

# A hybrid approach for state estimation: combining moving horizon estimation and particle filtering

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# Outline

- 1 State Estimation of Linear Systems
  - Limitations
- 2 Moving Horizon Estimation (MHE)
- 3 Particle Filtering
- 4 Combining Particle Filtering and MHE
- 5 Conclusions

# The conditional density function

For the linear, time invariant model with Gaussian noise,

$$\begin{aligned}x(k + 1) &= Ax + Bu + Gw \\ y &= Cx + v\end{aligned}$$

$$w \sim N(0, Q) \quad v \sim N(0, R) \quad x(0) \sim N(\bar{x}_0, Q_0)$$

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We can compute the conditional density function exactly

$$\begin{aligned}p_{x|Y}(x|Y(k-1)) &= N(\hat{x}^-, P^-) && \text{(before } y(k)) \\ p_{x|Y}(x|Y(k)) &= N(\hat{x}, P) && \text{(after } y(k))\end{aligned}$$

# Mean and covariance before and after measurement

## Forecast

$$\begin{aligned}\hat{x}^-(k+1) &= A\hat{x} + Bu && \text{(estimate)} \\ P^-(k+1) &= APA' + GQG' && \text{(covariance)} \\ \hat{x}^-(0) &= \bar{x}_0 \quad P^-(0) = Q_0 && \text{(initial condition)}\end{aligned}$$

# Mean and covariance before and after measurement

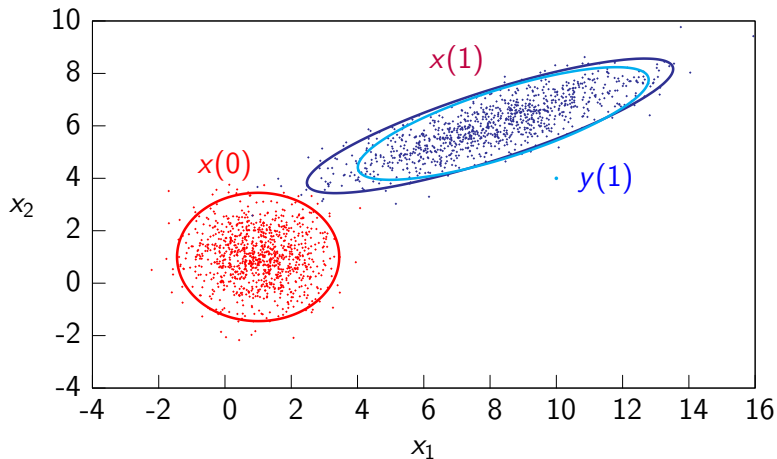
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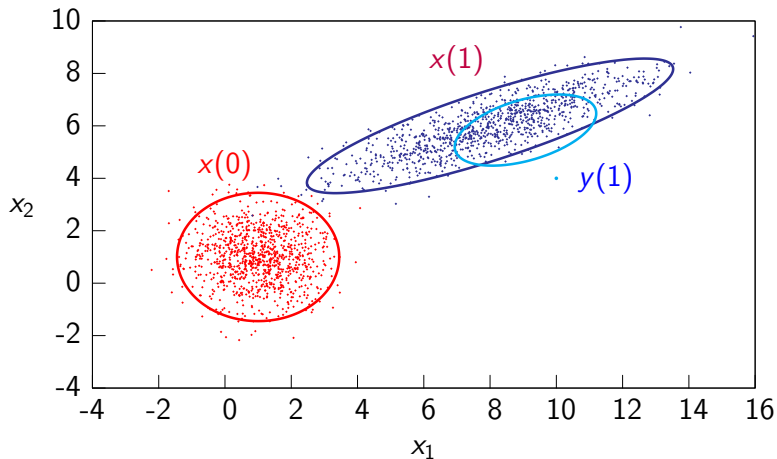
## Correction

$$\begin{aligned}\hat{x} &= \hat{x}^- + L(y - C\hat{x}^-) && \text{(estimate)} \\ L &= P^-C'(R + CP^-C')^{-1} && \text{(gain)} \\ P &= P^- - LCP^- && \text{(covariance)}\end{aligned}$$

