

# Graphical Models for Sequential Data Modeling and Forecasting

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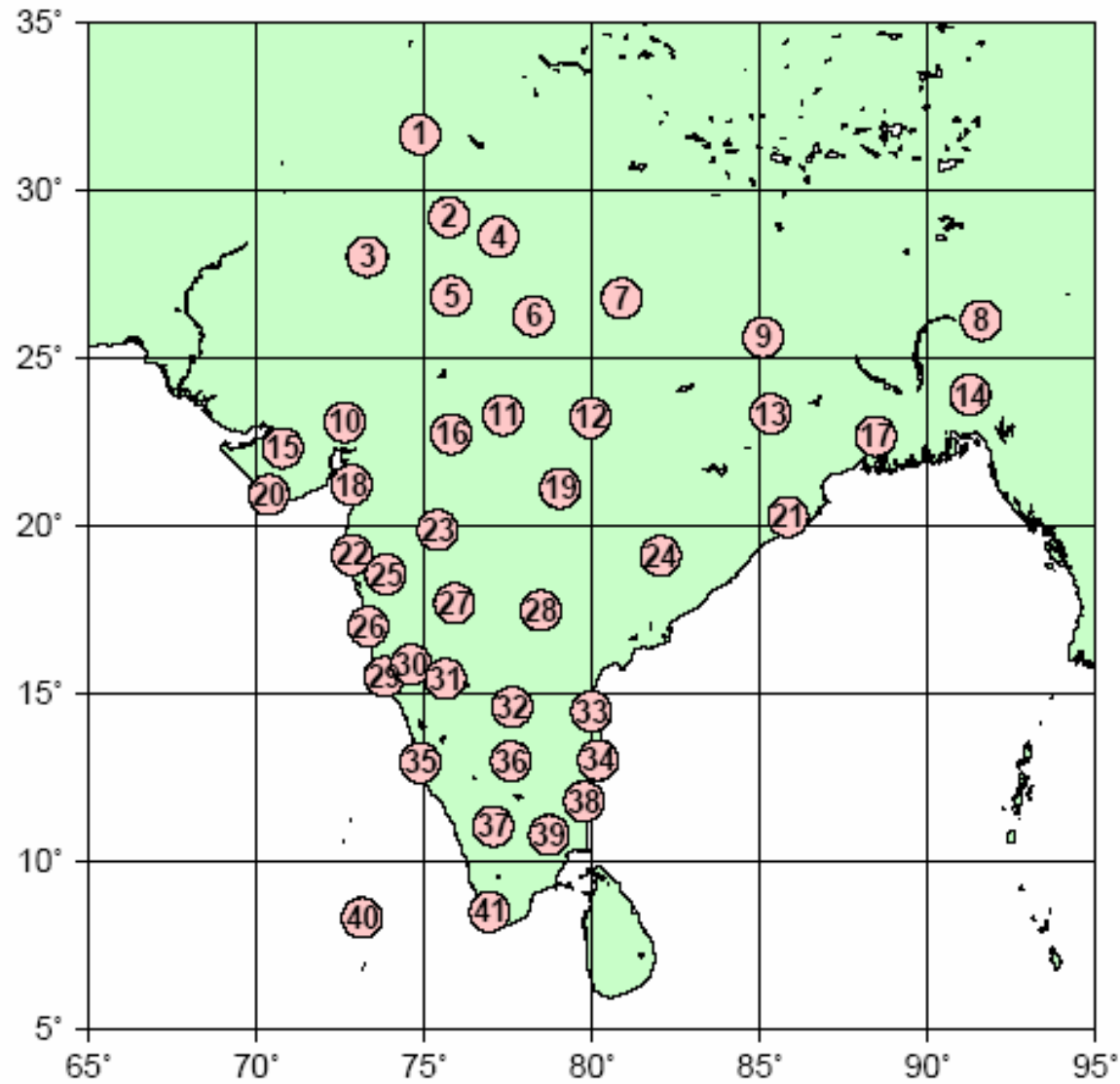
# Collaborators

- UC Irvine, computer science
  - Scott Gaffney, Sergey Kirshner
- Atmospheric science
  - Andy Robertson, Suzana Camargo, Michael Ghil

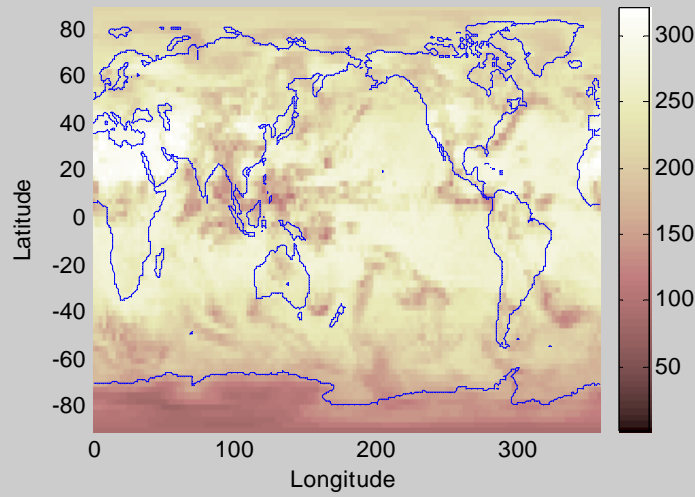
# Outline

- Graphical models
  - a framework for working with sets of random variables
  - Modeling sequential data
  - Estimating graphical models from data
- Examples
  - Cyclone clustering
  - Precipitation modeling with hidden Markov models
- Research problems, future directions

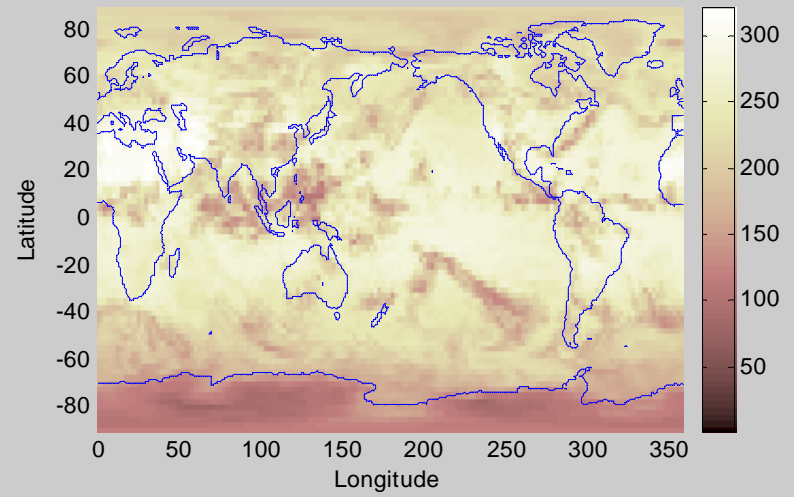
# India 1973-03 NCDC GSOD Rainfall Stations



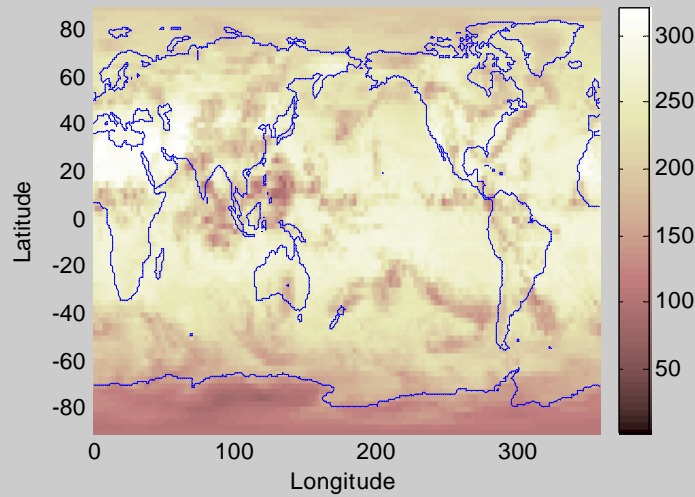
OLR Data on 30-Jun-2000



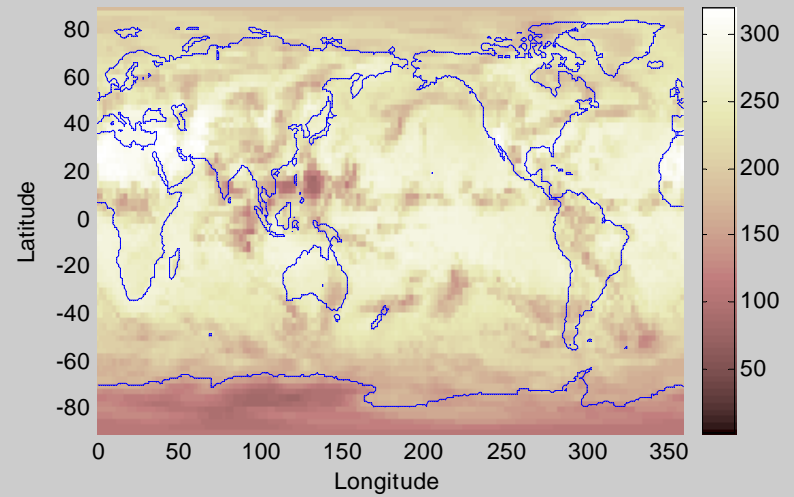
OLR Data on 01-Jul-2000



OLR Data on 02-Jul-2000



OLR Data on 03-Jul-2000



# Prediction and Uncertainty

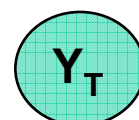
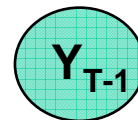
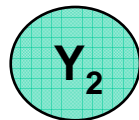
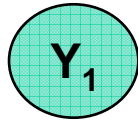
- Uncertainty is ever-present in climate science
  - Model uncertainty
    - which model is more likely given observed data?
  - Forecasting and prediction
    - Distributions over future outcomes
  - Modeling unobserved phenomena
  - Measurement error
- Probability is the language of uncertainty
  - Graphical models are a systematic framework for handling large numbers of random variables

# Preliminaries

- Variables
  - $Y = y$  : observed variable
  - $S = s$  : unobserved state variable
  - $P(S = s | Y = y) = P(s|y)$
- Joint probability densities or distributions
  - e.g.,  $p(\mathbf{S}) = p(S_1, S_2, \dots, S_T)$
  - If we know the joint density, we can compute any quantity of interest
    - .... But working with the joint density is hard
- Examples
  - $\mathbf{S}$  discrete:  $P(\mathbf{S})$  is a table containing  $O(K^T)$  numbers
  - $\mathbf{S}$  continuous:  $P(\mathbf{S})$  is a function over a T-dimensional space

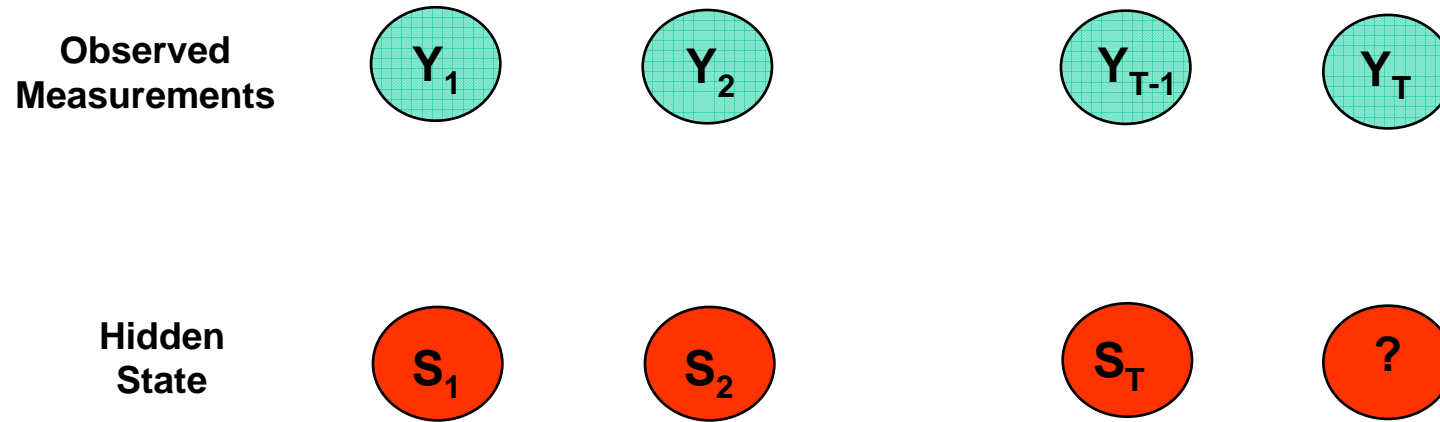
# Sequential Data

Observed  
Measurements

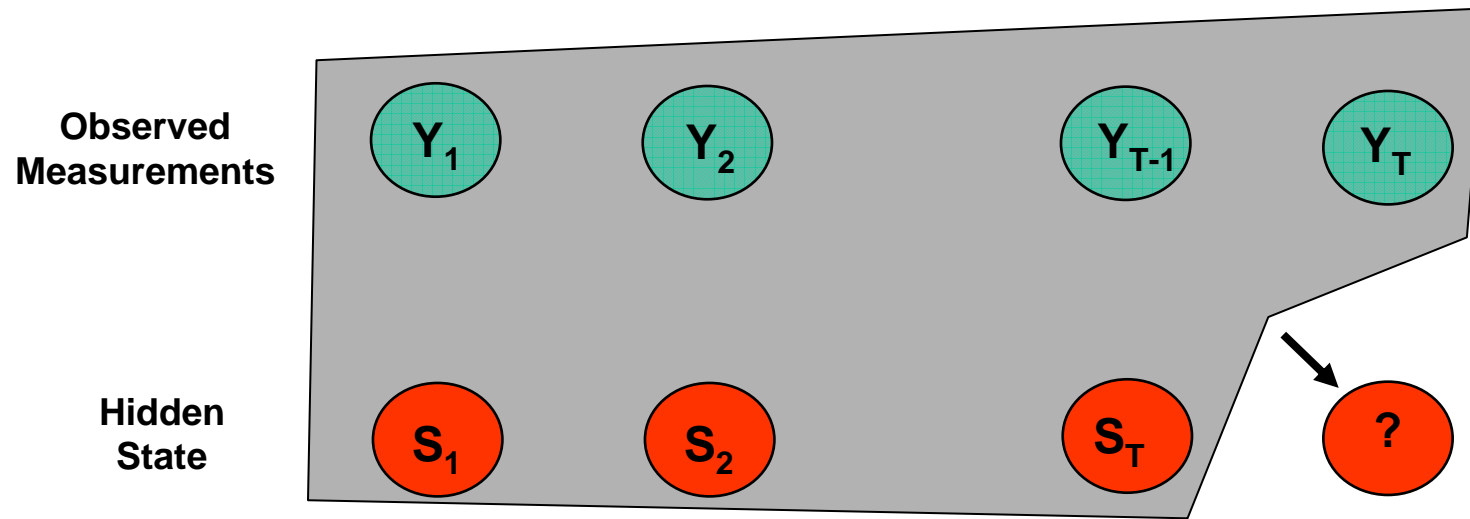




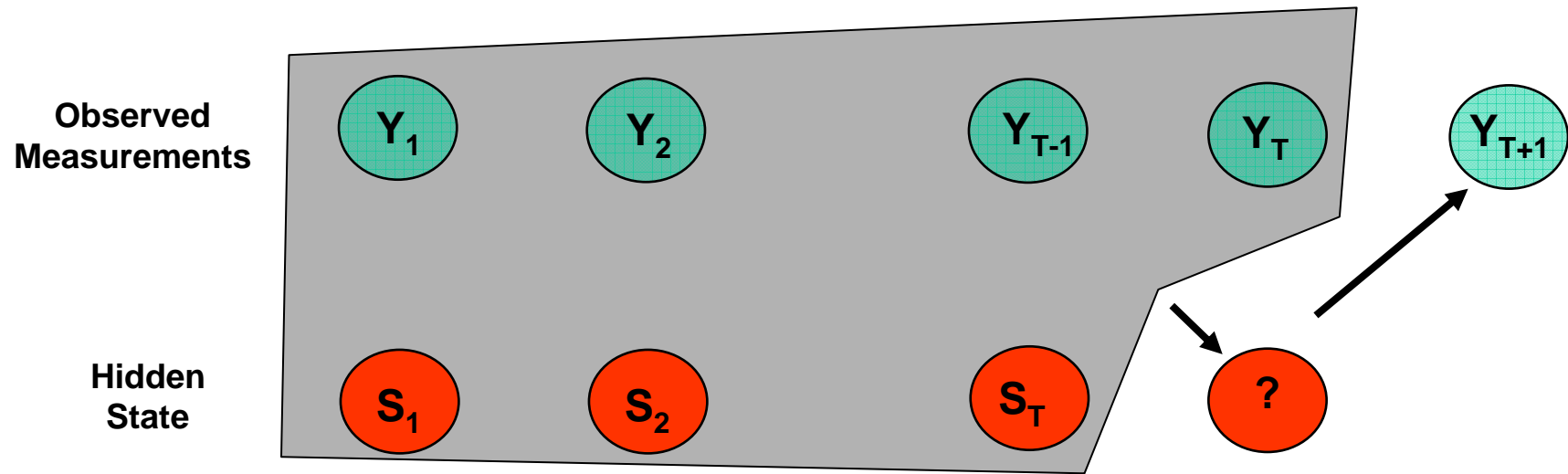
# Sequential Data



# Sequential Data



# Sequential Data



# Conditional Probabilities

- Many problems of interest involve computing conditional probabilities, densities, or expectation

- Prediction

$$E [ y_{T+1} \mid y_T, \dots, y_1 ]$$

- State Estimation

$$\arg \max \{ P(s_1, \dots, s_T \mid y_1, \dots, y_T) \}$$

- Parameter Estimation

$$P(\theta \mid y_1, \dots, y_T)$$

- Note:

- Computing  $P(s_{T+1} \mid s_1 = s)$  has time complexity  $O(K^T)$

# Two Problems

- Problem 1: Computational Complexity
  - computations scale as  $O(K^N)$
- Problem 2: Model Specification
  - To specify  $p(U)$  we need a table of  $K^N$  numbers
  - Where do these numbers come from?

# Two Key Ideas

- Problem 1: Computational Complexity
  - Idea:
    - Represent dependency structure as a graph and exploit sparseness in computation
- Problem 2: Model Specification
  - Idea:
    - learn models from data using statistical learning principles

“...probability theory is more fundamentally concerned with the structure of reasoning and causation than with numbers.”

**Glenn Shafer and Judea Pearl**  
***Introduction to Readings in Uncertain Reasoning,***  
**Morgan Kaufmann, 1990**

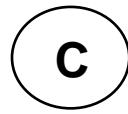
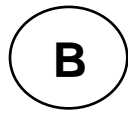
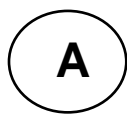
# Graphical Models

- Dependency structure encoded by an acyclic directed graph
  - Node  $\leftrightarrow$  random variable
  - Edges encode dependencies
    - Absence of edge  $\rightarrow$  conditional independence
  - Directed and undirected versions
- Why is this useful?
  - A language for communication
  - A language for computation
- Origins:
  - Wright 1920's
  - 1988
    - Spiegelhalter and Lauritzen in statistics
    - Pearl in computer science
  - Aka Bayesian networks, belief networks, causal networks, etc



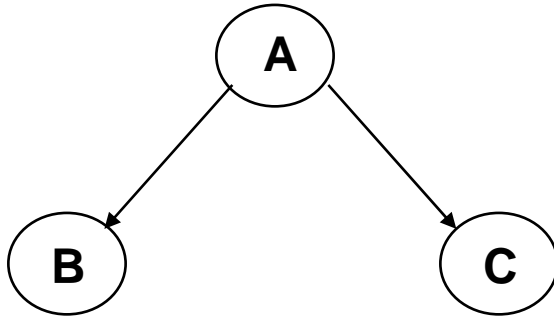


# Examples of 3-way Graphical Models



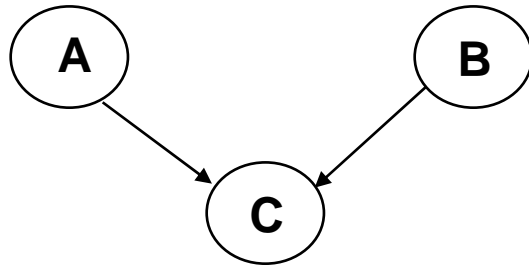
**Marginal Independence:**  
 $p(A,B,C) = p(A) p(B) p(C)$

# Examples of 3-way Graphical Models



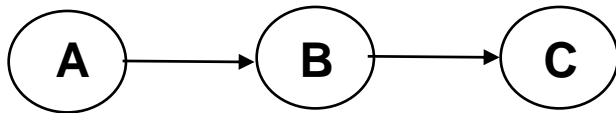
**Conditionally independent effects:**  
 $p(A,B,C) = p(B|A)p(C|A)p(A)$

# Examples of 3-way Graphical Models



**Independent Causes:**  
 $p(A,B,C) = p(C|A,B)p(A)p(B)$

# Examples of 3-way Graphical Models

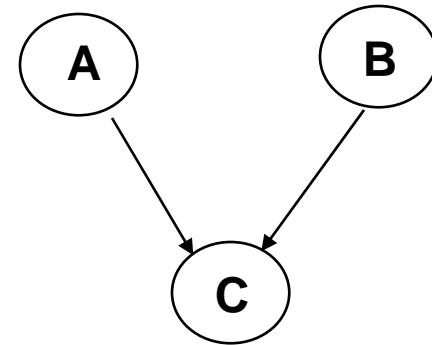


**Markov dependence:**

$$p(A,B,C) = p(C|B) p(B|A)p(A)$$

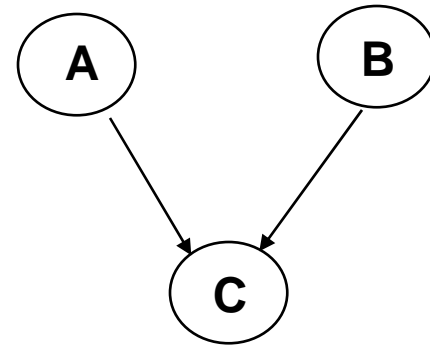
# Directed Graphical Models

$$p(A,B,C) = p(C|A,B)p(A)p(B)$$



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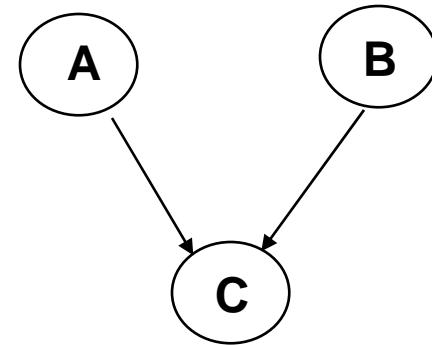


In general,

$$p(X_1, X_2, \dots, X_N) = \prod p(X_i | \text{parents}(X_i))$$

# Directed Graphical Models

$$p(A,B,C) = p(C|A,B)p(A)p(B)$$

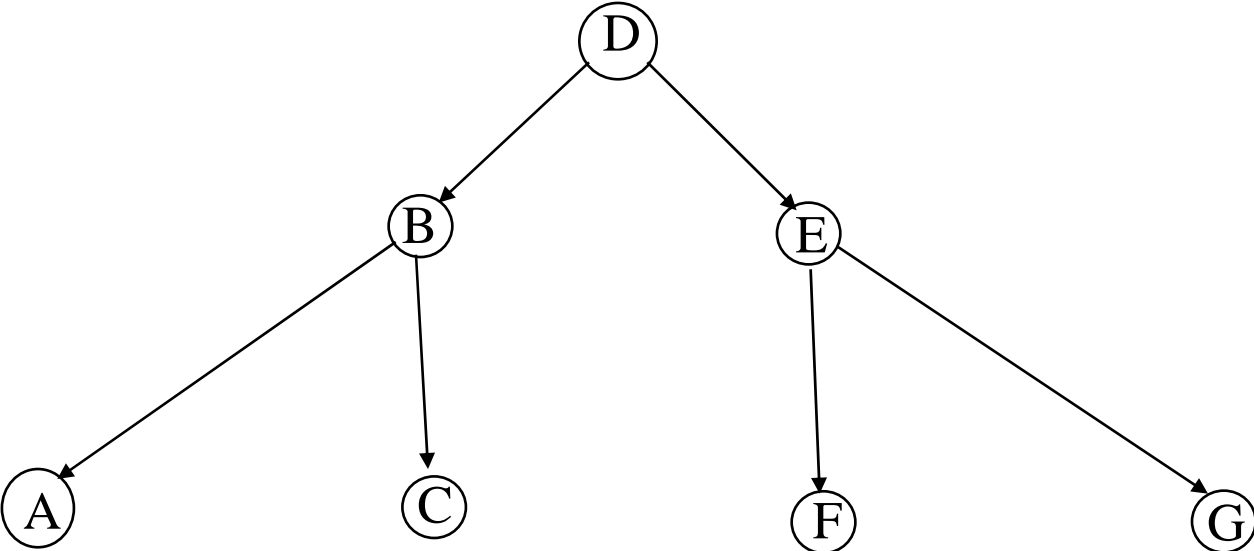


In general,

$$p(X_1, X_2, \dots, X_N) = \prod p(X_i \mid \text{parents}(X_i))$$

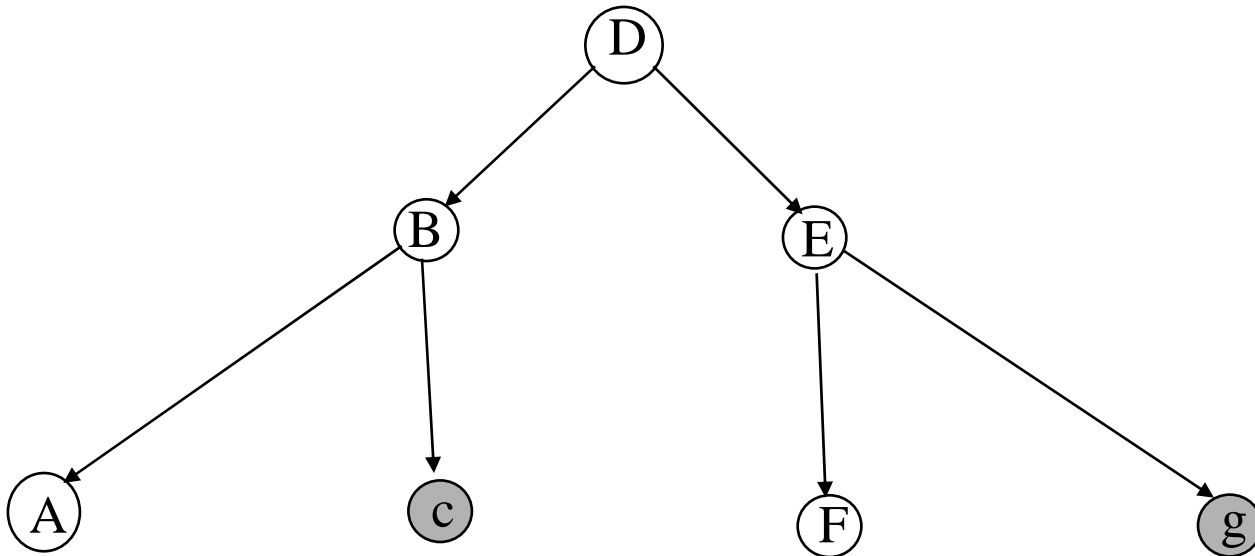
- Probability model has simple factored form
- Directed edges => direct dependence
- Absence of an edge => conditional independence
- Also known as belief networks, Bayesian networks, causal networks

