

Topics in Reinforcement Learning: Rollout and Approximate Policy Iteration

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Links to Class Notes, Videolectures, and Slides at
<http://web.mit.edu/dimitrib/www/RLbook.html>

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Lecture 12
Aggregation Methods

- 1 Introduction to Aggregation
- 2 Aggregation with Representative States: A Form of Discretization
- 3 Aggregation with Representative Features
- 4 Examples of Feature-Based Aggregation
- 5 What is the Aggregate Problem and How Do We Solve It?
- 6 Simulation-Based Solution of the Aggregate Problem
- 7 Variants of Aggregation

Aggregation within the Approximation in Value Space Framework

Approximate minimization

$$\min_{u \in U(i)} \sum_{j=1}^n p_{ij}(u) (g(i, u, j) + \alpha \tilde{J}(j))$$

First Step “Future”

Approximations:

Replace $E\{\cdot\}$ with nominal values
(certainty equivalence)
Adaptive simulation
Monte Carlo tree search

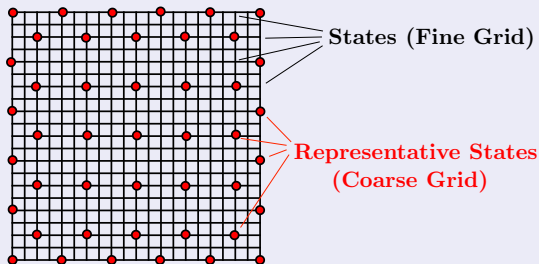
Computation of \tilde{J} :

Problem approximation
Rollout
Approximate PI
Parametric approximation
Aggregation

- Aggregation is a form of **problem approximation**. We approximate our DP problem with a “smaller/easier” version, which we solve optimally to obtain \tilde{J} .
- **Is related to feature-based parametric approximation** (e.g., when \tilde{J} is piecewise constant, the features are 0-1 membership functions).
- **Can be combined with (global) parametric approximation** (like a neural net) in two ways. Either **use the neural net to provide features**, or **add a local parametric correction** to a \tilde{J} obtained by a neural net.
- Several versions: **multistep lookahead, finite horizon, etc ...**

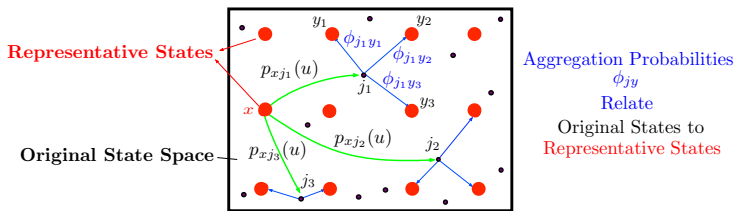
Illustration: A Simple Classical Example of Approximation

Approximate the state space with a coarse grid of states



- Introduce a “small” set of “representative” states to form a **coarse grid**.
- Approximate the original DP problem with a coarse-grid DP problem, called **aggregate problem** (need transition probs. and cost from rep. states to rep. states).
- Solve the aggregate problem by **exact DP**.
- “Extend” the **optimal cost function of the aggregate problem** to an approximately optimal cost function for the original fine-grid DP problem.
- For example extend the solution by a **nearest neighbor/piecewise constant scheme** (a fine grid state takes the cost value of the “nearest” coarse grid state).

Approximate the Problem by “Projecting” it onto Representative States



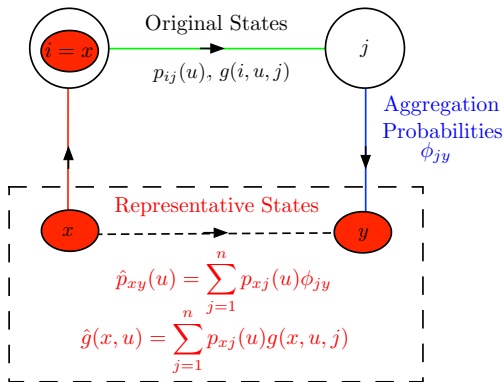
- Introduce a finite subset of “representative states” $\mathcal{A} \subset \{1, \dots, n\}$. We denote them by x and y .
- Original system states j are related to rep. states $y \in \mathcal{A}$ with **aggregation probabilities** ϕ_{jy} (“weights” satisfying $\phi_{jy} \geq 0$, $\sum_{y \in \mathcal{A}} \phi_{jy} = 1$).
- Aggregation probabilities express “similarity” or “proximity” of original to rep. states.
- **Aggregate dynamics**: Transition probabilities between rep. states x, y

