2019

Filters for dynamic models

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Outline

1. Objective & main principles
2. Model specification
3. Filter and smoother using Gaussian dynamic linear models
4. Filter and smoother using non-linear models
5. Conclusion

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1. Objective & main principles
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1. Objective & main principles

Data assimilation aims at improving model performance by assimilating data into the model

Two approaches

- Parameter estimation
  - Data are used for estimating model parameters
  - See the courses on parameter estimation
- Filter and smoother
  - Data are used to update model state variables
  - Sequential approach (update done each time a data is available

Two approaches

- Parameter estimation
  - Data are used for estimating model parameters
  - See the courses on parameter estimation

- Filter and smoother
  - Data are used to update model state variables
  - Sequential approach (update done each time a data is available)

$$Z(t+1) = Z(t) + g[\, X(t), \theta \,]$$

State variable **Input variable** **Parameters**

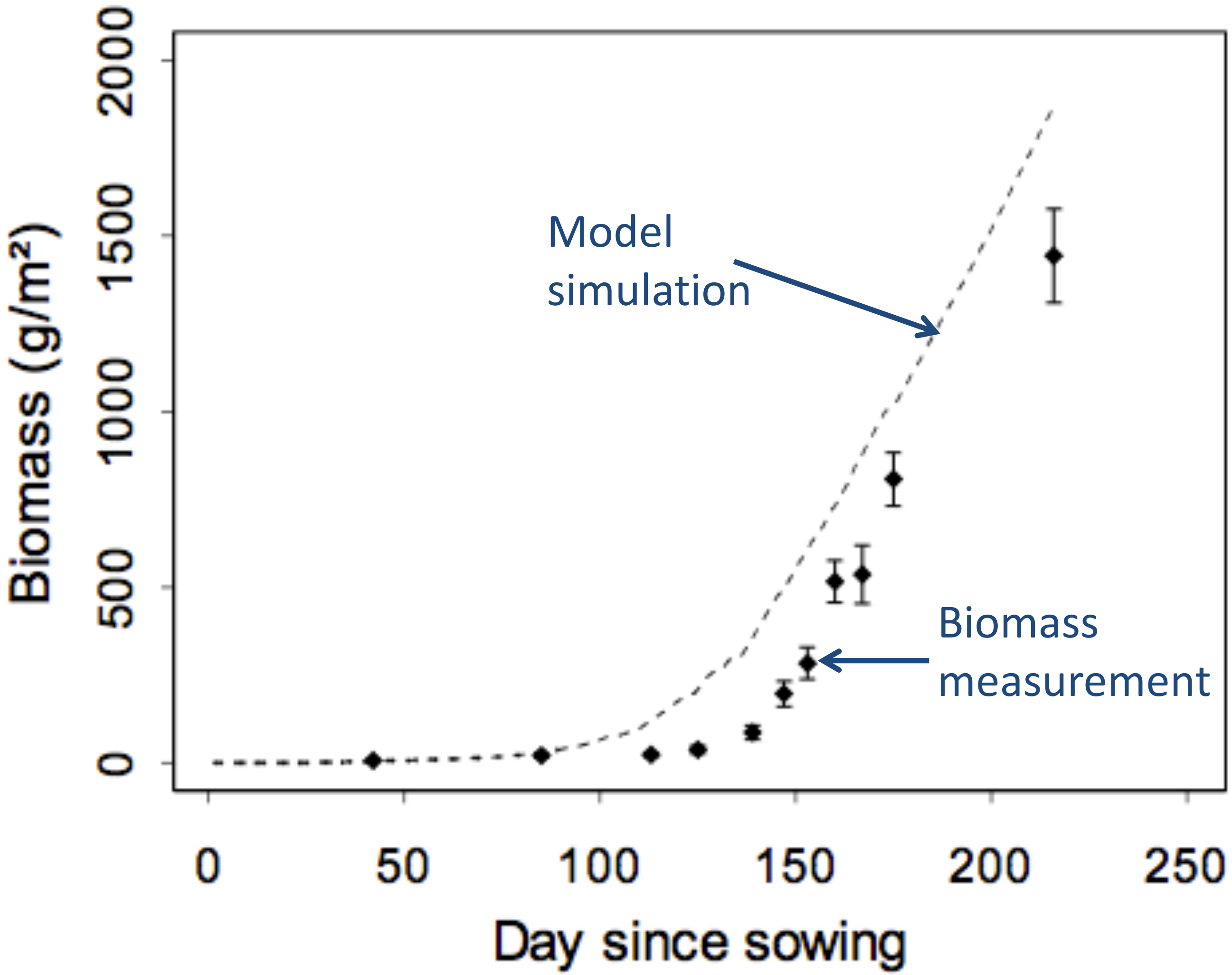
$$Z(t+1) = Z(t) + g[\,X(t), \theta\,]$$

State variable — $Z(t)$

Input variable — $X(t)$

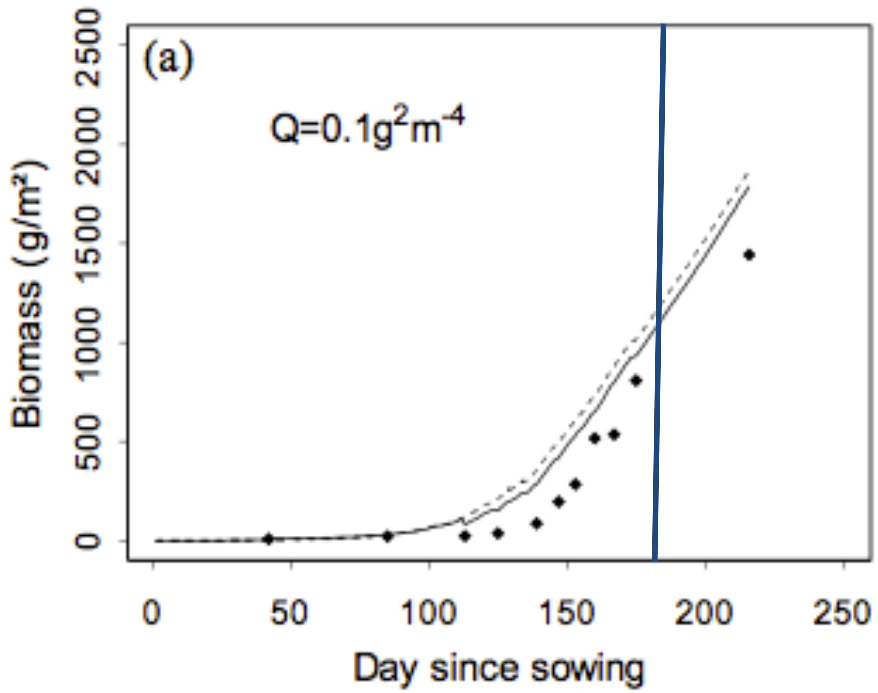
Parameters — θ

Wheat biomass simulation

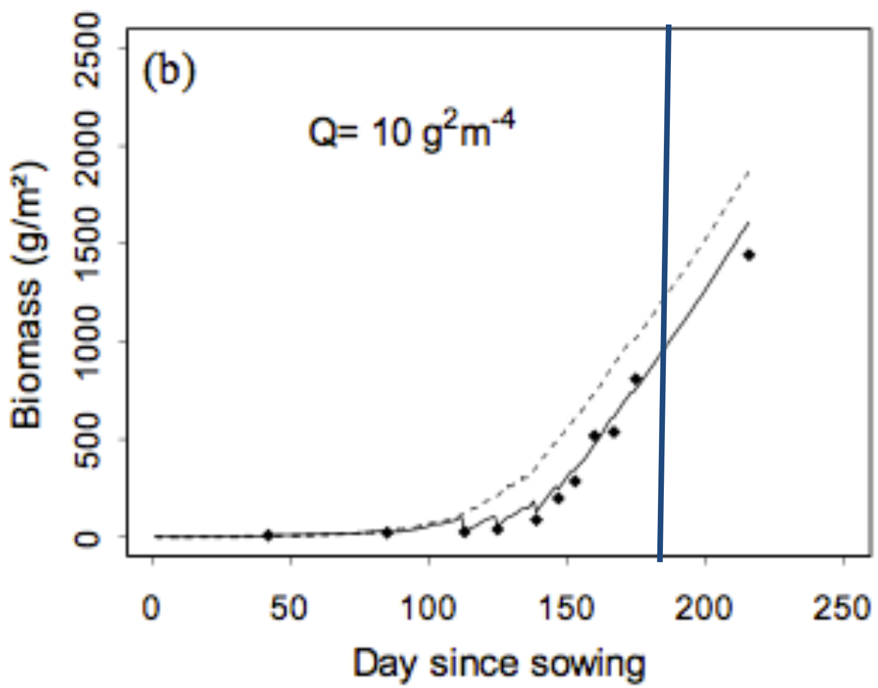


Filtering for improving wheat biomass simulation

Hypothesis 1: Low level of uncertainty

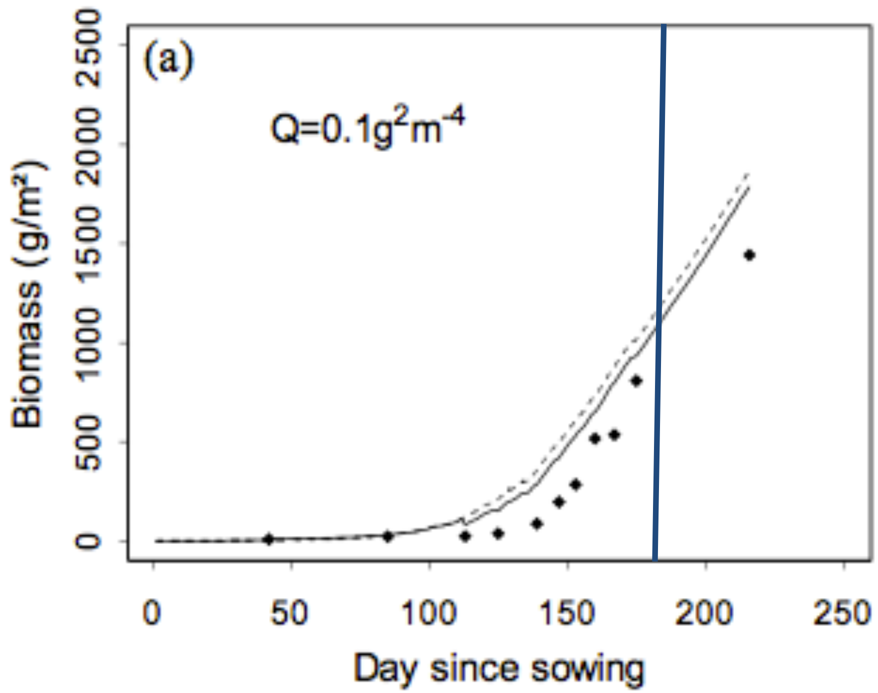


Hypothesis 2: High level of uncertainty



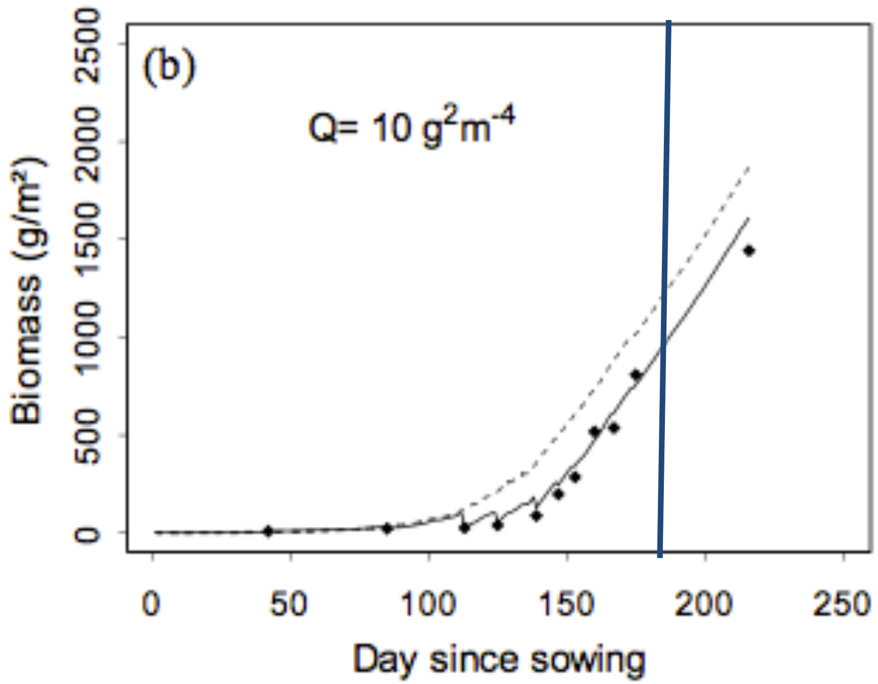
Filtering for improving wheat biomass simulation

