15-780: Grad AI
Lecture 21: Bayesian learning, MDPs

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Admin

- Reminder: project milestone reports due today
- Reminder: HW5 out

Review: numerical integration

- Parallel importance sampling
  - allows ZR(x) instead of R(x)
  - biased, but asymptotically unbiased
- Sequential sampling (for chains, trees)
- Parallel IS + ***resampling*** for sequential problems = ***particle filter***

Review: MCMC

- Metropolis-Hastings: randomized search procedure for high R(x)
- Leads to ***stationary distribution*** = R(x)
- Repeatedly tweak current x to get x'
  - If R(x') ≥ R(x), move to x'
  - If R(x') << R(x), stay at x
  - randomize in between
- Requires good one-step proposal Q(x' | x) to get acceptable acceptance rate and mixing rate

Review: Gibbs

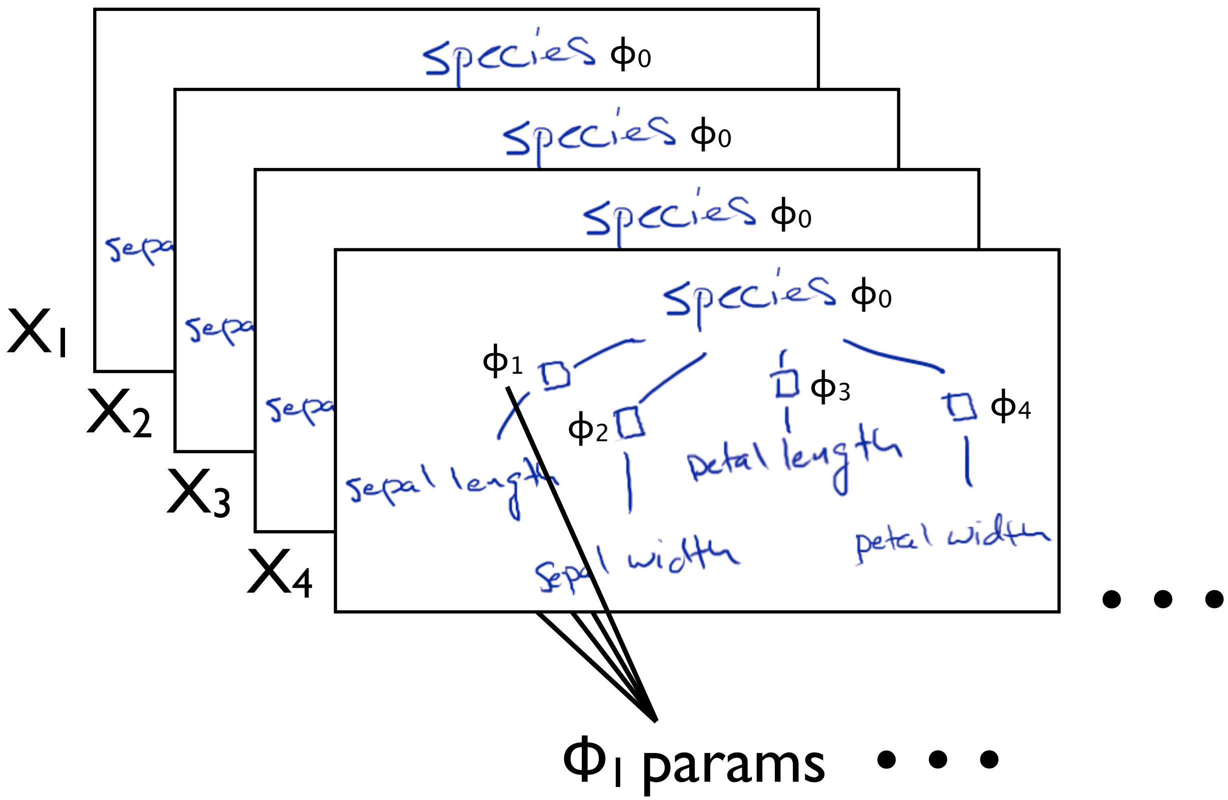
- Special case of MH for $\mathbf{x}$ divided into blocks
- Proposal Q:
  - pick a block i uniformly (or round robin, or any other fair schedule)
  - sample $\mathbf{x}_{B(i)} \sim P(\mathbf{x}_{B(i)} \mid \mathbf{x}_{\neg B(i)})$
- Acceptance rate = 100%

Review: Learning

- $P(M \mid \mathbf{X}) = P(\mathbf{X} \mid M)\, P(M) \,/\, P(\mathbf{X})$
- $P(M \mid \mathbf{X}, \mathbf{Y}) = P(\mathbf{Y} \mid \mathbf{X}, M)\, P(\mathbf{X} \mid M) \,/\, P(\mathbf{Y} \mid M)$
- Example: framlings
- Version space algorithm: when prior is uniform and likelihood is 0 or 1

Bayesian Learning

Recall iris example



- $\mathscr{H}$ = factor graphs of given structure
- Need to specify entries of ϕs

Factors

ϕ_0

setosa	p
versicolor	q
virginica	$1-p-q$

$\phi_1 - \phi_4$

	lo	m	hi
set.	p_i	q_i	$1-p_i-q_i$
vers.	r_i	s_i	$1-r_i-s_i$
vir.	u_i	v_i	$1-u_i-v_i$

Continuous factors

ϕ_1

	lo	m	hi
set.	p_l	q_l	$1-p_l-q_l$
vers.	r_l	s_l	$1-r_l-s_l$
vir.	u_l	v_l	$1-u_l-v_l$

Discretized petal length

$$\Phi_1(\ell, s) = \exp(-(\ell - \ell_s)^2 / 2\sigma^2)$$

parameters ℓ_{set}, ℓ_{vers}, ℓ_{vir}; constant σ^2

Continuous petal length

Simpler example

H	p
T	$1-p$

Coin toss

Parametric model class

- $\mathscr{H}$ is a ***parametric*** model class: each H in $\mathscr{H}$ corresponds to a vector of parameters $\theta = (p)$ or $\theta = (p, q, p_1, q_1, r_1, s_1, \ldots)$
- H_θ: $\mathbf{X} \sim P(\mathbf{X} \mid \theta)$ (or, $Y \sim P(Y \mid \mathbf{X}, \theta)$)
- Contrast to ***discrete*** $\mathscr{H}$, as in version space
- Could also have ***mixed*** $\mathscr{H}$: discrete choice among parametric (sub)classes

Continuous prior

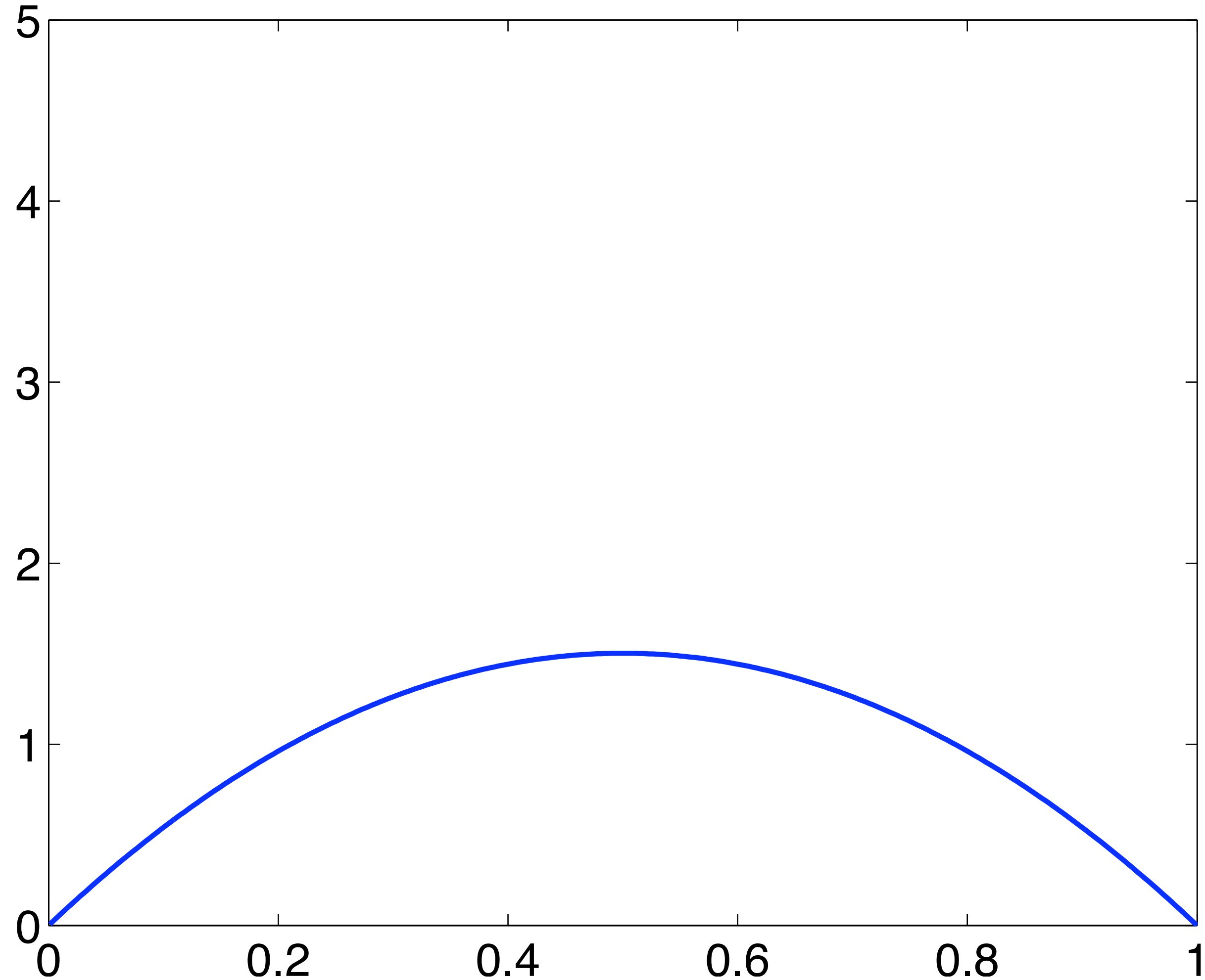
- E.g., for coin toss, p ~ Beta(a, b):

