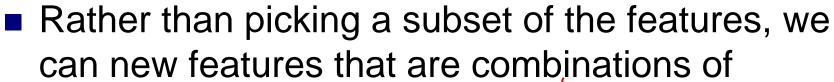
Dimensionality reduction (cont.)

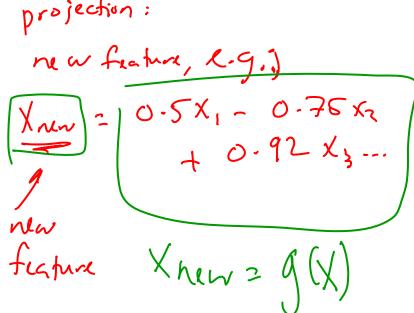
Machine Learning – 10701/15781
Carlos Guestrin
Carnegie Mellon University

April 25th, 2007

Lower dimensional projections



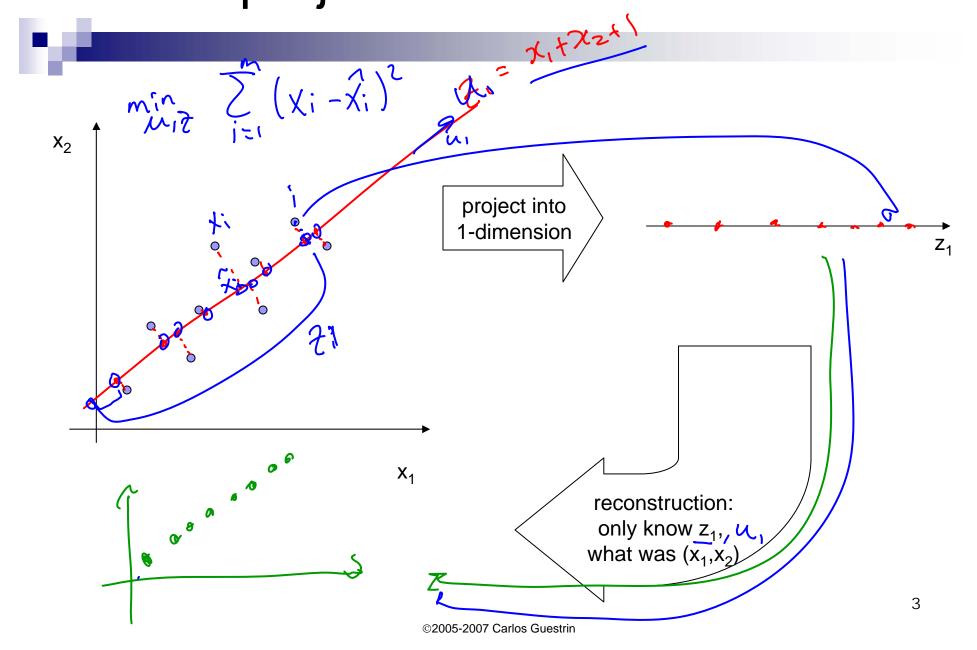
existing features



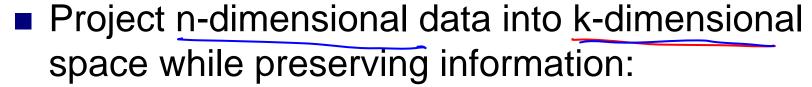
Let's see this in the unsupervised setting

just **X**, but no Y

Linear projection and reconstruction



Principal component analysis – basic idea

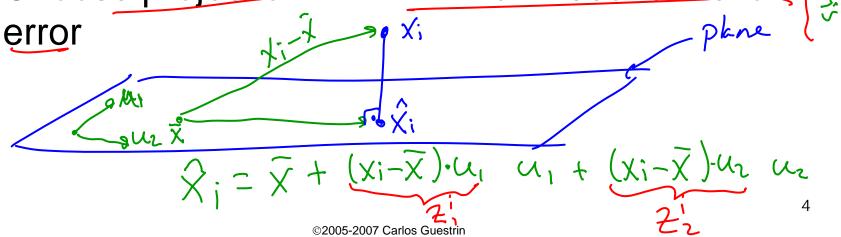


□ e.g., project space of 10000 words into 3-dimensions

□ e.g., project 3-d into 2-d

2D plane
U17 U2:
U1. U2=0 \$

Choose projection with minimum reconstruction



Linear projections, a review



- Project a point into a (lower dimensional) space:
 - \square point: $\mathbf{x} = (x_1, ..., x_n)$