Hypothesis 1: Low level of uncertainty



Small correction of the simulated biomass

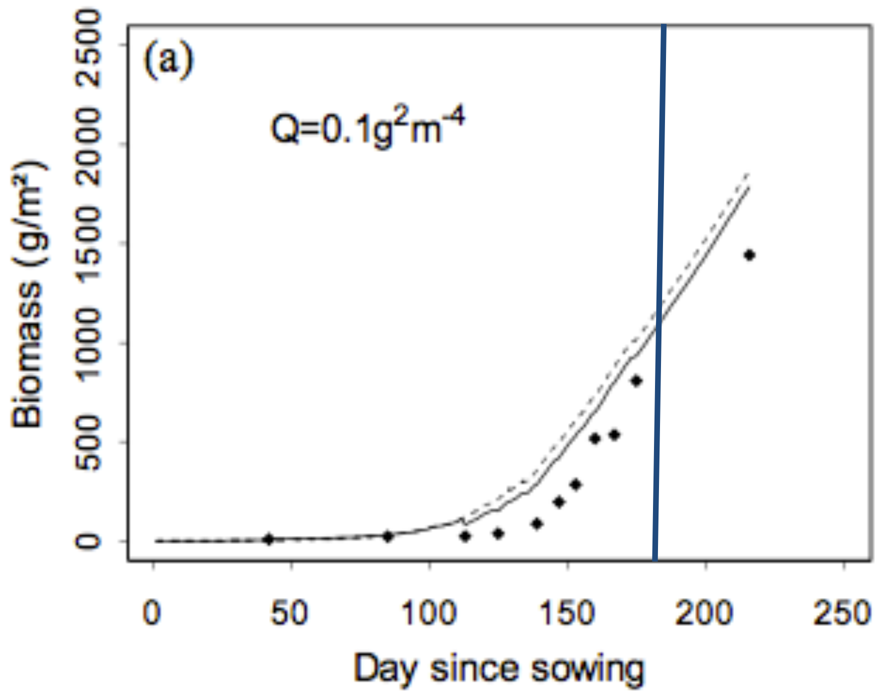
Hypothesis 2: High level of uncertainty



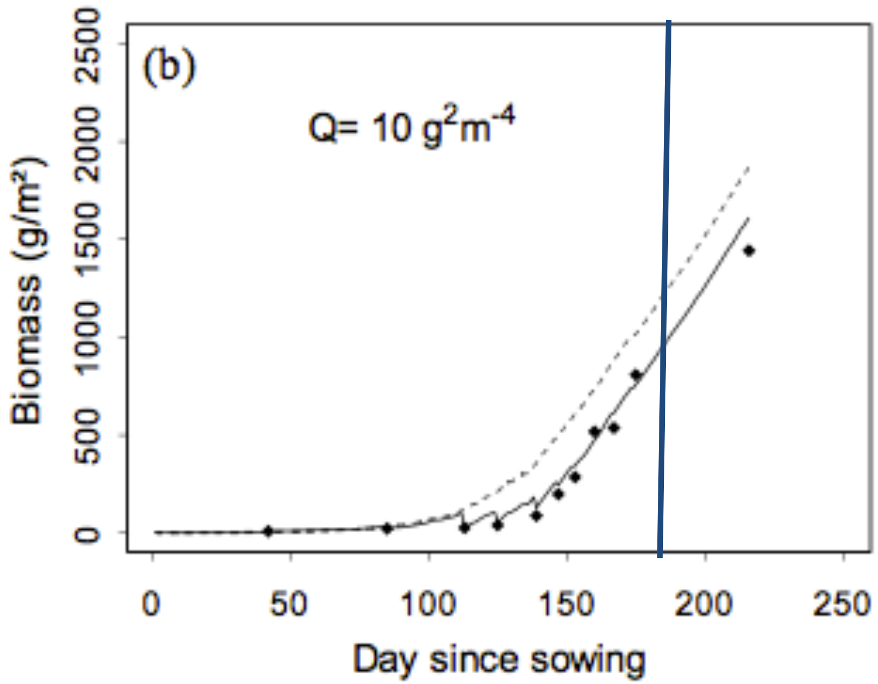
Strong correction of the simulated biomass

Filtering for improving wheat biomass simulation

Hypothesis 1: Low level of uncertainty



Hypothesis 2: High level of uncertainty



Sequential updating of the simulated wheat biomass leading to an improved prediction of final biomass

Main principles of data assimilation (1)

- Level of correction depends on
  - Error of measurements
  - Uncertainty in model predictions

- Low error of measurement

+ High model uncertainty → **Strong correction**

- High error of measurement

+ Low model uncertainty → **Small correction**

Main principles of data assimilation (2)

- Filtering: Updating state variable sequentially in time

Simulation t ⟶ Simulation t+1 ⟶ Simulation t+2 ⟶ Simulation t+3

Main principles of data assimilation (2)

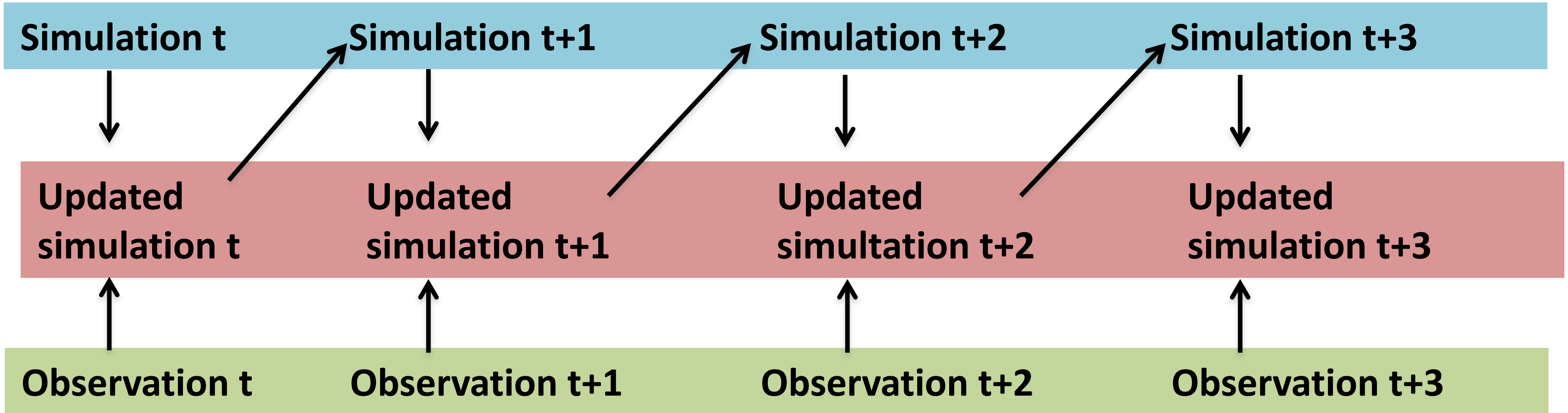
- Filtering: Updating state variable sequentially in time

Simulation t → **Simulation t+1** → **Simulation t+2** → **Simulation t+3**

Observation t **Observation t+1** **Observation t+2** **Observation t+3**

Main principles of data assimilation (2)

- Filtering: Updating state variable sequentially in time



Main principles of data assimilation (3)

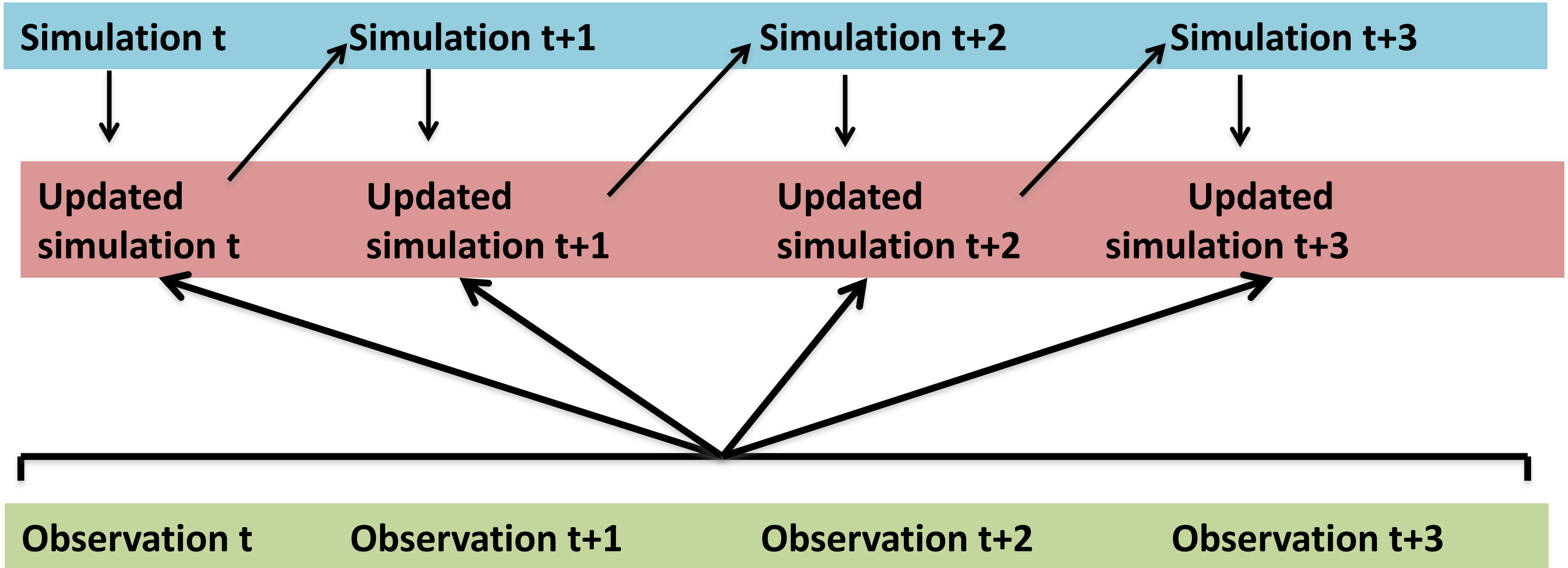
- Smoothing: Updating state variable using all observations

Simulation t → **Simulation t+1** → **Simulation t+2** → **Simulation t+3**

Observation t **Observation t+1** **Observation t+2** **Observation t+3**

Main principles of data assimilation (3)

- Smoothing: Updating state variable using all observations



Summary

- **Filter and smoother** are two tools for updating dynamic state variables

- State variables are updated sequentially in time using data

- Measurement and model errors are both taken into account

Summary

- The use of filtering and smoothing is currently limited in agriculture and environmental science
- The increase in detection and transmission capability makes this approach attractive for improving predictions of system models.
- Due to the recent development of new algorithms and of efficient tools, such as those available in R, the application of filtering and smoothing is now relatively easy.

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Model specification

Two equations

- **Observation equation**

Relates an observation collected at time t to the model state variable(s)

- **System equation**

Describes the dynamic behavior of the state variables. It relates the values of the vector of the state variables at time t to the values at time t-1

Observation equation

$$Y_t = f\left(Z_t, X_t^{(y)}, \delta, \varepsilon_t\right)$$

State variable at time t

Input variable at time t

Fixed parameters

Random term accounting for the **imperfection** of the relationship

System equation

$$Z_t = g\left(Z_{t-1}, X_t^{(z)}, \theta, \eta_{t-1}\right)$$

- Z_t: State variable at time t
- Z_{t-1}: State variable at time t-1
- $X_t^{(z)}$: Input variable at time t
- θ: Fixed parameters
- η_{t-1}: Random term describing **model error**

Model specification

- **Observation equation**

$$Y_t = f\left(Z_t, X_t^{(y)}, \delta, \varepsilon_t\right)$$

- **System equation**

$$Z_t = g\left(Z_{t-1}, X_t^{(z)}, \theta, \eta_{t-1}\right)$$

Example 1: Random walk model

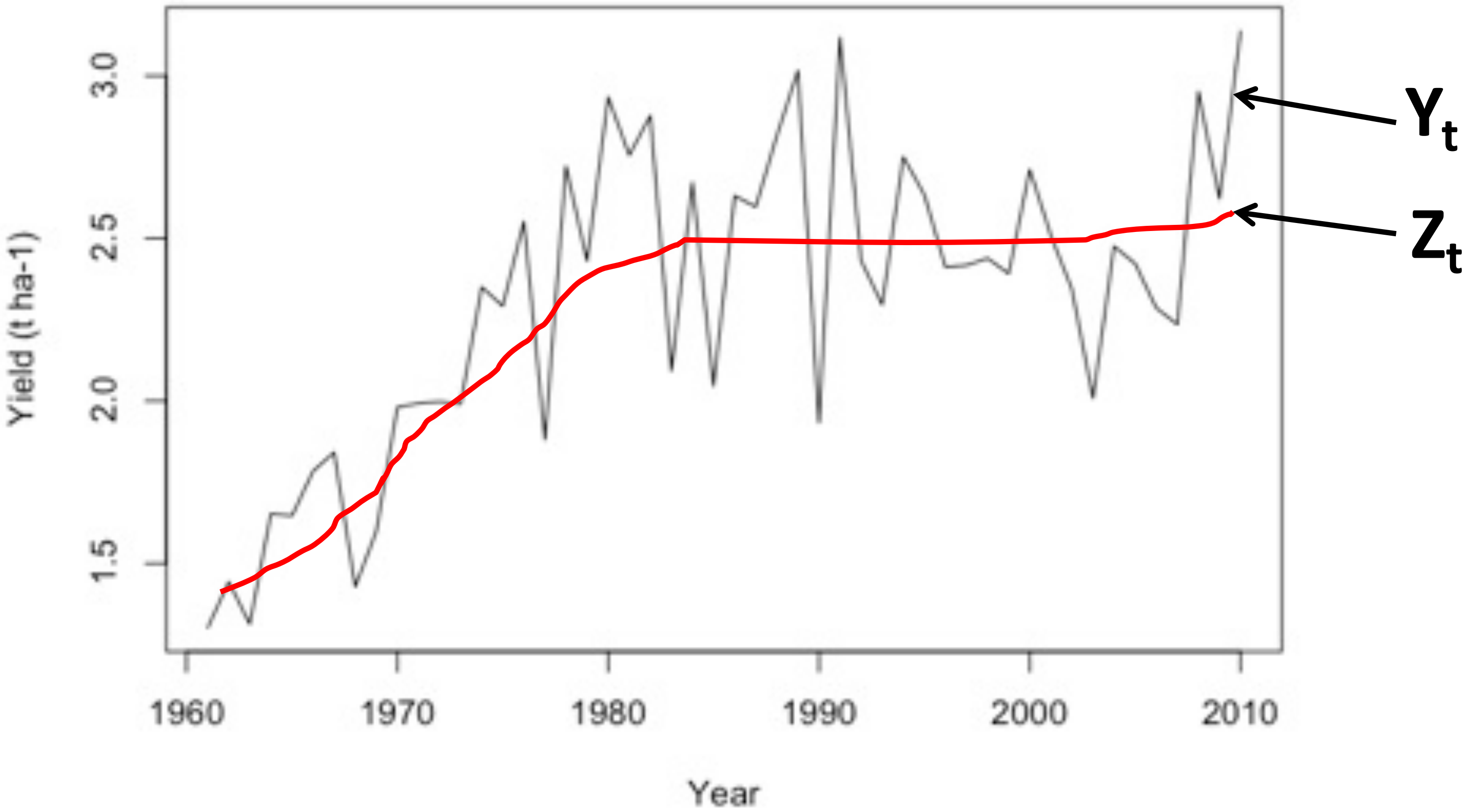
- **Observation equation**

$$Y_t = Z_t + \varepsilon_t \qquad \varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$$