# Example



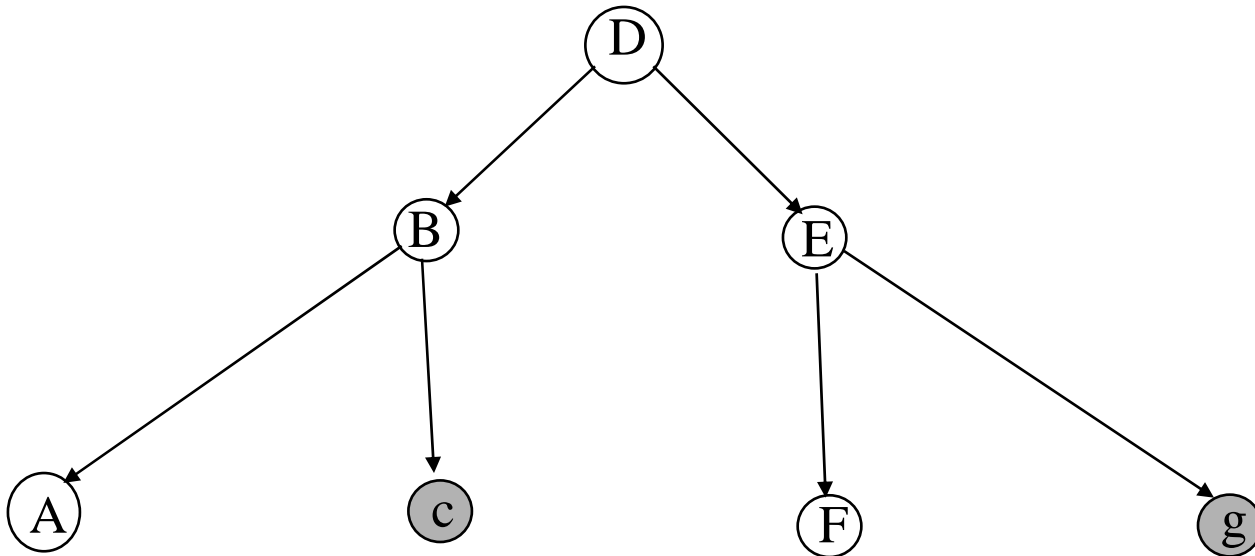


# Example



Say we want to compute  $p(a \mid c, g)$

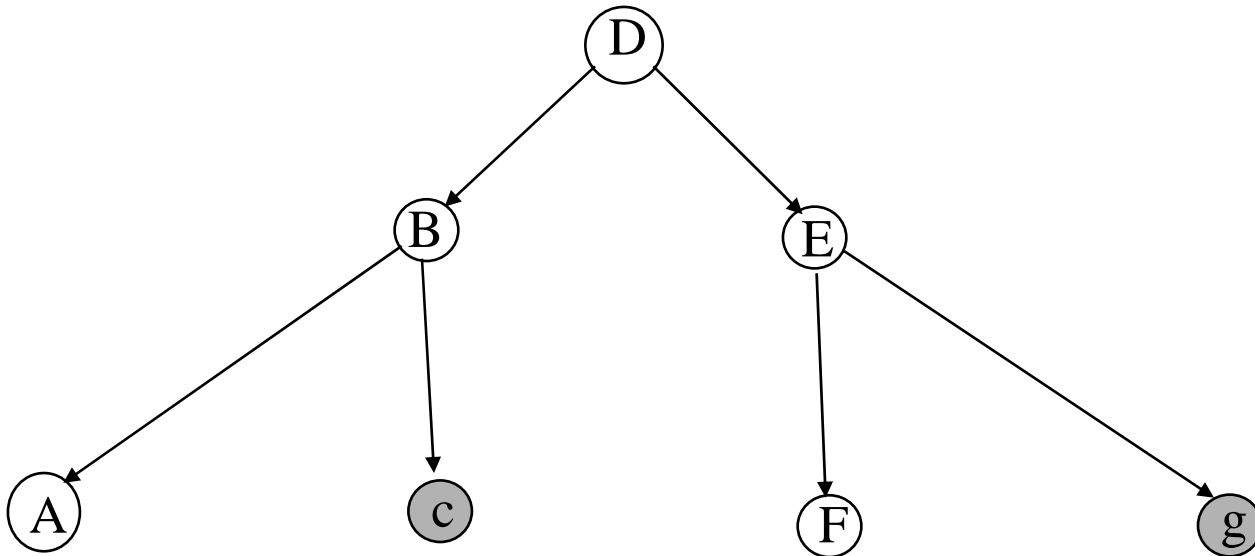
# Example



Direct calculation:  $p(a|c,g) = \sum_{bdef} p(a,b,d,e,f | c,g)$

Complexity of the sum is  $O(K^4)$

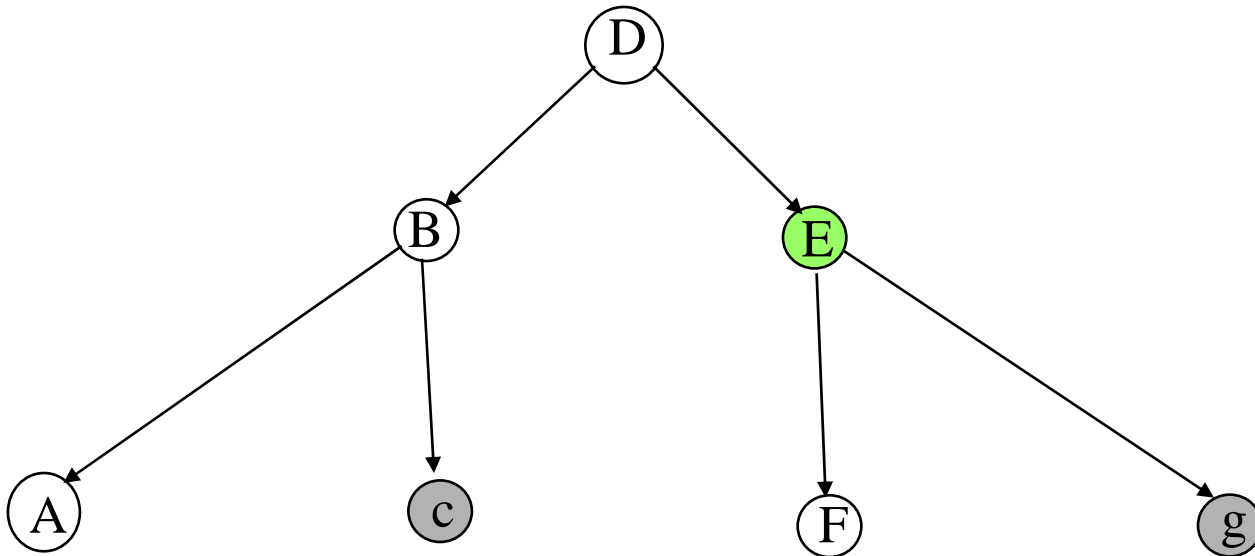
# Example



Reordering:

$$\sum_d p(a|b) \sum_d p(b|d,c) \sum_e p(d|e) \sum_f p(e,f |g)$$

# Example

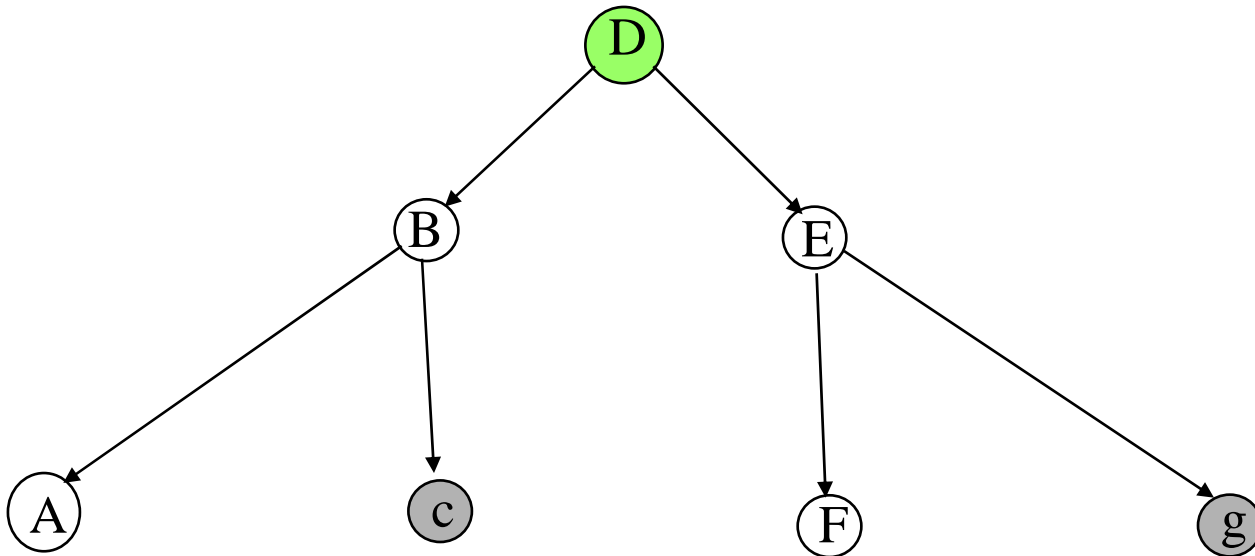


Reordering:

$$\sum_b p(a|b) \sum_d p(b|d,c) \sum_e p(d|e) \sum_f p(e,f|g)$$

$p(e|g)$

# Example

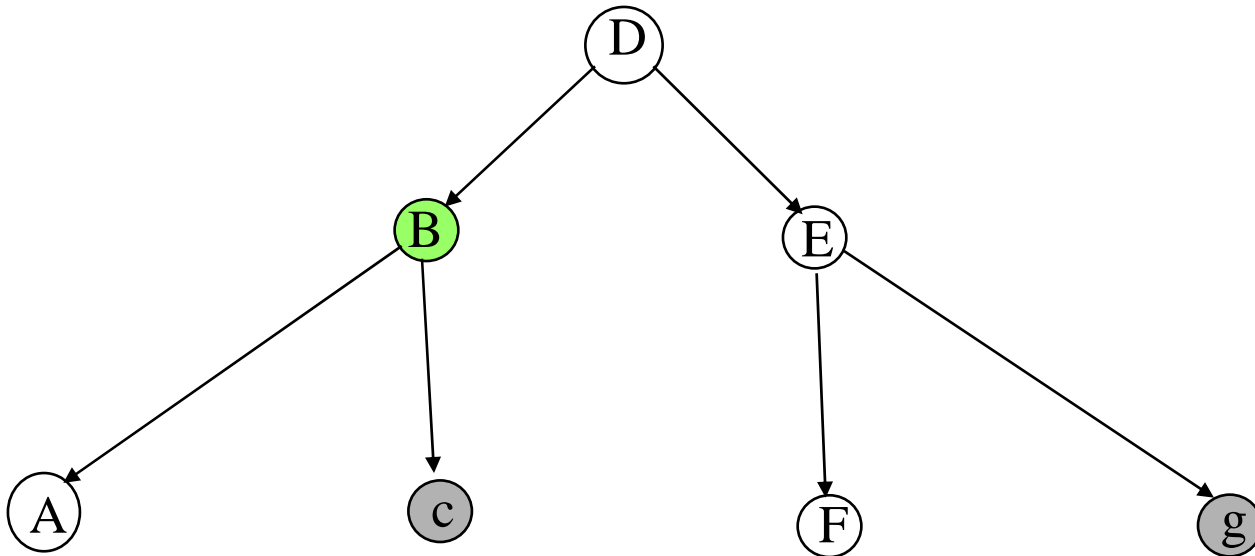


Reordering:

$$\sum_b p(a|b) \sum_d p(b|d,c) \sum_e p(d|e) p(e|g)$$

$p(d|g)$

# Example

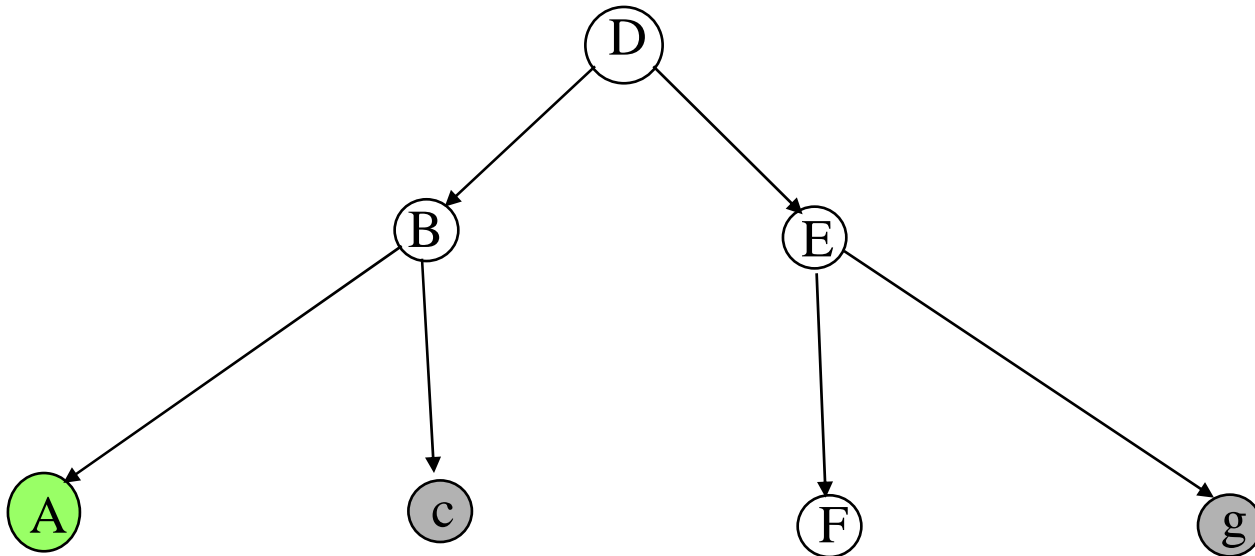


Reordering:

$$\sum_b p(a|b) \sum_d p(b|d,c) p(d|g)$$

$$p(b|c,g)$$

# Example



Reordering:

$$\sum_b p(a|b) p(b|c,g)$$

$$p(a|c,g)$$

Complexity is  $O(K)$ , compared to  $O(K^4)$

# Probability Calculations on Graphs

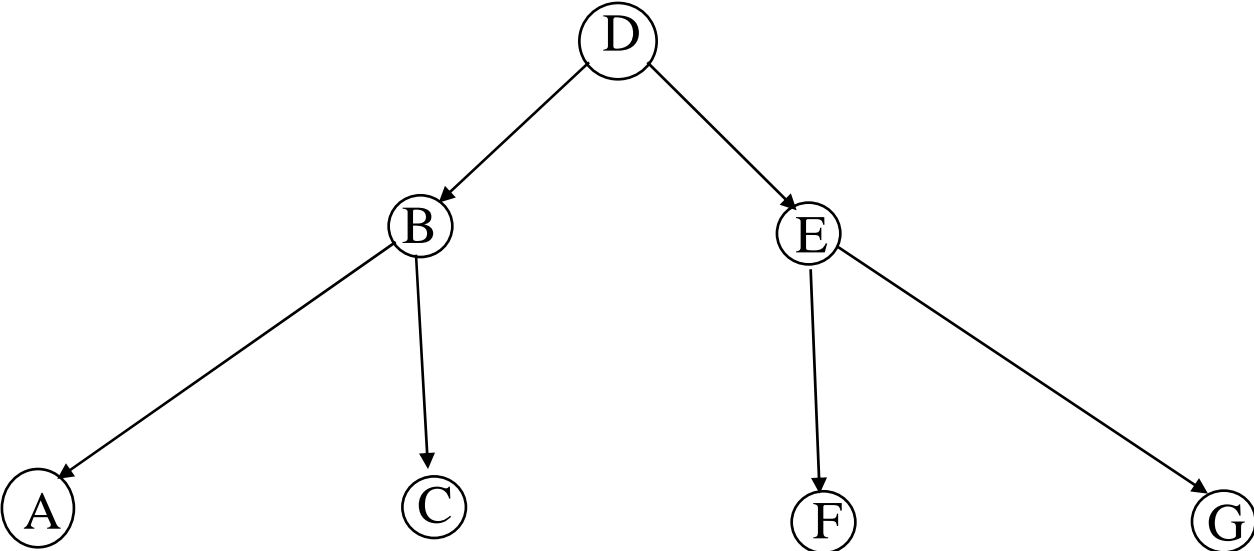
- Structure of the graph -> reveals order in which variables can be eliminated
- Complexity is typically  $O(K^{\max(\text{number of parents})})$ 
  - If single parents (e.g., tree), ->  $O(K)$
  - The sparser the graph the lower the complexity
- Technique can be “automated”
  - i.e., a fully general algorithm for arbitrary graphs
  - For continuous variables:
    - replace sum with integral
  - For identification of most likely values
    - Replace sum with max operator



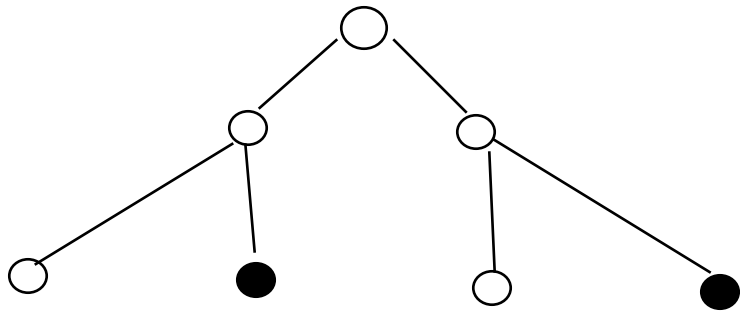
# Inference in Graphical Models

- “Inference” = calculating  $p(\text{one variable} \mid \text{values of others})$
- Assume the graph has no loops after arrows are “dropped”
- Message Passing (MP) Algorithm
  - Pearl, 1988; Lauritzen and Spiegelhalter, 1988
  - Declare 1 node (any node) to be a root
  - Schedule two phases of message-passing
    - nodes pass messages up to the root
    - messages are distributed back to the leaves
  - In time  $O(N)$ , we can compute  $P(\dots)$

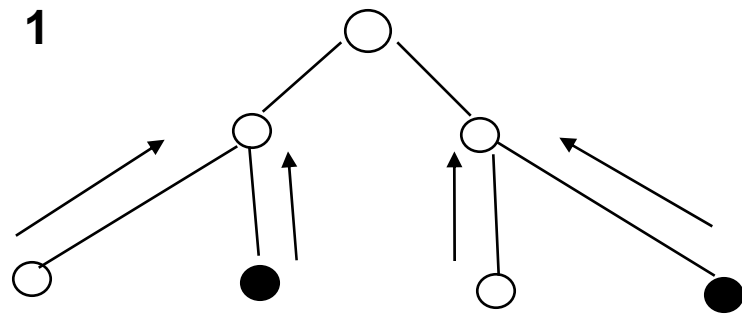
# Example



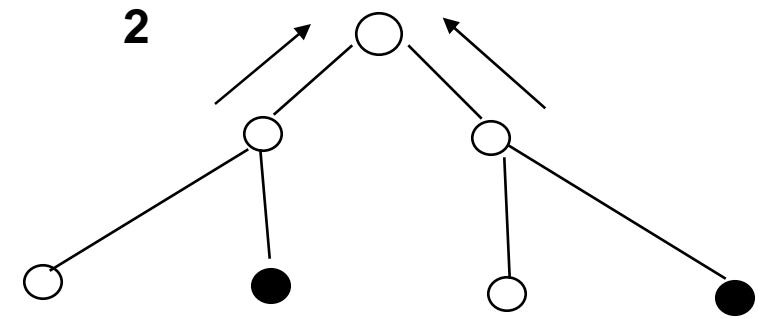
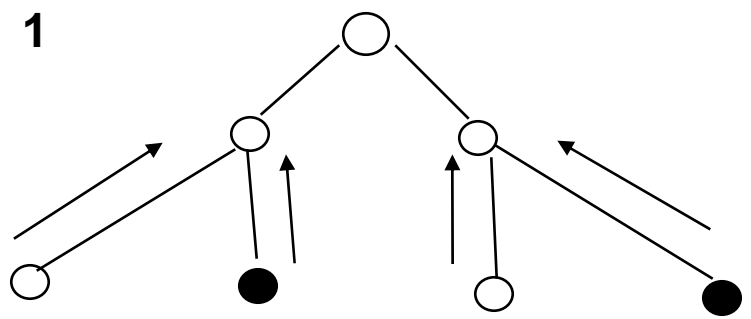
# Sketch of the MP algorithm in action



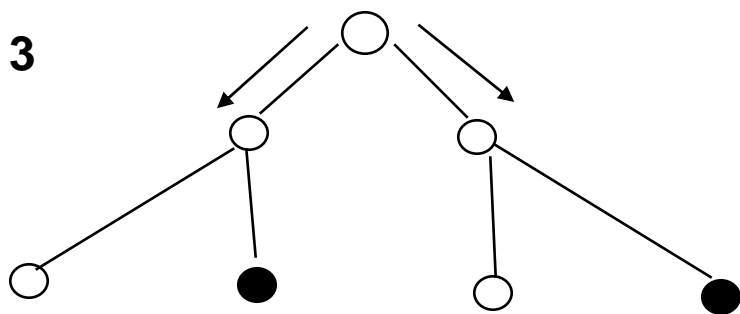
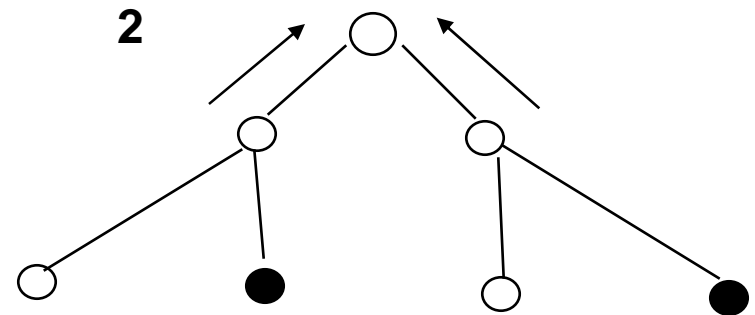
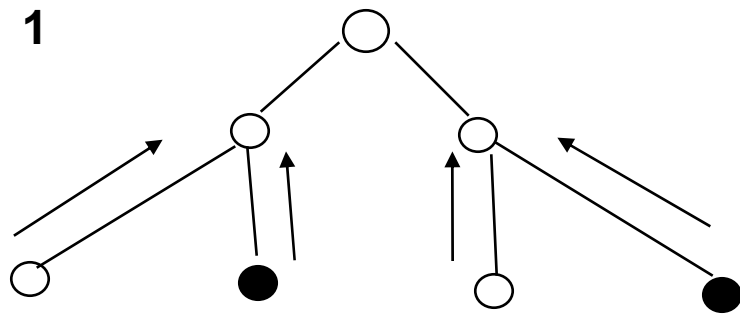
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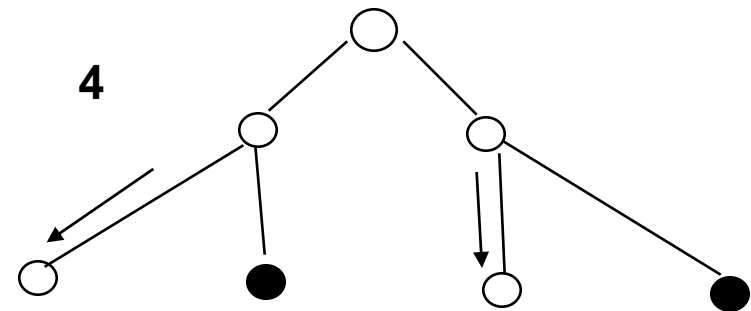
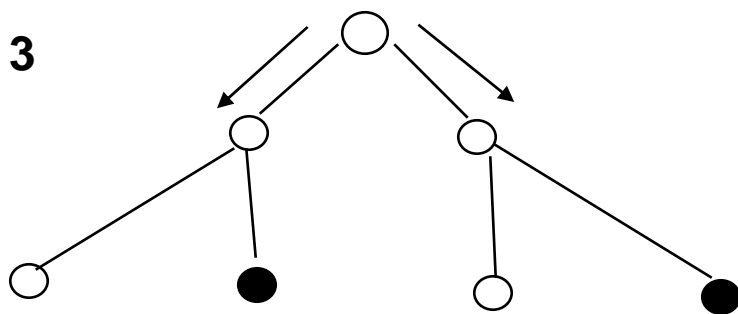
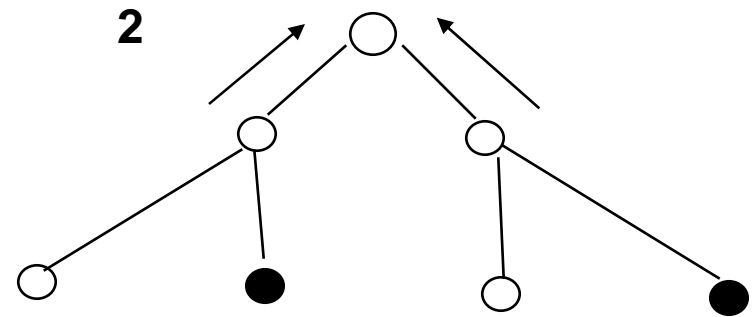
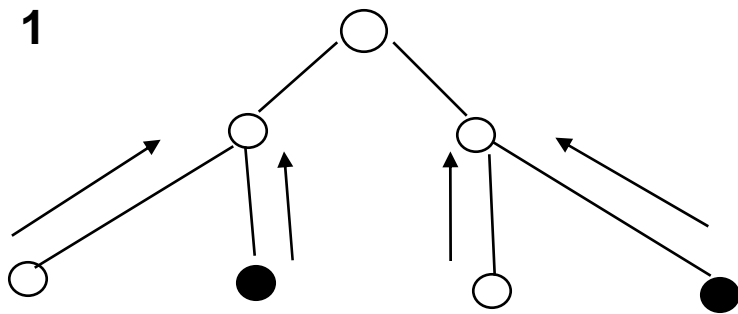
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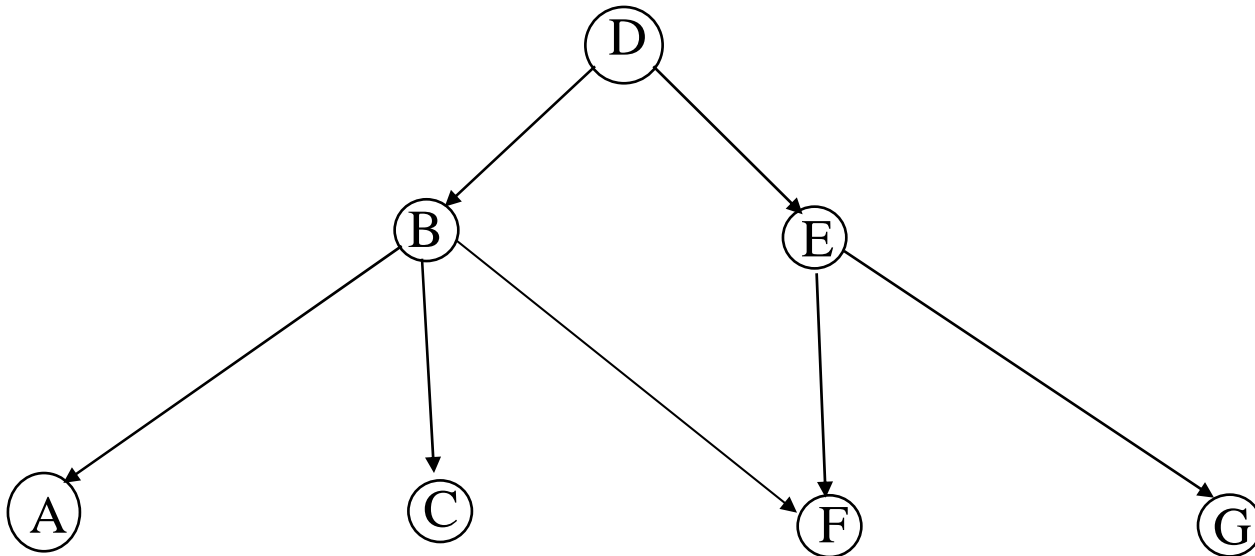


# Complexity of the MP Algorithm

- Efficient
  - Complexity scales as  $O(N K^m)$ 
    - $N$  = number of variables
    - $K$  = arity of variables
    - $m$  = maximum number of parents for any node
  - Compare to  $O(K^N)$  for brute-force method

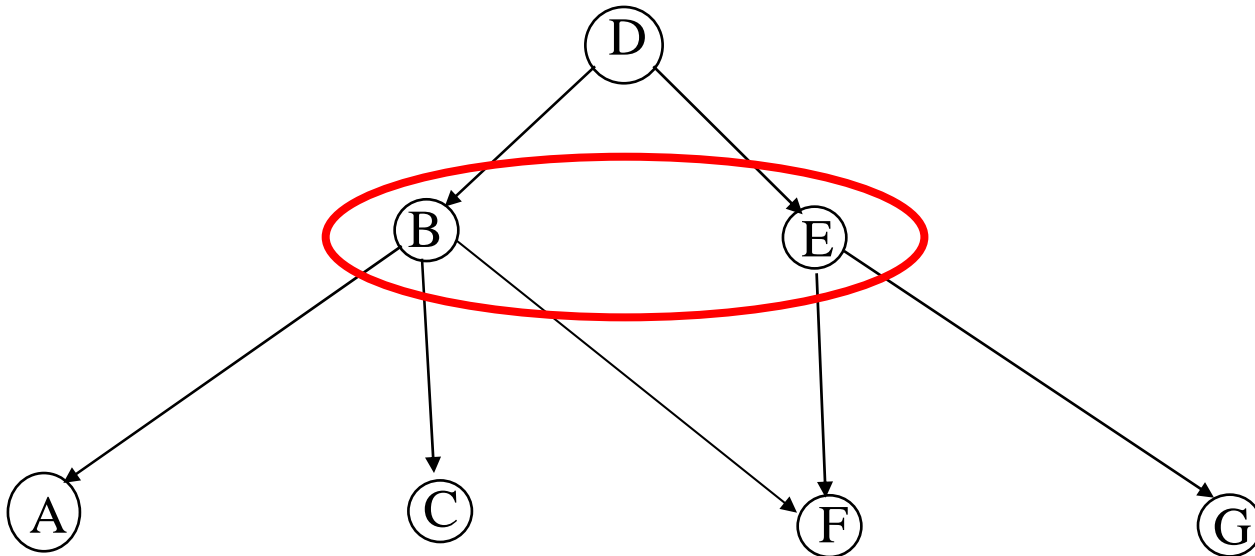


# Graphs with "loops"



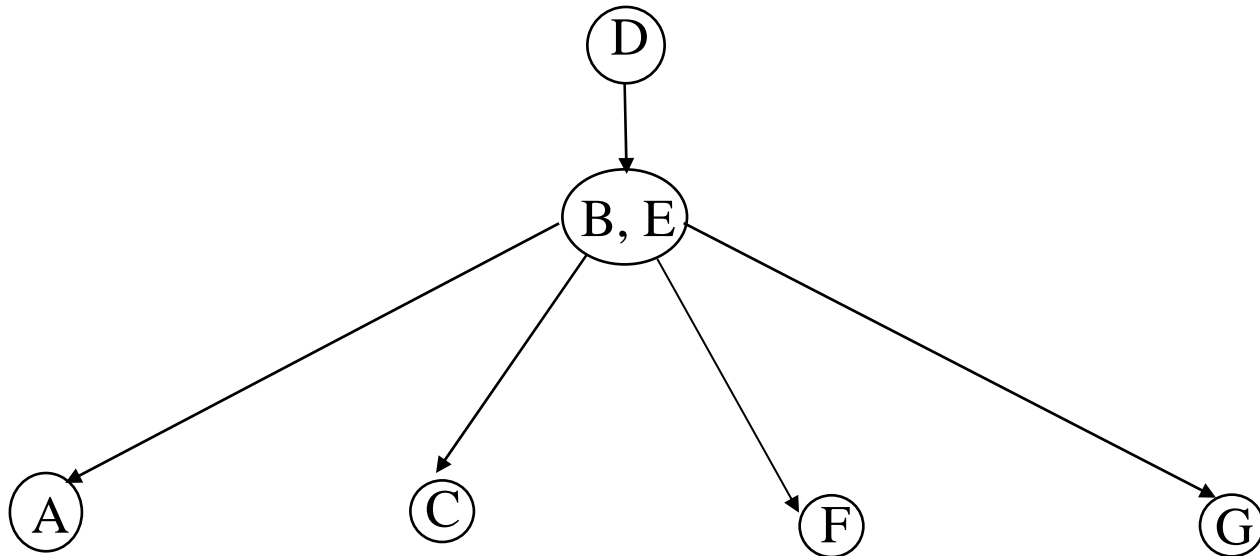
Message passing algorithm does not work when there are multiple paths between 2 nodes