$$\hat{p}_{xy}(u) = \sum_{j=1}^n p_{xj}(u) \phi_{jy}$$

- **Expected cost** at rep. state x under control u :

$$\hat{g}(x, u) = \sum_{j=1}^n p_{xj}(u) g(x, u, j)$$

The Aggregate Problem



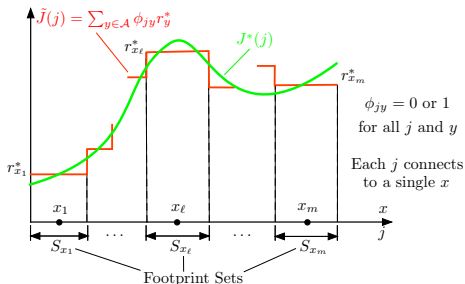
- If r_x^* , $x \in \mathcal{A}$, are the optimal costs of the aggregate problem, approximate the optimal cost function of the original problem by

$$\tilde{J}(j) = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*, \quad j = 1, \dots, n, \quad (\text{interpolation})$$

- If $\phi_{jy} = 0$ or 1 for all j and y , $\tilde{J}(j)$ is piecewise constant. It is constant on each set

$$S_y = \{j \mid \phi_{jy} = 1\}, \quad y \in \mathcal{A}, \quad (\text{called the footprint of } y)$$

The Piecewise Constant Case ($\phi_{jy} = 0$ or 1 for all j, y)



The approximate cost function $\tilde{J} = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*$ is constant within $S_y = \{j \mid \phi_{jy} = 1\}$.

Approximation error for the piecewise constant case ($\phi_{jy} = 0$ or 1 for all j, y)

Consider the footprint sets

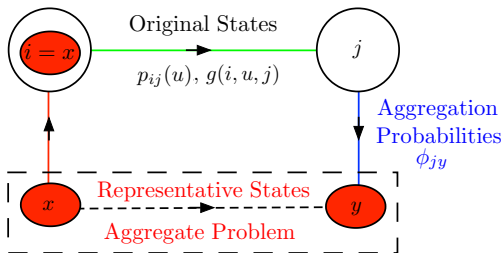
$$S_y = \{j \mid \phi_{jy} = 1\}, \quad y \in \mathcal{A}$$

The $(J^* - \tilde{J})$ error is small if J^* varies little within each S_y . In particular,

$$|J^*(j) - \tilde{J}(j)| \leq \frac{\epsilon}{1 - \alpha}, \quad j \in S_y, y \in \mathcal{A},$$

where $\epsilon = \max_{y \in \mathcal{A}} \max_{i, j \in S_y} |J^*(i) - J^*(j)|$ is the max variation of J^* within the S_y .

Solution of the Aggregate Problem



Data of aggregate problem (it is stochastic even if the original is deterministic)

$$\hat{p}_{xy}(u) = \sum_{j=1}^n p_{xj}(u) \phi_{jy}, \quad \hat{g}(x, u) = \sum_{j=1}^n p_{xj}(u) g(x, u, j), \quad \tilde{J}(j) = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*$$

Exact methods

Once the aggregate model is computed (i.e., its transition probs. and cost per stage), **any exact DP method can be used**: VI, PI, optimistic PI, or linear programming.

Model-free simulation methods - Needed for large n , even if model is available

Given a simulator for the original problem, we can obtain a simulator for the aggregate problem. Then **use an (exact) model-free method** to solve the aggregate problem.

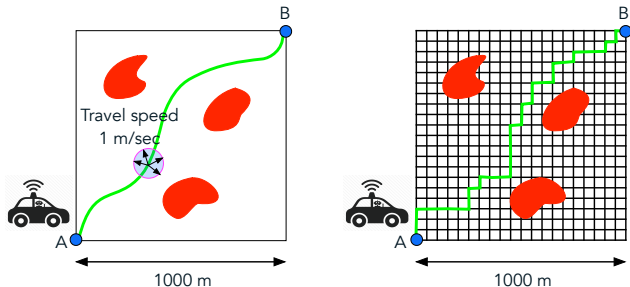
Continuous state space

- The rep. states approach **applies with no modification to continuous spaces discounted problems**.
- **The number of rep. states should be finite.**
- **The cost per stage should be bounded** for the “good”/contraction mapping-based theory to apply to the original DP problem.
- A simulation/model-free approach may still be used for the aggregate problem.
- We thus obtain **a general discretization method** for continuous-spaces discounted problems.

Discounted POMDP with a belief state formulation

- Discounted POMDP models with belief states, fit neatly into the continuous state discounted aggregation framework.
- **The aggregate/rep. states POMDP problem is a finite-state MDP** that can be solved for r^* with any (exact) model-based or model-free method (VI, PI, etc).
- The optimal aggregate cost r^* **yields an approximate cost function** $\tilde{J}(j) = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*$, which defines a one-step or multistep lookahead suboptimal control scheme for the original POMDP.

