7. Boosting and Bagging

Bagging

Bagging

- So far: Boosting as an **ensemble** learning method, i.e.: a combination of (weak) learners
- A different way to combine classifiers is known as **bagging ("bootstrap aggregating")**
- **Idea:** sample M "bootstrap" data sets (sub sets) **with replacement** from the training set and train different models
- Overall classifier is then the **average** over all models:

$$\bar{y}(\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} y_m(\mathbf{x})$$

Bagging

Bagging reduces the expected error. E.g. in regression: $$y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$$

prediction ground truth error

- Expected error: $E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$
- Average error over all (weak) learners:

$$E_{AV} = \frac{1}{M}\sum_{m=1}^{M} E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$$

- Average error of committee:

$$E_{COM} = E_x\left[(\bar{y}(\mathbf{x}) - h(\mathbf{x}))^2\right]$$

Bagging

Bagging reduces the expected error. E.g. in regression:

$$y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$$

prediction ground truth error

- Expected error: $E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$
- Average error over all weak learners (indep.):

$$E_{AV} = \frac{1}{M}\sum_{m=1}^{M} E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$$

- In contrast: average error of committee:

$$E_{COM} = E_x\left[\left(\frac{1}{M}\sum_{m=1}^{M} y_m(\mathbf{x}) - h(\mathbf{x})\right)^2\right]$$

Bagging

Bagging reduces the expected error. E.g. in regression: $$y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$$

- Expected error: $E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$
- Average error over all (weak) learners:

$$E_{AV} = \frac{1}{M}\sum_{m=1}^{M} E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$$

- Average error of committee if learners are uncorrelated:

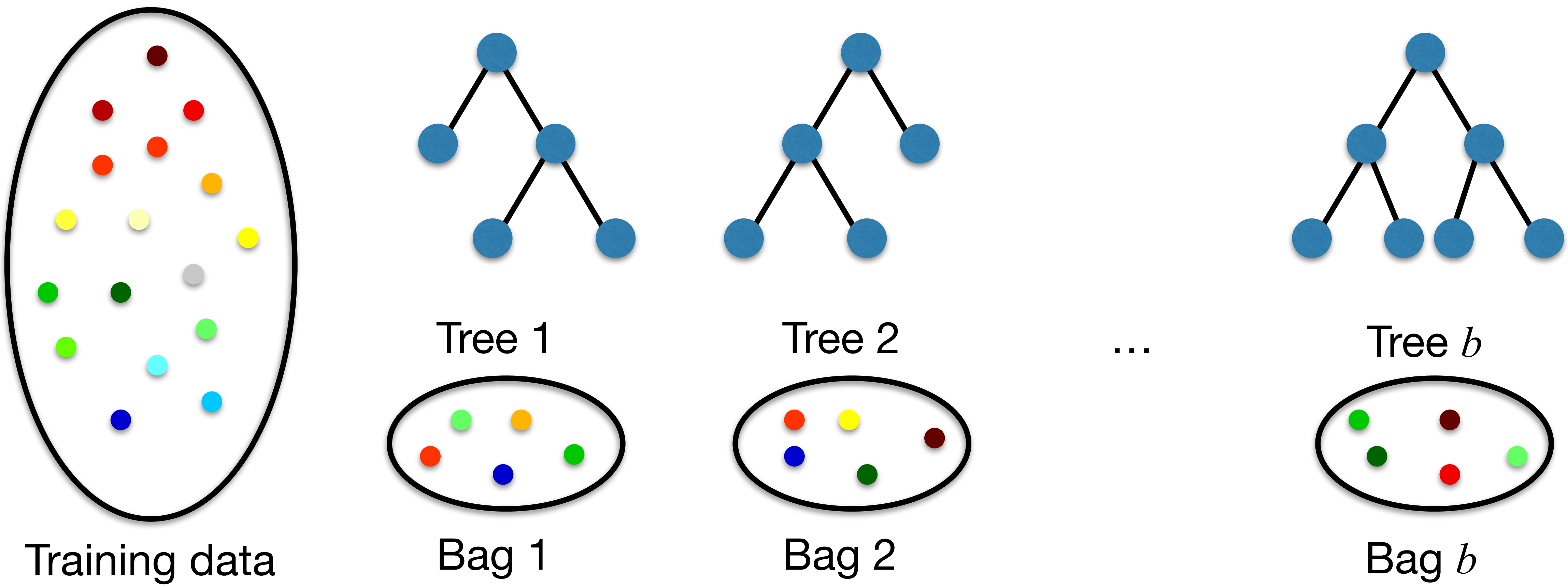
$$E_{COM} = \frac{1}{M}E_{AV}$$

Random Forests

Given: training set of size N $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ $\mathbf{x}_i \in \mathbb{R}^d$

