Bayesian Networks Part 3

CS 760@UW-Madison

Goals for the lecture

you should understand the following concepts

- structure learning as search
- Kullback-Leibler divergence
- the Sparse Candidate algorithm

- the Tree Augmented Network (TAN) algorithm

Heuristic search for structure learning

- each state in the search space represents a DAG Bayes net structure
- to instantiate a search approach, we need to specify
  - scoring function
  - state transition operators
  - search algorithm

Scoring function decomposability

- when the appropriate priors are used, and all instances in D are complete, the scoring function can be decomposed as follows

$$\text{score}(G, D) = \sum_i \text{score}(X_i, Parents(X_i) : D)$$

- thus we can
  - score a network by summing terms over the nodes in the network
  - efficiently score changes in a *local* search procedure

Scoring functions for structure learning

- Can we find a good structure just by trying to maximize the likelihood of the data?

$$\arg\max_{G,\theta_G} \log P(D \mid G, \theta_G)$$

- If we have a strong restriction on the the structures allowed (e.g. a tree), then maybe.

- Otherwise, no! Adding an edge will never decrease likelihood. Overfitting likely.

Scoring functions for structure learning

- there are many different scoring functions for BN structure search
- one general approach

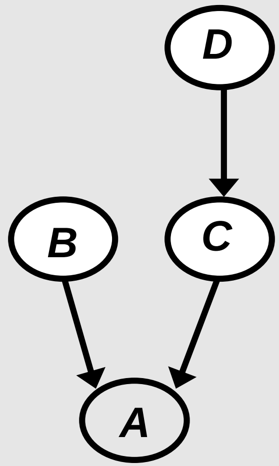
$$\arg\max_{G,\theta_G} \log P(D \mid G, \theta_G) - \underbrace{f(m)\,|\theta_G|}_{\text{complexity penalty}}$$

Akaike Information Criterion (AIC): $f(m) = 1$

Bayesian Information Criterion (BIC): $f(m) = \frac{1}{2}\log(m)$

Structure search operators

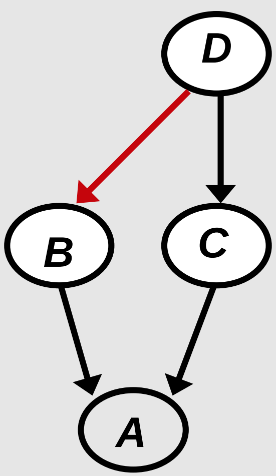
given the current network
at some stage of the search,
we can…

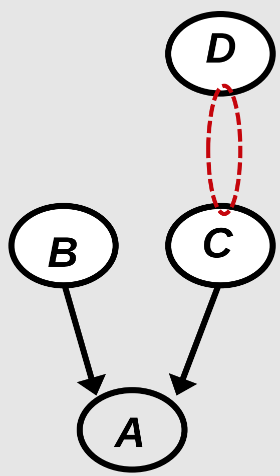


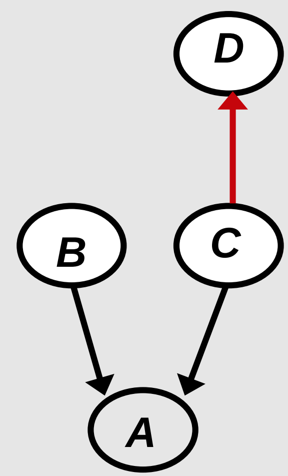
add an edge

delete an edge

reverse an edge







Bayesian network search: *hill-climbing*

given: data set D, initial network B_0

$i = 0$
$B_{best} \leftarrow B_0$
while stopping criteria not met
{
  for each possible operator application a
  {
    $B_{new} \leftarrow$ apply(a, B_i)
    if score(B_{new}) > score(B_{best})
      $B_{best} \leftarrow B_{new}$
  }
  $++i$
  $B_i \leftarrow B_{best}$
}
return B_i