1 K-dian

- select a basis set of basis vectors $(\mathbf{u}_1, \dots, \mathbf{u}_{\nu})$
 - we consider orthonormal basis:

$$\square$$
 $\mathbf{u}_i \leq \mathbf{u}_i = 1$, and $\mathbf{u}_i \leq \mathbf{u}_j = 0$ for $i \neq j$

- \square select a center $-\overline{x}$, defines offset of space
- best coordinates in lower dimensional space defined by dot-products: $(z_1,...,z_k)$, $z_i = (\mathbf{x} - \overline{\mathbf{x}}) \leq \mathbf{u}_i$ $\geq_i = (\mathbf{x} - \overline{\mathbf{x}}) \cdot \mathbf{u}_i$
 - minimum squared error

PCA finds projection that minimizes reconstruction error

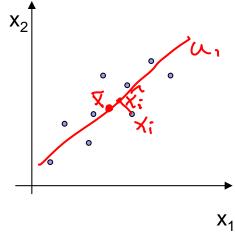


Will represent each point as a projection:

$$\bar{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^k z^i_j \mathbf{u}_j \quad \text{where: } \bar{\mathbf{x}} = \frac{1}{m} \sum_{i=1}^m \mathbf{x}^i \quad \text{and} \quad z^i_j = (\mathbf{x}^i - \bar{\mathbf{x}}) \cdot \mathbf{u}_j$$

- PCA:
 - □ Given $k \le n$, find $(\mathbf{u}_1, ..., \mathbf{u}_k)$ minimizing reconstruction error:

$$error_k = \sum_{i=1}^m (\mathbf{x}^i - \hat{\mathbf{x}}^i)^2$$



Understanding the reconstruction

error

can be represented exactly by n-basis

Note that xⁱ can be represented exactly by n-dimensional projection:

$$\mathbf{x}^i = \bar{\mathbf{x}} + \sum_{j=1}^n z_j^i \mathbf{u}_j$$

$$\hat{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^k z_j^i \mathbf{u}_j$$

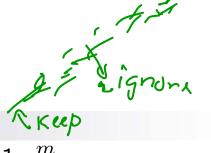
$$\mathbf{z}_j^i = (\mathbf{x}^i - \bar{\mathbf{x}}) \cdot \mathbf{u}_j$$

□Given $k \le n$, find $(\mathbf{u}_1, ..., \mathbf{u}_k)$ minimizing reconstruction error:

$$error_k = \sum_{i=1}^m (\mathbf{x}^i - \hat{\mathbf{x}}^i)^2$$

Rewriting error: $Crror_{k} = \sum_{j=1}^{\infty} (x^{j} - \hat{x}^{j})^{j} = \sum_{j=1}^{\infty} (x^{j$

Reconstruction error and covariance matrix



$$error_{k} = \sum_{i=1}^{m} \sum_{j=k+1}^{n} [u_{j} \cdot (x^{i} - \bar{x})]^{2}$$

$$= \sum_{i=1}^{m} \sum_{j=k+1}^{n} [u_{j} \cdot (x^{i} - \bar{x})]^{2} [(x^{i} - \bar{x}) \cdot u_{j}]$$

$$= \sum_{i=1}^{n} \sum_{j=k+1}^{n} [u_{j} \cdot (x^{i} - \bar{x})] [(x^{i} - \bar{x}) \cdot u_{j}]$$

$$= \sum_{i=1}^{n} u_{j} [(x^{i} - \bar{x}) \cdot u_{j}]$$

$$= \sum_{j=k+1}^{n} u_{j} [(x^{i} - \bar{x}) \cdot u_{j}]$$

$$\mathbf{\Sigma} = \frac{1}{m} \sum_{i=1}^{m} (\mathbf{x}^i - \bar{\mathbf{x}}) (\mathbf{x}^i - \bar{\mathbf{x}})^T$$

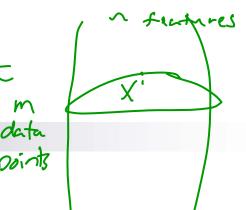
Minimizing reconstruction error and eigen vectors z, then $u_j \in u_j = \lambda_j \in S$

Minimizing reconstruction error equivalent to picking orthonormal basis (**u**₁,...,**u**_n) minimizing:

Minimizing reconstruction error equivalent to picking $(\mathbf{u}_{k+1},...,\mathbf{u}_n)$ to be eigen vectors with smallest eigen values

ligen Value

Basic PCA algoritm



- Start from m by n data matrix X
- Recenter: subtract mean from each row of X

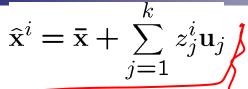
$$\square X_c \leftarrow X - \overline{X}$$