$$P(p \mid a, b) = \frac{1}{B(a,b)} p^{a-1}(1-p)^{b-1}$$

- Specifying, e.g., a = 2, b = 2:

$$P(p) = 6p(1-p)$$

Prior for p



Coin toss, cont'd

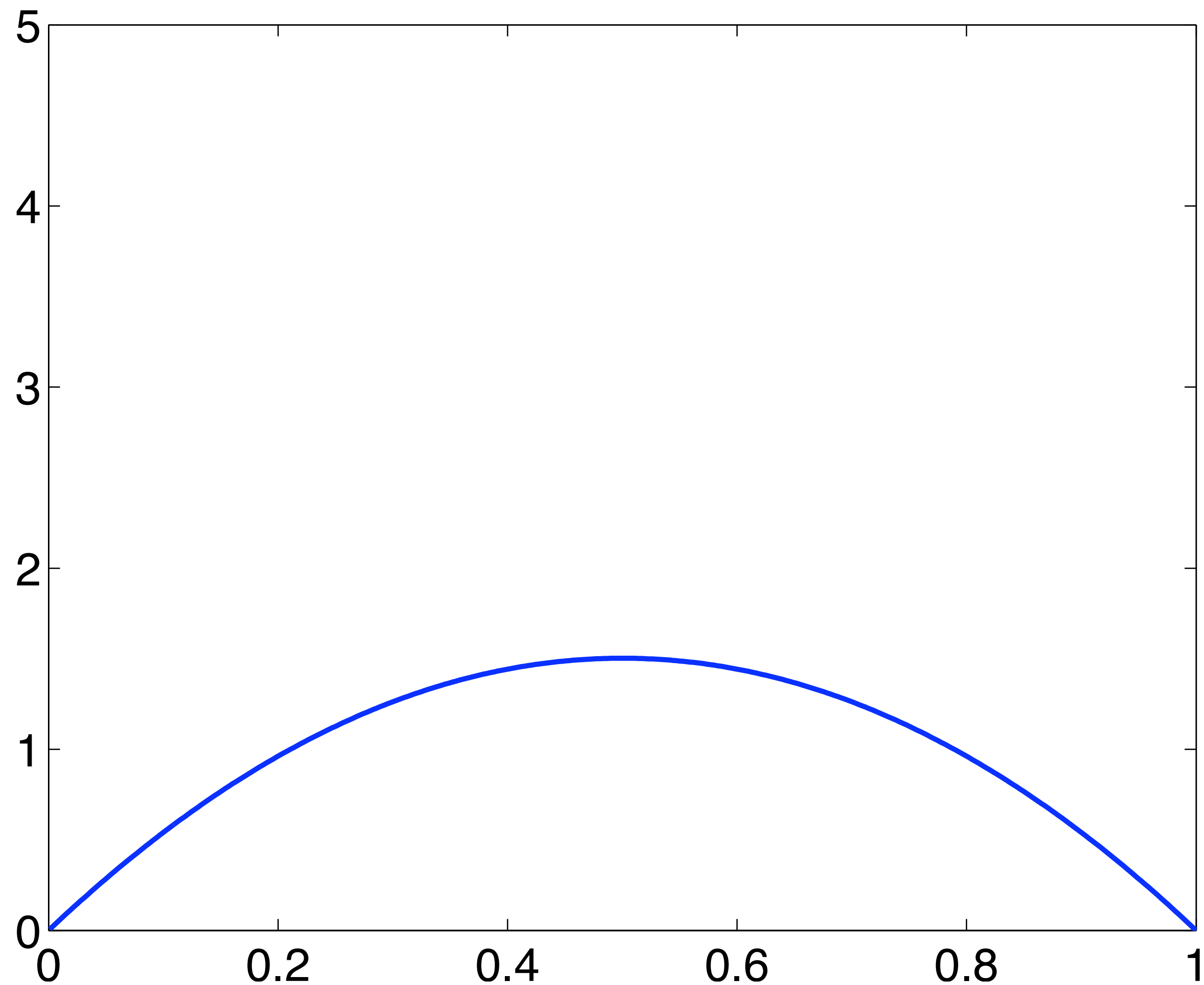
- Joint dist'n of parameter p and data x_i:

$$
\begin{aligned}
P(p, \mathbf{x}) &= P(p) \prod_i P(x_i \mid p) \\
&= 6p(1-p) \prod_i p^{x_i} (1-p)^{1-x_i}
\end{aligned}
$$

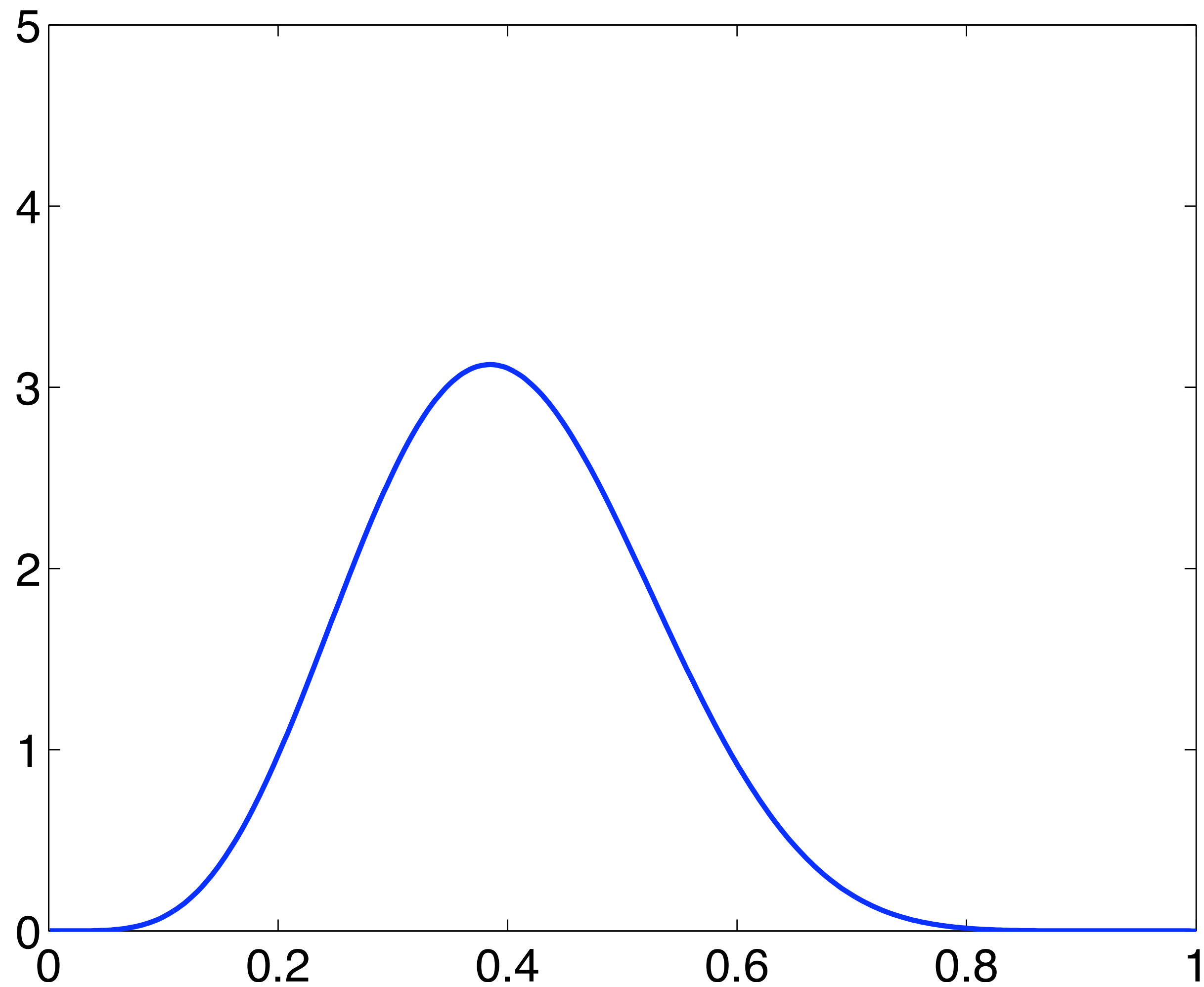
Coin flip posterior

$$
\begin{aligned}
P(p \mid \mathbf{x}) &= P(p) \prod_i P(x_i \mid p) / P(\mathbf{x}) \\
&= \frac{1}{Z} p(1-p) \prod_i p^{x_i} (1-p)^{1-x_i} \\
&= \frac{1}{Z} p^{1+\sum_i x_i} (1-p)^{1+\sum_i (1-x_i)} \\
&= \mathrm{Beta}(2 + \textstyle\sum_i x_i,\, 2 + \sum_i (1-x_i))
\end{aligned}
$$