1. Randomly sample $n \leq N$ elements from training set **with replacement (repetitions likely)**
2. Randomly select a subset of p features ($p<d$)
3. Pick from those the feature that produces the best **split** of the data
4. Perform the split and go back to 2.
5. If maximum tree depth is reached:
6. If number of trees M is reached then stop.
7. Else: go to 1. building a new tree.

Random Forests



- Each bag is a subset of the entire training data
- Repetitions are very likely

Note: in this figure, repetitions are not shown

Performance of Random Forests

The error rate depends on two main aspects:

- the **correlation** between any two trees:
  high correlation → high error rate
- the **strength** of each tree (low error per tree)
  higher strength → lower overall error rate

These values are mainly influenced by p:

- If p is low: correlation and strength are low
- If p is high: correlation and strength are high

There is usually an “optimal range” of p

Splitting Criterion

- **Aim**: split such that both data sub sets contain samples that are as **pure** as possible
- Possible impurity values:
  - misclassification error: let π be the prob of class 1 (binary classification), i.e. $\pi = P(y = 1|\Omega)$ data subset then use $\min(\pi, 1 - \pi)$
  - Gini index: $2\pi(1 - \pi)$
  - Deviance: $-\pi \log \pi - (1 - \pi) \log(1 - \pi)$
  - For regression trees we can use the mean-squared error

Properties of Random Forests

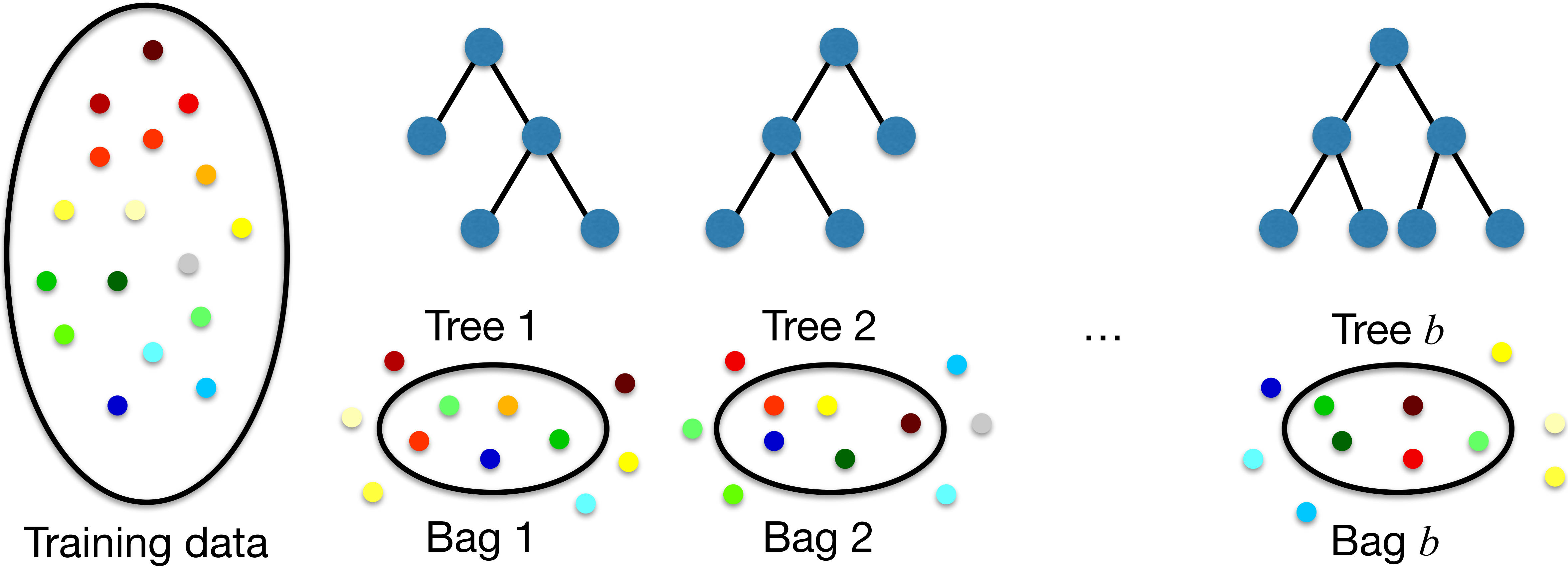
- They reduce the **variance** of the classification estimate, by training several trees on randomly sampled subsets of the data ("**bagging**")
- They tend to give **uncorrelated** trees by randomly sampling the features (splits)
- They can **not overfit**! One can use as many trees as required
- Only restriction is memory
- Random Forests have very good accuracy and are widely used, e.g. for body pose recognition

