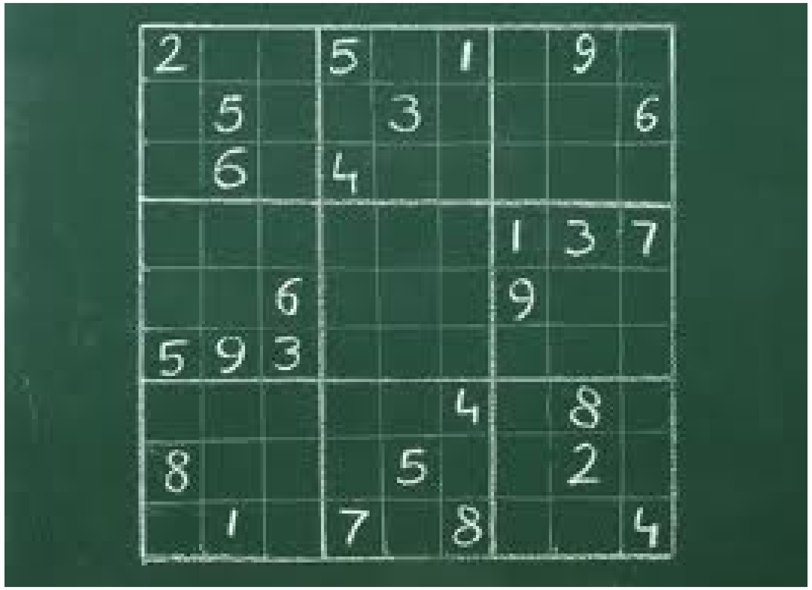
Lecture 4.2: CSPs I



Question

Find two neighboring countries, one that begins with an A and the other that speaks Hungarian.

Course plan

Search problems

Markov decision processes

Adversarial games

Constraint satisfaction problems

Bayesian networks

Reflex **States** **Variables** **Logic**

"Low-level intelligence" "High-level intelligence"

Machine learning

- Now we begin our tour of variable-based models with constraint satisfaction problems.

Review of search

[Modeling]

Framework search problems

Objective minimum cost paths

[Inference]

Tree-based backtracking search

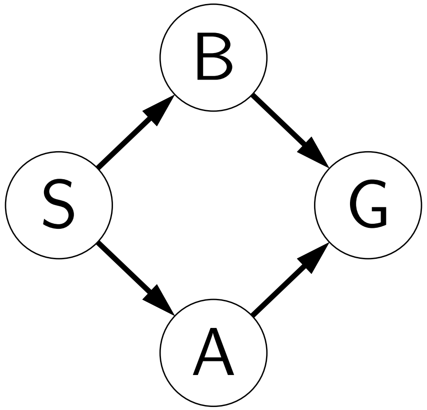
Graph-based DP, UCS, A*

[Learning]

Methods structured Perceptron

- **Modeling**: In the context of state-based models, we seek to find minimum cost paths.
- **Inference**: To compute these solutions, we can either work on the search tree or on the state graph. In the former case, we end up with recursive procedures which take exponential time but require very little memory (generally linear in the size of the solution). In the latter case, where we are fortunate to have few enough states to fit into memory, we can work directly on the graph, which can often yield an exponential savings in time.
- Given that we can find the optimal solution with respect to a fixed model, the final question is where this model actually comes from. **Learning** provides the answer: from data. You should think of machine learning as not just a way to do binary classification, but more as a way of life, which can be used to support a variety of different models.

State-based models: takeaway 1



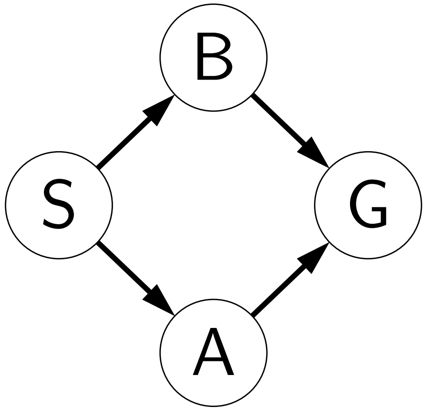
Key idea: specify locally, optimize globally

Modeling: specifies local interactions

Inference: find globally optimal solutions

- One high-level takeaway is the motto: specify locally, optimize globally. When we're building a search problem, we only need to specify how the states are connected through actions and what the local action costs are; we need not specify the long-term consequences of taking an action. It is the job of the inference to take all of this local information into account and produce globally optimal solutions (minimum cost paths).
- This separation is quite powerful in light of modeling and inference: having to worry only about local interactions makes modeling easier, but we still get the benefits of a globally optimal solution via inference which are constructed independent of the domain-specific details.
- We will see this local specification + global optimization pattern again in the context of variable-based models.

State-based models: takeaway 2



Key idea: state

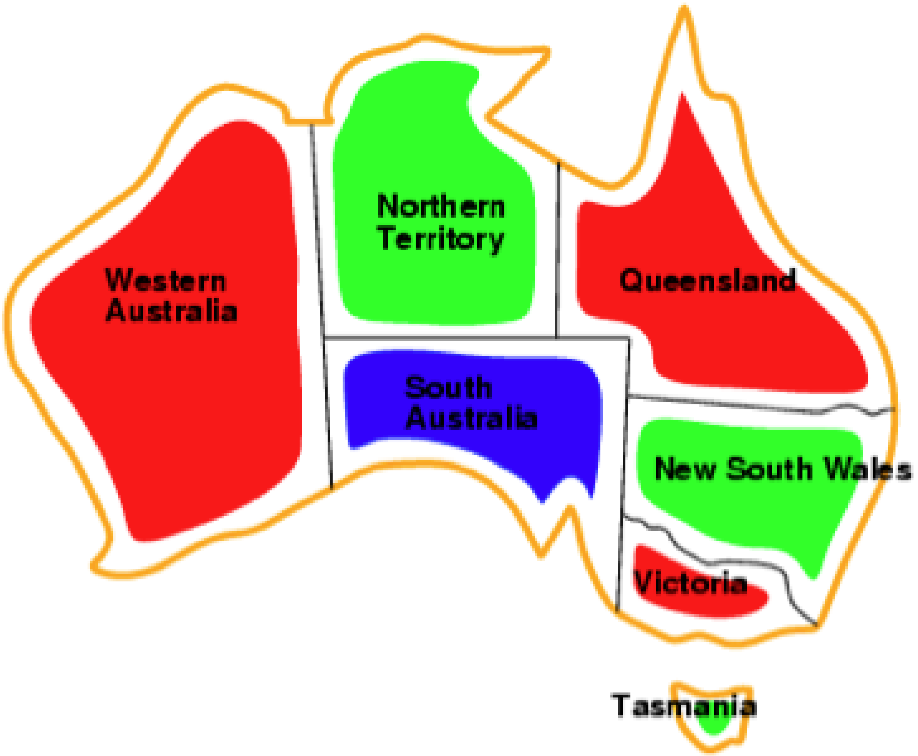
A **state** is a summary of all the past actions sufficient to choose future actions **optimally**.