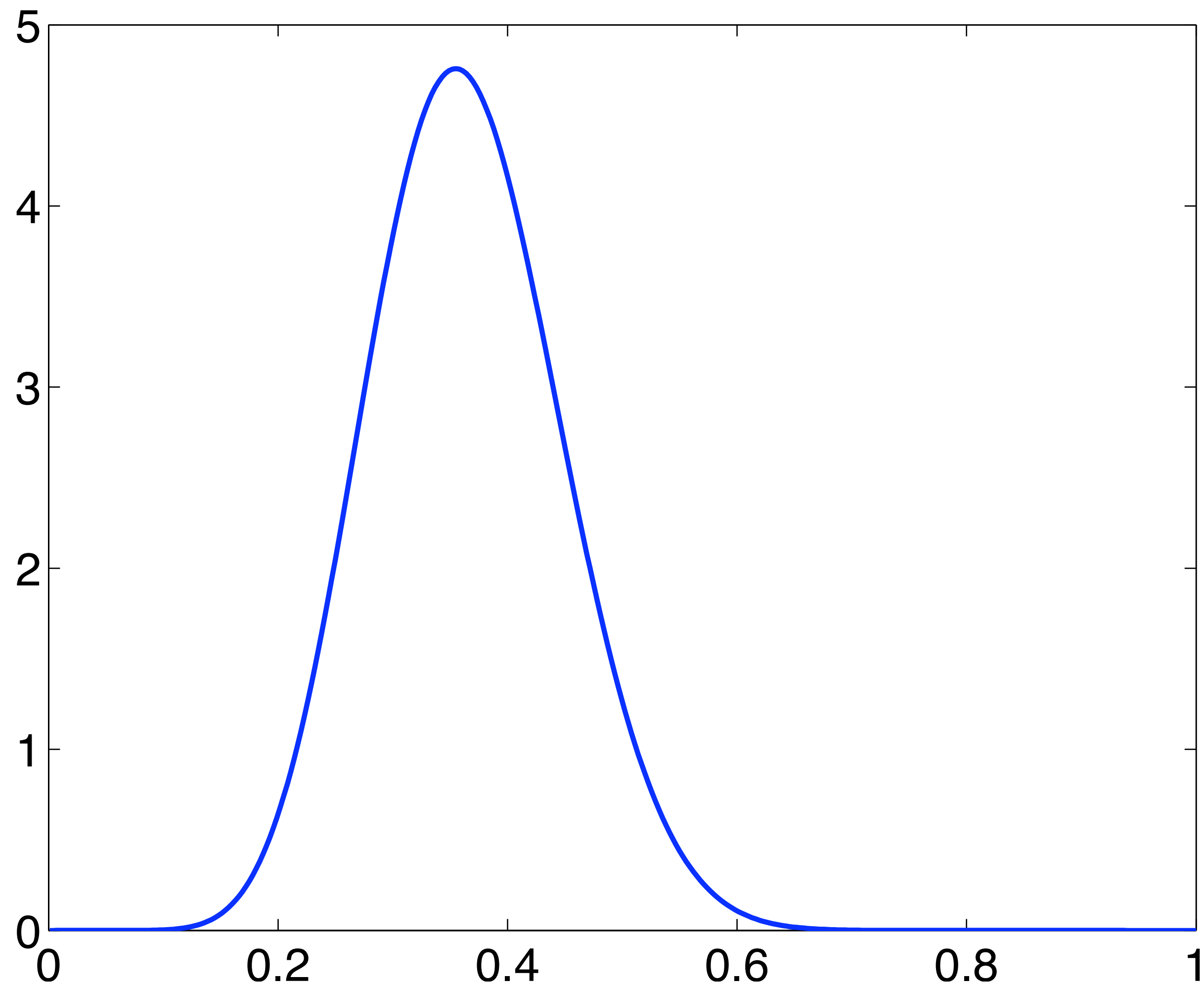
Prior for p



Posterior after 4 H, 7 T



Posterior after 10 H, 19 T



Predictive distribution

- Posterior is nice, but doesn't tell us directly what we need to know
- We care more about $P(x_{N+1} \mid x_1, \ldots, x_N)$
- By law of total probability, conditional independence:

$$
\begin{aligned}
P(x_{N+1} \mid \mathbf{D}) &= \int P(x_{N+1}, \theta \mid \mathbf{D}) d\theta \\
&= \int P(x_{N+1} \mid \theta) P(\theta \mid \mathbf{D}) d\theta
\end{aligned}
$$

Coin flip example

- After 10 H, 19 T: $p \sim \text{Beta}(12, 21)$
- $E(x_{N+1} \mid p) = p$
- $E(x_{N+1} \mid \theta) = E(p \mid \theta) = a/(a+b) = 12/33$
- So, predict 36.4% chance of H on next flip

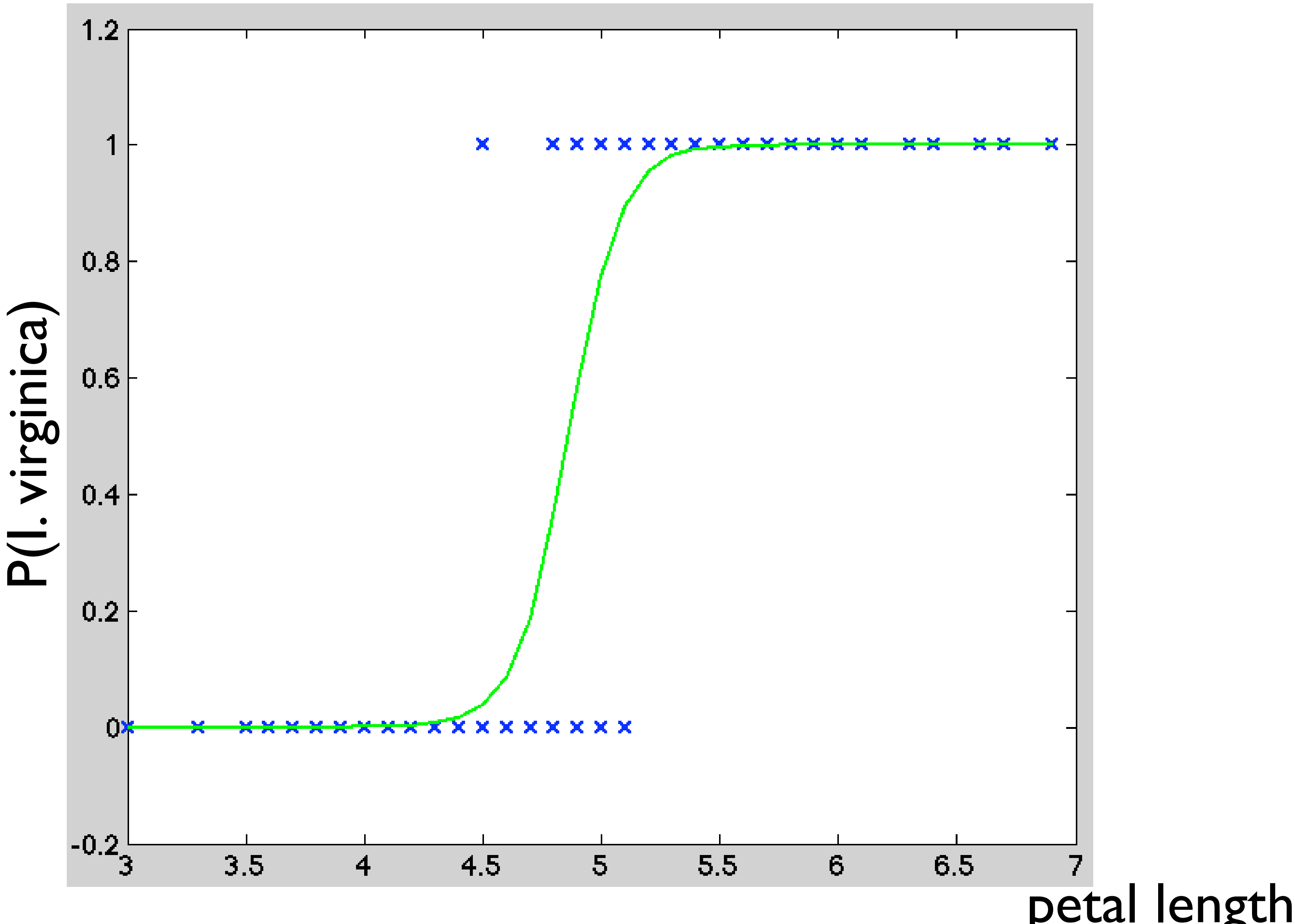
Approximate Bayes

Approximate Bayes

- Coin flip example was easy
- In general, computing posterior (or predictive distribution) may be hard
- Solution: use the approximate integration techniques we've studied!