# Graphs with "loops"

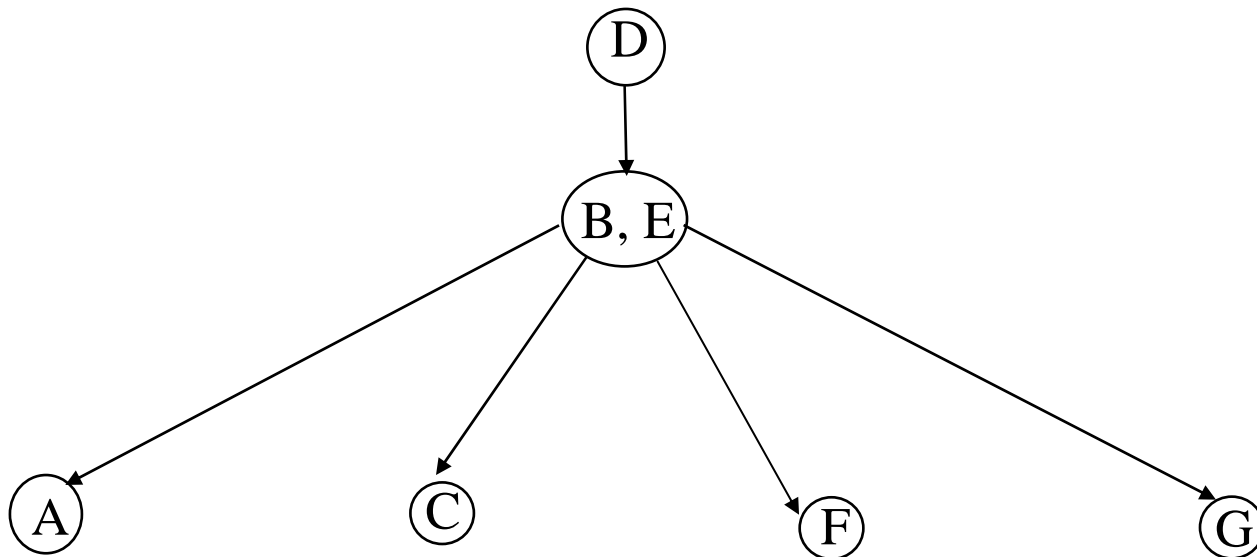


General approach: "cluster" variables together to convert graph to a tree

# Junction Tree



# Junction Tree



Good news: can perform MP algorithm on this tree

Bad news: complexity is now  $O(K^2)$

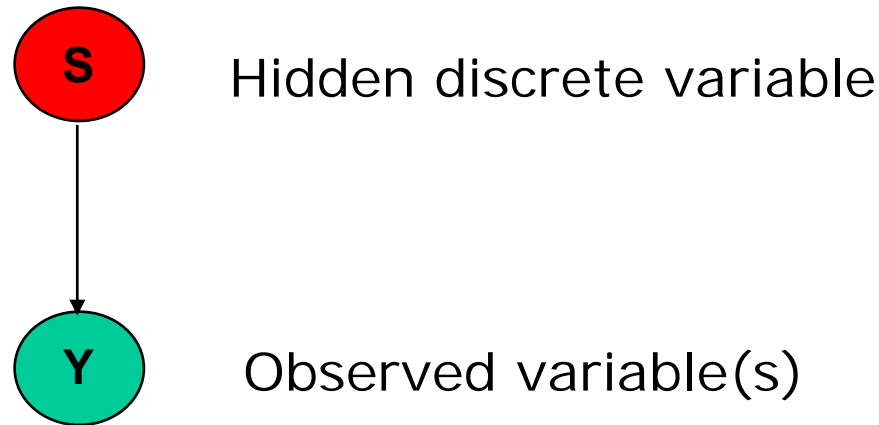
# Additional Topics

- Continuous-valued variables
  - Gaussian models
    - Tractable closed-form updating equations
  - Non-parametric models (kernel density)
    - Efficient algorithms exist for sparse graphs
- Undirected graphs:
  - Similar representation and semantics
  - Special case: Markov random field (Ising model)
    - Inference in general is intractable

# Hidden Variable Models

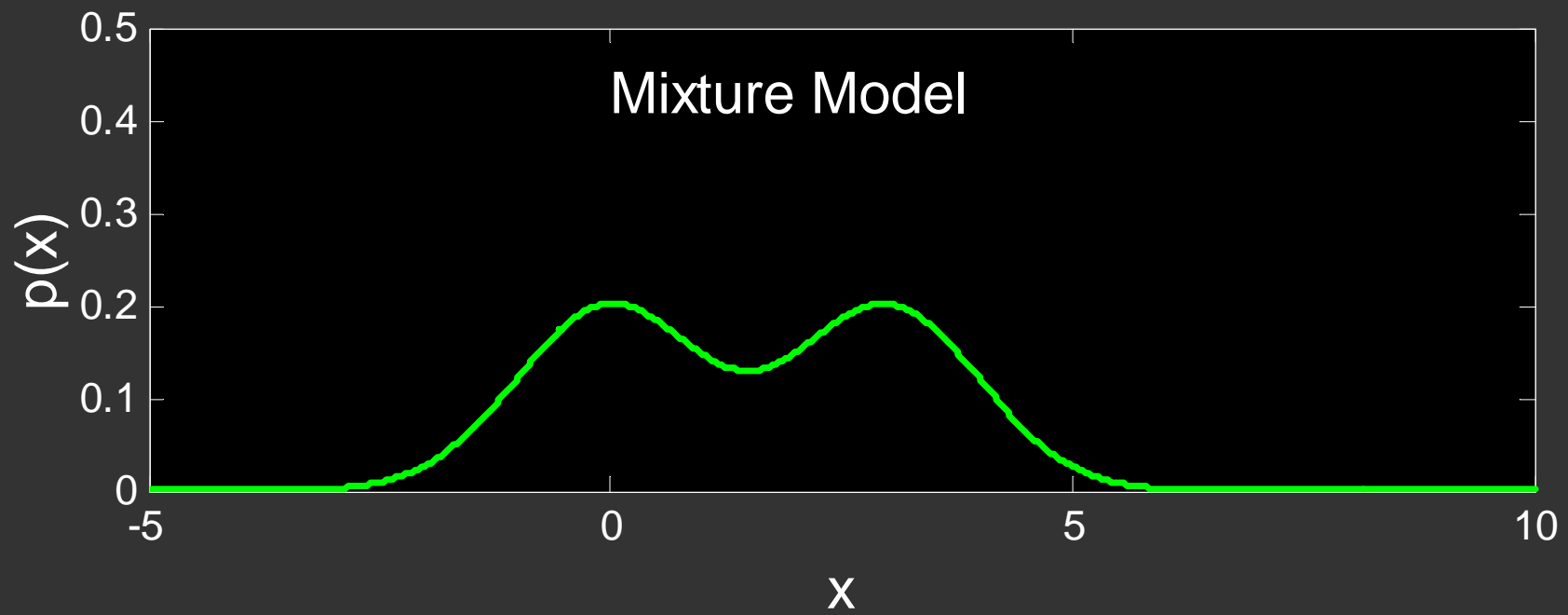
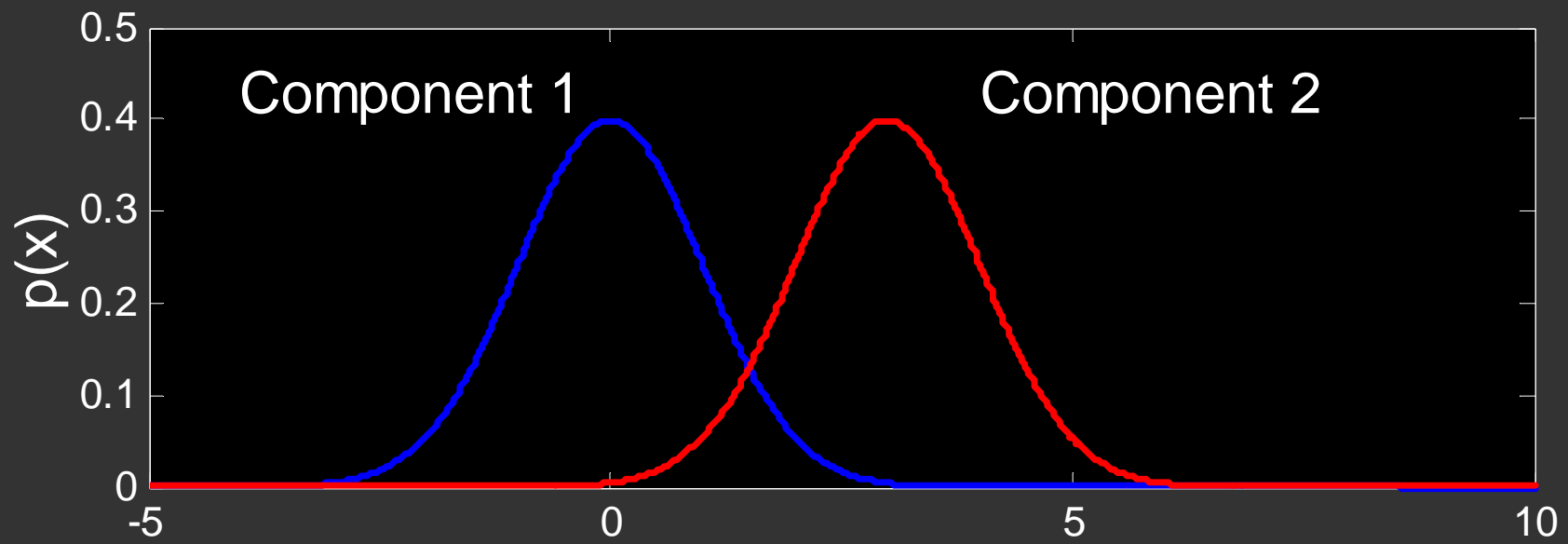
# Mixture Models

$$p(Y) = \sum_k p(Y | S=k) p(S=k)$$

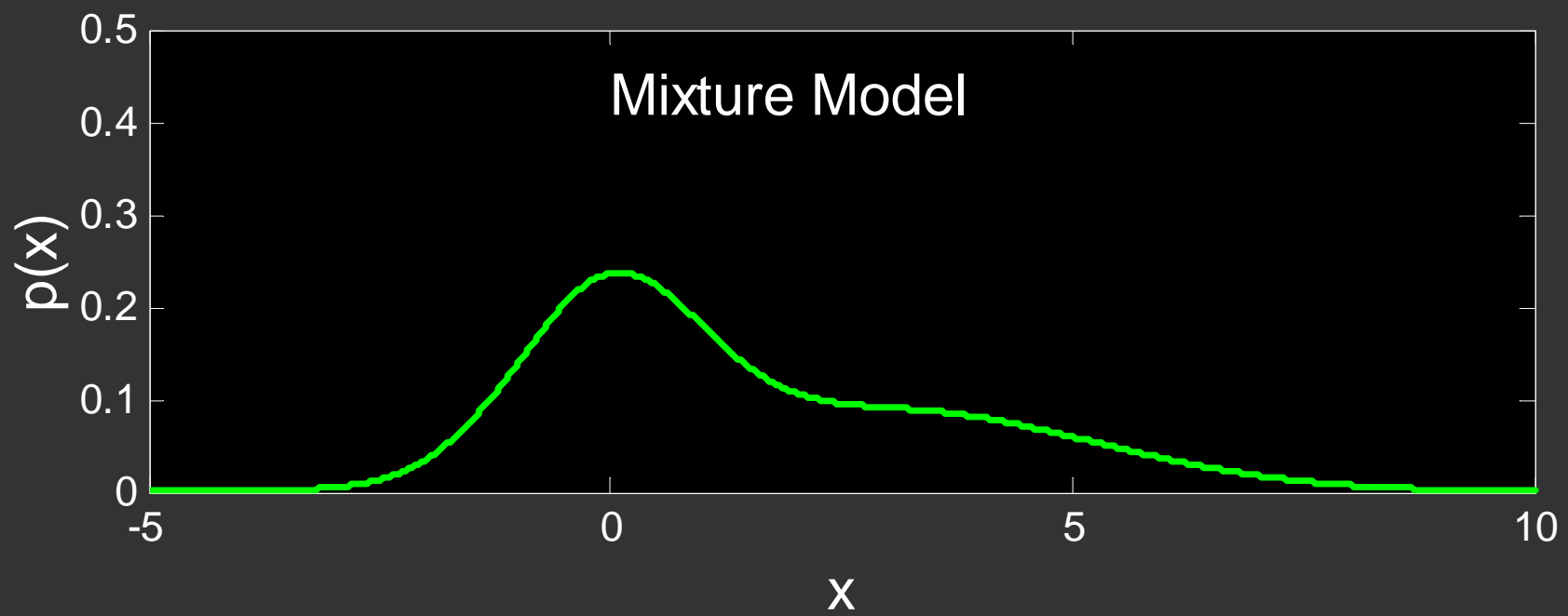
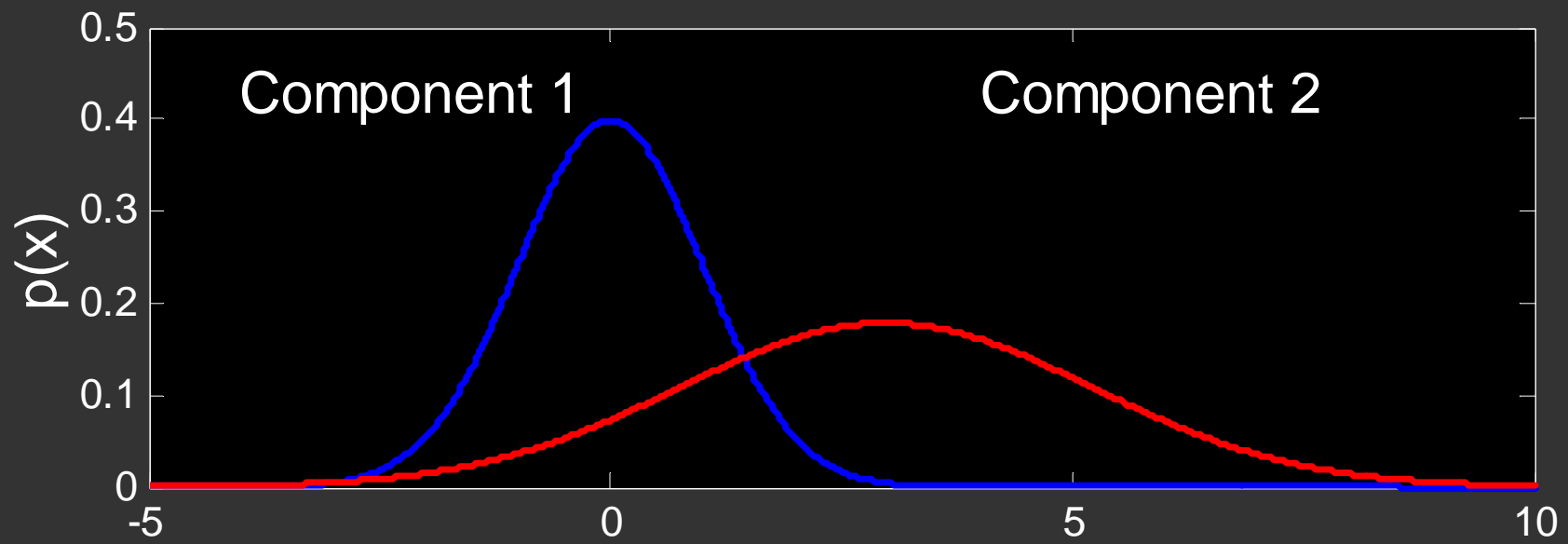


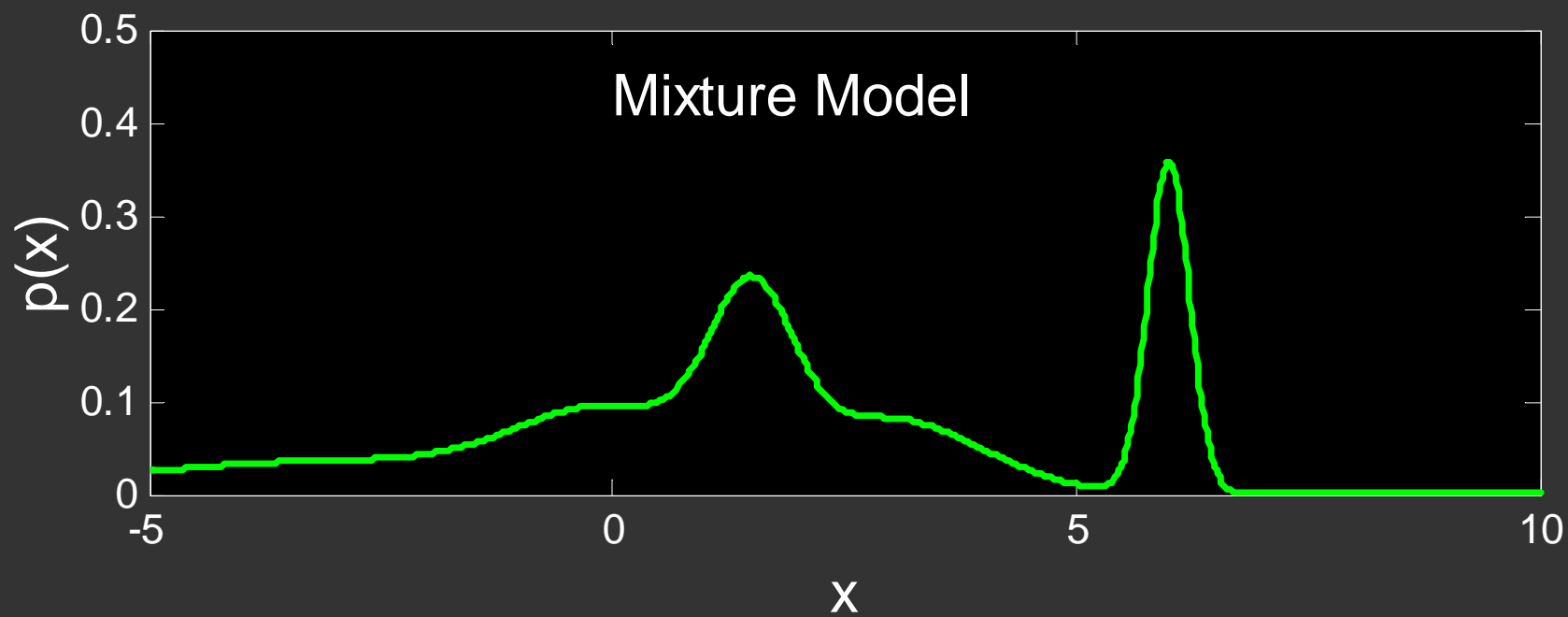
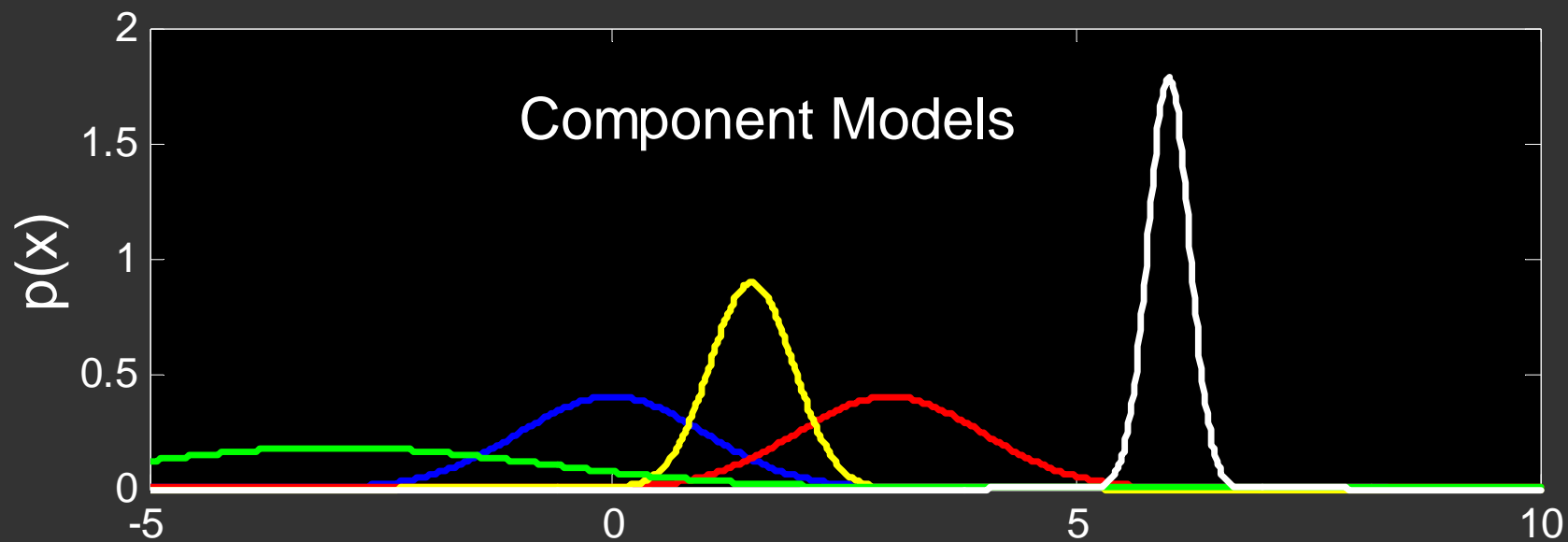
Motivation:

1. models a true process (e.g., fish example)
2. approximate state-based representation (e.g., regimes in climate data)

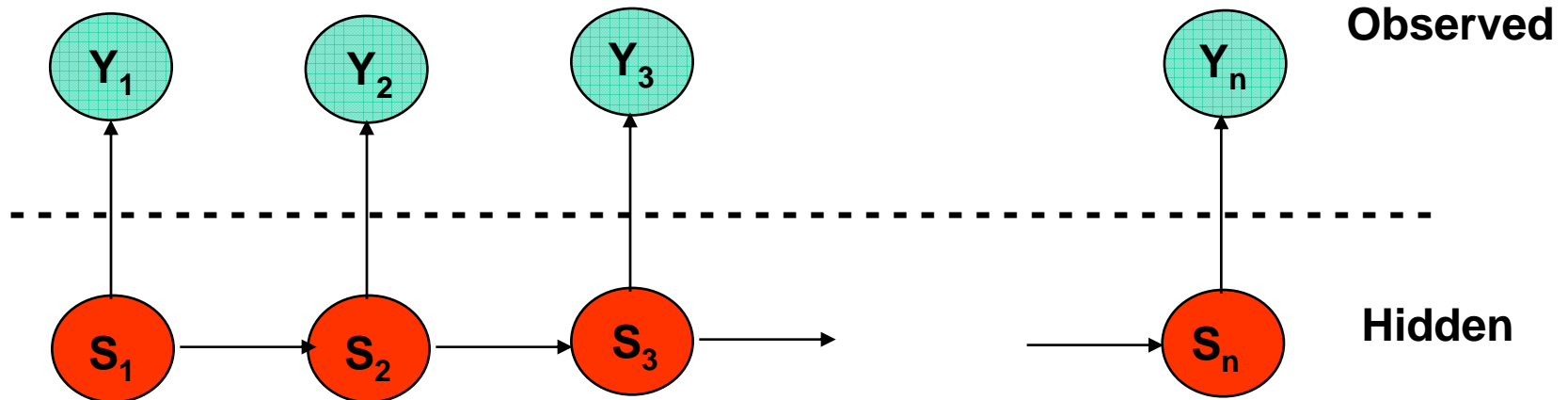




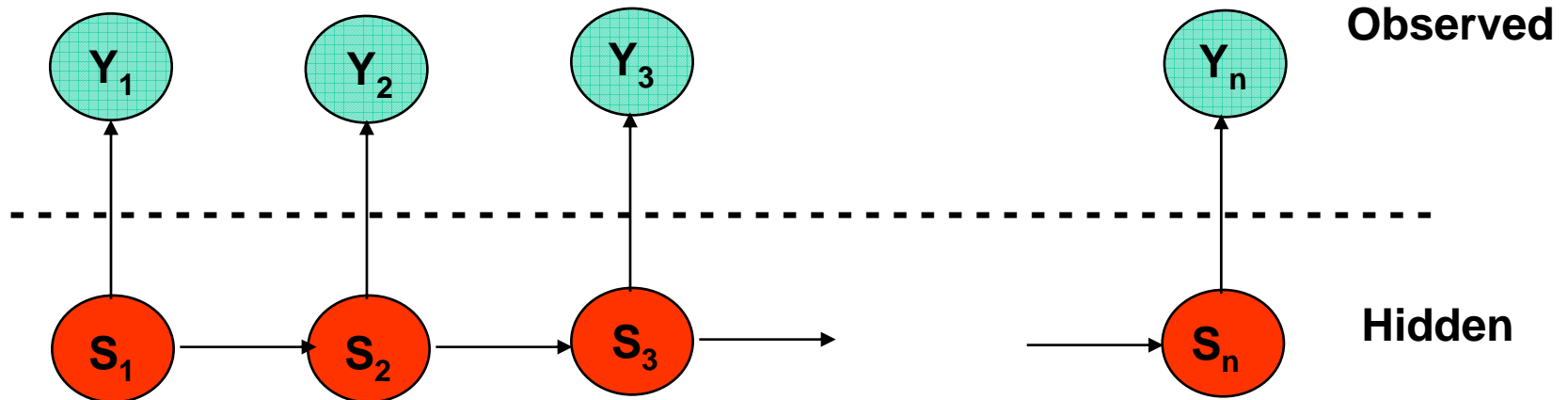




# Hidden Markov Model (HMM)



# Hidden Markov Model (HMM)



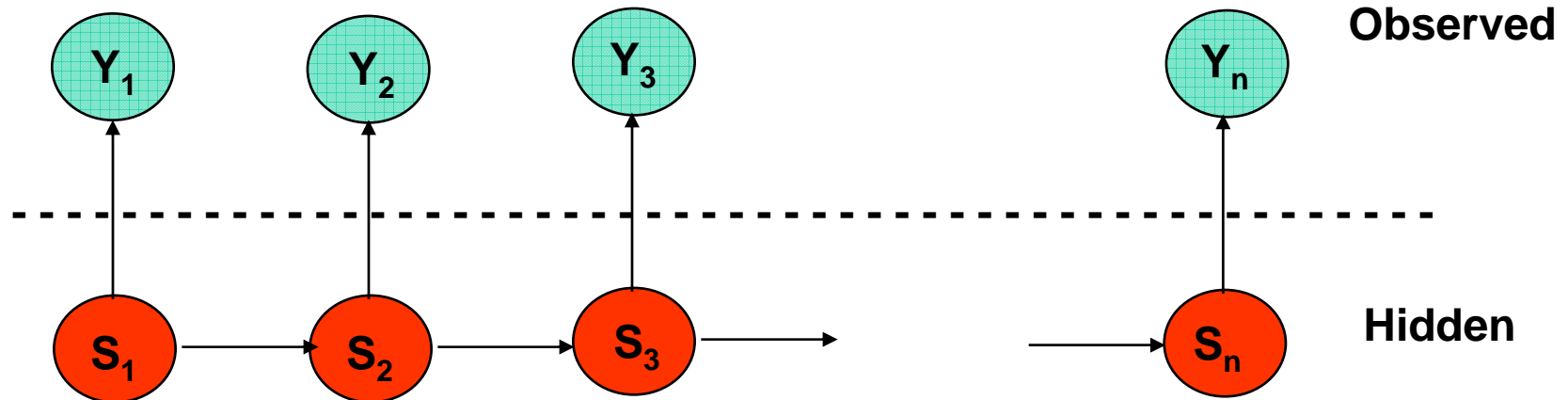
Two key independence assumptions

$$P(s_1, \dots, s_n, y_1, \dots, y_n) = \prod p(s_t | s_{t-1}) p(y_i | s_i)$$

State dynamics

Observation model

# Comments on HMMs

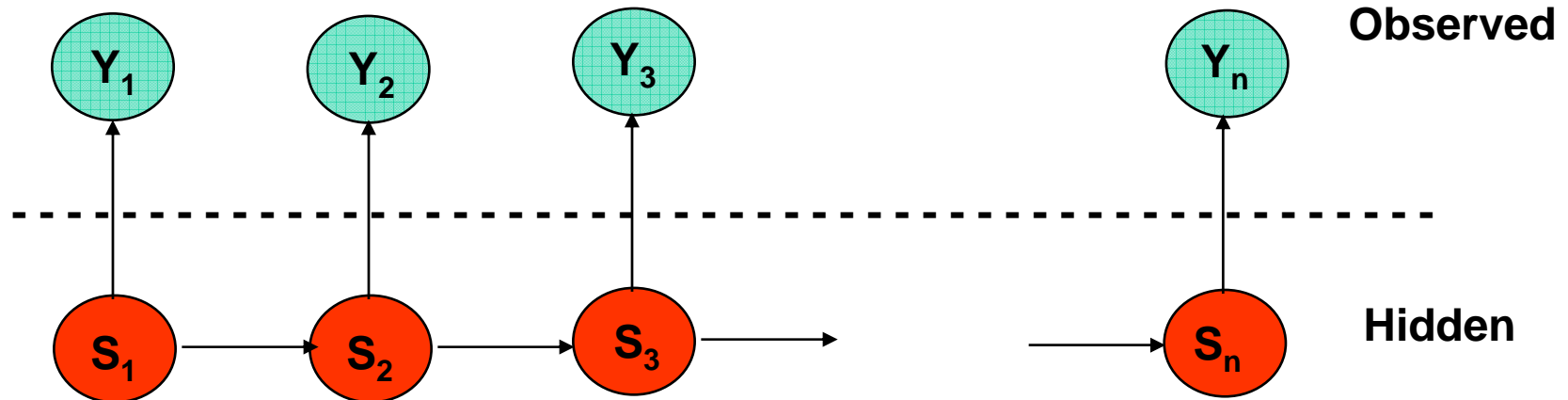


Motivation?

- S discrete:
  - > can provide non-linear switching
  - > can encode low-dim time-dependence for high-dim Y
- S is continuous, Gaussian dependencies, we have a Kalman filter

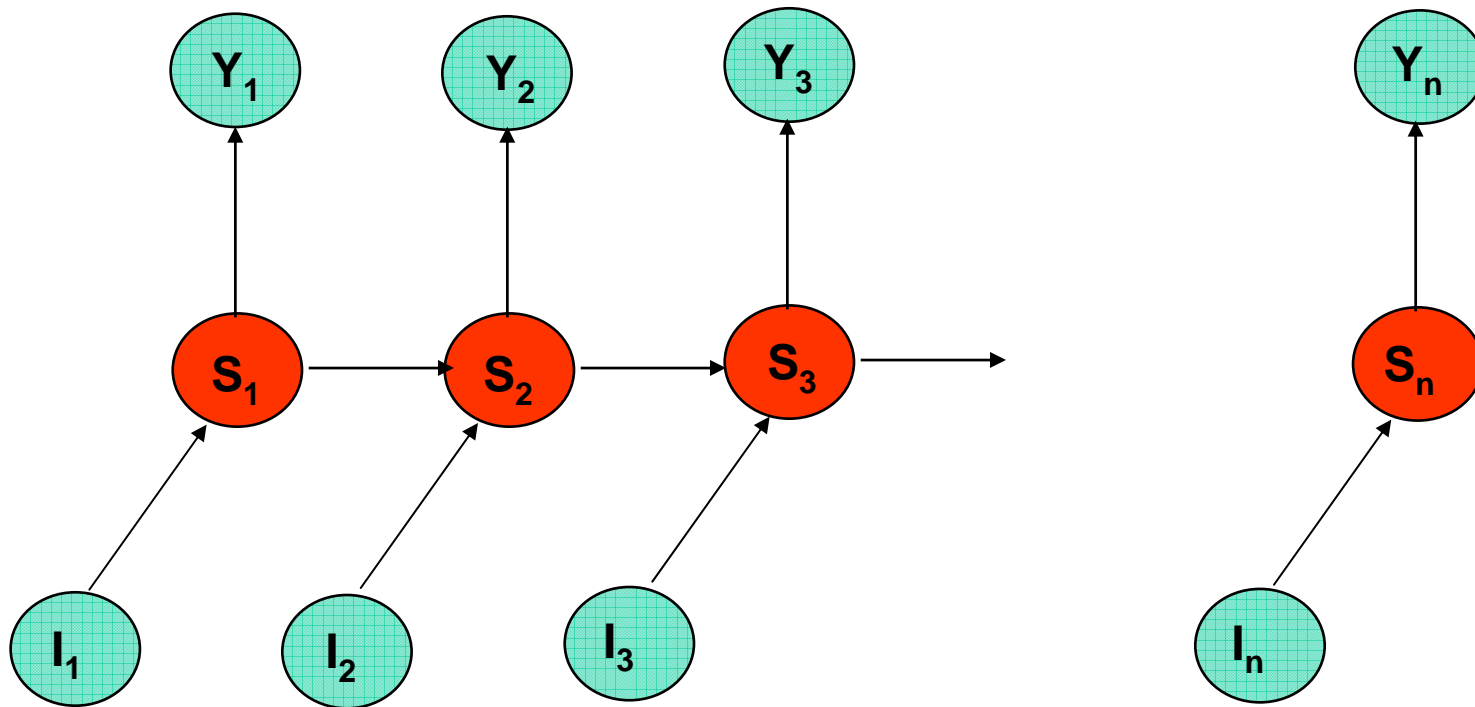
Widely used in speech recognition, protein sequence modeling, ...