Mindset: move through states (nodes) via actions (edges)

- The second high-level takeaway which is core to state-based models is the notion of **state**. The state, which summarizes previous actions, is one of the key tools that allows us to manage the exponential search problems frequently encountered in AI. We will see the notion of state appear again in the context of conditional independence in variable-based models.
- With states, we were in the mindset of thinking about taking a sequence of actions (where order is important) to reach a goal. However, in some tasks, order is irrelevant. In these cases, maybe search isn't the best way to model the task. Let's see an example.

Question: how can we color each of the 7 provinces {red,green,blue} so that no two neighboring provinces have the same color?

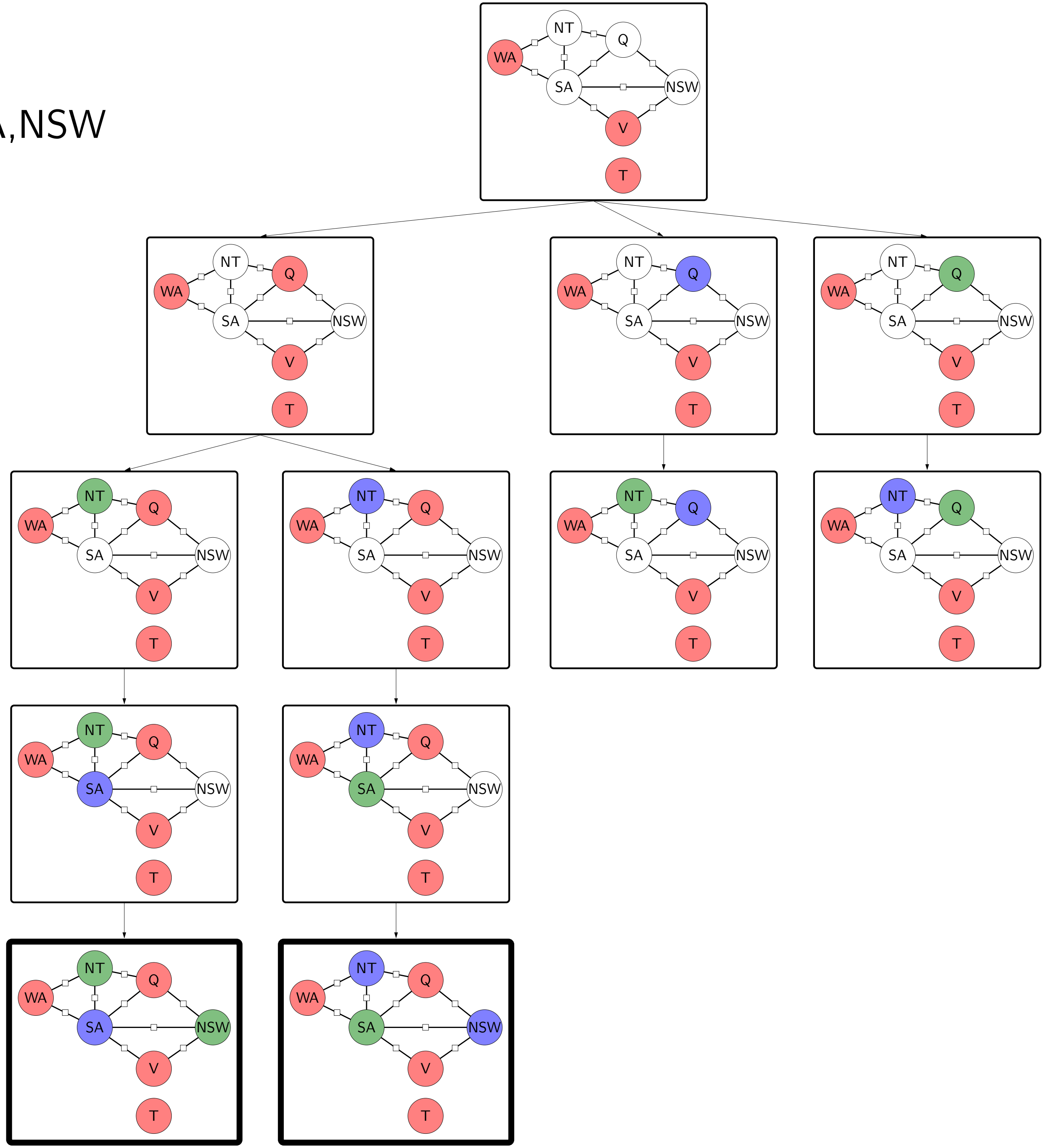
Map coloring



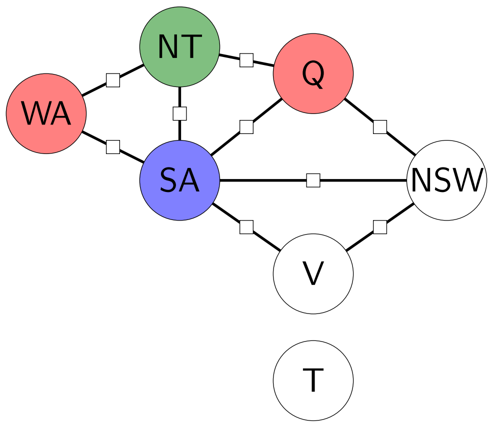
(one possible solution)

Search

WA,V,T,Q,NT,SA,NSW



As a search problem



- State: partial assignment of colors to provinces
- Action: assign next uncolored province a compatible color

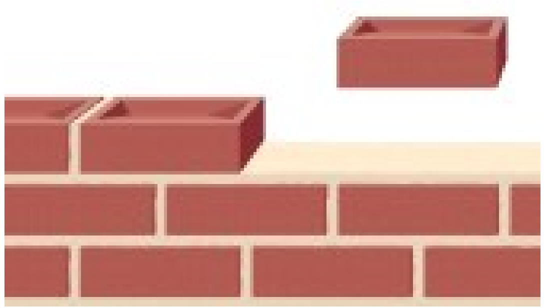
What's missing? There's more problem structure!