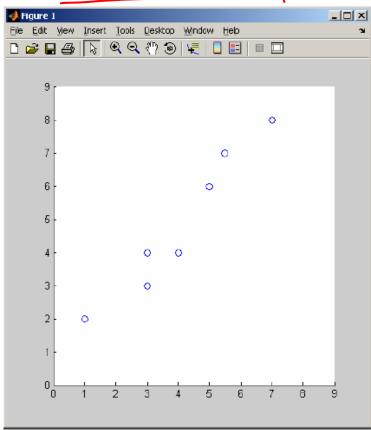
Compute covariance matrix:

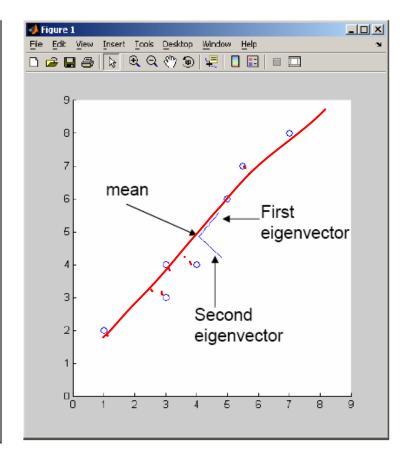
$$\square \wedge \Sigma \leftarrow 1/m X_c^T X_c$$

- Find eigen vectors and values of Σ
- Principal components: k eigen vectors with highest eigen values

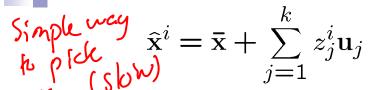
PCA example



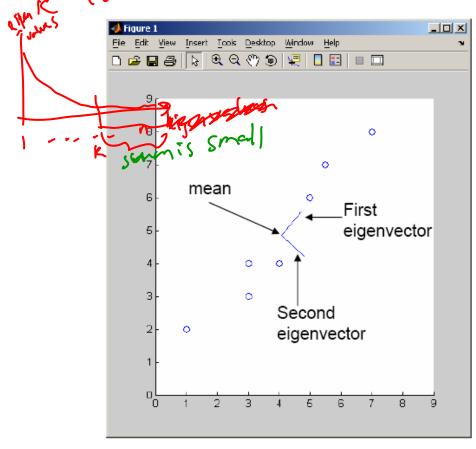


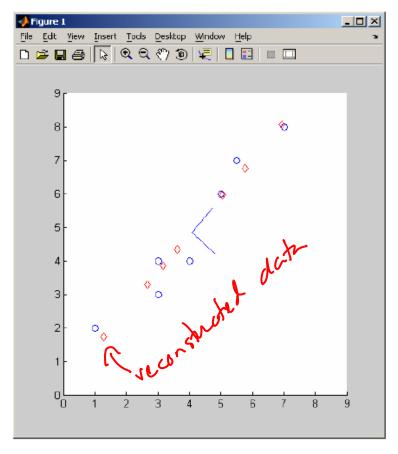


PCA example – reconstruction



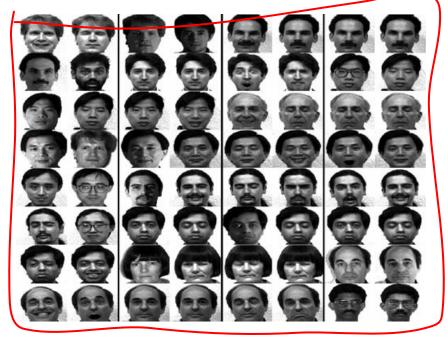
only used first principal component





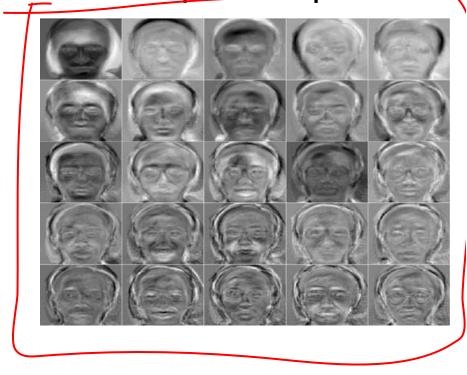
Eigenfaces [Turk, Pentland '91]





Xi= 1 Pixely

Principal components:



Eigenfaces reconstruction

Each image corresponds to adding 8 principal components:



Relationship to Gaussians

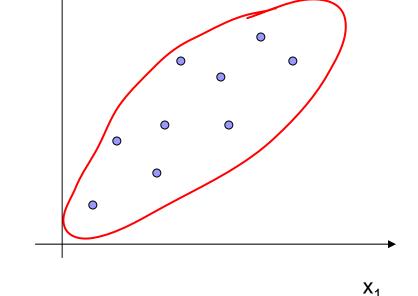
Gaussian discribes data



$$\neg \square \underline{\mathbf{x}} \sim \mathsf{N}(\overline{\mathbf{x}};\Sigma)$$

