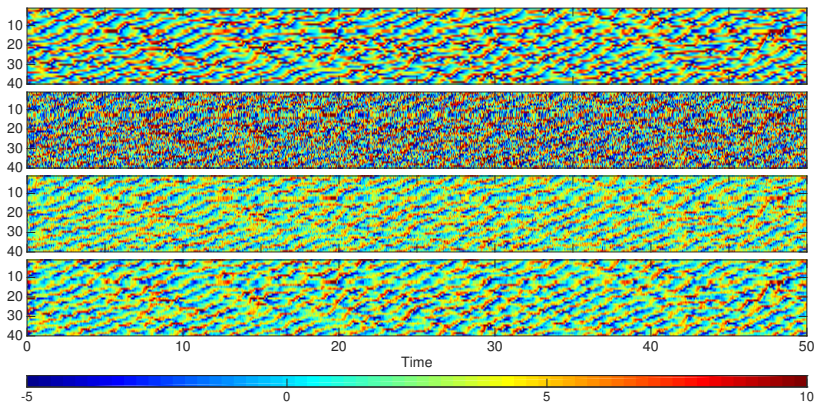
$$\begin{aligned}x_k &= f(x_{k-1}) + \eta_k & \eta_k &\in N(0, Q) \\y_k &= h(x_k) + \nu_k & \nu_k &\in N(0, R)\end{aligned}$$

Possible obstructions.

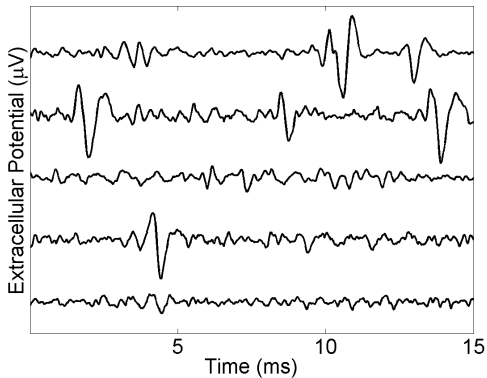
- ▶ The observations y_k mix system noise η_k with obs noise ν_k .
- ▶ Model error
 - ▶ Q and R may be unknown
 - ▶ Known model with unknown parameters
 - ▶ Wrong model, even with best fit parameters
 - ▶ Have model for some, not all of the variables

EXAMPLE 1. LORENZ 96

$$\frac{dx^i}{dt} = -x^{i-2}x^{i-1} + x^{i-1}x^{i+1} - x^i + F$$



EXAMPLE 2. MEA RECORDINGS



TWO STEPS TO FIND $p(x_k | y_1, \dots, y_k)$

- ▶ Assume we have $p(x_{k-1} | y_1, \dots, y_{k-1})$
- ▶ **Forecast Step:** Find $p(x_k | y_1, \dots, y_{k-1})$
- ▶ **Assimilation Step:** Perform a Bayesian update,

$$p(x_k | y_1, \dots, y_k) \propto p(x_k | y_1, \dots, y_{k-1})p(y_k | x_k, y_1, \dots, y_{k-1})$$

$$\text{Posterior} \propto \text{Prior} \times \text{Likelihood}$$

BEST POSSIBLE SCENARIO

$$x_k = f(x_{k-1}) + \eta_k \quad \eta_k \in N(0, Q)$$

$$y_k = h(x_k) + \nu_k \quad \nu_k \in N(0, R)$$

f and h are linear, all parameters known.

$$x_k = F_{k-1}x_{k-1} + \eta_k \quad \eta_k \in N(0, Q)$$

$$y_k = H_k x_k + \nu_k \quad \nu_k \in N(0, R)$$

KALMAN FILTER

- Assume linear dynamics/obs and additive Gaussian noise

$$x_k = F_{k-1}x_{k-1} + \eta_k \quad \eta_k \sim \mathcal{N}(0, Q)$$

$$y_k = H_k x_k + \nu_k \quad \nu_k \sim \mathcal{N}(0, R)$$

- observability condition for linear systems:

$$\tilde{H}_k^\ell = \begin{pmatrix} H_k \\ H_{k+1}F_k \\ \vdots \\ H_{k+\ell+1}F_{k+\ell} \cdots F_k \end{pmatrix}$$