- Variable ordering doesn't affect correctness, but can affect runtime
- Variables are interdependent in a local way

- We can certainly use search to find an assignment of colors to the provinces of Australia. Let's fix an arbitrary ordering of the provinces. Each state contains an assignment of colors to a subset of the provinces (a **partial assignment**), and each action chooses a color for the next unassigned province as long as the color isn't already assigned to one of its neighbors. In this way, all the leaves of the search tree are solutions (18 of them). (In the slide, in the interest of space, we've only shown the subtree rooted at a partial assignment to 3 variables.)
- This is a fine way to solve this problem, and in general, it shows how powerful search is: we don't actually need any new machinery to solve this problem. But the question is: can we do better?
- First, the particular search tree that we drew had several dead ends; it would be better if we could detect these earlier. We will see in this lecture that the fact that **the order in which we assign variables doesn't matter for correctness** gives us the flexibility to dynamically choose a better ordering of the variables. That, with a bit of lookahead will allow us to dramatically improve the efficiency over naive tree search.
- Second, it's clear that Tasmania's color can be any of the three colors regardless of the colors on the mainland. This is an instance of **independence**, and next time, we'll see how to exploit these observations systematically.

Variable-based models

A new framework...



Key idea: variables

- Solutions to problems $\Rightarrow$ assignments to variables (modeling).
- Decisions about variable ordering, etc. chosen by inference.

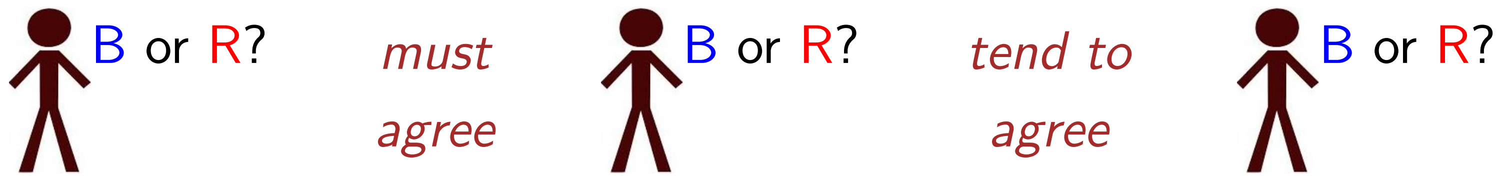
- With that motivation in mind, we now embark on our journey into variable-based models. Variable-based models is an umbrella term that includes constraint satisfaction problems (CSPs), Markov networks, Bayesian networks, hidden Markov models (HMMs), conditional random fields (CRFs), etc., which we'll get to later in the course. The term graphical models can be used interchangeably with variable-based models, and the term probabilistic graphical models (PGMs) generally encompasses both Markov networks (also called undirected graphical models) and Bayesian networks (directed graphical models).
- The unifying theme is the idea of thinking about solutions to problems as assignments of values to variables (this is the modeling part). All the details about how to find the assignment (in particular, which variables to try first) are delegated to inference. So the advantage of using variable-based models over state-based models is that it's making the algorithms do more of the work, freeing up more time for modeling.
- An apt analogy is programming languages. Solving a problem directly by implementing an ad-hoc program is like using assembly language. Solving a problem using state-based models is like using C. Solving a problem using variable-based models is like using Python. By moving to a higher language, you might forgo some amount of ability to optimize manually, but the advantage is that (i) you can think at a higher level and (ii) there are more opportunities for optimizing automatically.
- Once the different modeling frameworks become second nature, it is almost as if they are invisible. It's like when you master a language, you can "think" in it without constantly referring to the framework.

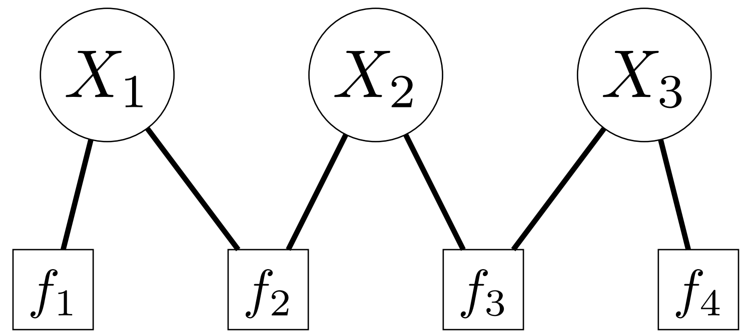
Roadmap

Factor graphs

Dynamic ordering

Factor graph (example)





x_1	$f_1(x_1)$
R	0
B	1

x_1	x_2	$f_2(x_1, x_2)$
R	R	1
R	B	0
B	R	0
B	B	1

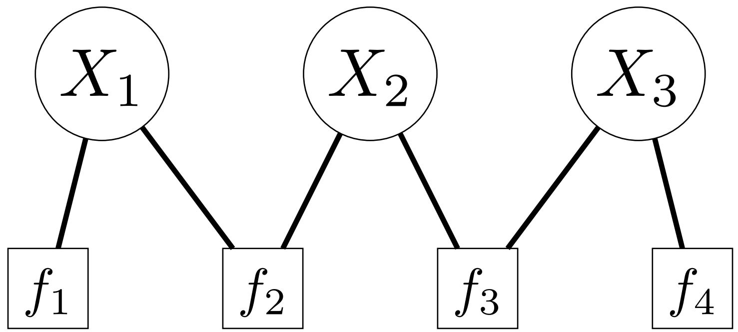
x_2	x_3	$f_3(x_2, x_3)$
R	R	3
R	B	2
B	R	2
B	B	3

x_3	$f_4(x_3)$
R	2
B	1

$f_2(x_1, x_2) = [x_1 = x_2]$ $\quad$ $f_3(x_2, x_3) = [x_2 = x_3] + 2$

- The most important concept for the next three weeks will be that of a **factor graph**. But before we define it formally, let us consider a simple example.
- Suppose there are three people, each of which will vote for a color, red or blue. We know that Person 1 is leaning pretty set on blue, and Person 3 is leaning red. Person 1 and Person 2 must have the same color, while Person 2 and Person 3 would weakly prefer to have the same color.
- We can model this as a factor graph consisting of three **variables**, X_1, X_2, X_3, each of which must be assigned red (R) or blue (B).
- We encode each of the constraints/preferences as a **factor**, which assigns a non-negative number based on the assignment to a subset of the variables. We can either describe the factor as an explicit table, or via a function (e.g., $[x_1 = x_2]$).