Equivalent to weighted sum of simple Gaussians:

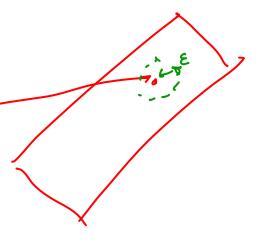
$$\mathbf{x} = \bar{\mathbf{x}} + \sum_{j=1}^{n} z_j \mathbf{u}_j; \quad z_j \sim N(0; \sigma_j^2)$$



 Selecting top k principal components equivalent to lower dimensional Gaussian approximation:

$$\mathbf{x} \approx \mathbf{\bar{x}} + \sum_{j=1}^{k} z_j \mathbf{u}_j + \varepsilon; \quad z_j \sim N(0; \sigma_j^2)$$

 \square $\varepsilon \sim N(0; \sigma^2)$, where σ^2 is defined by error_k



Scaling up



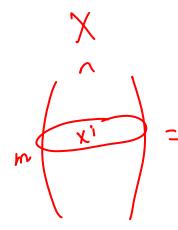
- Covariance matrix can be really big!
 - \square Σ is n by n
 - \square 10000 features $\rightarrow |\Sigma|$
 - □ finding eigenvectors is very slow...
- Use singular value decomposition (SVD)
 - ☐ finds to k eigenvectors
 - □ great implementations available, e.g., Matlab svd

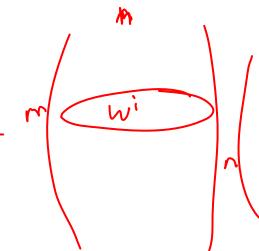
SVD

X = (x)

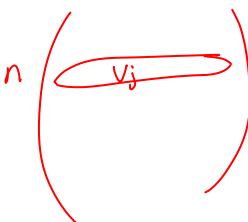
- Write X = W S V^T
 - \square X \leftarrow data matrix, one row per datapoint
 - \square **W** \leftarrow weight matrix, one row per datapoint coordinate of \mathbf{x}^i in eigenspace
 - □ S ← singular value matrix, diagonal matrix
 - in our setting each entry is eigenvalue λ_i
 - □ V^T ← singular vector matrix
 - \blacksquare in our setting each row is eigenvector \boldsymbol{v}_j











PCA using SVD algoritm



- Start from m by n data matrix X
- Recenter: subtract mean from each row of X

$$\square X_c \leftarrow X - \overline{X}$$

- Call SVD algorithm on X_c ask for k singular vectors
- Principal components: k singular vectors with highest singular values (rows of V^T)
 - ☐ Coefficients become:

$$2j = (\chi^i - \overline{\chi}).V$$

Using PCA for dimensionality reduction in classification

- Want to learn f:X[→]Y
 - \square **X**=< $X_1,...,X_n$ >
 - □ but some features are more important than others
- **Approach**: Use PCA on **X** to select a few important features \mathcal{M}_{1} \mathcal{M}_{K}

rather than learning
$$f(X) \mapsto Y$$

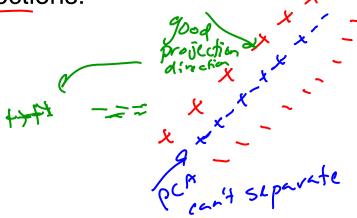
$$f(X, \dots, X_n) \mapsto Y$$

you learn
$$f(z_1, \dots, z_k) \mapsto y$$

$$\overline{z_i} = (x - \overline{x}) \cdot u_i$$

PCA for classification can lead to problems...

Direction of maximum variation may be unrelated to "discriminative" directions:



- PCA often works very well, but sometimes must use more advanced methods
 - e.g., Fisher linear discriminant

What you need to know

- NA.
 - Dimensionality reduction
 - ☐ why and when it's important
 - Simple feature selection
 - Principal component analysis
 - minimizing reconstruction error
 - □ relationship to covariance matrix and eigenvectors
 - □ using SVD
 - □ problems with PCA

Announcements



- Homework 5:
 - □ Extension: Due Friday at 10:30am
 - □ Hand in to Monica, Wean 4619
- Project:
 - □ Poster session: Friday May 4th 2-5pm, NSH Atrium
 - please arrive a 15mins early to set up
 - □ Paper: Thursday May 10th by 2pm
 - electronic submission by email to instructors list
 - maximum of 8 pages, NIPS format
 - no late days allowed
- FCEs!!!!
 - □ Please, please, please, please, please, please give us your feedback, it helps us improve the class! ☺
 - http://www.cmu.edu/fce