Advantages of Random Forests

- One of the best classifiers in general
- Runs very **efficiently** on large data sets
- Can handle thousands of **feature dimensions**
- Can provide **importance** of variables
- Generates an **unbiased** estimate of the error
- Can deal with missing data
- Implicitly generates **proximities** of pairs of data samples, useful e.g. for clustering
- Can be extended to unlabeled data

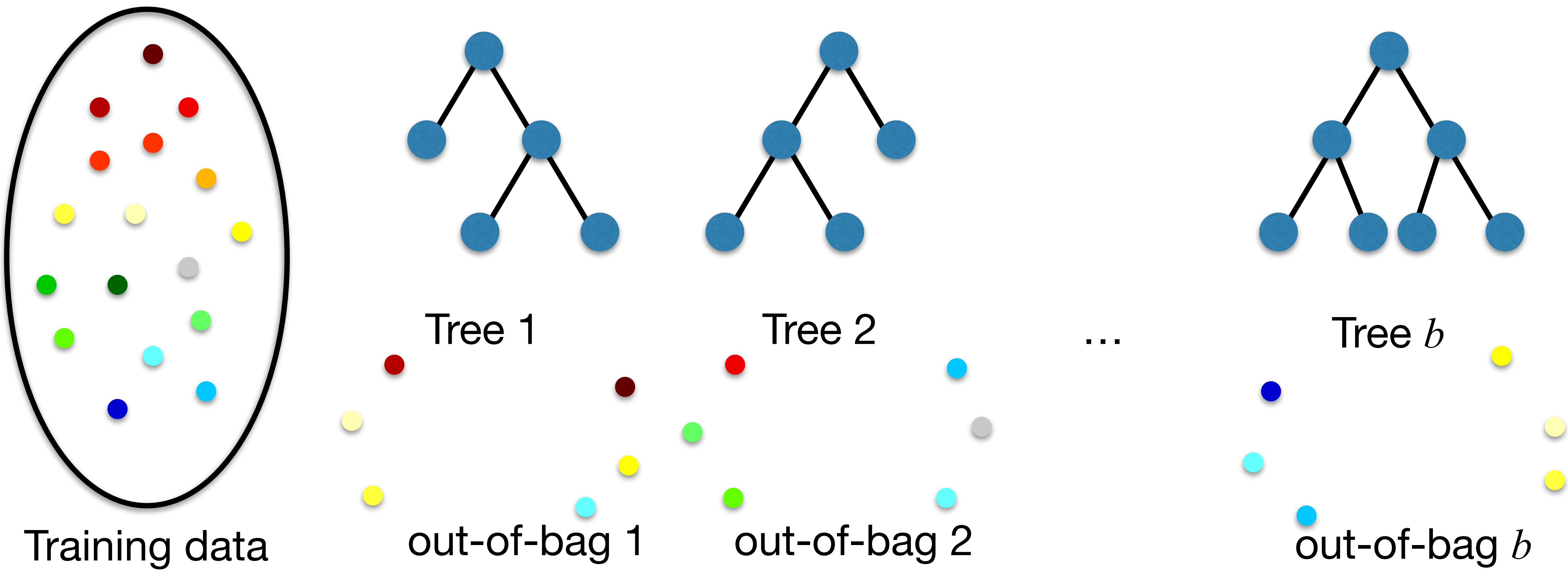
Out-of-Bag (OOB) Error

- All samples that are not used to train a tree are called the **out-of-bag data**
- These samples can be used to evaluate the overall random forest **without** an additional validation set