# Probability Computation



- Computing  $p(S_n | y_1, \dots, y_n)$ 
  - Recursively compute
    - $p(S_1 | y_1)$
    - $p(S_2 | y_2, S_1)$  weighted by  $p(S_1 | y_1)$
    - and so on..
  - This is the MP algorithm, with  $S_1$  as the root node

# Generalizing HMMs



Inputs  $I$  provide context to influence switching, e.g., downscaling

$I$  = observed atmospheric measurements

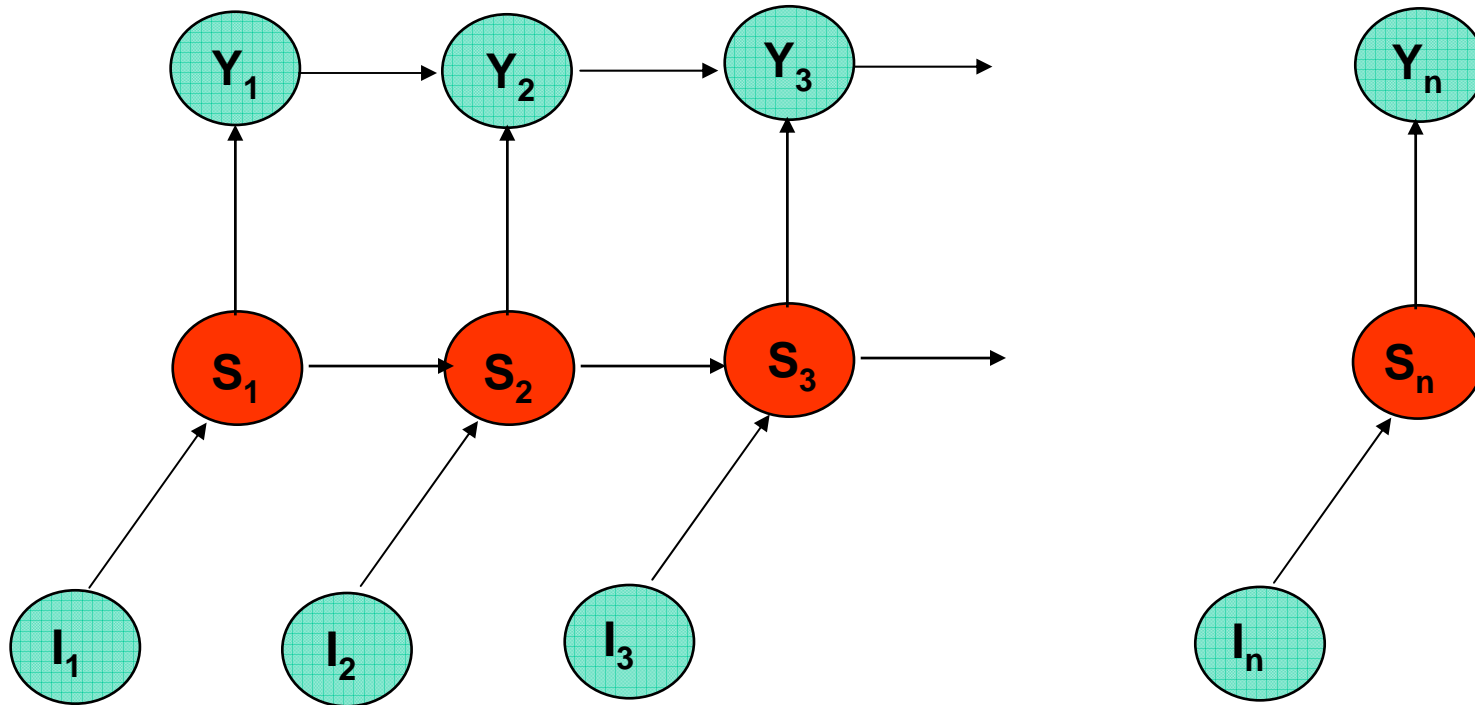
$S$  = "weather regimes"

$Y$  = observed rainfall

(Guttorp and Charles, 1994)

Model is still a tree -> inference is still linear

# Generalizing HMMs

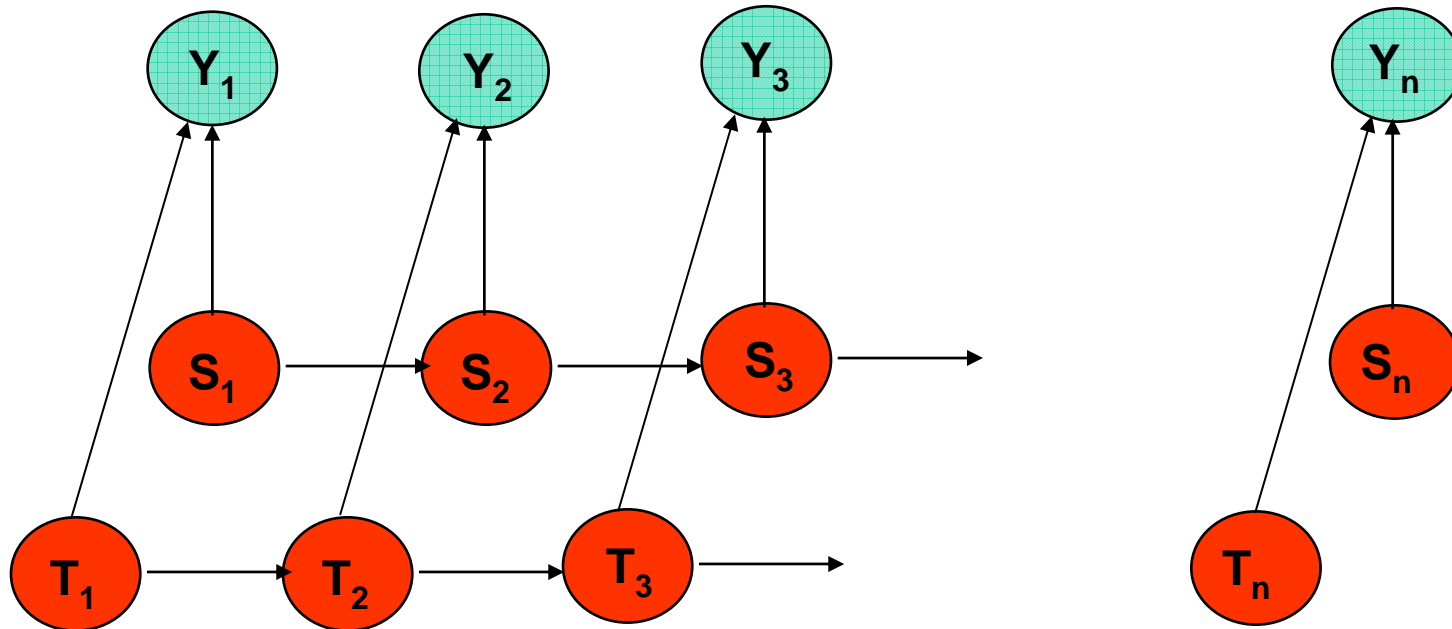


Add direct dependence between  $Y$ 's to better model persistence

Can merge each  $S_t$  and  $Y_t$  to construct a junction tree



# Generalizing HMMs



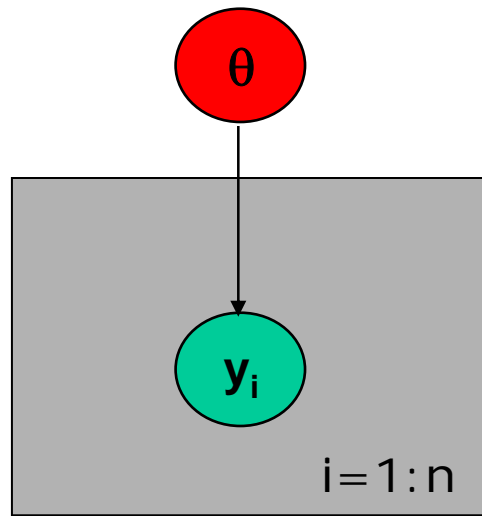
Two independent state variables,  
e.g., two processes evolving at different time-scales

# Comments on HMMs

- Non-Gaussian state-space models
  - Non-linear dynamical model for  $p(s_t | s_{t-1})$
  - Complicates probability calculations and estimation
- Integrating different measurements
  - $y$  variables can include, e.g., remote-sensing, station data,
  - Conditional independence for  $p(y_i | s_i)$
- Handling missing data
  - e.g., missing measurements  $y$  (station data)
  - average over missing data, conditioned on observed data – calculations are straightforward

# Learning Model Parameters from Data

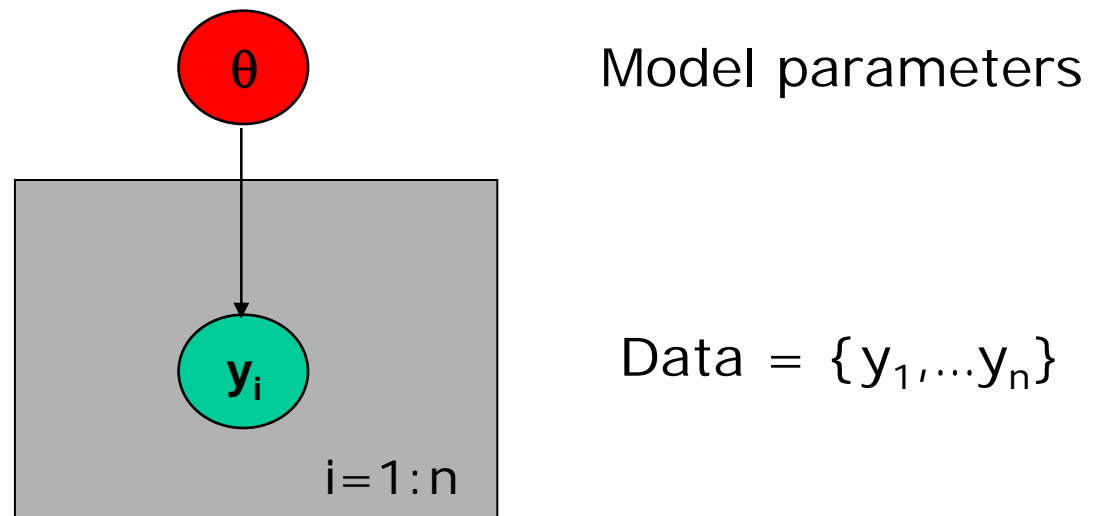
# Data and Plates



Model parameters

Data =  $\{y_1, \dots, y_n\}$

# Maximum Likelihood

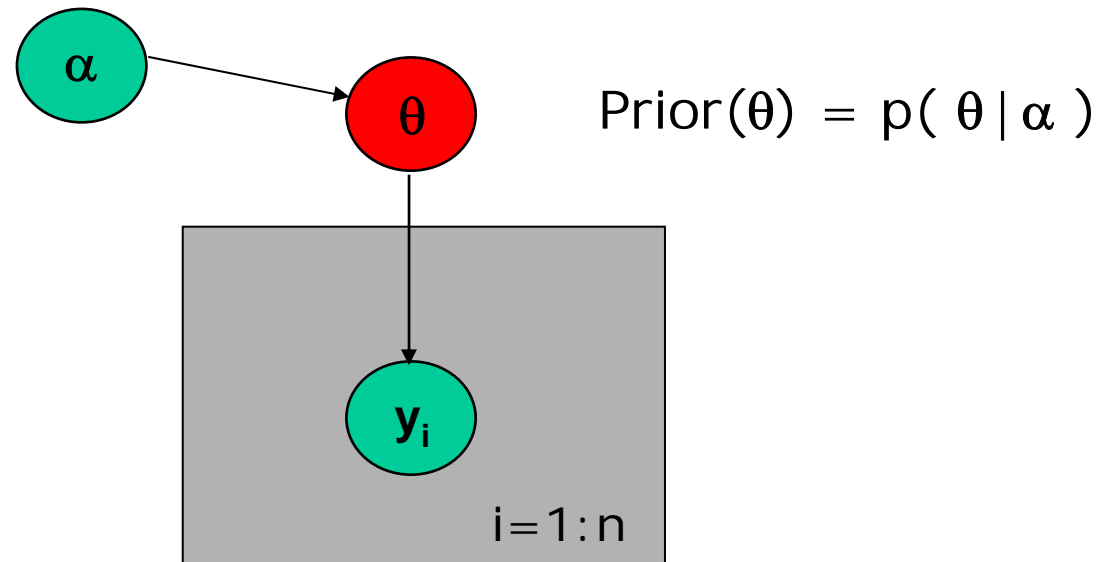


$$\text{Likelihood}(\theta) = p(\text{Data} \mid \theta) = \prod p(y_i \mid \theta)$$

Maximum Likelihood:

$$\theta_{\text{ML}} = \arg \max \{ \text{Likelihood}(\theta) \}$$

# Bayesian Estimation



Maximum A Posteriori:

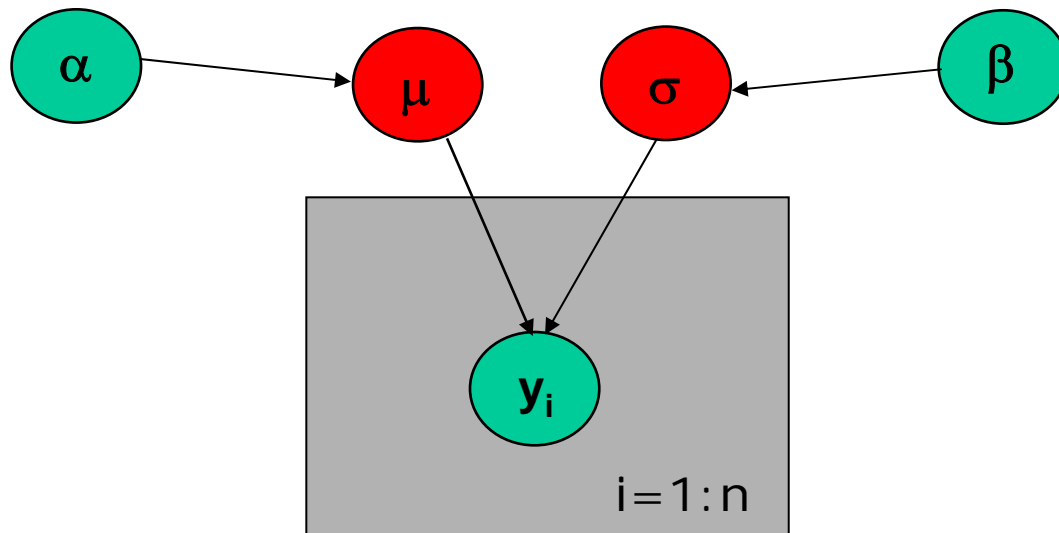
$$\theta_{\text{MAP}} = \arg \max \{ \text{Likelihood}(\theta) \times \text{Prior}(\theta) \}$$

Fully Bayesian:

$$p(\theta | \text{Data}) = p(\text{Data} | \theta) p(\theta) / p(\text{Data})$$

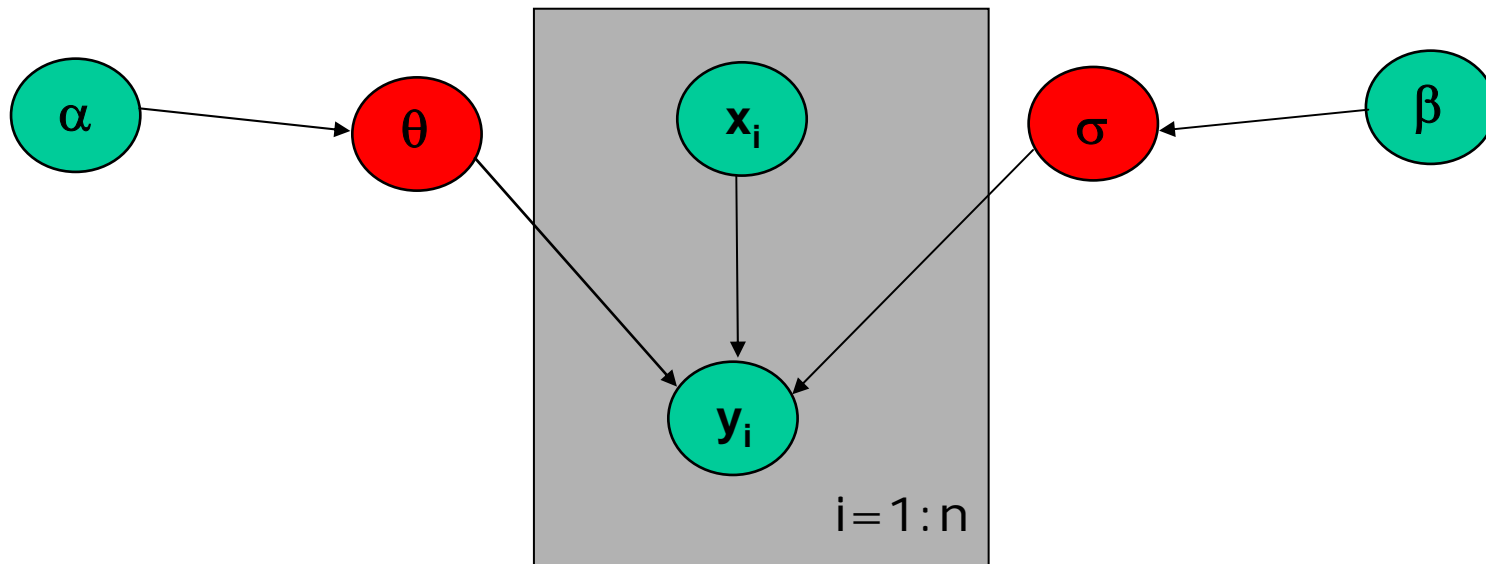
Note: "learning"  $\leftrightarrow$  inference in a graphical model

# Example: Gaussian Model



Note: priors and parameters are assumed independent here

# Example: Bayesian Regression

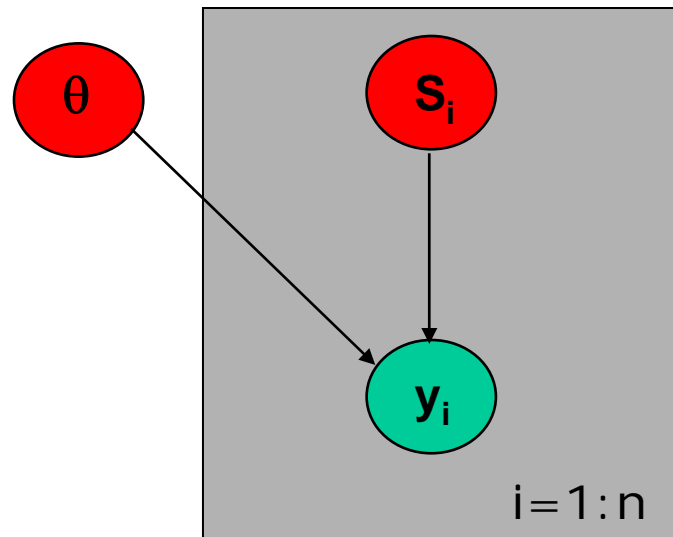


Model:  $y_i = f[x_i; \theta] + e, \quad e \sim N(0, \sigma^2)$

$$p(y_i | x_i) = N(f[x_i; \theta], \sigma^2)$$



# Mixture Model



$$\text{Likelihood}(\theta) p(\theta) = p(\text{Data} \mid \theta) p(\theta)$$

$$= p(\theta) \prod_i p(y_i \mid \theta)$$

$$= p(\theta) \prod_i \left[ \sum_k p(y_i \mid s_i = k, \theta) p(s_i = k) \right]$$

# Estimation with Missing Data

Dempster, Laird, Rubin, 1977

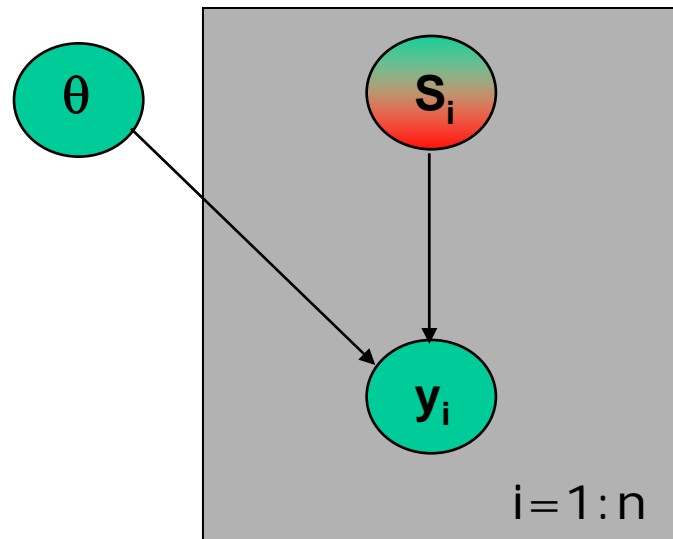
- Guess at some initial parameters  $\theta^0$
- E-step
  - For each case, and each unknown variable compute  $p(S \mid \text{known data}, \theta^0)$
- M-step:
  - Maximize  $p(\theta \mid \text{data})$  using  $p(S \mid \dots)$
  - This yields new parameter estimates  $\theta^1$
- This is the EM algorithm:
  - converges to a (local) maximum of  $p(\theta \mid \text{data})$

# Estimation with Missing Data

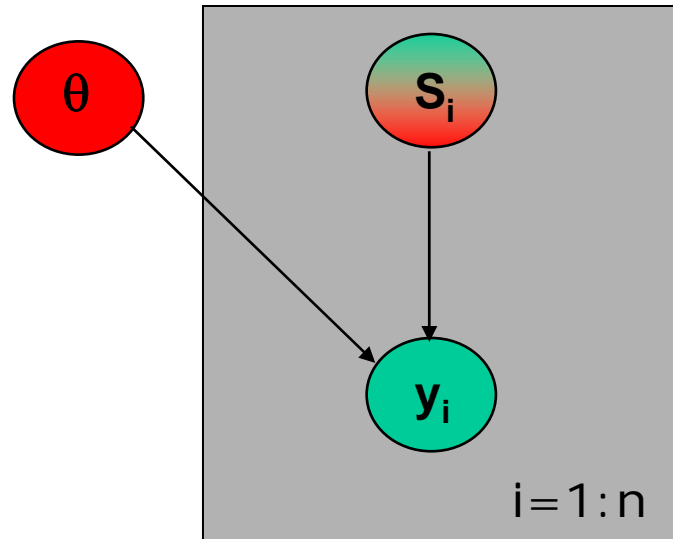
Dempster, Laird, Rubin, 1977

- Guess at some initial parameters  $\theta^0$
- E-step (Computation in a graph)
  - For each case, and each unknown variable compute  $p(S \mid \text{known data}, \theta^0)$
- M-step: (Multivariate optimization)
  - Maximize  $p(\theta \mid \text{data})$  using  $p(S \mid \dots)$
  - This yields new parameter estimates  $\theta^1$
- This is the EM algorithm:
  - converges to a (local) maximum of  $p(\theta \mid \text{data})$