Large  $R$ , ignore the measurement, trust the forecast

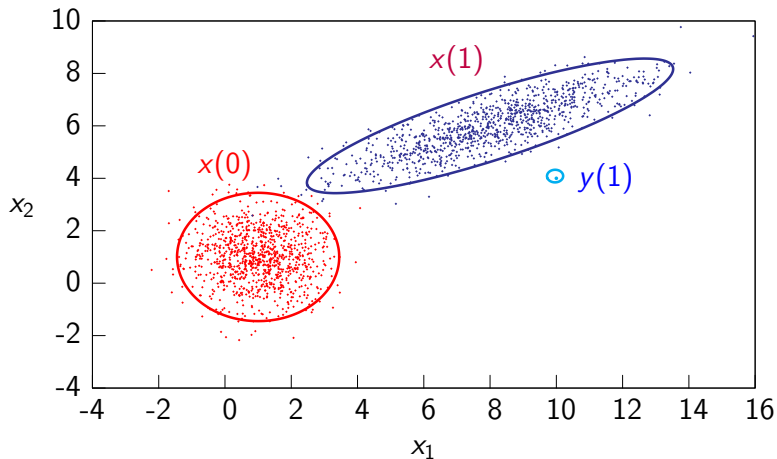


## Medium $R$ , blend the measurement and the forecast

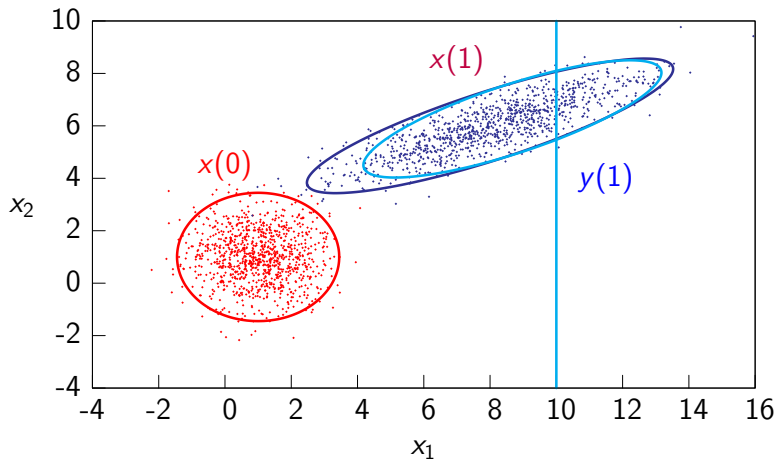




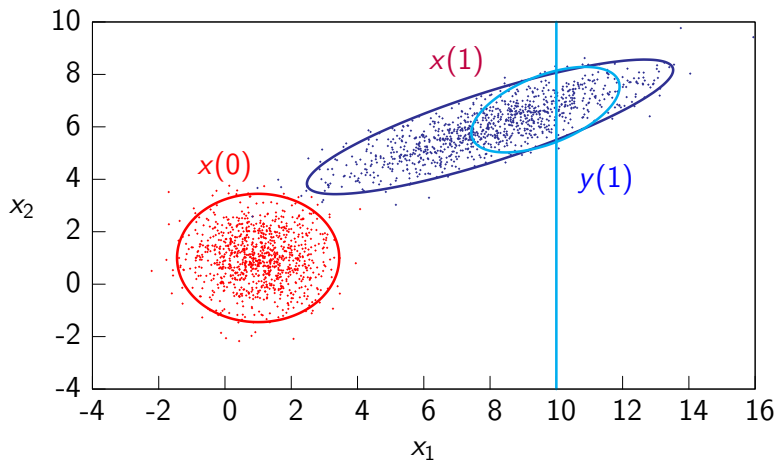
# Small $R$ , trust the measurement, override the forecast