Out-of-Bag (OOB) Error

- All samples that are not used to train a tree are called the **out-of-bag data**
- This is done by evaluating each tree with its own out-of-bag data



Variable Importance

Idea: rate variables (features) according to their potential to change the tree structure

Method:

1. compute **tree impurity** ι_m (sum of node impurities of leaf nodes per tree) for each tree $m=1,\ldots,M$
2. for all features $j=1,\ldots,d$: **permute** the jth feature value in the out-of-bag data
3. compute tree impurity of the **permuted** data ι_{jm}
4. compute the **difference** of tree impurity:

$$\delta_{mj} = \iota_{mj} - \iota_m$$

Variable Importance

Idea: rate variables (features) according to their potential to change the tree structure

Method:

1. compute **tree impurity** ι_m (sum of node impurities of leaf nodes per tree) for each tree $m=1,\ldots,M$
2. for all features $j=1,\ldots,d$: **permute** the jth feature value in the out-of-bag data
3. compute tree impurity of the **permuted** data ι_{jm}
4. compute the **difference** of tree impurity
5. variable importance is: $$\frac{\bar{\delta}_j}{\sqrt{\frac{1}{M}\sum_m(\delta_{mj}-\bar{\delta}_m)^2}}$$

mean

standard deviation

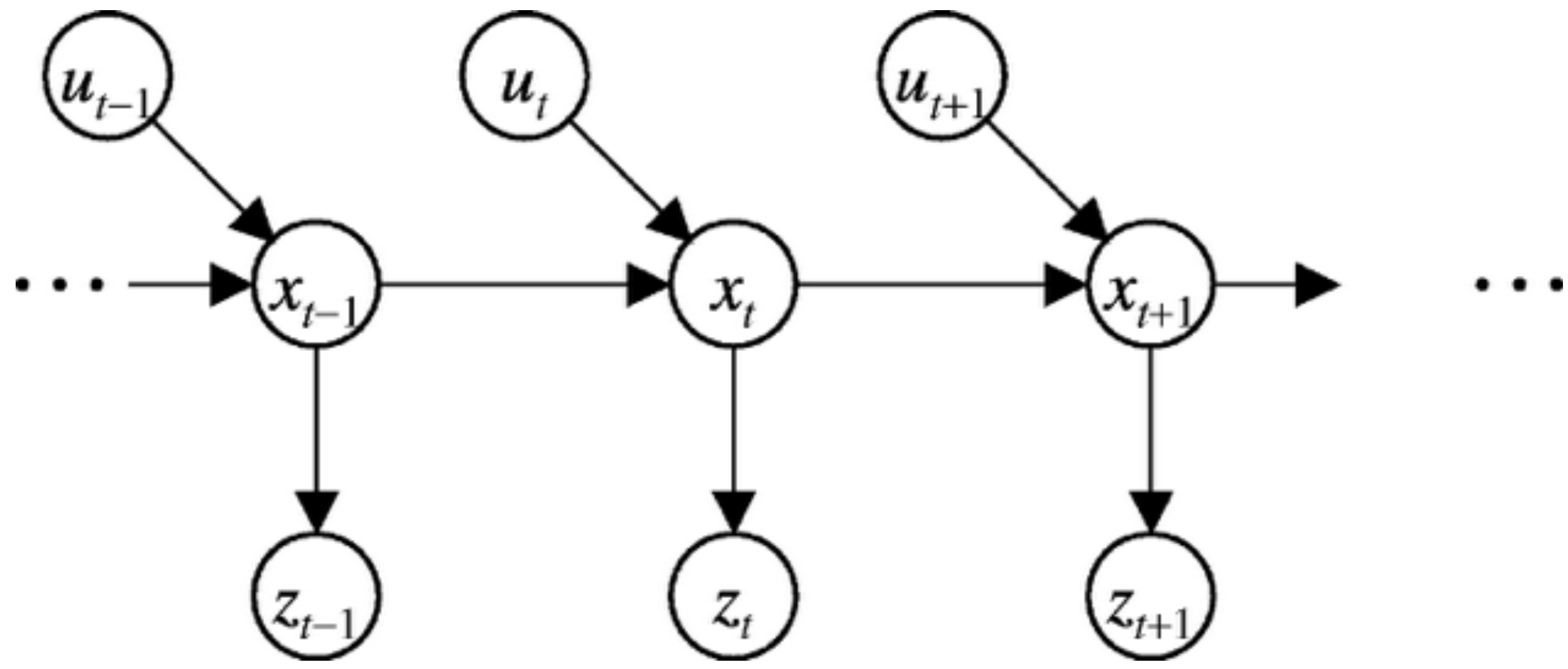
Summary

- Boosting uses **weak** classifiers and turns them into a **strong** one (arbitrarily small training error!)
- AdaBoost minimizes the **exponential** loss
- To be more robust against outliers, we can use **LogitBoost**
- Face detection can be done with Boosting
- Bagging reduces the overall committee error
- Random Forests are an example of bagging with a very good performance

8. Sequential Data

Bayes Filter (Rep.)

We can describe the overall process using a *Dynamic Bayes Network*:



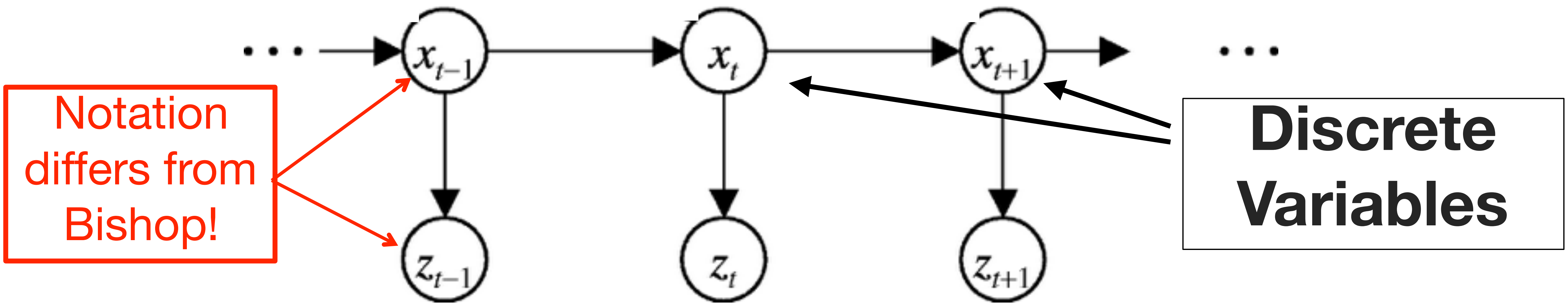
- This incorporates the following Markov assumptions:

$$p(z_t \mid x_{0:t}, u_{1:t}, z_{1:t}) = p(z_t \mid x_t)$$ (measurement)

$$p(x_t \mid x_{0:t-1}, u_{1:t}, z_{1:t}) = p(x_t \mid x_{t-1}, u_t)$$ (state)

Bayes Filter Without Actions

Removing the action variables we obtain:



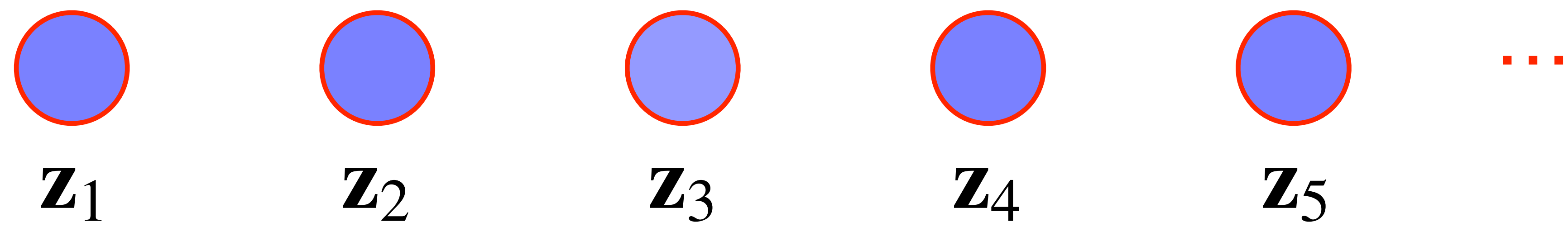
- This incorporates the following Markov assumptions:

$$p(z_t \mid x_{0:t}, \qquad z_{1:t}) = p(z_t \mid x_t) \quad \text{(measurement)}$$