Bayes as numerical integration

- Parameters θ, data $\mathbf{D}$
- $P(\theta \mid \mathbf{D}) = P(\mathbf{D} \mid \theta)\, P(\theta) \,/\, P(\mathbf{D})$
- Usually, $P(\theta)$ is simple; so is $Z\, P(\mathbf{D} \mid \theta)$
- So, $P(\theta \mid \mathbf{D}) \propto Z\, P(\mathbf{D} \mid \theta)\, P(\theta)$
  - similarly for conditional model: if $\mathbf{X} \perp \theta$,
  - $P(\theta \mid \mathbf{X}, \mathbf{Y}) \propto Z\, P(\mathbf{Y} \mid \theta, \mathbf{X})\, P(\theta)$
- Perfect for MH



$$
\begin{aligned}
P(y \mid x) &= \sigma(ax + b) \\
\sigma(z) &= 1/(1 + exp(-z))
\end{aligned}
$$

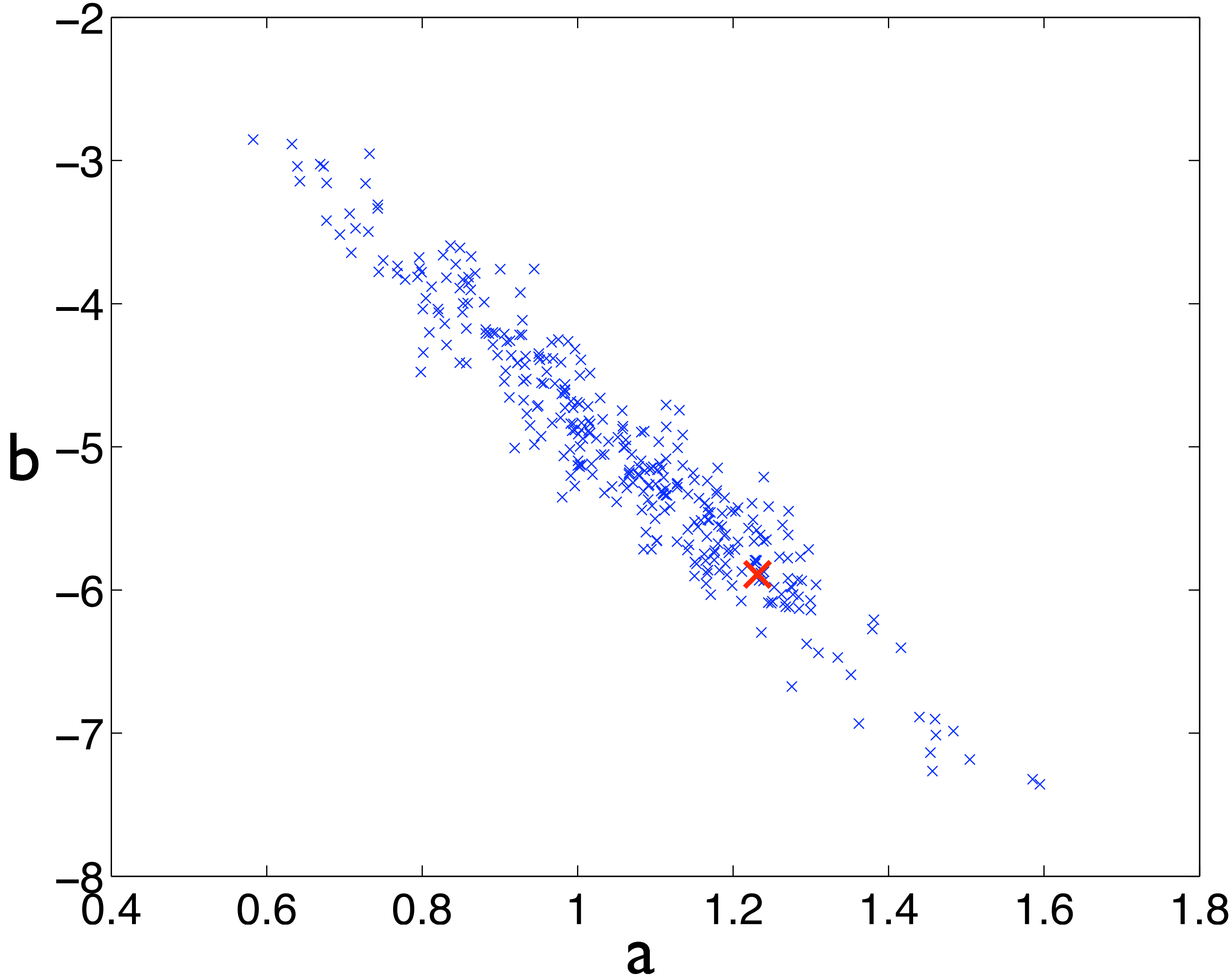
Posterior

$$P(a, b \mid x_i, y_i) =$$

$$ZP(a, b) \prod_i \sigma(ax_i + b)^{y_i} \sigma(-ax_i - b)^{1 - y_i}$$

$$P(a, b) = N(0, I)$$

Sample from posterior



Predictive distribution

- For each θ in sample, predict $P(X)$ or $P(Y \mid X)$
- Average predictions over all θ in sample

Cheaper approximations

Getting cheaper

- Maximum a posteriori (MAP)
- Maximum likelihood (MLE)
- Conditional MLE / MAP

- Instead of true posterior, just use single most probable hypothesis

MAP

$$\arg\max_{\theta} P(D \mid \theta)P(\theta)$$

- Summarize entire posterior density using the maximum

MLE

$$\arg\max_{\theta} P(D \mid \theta)$$

- Like MAP, but ignore prior term
  - often prior is overwhelmed if we have enough data