Factor graph



Definition: factor graph

Variables:

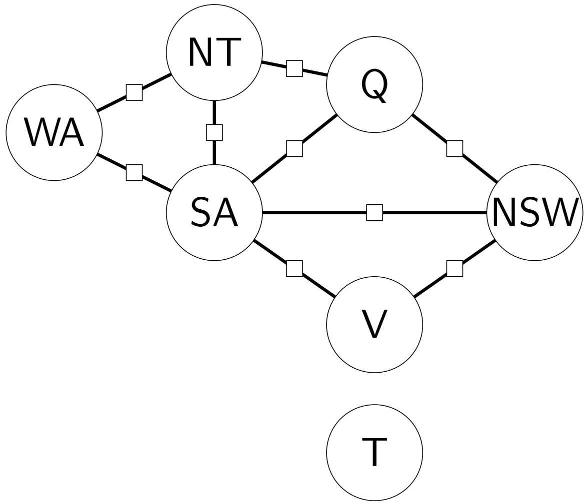
$$X = (X_1, \ldots, X_n), \text{ where } X_i \in \text{Domain}_i$$

Factors:

$$f_1, \ldots, f_m, \text{ with each } f_j(X) \geq 0$$

- Now we proceed to the general definition. A factor graph consists of a set of variables and a set of factors: (i) n variables $X_1, \dots, X_n$, which are represented as circular nodes in the graphical notation; and (ii) m factors (also known as potentials) $f_1, \dots, f_m$, which are represented as square nodes in the graphical notation.
- Each variable X_i can take on values in its **domain** Domain_i. Each factor f_j is a function that takes an assignment x to all the variables and returns a non-negative number representing how good that assignment is (from the factor's point of view). Usually, each factor will depend only on a small subset of the variables.

Example: map coloring



Variables:

$$X = (\text{WA}, \text{NT}, \text{SA}, \text{Q}, \text{NSW}, \text{V}, \text{T})$$

$$\text{Domain}_i \in \{\text{R}, \text{G}, \text{B}\}$$

Factors:

$$f_1(X) = [\text{WA} \neq \text{NT}]$$

$$f_2(X) = [\text{NT} \neq \text{Q}]$$

...

- Notation: we use $[\text{condition}]$ to represent the indicator function which is equal to 1 if the condition is true and 0 if not. Normally, this is written $\mathbf{1}[\text{condition}]$, but we drop the $\mathbf{1}$ for succinctness.

Factors

Definition: scope and arity

Scope of a factor f_j: set of variables it depends on.

Arity of f_j is the number of variables in the scope.

Unary factors (arity 1); **Binary** factors (arity 2).

Example: map coloring

- Scope of $f_1(X) = [\text{WA} \neq \text{NT}]$ is $\{\text{WA}, \text{NT}\}$
- f_1 is a binary factor

- The key aspect that makes factor graphs useful is that each factor f_j only depends on a subset of variables, called the **scope**. The arity of the factors is generally small (think 1 or 2).

Assignment weights (example)

x_1	$f_1(x_1)$
R	0
B	1

x_1	x_2	$f_2(x_1, x_2)$
R	R	1
R	B	0
B	R	0
B	B	1

x_2	x_3	$f_3(x_2, x_3)$
R	R	3
R	B	2
B	R	2
B	B	3

x_3	$f_4(x_3)$
R	2
B	1

x_1	x_2	x_3	Weight
R	R	R	$0 \cdot 1 \cdot 3 \cdot 2 = 0$
R	R	B	$0 \cdot 1 \cdot 2 \cdot 1 = 0$
R	B	R	$0 \cdot 0 \cdot 2 \cdot 2 = 0$
R	B	B	$0 \cdot 0 \cdot 3 \cdot 1 = 0$
B	R	R	$1 \cdot 0 \cdot 3 \cdot 2 = 0$
B	R	B	$1 \cdot 0 \cdot 2 \cdot 1 = 0$
B	B	R	$1 \cdot 1 \cdot 2 \cdot 2 = 4$
B	B	B	$1 \cdot 1 \cdot 3 \cdot 1 = 3$

- A factor graph specifies all the local interactions between variables. We wish to find a global solution. A solution is called an **assignment**, which specifies a value for each variable.
- Each assignment is associated with a weight, which is just the product over each factor evaluated on that assignment. Intuitively, each factor contributes to the weight. Note that any factor has veto power: if it returns zero, then the entire weight is irrecoverably zero.
- In this setting, the maximum weight assignment is $(\mathsf{B}, \mathsf{B}, \mathsf{R})$, which has a weight of 4. You can think of this as the optimal configuration or the most likely outcome.