Must be full rank for some $\ell \Rightarrow$ KF guaranteed to work

KALMAN FILTER

- Assume linear dynamics/obs and additive Gaussian noise

$$x_k = F_{k-1}x_{k-1} + \eta_k \quad \eta_k \sim \mathcal{N}(0, Q)$$

$$y_k = H_k x_k + \nu_k \quad \nu_k \sim \mathcal{N}(0, R)$$

- Assume current estimate is Gaussian:

$$p(x_{k-1} | y_1, \dots, y_{k-1}) = \mathcal{N}(x_{k-1}^a, P_{k-1}^a)$$

- **Forecast:** Linear combinations of Gaussians

- **Prior:** $p(x_k | y_1, \dots, y_{k-1}) = \mathcal{N}(x_k^f, P_k^f)$

- $x_k^f = F_{k-1}x_{k-1}^a$

- $P_k^f = F_{k-1}P_{k-1}F_{k-1}^\top + Q$

- **Likelihood:** $p(y_k | x_k, y_1, \dots, y_{k-1}) = \mathcal{N}(y_k^f, P_k^y)$

- $y_k^f = H_k x_k^f$

- $P_k^y = H_k P_k^f H_k^\top + R$

KALMAN FILTER

► Forecast: Linear combinations of Gaussians

► Prior: $p(x_k | y_1, \dots, y_{k-1}) = \mathcal{N}(x_k^f, P_k^f)$

► $x_k^f = F_{k-1} x_{k-1}^a$

► $P_k^f = F_{k-1} P_{k-1} F_{k-1}^\top + Q$

► Likelihood: $p(y_k | x_k, y_1, \dots, y_{k-1}) = \mathcal{N}(y_k^f, P_k^y)$

► $y_k^f = H_k x_k^f$

► $P_k^y = H_k P_k^f H_k^\top + R$

► **Assimilation:** Product of Gaussians (complete the square)

$$p(x_k | y_1, \dots, y_k) = \mathcal{N}(x_k^f, P_k^f) \times \mathcal{N}(y_k^f, P_k^y) = \mathcal{N}(x_k^a, P_k^a)$$

► Define the **Kalman gain:** $K_k = P_k^f H_k^\top (P_k^y)^{-1}$

► $x_k^a = x_k^f + K_k (y_k - y_k^f)$

► $P_k^a = (I - K_k H_k) P_k^f$

KALMAN FILTER SUMMARY

forecast

$$x_k^f = F_{k-1} x_{k-1}^a$$

covariance update

$$P_k^f = F_{k-1} P_{k-1}^a F_{k-1}^T + Q_{k-1}$$

$$P_k^y = H_k P_k^f H_k^T + R_{k-1}$$

Kalman gain

$$K_k = P_k^f H_k^T (P_k^y)^{-1}$$

$$\epsilon_k = y_k - y_k^f = y_k - H_k x_k^f$$

assimilation step

$$x_k^a = x_k^f + K_k \epsilon_k$$

$$P_k^a = (I - K_k H_k) P_k^f$$

WHAT ABOUT NONLINEAR SYSTEMS?

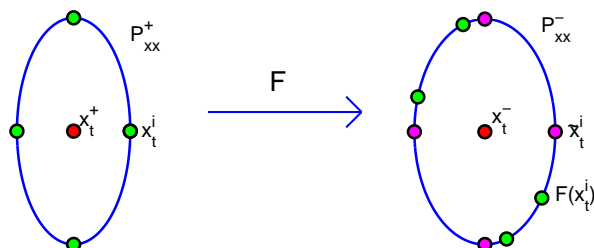
- ▶ Consider a system of the form:

$$x_{k+1} = f(x_k) + \eta_{k+1} \quad \eta_{k+1} \sim \mathcal{N}(0, Q)$$

$$y_{k+1} = h(x_{k+1}) + \nu_{k+1} \quad \nu_{k+1} \sim \mathcal{N}(0, R)$$

- ▶ More complicated observability condition (Lie derivatives)
- ▶ **Extended Kalman Filter (EKF):**
 - ▶ Linearize $F_k = Df(\hat{x}_k^a)$ and $H_k = Dh(\hat{x}_k^f)$
- ▶ Problem: State estimate \hat{x}_k^a may not be well localized
- ▶ Solution: Ensemble Kalman Filter (EnKF)

ENSEMBLE KALMAN FILTER (ENKF)



Calculate $y_t^i = H(F(x_t^i))$. Set $y_t^f = \frac{1}{2n} \sum_i y_t^i$.

$$P_{yy} = (2n - 1)^{-1} \sum (y_t^i - y_t^f)(y_t^i - y_t^f)^T + R$$

$$P_{xy} = (2n - 1)^{-1} \sum (F(x_t^i) - x_t^f)(y_t^i - y_t^f)^T$$

$$K = P_{xy} P_{yy}^{-1} \text{ and } P_{xx}^a = P_{xx}^f - K P_{yy} K^T$$

$$x_{t+1}^a = x_t^f + K(y_t - y_t^f)$$

PARAMETER ESTIMATION

- ▶ When the model has parameters p ,

$$x_{k+1} = f(x_k, p) + \eta_{k+1}$$

- ▶ Can *augment* the state $\tilde{x}_k = [x_k, p_k]$
- ▶ Introduce trivial dynamics for p