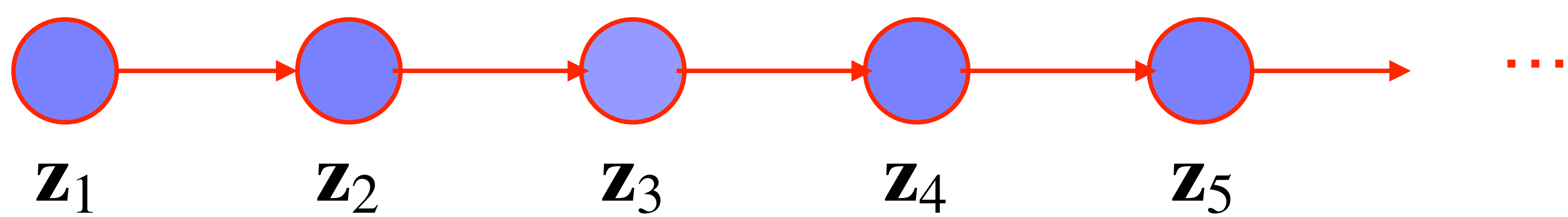
$$p(x_t \mid x_{0:t-1}, \qquad z_{1:t}) = p(x_t \mid x_{t-1} \qquad) \quad \text{(state)}$$

A Model for Sequential Data

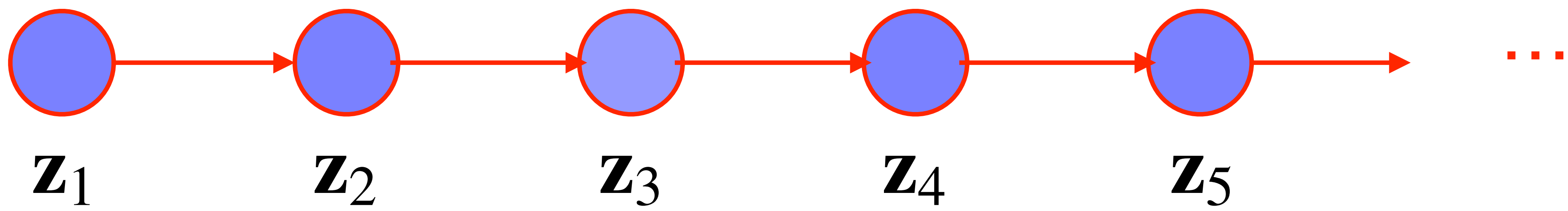
- Observations in sequential data should not be modeled as independent variables such as:



- Examples: weather forecast, speech, hand-written text, etc.
- The observation at time t depends on the observation(s) of (an) earlier time step(s):