Bayesian network search: the *Sparse Candidate* algorithm [Friedman et al., *UAI* 1999]

given: data set D, initial network B_0, parameter k

$i = 0$

repeat

{

$++i$

// restrict step

select for each variable X_j a set C_j^i of candidate parents ($|C_j^i| \leq k$)

// maximize step

find network B_i maximizing score among networks where $\forall X_j$, Parents(X_j) $\subseteq C_j^i$

} until convergence

return B_i

The *restrict* step in Sparse Candidate

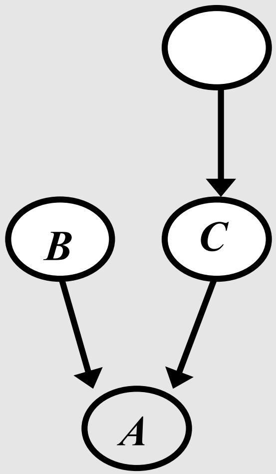
- to identify candidate parents in the <u>first</u> iteration, can compute the *mutual information* between pairs of variables

$$I(X,Y) = \sum_{x \in \text{values}(X)} \sum_{y \in \text{values}(Y)} P(x,y) \log_2 \frac{P(x,y)}{P(x)P(y)}$$

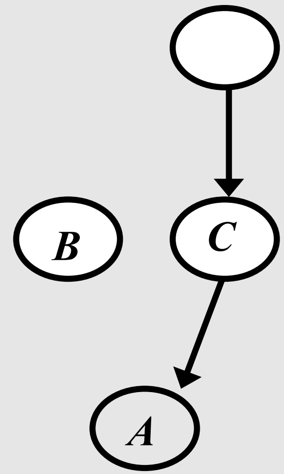
The *restrict* step in Sparse Candidate

- Suppose:

true distribution

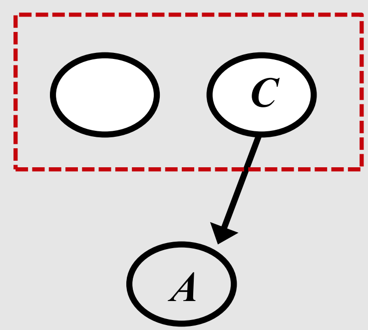


current network



we're selecting two candidate parents for A, and $I(A, C) > I(A, D) > I(A, B)$

- with mutual information, the candidate parents for A would be C and D



- how could we get B as a candidate parent?

The *restrict* step in Sparse Candidate

- *Kullback-Leibler* (KL) *divergence* provides a distance measure between two distributions, P and Q

$$D_{KL}(P(X)\,||\,Q(X)) = \sum_{x} P(x) \log \frac{P(x)}{Q(x)}$$

- mutual information can be thought of as the KL divergence between the distributions