$$x_{k+1} = f(x_k, p_k) + \eta_{k+1}$$

$$p_{k+1} = p_k + \eta_{k+1}^p$$

- ▶ Need to tune the covariance of η_{k+1}^p

EXAMPLE OF PARAMETER ESTIMATION

Consider the Hodgkin-Huxley neuron model, expanded to a network of n equations

$$\begin{aligned}\dot{V}_i &= -g_{Na}m^3h(V_i - E_{Na}) - g_Kn^4(V_i - E_K) - g_L(V_i - E_L) \\ &\quad + I + \sum_{j \neq i}^n \Gamma_{HH}(V_j)V_j\end{aligned}$$

$$\dot{m}_i = a_m(V_i)(1 - m_i) - b_m(V_i)m_i$$

$$\dot{h}_i = a_h(V_i)(1 - h_i) - b_h(V_i)h_i$$

$$\dot{n}_i = a_n(V_i)(1 - n_i) - b_n(V_i)n_i$$

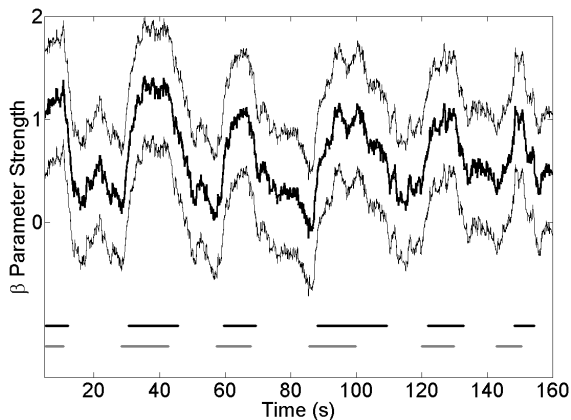
$$\Gamma_{HH}(V_j) = \beta_{ij}/(1 + e^{-10(V_j+40)})$$

Only observe the voltages V_i , recover the hidden variables and the connection parameters β

EXAMPLE OF PARAMETER ESTIMATION

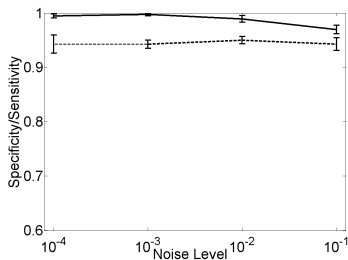
Can even turn connections on and off (grey dashes)

Variance estimate \Rightarrow statistical test (black dashes)

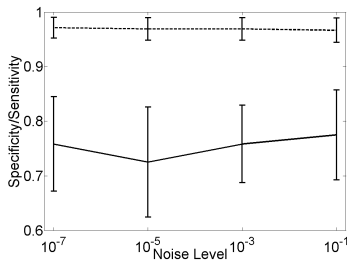


LINK DETECTION FROM NETWORKS OF MODEL NEURONS

Network of Hindmarsh-Rose
neurons, modeled by
Hindmarsh-Rose



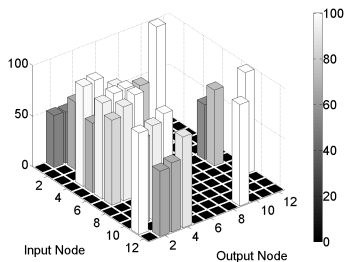
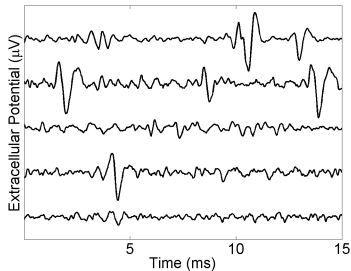
Network of Hodgkin-Huxley
neurons, modeled by
Hindmarsh-Rose



Sensitivity = true positive rate

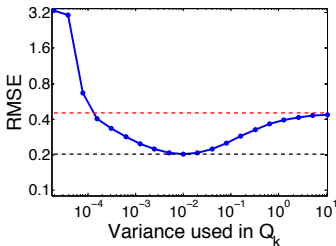
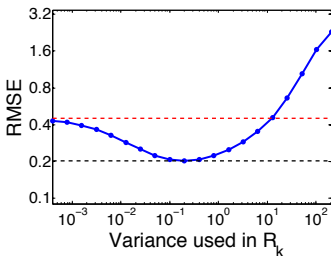
Specificity = true negative rate

LINK DETECTION FROM MEA RECORDINGS



ENKF: WRONG Q AND R

- ▶ Simple example with full observation and diagonal noise covariances
- ▶ Red indicates RMSE of unfiltered observations
- ▶ Black is RMSE of 'optimal' filter (true covariances known)