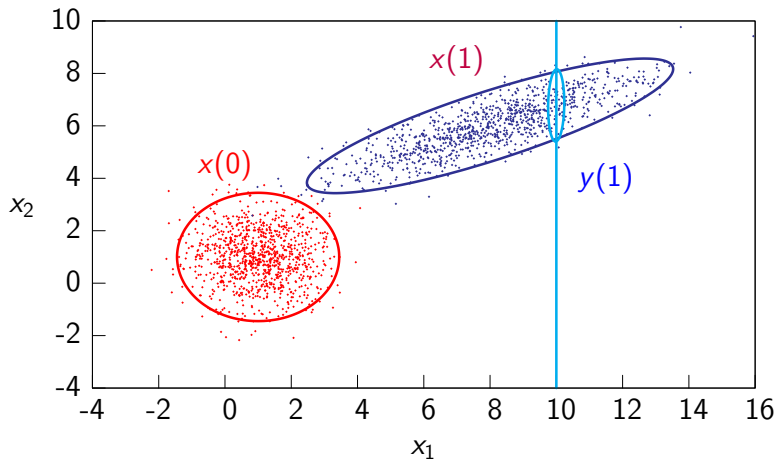
# Large $R$ , $y$ measures $x_1$ only



# Medium $R$ , $y$ measures $x_1$ only



# Small $R$ , $y$ measures $x_1$ only



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- What about nonlinear models?
  - ▶ Almost all physical models in chemical and biological applications are nonlinear differential equations or nonlinear Markov processes.
  - ▶ Linearizing the nonlinear model and using the standard update formulas (extended Kalman filter) is the standard industrial approach.



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*Many of these difficulties arise from its use of linearization.*

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## Options for handling constraints and nonlinearity in state estimation

- 1 Optimization (moving horizon estimation (MHE))
- 2 Sampling (particle filtering)

# Full information estimation

Nonlinear model, Gaussian noise,

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Maximizing the conditional density function

$$\max_{X(T)} p_{X|Y}(X(T)|Y(T))$$

# Equivalent optimization problem

Using the model and taking logarithms

$$\min_{x(T)} V_0(x_0) + \sum_{j=1}^{T-1} L_w(w_j) + \sum_{j=0}^T L_v(y_j - h(x_j))$$

subject to  $x(j+1) = F(x, u) + w$  ( $G(x, u) = l$ )

$$V_0(x) := -\log(p_{x_0}(x))$$

$$L_w(w) := -\log(p_w(w)) \quad L_v(v) := -\log(p_v(v))$$



# Arrival cost and moving horizon estimation

Most recent  $N$  states  $X(T - N : T) := \{x_{T-N} \dots x_T\}$

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Optimization problem

$$\min_{X(T-N:T)} \underbrace{V_{T-N}(x_{T-N})}_{\text{arrival cost}} + \sum_{j=T-N}^{T-1} L_w(w_j) + \sum_{j=T-N}^T L_v(y_j - h(x_j))$$

subject to  $x(j+1) = F(x, u) + w$ .

# Arrival cost approximation

The statistically correct choice for the **arrival cost** is the conditional density of  $x_{T-N} | Y(T - N - 1)$

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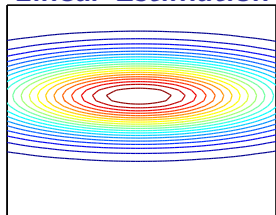
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Arrival cost approximations (Rao et al., 2003)

- uniform prior (and large  $N$ )
- EKF covariance formula
- MHE smoothing

# The challenge of nonlinear estimation

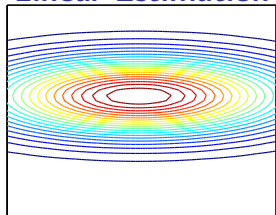
## Linear Estimation



Estimation Possibilities:

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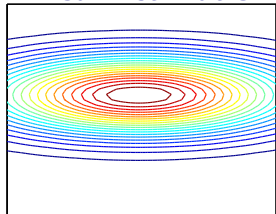


Estimation Possibilities:

- 1 *one* state is the optimal estimate
- 2 *infinitely many* states are optimal estimates (unobservable)

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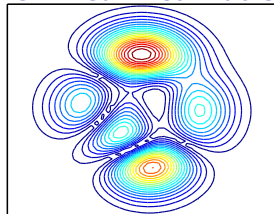
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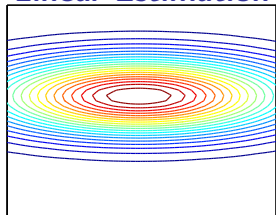