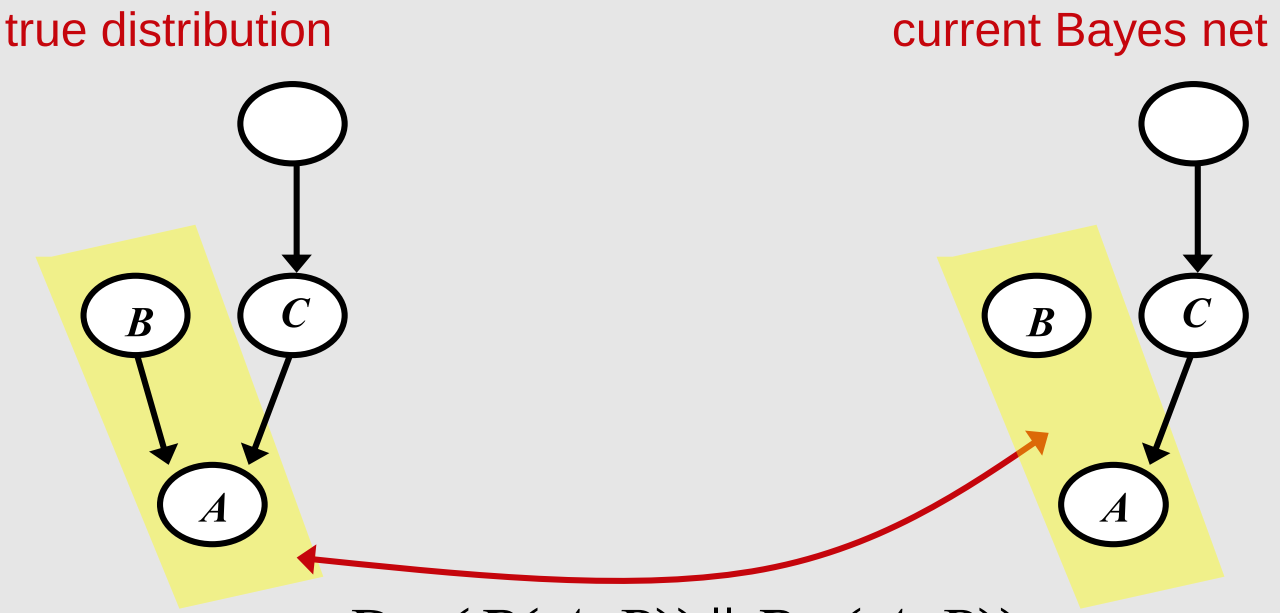
$$P(X,Y)$$

$$P(X)P(Y)$$ (assumes X and Y are independent)

The *restrict* step in Sparse Candidate

- we can use KL to assess the discrepancy between the network's $P_{net}(X, Y)$ and the empirical $P(X, Y)$

$$M(X,Y) = D_{KL}(P(X,Y)) \| P_{net}(X,Y))$$



$$D_{KL}(P(A,B)) \| P_{net}(A,B))$$

- can estimate $P_{net}(X, Y)$ by sampling from the network (i.e. using it to generate instances)

The *restrict* step in Sparse Candidate

given: data set D, current network B_i, parameter k

for each variable X_j

{

calculate M(X_j , X_l) for all $X_j \neq X_l$ such that $X_l \notin$ Parents(X_j)

choose highest ranking $X_1 \ldots X_{k-s}$ where $s = |$ Parents(X_j) $|$

// include current parents in candidate set to ensure monotonic

// improvement in scoring function

$C_j^i =$Parents(X_j) ∪ $X_1 \ldots X_{k-s}$

}

return { C_j^i } for all X_j

The *maximize* step in Sparse Candidate

- hill-climbing search with *add-edge*, *delete-edge*, *reverse-edge* operators
- test to ensure that cycles aren’t introduced into the graph

Efficiency of Sparse Candidate

n = number of variables

	possible parent sets for each node	changes scored on first iteration of search	changes scored on subsequent iterations
ordinary greedy search	$O(2^n)$	$O(n^2)$	$O(n)$
greedy search w/at most k parents	$O\left(\binom{n}{k}\right)$	$O(n^2)$	$O(n)$
Sparse Candidate	$O(2^k)$	$O(kn)$	$O(k)$

after we apply an operator, the scores will change only for edges from the parents of the node with the new impinging edge