ENKF: WRONG Q AND R

Standard Kalman Update:

$$P_k^f = F_{k-1} P_{k-1}^a F_{k-1}^T + Q_{k-1}$$

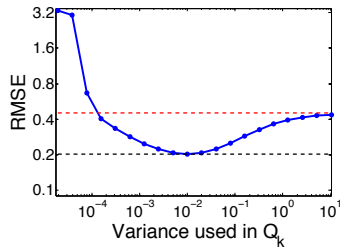
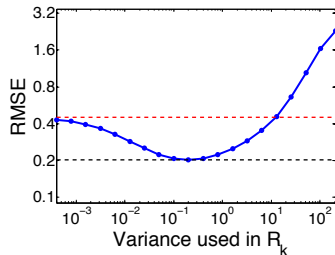
$$P_k^y = H_k P_k^f H_k^T + R_{k-1}$$

$$K_k = P_k^f H_k^T (P_k^y)^{-1}$$

$$P_k^a = (I - K_k H_k) P_k^f$$

$$\epsilon_k = y_k - y_k^f = y_k - H_k x_k^f$$

$$x_k^a = x_k^f + K_k \epsilon_k$$



ADAPTIVE FILTER: ESTIMATING Q AND R

- Innovations contain information about Q and R

$$\begin{aligned}
 \epsilon_k &= y_k - y_k^f \\
 &= h(x_k) + \nu_k - h(x_k^f) \\
 &= h(f(x_{k-1}) + \eta_k) - h(f(x_{k-1}^a)) + \nu_k \\
 &\approx H_k F_{k-1} (x_{k-1} - x_{k-1}^a) + H_k \eta_k + \nu_k
 \end{aligned}$$

- IDEA: Use innovations to produce samples of Q and R :

$$\begin{aligned}
 \mathbb{E}[\epsilon_k \epsilon_k^T] &\approx HP^f H^T + R \\
 \mathbb{E}[\epsilon_{k+1} \epsilon_k^T] &\approx HFP^e H^T - HFK \mathbb{E}[\epsilon_k \epsilon_k^T] \\
 P^e &\approx FP^a F^T + Q
 \end{aligned}$$

- In the linear case this is rigorous and was first solved by Mehra in 1970

ADAPTIVE FILTER: ESTIMATING Q AND R

- To find Q and R we estimate H_k and F_{k-1} from the ensemble and invert the equations:

$$\begin{aligned}\mathbb{E}[\epsilon_k \epsilon_k^T] &\approx HP^f H^T + R \\ \mathbb{E}[\epsilon_{k+1} \epsilon_k^T] &\approx HFP^e H^T - HFK \mathbb{E}[\epsilon_k \epsilon_k^T]\end{aligned}$$

- This gives the following *empirical* estimates of Q_k and R_k :

$$\begin{aligned}P_k^e &= (H_{k+1} F_k)^{-1} (\epsilon_{k+1} \epsilon_k^T + H_{k+1} F_k K_k \epsilon_k \epsilon_k^T) H_k^{-T} \\ Q_k^e &= P_k^e - F_{k-1} P_{k-1}^a F_{k-1}^T \\ R_k^e &= \epsilon_k \epsilon_k^T - H_k P_k^f H_k^T\end{aligned}$$

- P_k^e is an empirical estimate of the background covariance

ADAPTIVE ENKF

We combine the estimates of Q and R with a moving average

Original Kalman Eqs.

$$P_k^f = F_{k-1} P_{k-1}^a F_{k-1}^T + Q_{k-1}$$

$$P_k^y = H_k P_k^f H_k^T + R_{k-1}$$

$$K_k = P_k^f H_k^T (P_k^y)^{-1}$$

$$P_k^a = (I - K_k H_k) P_k^f$$

$$\epsilon_k = y_k - y_k^f$$

$$x_k^a = x_k^f + K_k \epsilon_k$$

Our Additional Update

$$P_{k-1}^e = F_{k-1}^{-1} H_k^{-1} \epsilon_k \epsilon_{k-1}^T H_{k-1}^{-T}$$

$$+ K_{k-1} \epsilon_{k-1} \epsilon_{k-1}^T H_{k-1}^{-T}$$

$$Q_{k-1}^e = P_{k-1}^e - F_{k-2} P_{k-2}^a F_{k-2}^T$$

$$R_{k-1}^e = \epsilon_{k-1} \epsilon_{k-1}^T - H_{k-1} P_{k-1}^f H_{k-1}^T$$

$$Q_k = Q_{k-1} + (Q_{k-1}^e - Q_{k-1})/\tau$$

$$R_k = R_{k-1} + (R_{k-1}^e - R_{k-1})/\tau$$

ADAPTIVE FILTER: APPLICATION TO LORENZ-96

- ▶ We will apply the adaptive EnKF to the 40-dimensional Lorenz96 model integrated over a time step $\Delta t = 0.05$

$$\frac{dx^i}{dt} = -x^{i-2}x^{i-1} + x^{i-1}x^{i+1} - x^i + F$$

- ▶ We augment the model with Gaussian white noise

$$\begin{aligned} x_k &= f(x_{k-1}) + \eta_k & \eta_k &= \mathcal{N}(0, Q) \\ y_k &= h(x_k) + \nu_k & \nu_k &= \mathcal{N}(0, R) \end{aligned}$$