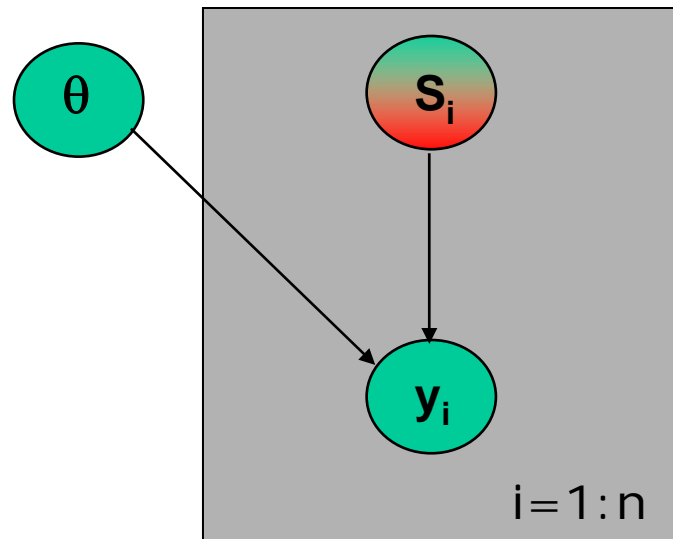
# E-Step



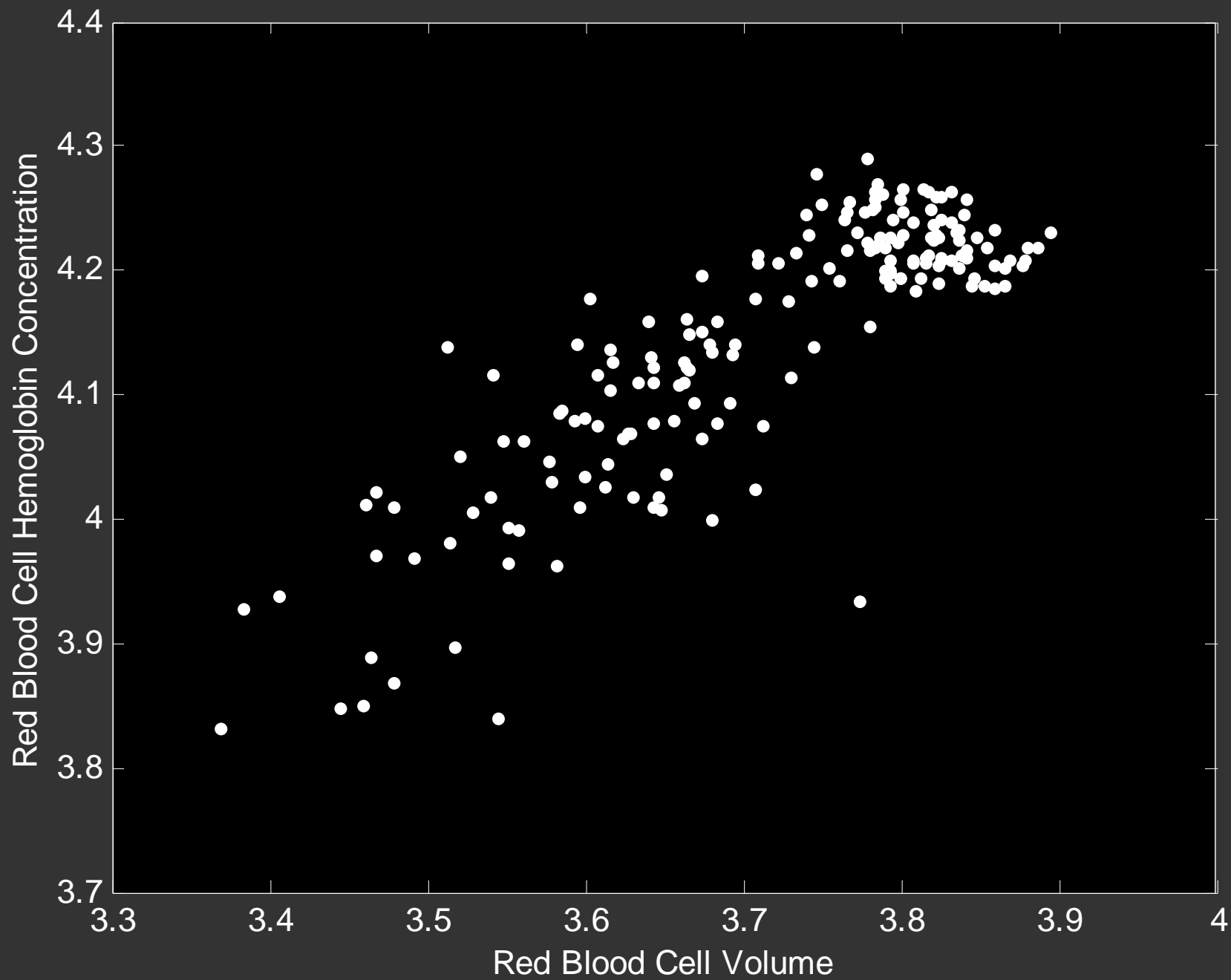
# M-Step



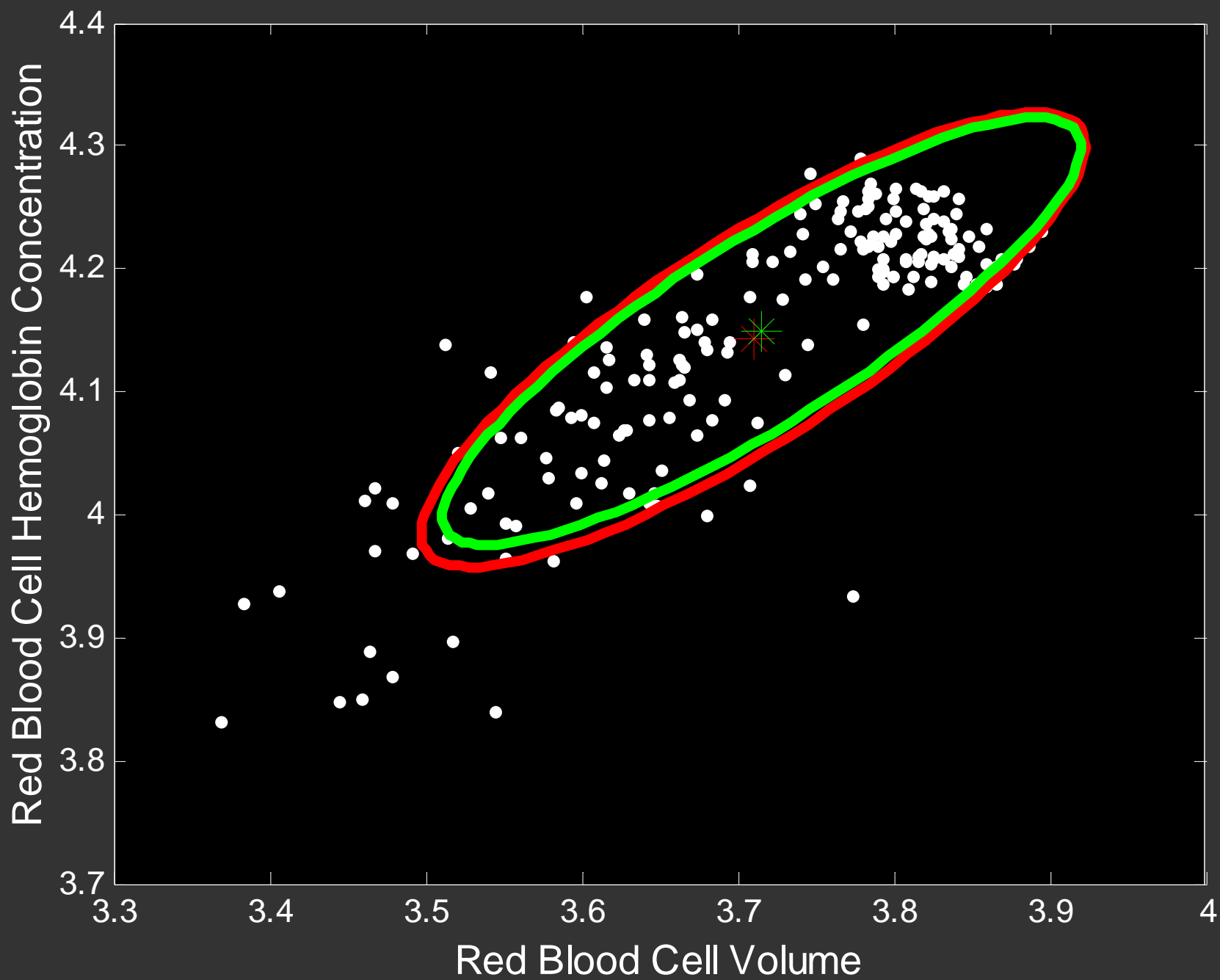
# E-Step



# ANEMIA PATIENTS AND CONTROLS

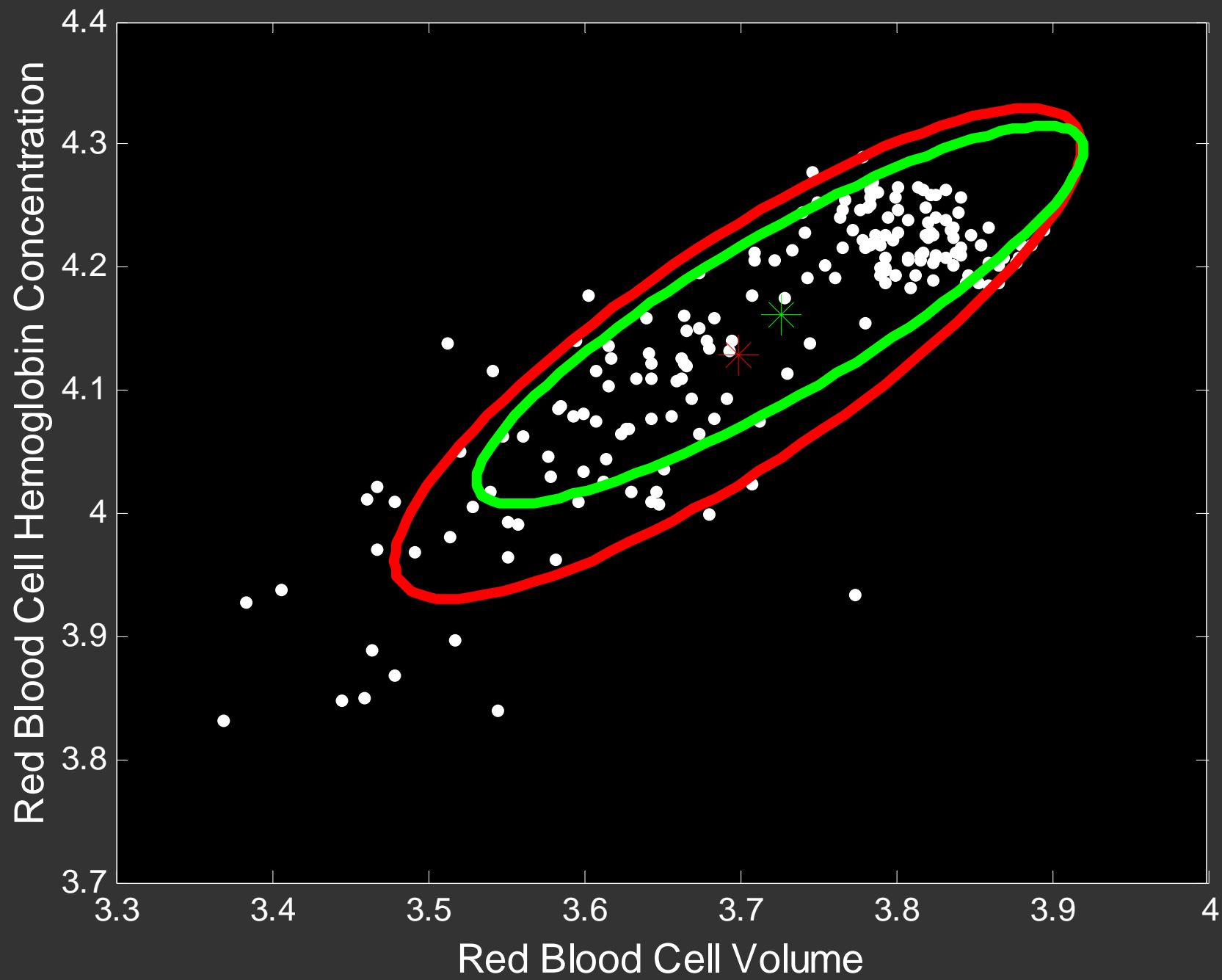


EM ITERATION 1

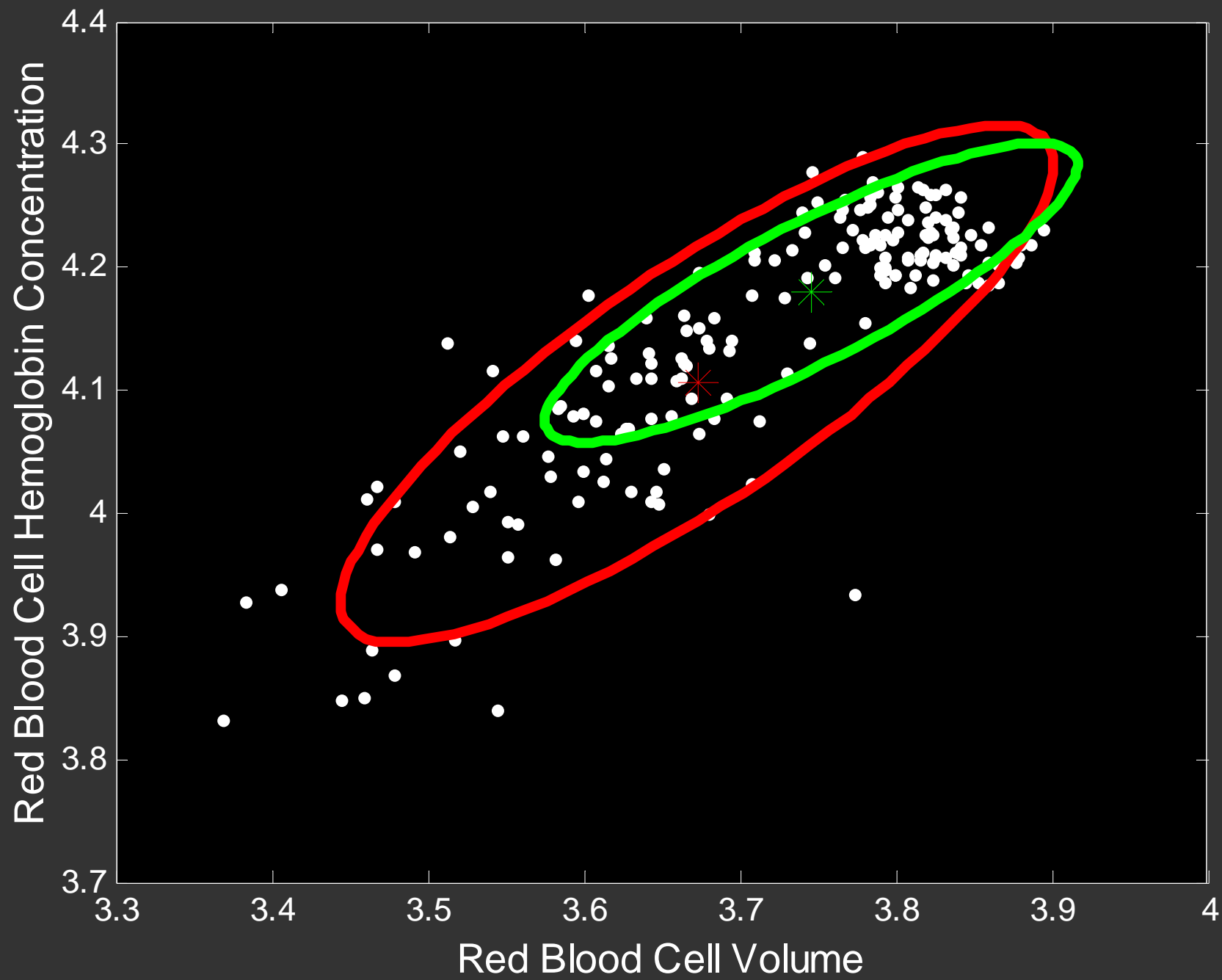




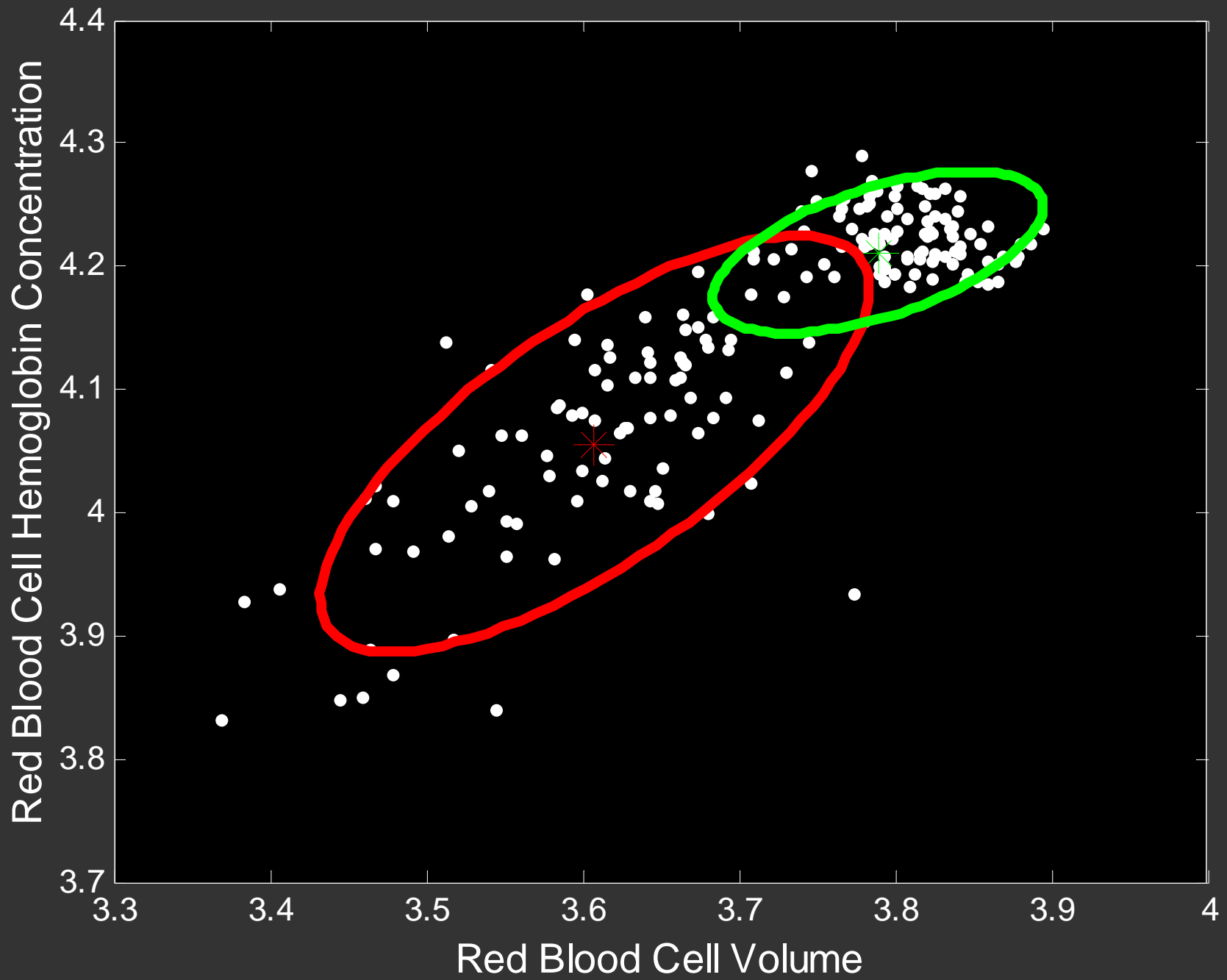
EM ITERATION 3



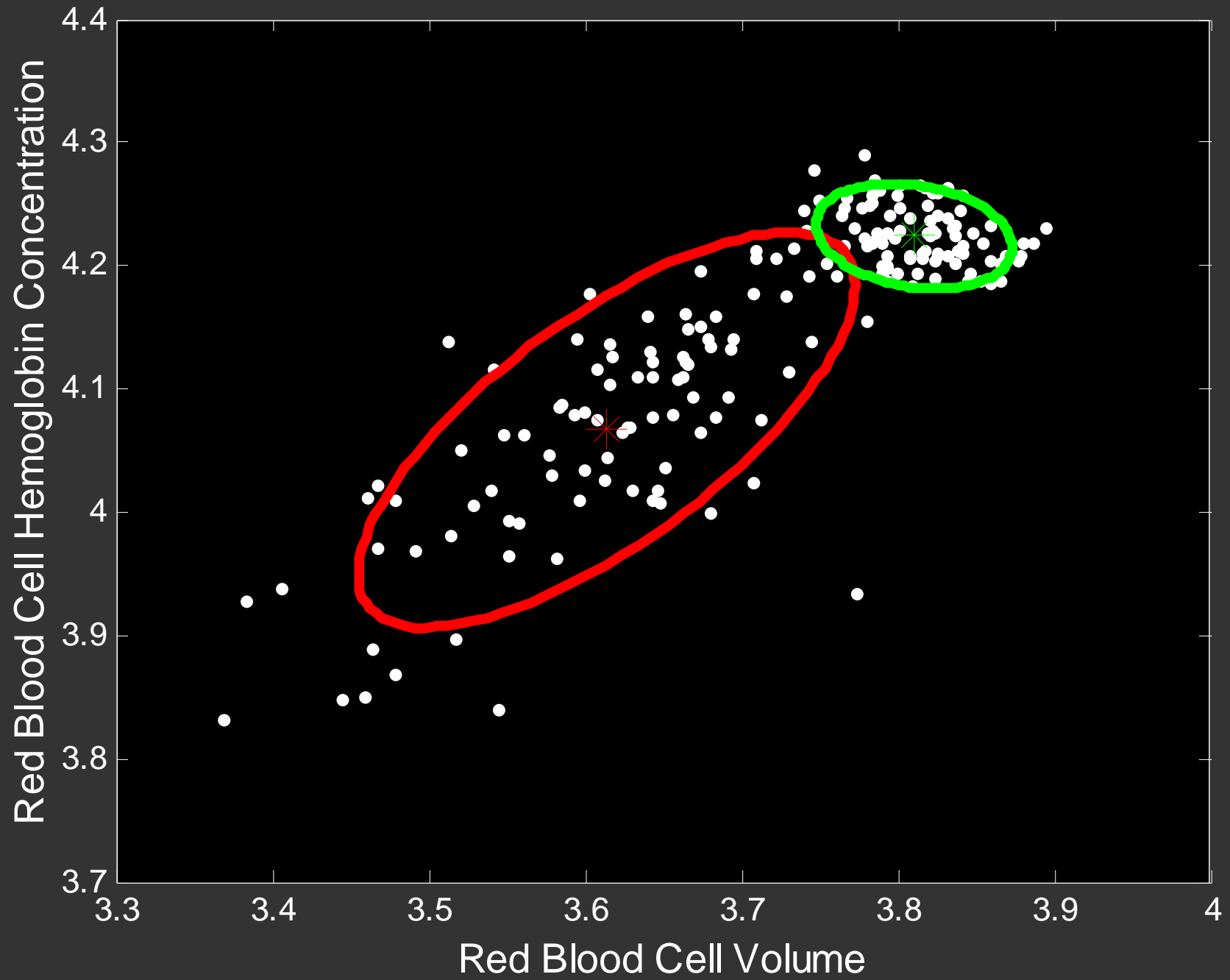
EM ITERATION 5



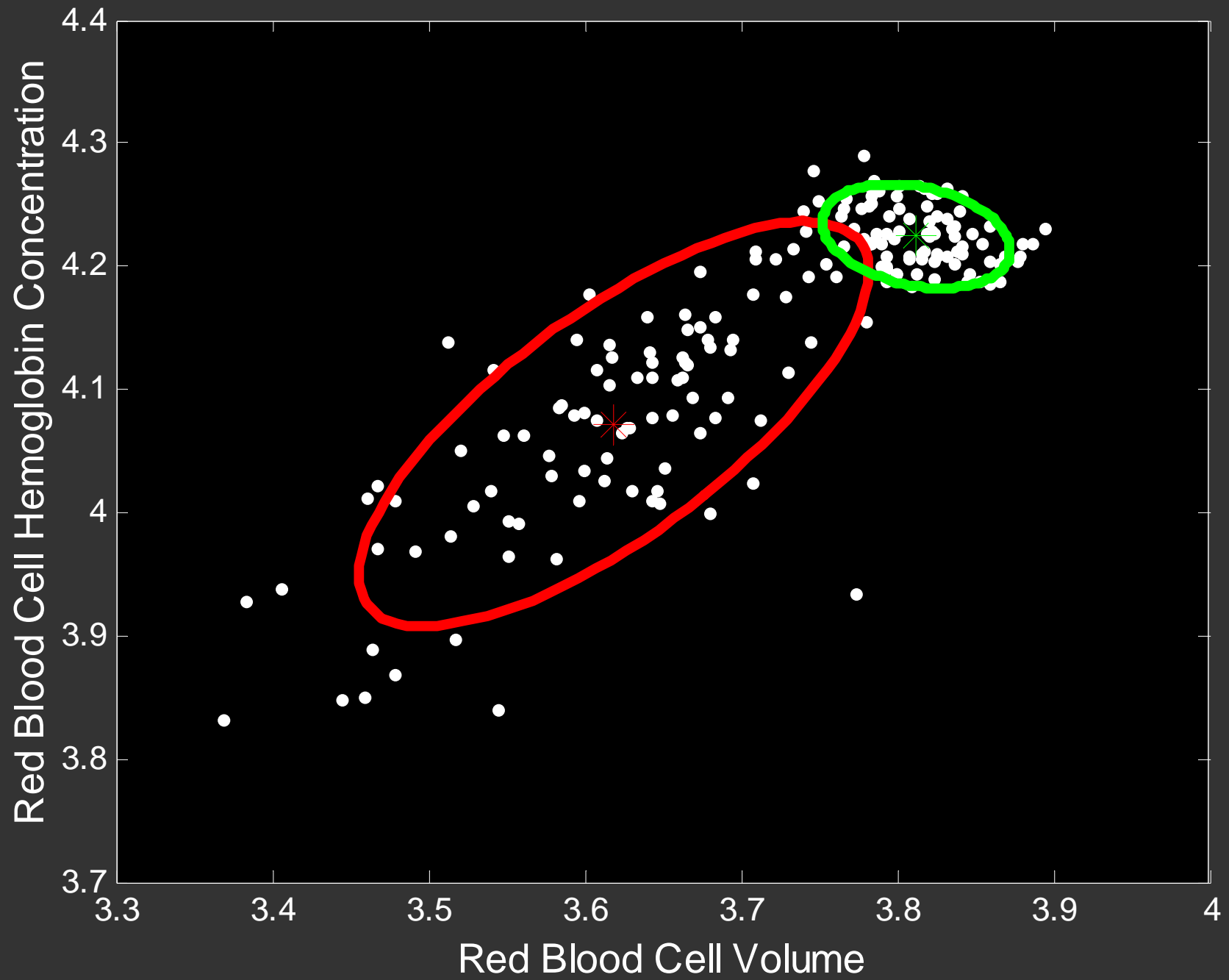
EM ITERATION 10



EM ITERATION 15

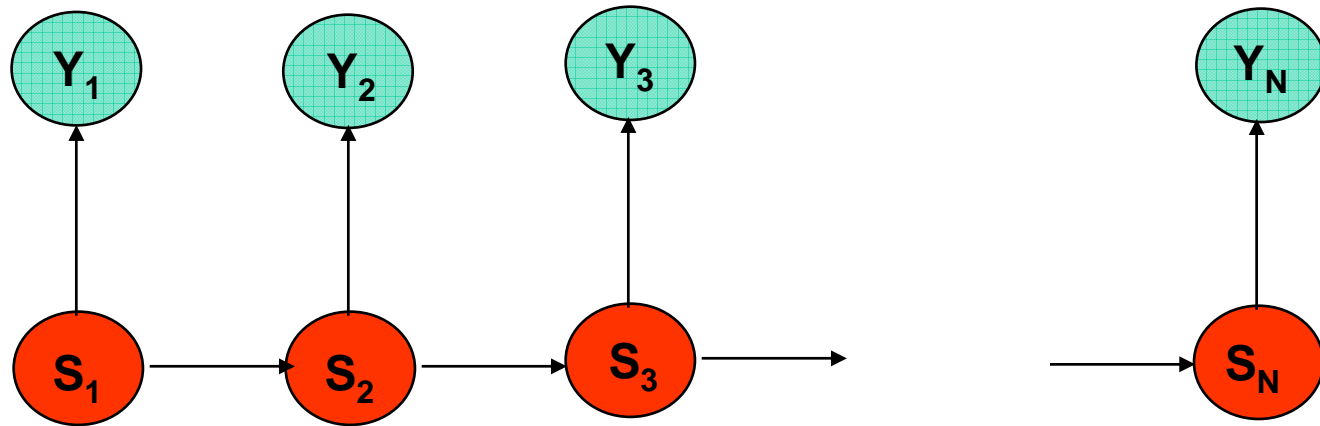


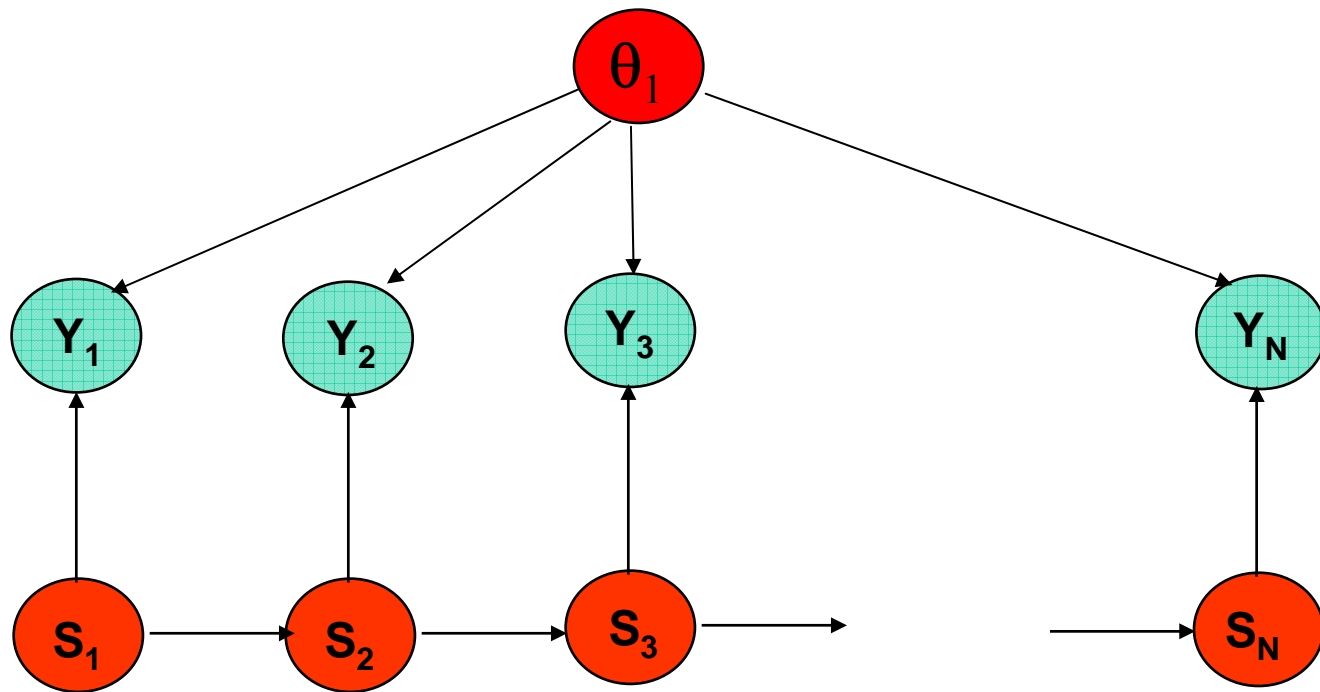
EM ITERATION 25



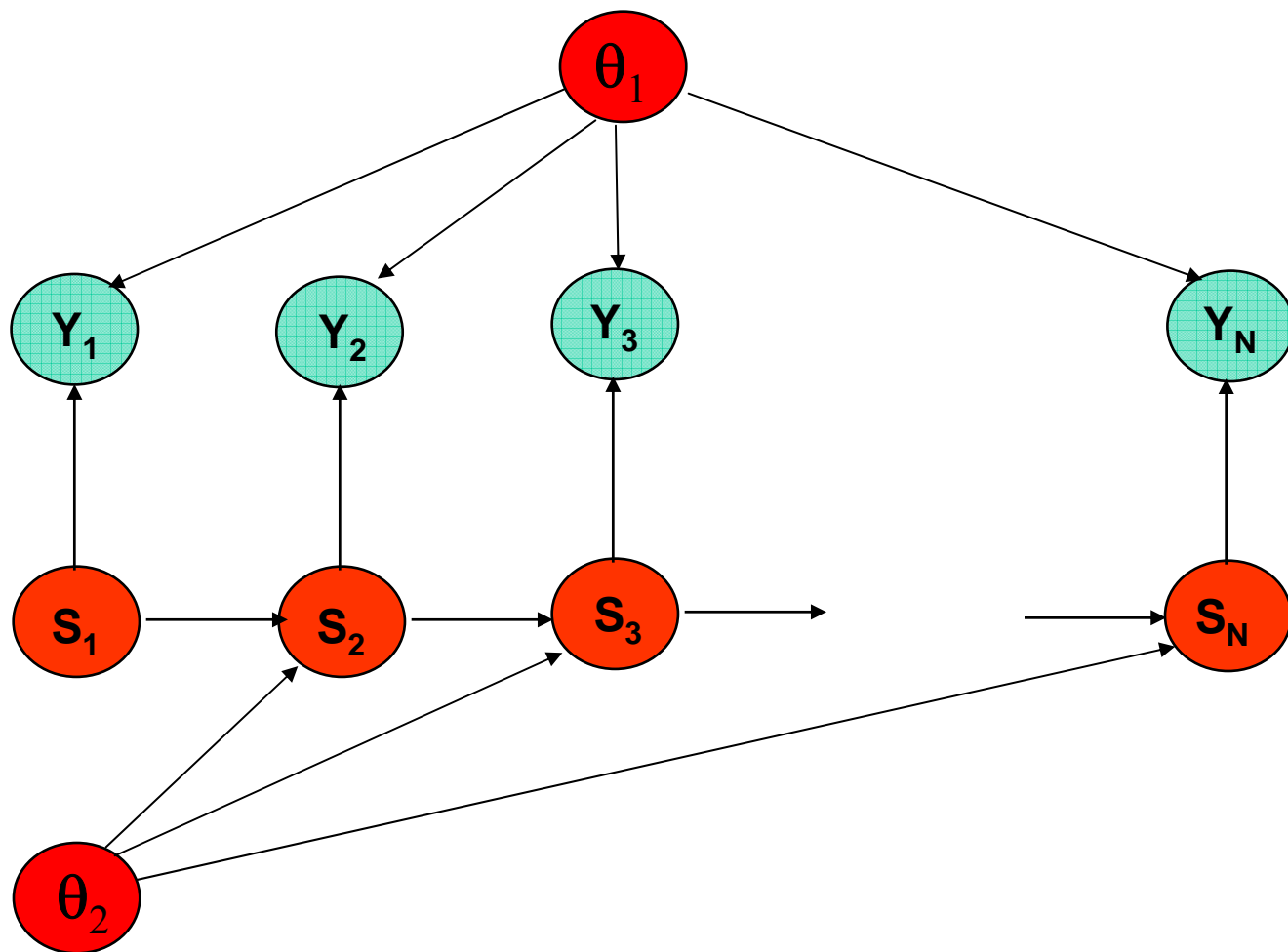


# HMMs



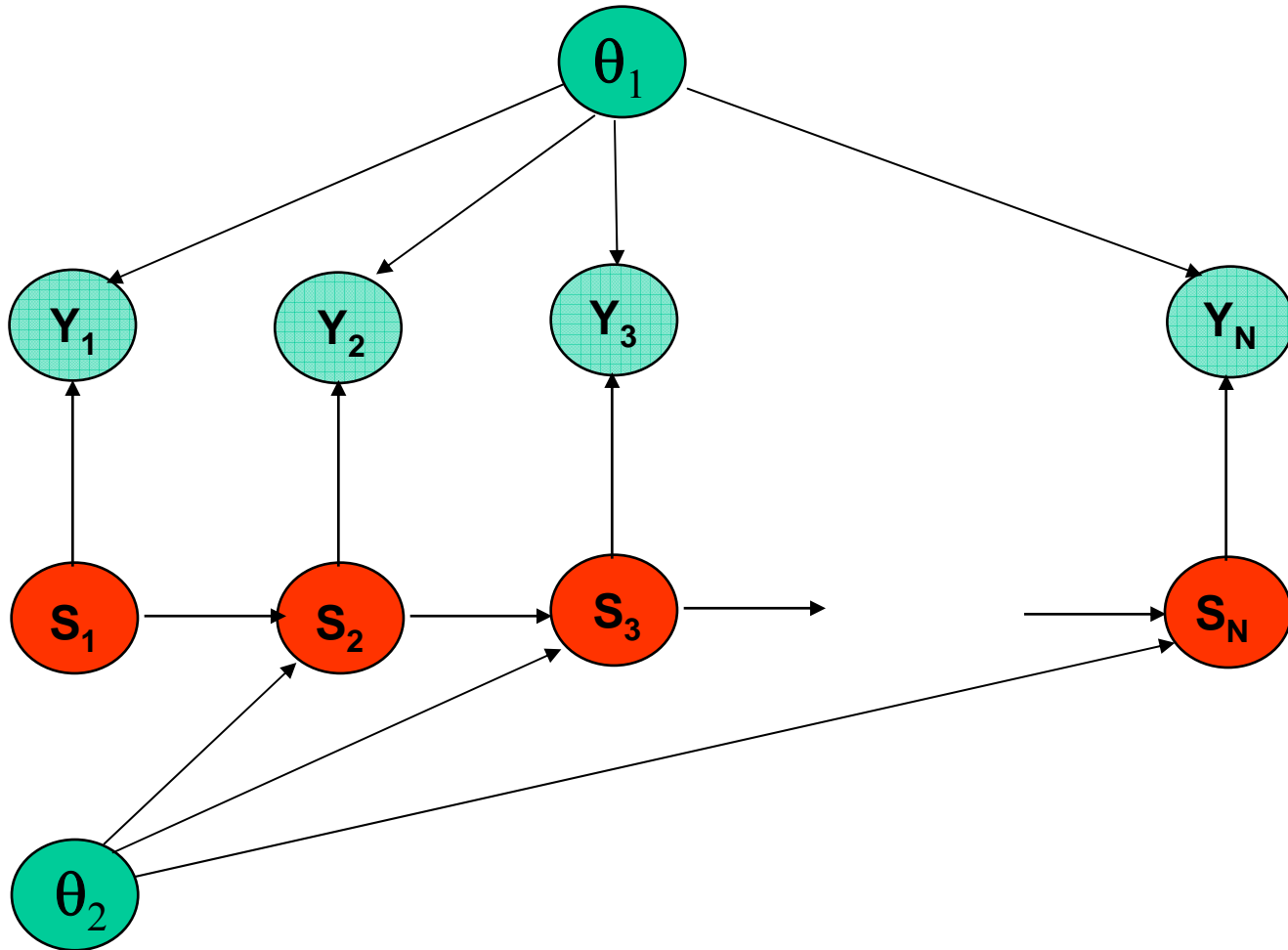






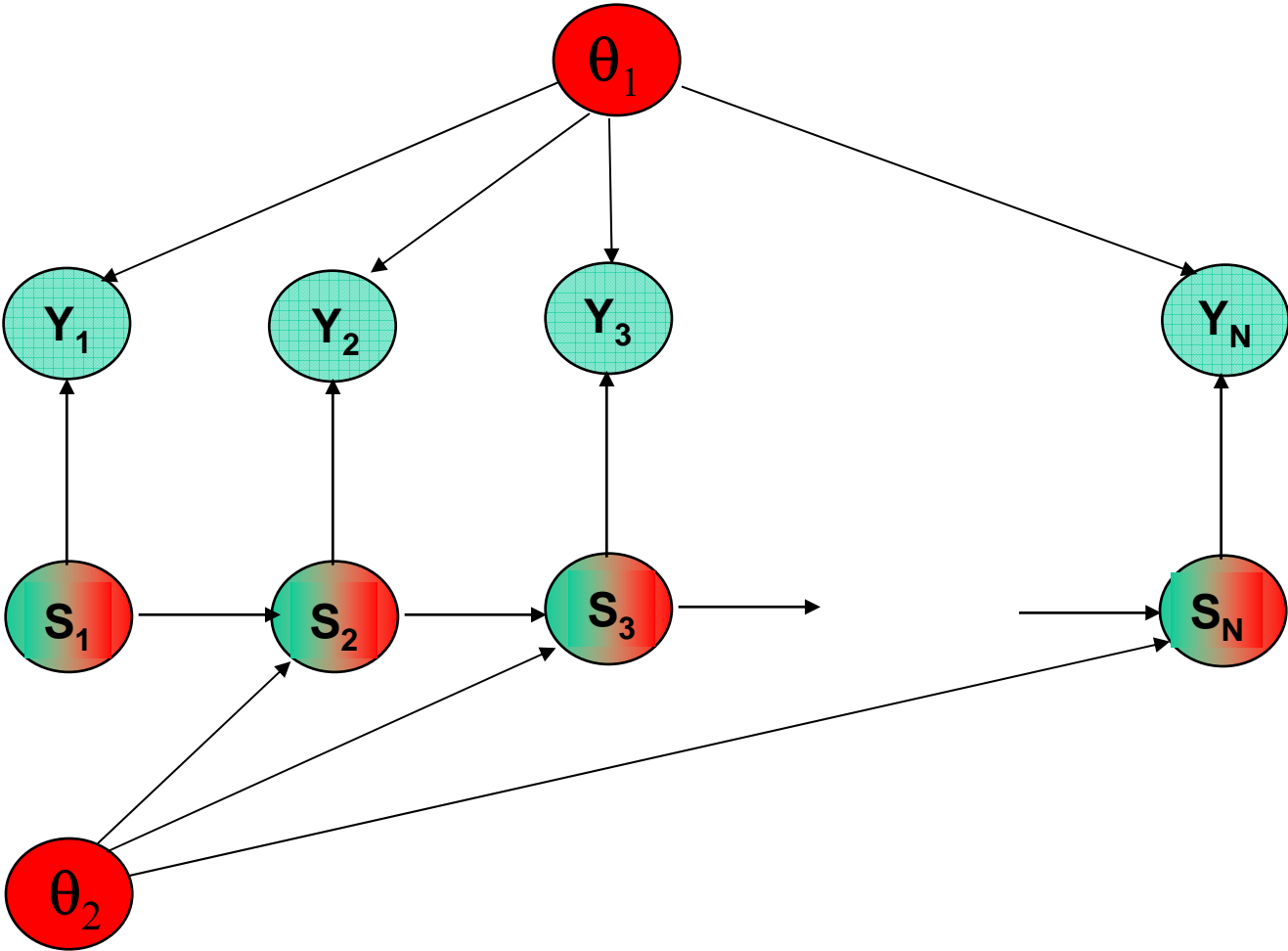
# E-Step

Compute  $p(\mathbf{s} \mid \theta, \mathbf{y})$ , linear time



# M-Step

Find  $\theta$  that maximizes  $p(\mathbf{y}|\theta)p(\theta) = \sum p(\mathbf{y},\mathbf{s}|\theta) p(\theta)$



Example 1:

## Simulating and Forecasting Seasonal Rainfall Data

Joint work with:

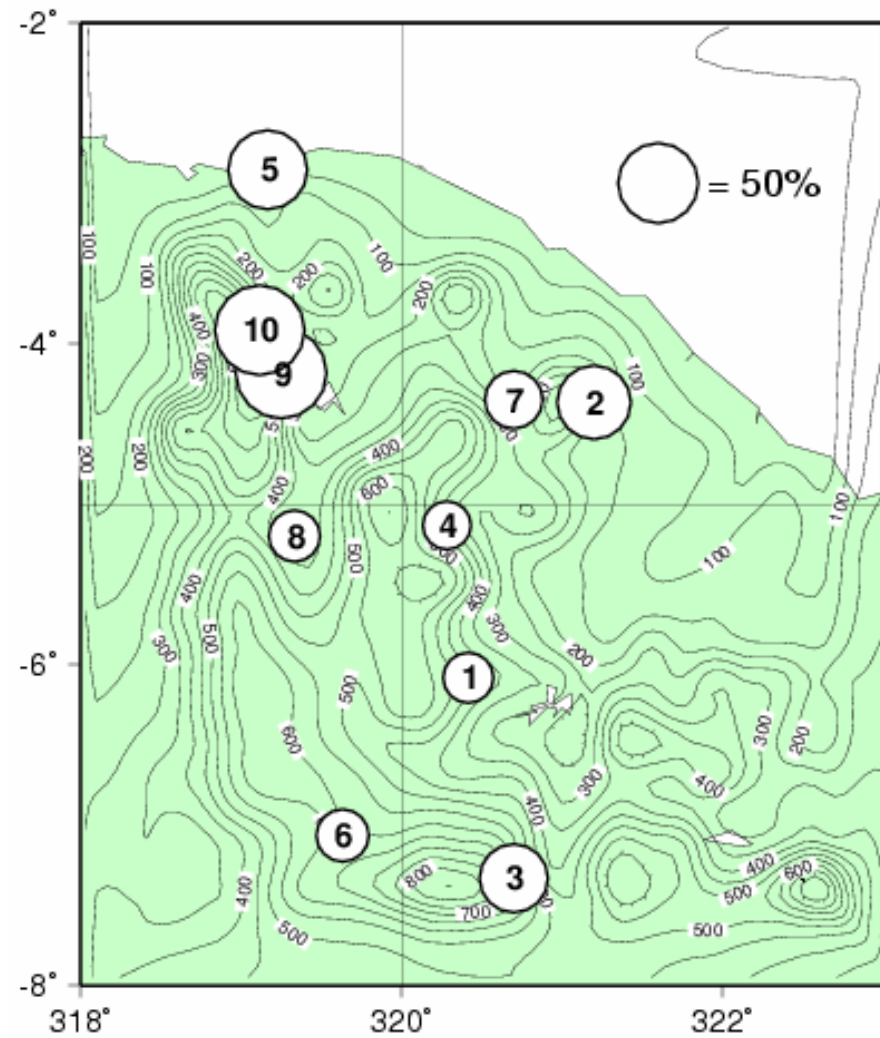
Andy Robertson, International Research Institute for Climate Prediction  
Sergey Kirshner, Department of Computer Science, UC Irvine

Robertson, Kirshner, Smyth, Hidden Markov models for modeling daily rainfall occurrence over Brazil, *Journal of Climate*, 17(22):4407-4424, November 2004.