Assignment weights

Definition: assignment weight

Each **assignment** $x = (x_1, \dots, x_n)$ has a **weight**:

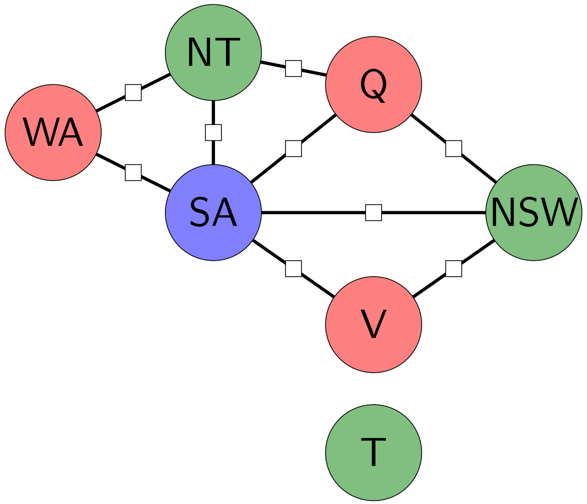
$$\text{Weight}(x) = \prod_{j=1}^{m} f_j(x)$$

Objective: find the maximum weight assignment

$$\arg\max_x \text{Weight}(x)$$

- Formally, the **weight** of an assignment x is the product of all the factors applied to that assignment ($\prod_{j=1}^{m} f_j(x)$). Think of all the factors chiming in on their opinion of x. We multiply all these opinions together to get the global opinion.
- Our objective will be to find the **maximum weight assignment**.
- Note: do not confuse the term "weight" in the context of factor graphs with the "weight vector" in machine learning.

Example: map coloring



Assignment:

$$x = \{\text{WA} : \text{R}, \text{NT} : \text{G}, \text{SA} : \text{B}, \text{Q} : \text{R}, \text{NSW} : \text{G}, \text{V} : \text{R}, \text{T} : \text{G}\}$$

Weight:

$$\text{Weight}(x) = 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 = 1$$

Assignment:

$$x' = \{\text{WA} : \text{R}, \text{NT} : \text{R}, \text{SA} : \text{B}, \text{Q} : \text{R}, \text{NSW} : \text{G}, \text{V} : \text{R}, \text{T} : \text{G}\}$$

Weight:

$$\text{Weight}(x') = 0 \cdot 0 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 = 0$$

- In the map coloring example, each factor only looks at the variables of two adjacent provinces and checks if the colors are different (returning 1) or the same (returning 0). From a modeling perspective, this allows us to specify local interactions in a modular way. A global notion of consistency is achieved by multiplying together all the factors.
- Again note that the factors are multiplied (not added), which means that any factor has veto power: a single zero causes the entire weight to be zero.

Constraint satisfaction problems

Definition: constraint satisfaction problem (CSP)

A CSP is a factor graph where all factors are **constraints**:

$$f_j(x) \in \{0, 1\} \text{ for all } j = 1, \dots, m$$

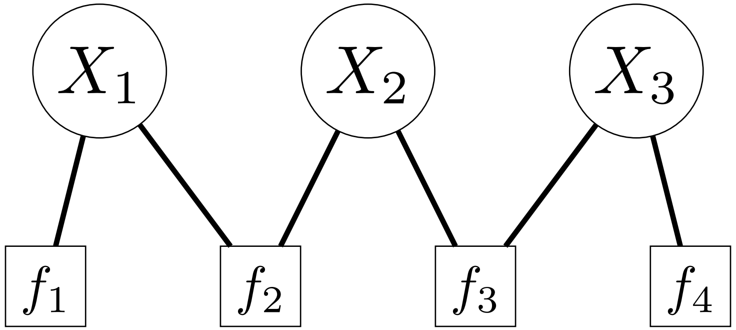
The constraint is satisfied iff $f_j(x) = 1$.

Definition: consistent assignments

An assignment x is **consistent** iff $\text{Weight}(x) = 1$ (i.e., **all** constraints are satisfied).

- Constraint satisfaction problems are just a special case of factor graphs where each of the factors returns either 0 or 1. Such a factor is a **constraint**, where 1 means the constraint is satisfied and 0 means that it is not.
- In a CSP, all assignments have either weight 1 or 0. Assignments with weight 1 are called **consistent** (they satisfy all the constraints), and the assignments with weight 0 are called inconsistent. Our goal is to find any consistent assignment (if one exists).

Summary so far



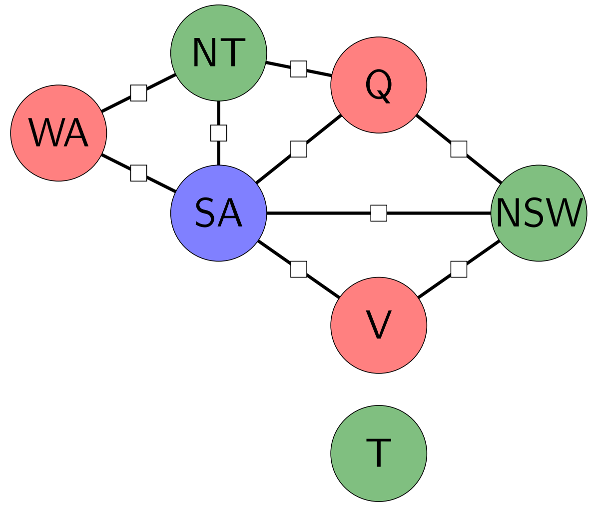
Factor graph (general)	**CSP** (all or nothing)
variables	variables
factors	constraints
assignment weight	consistent or inconsistent

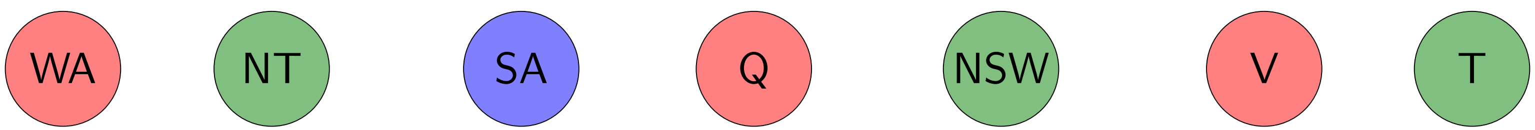
Roadmap

Factor graphs

Dynamic ordering

Extending partial assignments



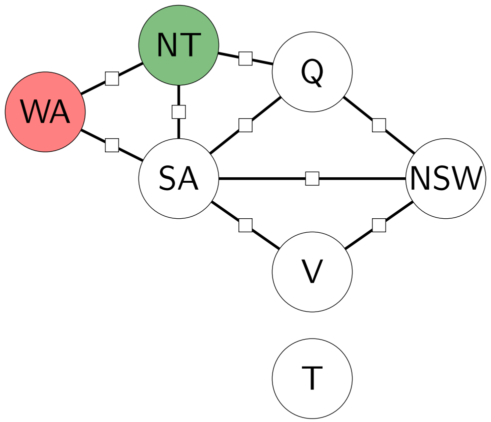


WA	NT	SA	Q	NSW	V	T
	[WA $\neq$ NT]	[WA $\neq$ SA] [NT $\neq$ SA]	[NT $\neq$ Q] [SA $\neq$ Q]	[SA $\neq$ NSW] [Q $\neq$ NSW]	[SA $\neq$ V] [NSW $\neq$ V]	

- The general idea, as we've already seen in our search-based solution is to work with **partial assignments**. We've defined the weight of a full assignment to be the product of all the factors applied to that assignment.
- We extend this definition to partial assignments: The weight of a partial assignment is defined to be the product of all the factors whose scope includes only assigned variables. For example, if only WA and NT are assigned, the weight is just value of the single factor between them.
- When we assign a new variable a value, the weight of the new extended assignment is defined to be the original weight times all the factors that depend on the new variable and only previously assigned variables.