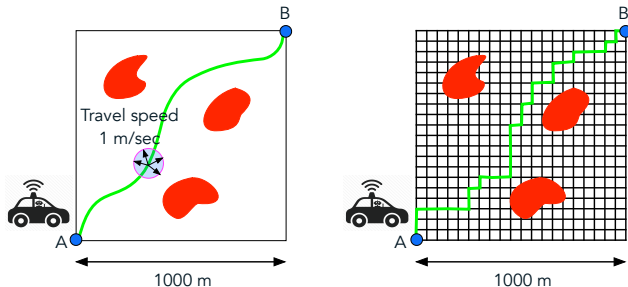
A Challenge Question - Think for Five Mins



Discretizing Continuous Motion

- A self-driving car wants to drive from A to B through obstacles. Find the fastest route.
- Car speed is 1 m/sec in any direction.
- We discretize the space with a fine square grid; restrict directions of motion to horizontal and vertical.
- We take the discretized shortest path solution as an approximation to the continuous shortest path solution.
- Is this a good approximation?

Answer to the Challenge Question



Discretizing Continuous Motion

- The discretization is **FLAWED**.
- **Example:** Assume all motion costs 1 per meter, and no obstacles.
- The continuous optimal solution (the straight A-to-B line) has length $\sqrt{2}$ kilometers.
- The discrete optimal solution has length 2 kilometers **regardless of how fine the discretization is**.
- Here the state space is discretized finely **but the control space is not**.
- This is not an issue in POMDP (the control space is finite).

From Representative States to Representative Features

The main difficulty with rep. states/discretization schemes:

- It may not be easy to find a set of rep. states and corresponding piecewise constant or linear functions that approximate well J^* .
- Too many rep. states may be required for good approximate costs $\tilde{J}(j)$.

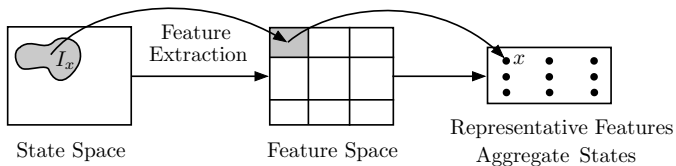
Suppose we have a good feature vector $F(i)$: We discretize the feature space

- We introduce representative features that span adequately the feature space

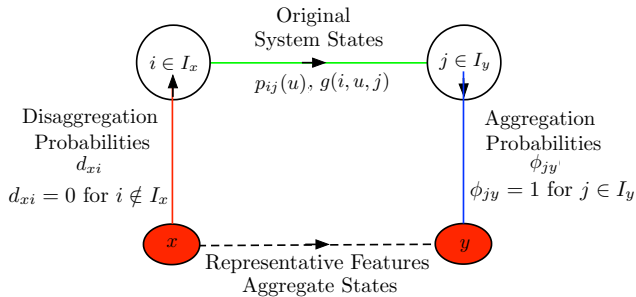
$$\mathcal{F} = \{F(i) \mid i = 1, \dots, n\}$$

- We aim for an aggregate problem whose states are the rep. features.
- We associate each rep. feature x with a subset of states I_x that nearly map onto feature x , i.e.,
$$F(i) \approx x, \quad \text{for all } i \in I_x$$
- This is done with the help of weights d_{xi} (called disaggregation probabilities) that are 0 outside of I_x .
- As before, we associate each state j with rep. features y using aggregation probabilities ϕ_{jy} .
- We construct an aggregate problem using d_{xi} , ϕ_{jy} , and the original problem data.

Illustration of Feature-Based Aggregation Framework

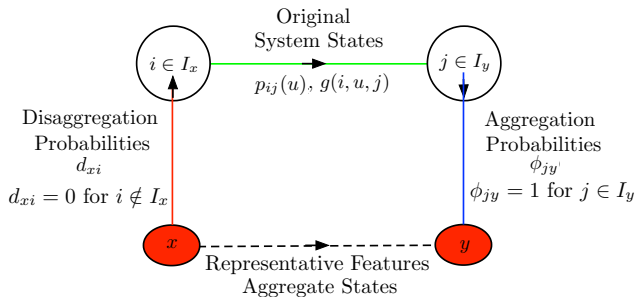


Representative feature formation



Transition diagram for the aggregate problem

Working Break: Feature Formation Methods in Aggregation



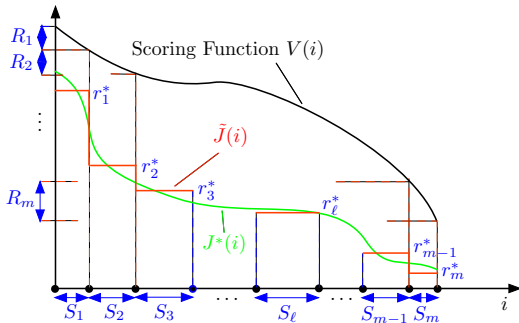
Question 1: Why is the rep. states model a special case of the rep. features model?