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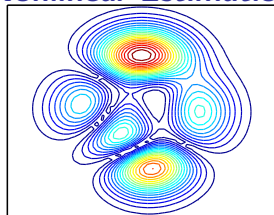
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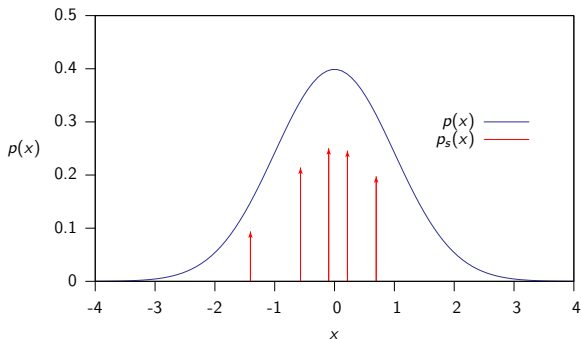
Estimation Possibilities:

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- 3 *finitely many* states are locally optimal estimates



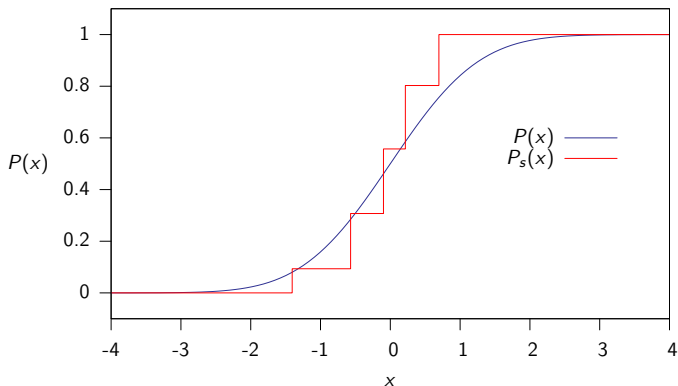
# Particle filtering — sampled densities

$$p_s(x) = \sum_{i=1}^s w_i \delta(x - x_i) \quad x_i \text{ samples (particles)} \quad w_i \text{ weights}$$



Exact density  $p(x)$  and a sampled density  $p_s(x)$  with five samples for  $\xi \sim N(0, 1)$

# Convergence — cumulative distributions



Corresponding exact  $P(x)$  and sampled  $P_s(x)$  cumulative distributions

# Importance sampling

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Both  $\bar{p}_s(x)$  and  $p_s(x)$  are *unbiased* and *converge* to  $p(x)$  as sample size increases (Smith and Gelfand, 1992).

# Importance sampled particle filter (Arulampalam et al., 2002)

$$p(x(k+1)|Y(k+1)) = \{x_i(k+1), \bar{w}_i(k+1)\}$$



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$$w_i(k+1) = w_i(k) \frac{p(y(k+1)|x_i(k+1))p(x_i(k+1)|x_i(k))}{q(x_i(k+1)|x_i(k), y(k+1))}$$

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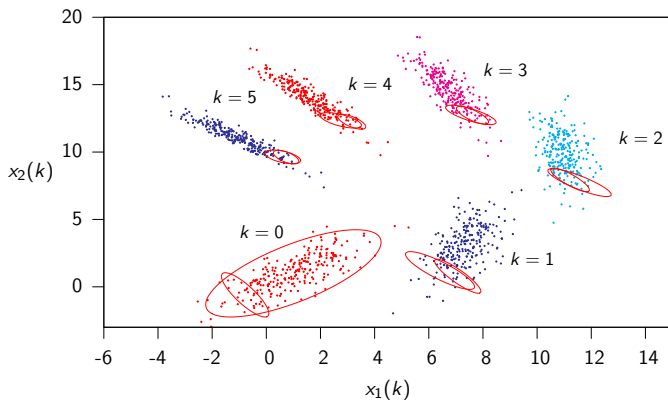
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The importance sampled particle filter *converges* to the conditional density with increasing sample size. It is *biased* for finite sample size.

# Research challenge — placing the particles

- Optimal importance function (Doucet et al., 2000). Restricted to linear measurement  $y = Cx + v$ .
- Resampling
- Curse of dimensionality

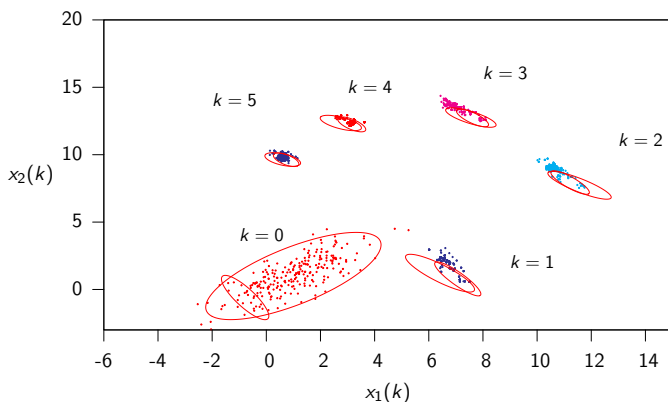
# Optimal importance function



Particles' locations versus time using the optimal importance function; 250 particles.