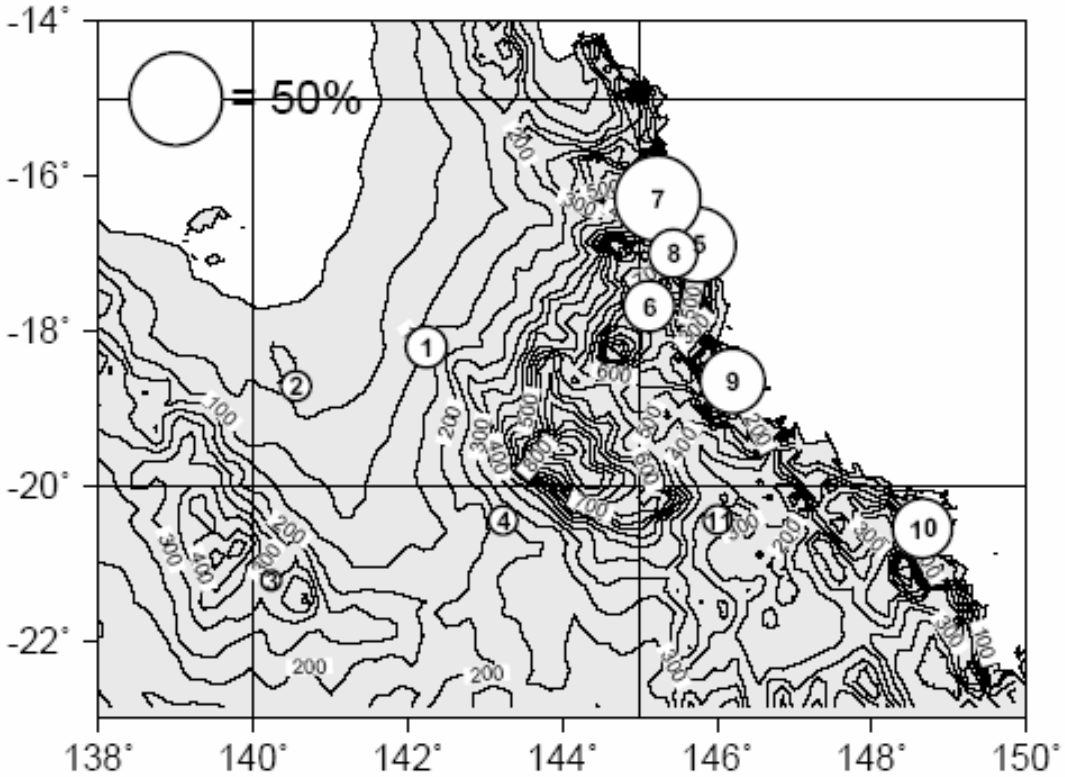
# Spatio-Temporal Rainfall Data

Northeast Brazil 1975-2002

90-day time series  
24 years  
10 stations



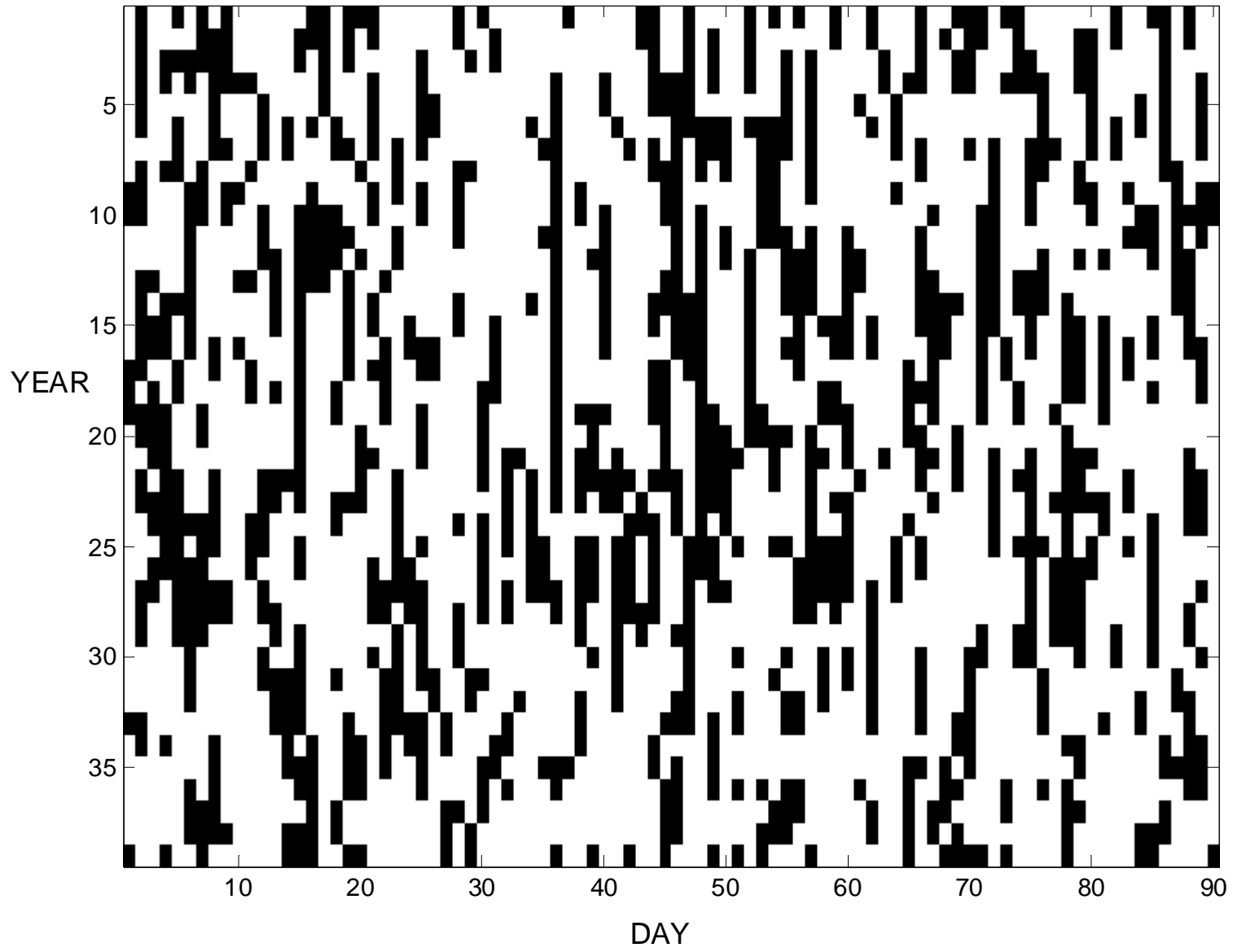
# N. Queensland Rainfall Station Oct-Apr Climatology



# Modeling Goals

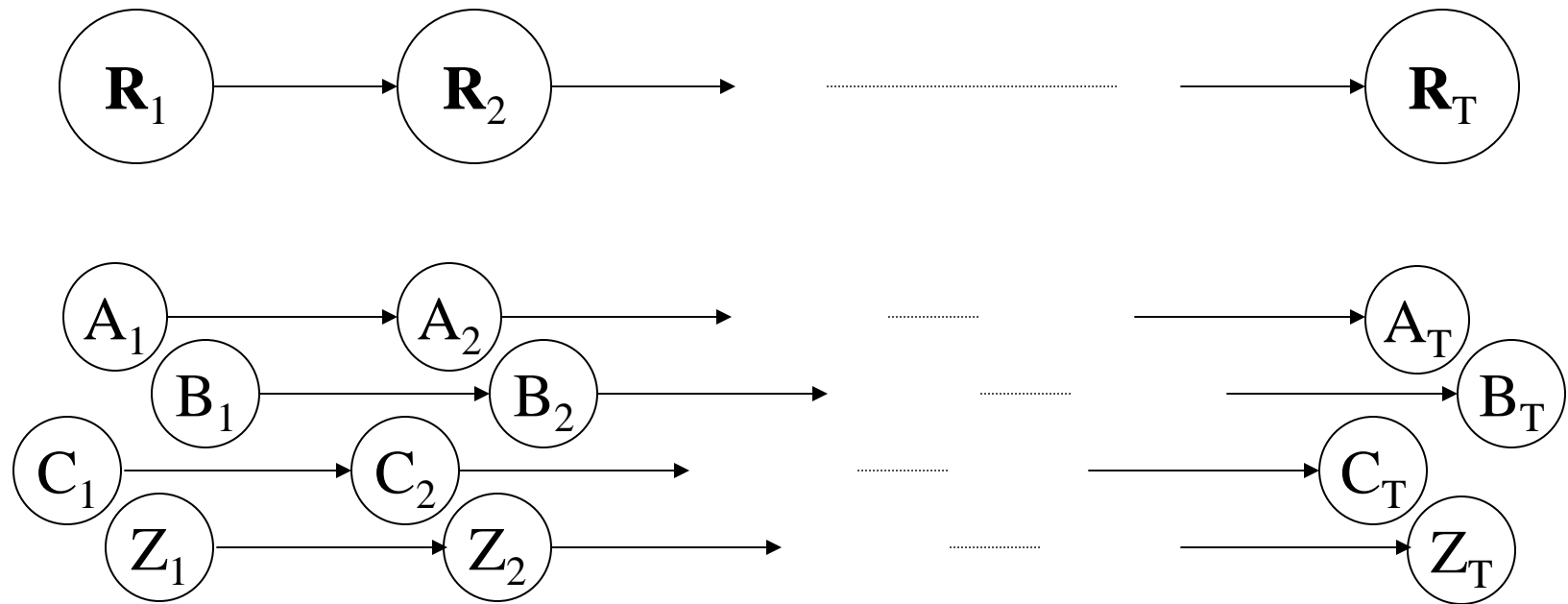
- “Downscaling”
  - From GCM output to daily local time-series for crop yield models
- Prediction
  - e.g., “hindcasting” of missing data
- Understanding
  - Relation of precip interannual variability to climate change

DATA FOR ONE RAIN-STATION





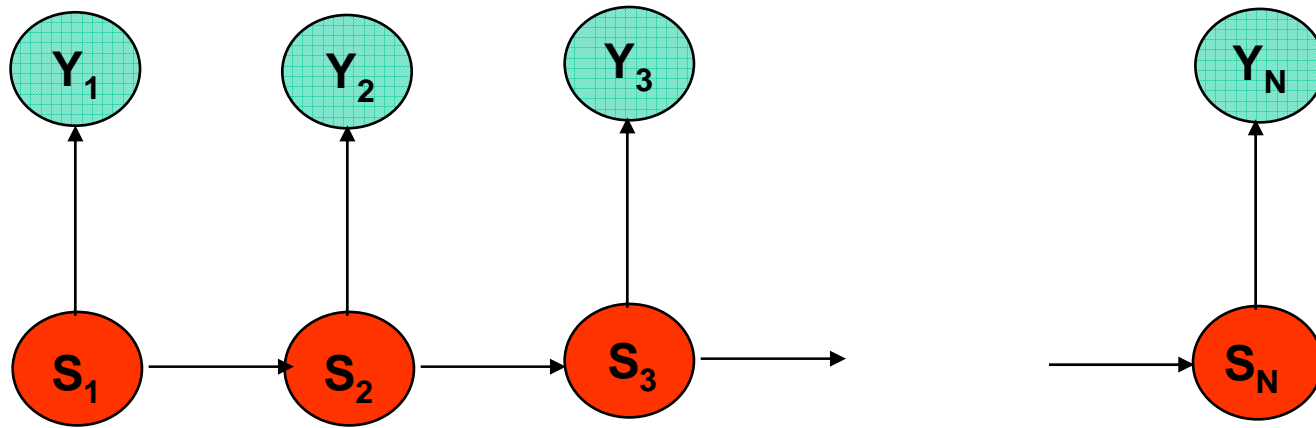
# Weather Generator



$$P(\mathbf{R}_{1:T}) = P(\mathbf{R}_1) \prod_{t=2}^T P(\mathbf{R}_t | \mathbf{R}_{t-1}) = \prod_{c \in \{A, \dots, Z\}} \left( P(c_1) \prod_{t=2}^T P(c_t | c_{t-1}) \right)$$

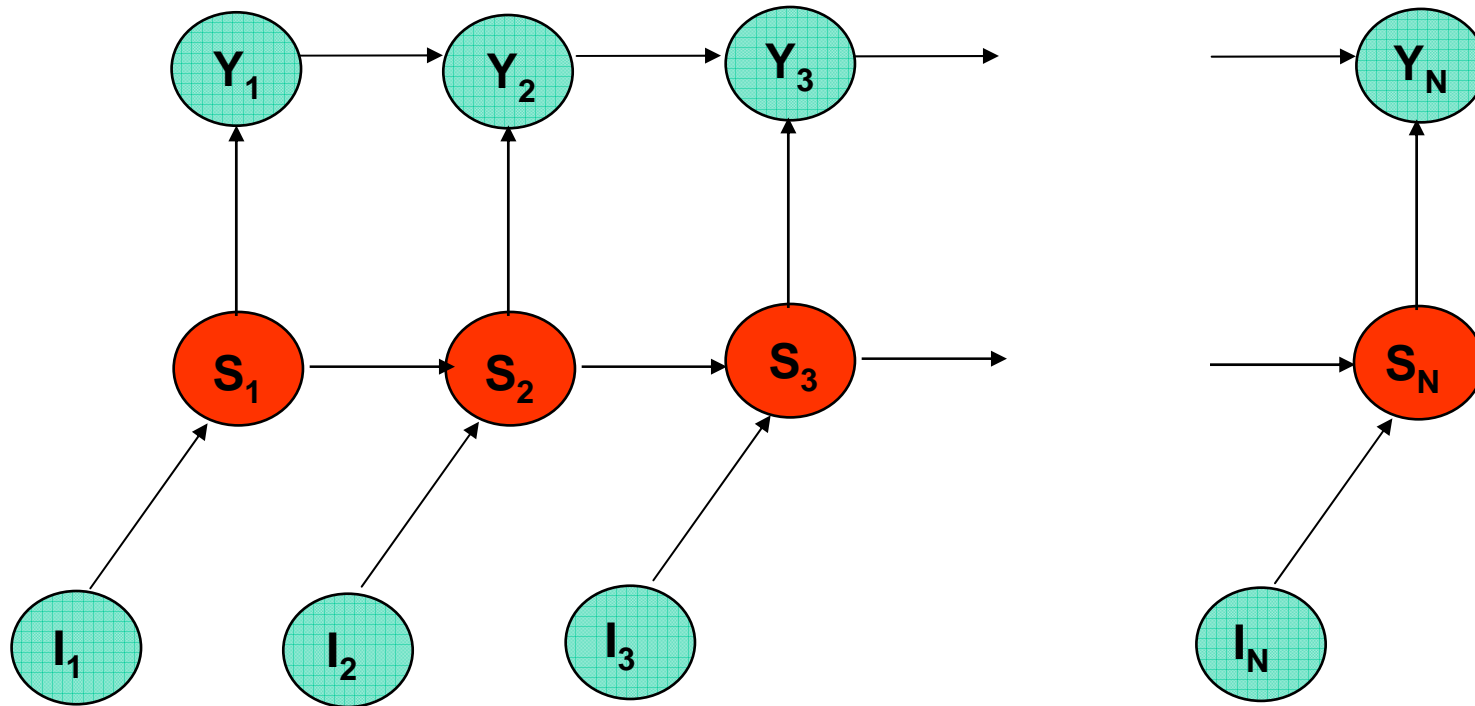
- Does not take spatial correlation into account

# HMMs for Rainfall Modeling



- $S$  = unobserved weather state
- $Y$  = spatial rainfall pattern ("outputs")

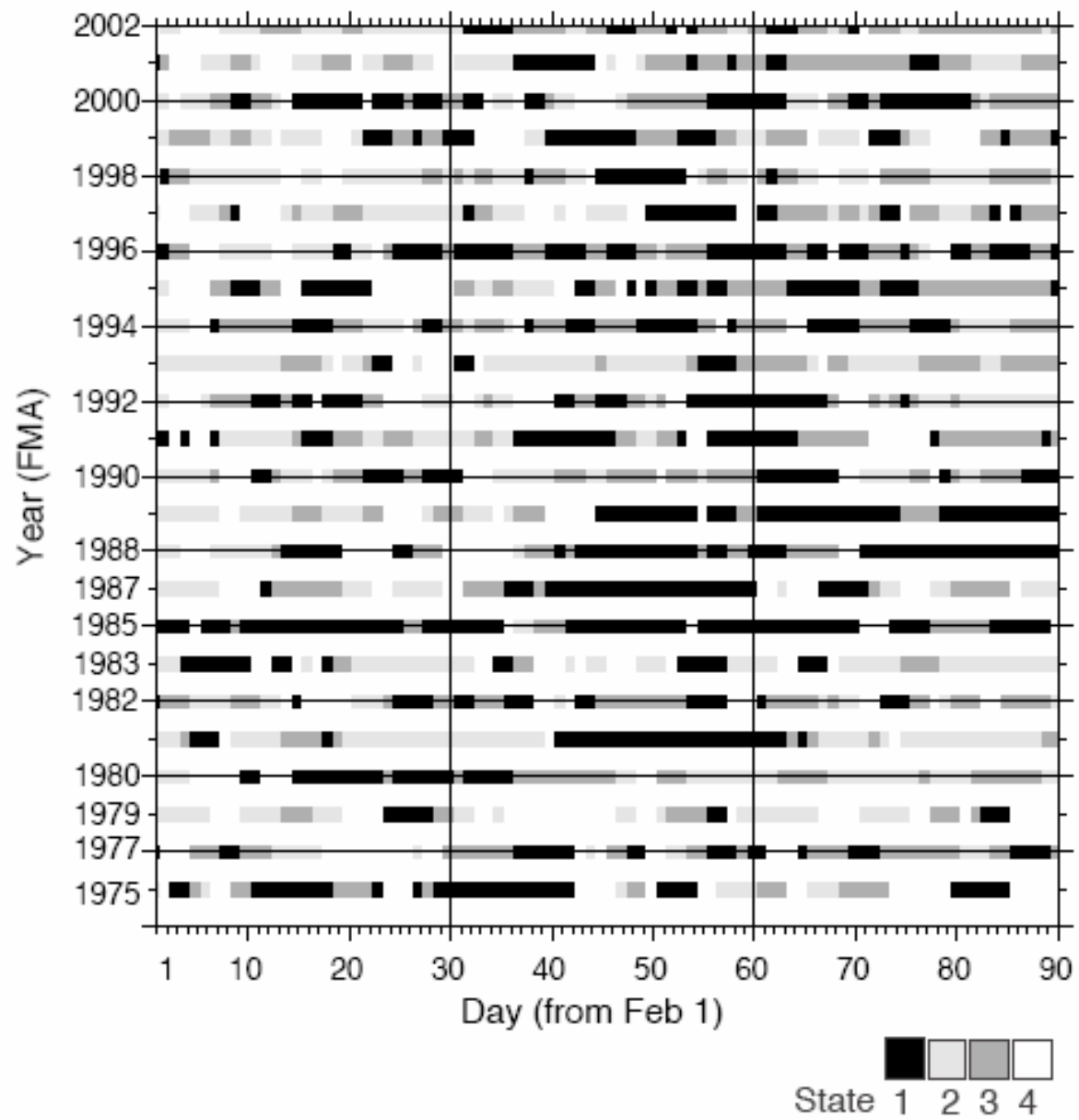
# HMMs for Rainfall Modeling



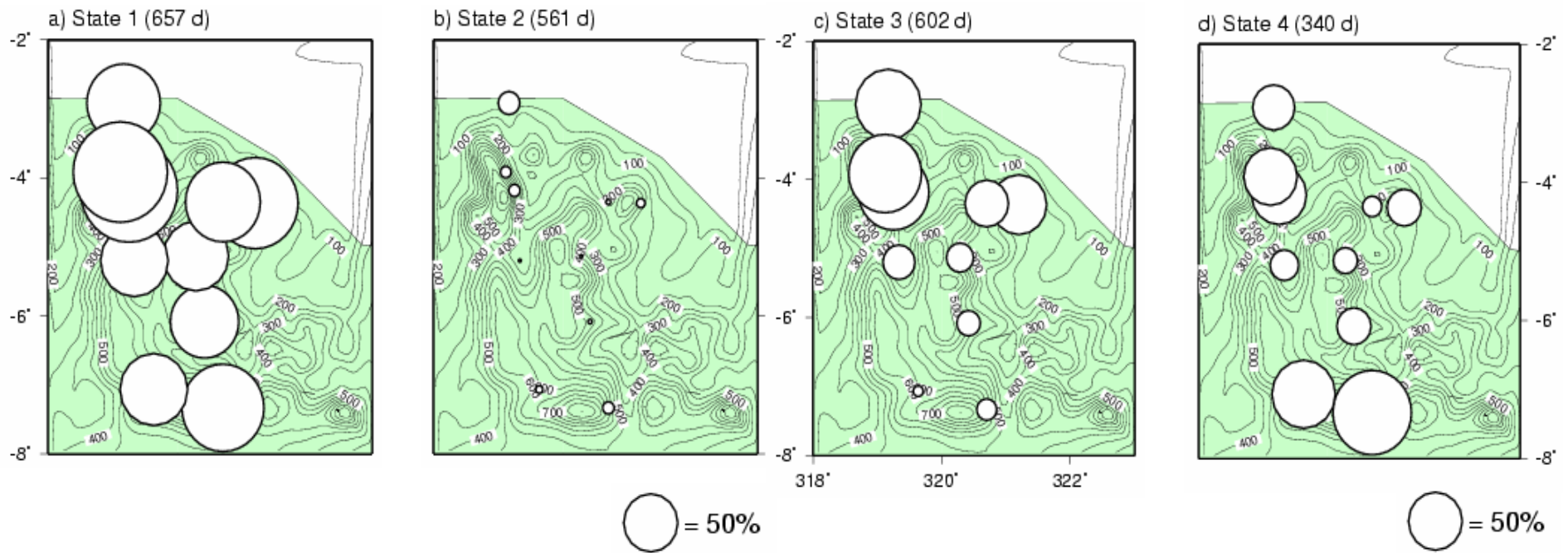
- $S$  = unobserved weather state
- $Y$  = spatial rainfall pattern ("outputs")
- $I$  = atmospheric variables ("inputs")