- **System equation**

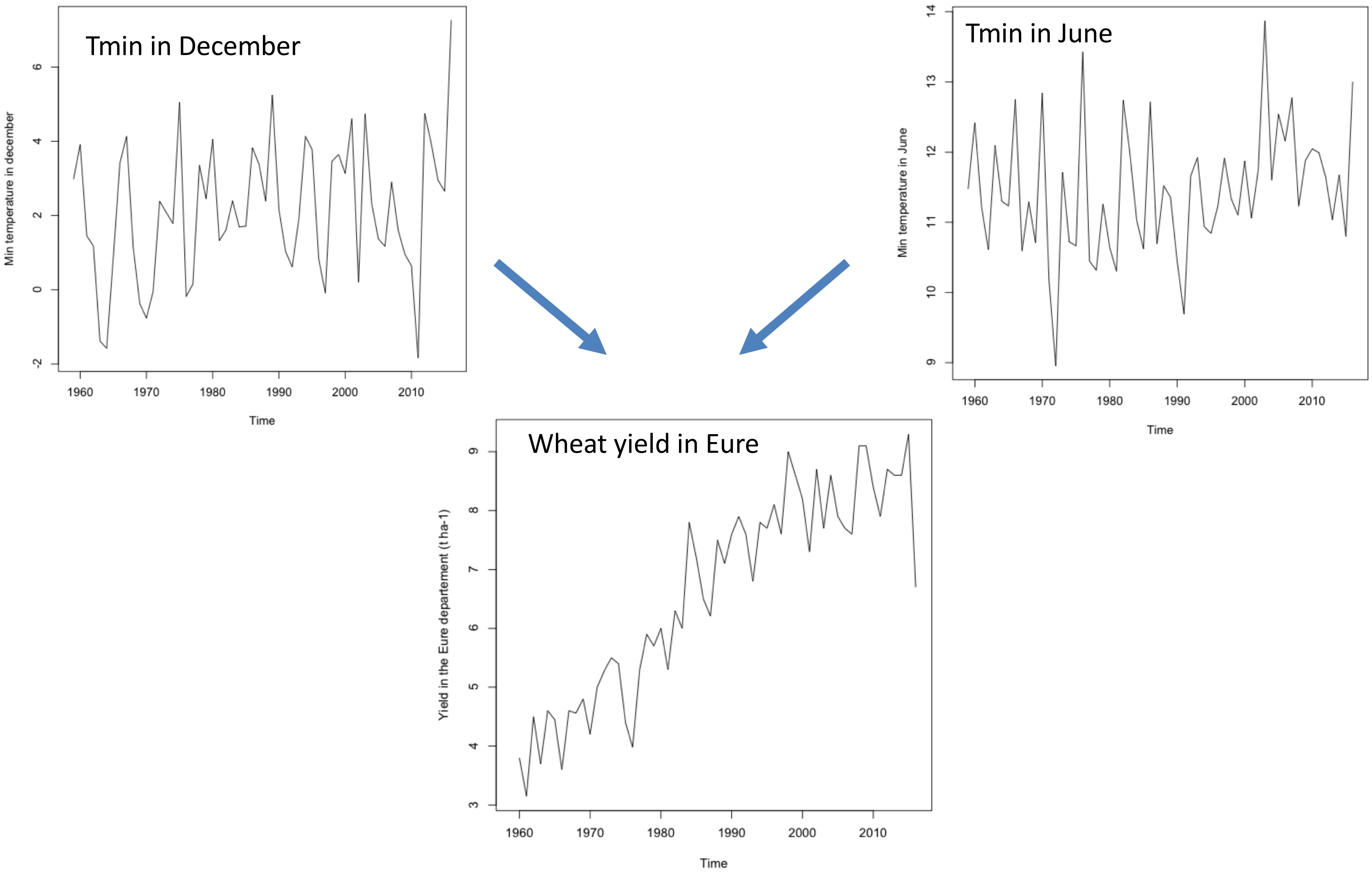
$$Z_t = Z_{t-1} + \eta_{t-1} \qquad \eta_{t-1} \sim N\left(0, \sigma_\eta^2\right)$$

Example 1: Random walk model



Wheat yield data in Greece (FAO)

Example 2: Autoregressive model with covariates



Example 3: Soil water content

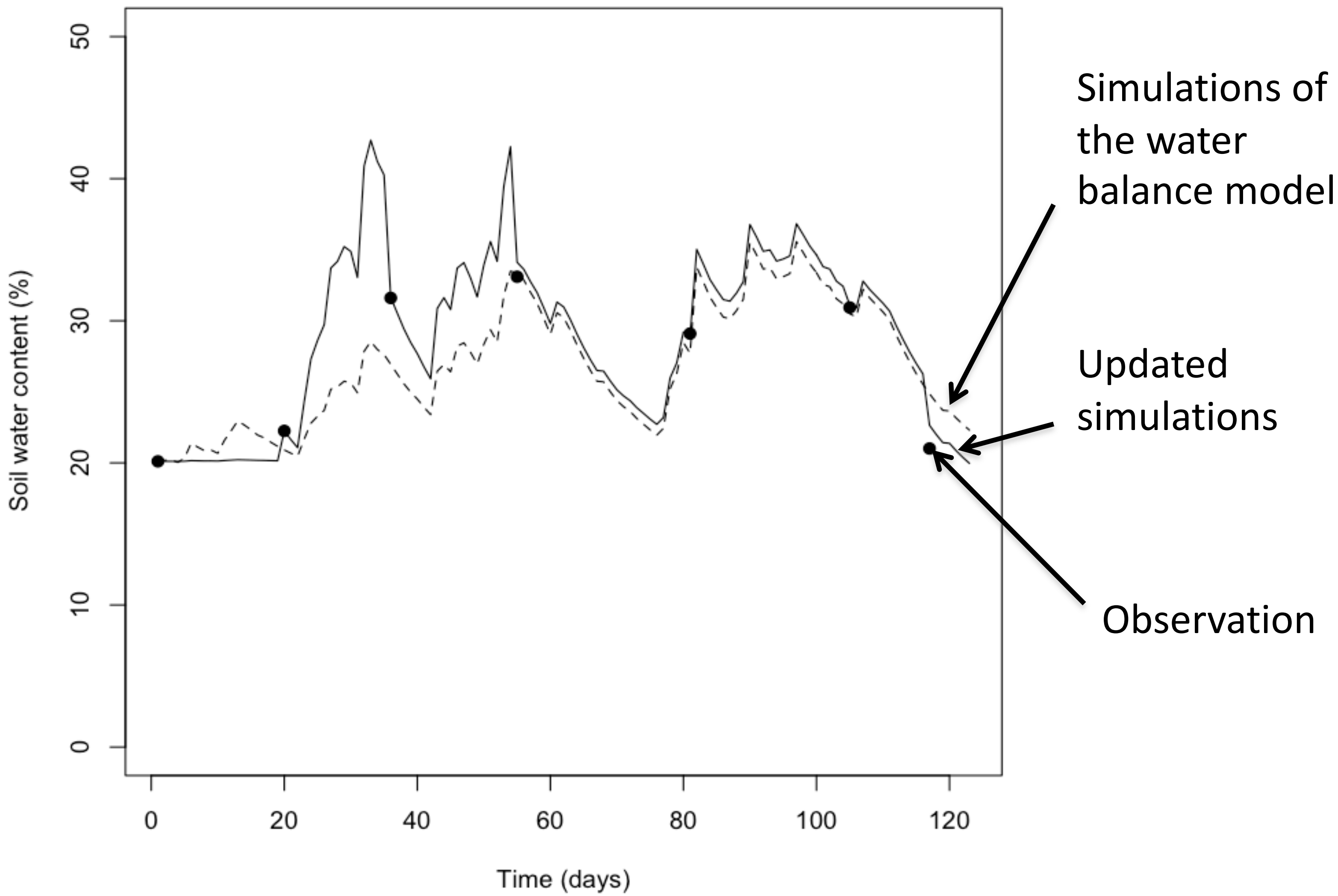
- Observation equation

The amount of water in the soil is measured several times every year.

- System equation

The water balance has a single state variable, the amount of water at the beginning of the day in a grassland.

Example 3: Soil water content



Example 4: Nonlinear population model

- This model is a dynamic model of a weed infestation of blackgrass (*A. myosuroides*) and it damage effect on wheat yield. It is based on weed model of Munier-Jolain et al. (2002) that included classical ecological concepts (survival, reproduction, fluxes between classes) often used to described population dynamic.

- The system is represented by 4 dynamic state variables: weed density at emergence (d, plants.m^{-2}), seed production (S, seeds.m^{-2}), surface seed bank after tillage (SSBa, seeds.m^{-2}), depth seed bank after tillage (DSBa, seeds.m^{-2}).

Example 4: Nonlinear population model

Four dynamic state variables

$$Z_t = \begin{pmatrix} d_t \\ SSB_t \\ DSB_t \\ S_t \end{pmatrix}$$

Example 4: Nonlinear population model

- Observation equation

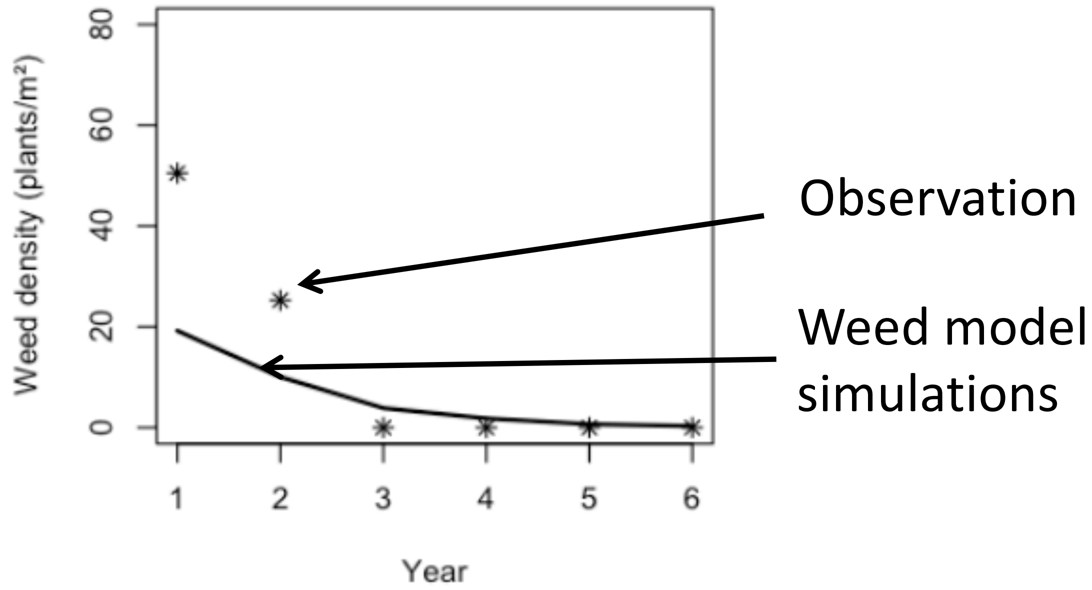
Measurements Y_t correspond to count data (number of weed plants in a plot)

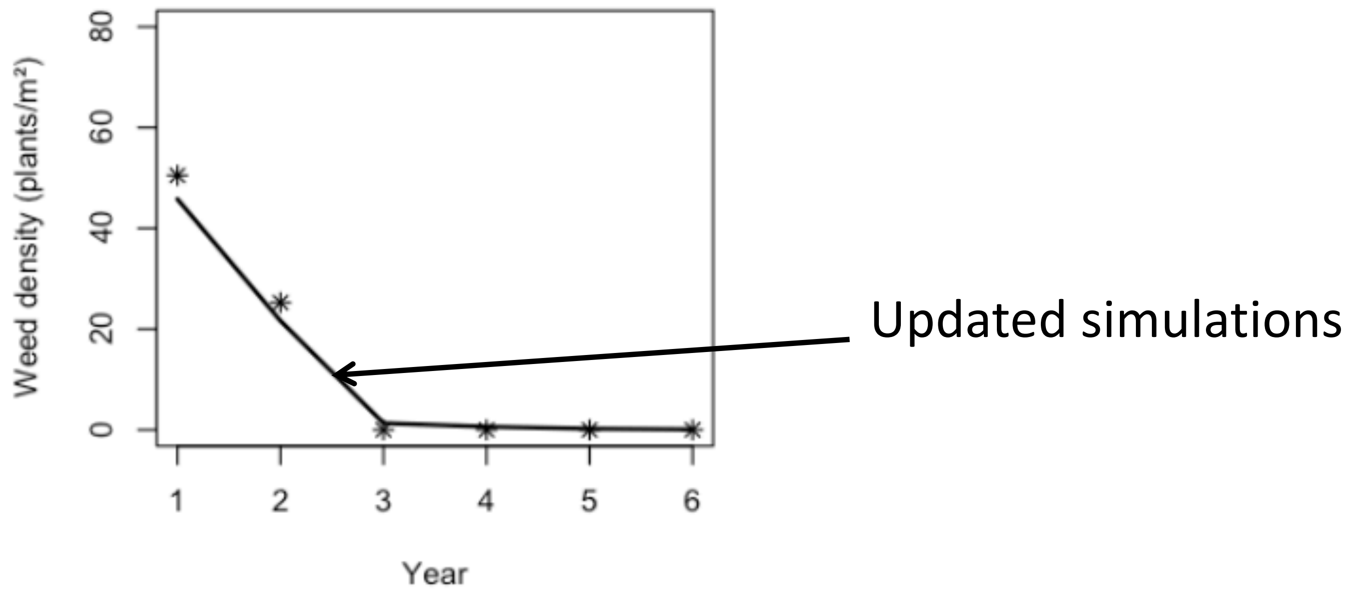
Measurements collected in a given plot were related to the weed density simulated by the model for the same plot using a Poisson probability density

- System equation

The values of the four state variables Z_t at year *t* are related to their values Z_{t-1} at year *t*-1 using a complex nonlinear function

Example 4: Nonlinear population model





Summary

- Use of two equations
  - Observation equation
  - System equation
- Very flexible
  - Data: continuous, binary, count
  - One or several state variables
- From simple to complex models
  - Linear Gaussian models
  - Nonlinear models

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Filter and smoother using Gaussian dynamic linear models

Gaussian linear model

- Observation equation

$$Y_t = f\left(Z_t, X_t^{(y)}, \delta, \varepsilon_t\right)$$

***f* is linear**

ε_t **is Gaussian**

- System equation

$$Z_t = g\left(Z_{t-1}, X_t^{(z)}, \theta, \eta_{t-1}\right)$$

***g* is linear**

η_{t-1} **is Gaussian**

Gaussian linear model

- Observation equation

$$Y_t = FZ_t + \varepsilon_t$$

F is a matrix and ε_t is a Gaussian random term. If Y_t includes N measurements and if Z_t includes m states variables, F is a (N x m) matrix, $\varepsilon_t \sim N(0,V)$, and V is a (N x N) variance-covariance matrix.