Dependent factors

- Partial assignment (e.g., $x = \{\text{WA} : \text{R}, \text{NT} : \text{G}\}$)



Definition: dependent factors

Let $D(x, X_i)$ be the set of factors depending on X_i and x but not on unassigned variables.

$$D(\{\text{WA} : \text{R}, \text{NT} : \text{G}\}, \text{SA}) = \{[\text{WA} \neq \text{SA}], [\text{NT} \neq \text{SA}]\}$$

- Formally, we will use $D(x, X_i)$ to denote this set of these factors, which we will call **dependent factors**.
- For example, if we assign SA, then $D(x, \text{SA})$ contains two factors: the one between SA and WA and the one between SA and NT.

Backtracking search

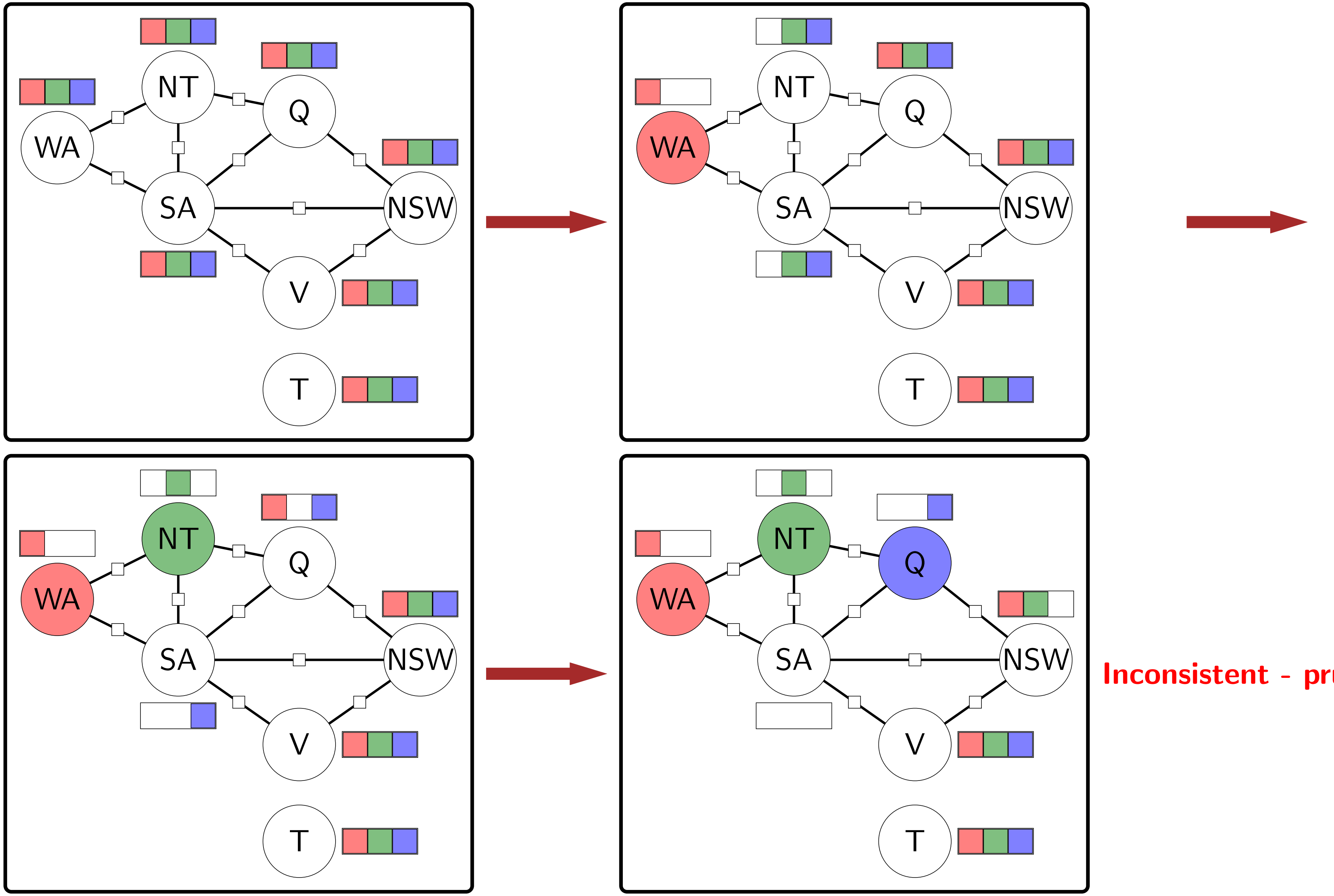
Algorithm: backtracking search

Backtrack($x, w,$ Domains):

- If x is complete assignment: update best and return
- Choose unassigned **VARIABLE** X_i
- Order **VALUES** Domain$_i$ of chosen X_i
- For each value v in that order:
  - $\delta \leftarrow \prod_{f_j \in D(x, X_i)} f_j(x \cup \{X_i : v\})$
  - If $\delta = 0$: continue
  - Domains$' \leftarrow$ Domains via **LOOKAHEAD**
  - Backtrack($x \cup \{X_i : v\}, w\delta,$ Domains$'$)