Markov Decision Processes (MDPs)

Machine Learning – 10701/15781
Carlos Guestrin
Carnegie Mellon University

April 25th, 200

Thus far this semester



- Regression:
- Classification:
- Density estimation:

Learning to act



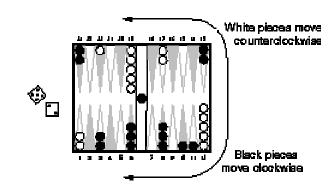
[Ng et al. '05]

- Reinforcement learning
- An agent
 - Makes sensor observations
 - Must select action
 - □ Receives rewards
 - positive for "good" states
 - negative for "bad" states

Learning to play backgammon

[Tesauro '95]

- Combines reinforcement learning with neural networks
- Played 300,000 games against itself
- Achieved grandmaster level!



Roadmap to learning about reinforcement learning

- When we learned about Bayes nets:
 - ☐ First talked about formal framework:
 - representation
 - inference
 - □ Then learning for BNs
- For reinforcement learning:
 - □ Formal framework
 - Markov decision processes
 - □ Then learning





States and actions



- State space:
 - ☐ Joint state **x** of entire system

- Action space:
 - □ Joint action $\mathbf{a} = \{a_1, ..., a_n\}$ for all agents



States change over time

- Like an HMM, state changes over time
- Next state depends on current state and action selected
 - e.g., action="build castle" likely to lead to a state where you have a castle
- Transition model:
 - \square Dynamics of the entire system $P(\mathbf{x}'|\mathbf{x},\mathbf{a})$



Some states and actions are better than others

- м
 - Each state x is associated with a reward
 - □ positive reward for successful attack
 - negative for loss
 - Reward function:
 - \Box Total reward R(**x**)

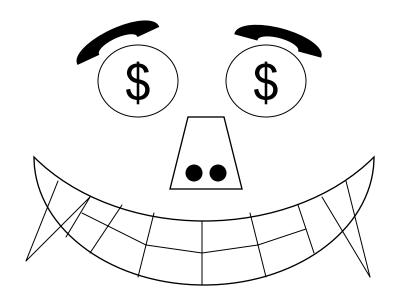


Discounted Rewards

An assistant professor gets paid, say, 20K per year.

How much, in total, will the A.P. earn in their life?

$$20 + 20 + 20 + 20 + 20 + \dots = Infinity$$



What's wrong with this argument?

Discounted Rewards



"A reward (payment) in the future is not worth quite as much as a reward now."

- □ Because of chance of obliteration
- □ Because of inflation

Example:

Being promised \$10,000 next year is worth only 90% as much as receiving \$10,000 right now.

Assuming payment n years in future is worth only $(0.9)^n$ of payment now, what is the AP's Future Discounted Sum of Rewards?

Discount Factors

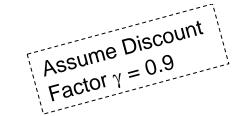


People in economics and probabilistic decision-making do this all the time.

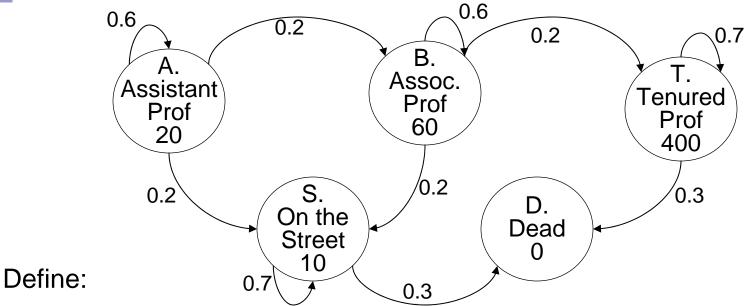
The "Discounted sum of future rewards" using discount factor γ " is

```
(reward now) + \gamma (reward in 1 time step) + \gamma^2 (reward in 2 time steps) + \gamma^3 (reward in 3 time steps) + \gamma^3 (reward in 3 time steps) + \gamma^3 (infinite sum)
```

The Academic Life







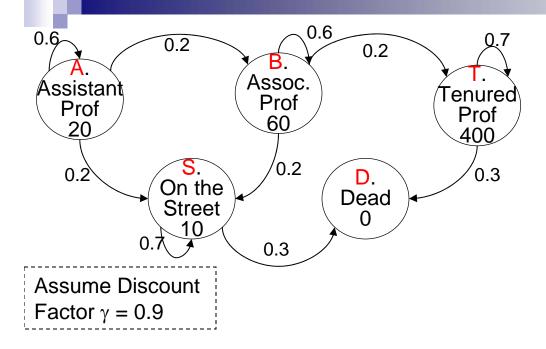
 V_A = Expected discounted future rewards starting in state A

V_B = Expected discounted future rewards starting in state B

$$V_T =$$
 " " " " T $V_S =$ " " " " " S $V_D =$ " " " " D

How do we compute V_A , V_B , V_T , V_S , V_D ?