- System equation

$$Z_t = GZ_{t-1} + \eta_{t-1}$$

G is a (m x m) matrix, $\eta_t \sim N(0,W)$, and W is a (m x m) variance-covariance matrix.

Example 1: Random walk model

- Observation equation

$$Y_t = Z_t + \varepsilon_t$$

f **= identity**

$$\varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$$

- System equation

$$Z_t = Z_{t-1} + \eta_{t-1}$$

g **= identity**

$$\eta_{t-1} \sim N\left(0, \sigma_\eta^2\right)$$

Kalman filter using Gaussian linear models

- Expected value and variance **before** update at time t

$$Y_{1:t-1} = \left(Y_1, \ldots, Y_{t-1}\right)$$

$$E\left(Z_t \middle| Y_{1:t-1}\right) \qquad V\left(Z_t \middle| Y_{1:t-1}\right)$$

- Expected value and variance **after** update at time t

$$Y_{1:t} = \left(Y_1, \ldots, Y_{t-1}, Y_t\right)$$

$$E\left(Z_t \middle| Y_{1:t}\right) \qquad V\left(Z_t \middle| Y_{1:t}\right)$$

Kalman smoother using Gaussian linear models

- Expected value and variance **before** update at time t

$$Y_{1:t-1} = \left(Y_1, \ldots, Y_{t-1}\right)$$

$$E\left(Z_t \middle| Y_{1:t-1}\right) \qquad V\left(Z_t \middle| Y_{1:t-1}\right)$$

- Expected value and variance **after** update at time t

$$Y_{1:t} = \left(Y_1, \ldots, Y_{t-1}, Y_t\right)$$

$$E\left(Z_t \middle| Y_{1:t}\right) \qquad V\left(Z_t \middle| Y_{1:t}\right)$$

Example 1: Random walk model (t=1)

- Observation equation

$$Y_1 = Z_1 + \varepsilon_1 \qquad \varepsilon_1 \sim N\left(0, \sigma_\varepsilon^2\right)$$

- System equation

$$Z_1 = Z_0 + \eta_0 \qquad \eta_0 \sim N\left(0, \sigma_\eta^2\right)$$

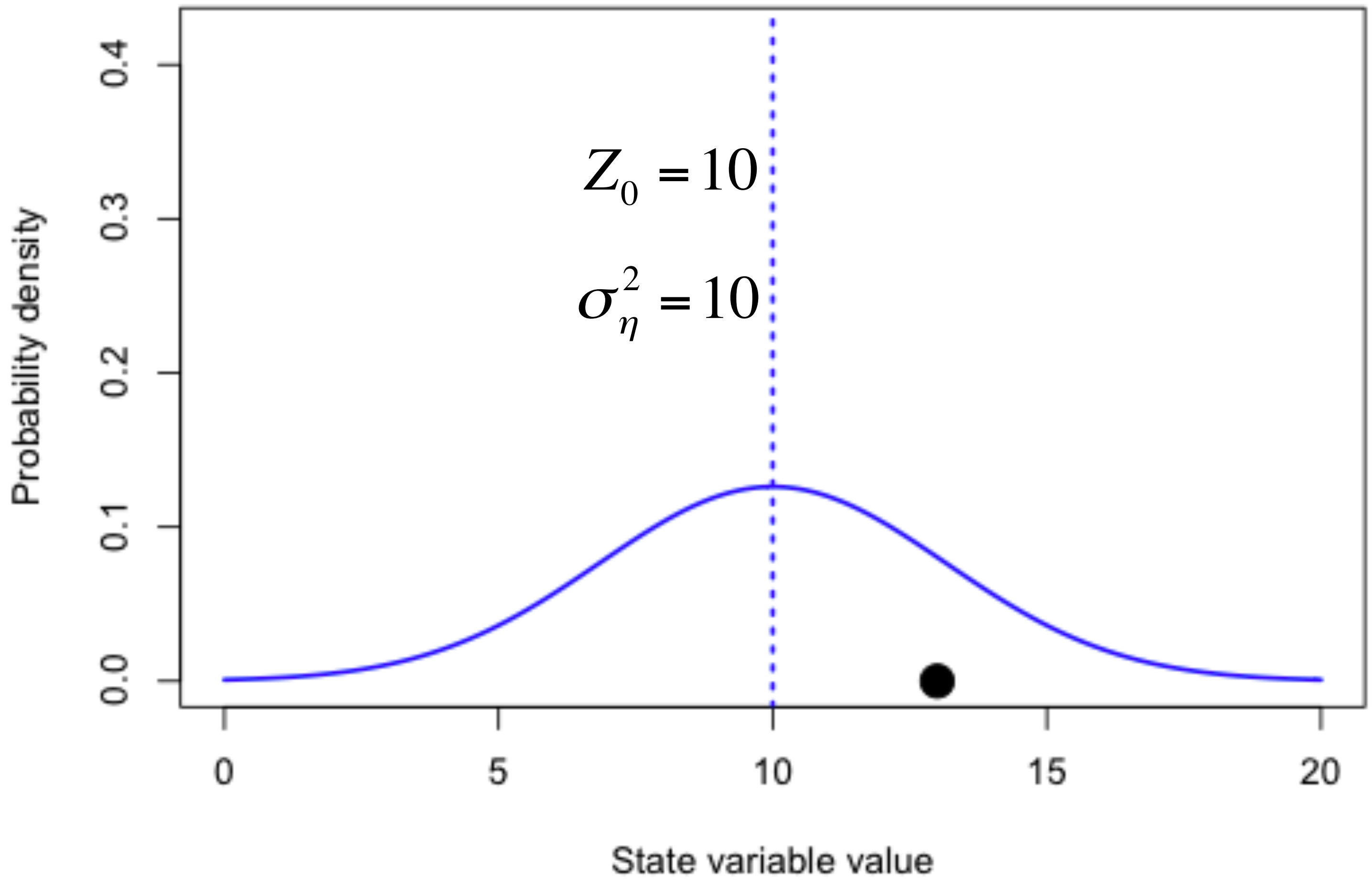
Example 1: Random walk model Kalman filter (t=1)

$$E\left(Z_1 \mid Y_1\right) = Z_0 + K\left(Y_1 - Z_0\right)$$

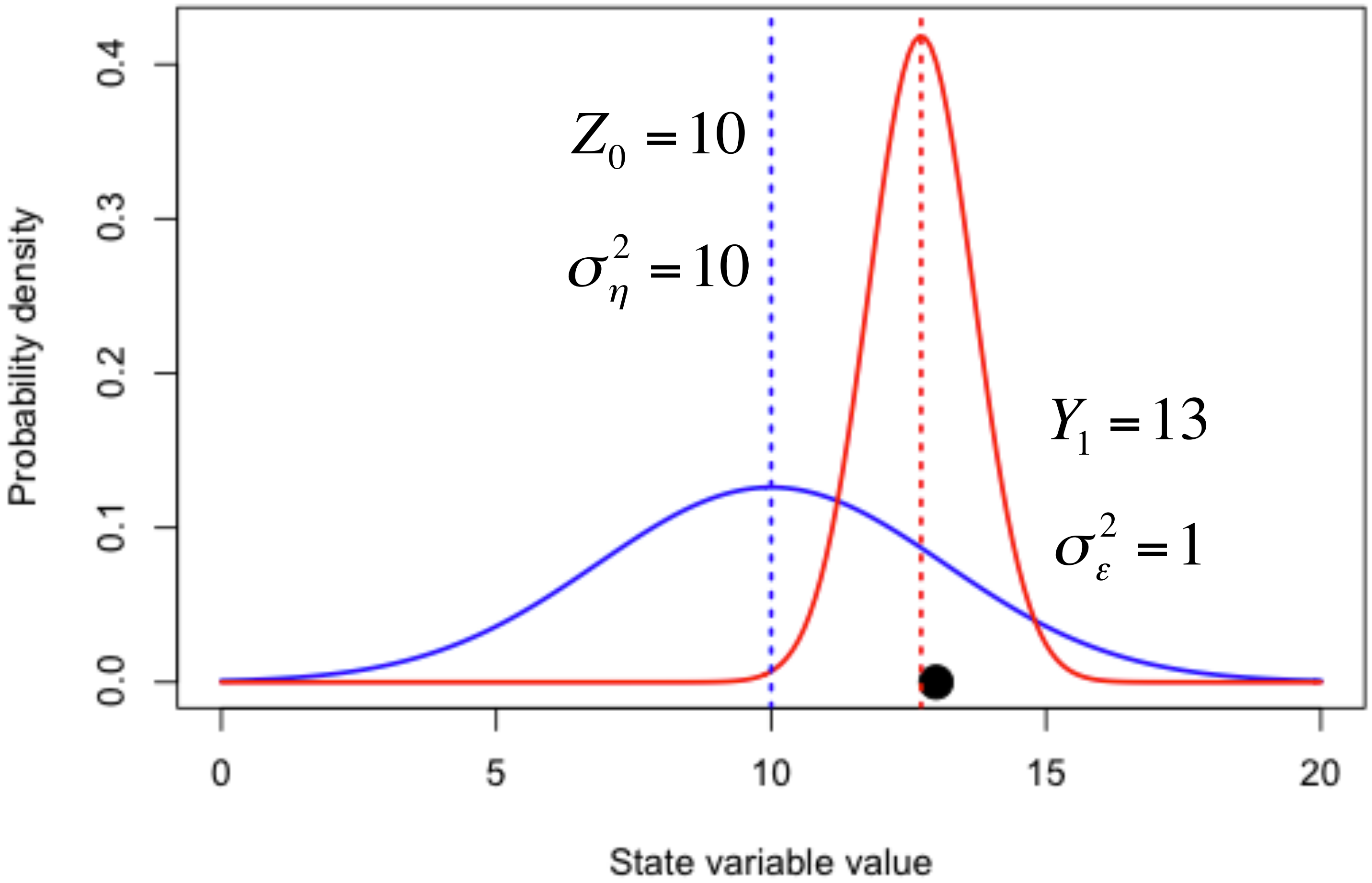
$$V\left(Z_1 \mid Y_1\right) = \left(1 - K\right)\sigma_\eta^2$$

$$K = \frac{\sigma_\eta^2}{\sigma_\eta^2 + \sigma_\varepsilon^2}$$

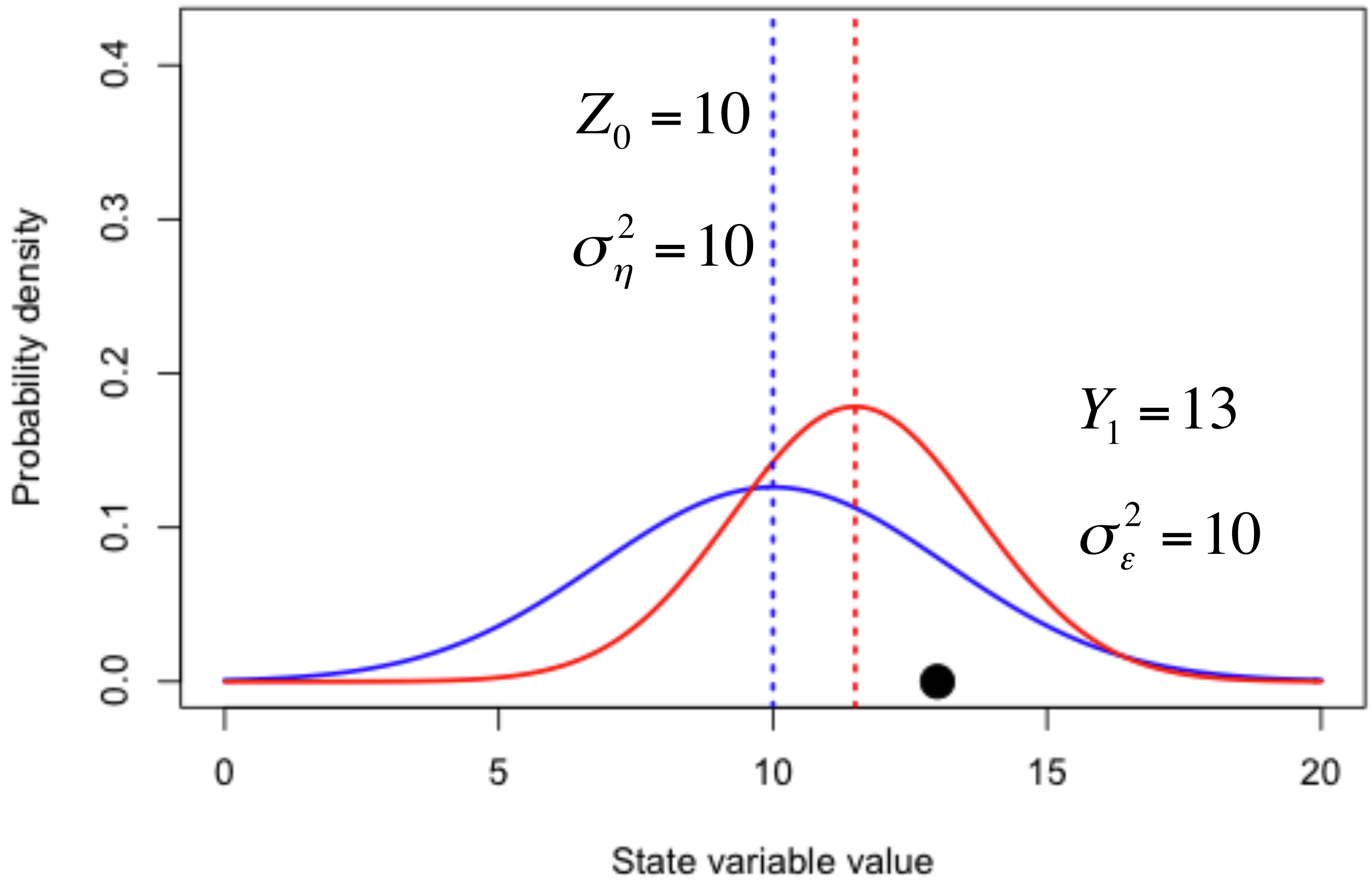
Example 1: Random walk model Kalman filter (t=1)