Ellipses show the 95% contour of the true conditional densities before and after measurement.

# Resampling



Particles' locations versus time using the optimal importance function with resampling; 250 particles.

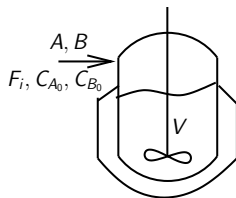
# The MHE and particle filtering hybrid approach

## Hybrid implementation

- Use the MHE optimization to locate/relocate the samples
- Use the PF to obtain fast state estimates between MHE optimizations

# Application: Semi-Batch Reactor

- Reaction:  $2A \rightarrow B$
- $k = 0.16$
- Measurement is  $C_A + C_B$
- $x_0 = [3 \quad 1]^T$



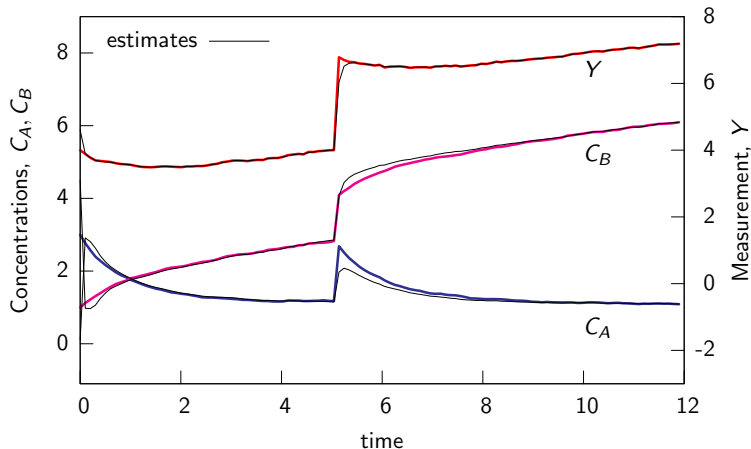
$$\begin{aligned}\frac{dC_A}{dt} &= -2kC_A^2 + \frac{F_i}{V}C_{A_0} & \Delta t &= 0.1 \\ \frac{dC_B}{dt} &= kC_A^2 + \frac{F_i}{V}C_{B_0}\end{aligned}$$

- Noise covariances  $Q_w = \text{diag}(0.01^2, 0.01^2)$  and  $R_v = 0.01^2$
- **Bad Prior:**  $\bar{x}_0 = [0.1 \quad 4.5]^T$  with a large  $P_0$
- **Unmodelled Disturbance:**  $C_{A_0}, C_{B_0}$  is pulsed at  $t_k = 5$



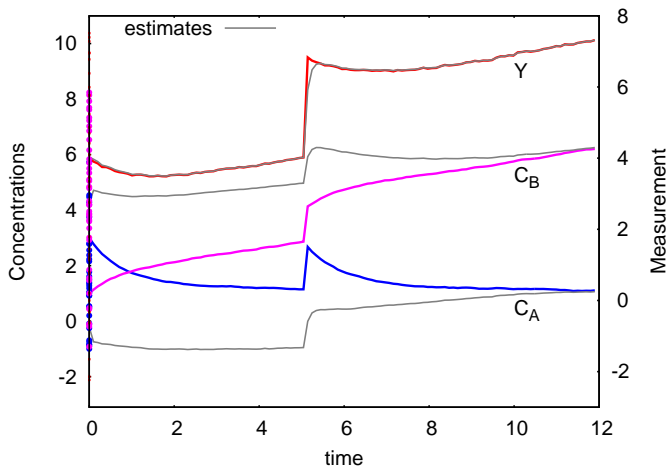
# Using only MHE

- MHE implemented with  $N = 15$  ( $t = 1.5$ ) and a smoothed prior
- MHE recovers robustly from bad priors and unmodelled disturbances