Assume the following general principle for feature-based aggregation:

Choose features so that **states i with similar features $F(i)$ have similar $J^*(i)$** , i.e., $J^*(i)$ changes little within each of the "footprint" sets $I_x = \{i \mid d_{xi} > 0\}$ and $S_y = \{j \mid \phi_{jy} > 0\}$.

Question 2: Can you think of examples of useful features for aggregation schemes?

Feature Formation Using Scoring Functions



Idea: Suppose that we have a **scoring function** $V(i)$ with $V(i) \approx J^*(i)$. Then **group together states with similar score**.

- We partition the range of values of V into m disjoint intervals R_1, \dots, R_m .
- We define a feature vector $F(i)$ according to

$$F(i) = \ell, \quad \text{all } i \text{ such that } V(i) \in R_\ell, \quad \ell = 1, \dots, m$$

- Defines a partition of the state space into the footprints $S_\ell = I_\ell = \{i \mid F(i) = \ell\}$.

Examples of Scoring Functions

- Cost functions of heuristics or policies.
- Approximate cost functions produced by neural networks.

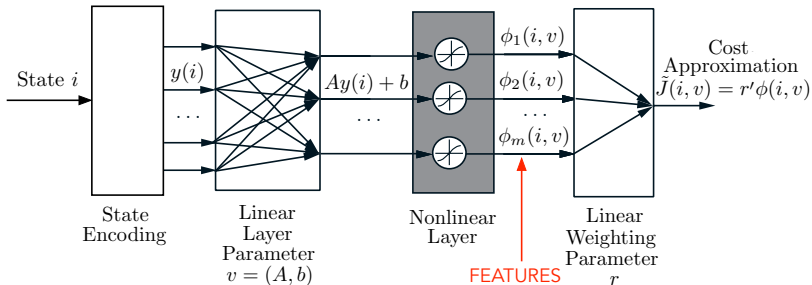
Let the scoring function be the cost function J_μ of a policy μ

Let's compare with rollout:

- Rollout uses as cost approximation $\tilde{J} = J_\mu$.
- Score-based aggregation uses J_μ as scoring function to form features. The resulting \tilde{J} is a "nonlinear function of J_μ " that aims to approximate J^* .
- If the scoring function quantization were so fine as to have a single feature value per interval R_ℓ , we would have $\tilde{J} = J^*$ (much better than rollout).
- Score-based aggregation can be viewed as a more sophisticated form of rollout.
- Score-based aggregation is more computation-intensive, less suitable for on-line implementation.

It is possible to use multiple scoring functions to generate more complex feature maps.

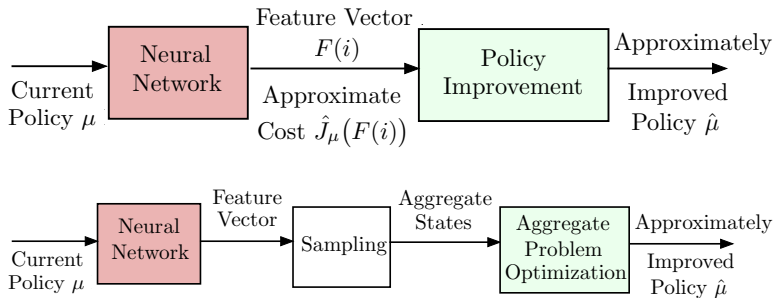
Feature Formation Using Neural Networks



Suppose we have trained a NN that provides an approximation $\hat{J}(i) = r'\phi(i, v)$

- Features from the NN can be used to define rep. features.
- Training of the NN yields lots of state-feature pairs.
- Rep. features and footprint sets of states can be obtained from the NN training set data, perhaps supplemented with additional (state,feature) pair data.
- NN features may be supplemented by handcrafted features.
- Feature-based aggregation yields a nonlinear function \tilde{J} of the features that approximates J^* (not \hat{J}).