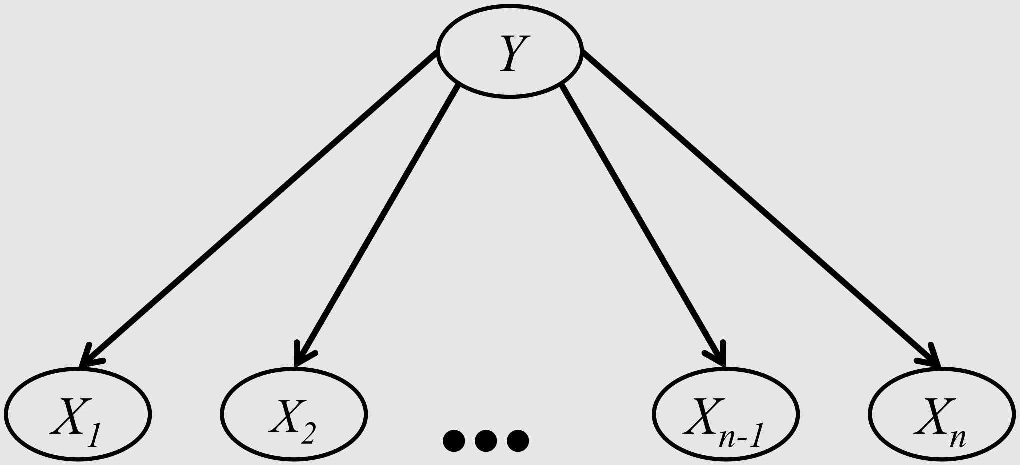
Bayes nets for classification

- the learning methods for BNs we've discussed so far can be thought of as being unsupervised
  - the learned models are not constructed to predict the value of a special class variable
  - instead, they can predict values for arbitrarily selected query variables

- now let's consider BN learning for a standard supervised task (learn a model to predict Y given $X_1 \ldots X_n$)

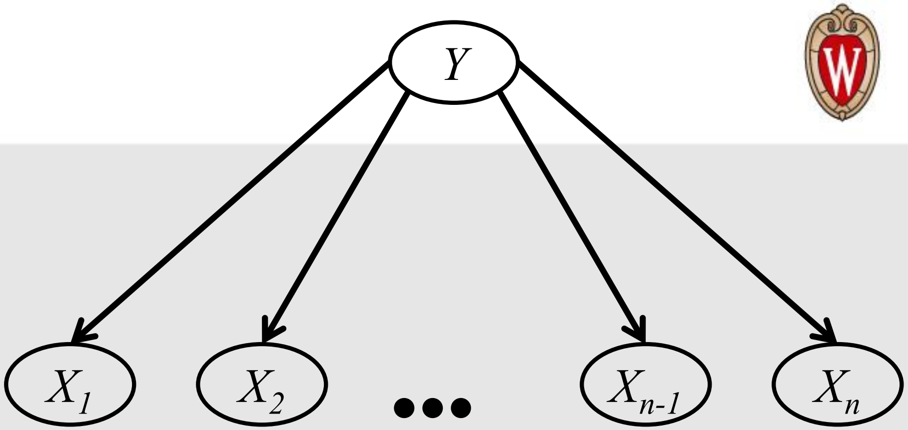
Naïve Bayes

- one very simple BN approach for supervised tasks is *naïve Bayes*
- in naïve Bayes, we assume that all features X_i are conditionally independent given the class Y



$$P(X_1,...,X_n,Y) = P(Y)\prod_{i=1}^{n} P(X_i \mid Y)$$

Naïve Bayes



Learning

- estimate $P(Y = y)$ for each value of the class variable Y
- *estimate* $P(X_i = x \mid Y = y)$ *for each* X_i

Classification: use Bayes' Rule

$$P(Y = y \mid \boldsymbol{x}) = \frac{P(y)P(\boldsymbol{x} \mid y)}{\sum_{y'} P(y')P(\boldsymbol{x} \mid y')} = \frac{P(y)\prod_{i=1}^{n} P(x_i \mid y)}{\sum_{y'}\left(P(y')\prod_{i=1}^{n} P(x_i \mid y') \right)}$$