- Now we are ready to present the full backtracking search, which is a recursive procedure that takes in a partial assignment x, its weight w, and the domains of all the variables Domains $= (\text{Domain}_1, \dots, \text{Domain}_n)$.
- If the assignment x is complete (all variables are assigned), then we update our statistics based on what we're trying to compute: We can increment the total number of assignments seen so far, check to see if x is better than the current best assignment that we've seen so far (based on w), etc. (For CSPs where all the weights are 0 or 1, we can stop as soon as we find one consistent assignment, just as in DFS for search problems.)
- Otherwise, we choose an **unassigned variable** X_i. Given the choice of X_i, we choose an **ordering of the values** of that variable X_i. Next, we iterate through all the values $v \in \text{Domain}_i$ in that order. For each value v, we compute δ, which is the product of the dependent factors $D(x, X_i)$; recall this is the multiplicative change in weight from assignment x to the new assignment $x \cup \{X_i : v\}$. If $\delta = 0$, that means a constraint is violated, and we can ignore this partial assignment completely, because multiplying more factors later on cannot make the weight non-zero.
- We then perform **lookahead**, removing values from the domains Domains to produce Domains$'$. This is not required (we can just use Domains$'$ = Domains), but it can make our algorithm run faster. (We'll see one type of lookahead in the next slide.)
- Finally, we recurse on the new partial assignment $x \cup \{X_i : v\}$, the new weight $w\delta$, and the new domain Domains$'$.
- If we choose an unassigned variable according to an arbitrary fixed ordering, order the values arbitrarily, and do not perform lookahead, we get the basic tree search algorithm that we would have used if we were thinking in terms of a search problem. We will next start to improve the efficiency by exploiting properties of the CSP.

Lookahead: forward checking (example)



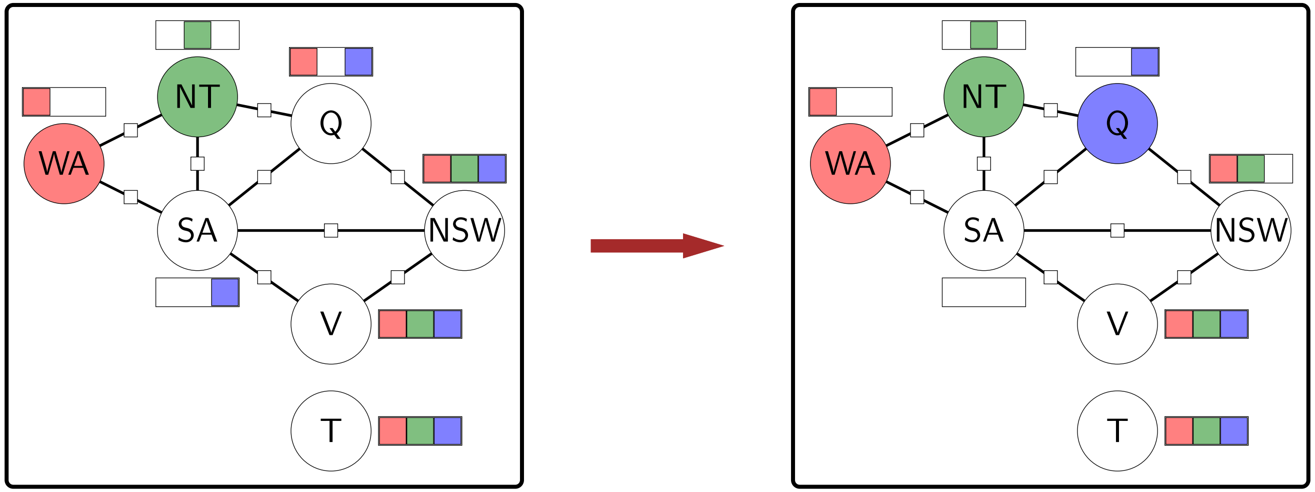
Inconsistent - prune!

- First, we will look at **forward checking**, which is a way to perform a one-step lookahead. The idea is that as soon as we assign a variable (e.g., WA $=$ R), we can pre-emptively remove inconsistent values from the domains of neighboring variables (i.e., those that share a factor).
- If we keep on doing this and get to a point where some variable has an empty domain, then we can stop and backtrack immediately, since there's no possible way to assign a value to that variable which is consistent with the previous partial assignment.
- In this example, after Q is assigned blue, we remove inconsistent values (blue) from SA's domain, emptying it. At this point, we need not even recurse further, since there's no way to extend the current assignment. We would then instead try assigning Q to red.

Lookahead: forward checking

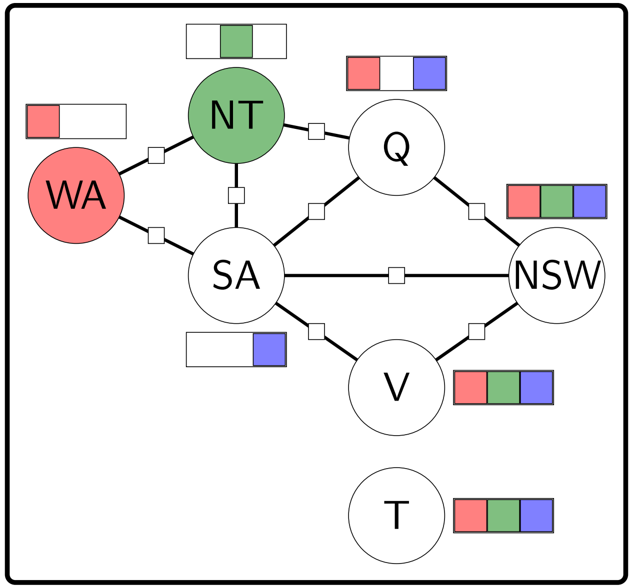
Key idea: forward checking (one-step lookahead)

- After assigning a variable X_i, eliminate inconsistent values from the domains of X_i's neighbors.
- If any domain becomes empty, don't recurse.
- When unassign X_i, restore neighbors' domains.



- When unassigning a variable, remember to restore the domains of its neighboring variables!
- The simplest way to implement this is to make a copy of the domains of the variables before performing forward checking. This is foolproof, but can be quite slow.
- A fancier solution is to keep a counter (initialized to be zero) c_{iv} for each variable X_i and value v in its domain. When we remove a value v from the domain of X_i, we increment c_{iv}. An element is deemed to be "removed" when $c_{iv} > 0$. When we want to un-remove a value, we decrement c_{iv}. This way, the remove operation is reversible, which is important since a value might get removed multiple times due to multiple neighboring variables.
- In the next lecture, we will look at arc consistency, which will allow us to lookahead even more.