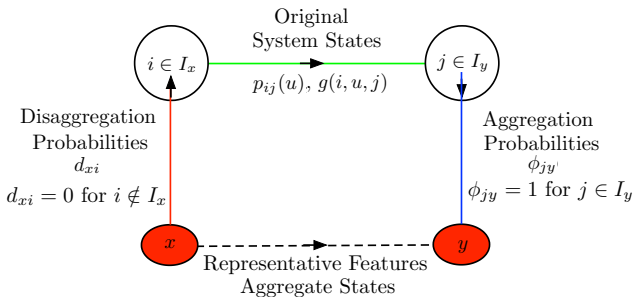
Policy Iteration with Neural Nets, and Feature-Based Aggregation



Several options for implementation of mixed NN/aggregation-based PI

- The NN-based feature construction process may be performed multiple times, each time followed by an aggregate problem solution that constructs a new policy.
- Alternatively: The NN training and feature construction may be done only once with some "good" policy.
- After each cycle of NN-based feature formation, we may add problem-specific handcrafted features, and/or features from previous cycles.
- Note: Deep NNs may produce fewer and more sophisticated final features

A Simple Version of the Aggregate Problem



Patterned after the simpler rep. states model.

Aggregate dynamics and costs

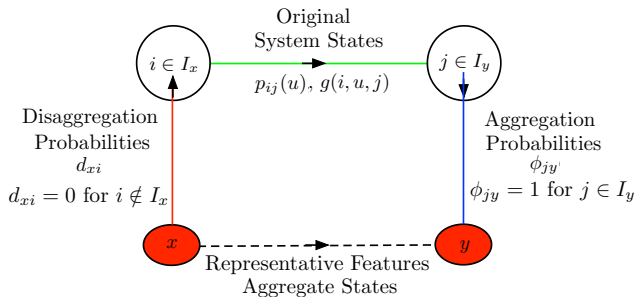
- **Aggregate dynamics:** Transition probabilities between rep. features x, y

$$\hat{p}_{xy}(u) = \sum_{i \in I_x} d_{xi} \sum_{j=1}^n p_{ij}(u) \phi_{jy}$$

- **Expected cost per stage:**

$$\hat{g}(x, u) = \sum_{i \in I_x} d_{xi} \sum_{j=1}^n p_{xj}(u) g(x, u, j)$$

The **Flaw** of the Simple Version of the Aggregate Problem



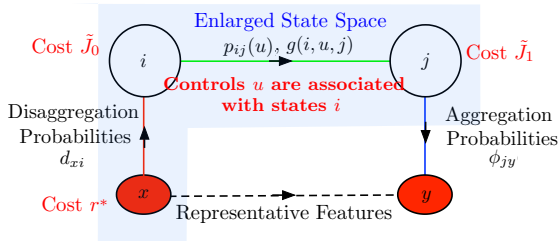
There is an implicit assumption in the aggregate dynamics and cost formulas

$$\hat{p}_{xy}(u) = \sum_{i \in I_x} d_{xi} \sum_{j=1}^n p_{ij}(u) \phi_{jy}, \quad \hat{g}(x, u) = \sum_{i \in I_x} d_{xi} \sum_{j=1}^n p_{xj}(u) g(x, u, j)$$

For a given rep. feature x , the same control u is applied at all states i in the footprint I_x .

So the simple aggregate problem is legitimate, but **the approximation \tilde{J} of J^* may not be very good**. We will address this issue in the next lecture.

More Accurate Version: The Enlarged Aggregate Problem



Bellman equations for the enlarged problem

$$r_x^* = \sum_{i=1}^n d_{xi} \tilde{J}_0(i), \quad x \in \mathcal{A},$$

$$\tilde{J}_0(i) = \min_{u \in U(i)} \sum_{j=1}^n p_{ij}(u) (g(i, u, j) + \alpha \tilde{J}_1(j)), \quad i = 1, \dots, n,$$

$$\tilde{J}_1(j) = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*, \quad j = 1, \dots, n$$

r^* solves uniquely the composite Bellman equation $r^* = Hr^*$:

$$r_x^* = (Hr^*)(x) = \sum_{i=1}^n d_{xi} \min_{u \in U(i)} \sum_{j=1}^n p_{ij}(u) \left(g(i, u, j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y^* \right), \quad x \in \mathcal{A}$$

Approximation error for the piecewise constant case ($\phi_{jy} = 0$ or 1 for all j, y)

Consider the footprint sets

$$S_y = \{j \mid \phi_{jy} = 1\}, \quad y \in \mathcal{A}$$

The $(J^* - \tilde{J})$ error is small if J^* varies little within each S_y . In particular,

$$|J^*(j) - r_y^*| \leq \frac{\epsilon}{1 - \alpha}, \quad j \in S_y, y \in \mathcal{A},$$

where $\epsilon = \max_{y \in \mathcal{A}} \max_{i, j \in S_y} |J^*(i) - J^*(j)|$ is the max variation of J^* within S_y .