Naïve Bayes vs. BNs learned with an unsupervised structure search

test-set error on 25 classification data sets from the UC-Irvine Repository

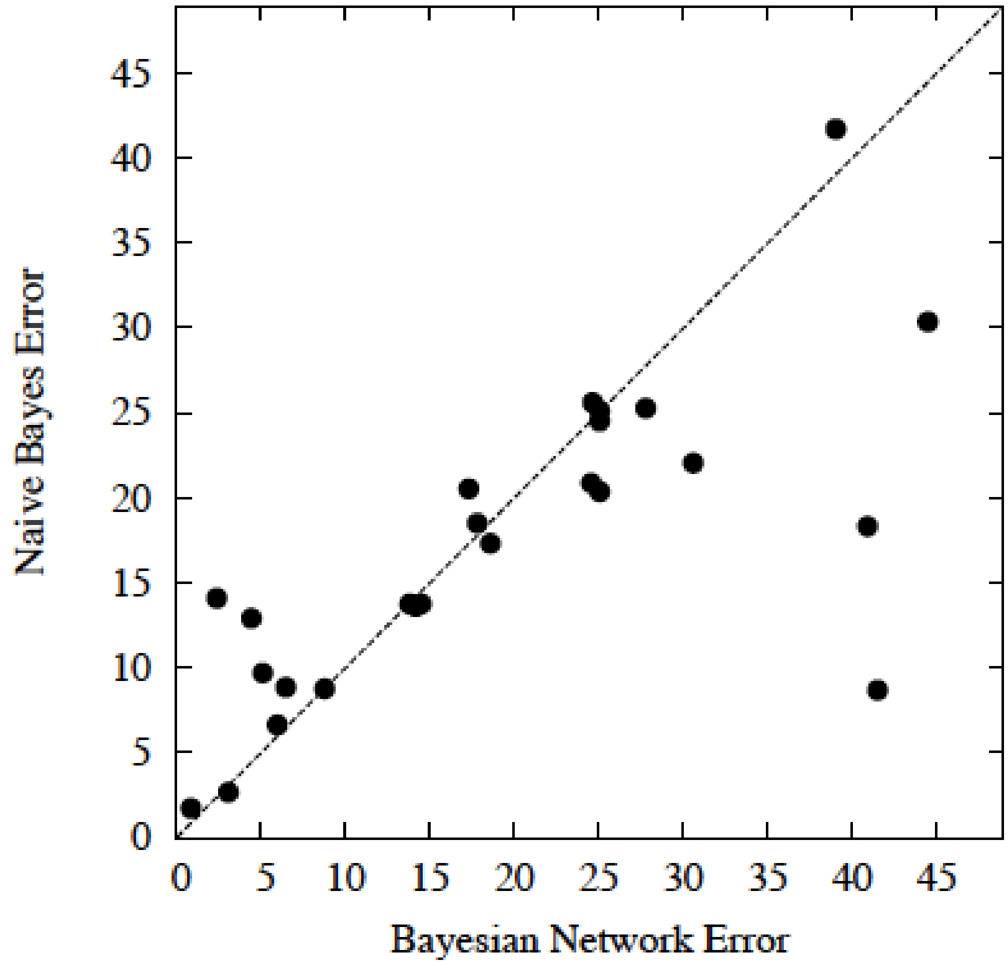


Figure from Friedman et al., *Machine Learning* 1997

The Tree Augmented Network (TAN) algorithm
[Friedman et al., *Machine Learning* 1997]

- learns a tree structure to augment the edges of a naïve Bayes network

- algorithm
  1. compute weight $I(X_i, X_j \mid Y)$ for each possible edge (X_i, X_j) between features
  2. find maximum weight spanning tree (MST) for graph over $X_1 \ldots X_n$
  3. assign edge directions in MST
  4. construct a TAN model by adding node for Y and an edge from Y to each X_i