Computing the Future Rewards of an Academic



Joint Decision Space

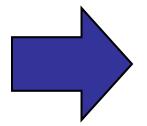
Markov Decision Process (MDP) Representation:

- State space:
 - □ Joint state **x** of entire system
- Action space:
 - □ Joint action $\mathbf{a} = \{a_1, ..., a_n\}$ for all agents
- Reward function:
 - \square Total reward R(\mathbf{x} , \mathbf{a})
 - sometimes reward can depend on action
- Transition model:
 - \square Dynamics of the entire system $P(\mathbf{x}'|\mathbf{x},\mathbf{a})$



Policy

Policy: $\pi(\mathbf{x}) = \mathbf{a}$



At state **x**, action **a** for all agents

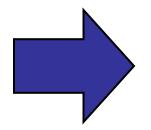


 $\pi(\mathbf{x}_1)$ = one peasant builds barrack, other gets gold

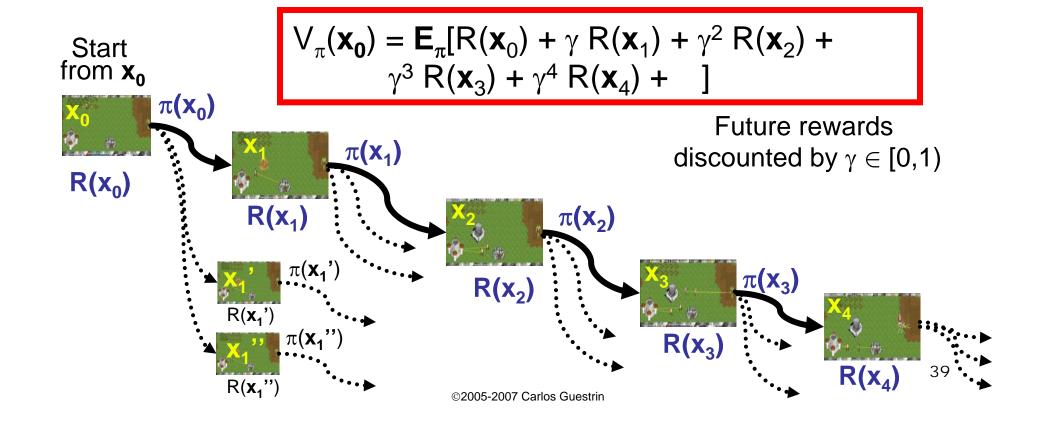
$$\pi(\mathbf{x}_2)$$
 = peasants get gold, footmen attack

Value of Policy

Value: $V_{\pi}(\mathbf{x})$



Expected longterm reward starting from **x**



Computing the value of a policy



$$V_{\pi}(\mathbf{x_0}) = \mathbf{E}_{\pi}[R(\mathbf{x_0}) + \gamma R(\mathbf{x_1}) + \gamma^2 R(\mathbf{x_2}) + \gamma^3 R(\mathbf{x_3}) + \gamma^4 R(\mathbf{x_4}) +]$$

- Discounted value of a state:
 - \square value of starting from x_0 and continuing with policy π from then on

$$V_{\pi}(x_0) = E_{\pi}[R(x_0) + \gamma R(x_1) + \gamma^2 R(x_2) + \gamma^3 R(x_3) + \cdots]$$

= $E_{\pi}[\sum_{t=0}^{\infty} \gamma^t R(x_t)]$

A recursion!

Computing the value of a policy 1 – the matrix inversion approach

$$V_{\pi}(x) = R(x) + \gamma \sum_{x'} P(x' \mid x, a = \pi(x)) V_{\pi}(x')$$

Solve by simple matrix inversion:

Computing the value of a policy 2 – iteratively

$$V_{\pi}(x) = R(x) + \gamma \sum_{x'} P(x' \mid x, a = \pi(x)) V_{\pi}(x')$$

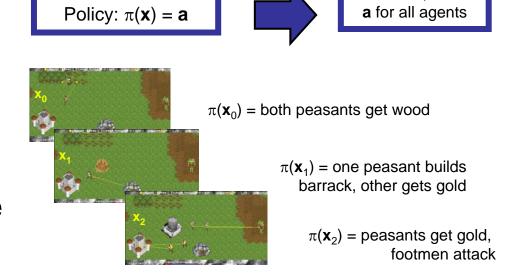
- If you have 1000,000 states, inverting a 1000,000x1000,000 matrix is hard!
- Can solve using a simple convergent iterative approach: (a.k.a. dynamic programming)
 - ☐ Start with some guess V₀
 - □ Iteratively say:

$$V_{t+1} = R + \gamma P_{\pi} V_{t}$$

- □ Stop when $||V_{t+1}-V_t||_{\infty} \le \varepsilon$
 - means that $||V_{\pi}-V_{t+1}||_{\infty} \le \varepsilon/(1-\gamma)$

But we want to learn a Policy

- So far, told you how good a policy is...
- But how can we choose the best policy???
- Suppose there was only one time step:
 - □ world is about to end!!!
 - select action that maximizes reward!



At state x, action

Another recursion!



- Two time steps: address tradeoff
 - □ good reward now
 - better reward in the future

Unrolling the recursion



- Choose actions that lead to best value in the long run
 - □ Optimal value policy achieves optimal value V*

$$V^*(x_0) = \max_{a_0} R(x_0, a_0) + \gamma E_{a_0} [\max_{a_1} R(x_1) + \gamma^2 E_{a_1} [\max_{a_2} R(x_2) + \cdots]]$$

Bellman equation



• Evaluating policy π :

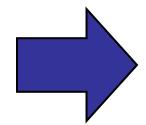
$$V_{\pi}(x) = R(x) + \gamma \sum_{x'} P(x' \mid x, a = \pi(x)) V_{\pi}(x')$$

Computing the optimal value V* - Bellman equation

$$V^*(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V^*(\mathbf{x}')$$

Optimal Long-term Plan

Optimal value function V*(x)



Optimal Policy: $\pi^*(\mathbf{x})$

$$Q^*(\mathbf{x}, \mathbf{a}) = R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V^*(\mathbf{x}')$$

Optimal policy:

$$\pi^*(\mathbf{x}) = \underset{\mathbf{a}}{\operatorname{arg\,max}} \, Q^*(\mathbf{x}, \mathbf{a})$$

Interesting fact — Unique value



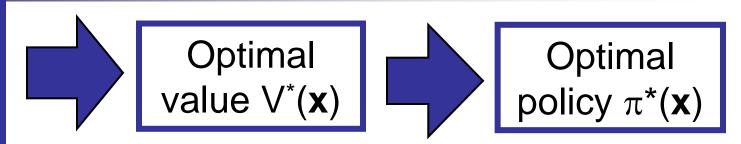
$$V^*(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V^*(\mathbf{x}')$$

- Slightly surprising fact: There is only one V* that solves Bellman equation!
 - □ there may be many optimal policies that achieve V*
- Surprising fact: optimal policies are good everywhere!!!

$$V_{\pi^*}(x) \geq V_{\pi}(x), \ \forall x, \ \forall \pi$$

Solving an MDP

Solve Bellman equation



$$V^*(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V^*(\mathbf{x}')$$

Bellman equation is non-linear!!!

Many algorithms solve the Bellman equations:

- Policy iteration [Howard '60, Bellman '57]
- Value iteration [Bellman '57]
- Linear programming [Manne '60]

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Value iteration (a.k.a. dynamic programming) — the simplest of all

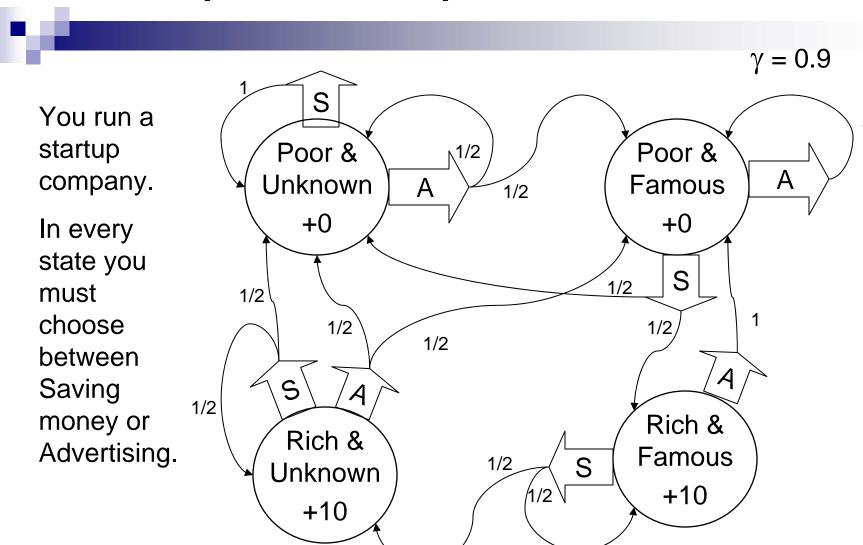
$$V^*(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V^*(\mathbf{x}')$$