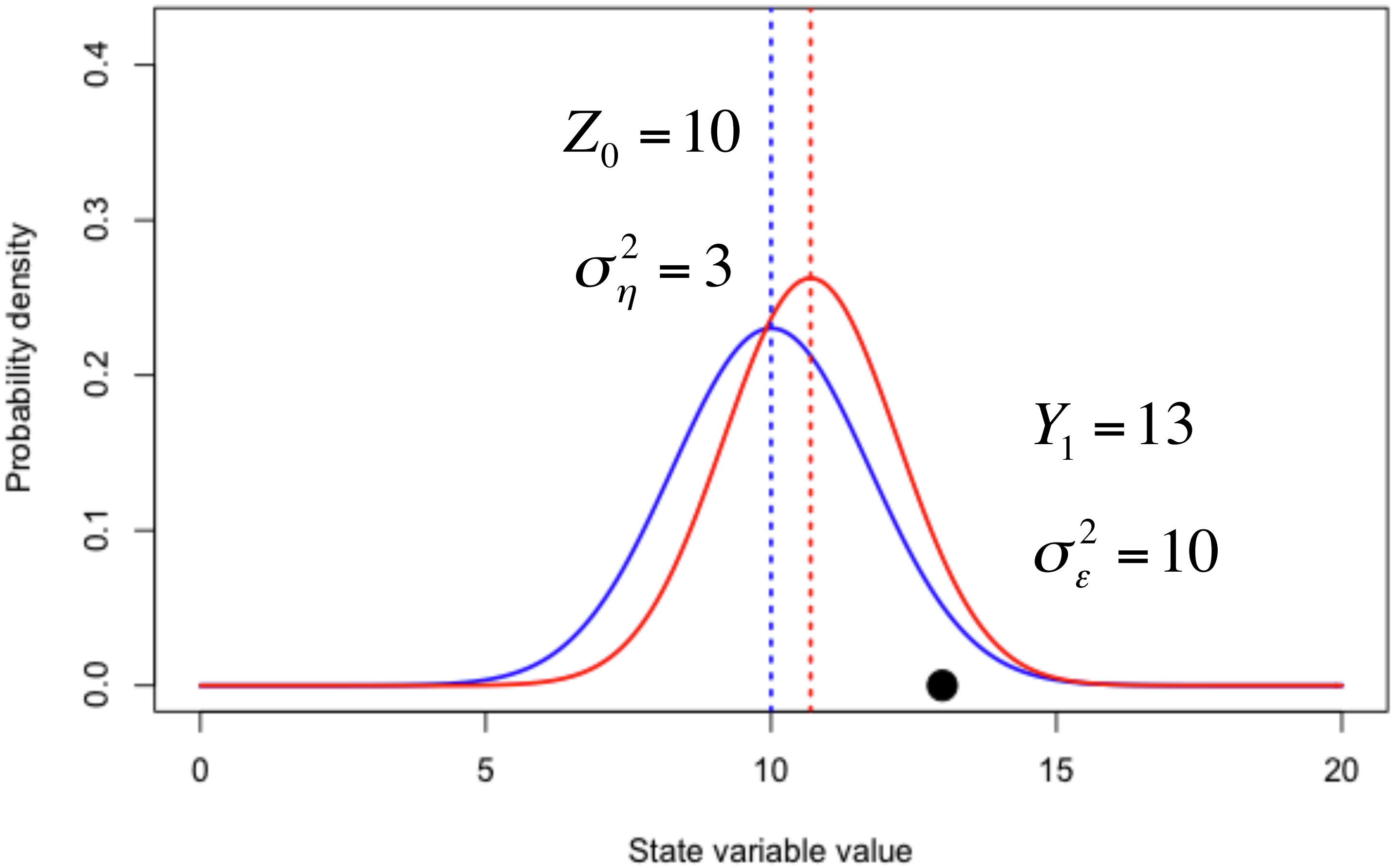
Example 1: Random walk model
Kalman filter (t=1)



Example 1: Random walk model
Kalman filter (t=1)



Example 1: Random walk model
Kalman filter (t=1)



Example 1: Random walk model (t=1, …, N)

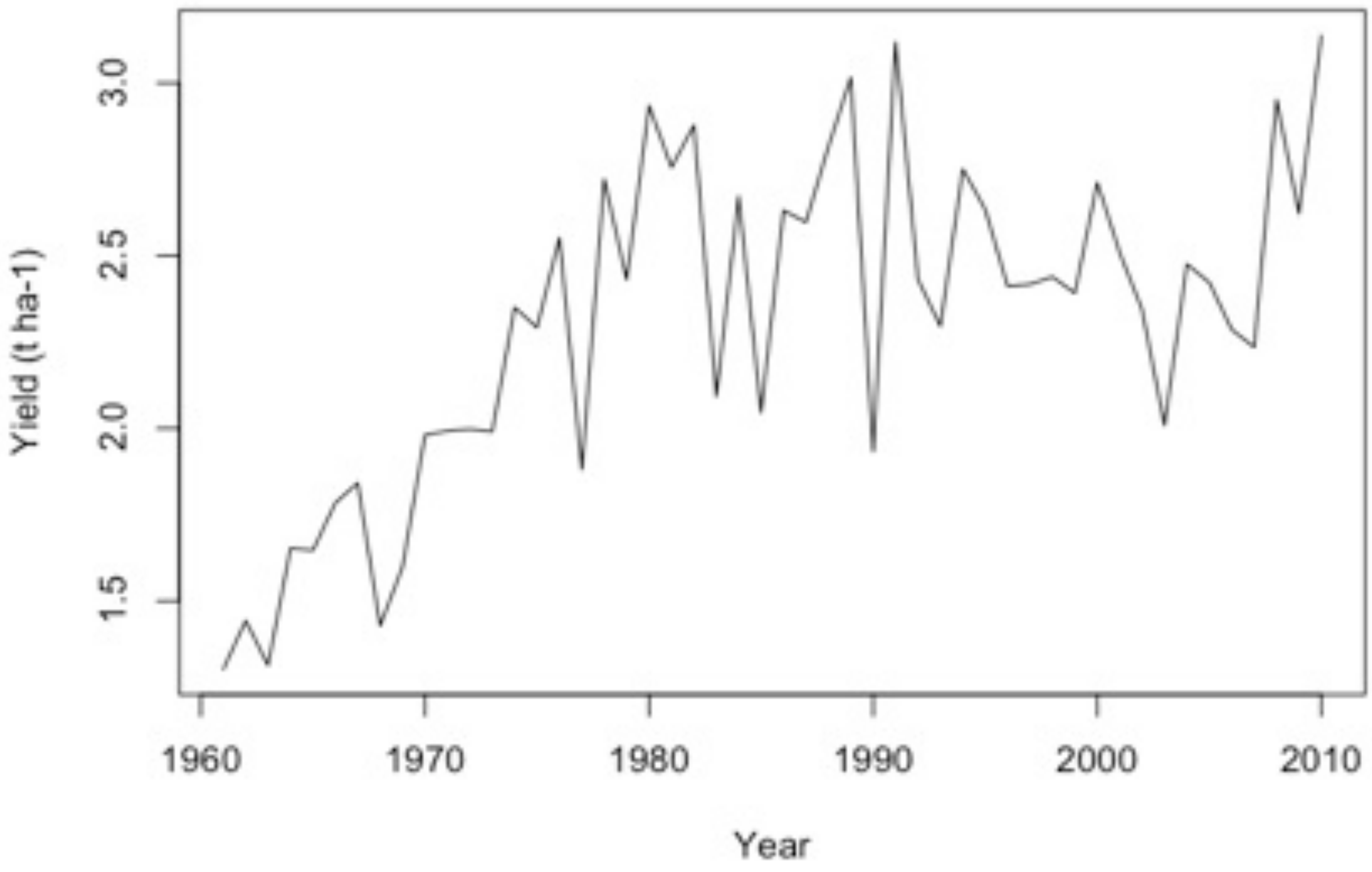
- Observation equation

$$Y_t = Z_t + \varepsilon_t \qquad \varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$$

- System equation

$$Z_t = Z_{t-1} + \eta_{t-1} \qquad \eta_{t-1} \sim N\left(0, \sigma_\eta^2\right)$$

Example 1: Random walk model (t=1, ..., N)



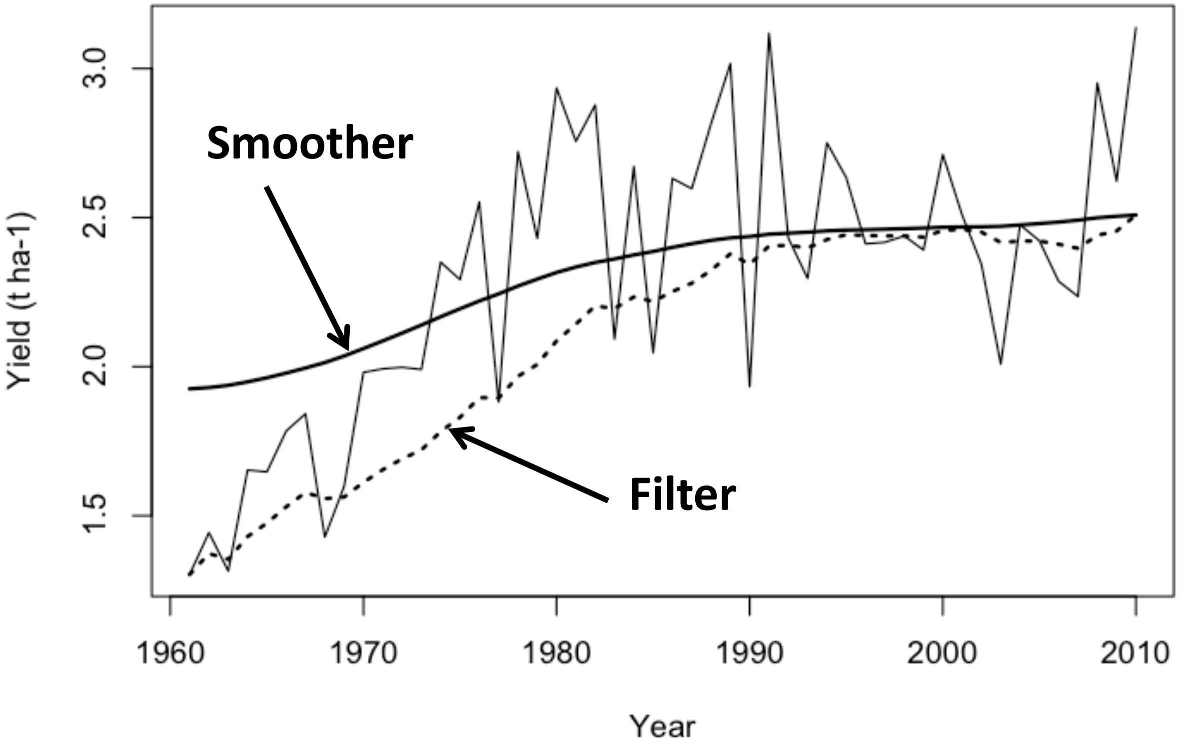
Example 1: Random walk model (t=1, …, N)

$$E\left(Z_t \mid Y_{1:t}\right) = E\left(Z_{t-1} \mid Y_{1:t-1}\right) + K\left(Y_t - E\left(Z_{t-1} \mid Y_{1:t-1}\right)\right)$$

$$V\left(Z_t \mid Y_{1:t}\right) = \left(1 - K\right)\sigma_\eta^2$$

$$K = \frac{\sigma_\eta^2}{\sigma_\eta^2 + \sigma_\varepsilon^2}$$

$$\sigma_{\eta}^{2} = 0.007 \qquad \sigma_{\varepsilon}^{2} = 1$$



Parameter estimation for Gaussian linear models

- Results of the Kalman filter depends on key parameters
  - Variance of model errors
  - Variance of the observation equation

- These parameters can be estimated from data
  - Maximum likelihood
  - Bayesian method

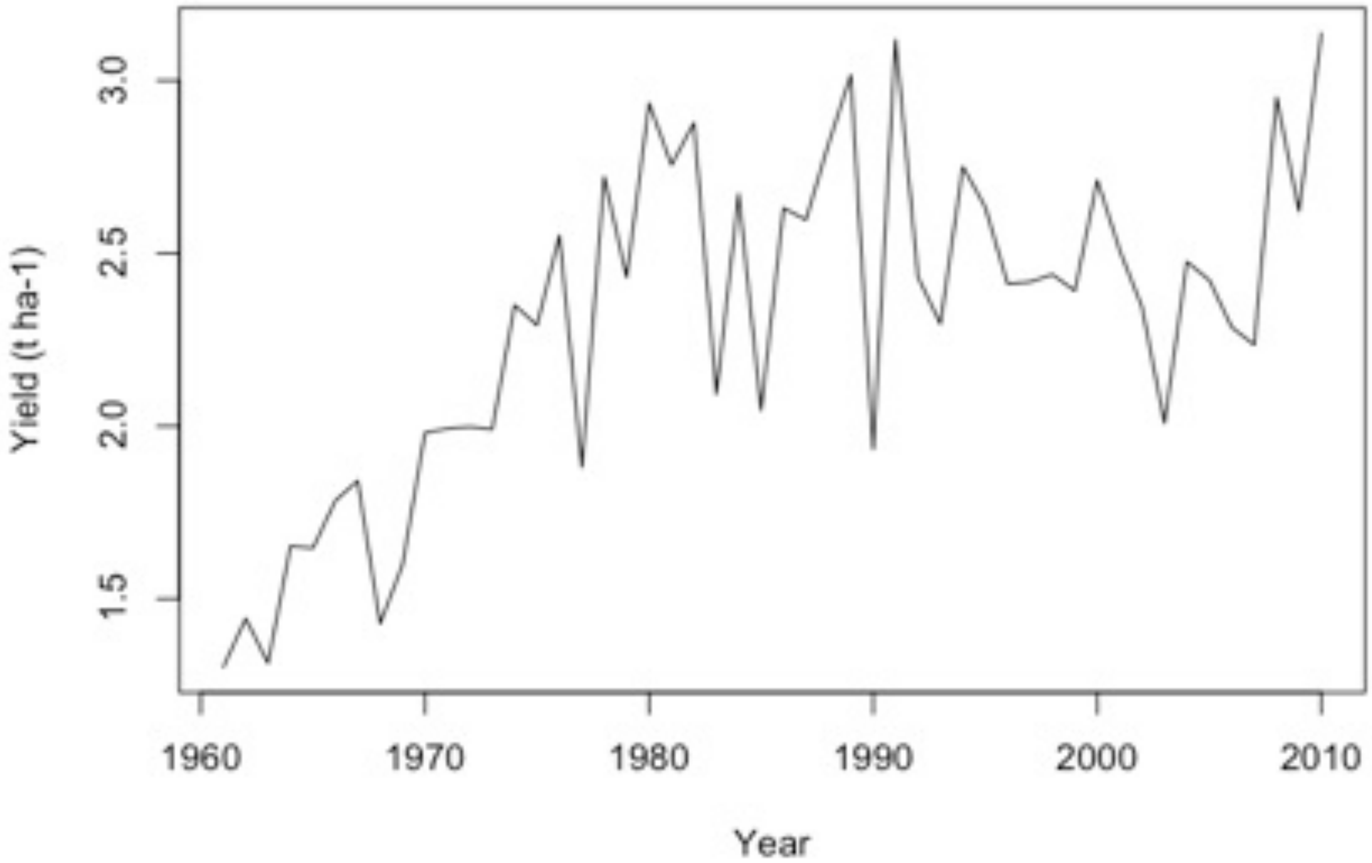
Example 1: Random walk model (t=1, …, N)