Conditional mutual information in TAN

conditional mutual information is used to calculate edge weights

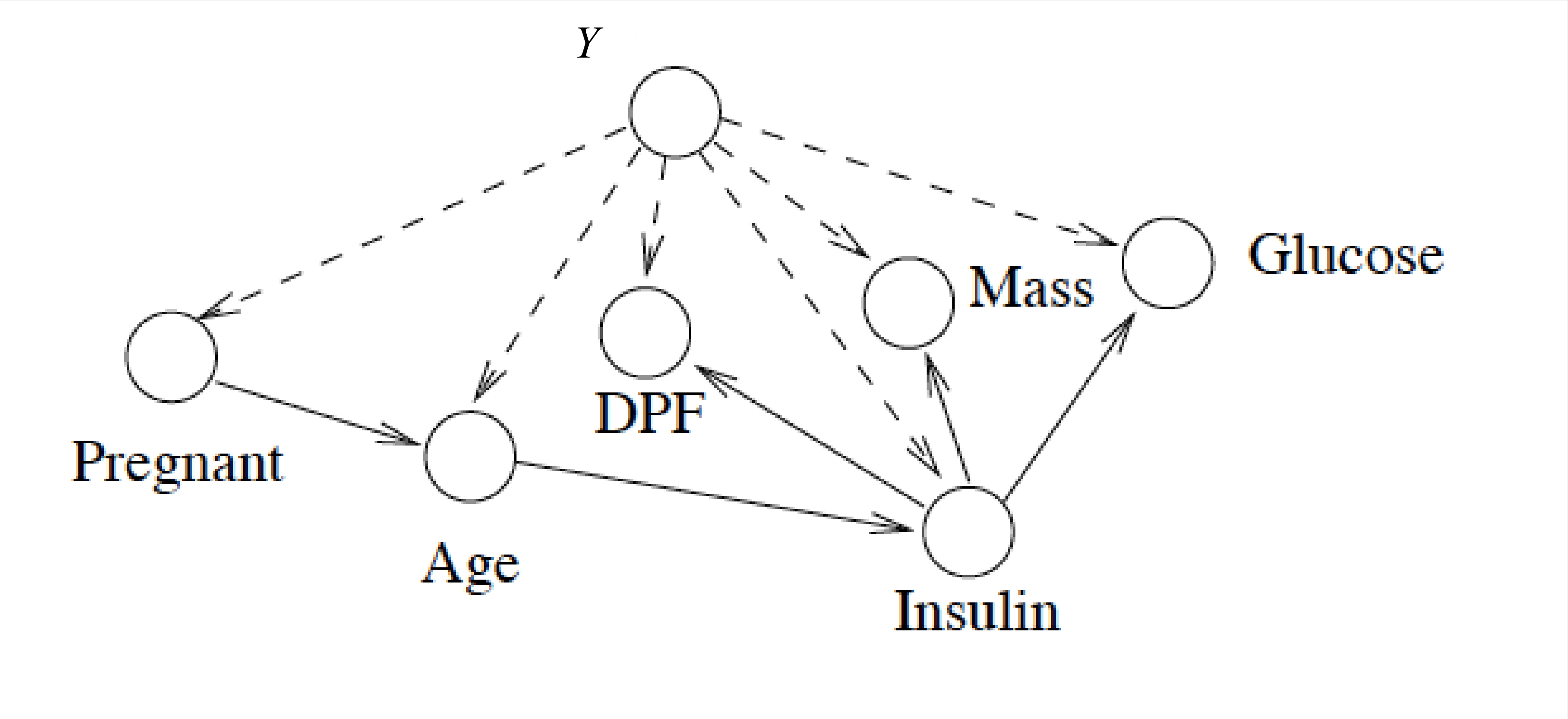
$$I(X_i, X_j \mid Y) =$$

$$\sum_{x_i \in \text{values}(X_i)} \sum_{x_j \in \text{values}(X_j)} \sum_{y \in \text{values}(Y)} P(x_i, x_j, y) \log_2 \frac{P(x_i, x_j \mid y)}{P(x_i \mid y) P(x_j \mid y)}$$

"how much information X_i provides about X_j when the value of Y is known"

Example TAN network

class variable



naïve Bayes edges

edges determined by MST

TAN vs. Chow-Liu

- TAN is focused on learning a Bayes net specifically for classification problems
- the MST includes only the feature variables (the class variable is used only for calculating edge weights)
- conditional mutual information is used instead of mutual information in determining edge weights in the undirected graph
- the directed graph determined from the MST is added to the $Y \rightarrow X_i$ edges that are in a naïve Bayes network