- ▶ The Adaptive EnKF uses $F = 8$
- ▶ We will consider model error where the true $F^i = \mathcal{N}(8, 16)$

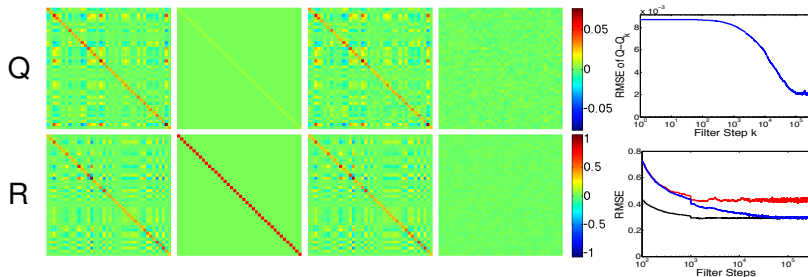
RECOVERING Q AND R , PERFECT MODEL

True Covariance

Initial Guess

Final Estimate

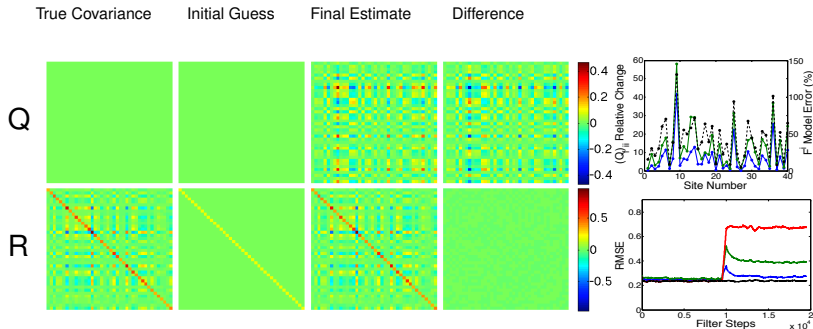
Difference



RMSE (bottom right) for the initial guess covariances (red) the true Q and R (black) and the adaptive filter (blue)

COMPENSATING FOR MODEL ERROR

The adaptive filter compensates for errors in the forcing F^i



RMSE (bottom right) for the initial guess covariances (red) the perfect model (black) and the adaptive filter (blue)

ESTIMATING UNMODELED DYNAMICS

Multiple models approach: Run m subfilters in parallel

$$\begin{aligned}\dot{w} &= F(w) + \eta_t \\ \begin{bmatrix} y \\ \vdots \\ y \\ S \end{bmatrix} &= H(w) + \nu_t\end{aligned}$$

where

$$w = \begin{bmatrix} x^1 \\ \vdots \\ x^m \\ c^1 \\ \vdots \\ c^m \\ d \end{bmatrix}, F = \begin{bmatrix} f(x, p_1) \\ \vdots \\ f(x, p_m) \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, H(w) = \begin{bmatrix} h(x^1) \\ \vdots \\ h(x^m) \\ \sum_{i,j} c_j^i x_j^i + d \end{bmatrix}$$

Learn c_j^i and d from training data S , then can predict unmodeled S .

SELECTING THE ASSIMILATION MODEL

- Assume a generic spiking neuron model (Hindmarsh-Rose)

$$\dot{\mathbf{V}} = \mathbf{y} - a\mathbf{V}^3 + b\mathbf{V}^2 - \mathbf{z} + I$$

$$\dot{\mathbf{y}} = c - d\mathbf{V}^2 - \mathbf{y}$$

$$\dot{\mathbf{z}} = \tau(s(\mathbf{V} + 1) - \mathbf{z})$$

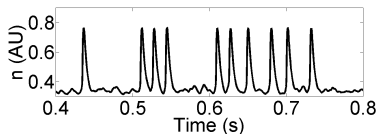
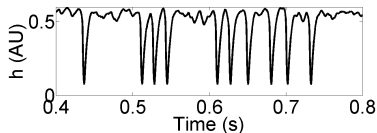
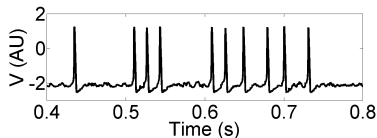
\mathbf{V} neuron potential, \mathbf{y} fast scale dynamics, \mathbf{z} slow scale dynamics