Choosing an unassigned variable



Which variable to assign next?

Key idea: most constrained variable

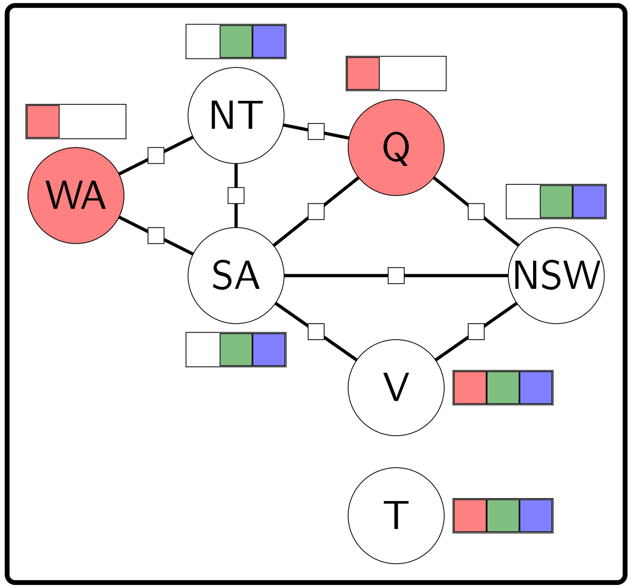
Choose variable that has the fewest consistent values.

This example: SA (has only one value)

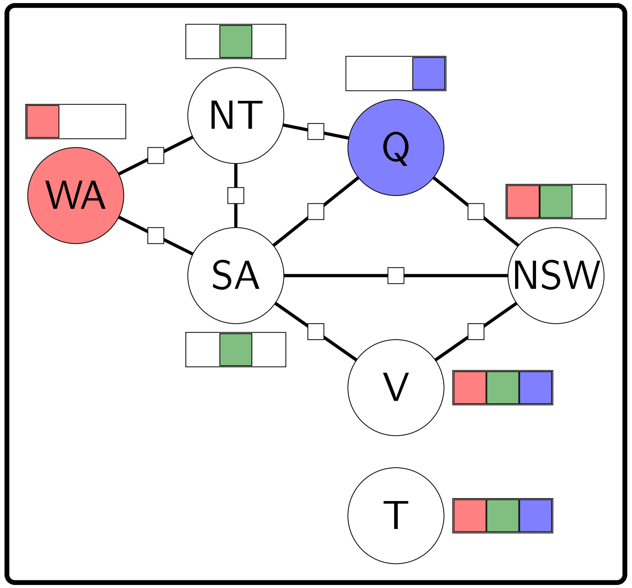
- Now let us look at the problem of choosing an unassigned variable. Intuitively, we want to choose the variable which is most constrained, that is, the variable whose domain has the fewest number of remaining valid values (based on forward checking), because those variables yield smaller branching factors.

Order values of a selected variable

What values to try for Q?



$2+2+2=6$ consistent values



$1+1+2=4$ consistent values

Key idea: least constrained value

Order values of selected X_i by decreasing number of consistent values of neighboring variables.

- Once we've selected an unassigned variable X_i, we need to figure out which order to try the different values in. Here the principle we will follow is to first try values which are less constrained.
- There are several ways we can think about measuring how constrained a variable is, but for the sake of concreteness, here is the heuristic we'll use: just count the number of values in the domains of all neighboring variables (those that share a factor with X_i).
- If we color Q red, then we have 2 valid values for NT, 2 for SA, and 2 for NSW. If we color Q blue, then we have only 1 for NT, 1 for SA, and 2 for NSW. Therefore, red is preferable (6 total valid values versus 4).
- The intuition is that we want values which impose the fewest number of constraints on the neighbors, so that we are more likely to find a consistent assignment.

When to fail?

Most constrained variable (MCV):

- Must assign **every** variable
- If going to fail, fail early $\Rightarrow$ more pruning

Least constrained value (LCV):

- Need to choose **some** value
- Choosing value most likely to lead to solution

- The most constrained variable and the least constrained value heuristics might seem conflicting, but there is a good reason for this superficial difference.
- An assignment involves **every** variable whereas for each variable we only need to choose **some** value. Therefore, for variables, we want to try to detect failures early on if possible (because we'll have to confront those variables sooner or later), but for values we want to steer away from possible failures because we might not have to consider those other values.

When do these heuristics help?

- Most constrained variable: useful when **some** factors are constraints (can prune assignments with weight 0)

$$[x_1 = x_2] \qquad\qquad [x_2 \neq x_3] + 2$$

- Least constrained value: useful when **all** factors are constraints (all assignment weights are 1 or 0)

$$[x_1 = x_2] \qquad\qquad [x_2 \neq x_3]$$

- Forward checking: need to actually prune domains to make heuristics useful!

- Most constrained variable is useful for finding maximum weight assignments in any factor graph as long as there are some factors which are constraints, because we only save work if we can prune away assignments with zero weight, and this only happens with violated constraints (weight 0).
- On the other hand, least constrained value only makes sense if all the factors are constraints (CSPs). In general, ordering the values makes sense if we're going to just find the first consistent assignment. If there are any non-constraint factors, then we need to look at all consistent assignments to see which one has the maximum weight. Analogy: think about when depth-first search is guaranteed to find the minimum cost path.

Review: backtracking search

Algorithm: backtracking search

Backtrack(x, w, Domains):

- If x is complete assignment: update best and return
- Choose unassigned **VARIABLE** X_i
- Order **VALUES** Domain$_i$ of chosen X_i
- For each value v in that order:
  - $\delta \leftarrow \prod_{f_j \in D(x, X_i)} f_j(x \cup \{X_i : v\})$
  - If $\delta = 0$: continue
  - Domains$' \leftarrow$ Domains via **LOOKAHEAD**
  - Backtrack($x \cup \{X_i : v\}, w\delta$, Domains$'$)

Summary

- Factor graphs: modeling framework (variables, factors)

- Key property: ordering decisions pushed to algorithms

- Algorithms: backtracking search + dynamic ordering + lookahead

- Next time: better lookahead, modeling, approximate search