Implication

Choose representative features x so that J^* varies little over the footprint of x .

This is a generally valid qualitative guideline

Holds for the more general piecewise linear interpolation case.

Simulation-Based Asynchronous Value Iteration for the Aggregate Problem

A sampled version of VI for solving $r^* = Hr^*$: $r^{k+1} \approx (1 - \gamma^k)r^k + \gamma^k H(r^k)$ with

$$(Hr)(x) = \sum_{i=1}^n d_{xi} \min_{u \in U(i)} \sum_{j=1}^n p_{ij}(u) \left(g(i, u, j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y \right), \quad x \in \mathcal{A}$$

Note that H is a contraction.

At time k iterate for a single rep. feature x_k , and keep all other r_x^k unchanged:

$$r_{x_k}^{k+1} = (1 - \gamma^k)r_{x_k}^k + \gamma^k \min_{u \in U(i_k)} \sum_{j=1}^n p_{i_k j}(u) \left(g(i_k, u, j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y^k \right)$$

where i_k is a sample from I_{x_k} selected according to $d_{x_k i}$, and γ^k is a stepsize.

Convergence result [Tsitsiklis and Van Roy (1995)]

With $\gamma^k \rightarrow 0$ and other technical conditions, this iteration converges to the unique solution r^* . Some similarity with (exact) Q-learning proofs.

Simulation-Based Policy Iteration

Uses policy evaluation/policy improvement to generate policy/cost pairs $\{(\mu^k, r^k)\}$.
Converges monotonically ($r^{k+1} \leq r^k$) and **finitely** ($r^k = r^*$ for sufficiently large k).

Policy evaluation of current policy μ^k

Solve the (linear) composite Bellman equation $r^k = H_{\mu^k} r^k$ for μ^k , where

$$(H_{\mu^k} r)(x) = \sum_{i=1}^n d_{xi} \sum_{j=1}^n p_{ij}(\mu^k(i)) \left(g(i, \mu^k(i), j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y \right), \quad x \in \mathcal{A}$$

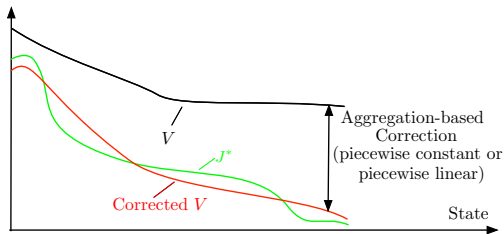
Two possibilities:

- **Iteratively**: Using a sampled version of VI with **sampling for both i and for j** .
- **By matrix inversion**: Write the equation $r^k = H_{\mu^k} r^k$ in matrix form as $r^k = A^k r^k + b^k$.
Evaluate A^k and b^k by simulation, and set $r^k = (I - A^k)^{-1} b^k$.

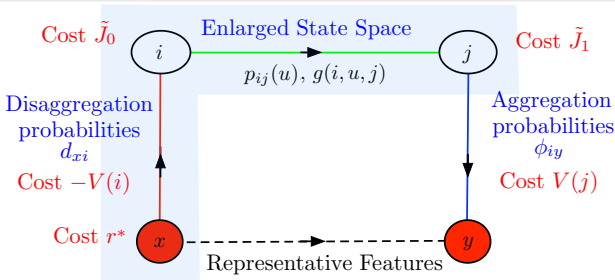
Policy improvement by one-step lookahead

$$\mu^{k+1}(i) = \arg \min_{u \in U(i)} \sum_{j=1}^n p_{ij}(u) \left(g(i, u, j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y^k \right), \quad i = 1, \dots, n$$

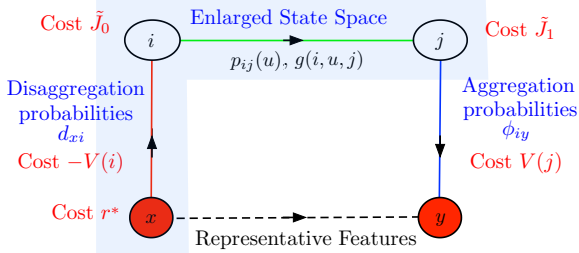
Biased Aggregation - Suppose we Know a Good Approximation $V \approx J^*$; How do we Correct it?