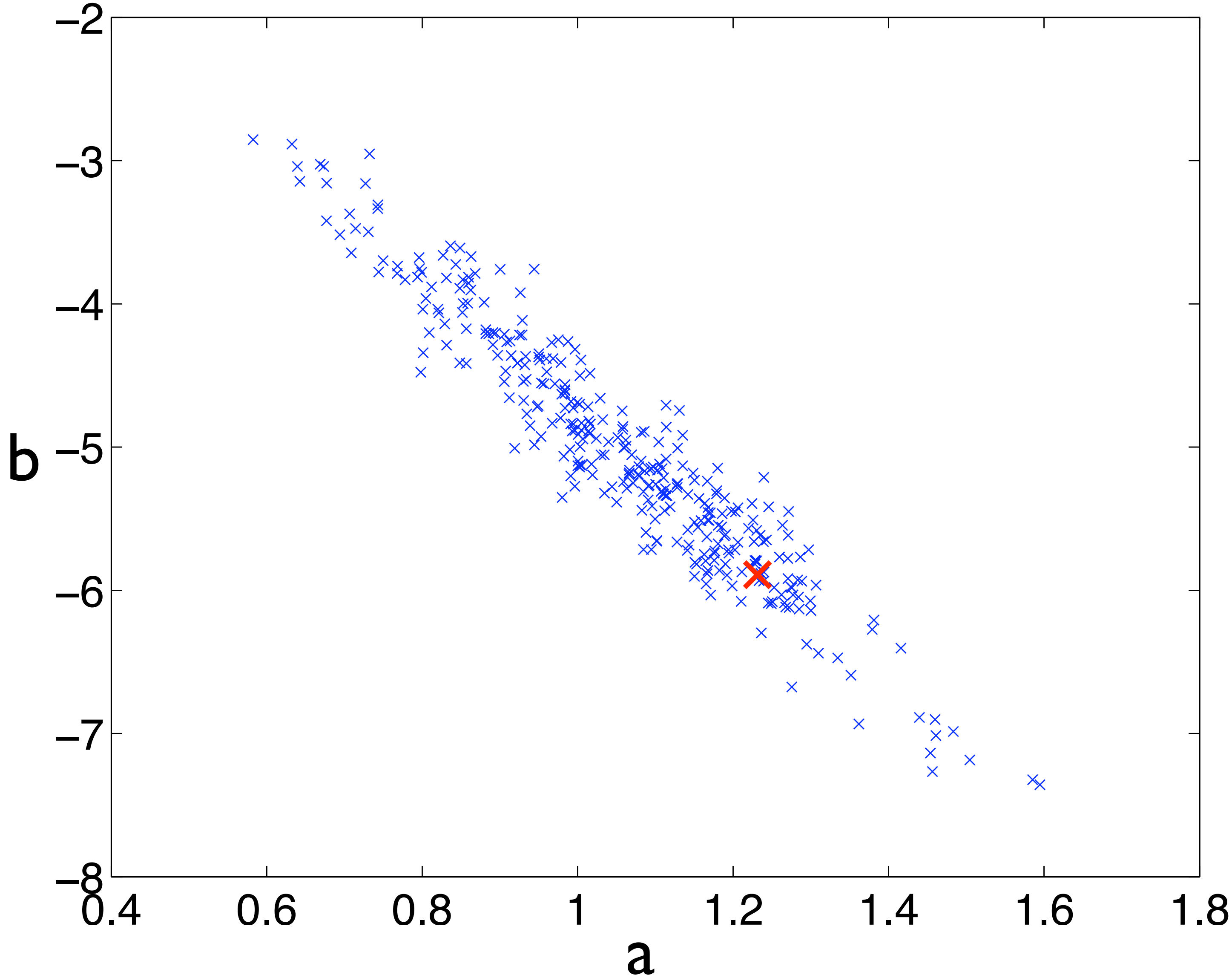
Conditional MLE, MAP

$$\arg\max_{\theta} P(\mathbf{y} \mid \mathbf{x}, \theta)$$

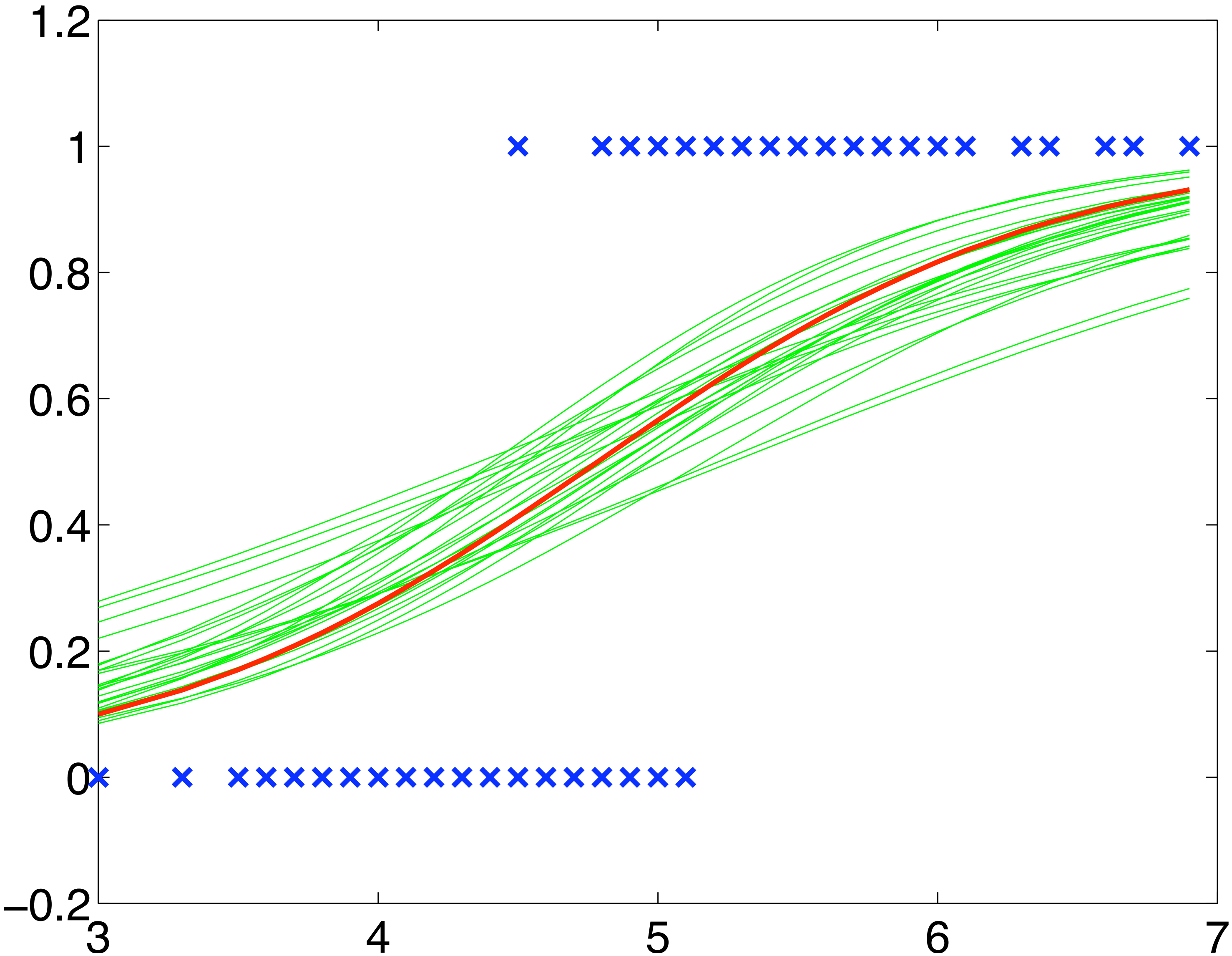
$$\arg\max_{\theta} P(\mathbf{y} \mid \mathbf{x}, \theta) P(\theta)$$

- Split D = (**x**, **y**)
- Condition on **x**, try to explain only **y**

Iris example: MAP vs. posterior



Irises: MAP vs. posterior

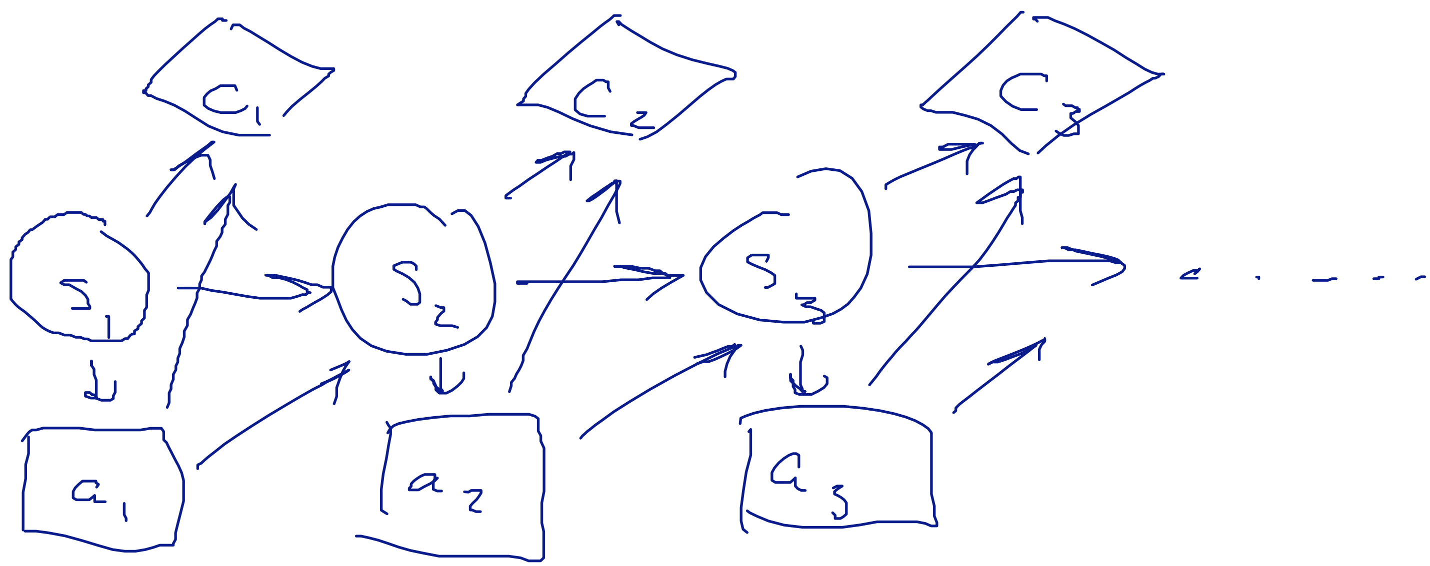


Too certain

- This behavior of MAP (or MLE) is typical: we are too sure of ourselves
- But, often gets better with more data
- Thm: MAP and MLE are consistent estimates of true θ, if "data per parameter" $\rightarrow \infty$

Sequential Decisions

Markov decision process: influence diagram

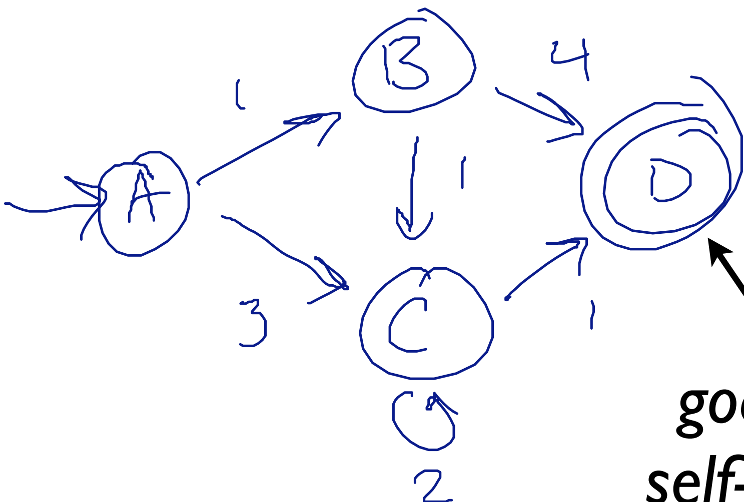


- States, actions, initial state s_1, (expected) costs $C(s,a) \in [C_{min}, C_{max}]$, transitions $T(s' \mid s, a)$

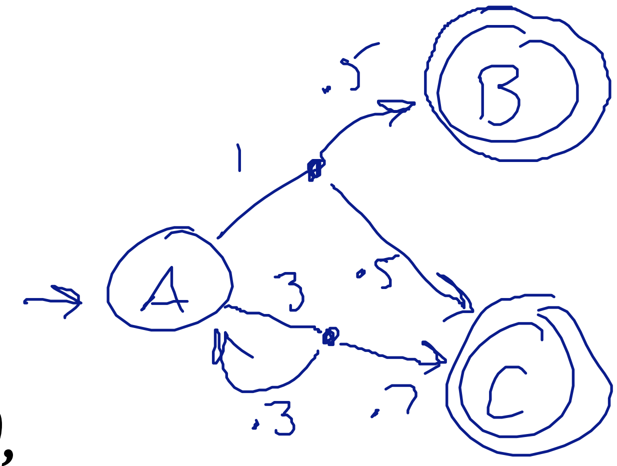
Influence diagrams

- Like a Bayes net, except:
  - diamond nodes are costs/rewards
    - must have no children
  - square nodes are decisions
    - we pick the CPTs (before seeing anything)
    - minimize expected cost
- Circles are ordinary r.v.s as before

Markov decision process: state space diagram



goal: all costs = 0, self-transition 100%



- States, actions, costs $C(s,a) \in [C_{min}, C_{max}]$, transitions $T(s' \mid s, a)$, initial state s_1

Choosing actions

- Execution trace: $\tau = (s_1, a_1, c_1, s_2, a_2, c_2, \ldots)$
  - $c_1 = C(s_1, a_1)$, $c_2 = C(s_2, a_2)$, etc.
  - $s_2 \sim T(s \mid s_1, a_1)$, $s_3 \sim T(s \mid s_2, a_2)$, etc.
- Policy $\pi: S \to A$
  - or randomized, $\pi(a \mid s)$
- Trace from π: $a_1 \sim \pi(a \mid s_1)$, etc.
  - τ is then an r.v. with known distribution
  - we'll write $\tau \sim \pi$ (rest of MDP implicit)

Choosing ***good*** actions

discount factor in (0,1)

- Value of a policy:

$$J^\pi = \frac{1-\gamma}{\gamma} \mathbb{E}\left[\sum_t \gamma^t c_t \,\middle|\, \tau \sim \pi\right]$$

- Objective:

$$J^* = \min_\pi J^\pi$$

$$\pi^* \in \arg\min_\pi J^\pi$$

Why a discount factor?