- **Goal:** Use multiple parameterized Hindmarsh-Rose models to reconstruct unmodeled neuronal quantities while assimilating recorded neuron potential

RECONSTRUCTING UNMODELED GATING VARIABLES

Observing Hodgkin-Huxley voltage, reconstruct unmodeled gating variables (assimilation model is Hindmarsh-Rose)

A. Hodgkin and A. Huxley, J. Physiology **117**, 500 (1952).

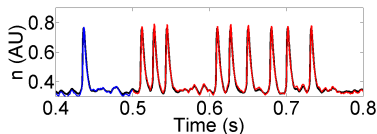
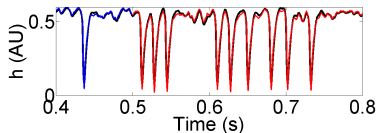
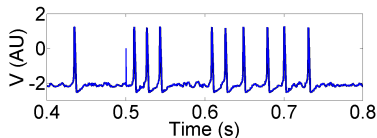


Actual

RECONSTRUCTING UNMODELED GATING VARIABLES

Observing Hodgkin-Huxley voltage, reconstruct unmodeled gating variables (assimilation model is Hindmarsh-Rose)

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Actual

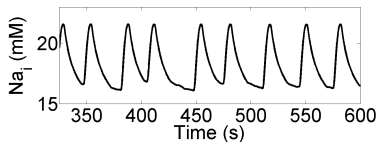
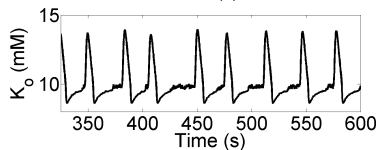
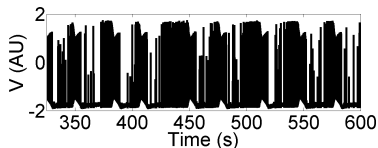
Observed

Predicted

RECONSTRUCTING UNMODELED IONIC DYNAMICS

Observing seizure voltage, reconstruct unmodeled potassium and sodium dynamics (assimilation model is Hindmarsh-Rose)

J. Cressman, G. Ullah, J. Ziburkus, S. Schiff, and E. Barreto, *Journal of Comp. Neuroscience* **26**, 159 (2009).

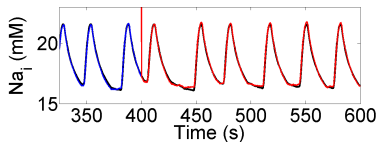
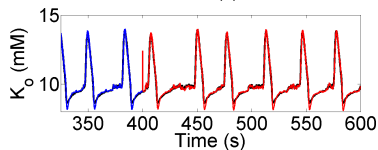
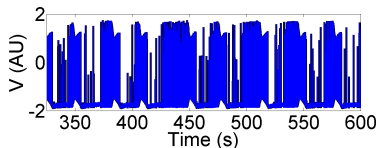


Actual

RECONSTRUCTING UNMODELED IONIC DYNAMICS

Observing seizure voltage, reconstruct unmodeled potassium and sodium dynamics (assimilation model is Hindmarsh-Rose)

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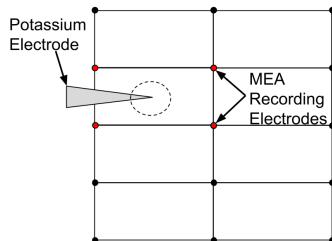
Actual

Observed

Predicted

RECONSTRUCTING EXTRACELLULAR POTASSIUM FROM AN *In Vitro* NETWORK

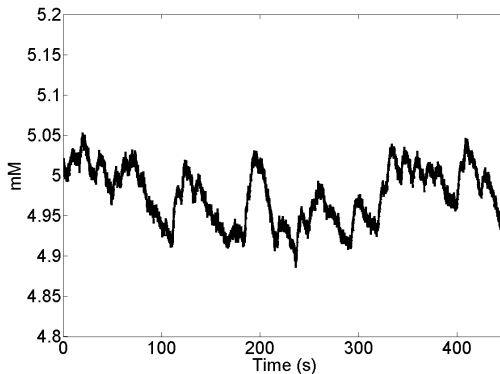
We want to track extracellular potassium dynamics in a network but measurements are difficult and spatially limited