TAN vs. Naïve Bayes

test-set error on 25 data sets from the UC-Irvine Repository

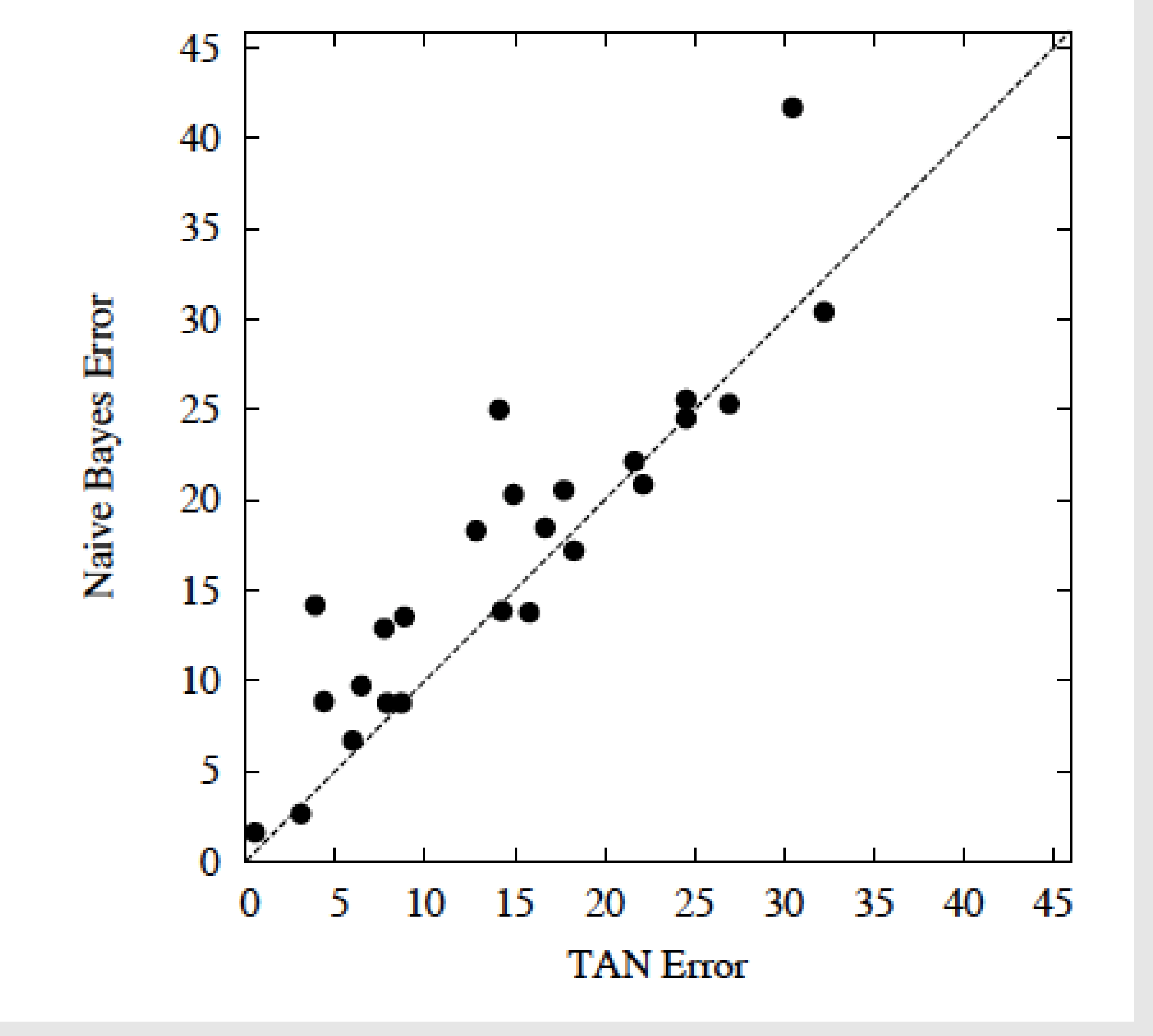
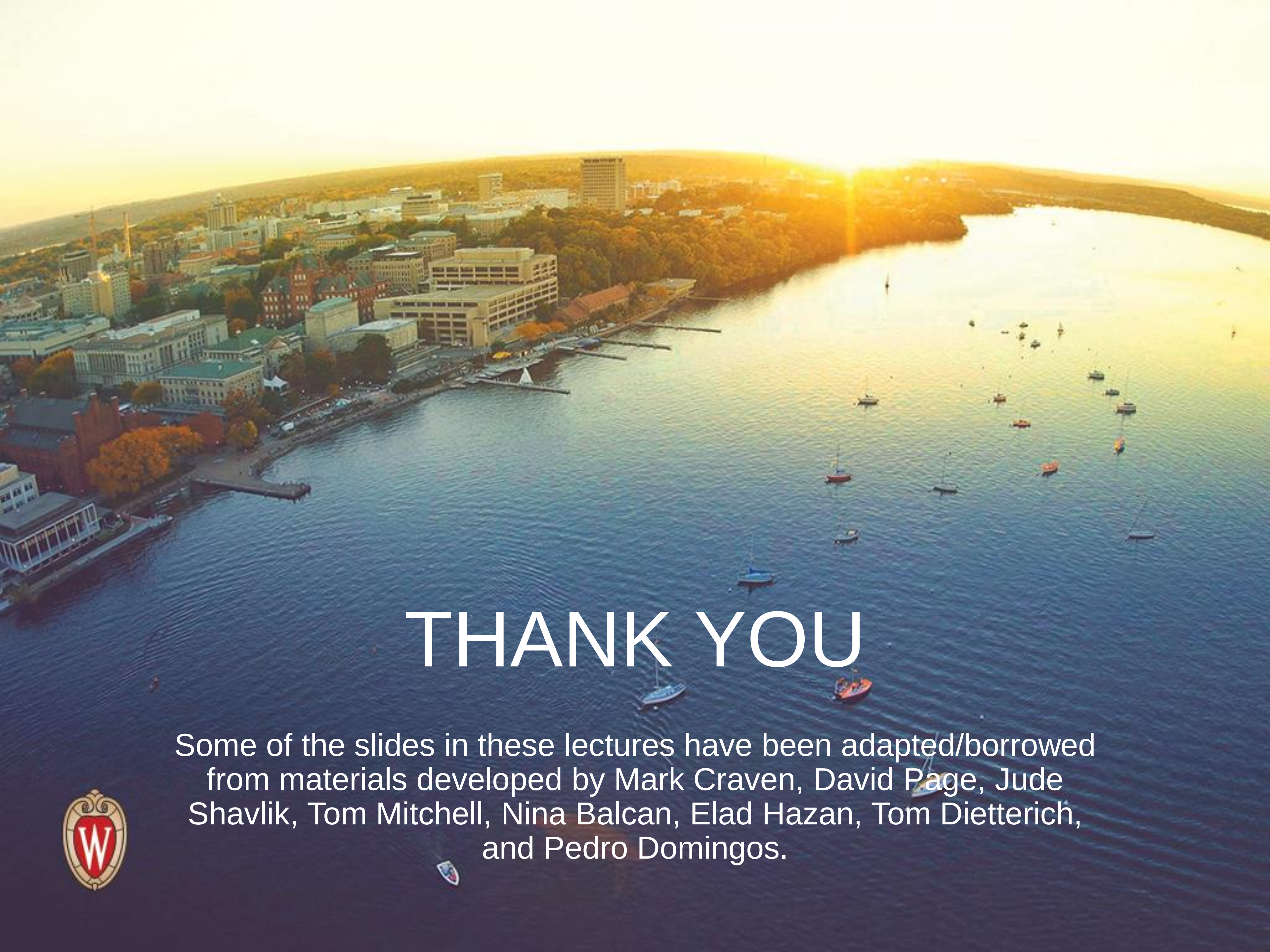


Figure from Friedman et al., *Machine Learning* 1997

Comments on Bayesian networks

- the BN representation has many advantages
  - easy to encode domain knowledge (direct dependencies, causality)
  - can represent uncertainty
  - principled methods for dealing with missing values
  - can answer arbitrary queries (in theory; in practice may be intractable)
- for supervised tasks, it may be advantageous to use a learning approach (e.g. TAN) that focuses on the dependencies that are most important
- although very simplistic, naïve Bayes often learns highly accurate models
- BNs are one instance of a more general class of *probabilistic graphical models*



THANK YOU

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, and Pedro Domingos.