- Observation equation

$$Y_t = Z_t + \varepsilon_t \qquad \varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$$

- System equation

$$Z_t = Z_{t-1} + \eta_{t-1} \qquad \eta_{t-1} \sim N\left(0, \sigma_\eta^2\right)$$



Yield (t ha-1)
1.5
2.0
2.5
3.0
1960
1970
1980
1990
2000
2010
Year

Example 1: Random walk model (t=1, …, N)

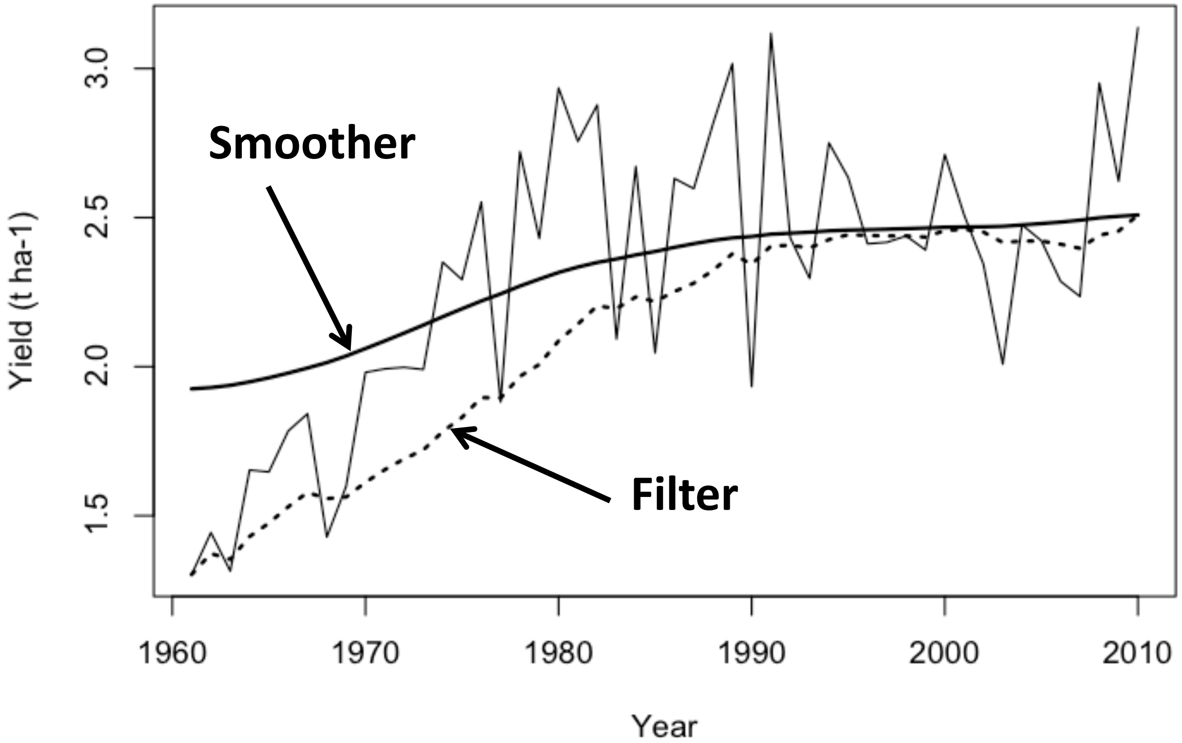
$$E\left(Z_t \mid Y_{1:t}\right) = E\left(Z_{t-1} \mid Y_{1:t-1}\right) + K\left(Y_t - E\left(Z_{t-1} \mid Y_{1:t-1}\right)\right)$$

$$V\left(Z_t \mid Y_{1:t}\right) = \left(1 - K\right)\sigma_\eta^2$$

$$K = \frac{\sigma_\eta^2}{\sigma_\eta^2 + \sigma_\varepsilon^2}$$

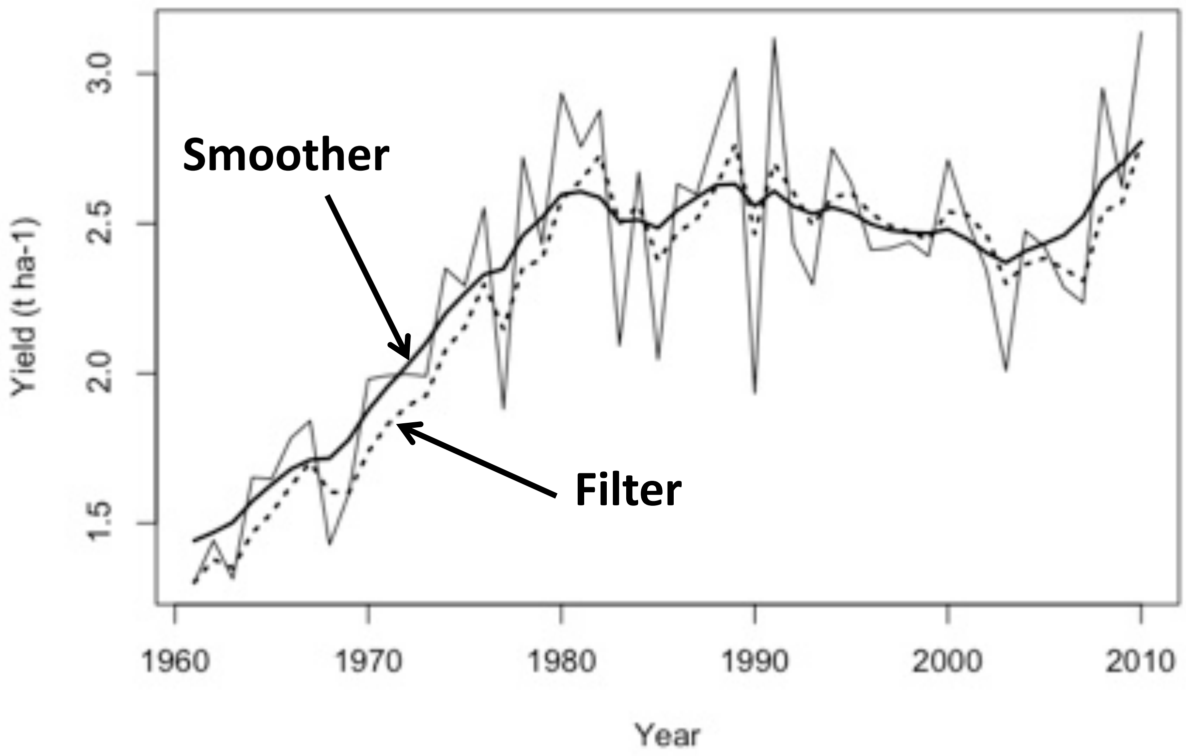
Arbitrary parameter values

$$\sigma_{\eta}^{2} = 0.007 \qquad \sigma_{\varepsilon}^{2} = 1$$

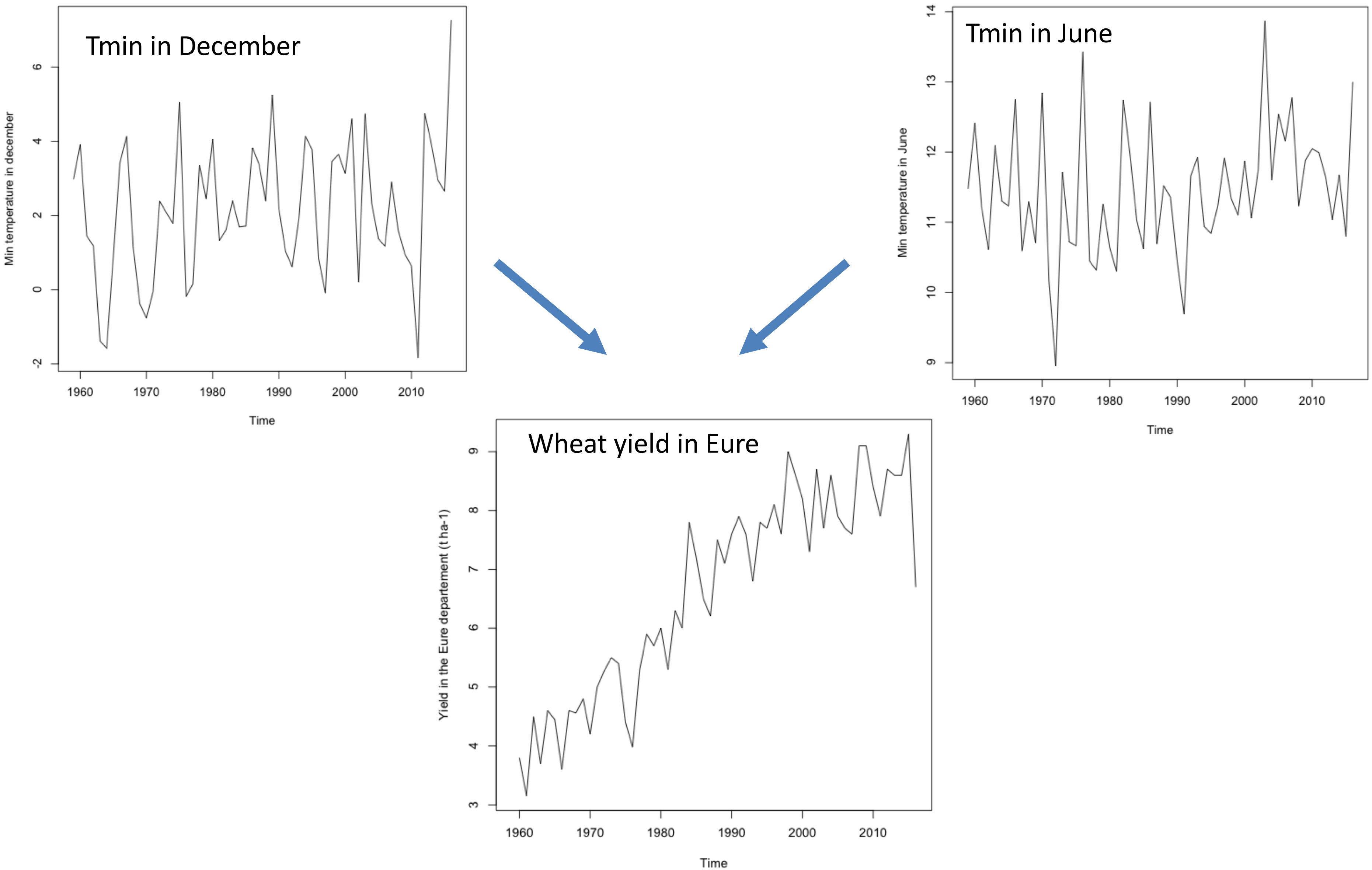


Maximum likelihood estimation

$$\sigma_{\eta}^{2} = 0.014 \qquad \sigma_{\varepsilon}^{2} = 0.07$$



Example 2: Autoregressive model with covariates



$$Y_t = Z_t + \varepsilon_t \qquad \varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$$

Model 1

$$Z_t = BZ_{t-1} + U + \eta_{t-1} \qquad \eta_{t-1} \sim N\left(0, \sigma_\eta^2\right)$$

Model 2

$$Z_t = BZ_{t-1} + C_1 X_{1,t} + C_2 X_{2,t} + U + \eta_{t-1}$$

Results obtained with the R MARSS package

```
modelY<-list(B="unconstrained")
t_Y<-MARSS(Yield,model=modelY)

X_m<-t(cbind(X_1,X_2))
model_YX<-list(B="unconstrained", C="unconstrained", c=X_m, Q=matrix(0.00579))
t_XY<-MARSS(Yield,model=model_YX)
t_XY
plot(Time, Yield, type="l", ylab="Yield in the Eure departement (t ha-1)")
lines(Time,t_XY$states, col="red")
lines(Time,t_XY$states-1.96*t_XY$states.se, col="blue", lty=2)
lines(Time,t_XY$states+1.96*t_XY$states.se, col="blue", lty=2)
```