Extracellular potassium is an **unmodeled variable**

RECONSTRUCTING EXTRACELLULAR POTASSIUM FROM AN *In Vitro* NETWORK

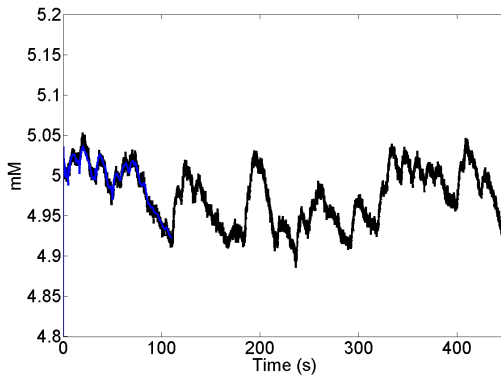
The local extracellular potassium in an MEA network can be reconstructed and predicted using our approach (assimilation model is Hindmarsh-Rose)



Actual

RECONSTRUCTING EXTRACELLULAR POTASSIUM FROM AN *In Vitro* NETWORK

The local extracellular potassium in an MEA network can be reconstructed and predicted using our approach (assimilation model is Hindmarsh-Rose)

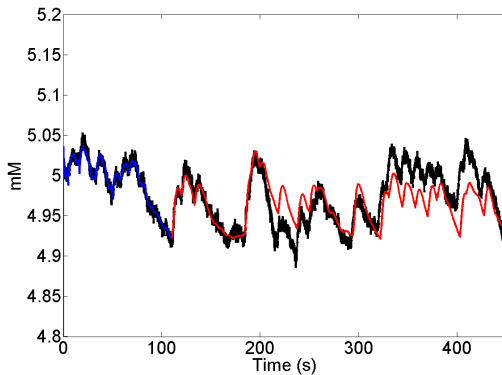


Actual

Observed

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Actual

Observed

Predicted

KALMAN-TAKENS FILTER: THROWING OUT THE MODEL...

- ▶ Starting with historical observations $\{y_0, \dots, y_n\}$
- ▶ Form Takens delay-embedding state vectors $x_i = (y_i, y_{i-1}, \dots, y_{i-d})^\top$
- ▶ Build an EnKF:
 - ▶ Apply analog forecast to each ensemble member
 - ▶ Use the observation function $Hx_i = y_i$
 - ▶ Crucial to estimate Q and R

NO MODEL: KALMAN-TAKENS FILTER

Reasons why this might not work:

- ▶ Nonparametric methods that depend on local reconstructions tend to fail in presence of observation noise
 - ▶ Takens' Theorem assumes no obs noise
 - ▶ Neighbors in reconstruction space are wrong
- ▶ Kalman filters depend on knowledge of model to advance dynamics
 - ▶ Filter equations need knowledge of dynamics to advance "background"

ENSEMBLE KALMAN FILTERING (ENKF)

At k th step:

- Form an ensemble of state vectors centered at best guess x_{k-1}^+ , with spread given by estimated covariance P_{k-1}^+
- Model f is applied to this ensemble and observed with function h . Form the *prior* state estimate x_k^- and the predicted observation y_k^-
- Construct the resulting covariance matrices P_k^{xy} and P_k^y
- Update the state and covariance estimates with the observation y_k

$$K_k = P_k^{xy} (P_k^y)^{-1}$$

$$P_k^+ = P_k^- - P_k^{xy} (P_k^y)^{-1} P_k^{yx}$$

$$x_k^+ = x_k^- + K_k (y_k - y_k^-).$$

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KALMAN-TAKENS FILTER

At k th step:

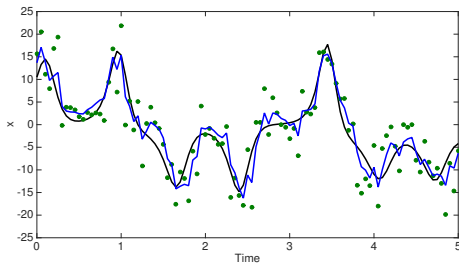
- ▶ Form ensemble of reconstructed states centered at delay-coordinate vector x_{k-1}^+ , with spread given by estimated covariance P_{k-1}^+
- ▶ Apply nonparametric prediction and observe with function h . Estimate *prior* state x_k^- and observation y_k^-
- ▶ Construct the resulting covariance matrices P_k^{xy} and P_k^y
- ▶ Update the state and covariance estimates with the observation y_k

$$K_k = P_k^{xy} (P_k^y)^{-1}$$

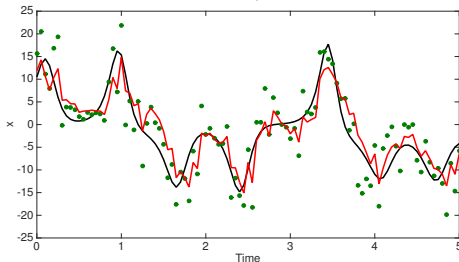
$$P_k^+ = P_k^- - P_k^{xy} (P_k^y)^{-1} P_k^{yx}$$