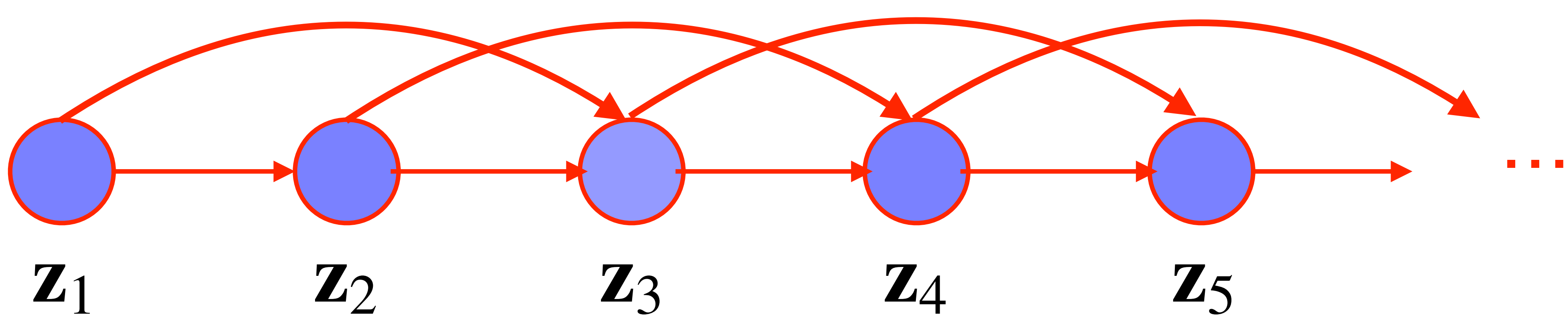
A Model for Sequential Data



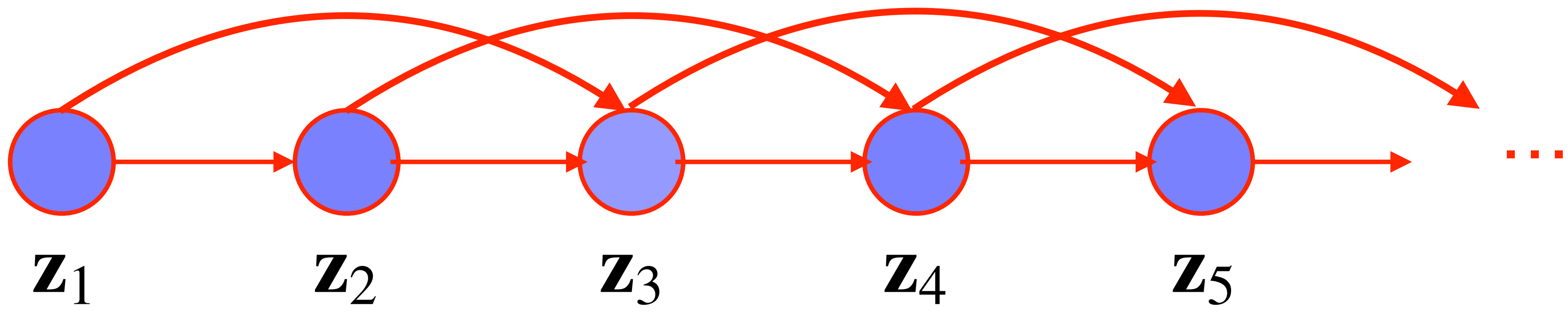
- The joint distribution is therefore (d-sep):

$$p(\mathbf{z}_1 \dots \mathbf{z}_n) = p(\mathbf{z}_1) \prod_{i=2}^{n} p(\mathbf{z}_i \mid \mathbf{z}_{i-1})$$

- **However:** often data depends on several earlier observations (not just one)