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- A1: to make the sums finite

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- A2: interest rate $1/\gamma - 1$ per period

Why a discount factor?

- A1: to make the sums finite
- A2: interest rate $1/\gamma - 1$ per period
- A3: model mismatch
  - probability $(1-\gamma)$ that something unexpected happens on each step and my plan goes out the window

Recursive expression

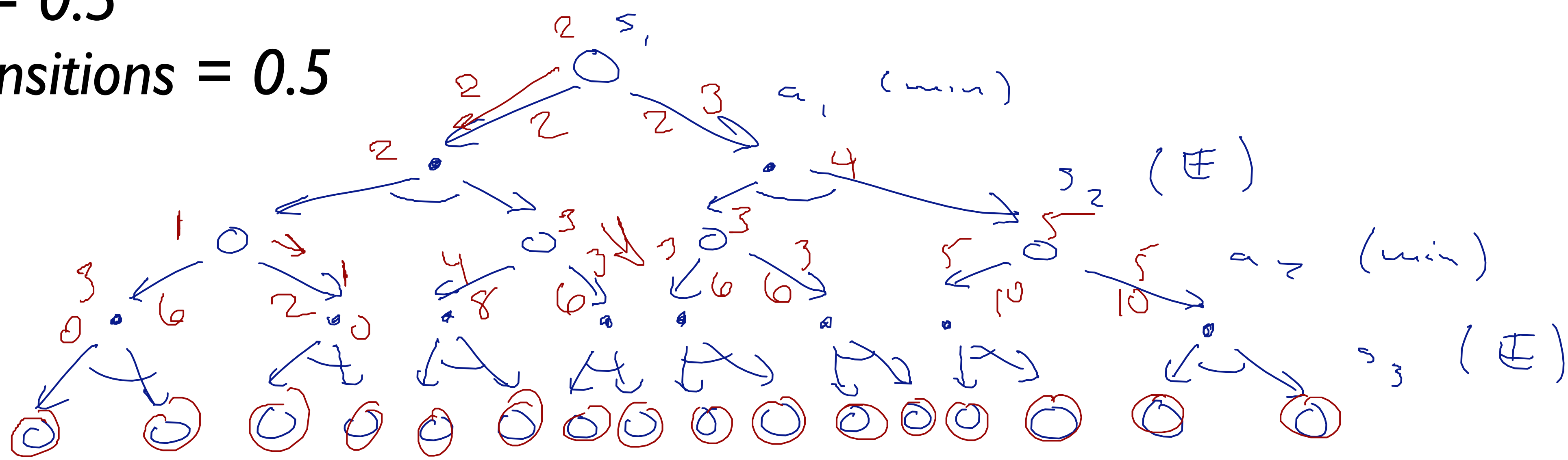
$$
\begin{aligned}
J^\pi &= \mathbb{E}\left[\frac{1-\gamma}{\gamma}\sum_t \gamma^t c_t \;\middle|\; \tau \sim \pi\right] \\
&= \mathbb{E}[J(\tau) \mid \tau \sim \pi] \\
J(\tau) &= \frac{1-\gamma}{\gamma}\;[\gamma c_1 + \gamma^2 c_2 + \gamma^3 c_3 + \ldots] \\
&= (1-\gamma)c_1 + \gamma\left[\frac{1-\gamma}{\gamma}(\gamma c_2 + \gamma^2 c_3 + \ldots)\right] \\
&= (1-\gamma)c_1 + \gamma J(\tau^+)
\end{aligned}
$$

$(1-\gamma)$ × immediate cost + γ × future cost

Tree search

$\gamma = 0.5$

transitions = 0.5



- Root node = current state
- Alternating levels: action and outcome
  - min and expectation
- Build out tree until goal or until γ^t small enough

Interpreting the result

- Number at each ○ node: optimal cost if starting from state s instead of s_1
  - call this $J^*(s)$—so, $J^* = J^*(s_1)$
  - ***state-value*** function
- Number at each · node: optimal cost if starting from parent's s, choosing incoming a
  - call this $Q^*(s,a)$
  - ***action-value*** function
- Similarly, $J^\pi(s)$ and $Q^\pi(s, a)$

The update equations

- For $\cdot$ node

$$Q^*(s,a) \quad = \quad (1-\gamma)C(s,a) + \gamma\mathbb{E}[J^*(s') \mid s' \sim T(\cdot \mid s,a)]$$

- For $\circ$ node

$$J^*(s) \quad = \quad \min_a \; Q^*(s,a)$$

(1–γ) × immediate cost + γ × future cost

Updates for a fixed policy

- For $\cdot$ node

$$Q^\pi(s,a) \quad = \quad (1-\gamma)C(s,a) + \gamma \mathbb{E}[J^\pi(s') \mid s' \sim T(\cdot \mid s,a)]$$

- For $\circ$ node

$$J^\pi(s) \quad = \quad \mathbb{E}[Q^\pi(s,a) \mid a \sim \pi(\cdot \mid s)]$$

(1–γ) × immediate cost + γ × future cost

Speeding it up

- Can't do DPLL-style pruning: outcome node depends on ***all*** children
- Can do some pruning: e.g., low-probability outcomes when branch is already clearly bad
- Or, use scenarios: subsample outcomes at each expectation node
  - with enough samples, good estimate of value of each expectation

Receding-horizon planning

- Stop building tree at 2k levels, evaluate leaf nodes with ***heuristic*** h(s)
  - or at 2k–1 levels, evaluate with h(s, a)
- Minimal guarantees, but often works well in practice
- Can also use adaptive horizon
- Just as in deterministic search, a good heuristic is essential!

Good heuristic

- Good heuristic: $h(s) \approx J^*(s)$ or $h(s, a) \approx Q^*(s,a)$
- If we have $h(s) = J^*(s)$, only need to build first two levels of tree (action and outcome) to choose optimal action at s_1
- With $h(s, a) = Q^*(s,a)$, only need to build first (action) level
- Often try to use $h \approx J^\pi$ or Q^π for some good π

Roll-outs

- Want $h(s) \approx J^{\pi}(s)$
- Starting from $s_1 = s$, sample $a_1 \sim \pi(a \mid s_1)$, set $c_1 = c(s_1,a_1)$, sample $s_2 \sim T(s' \mid s_1,a_1)$
- Repeat until goal (or until γ^t small)
- Take $h(s) = (1-\gamma)/\gamma \sum_t \gamma^t c_t$
- Used in ***UCT*** (best algorithm for Go)

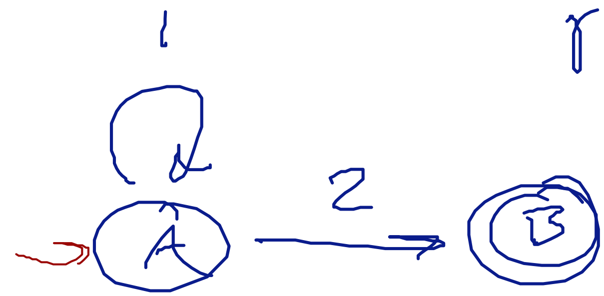
Dynamic programming

- If there are a small number of states and actions, makes sense to ***memoize*** tree search
  - compute an entire level of the tree at a time, working from bottom up
  - store only S × A numbers r.t. b^d

DP example: should I stay or should I go?

$(1-\gamma)1 + \gamma\frac{1}{3}$

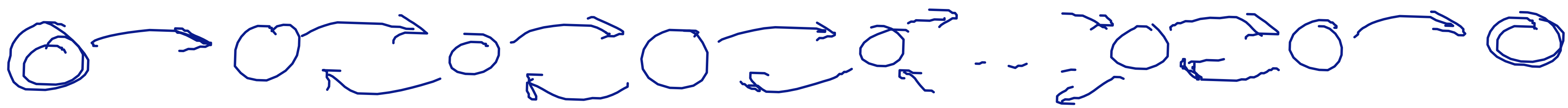
Q(A, stay)	Q(A, go)	J(A)
0	0	0
$1/3$	$2/3$	$1/3$
$5/9$	$2/3$	$5/9$
$\frac{1}{3} + \frac{2}{3}\cdot\frac{5}{9} = \frac{19}{27}$	$2/3$	$2/3$
$\frac{1}{3} + \frac{2}{3}\cdot\frac{2}{3} = 7/9$	$2/3$	$2/3$
$Q^*(A,s)$	$Q^*(A,g)$	$J^*(A)$