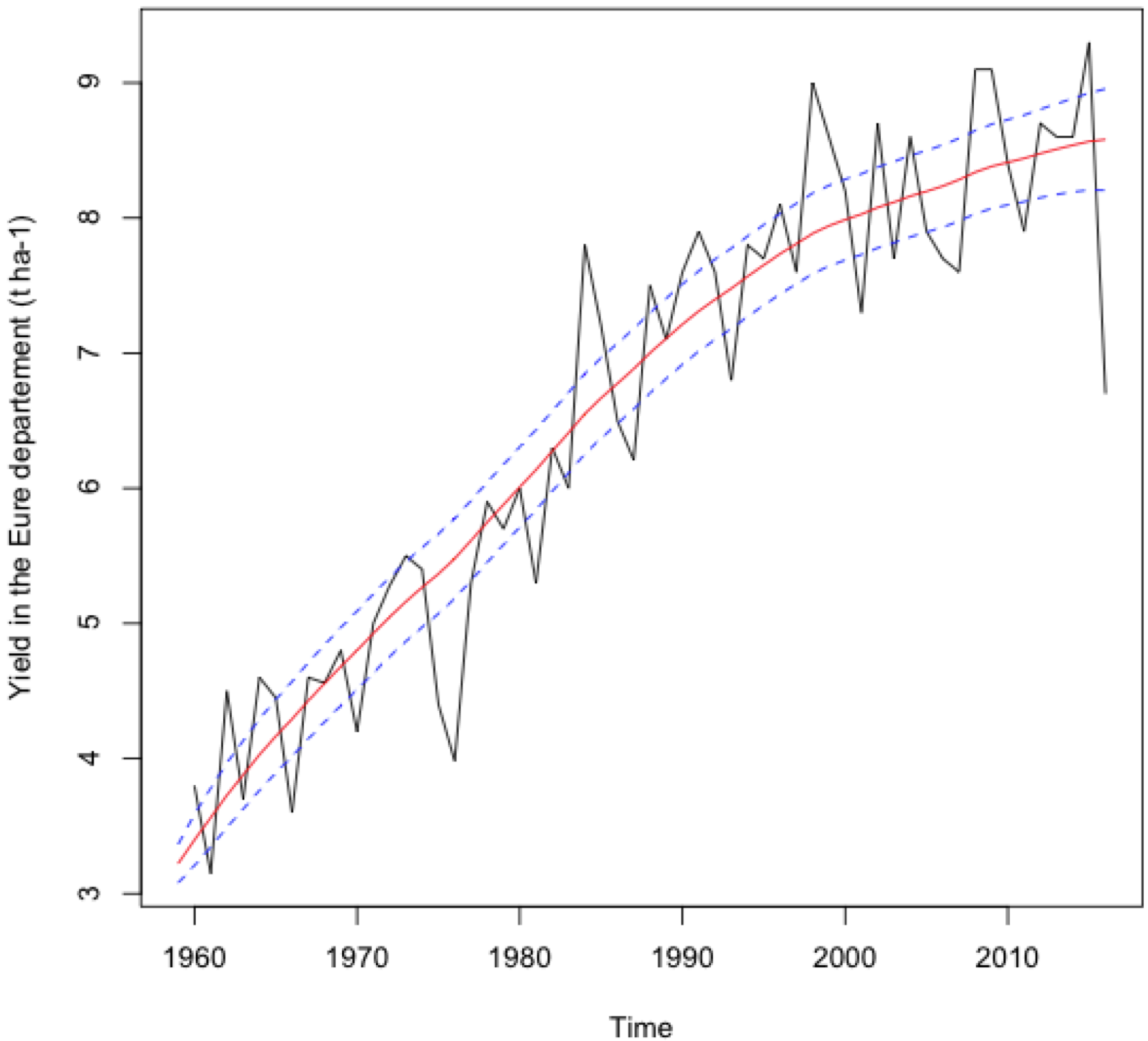
MODEL 1

```
MARSS fit is
Estimation method: kem
Convergence test: conv.test.slope.tol = 0.5, abstol = 0.001
Estimation converged in 194 iterations.
Log-likelihood: -55.35096
AIC: 120.7019   AICc: 121.8784

      Estimate
R.R    0.37139
B.B    0.97534
U.U    0.25489
Q.Q    0.00579
x0.x0  3.04248
Initial states (x0) defined at t=0

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

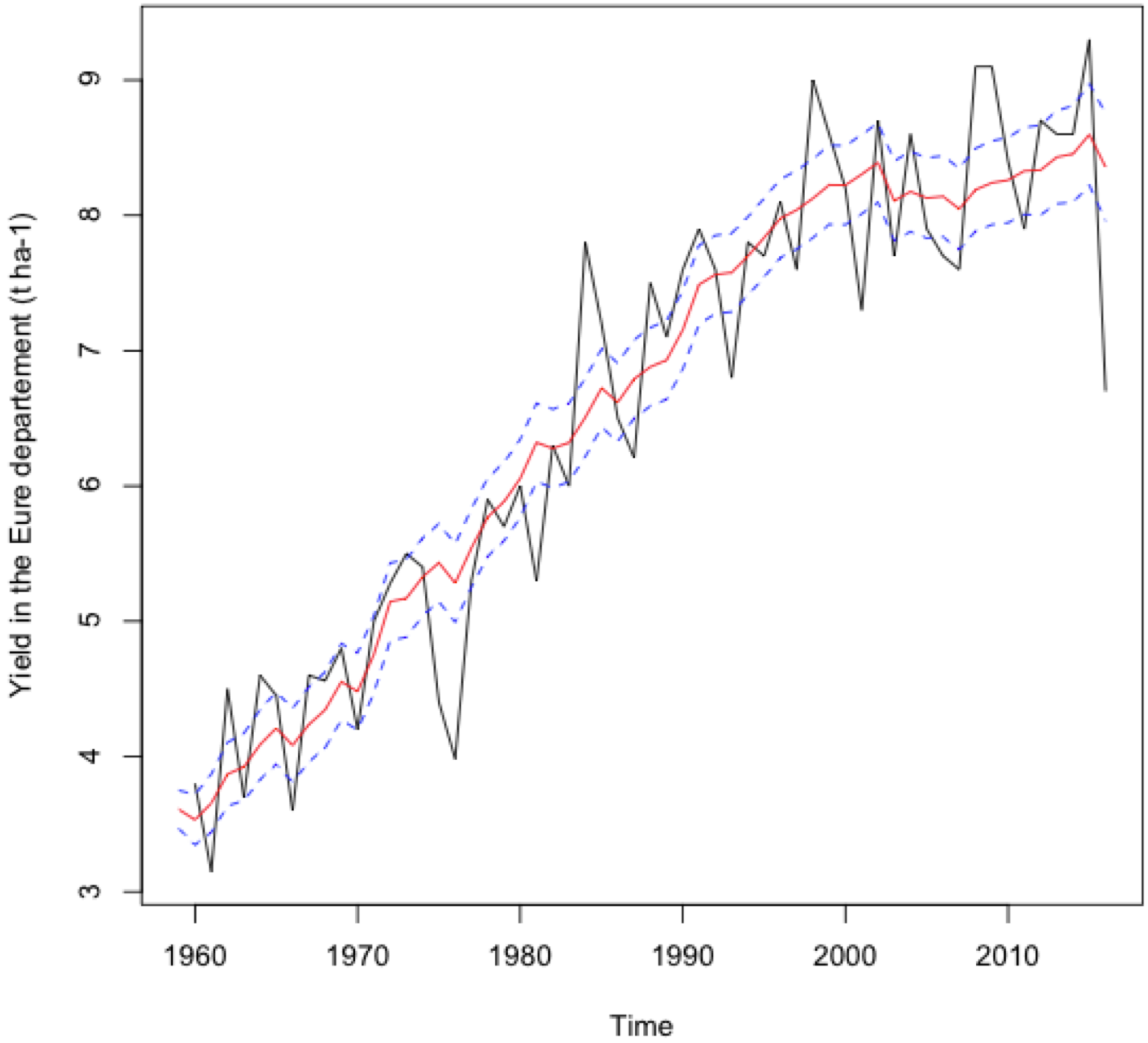
MODEL 2

```
MARSS fit is
Estimation method: kem
Convergence test: conv.test.slope.tol = 0.5, abstol = 0.001
Estimation converged in 265 iterations.
Log-likelihood: -52.30767
AIC: 116.6153   AICc: 118.2953

               Estimate
R.R              0.3332
B.B              1.0000
U.U              1.6376
x0.x0            3.5435
C.(X.Y1,X_1)    -0.0175
C.(X.Y1,X_2)    -0.1325
Initial states (x0) defined at t=0

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

MODEL 1


Yield in the Eure departement (t ha-1)
3
4
5
6
7
8
9
1960
1970
1980
1990
2000
2010
Time

MODEL 2



Yield in the Eure departement (t ha-1)
3
4
5
6
7
8
9
1960
1970
1980
1990
2000
2010
Time

Summary

- Kalman filter and smoother can be applied using dynamic linear gaussian models

- These models can handle a great diversity of situations (see practical session)

- They can be implemented using R (see practical session)

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Filter and smoothers using nonlinear models

- Nonlinear models are frequent in environmental science

$$Y_t \neq FZ_t + \varepsilon_t \qquad\qquad Z_t \neq GZ_{t-1} + \eta_{t-1}$$

- Kalman filter and smoother cannot be directly applied to nonlinear models

- Several methods are available for this type of model

Methods for nonlinear models

- Linearization (extended Kalman filter)
- Dynamic regression
- Methods based on Monte Carlo simulations
  - Ensemble Kalman filter
  - Particle filter

Linearization

Linearization can be applied to the following type of model:

- Observation equation

$$Y_t = FZ_t + \varepsilon_t$$

- System equation

$$Z_t = g\left(Z_{t-1}, X_t, \theta\right) + \eta_{t-1}$$

Linearization

Linearization of $$Z_t = g(Z_{t-1}, X_t, \theta) + \eta_{t-1}$$

The standard Kalman filter is applied to

$$Z_t \approx g(\hat{Z}_{t-1}, X_t, \theta) + H_{t-1}(Z_{t-1} - \hat{Z}_{t-1}) + w_{t-1}$$

H_t is a $(m \times m)$ matrix of partial derivatives of F with respect to the m elements of Z_t, $\hat{Z}_t$ is the predicted state variable at time t, $\hat{Z}_t = \hat{E}(Z_t | y_1, \ldots, y_t)$, w_t is a m-error term vector assumed to be normally distributed. The main drawback of this method is that the linearization has been shown to be a poor approximation in a number of applications. The linear approximation may not give a good description of how the model errors evolve over time.

Methods for nonlinear models

- Linearization (extended Kalman filter)
- Dynamic regression
- Methods based on Monte Carlo simulations
  - Ensemble Kalman filter
  - Particle filter

Dynamic regression

- The output of the nonlinear model as input of a regression model

Nonlinear model → Dynamic linear model

- Application of the standard Kalman filter

Dynamic regression

Observation equation

$$Y_t = \alpha_{0t} + \alpha_{1t} O_t + \varepsilon_t$$

with O_t is the output of the original nonlinear model

$$\varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$$

System equation

$$Z_t = Z_{t-1} + \eta_{t-1}$$

with $Z_t = \begin{pmatrix} \alpha_{0t} \\ \alpha_{1t} \end{pmatrix}$, $\eta_{t-1} \sim N\left(0, \Sigma\right)$, and $\Sigma = \begin{pmatrix} \sigma_{\alpha 0}^2 & 0 \\ 0 & \sigma_{\alpha 1}^2 \end{pmatrix}$

Dynamic regression

Observation equation

$Y_t = \alpha_{0t} + \alpha_{1t} O_t + \varepsilon_t$

with O_t is the output of the original nonlinear model,

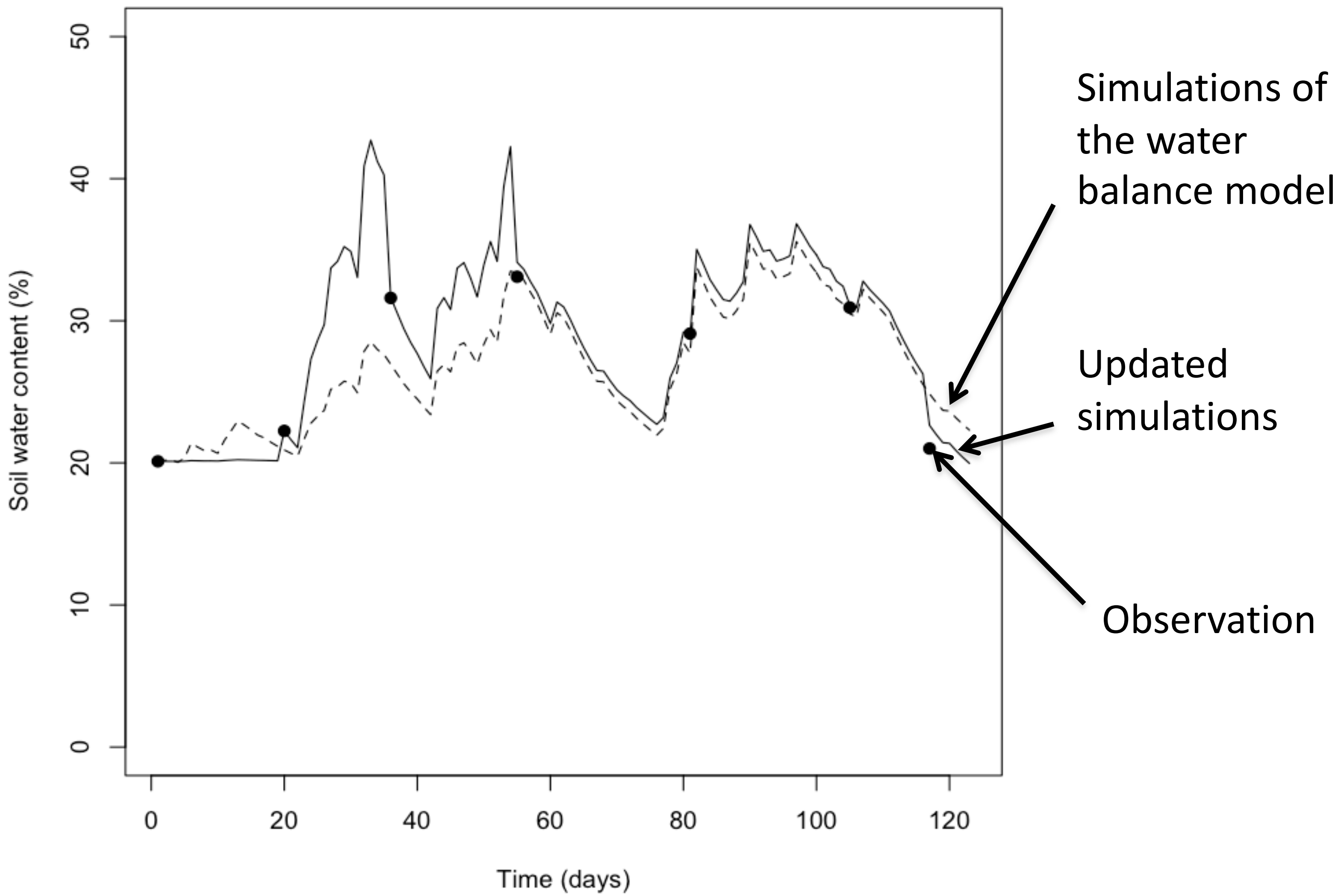
$\varepsilon_t \sim N\left(0, \sigma_\varepsilon^2\right)$

System equation

$Z_t = Z_{t-1} + \eta_{t-1}$

with $Z_t = \begin{pmatrix} \alpha_{0t} \\ \alpha_{1t} \end{pmatrix}$, $\eta_{t-1} \sim N(0, \Sigma)$, and $\Sigma = \begin{pmatrix} \sigma_{\alpha 0}^2 & 0 \\ 0 & \sigma_{\alpha 1}^2 \end{pmatrix}$

Example 3: Soil water content



Methods based on Monte Carlo simulations

- These methods use the original nonlinear model directly
- They require a large number of model simulations
- Random terms need to be inserted in the nonlinear model equations
- Several methods exist:
  - Ensemble Kalman filter
  - Particle filter