We add a "bias" function V to the cost structure of the enlarged aggregate problem



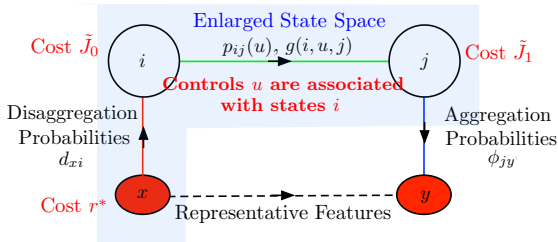
Some Results for Biased Aggregation



Let $(r^*, \tilde{J}_0, \tilde{J}_1)$ be the solution [note that $\tilde{J}_1(j) = V(j) + \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*$]

- When $V = J^*$ then $r^* = 0$, $\tilde{J}_0 = \tilde{J}_1 = J^*$, and any optimal policy for the aggregate problem is optimal for the original problem.
- When $V = J_\mu$ for some policy μ , the policy produced by aggregation is a rollout policy based on μ , when there is a single rep. feature. **Suggests that with multiple rep. features the aggregation/rollout policy should be much better than rollout.**
- Error bounds similar to the ones for the case $V = 0$ suggest to **choose rep. features and footprint sets within which $V - J^*$ varies little.**
- We do not know J^* , but we may use $T^k V$ (k value iterations on V) as an approximation. Then **use $V - T^k V$ as a scoring function to form rep. features.**

A Challenge Question - Deterministic Problems



How do VI and PI benefit from the problem being deterministic?

- VI form: $r_{x_k}^{k+1} = (1 - \gamma^k) r_{x_k}^k + \gamma^k \min_{u \in U(i)} \sum_{j=1}^n p_{ikj}(u) (g(i_k, u, j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y^k)$
- Policy evaluation: Solve the composite Bellman equation $r^k = H_{\mu^k} r^k$, where

$$(H_{\mu^k} r)(x) = \sum_{i=1}^n d_{xi} \sum_{j=1}^n p_{ij}(\mu^k(i)) \left(g(i, \mu^k(i), j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y \right), \quad x \in \mathcal{A}$$

- Policy improvement: $\mu^{k+1}(i) = \arg \min_{u \in U(i)} \sum_{j=1}^n p_{ij}(u) (g(i, u, j) + \alpha \sum_{y \in \mathcal{A}} \phi_{jy} r_y^k)$
- How about using representative states? Possibility of multistep lookahead?

For a deterministic problem, the simulation-based VI and PI are simplified

- The sampled version of VI has the form

$$r_{x_k}^{k+1} = (1 - \gamma^k)r_{x_k}^k + \gamma^k \min_{u \in U(i)} \left(g(i_k, u) + \alpha \sum_{y \in \mathcal{A}} \phi_{f(i_k, u)y} r_y^k \right)$$

- No expectation over j is required.
- If representative states are used, there is no need for sampling according to the probabilities $d_{x_k i}$ to obtain i_k (so $\gamma^k \equiv 1$).

Given r^* , consider ℓ -step lookahead minimization

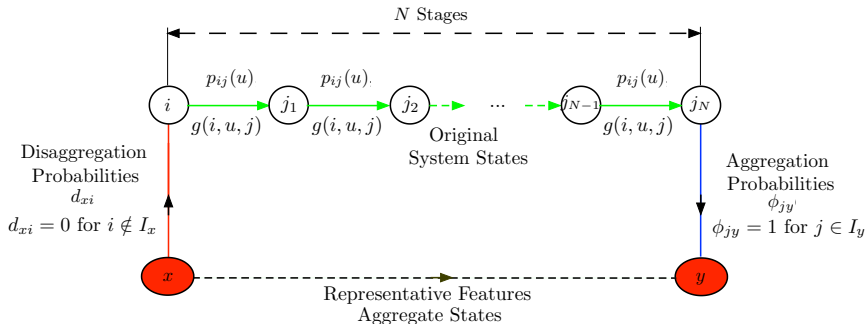
- At state i_0 we find

$$(u_0^*, \dots, u_{N-1}^*) \in \arg \min_{(u_0, \dots, u_{\ell-1})} \left(\sum_{k=0}^{\ell-1} \alpha^k g(i_k, u_k) + \alpha^\ell \sum_{y \in \mathcal{A}} \phi_{i_\ell y} r_y^* \right)$$

and apply $\tilde{\mu}(i_0) = u_0^*$.

- This is a shortest path problem, and its solution on-line may be fast.

N-Step Feature-Based Aggregation



- The composite system consists of $N + 2$ stochastic Bellman equations.
- Simulation-based version of VI is hard to implement.
- Simulation-based version of PI is possible, but policies are multistep.