A Model for Sequential Data

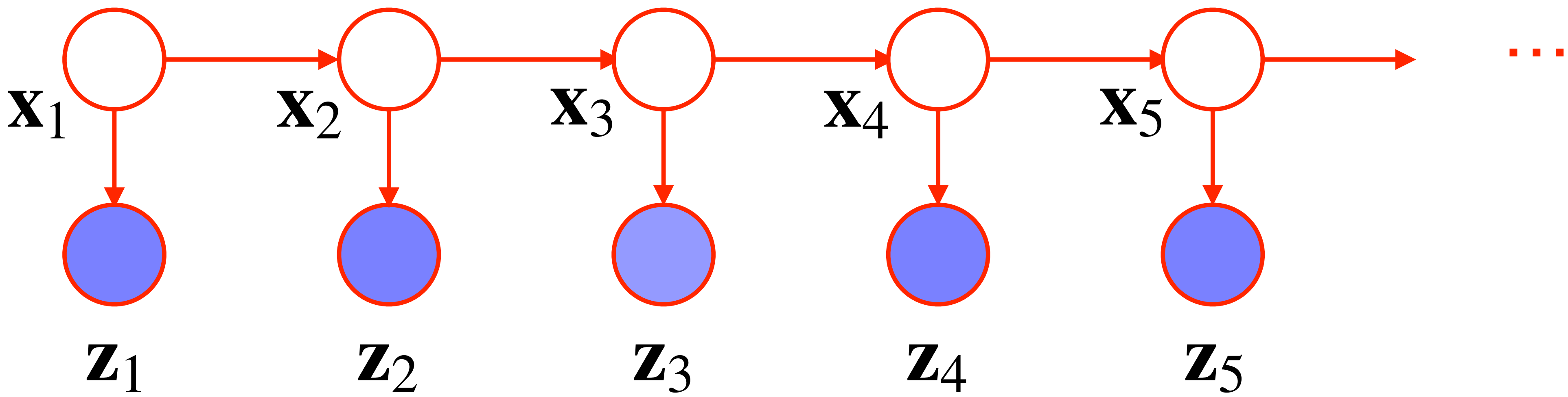


$$p(\mathbf{z}_1 \dots \mathbf{z}_n) = p(\mathbf{z}_1)p(\mathbf{z}_2 \mid \mathbf{z}_1) \prod_{i=3}^{n} p(\mathbf{z}_i \mid \mathbf{z}_{i-1}, \mathbf{z}_{i-2})$$

- **Problem:** number of stored parameters grows exponentially with the **order** of the Markov chain
- **Question:** can we model dependency of all previous observations with a limited number of parameters?

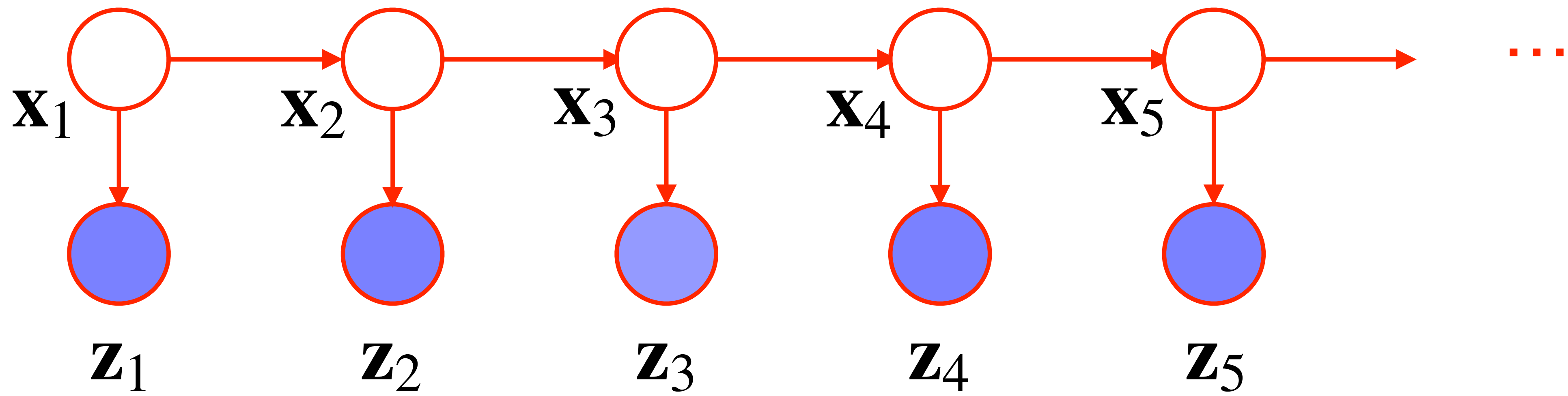
A Model for Sequential Data

Idea: Introduce **hidden** (unobserved) variables:



A Model for Sequential Data

Idea: Introduce **hidden** (unobserved) variables:



Now we have: $\mathrm{dsep}(\mathbf{x}_n, \{\mathbf{x}_1, \ldots, \mathbf{x}_{n-2}\}, \mathbf{x}_{n-1})$

$$\Leftrightarrow p(\mathbf{x}_n \mid \mathbf{x}_1, \ldots, \mathbf{x}_{n-2}, \mathbf{x}_{n-1}) = p(\mathbf{x}_n \mid \mathbf{x}_{n-1})$$

But: $\neg\mathrm{dsep}(\mathbf{z}_n, \{\mathbf{z}_1, \ldots, \mathbf{z}_{n-2}\}, \mathbf{z}_{n-1})$

$$\Leftrightarrow p(\mathbf{z}_n \mid \mathbf{z}_1, \ldots, \mathbf{z}_{n-2}, \mathbf{z}_{n-1}) \neq p(\mathbf{z}_n \mid \mathbf{z}_{n-1})$$

And: number of parameters is $nK(K\text{-}1) + const.$

Example

- Place recognition for mobile robots
- 3 different states: corridor, room, doorway
- Problem: misclassifications
- Idea: use information from previous time step