- Start with some guess V₀
- Iteratively say:

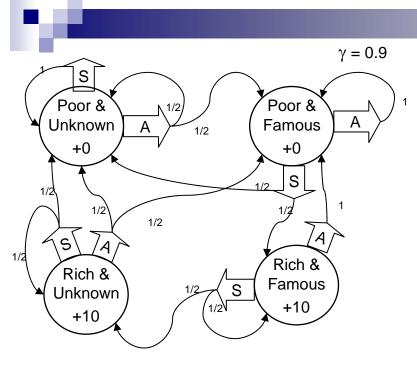
$$V_{t+1}(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V_t(\mathbf{x}')$$

- Stop when $||V_{t+1}-V_t||_{\infty} \leq \varepsilon$
 - \square means that $||V^*-V_{t+1}||_{\infty} \leq \varepsilon/(1-\gamma)$

A simple example



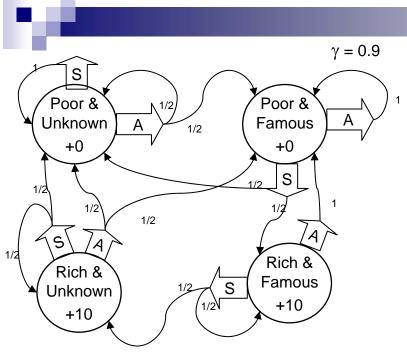
Let's compute $V_t(x)$ for our example



t	V _t (PU)	V _t (PF)	$V_t(RU)$	$V_t(RF)$
1				
2				
3				
4				
5				
6				

$$V_{t+1}(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V_t(\mathbf{x}')$$

Let's compute $V_t(x)$ for our example



t	V _t (PU)	V _t (PF)	V _t (RU)	V _t (RF)
1	0	0	10	10
2	0	4.5	14.5	19
3	2.03	6.53	25.08	18.55
4	3.852	12.20	29.63	19.26
5	7.22	15.07	32.00	20.40
6	10.03	17.65	33.58	22.43

$$V_{t+1}(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V_t(\mathbf{x}')$$

Policy iteration – Another approach for computing π^*



- Start with some guess for a policy π₀
- Iteratively say:
 - evaluate policy:

$$V_{t}(\mathbf{x}) = R(\mathbf{x}, \mathbf{a} = \pi_{t}(\mathbf{x})) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a} = \pi_{t}(\mathbf{x})) V_{t}(\mathbf{x}')$$

improve policy:

$$\pi_{t+1}(\mathbf{x}) = \max_{\mathbf{a}} R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V_t(\mathbf{x}')$$

- Stop when
 - policy stops changing
 - usually happens in about 10 iterations
 - \Box or $||V_{t+1}-V_t||_{\infty} \leq \varepsilon$
 - means that $||V^*-V_{t+1}||_{\infty} \leq \varepsilon/(1-\gamma)$

Policy Iteration & Value Iteration: Which is best ???

It depends.

Lots of actions? Choose Policy Iteration Already got a fair policy? Policy Iteration Few actions, acyclic? Value Iteration

Best of Both Worlds:

Modified Policy Iteration [Puterman] ...a simple mix of value iteration and policy iteration

3rd Approach

Linear Programming

LP Solution to MDP

[Manne '60]

Value computed by linear programming:

minimize:
$$\sum_{\mathbf{x}} V(\mathbf{x})$$

subject to:
$$\begin{cases} V(\mathbf{x}) \ge R(\mathbf{x}, \mathbf{a}) + \gamma \sum_{\mathbf{x}'} P(\mathbf{x}' | \mathbf{x}, \mathbf{a}) V(\mathbf{x}') \\ \forall \mathbf{x}, \mathbf{a} \end{cases}$$

- \blacksquare One variable $V(\mathbf{x})$ for each state
- One constraint for each state x and action a
- Polynomial time solution

What you need to know



- What's a Markov decision process
 - □ state, actions, transitions, rewards
 - □ a policy
 - □ value function for a policy
 - computing V_π
- Optimal value function and optimal policy
 - □ Bellman equation
- Solving Bellman equation
 - with value iteration, policy iteration and linear programming

Acknowledgment



- This lecture contains some material from Andrew Moore's excellent collection of ML tutorials:
 - □ http://www.cs.cmu.edu/~awm/tutorials