A simpler case: Deterministic problem and representative states (no features)

- Then each VI iteration involves solution of an N -stage deterministic DP (shortest path) problem: $r^{k+1} = H_N(r^k)$, where H_N is the N -stage DP operator.
- This algorithm embodies the idea of aggregation in both space and time.

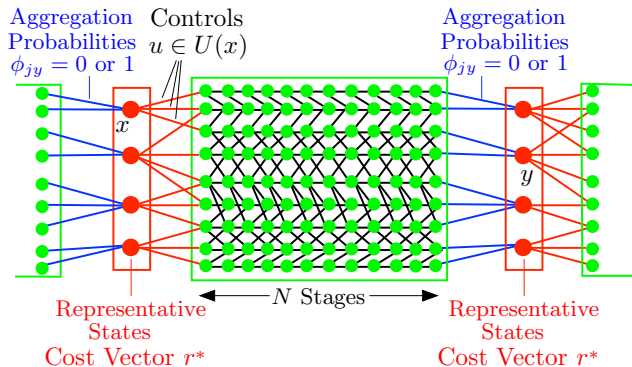
Spatio-Temporal Aggregation - Compressing Space and Time



Plan 5-day auto travel from Boston to San Francisco - How would you do it?

- **Select major stops/cities** (New York, Chicago, Salt Lake City, Phoenix, etc).
- **Select major stopping times** (times to stop for sleep, rest, etc).
- **Decide on space and time schedules at a coarse level.** Optimize the details later.
- We may view this as an example of reduction of a very large-scale shortest path problem to a manageable problem by **spacio-temporal aggregation**.

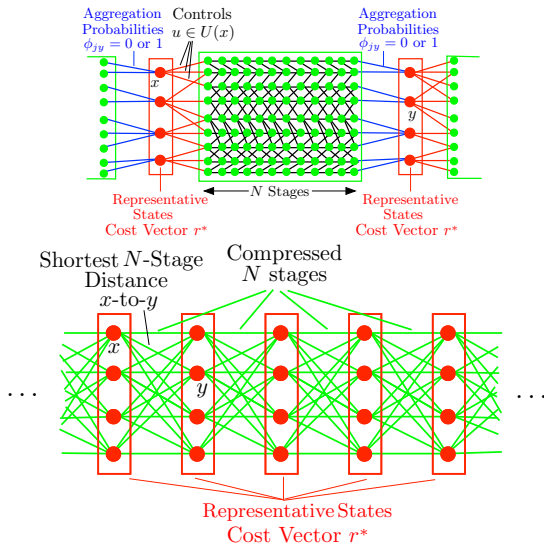
Deterministic Problems - N -Stage Aggregation with Representative States and Aggregation Probabilities $\phi_{jy} = 0$ or 1



An example of spacio-temporal aggregation

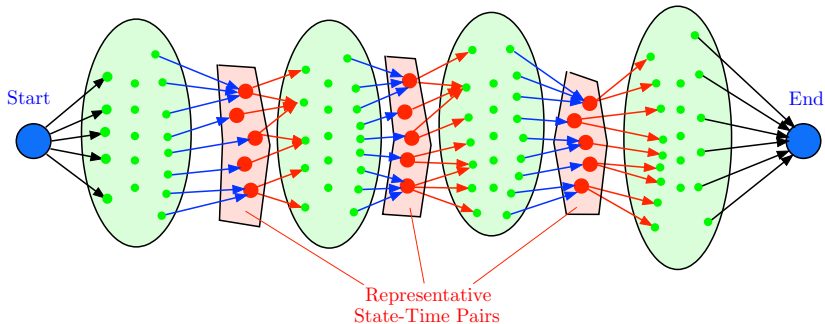
- The infinite horizon discounted aggregate problem decomposes into a sequence of (identical) N -stage shortest path problems.
- Compute shortest path from each rep. state x to each rep. state y .
- Construct a low-dimensional deterministic infinite horizon DP problem (the states are just the representative states).

Spatio-Temporal Decomposition



- Each N -stages block is "compressed" into an all-to-all shortest path problem.
- The compressed problem is a low-dimensional deterministic DP problem.

Spatio-Temporal Decomposition - Extension



Deterministic shortest path and finite horizon extensions

- Consider the **space-time tube** of a deterministic shortest path problem.
- Introduce **space-time barriers**, i.e., subsets of **representative state-time pairs** that “separate past from future” (think of the Boston-San Francisco travel).
- “Compress” the portions of the **space-time tube between two successive barriers into shortest path problems** between each state-time pair of the left barrier to each state-time pair of the right barrier.
- Form a “master” **shortest path problem of low dimension** that involves only the representative state-time pairs.

WE WILL GIVE AN OVERVIEW OF THE ENTIRE COURSE