# Modeling and Estimation

- Model
  - Transitions  $p(s_t | s_{t-1})$  are now  $p(s_t | s_{t-1}, i_{t-1})$
  - Parametrized by a logistic function
- Parameter estimation
  - EM algorithm can be derived from general principles
  - E-step:
    - linear in length of sequence
  - M-step:
    - No closed form solution with logistic function
    - Solve a numerical optimization problem at each M-step
- “Parsing”
  - Given a model, can estimate most likely state sequence in historical data
  - Assigns each day to its most likely state



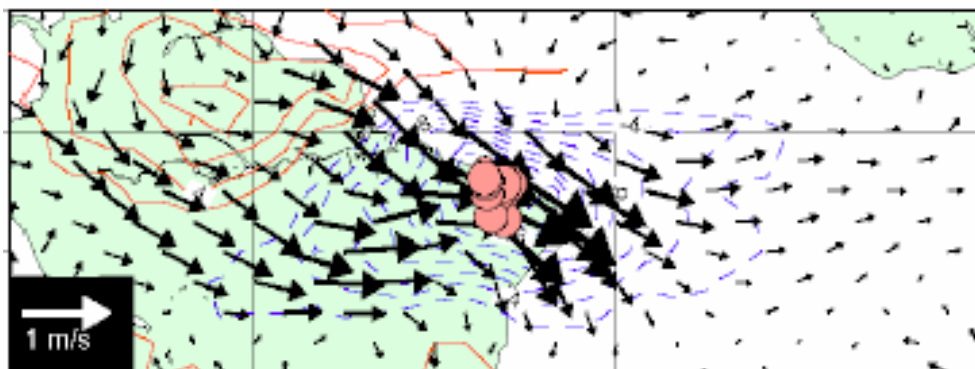
# Resulting Weather States



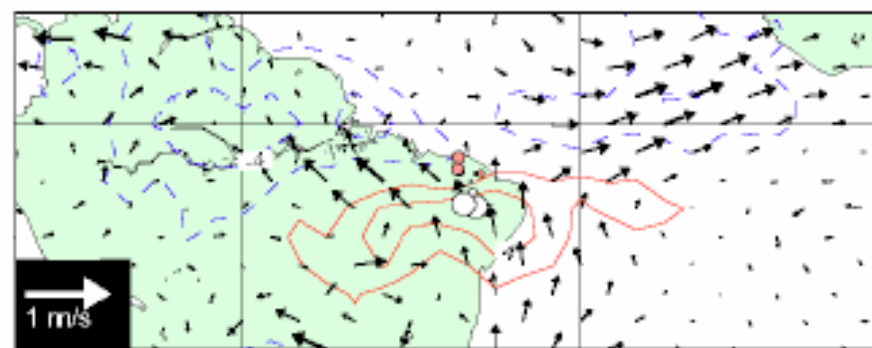
States provide an interpretable “view” of spatio-temporal relationships in the data

a) State 1 (657 d)

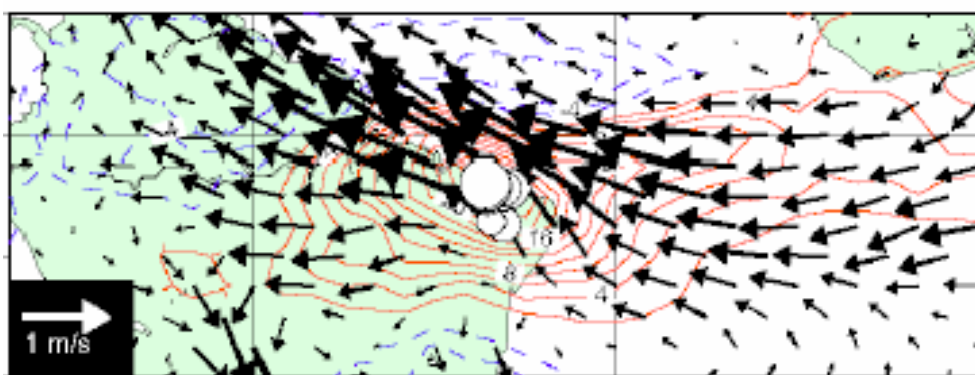
● = +50%    ○ = -50%



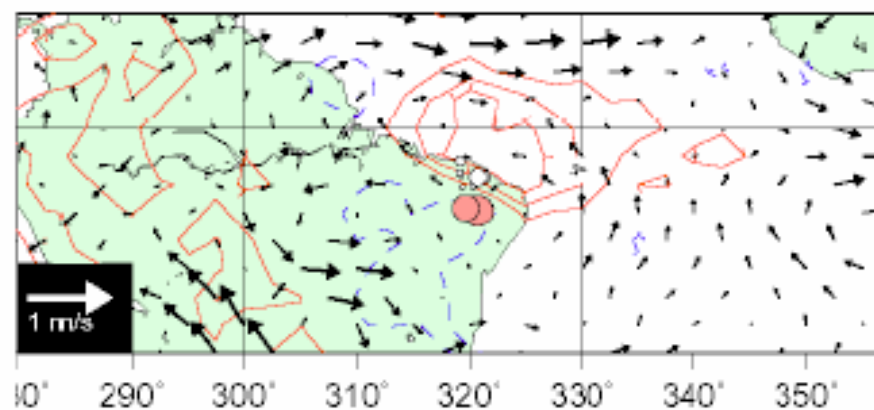
c) State 3 (602 d)



b) State 2 (561 d)

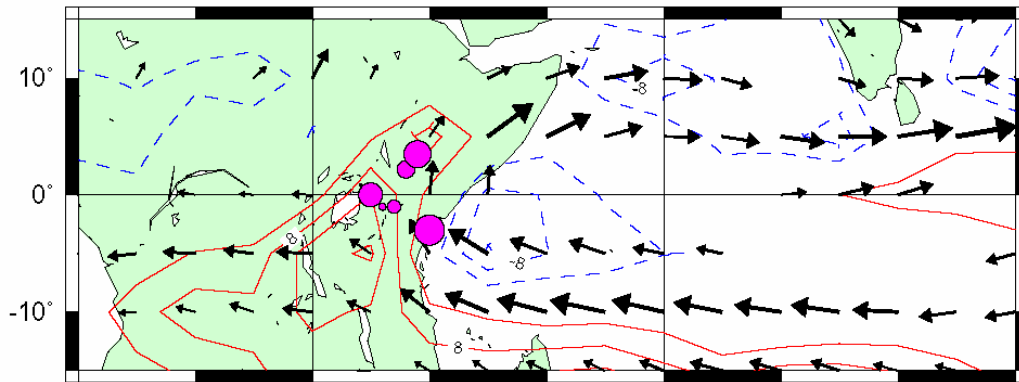


d) State 4 (340 d)

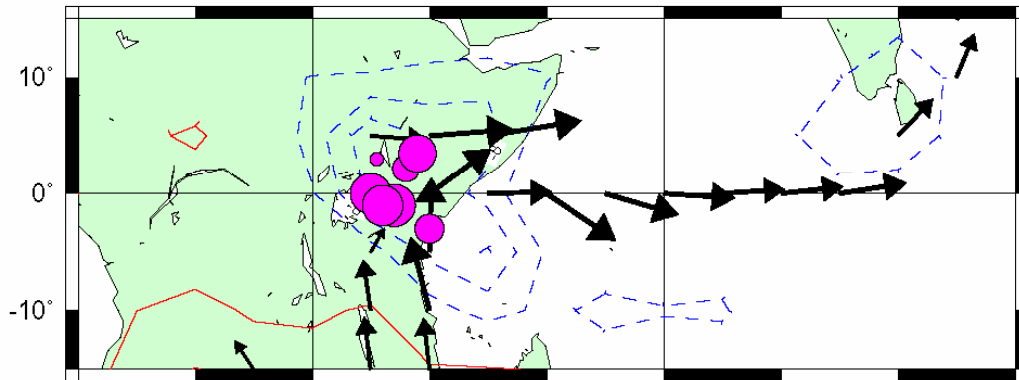


# Weather States for Kenya

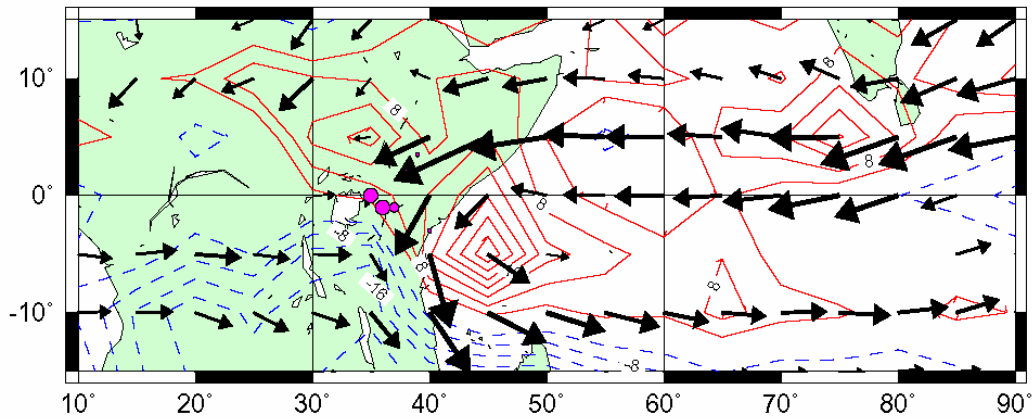
a) State 1 (830 d)



b) State 2 (1083 d) (winds x 3)

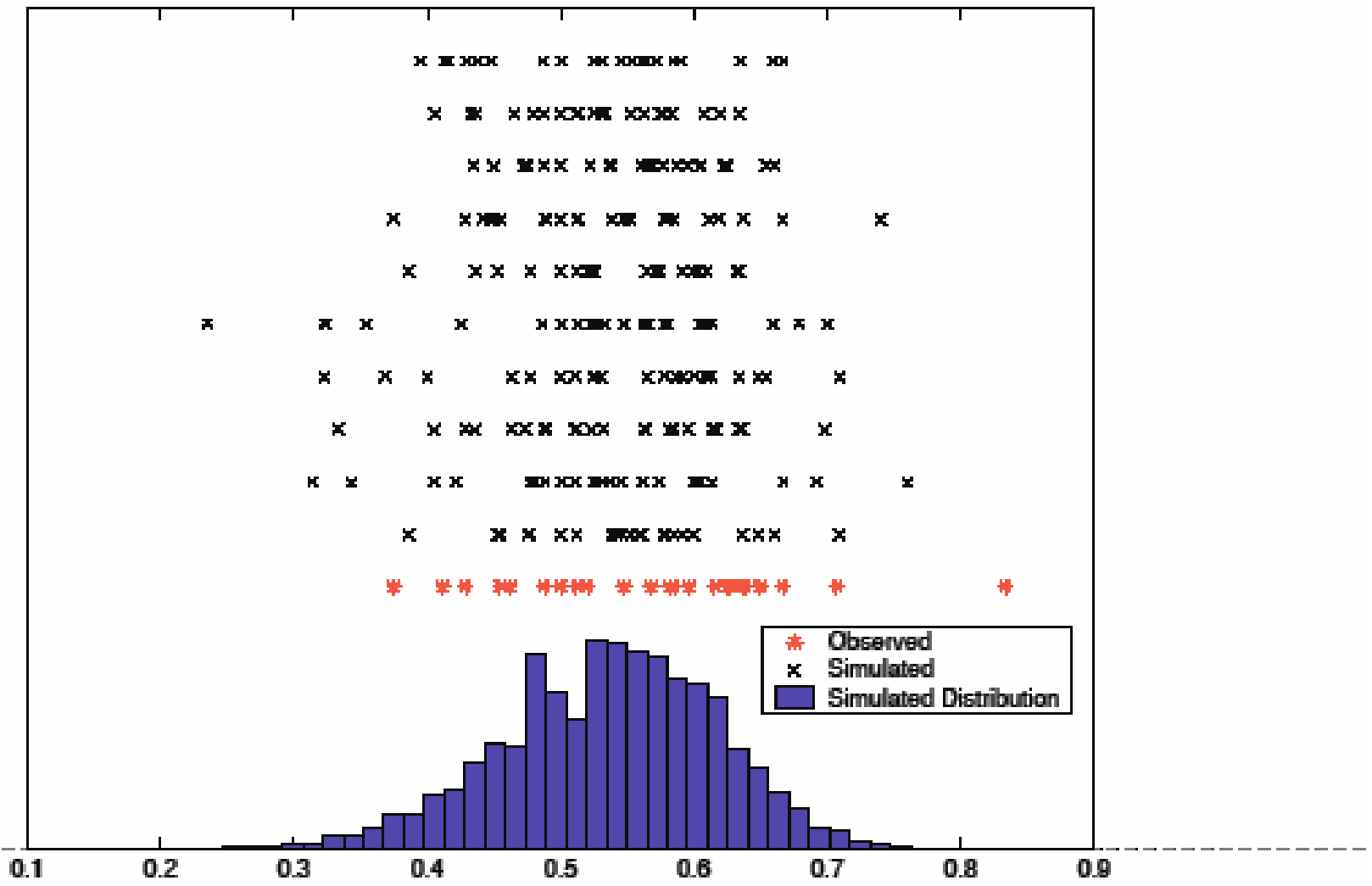


c) State 3 (755 d)

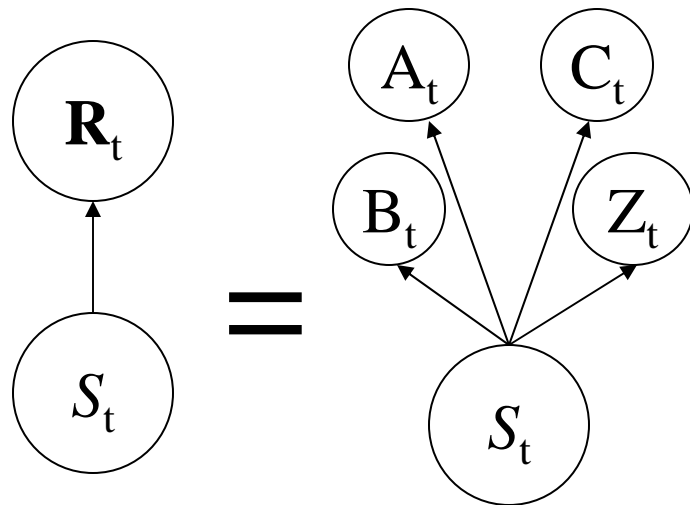
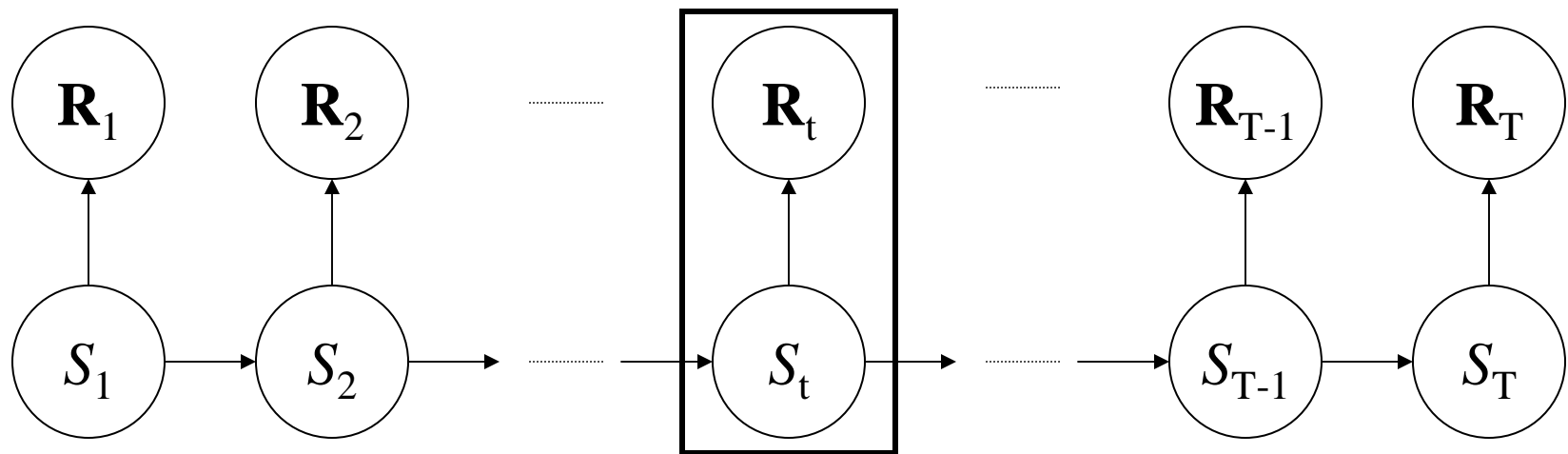




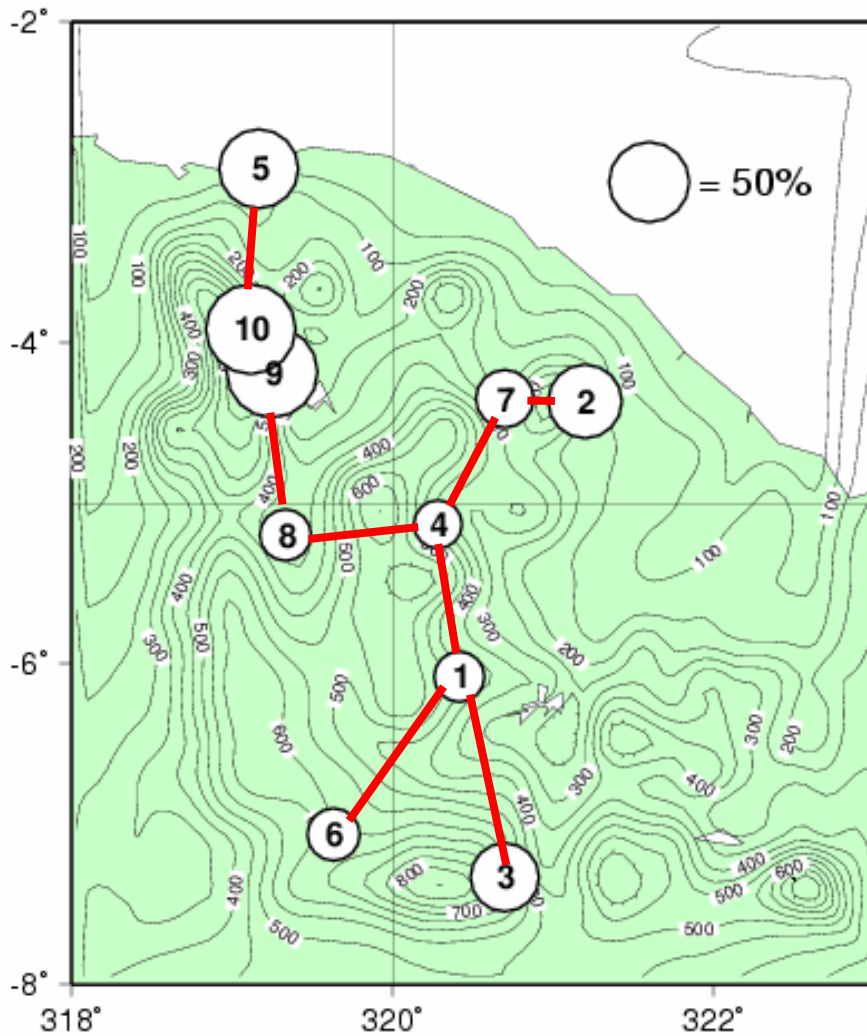
Annual Variability in Rainfall Persistence (Station 5)



# HMM-Conditional-Independence



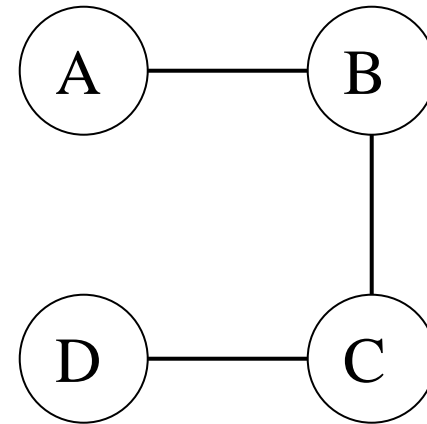
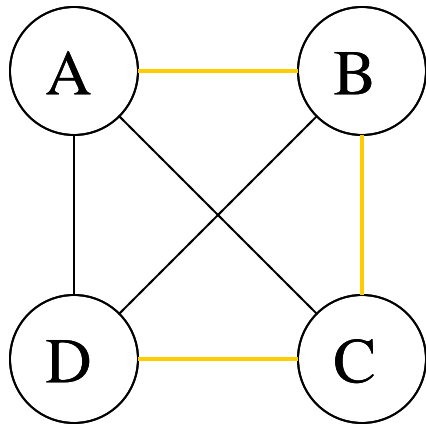
$$\begin{aligned} P(\mathbf{R}_t | S_t) &= P(A_t, \dots, Z_t | S_t) \\ &= \prod_{c \in \{A, \dots, Z\}} P(c_t / S_t) \end{aligned}$$



## Spatial Chow-Liu Trees

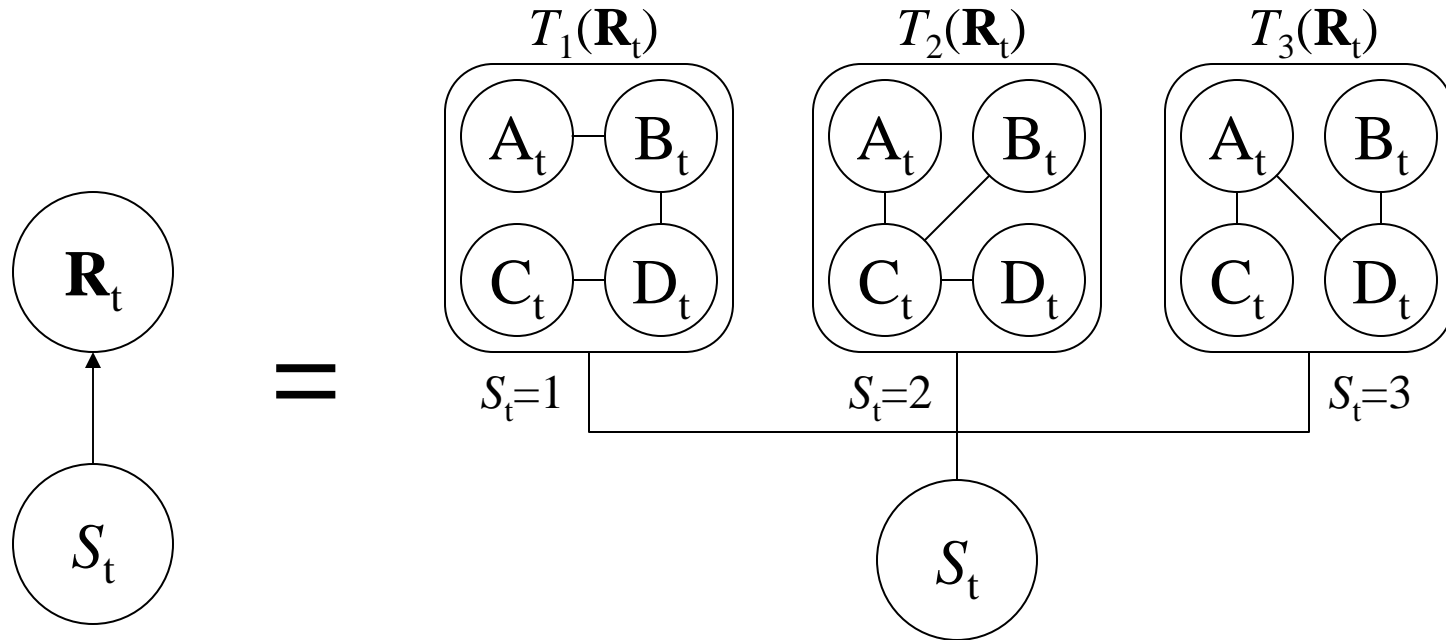
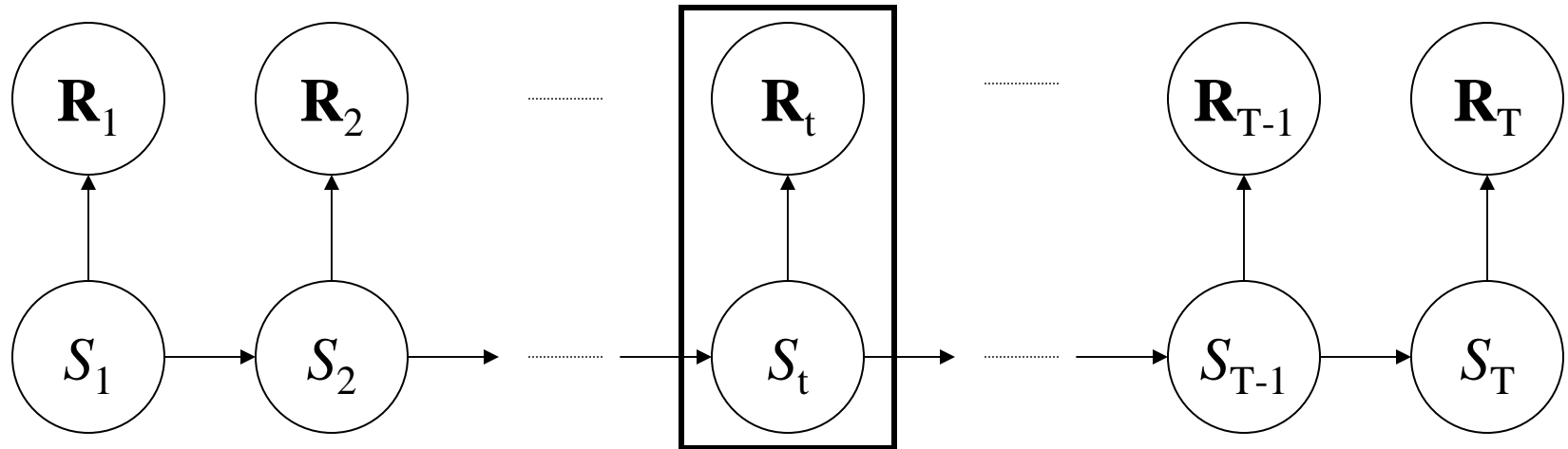
- Spatial distribution given a state is a tree structure
- Useful intermediate between full pair-wise model and conditional independence
- Topology learned from data
- Can use priors based on distance, topography
- Tree-structure over time also

# Illustration of CL-Tree Learning

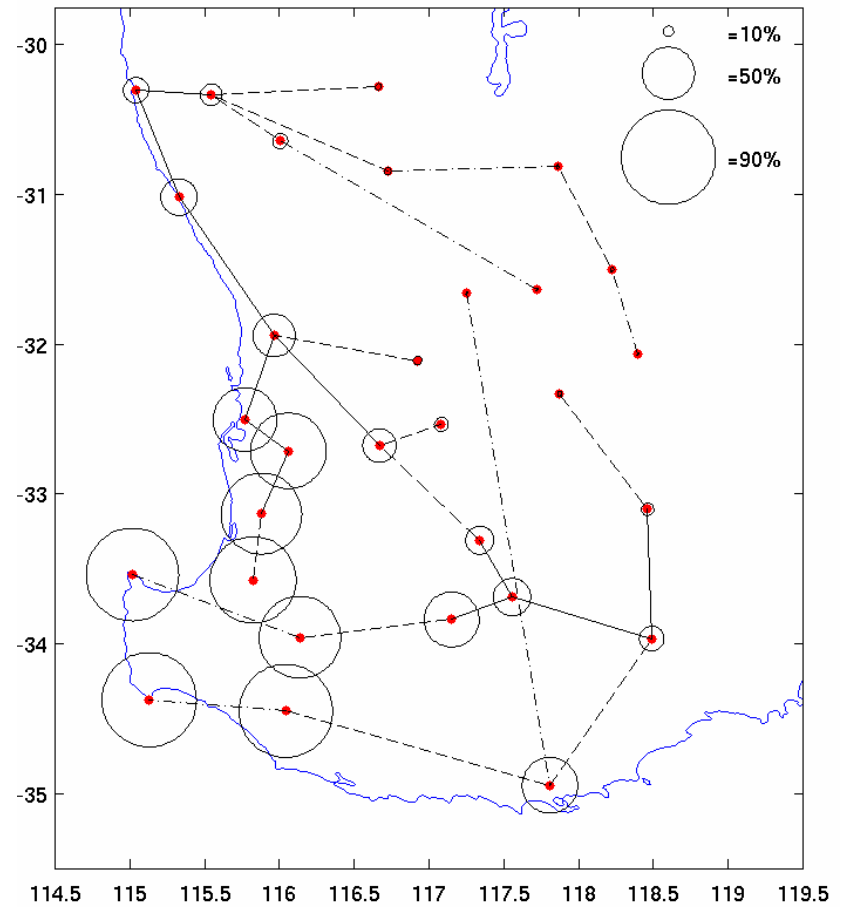
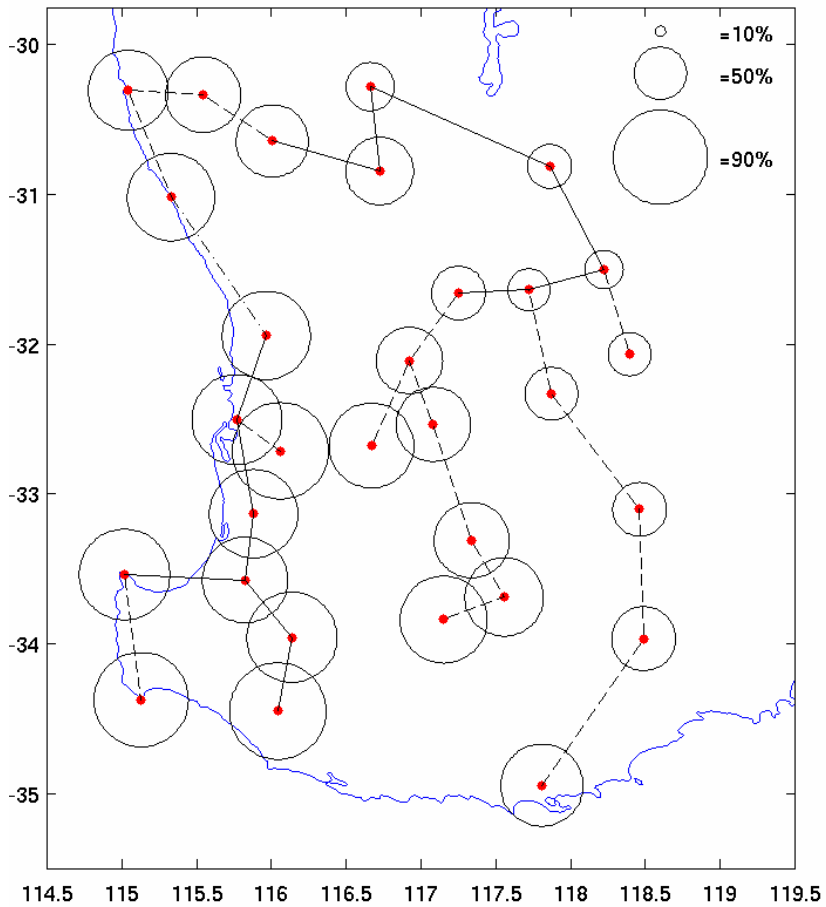