$$x_k^+ = x_k^- + K_k (y_k - y_k^-).$$

KALMAN-TAKENS FILTER: LORENZ 63



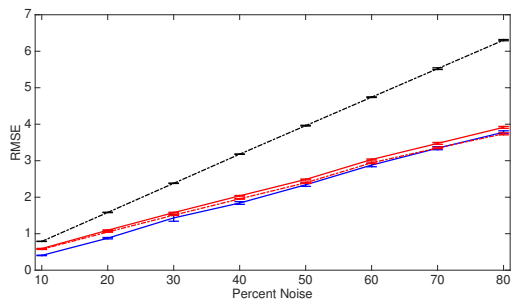
full model



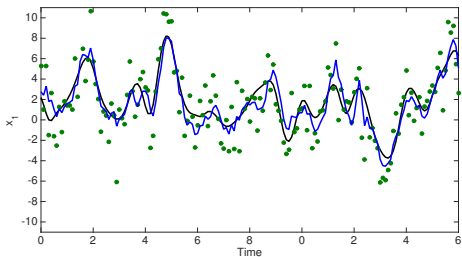
Kalman-Takens

KALMAN-TAKENS FILTER

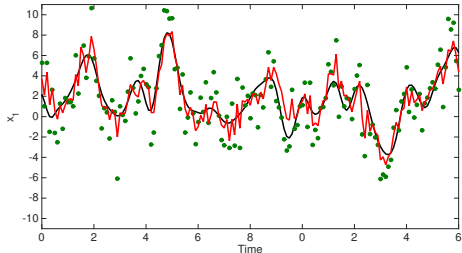
Comparison of Kalman-Takens (red) with full model (blue)



KALMAN-TAKENS FILTER: LORENZ 96

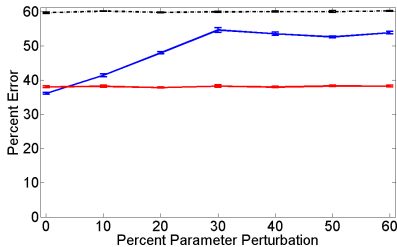


full model

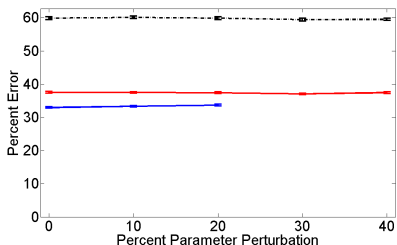


Kalman-Takens

KALMAN-TAKENS FILTER: MODEL ERROR

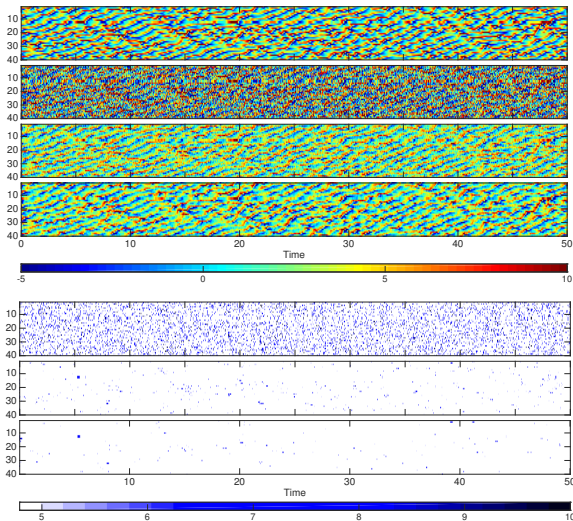


Lorenz 63



Lorenz 96

KALMAN-TAKENS FILTER: LORENZ 96

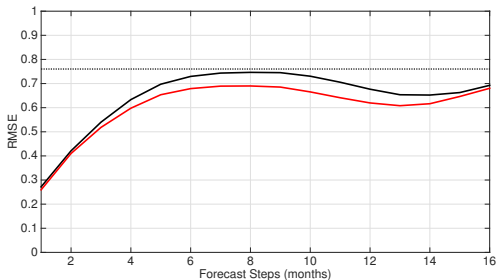


KALMAN-TAKENS FILTER: FORECAST ERROR

El Nino index

Training data: Jan. 1950 - Dec. 1999.

Forecasts after 2000



SUMMARY

- ▶ EnKF is a useful data assimilation technique for neurodynamics and other types of data
- ▶ Parameter estimation
- ▶ Adaptive QR is helpful when Q and R are unknown
- ▶ Difficulties
 - ▶ Model error
 - ▶ Unmodeled variables
 - ▶ No model
- ▶ Multimodel data assimilation
- ▶ Kalman-Takens filter

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- ▶ F. Hamilton, T. Berry, T. Sauer, [Kalman-Takens filtering in the presence of dynamical noise](#). To appear, Eur. Phys. J.