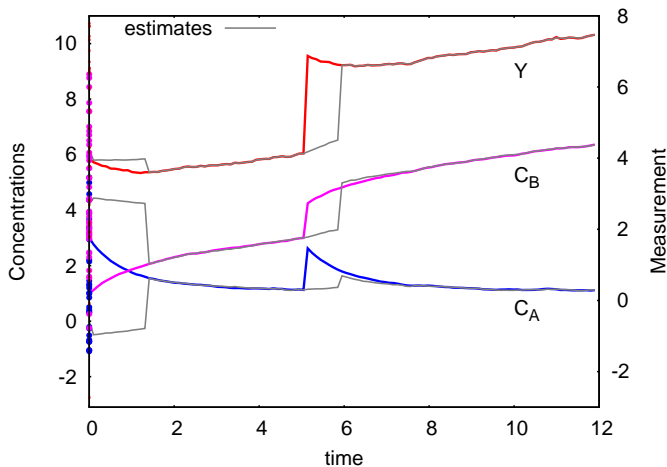
# Using only particle filter

- Particle filter implemented with the Optimal importance function:  $p(x_k|x_{k-1}, y_k)$ , 50 samples, Resampling
- The PF samples never recover from a bad  $\bar{x}_0$  and is unreliable



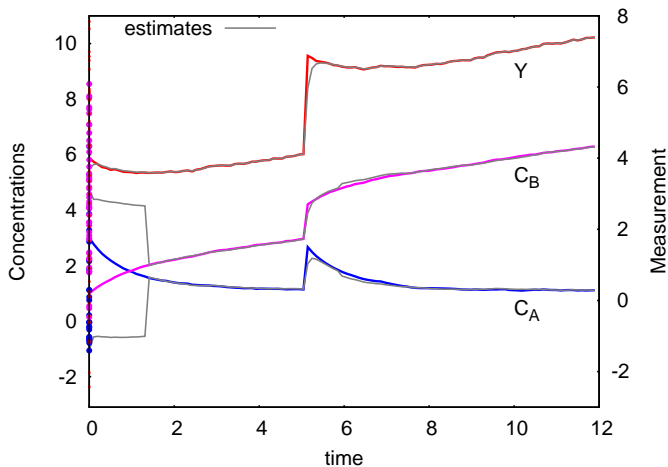
# MHE/PF hybrid with a simple importance function

- Importance function for PF:  $p(x_k|x_{k-1})$ , 50 samples
- The PF samples recover from a bad  $\bar{x}_0$  and the unmodelled disturbance only after the MHE relocates the samples



# MHE/PF hybrid with an optimal importance function

- The optimal importance function:  $p(x_k|x_{k-1}, y_k)$ , 50 samples
- MHE relocates the samples after a bad  $\bar{x}_0$ , but samples recover from the unmodelled disturbance without needing the MHE



# Conclusions

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- Hybrid MHE/PF methods can combine these complementary strengths.

# Future challenges

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- Nonlinear systems produce multi-modal densities. We need better solutions for handling these multi-modal densities in real time.

# Acknowledgments

- Professor Bhavik Bakshi of OSU for helpful discussion.
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# Further Reading I

- M. S. Arulampalam, S. Maskell, N. Gordon, and T. Clapp. A tutorial on particle filters for online nonlinear/non-Gaussian Bayesian tracking. *IEEE Trans. Signal Process.*, 50(2):174–188, February 2002.
- A. Doucet, S. Godsill, and C. Andrieu. On sequential Monte Carlo sampling methods for Bayesian filtering. *Stat. and Comput.*, 10:197–208, 2000.
- S. J. Julier and J. K. Uhlmann. Unscented filtering and nonlinear estimation. *Proc. IEEE*, 92(3):401–422, March 2004.
- C. V. Rao, J. B. Rawlings, and D. Q. Mayne. Constrained state estimation for nonlinear discrete-time systems: stability and moving horizon approximations. *IEEE Trans. Auto. Cont.*, 48(2):246–258, February 2003.
- A. F. M. Smith and A. E. Gelfand. Bayesian statistics without tears: A sampling-resampling perspective. *Amer. Statist.*, 46(2):84–88, 1992.