$\gamma = 2/3$

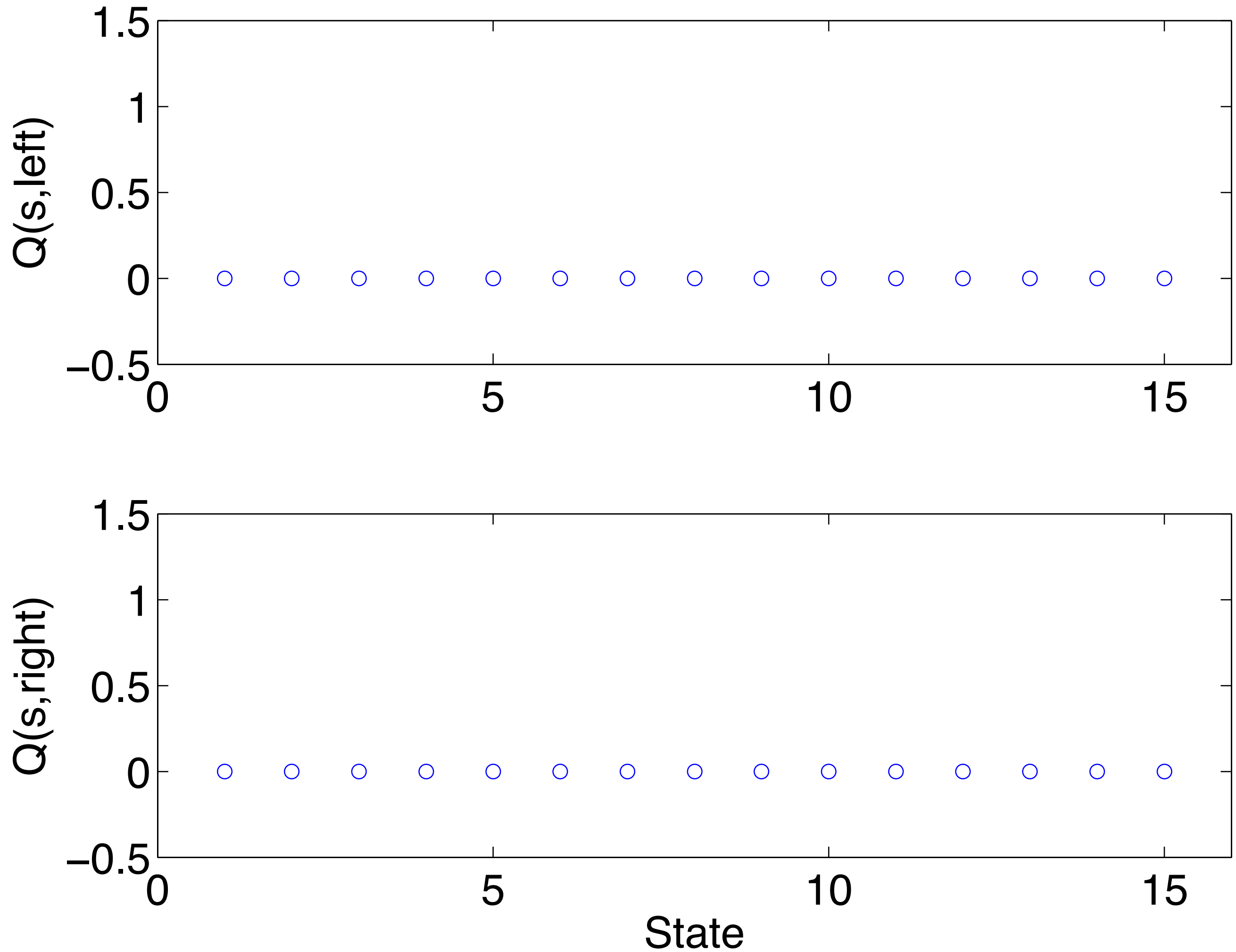
$u(s,a) = 0$

DP example 2

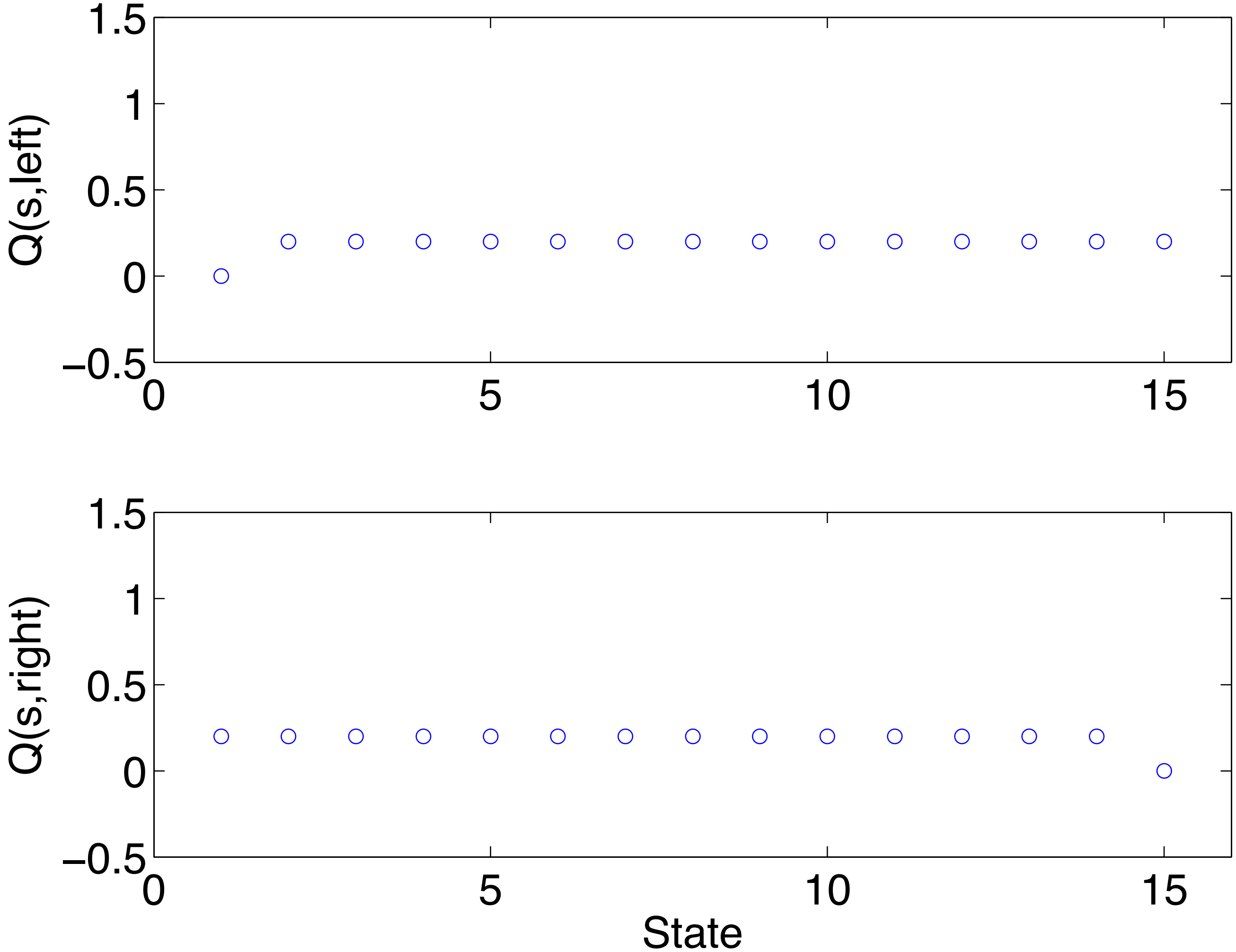


- each step costs 1
- discount 0.8

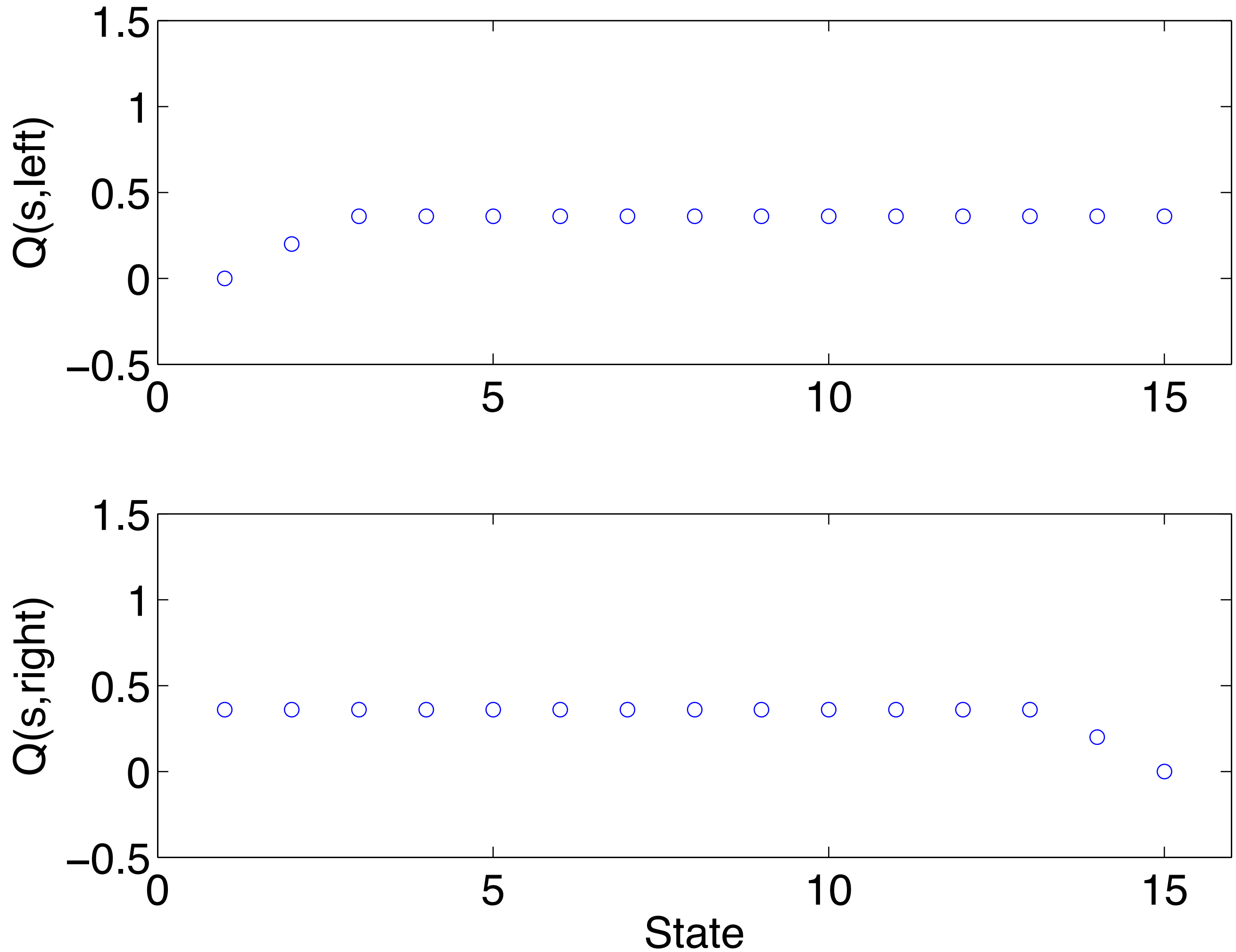
DP example 2—iteration 0



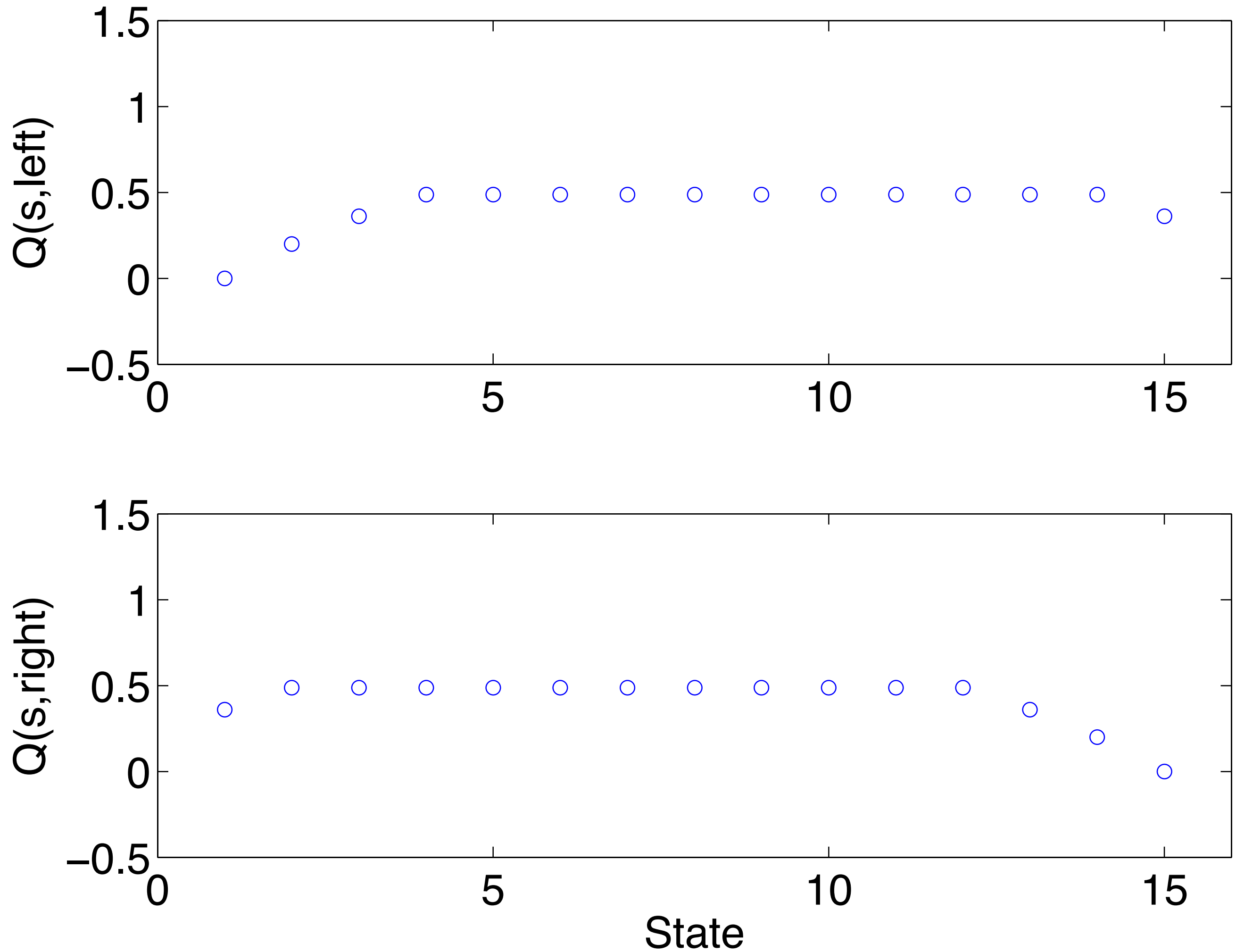
DP example 2—iteration 1



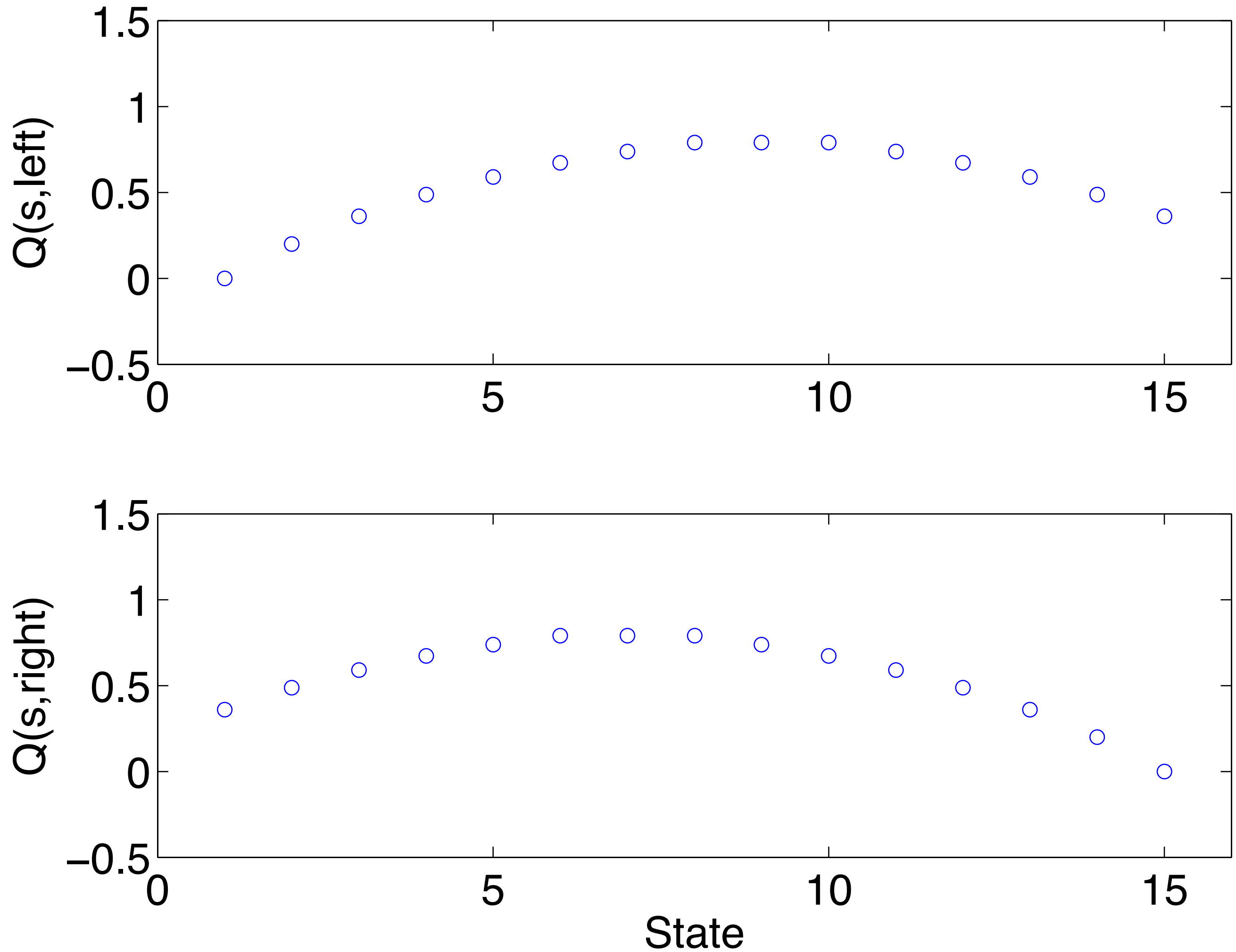
DP example 2—iteration 3



DP example 2—iteration 4



DP example 2—iteration 8



Discussion

- Terminology: backup, sweep, value iteration
- VI makes max error converge linearly to 0 at rate γ per sweep
- Works well for up to 1,000,000s of states, as long as we can evaluate min and expectation efficiently (e.g., few actions, sparse outcomes)
  - tricks: replace J(s) by backed up value immediately (not at end of sweep); schedule backups by ***priority*** = estimate of how much J(s) will change

Curse of dimensionality

- Sadly, 1,000,000s of states don't necessarily get us very far
- E.g., 10 state variables, each with 10 values: 10^{10} states
- See below for ways around the curse