Example 4: Nonlinear population model

Four dynamic state variables

$$Z_t = \begin{pmatrix} d_t \\ SSB_t \\ DSB_t \\ S_t \end{pmatrix}$$

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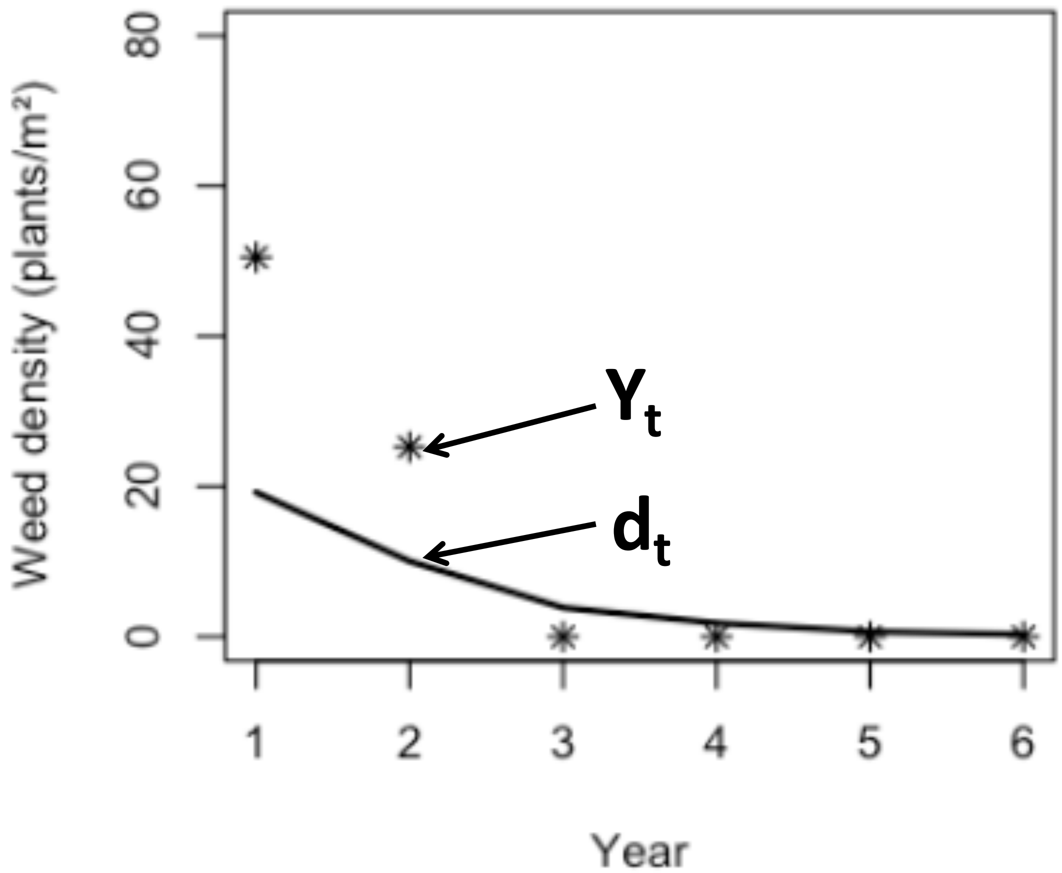
Example 4: Nonlinear population model

$$Z_t = \begin{pmatrix} d_t \\ SSB_t \\ DSB_t \\ S_t \end{pmatrix}$$

$$Z_t = g\left(Z_{t-1}, X_t, \theta\right)$$

Example 4: Nonlinear population model



Example 4: Nonlinear population model

- System equation

$$Z_t = g\left(Z_{t-1}, X_{t-1}, \theta\right) \times \eta_t$$

$\eta_t^{(k)}$~Gamma(λ, λ)

$$\eta_t = \begin{pmatrix} \eta_t^{(1)} \\ \eta_t^{(2)} \\ \eta_t^{(3)} \\ \eta_t^{(4)} \end{pmatrix}$$

Example 4: Nonlinear population model

- Observation equation

$$Y_t = \sum_{k=1}^{n} Y_{tk} \qquad P\left(Y_t \middle| d_t\right) = \frac{\exp\left(-d_t \times s \times n\right) \times \left(d_t \times s \times n\right)^{Y_t}}{Y_t!}$$

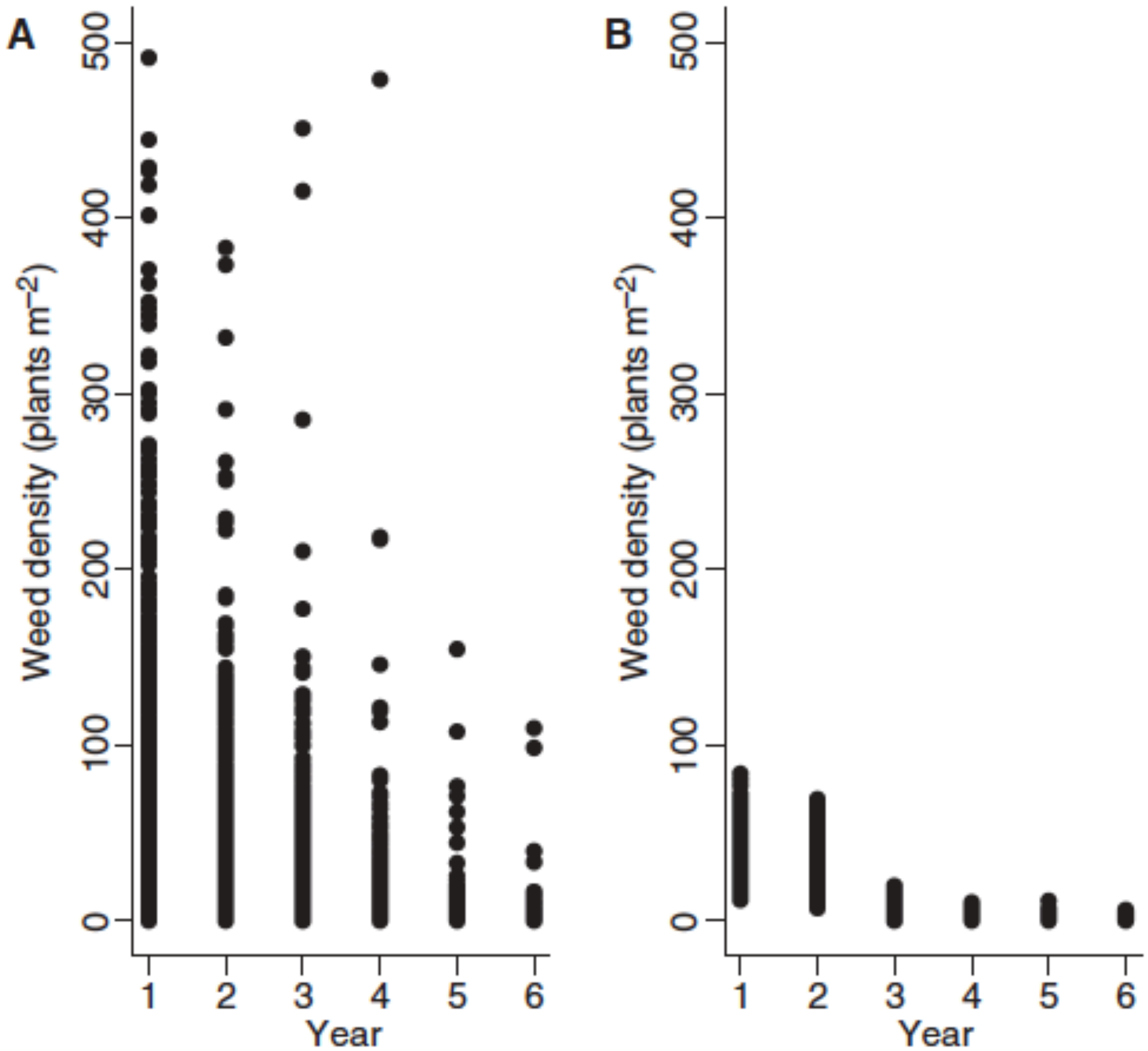
where $Y_t = \sum_{k=1}^{n} Y_{tk}$ is the total number of weed plants counted in year t in the n subplots taken in a given plot, Y_{tk} is the weed count in the k^{th} subplot, k=1, ..., n, s is the surface area of each subplot, d_t is the weed density before weed control computed by the model.

- System equation

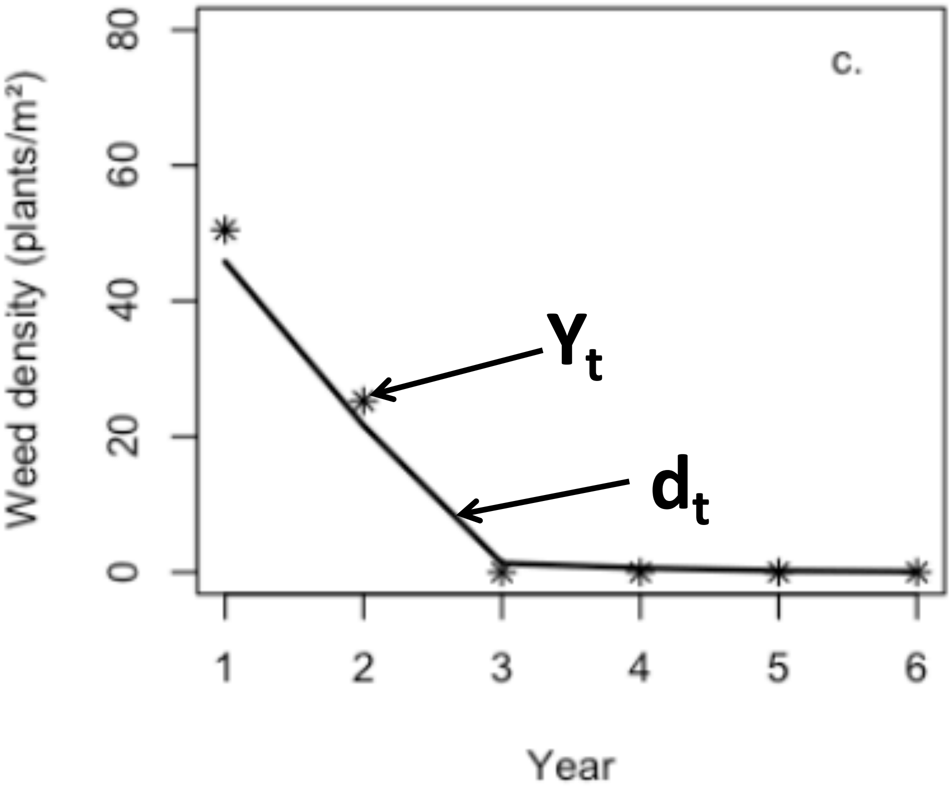
$$Z_t = g\left(Z_{t-1}, X_{t-1}, \theta\right) \times \eta_t \qquad \eta_t = \begin{pmatrix} \eta_t^{(1)} \\ \eta_t^{(2)} \\ \eta_t^{(3)} \\ \eta_t^{(4)} \end{pmatrix}$$

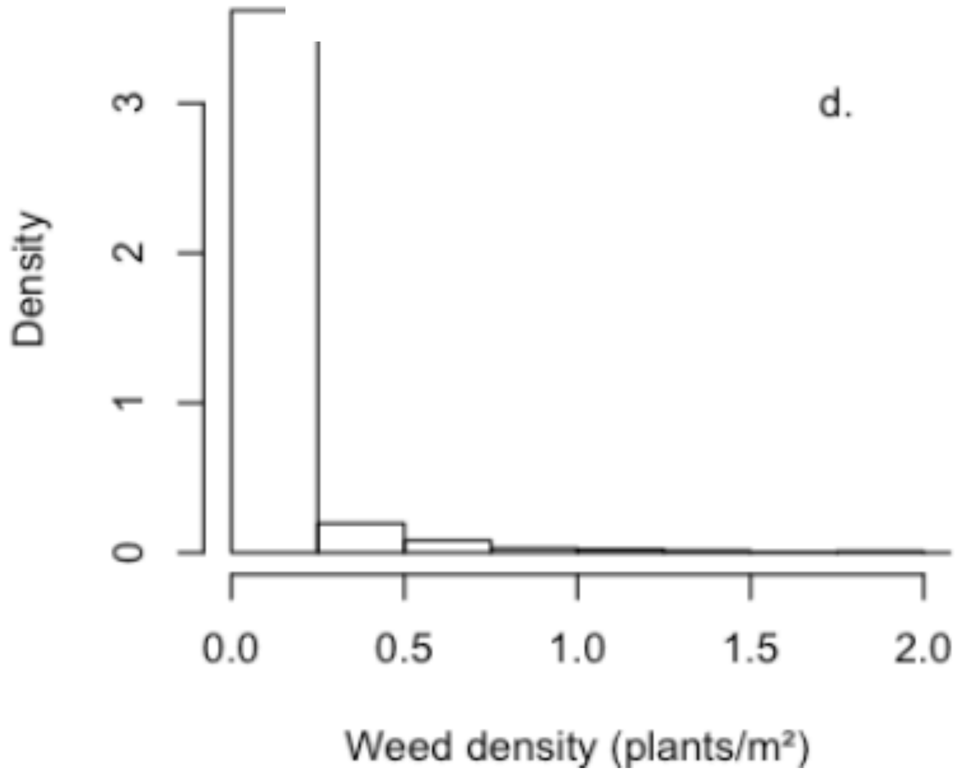
$\eta_t^{(k)}$~Gamma(λ, λ)

10,000 Monte Carlo simulations with the Weed model



Example 4: Nonlinear population model





t =6

Conclusion (1)

- Data assimilation is a powerful tool for updating dynamic models

- Filtering and smoothing allow one to combine a model and measurements in useful ways, taking into account the uncertainties in each.

- Filtering is useful for estimating sequentially in time the values of one or several state variables, whereas smoothing can be used to estimate past values of state variables using all available measurements.

Conclusion (2)

- To implement these methods, it is necessary to define the system models using two different equations; an observation equation (relating observation to state variables) and a system equation (describing the dynamic of the state variables).

Conclusion (3)

- Filtering and smoothing use these equations to calculate the expected values and variances of the state variables conditionally to one or several measurements.
- For linear Gaussian models, the expected values and variances can be computed analytically and the dlm R package makes the calculations very accessible.

Conclusion (4)

- For nonlinear models, a first option is to approximate the original model by a linear one and then to apply the standard Kalman filter and smoother.
- Another option is to use the original nonlinear model and to approximate the state variable expected values and variances with special algorithms based on Monte Carlo simulations.