<b>AB</b>	<b>(0.56, 0.11, 0.02, 0.31)</b>	<b>0.3126</b>
AC	(0.51, 0.17, 0.17, 0.15)	0.0229
AD	(0.53, 0.15, 0.19, 0.13)	0.0172
<b>BC</b>	<b>(0.44, 0.14, 0.23, 0.19)</b>	<b>0.0230</b>
BD	(0.46, 0.12, 0.26, 0.16)	0.0183
<b>CD</b>	<b>(0.64, 0.04, 0.08, 0.24)</b>	<b>0.2603</b>

# HMM-Chow-Liu



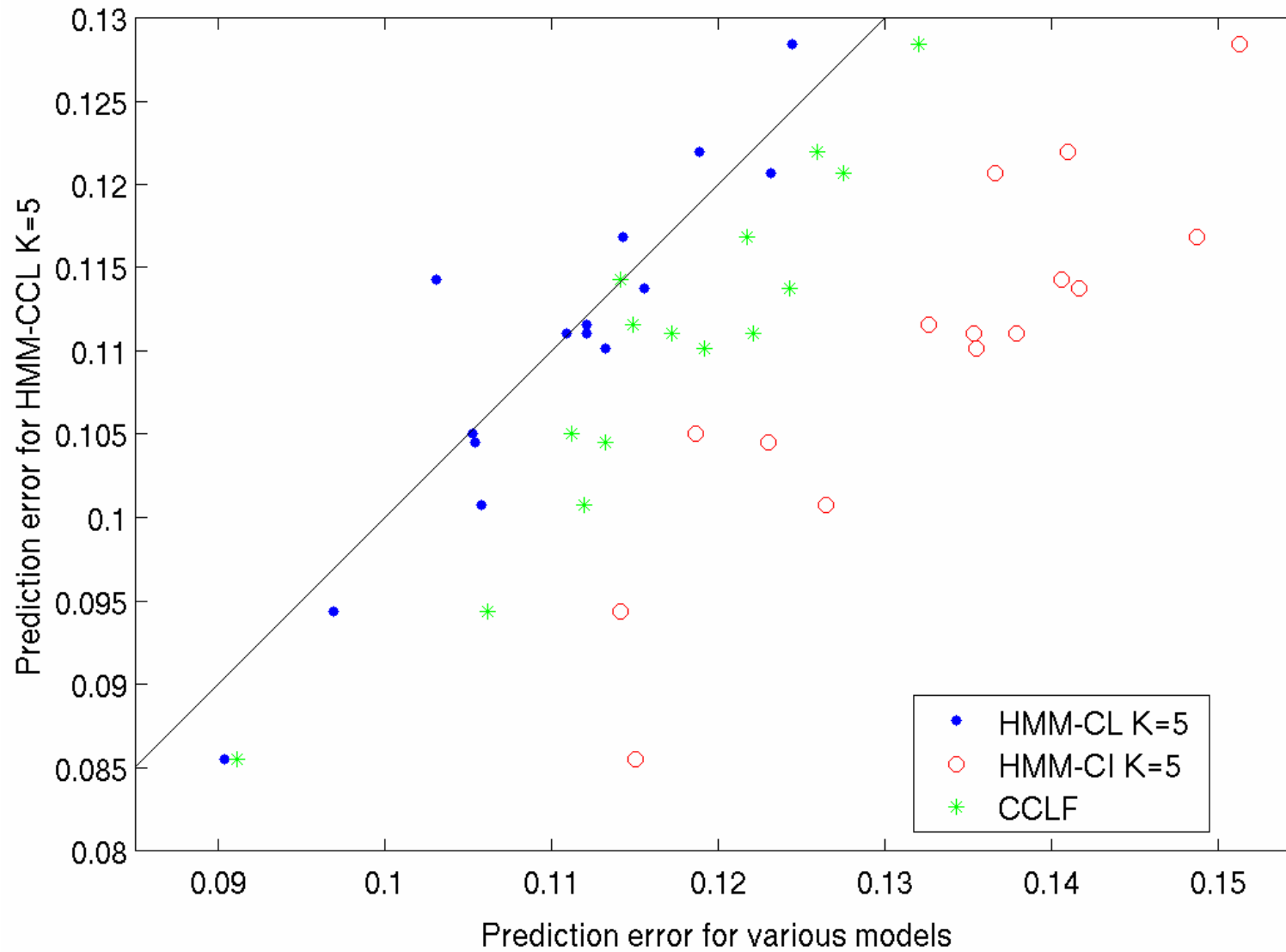
# Tree-Structured Weather States



# Evaluation

- HMM models with tree structures learned from historical precipitation data using EM
  - Brazil, Kenya, Senegal, Australia, Western US, ...
- Cross-validation to evaluate predictive power
  - Train on N-K seasons, predict data from other K seasons
  - Leave out single (1-day) station measurement and predict
  - Repeat, and look at average prediction accuracy
- Results
  - First-order Markov chains capture no spatial dependence
  - HMM with conditional-independence -> quite good
  - HMMs with tree-structures are most accurate

# Australia (predictive error)





Example 2:

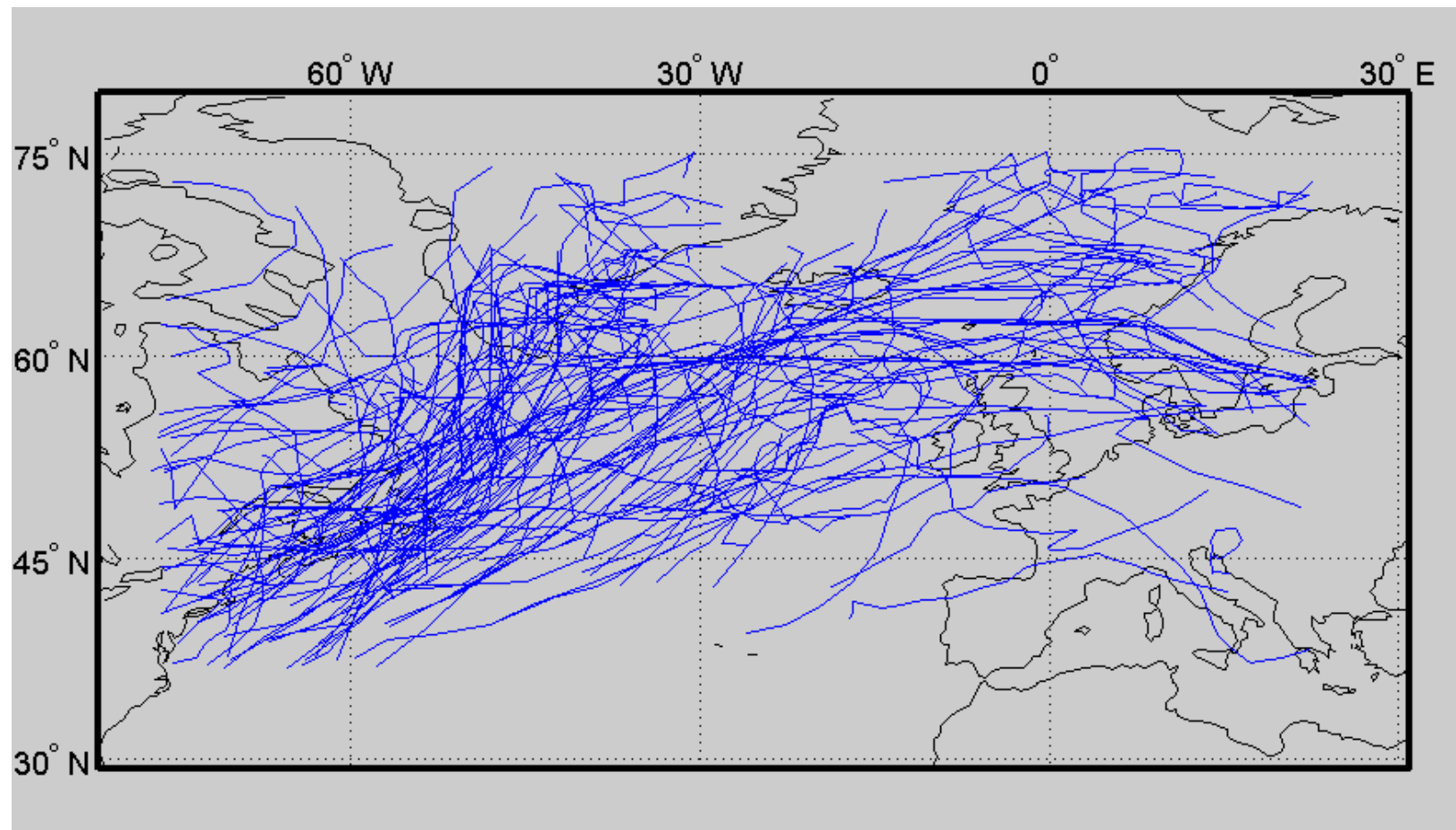
## Clustering Cyclone Trajectories

Joint work with:

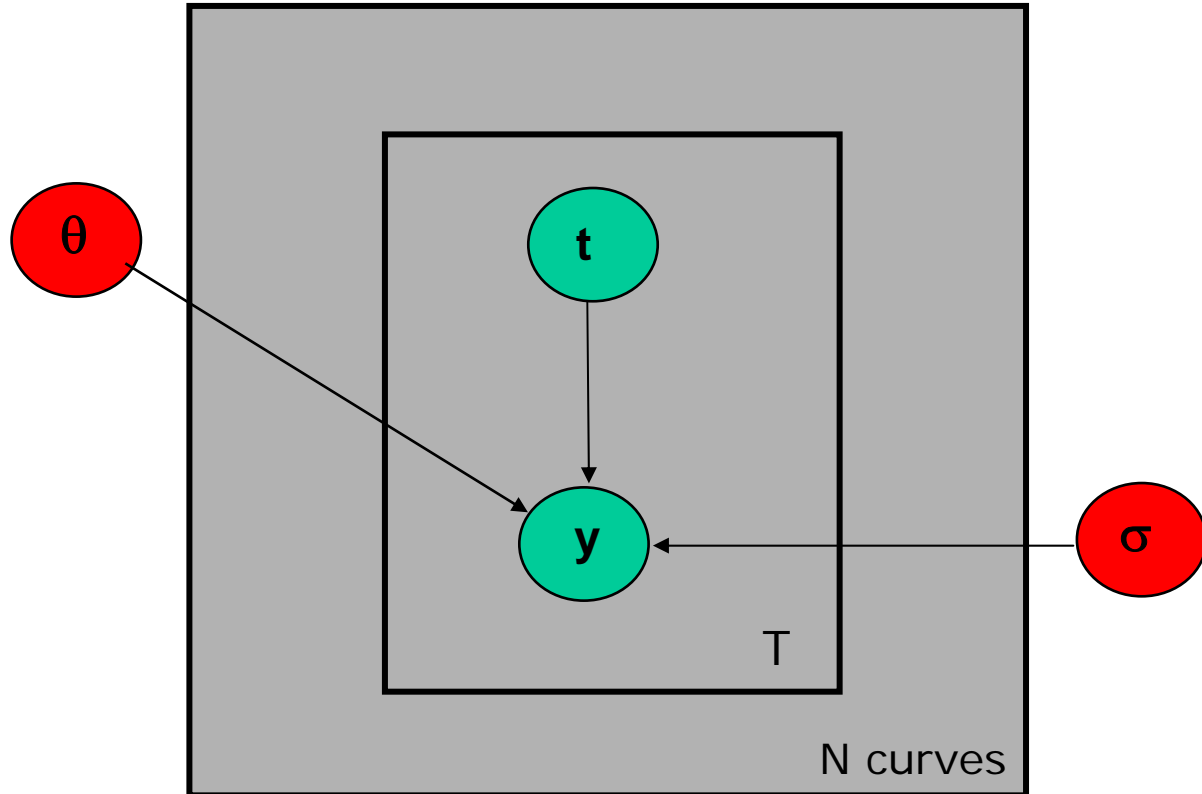
Suzana Camargo, Andy Robertson, International Research Institute for  
Climate Prediction

Scott Gaffney, Department of Computer Science, UC Irvine

# Storm Trajectories

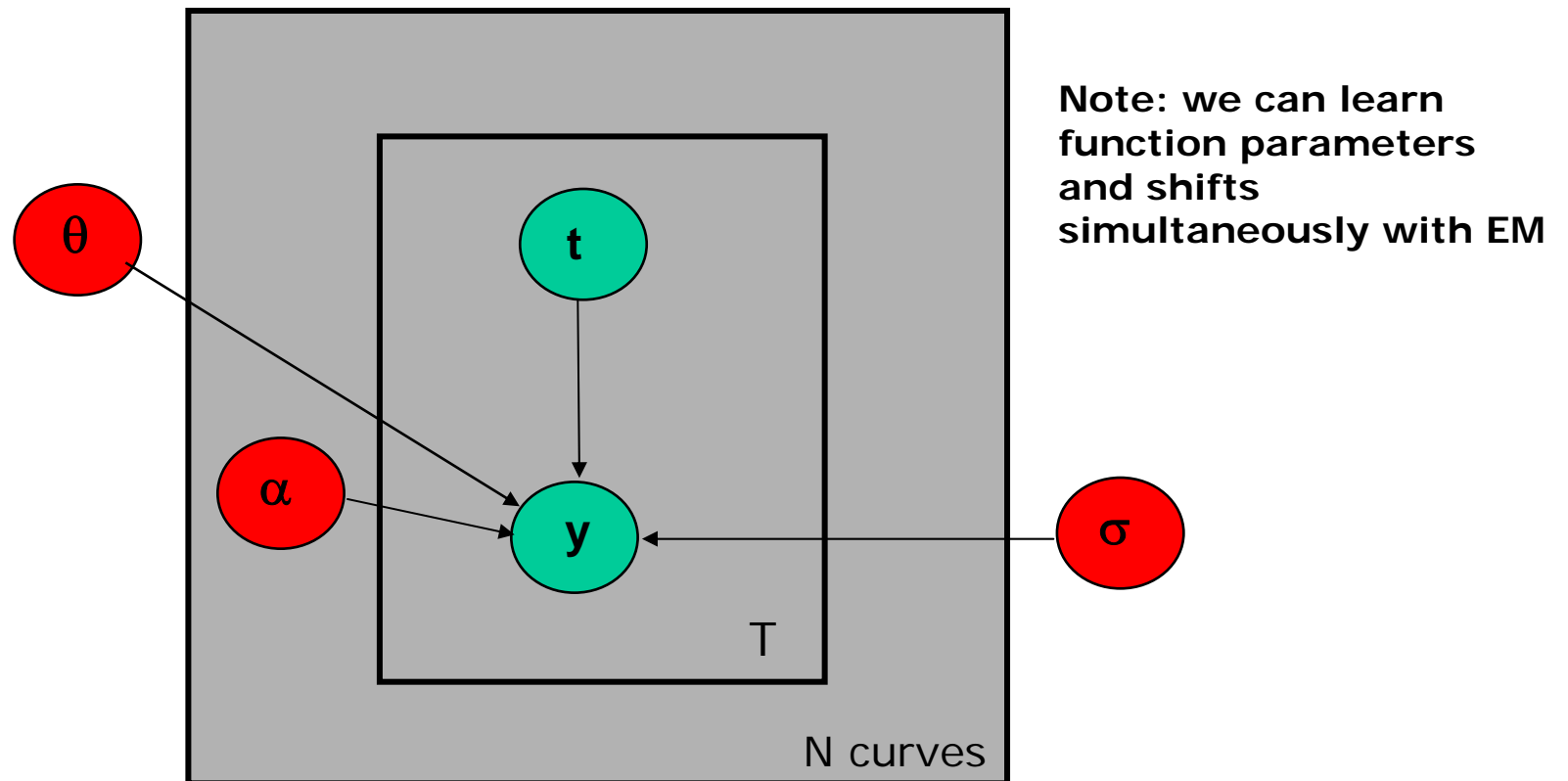


# Graphical Models for Sets of Trajectories



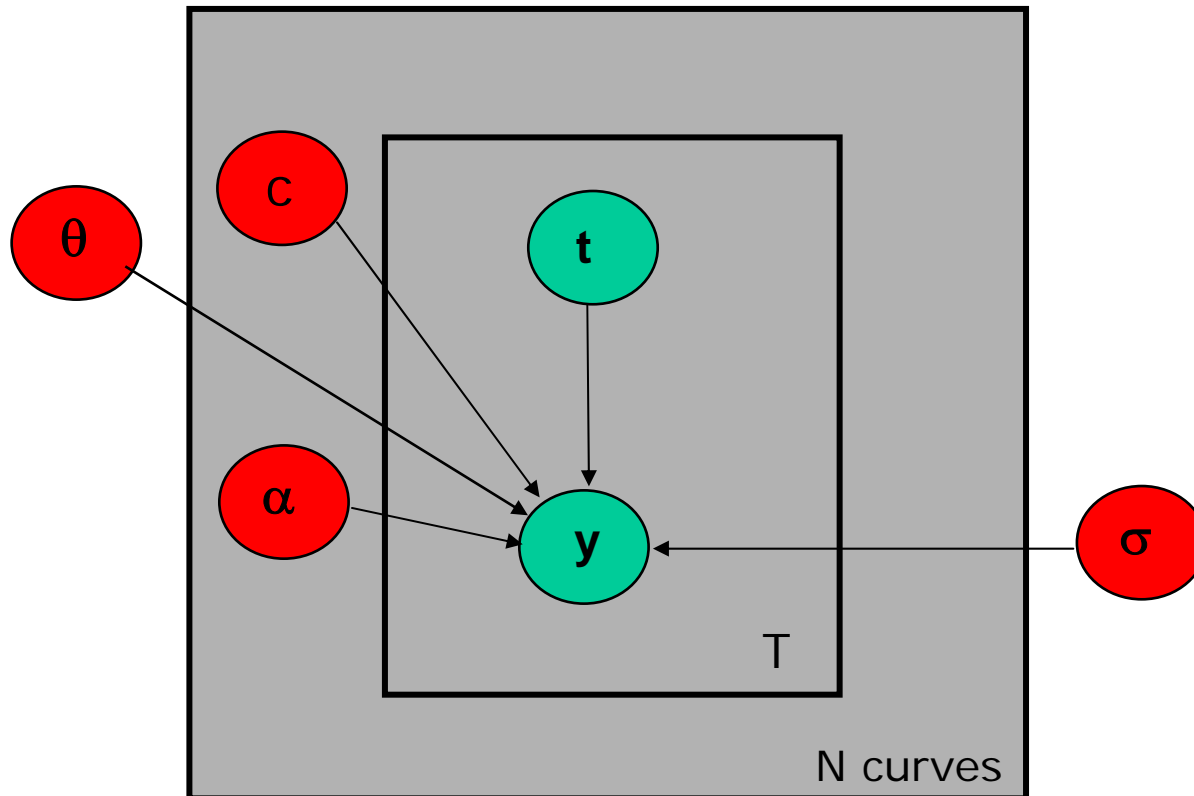
Each curve:  $P(\mathbf{y}_i \mid \mathbf{t}_i, \theta) = \text{product of Gaussians}$

# Curve-Specific Transformations



e.g.,  $y_i = at^2 + bt + c + \alpha_i$ ,  $\theta = \{a, b, c, \alpha_1, \dots, \alpha_N\}$

# Clustering: Mixtures of Trajectories

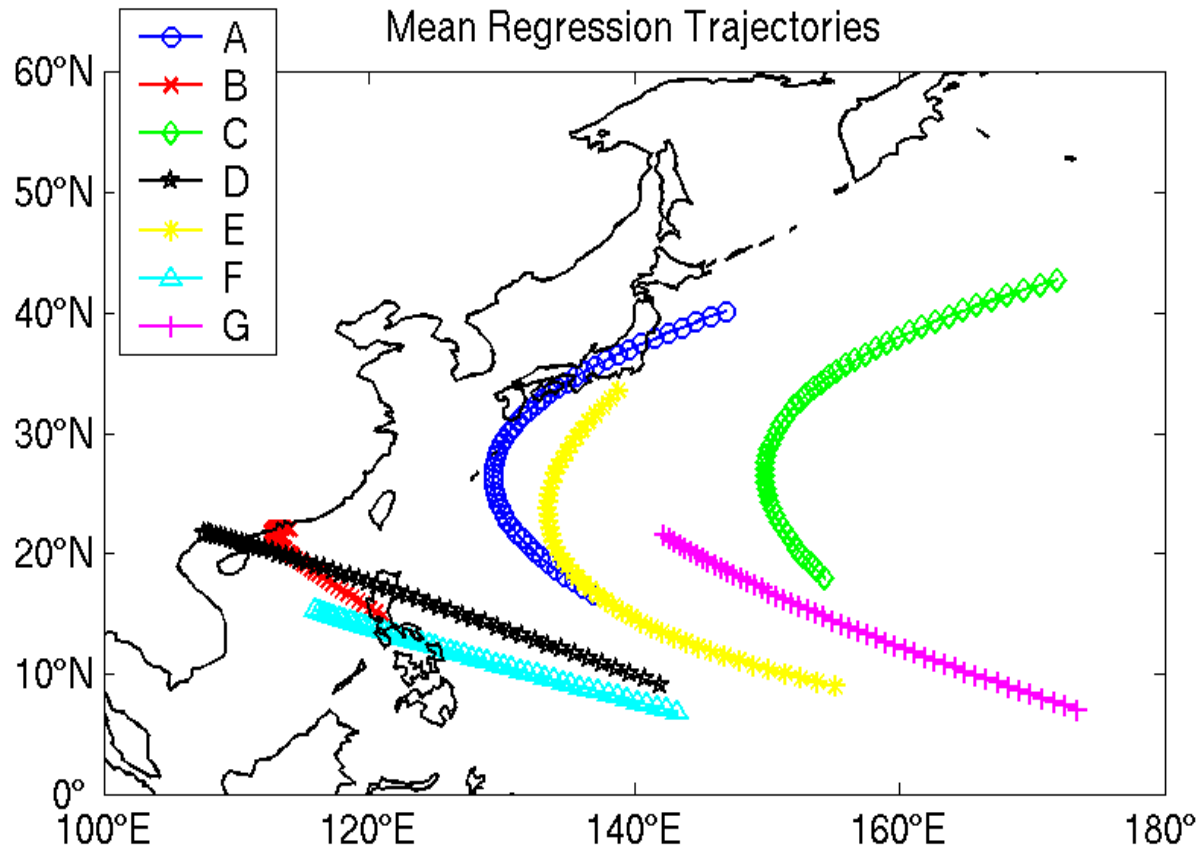


Each set of trajectory points comes from 1 of  $K$  models

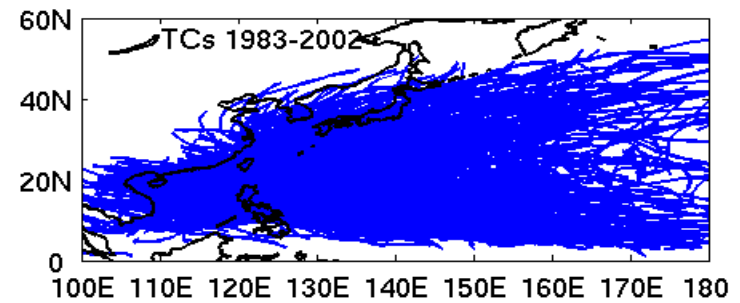
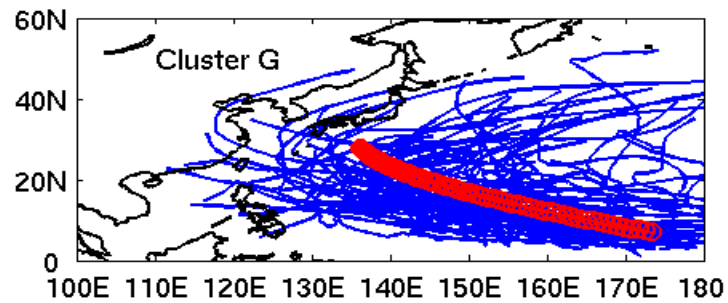
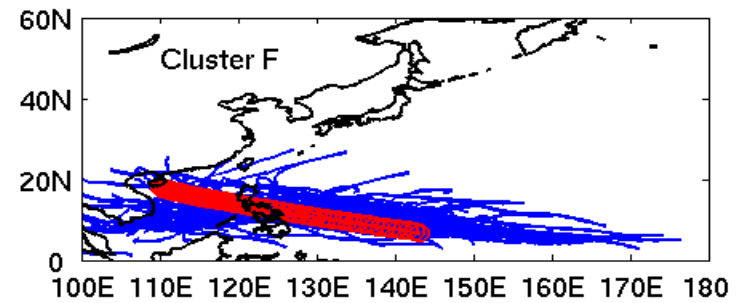
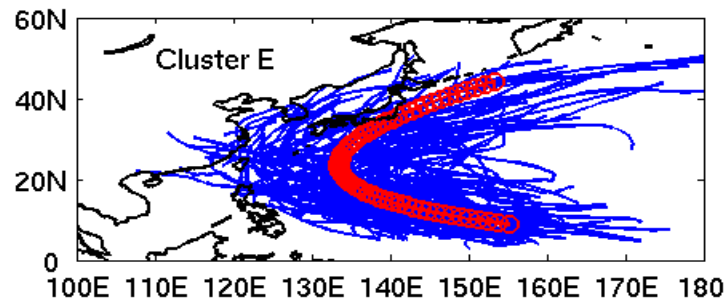
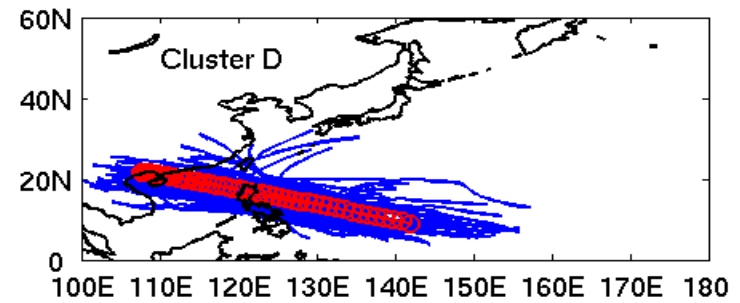
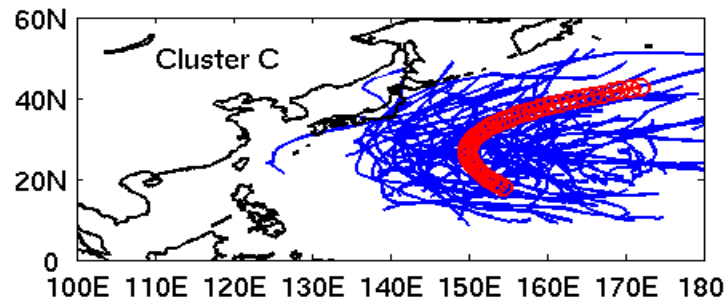
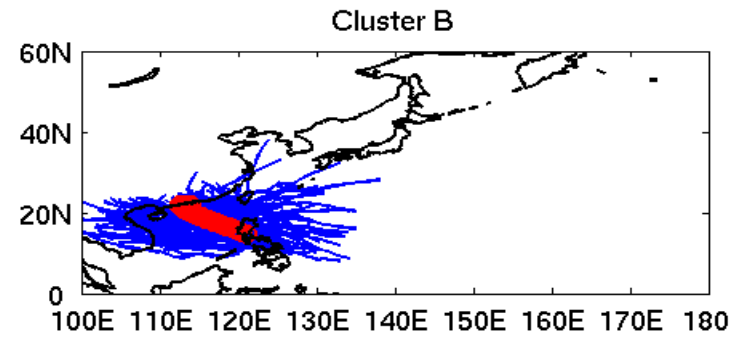
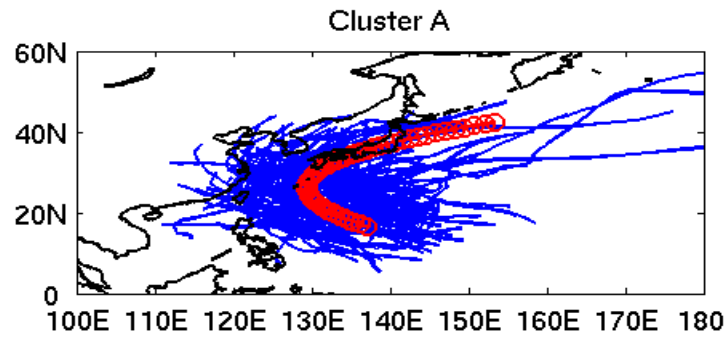
Model for group  $k$  is a Gaussian curve model

Marginal probability for a trajectory = mixture model

# Cluster Shapes for Pacific Cyclones



# TROPICAL CYCLONES Western North Pacific 1983-2002



# Topics not discussed....

- Learning model structure from data
  - Without hidden variables -> doable
  - With hidden variables -> difficult
- Non-Gaussian models for continuous data
  - Relatively little work
- Monte-Carlo sampling techniques
  - for probability calculation and forecasting
  - E.g., sequential importance sampling (“particle filtering”)
- Prediction using model-averaging
  - Bayesian approach:
    - Estimate model-combining weights using Bayesian estimation methods
  - Empirical approach:
    - Estimate model-combining weights that lead to the best prediction



# Looking to the future...

- Integration of different data sources for climate modeling
  - Temperature, precipitation, ground-cover, etc
  - Integrating satellite data with traditional data
    - e.g. MODIS data
- Leads to “large-scale structured stochastic models”
  - Multiple temporal scales, spatial scales, different variables
  - Issues
    - missing data
    - data on different time-scales/spatial grids
    - Variable selection, model selection...
    - Parameter/model/forecast uncertainty
- Graphical models provide a useful framework for
  - Thinking about model structure
  - General-purpose algorithms for estimation and prediction
  - Efficient computation
  - General “language” for Bayesian modeling (e.g., BUGS)

# References

- Papers from my Web page:
  - Rainfall modeling with HMMs
    - Robertson, Kirshner, Smyth, Hidden Markov models for modeling daily rainfall occurrence over Brazil, *Journal of Climate*, 17(22):4407-4424, November 2004.
  - Graphical models and HMMs
    - Smyth, Heckerman, Jordan, 1997, *Neural Computation*
- Other sources
  - Kevin Murphy:
    - Dynamic Bayesian Networks: Representation, Inference, and Learning, Phd thesis, EECS Department, UC Berkeley, 2002
    - Dynamic Bayesian Networks, draft book chapter.